



Full wwPDB EM Validation Report ⓘ

Jun 27, 2024 – 04:07 AM JST

PDB ID : 8JO0
EMDB ID : EMD-36451
Title : The Cryo-EM structure of a heptameric CED-4/CED-3 catalytic complex
Authors : Li, Y.; Shi, Y.
Deposited on : 2023-06-06
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

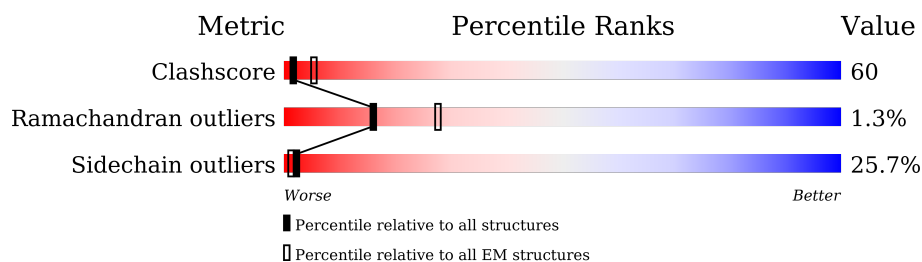
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	H	110	<div> <div>98%</div> <div> <div>35%</div> <div>55%</div> <div>9%</div> </div> </div>
1	I	110	<div> <div>98%</div> <div> <div>35%</div> <div>55%</div> <div>9%</div> </div> </div>
1	J	110	<div> <div>97%</div> <div> <div>35%</div> <div>55%</div> <div>9%</div> </div> </div>
1	K	110	<div> <div>95%</div> <div> <div>37%</div> <div>46%</div> <div>12%</div> <div>5%</div> </div> </div>
1	L	110	<div> <div>95%</div> <div> <div>37%</div> <div>45%</div> <div>13%</div> <div>5%</div> </div> </div>
1	M	110	<div> <div>95%</div> <div> <div>37%</div> <div>47%</div> <div>11%</div> <div>5%</div> </div> </div>
2	A	549	<div> <div>8%</div> <div> <div>20%</div> <div>36%</div> <div>15%</div> <div>29%</div> </div> </div>
2	B	549	<div> <div>8%</div> <div> <div>18%</div> <div>38%</div> <div>16%</div> <div>29%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	549	
2	D	549	
2	E	549	
2	F	549	
2	G	549	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATP	A	602	-	-	X	-
4	ATP	B	602	-	-	X	-
4	ATP	D	602	-	-	X	-
4	ATP	G	602	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27362 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Cell death protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	110	Total	C	N	O	S	0	0
			910	580	156	170	4		
1	I	110	Total	C	N	O	S	0	0
			910	580	156	170	4		
1	J	110	Total	C	N	O	S	0	0
			910	580	156	170	4		
1	K	105	Total	C	N	O	S	0	0
			870	552	150	164	4		
1	L	105	Total	C	N	O	S	0	0
			870	552	150	164	4		
1	M	105	Total	C	N	O	S	0	0
			870	552	150	164	4		

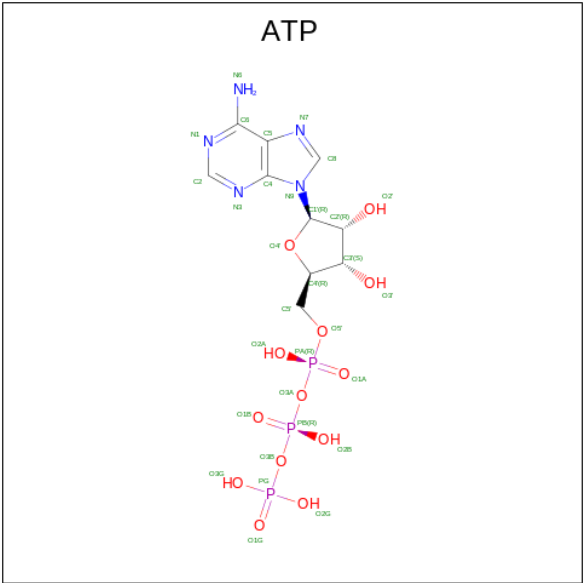
- Molecule 2 is a protein called Cell death protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	391	Total	C	N	O	S	0	0
			3114	1987	518	584	25		
2	B	391	Total	C	N	O	S	0	0
			3114	1987	518	584	25		
2	C	391	Total	C	N	O	S	0	0
			3114	1987	518	584	25		
2	D	391	Total	C	N	O	S	0	0
			3114	1987	518	584	25		
2	E	391	Total	C	N	O	S	0	0
			3114	1987	518	584	25		
2	F	391	Total	C	N	O	S	0	0
			3114	1987	518	584	25		
2	G	391	Total	C	N	O	S	0	0
			3114	1987	518	584	25		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	
3	B	1	Total	Mg	0
			1	1	
3	C	1	Total	Mg	0
			1	1	
3	D	1	Total	Mg	0
			1	1	
3	E	1	Total	Mg	0
			1	1	
3	F	1	Total	Mg	0
			1	1	
3	G	1	Total	Mg	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

Continued on next page...

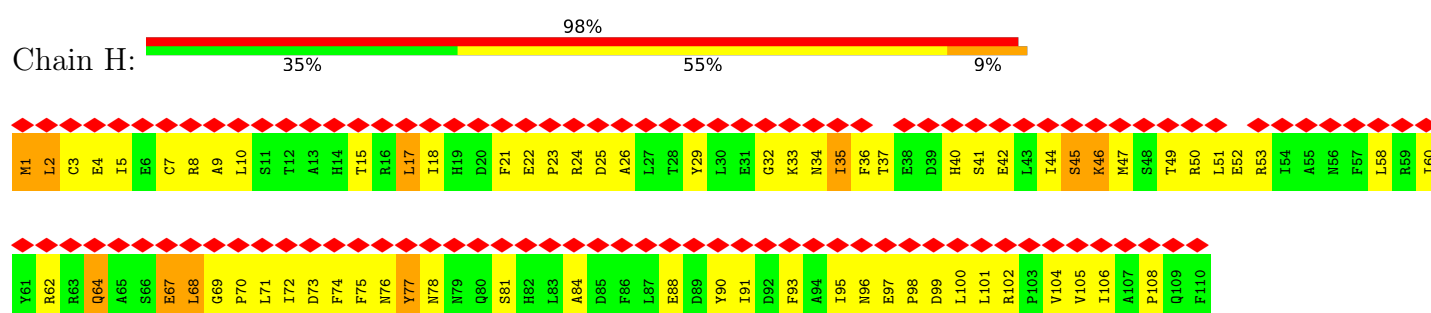
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
4	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	F	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	G	1	Total	C	N	O	P	0
			31	10	5	13	3	

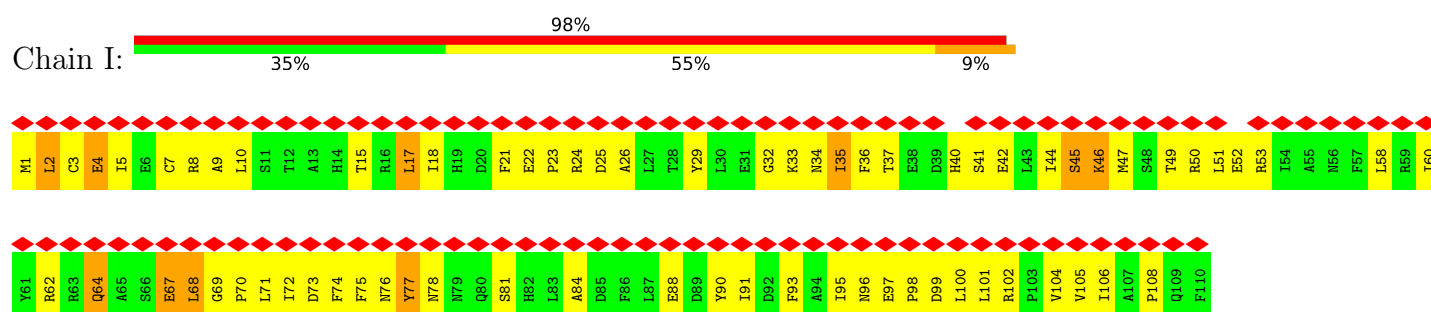
3 Residue-property plots

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

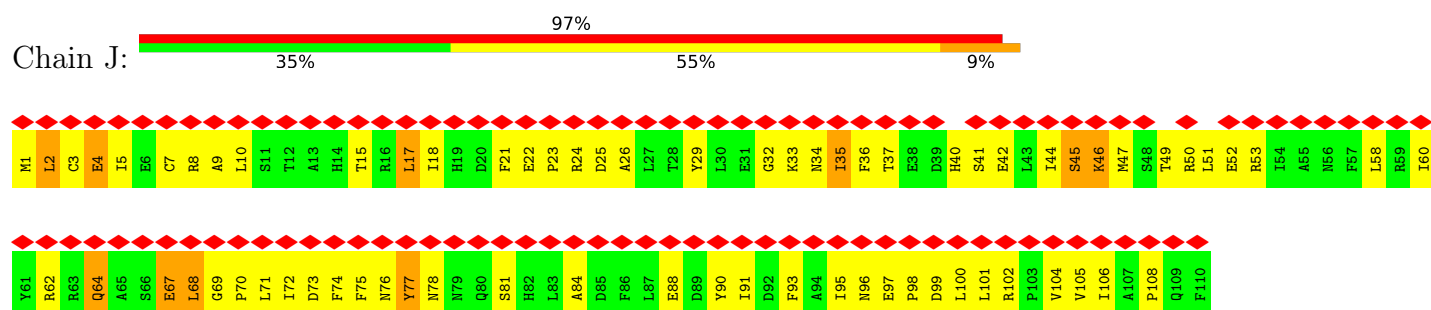
- Molecule 1: Cell death protein 4



- Molecule 1: Cell death protein 4

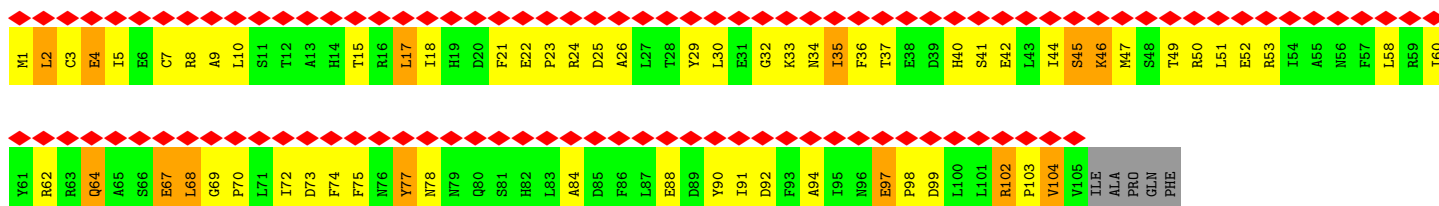


- Molecule 1: Cell death protein 4

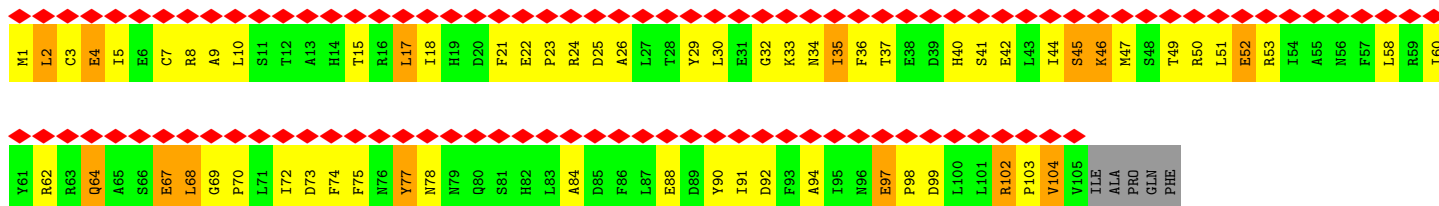


- Molecule 1: Cell death protein 4

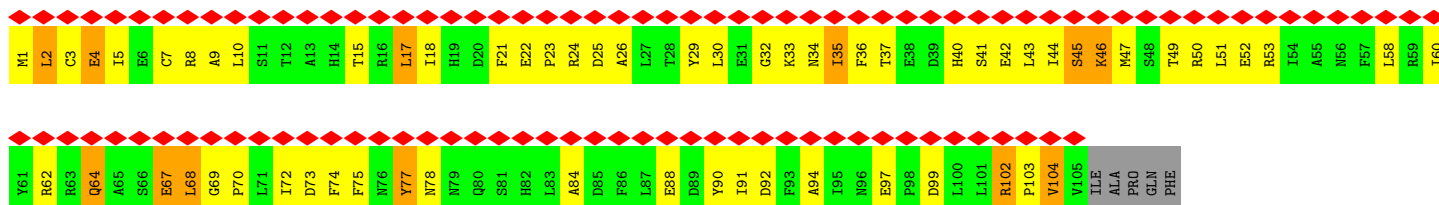




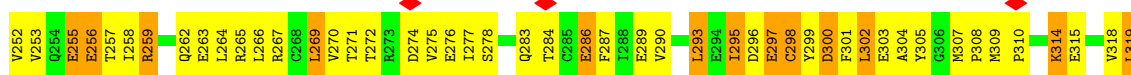
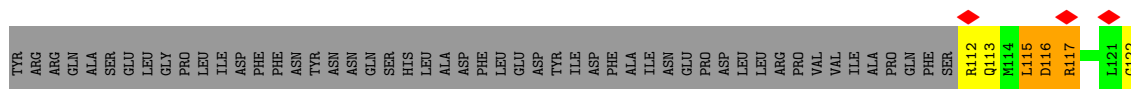
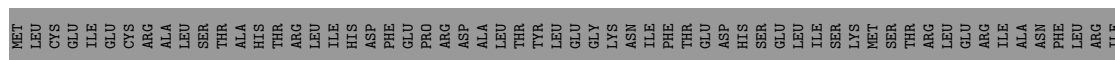
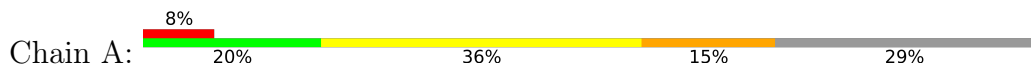
• Molecule 1: Cell death protein 4

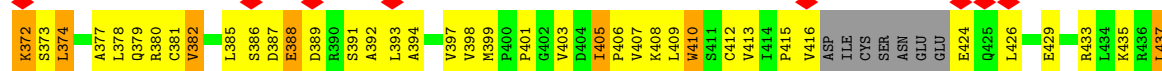


• Molecule 1: Cell death protein 4



• Molecule 2: Cell death protein 4









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67312	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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

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	H	0.38	0/930	0.54	0/1259
1	I	0.38	0/930	0.54	0/1259
1	J	0.38	0/930	0.54	0/1259
1	K	0.40	0/888	0.54	0/1201
1	L	0.39	0/888	0.54	0/1201
1	M	0.39	0/888	0.54	0/1201
2	A	0.47	0/3167	0.61	0/4276
2	B	0.47	0/3167	0.60	0/4276
2	C	0.47	0/3167	0.62	0/4276
2	D	0.48	0/3167	0.61	0/4276
2	E	0.42	0/3167	0.56	0/4276
2	F	0.37	0/3167	0.54	0/4276
2	G	0.36	0/3167	0.54	0/4276
All	All	0.43	0/27623	0.57	0/37312

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
2	A	0	1
2	B	0	1
2	D	0	1
2	E	0	1
2	F	0	1
2	G	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	449	MET	Peptide
2	B	449	MET	Peptide
2	D	449	MET	Peptide
2	E	449	MET	Peptide
2	F	449	MET	Peptide
2	G	449	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	910	0	889	77	0
1	I	910	0	889	77	0
1	J	910	0	889	74	0
1	K	870	0	849	68	0
1	L	870	0	849	70	0
1	M	870	0	849	67	0
2	A	3114	0	3165	433	0
2	B	3114	0	3165	462	0
2	C	3114	0	3165	435	0
2	D	3114	0	3165	472	0
2	E	3114	0	3165	409	0
2	F	3114	0	3165	336	0
2	G	3114	0	3165	376	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	31	0	12	9	0
4	B	31	0	12	9	0
4	C	31	0	12	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	31	0	12	11	0
4	E	31	0	12	8	0
4	F	31	0	12	5	0
4	G	31	0	12	10	0
All	All	27362	0	27453	3288	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 60.

All (3288) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:533:MET:HB3	2:D:540:TYR:CE2	1.21	1.66
2:C:305:TYR:CE2	2:C:334:MET:HE1	1.24	1.58
2:D:533:MET:CB	2:D:540:TYR:HE2	1.22	1.53
2:C:305:TYR:HB3	2:C:337:PHE:CZ	1.46	1.48
2:C:305:TYR:HE2	2:C:334:MET:CE	1.27	1.46
2:A:299:TYR:CE2	2:A:310:PRO:HG3	1.52	1.43
2:E:335:MET:CE	2:E:373:SER:HA	1.46	1.43
2:D:480:LEU:CD1	2:D:484:LEU:HD13	1.57	1.31
2:B:308:PRO:HB2	2:B:345:PHE:CZ	1.66	1.30
2:B:308:PRO:HB2	2:B:345:PHE:CE2	1.66	1.29
2:C:127:GLN:HG2	2:C:174:SER:CB	1.63	1.28
2:C:161:ALA:HB2	2:C:273:ARG:CD	1.64	1.28
2:A:367:THR:OG1	2:A:368:PRO:CD	1.81	1.27
2:C:530:PRO:HD2	2:C:531:LYS:NZ	1.51	1.26
2:B:143:LYS:HE2	2:B:286:GLU:CG	1.66	1.26
2:B:530:PRO:HD2	2:B:531:LYS:NZ	1.51	1.26
2:E:184:TYR:CD2	2:E:246:LEU:HD12	1.69	1.26
2:A:530:PRO:HD2	2:A:531:LYS:NZ	1.51	1.25
2:C:530:PRO:CD	2:C:531:LYS:NZ	2.00	1.25
2:B:211:LEU:HD11	2:B:239:LEU:CD2	1.66	1.25
2:C:211:LEU:HD11	2:C:239:LEU:CD2	1.66	1.25
2:D:530:PRO:HD2	2:D:531:LYS:NZ	1.51	1.25
2:A:211:LEU:HD11	2:A:239:LEU:CD2	1.66	1.25
2:A:530:PRO:CD	2:A:531:LYS:NZ	1.99	1.25
2:E:530:PRO:CD	2:E:531:LYS:NZ	1.99	1.25
2:B:530:PRO:CD	2:B:531:LYS:NZ	1.99	1.25
2:E:232:LYS:HD3	2:E:263:GLU:OE1	1.36	1.25
2:D:184:TYR:CD2	2:D:246:LEU:HD12	1.69	1.24
2:D:211:LEU:HD11	2:D:239:LEU:CD2	1.66	1.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:530:PRO:CD	2:D:531:LYS:NZ	2.00	1.24
2:E:530:PRO:HD2	2:E:531:LYS:NZ	1.50	1.24
2:G:211:LEU:HD11	2:G:239:LEU:CD2	1.66	1.24
2:D:232:LYS:HD3	2:D:263:GLU:OE1	1.36	1.23
2:E:211:LEU:HD11	2:E:239:LEU:CD2	1.66	1.23
2:A:464:LEU:HA	2:A:467:VAL:CG1	1.69	1.23
2:D:186:SER:OG	2:D:245:THR:HG23	1.34	1.23
2:A:232:LYS:HD3	2:A:263:GLU:OE1	1.36	1.22
2:F:211:LEU:HD11	2:F:239:LEU:CD2	1.66	1.22
2:B:258:ILE:HD13	2:B:277:ILE:CD1	1.68	1.22
2:B:232:LYS:HD3	2:B:263:GLU:OE1	1.36	1.22
2:B:366:ILE:CG2	2:C:279:ASN:HB2	1.69	1.22
2:D:232:LYS:HE3	2:D:260:TRP:CZ2	1.75	1.22
2:D:232:LYS:HE3	2:D:260:TRP:CE2	1.72	1.21
2:B:156:PHE:CE2	2:B:278:SER:HB2	1.74	1.20
2:E:131:TYR:CD2	2:E:301:PHE:HD1	1.59	1.20
2:C:232:LYS:HD3	2:C:263:GLU:OE1	1.36	1.19
2:A:131:TYR:CD2	2:A:301:PHE:HD1	1.59	1.19
2:D:131:TYR:CD2	2:D:301:PHE:HD1	1.59	1.19
2:B:258:ILE:CD1	2:B:277:ILE:HD12	1.71	1.19
2:A:299:TYR:HE2	2:A:310:PRO:CG	1.55	1.18
2:D:533:MET:HG3	2:D:540:TYR:OH	1.43	1.18
2:B:131:TYR:CD2	2:B:301:PHE:HD1	1.59	1.18
2:C:366:ILE:CG2	2:D:279:ASN:HB2	1.75	1.17
2:G:393:LEU:CG	2:G:437:LEU:HD11	1.73	1.17
2:D:355:LEU:HD11	2:D:462:MET:CE	1.76	1.16
2:B:366:ILE:HG22	2:C:279:ASN:HB2	1.22	1.15
2:D:355:LEU:HD11	2:D:462:MET:HE1	1.17	1.15
2:B:143:LYS:HE2	2:B:286:GLU:HG3	1.20	1.14
2:D:232:LYS:CE	2:D:260:TRP:CE2	2.30	1.14
2:D:305:TYR:CE2	2:D:334:MET:HE3	1.83	1.14
2:A:367:THR:OG1	2:A:368:PRO:HD2	1.41	1.14
2:A:382:VAL:CG2	2:A:393:LEU:HD13	1.77	1.14
2:B:533:MET:HB3	2:B:540:TYR:CE2	1.82	1.14
2:E:530:PRO:CD	2:E:531:LYS:HZ2	1.55	1.14
2:D:530:PRO:CD	2:D:531:LYS:HZ2	1.56	1.13
2:A:143:LYS:CE	2:A:286:GLU:HG2	1.78	1.13
2:E:143:LYS:CE	2:E:286:GLU:HG2	1.78	1.13
2:A:334:MET:HE2	2:A:334:MET:HA	1.24	1.12
2:A:406:PRO:HG2	2:A:526:PRO:CG	1.79	1.12
2:D:406:PRO:HG2	2:D:526:PRO:CG	1.79	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:PRO:HG2	2:B:526:PRO:CG	1.79	1.12
2:C:143:LYS:CE	2:C:286:GLU:HG2	1.78	1.12
2:D:143:LYS:CE	2:D:286:GLU:HG2	1.78	1.11
2:E:335:MET:HE1	2:E:373:SER:HA	1.16	1.11
2:B:143:LYS:CE	2:B:286:GLU:HG3	1.81	1.11
2:C:406:PRO:HG2	2:C:526:PRO:CG	1.79	1.11
2:D:477:ILE:HG13	2:D:543:LEU:HD21	1.29	1.11
2:E:406:PRO:HG2	2:E:526:PRO:CG	1.79	1.11
2:A:367:THR:HG1	2:A:368:PRO:HD2	1.09	1.11
2:G:393:LEU:HG	2:G:437:LEU:CD1	1.80	1.11
2:C:127:GLN:HG2	2:C:174:SER:HB2	1.20	1.10
2:D:127:GLN:HG2	2:D:174:SER:HB2	1.32	1.10
2:D:480:LEU:HD13	2:D:484:LEU:HD13	1.19	1.10
2:G:298:CYS:SG	2:G:333:LEU:HD11	1.91	1.10
2:B:302:LEU:HD13	2:B:307:MET:CG	1.81	1.10
2:C:531:LYS:H	2:C:531:LYS:HD2	1.16	1.10
2:B:484:LEU:HD11	2:B:530:PRO:O	1.50	1.09
2:C:530:PRO:CD	2:C:531:LYS:HZ2	1.58	1.09
2:F:140:VAL:CG2	2:F:288:ILE:HD12	1.82	1.09
2:A:366:ILE:CD1	2:A:372:LYS:HG2	1.82	1.09
2:D:484:LEU:HD11	2:D:533:MET:HG2	1.11	1.09
2:A:366:ILE:CG1	2:A:372:LYS:HE2	1.81	1.09
2:D:531:LYS:H	2:D:531:LYS:HD2	1.16	1.09
2:C:161:ALA:HB2	2:C:273:ARG:HD2	1.25	1.09
2:G:392:ALA:CB	2:G:433:ARG:HD3	1.82	1.09
2:A:530:PRO:CD	2:A:531:LYS:HZ3	1.58	1.08
2:E:335:MET:HE3	2:E:373:SER:HA	1.27	1.08
2:E:531:LYS:H	2:E:531:LYS:HD2	1.16	1.08
2:A:531:LYS:H	2:A:531:LYS:HD2	1.16	1.08
2:D:184:TYR:CE2	2:D:246:LEU:HD12	1.89	1.08
2:D:305:TYR:CE2	2:D:334:MET:CE	2.36	1.08
2:A:464:LEU:HA	2:A:467:VAL:HG12	1.12	1.07
2:B:399:MET:HG3	2:B:400:PRO:HD2	1.33	1.07
2:E:160:ARG:O	2:E:163:SER:HB3	1.53	1.06
2:E:184:TYR:CE2	2:E:246:LEU:HD12	1.89	1.06
2:A:464:LEU:CA	2:A:467:VAL:HG12	1.84	1.06
2:C:334:MET:HE2	2:C:334:MET:HA	1.29	1.06
2:C:305:TYR:HB3	2:C:337:PHE:CE2	1.91	1.05
2:D:484:LEU:HD11	2:D:533:MET:CG	1.85	1.05
2:F:140:VAL:HG23	2:F:288:ILE:CD1	1.86	1.05
2:A:131:TYR:HD2	2:A:301:PHE:CD1	1.74	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:534:GLN:HA	2:A:537:GLN:HB2	1.36	1.05
2:B:531:LYS:H	2:B:531:LYS:HD2	1.16	1.05
2:C:305:TYR:CB	2:C:337:PHE:CZ	2.38	1.05
2:B:131:TYR:HD2	2:B:301:PHE:CD1	1.74	1.05
2:E:159:GLY:N	2:E:165:LYS:HD3	1.69	1.05
2:A:530:PRO:HD3	2:A:531:LYS:HZ3	1.19	1.05
2:A:439:LYS:O	2:A:440:ARG:HG2	1.57	1.04
2:C:439:LYS:O	2:C:440:ARG:HG2	1.56	1.04
2:A:143:LYS:HE2	2:A:286:GLU:HG2	1.05	1.04
2:C:161:ALA:CB	2:C:273:ARG:CD	2.35	1.04
2:B:131:TYR:CD2	2:B:301:PHE:CD1	2.46	1.04
2:B:530:PRO:CD	2:B:531:LYS:HZ2	1.63	1.04
2:D:131:TYR:HD2	2:D:301:PHE:CD1	1.74	1.04
2:D:305:TYR:HE2	2:D:334:MET:CE	1.70	1.04
2:A:131:TYR:CD2	2:A:301:PHE:CD1	2.46	1.04
2:E:131:TYR:HD2	2:E:301:PHE:CD1	1.74	1.04
2:E:211:LEU:CD2	2:E:242:ARG:HG3	1.88	1.04
2:D:484:LEU:CD1	2:D:533:MET:HG2	1.88	1.03
2:B:308:PRO:CB	2:B:345:PHE:CE2	2.42	1.03
2:B:366:ILE:HG22	2:C:279:ASN:CB	1.87	1.03
2:B:302:LEU:CD1	2:B:307:MET:HG2	1.89	1.03
2:C:305:TYR:CE2	2:C:334:MET:CE	2.15	1.03
2:D:131:TYR:CD2	2:D:301:PHE:CD1	2.46	1.03
2:E:310:PRO:HB3	2:E:319:LEU:HD23	1.39	1.03
2:E:530:PRO:HD2	2:E:531:LYS:HZ2	1.09	1.03
2:D:143:LYS:HE2	2:D:286:GLU:HG2	1.05	1.03
2:E:131:TYR:CD2	2:E:301:PHE:CD1	2.46	1.03
2:C:143:LYS:HE2	2:C:286:GLU:HG2	1.05	1.02
2:E:406:PRO:HG2	2:E:526:PRO:HG2	1.40	1.02
2:F:397:VAL:HG22	2:F:464:LEU:HB3	1.03	1.02
2:B:484:LEU:O	2:B:487:ILE:HG22	1.59	1.02
2:C:134:GLU:O	2:C:138:ASP:HB3	1.59	1.02
2:B:134:GLU:O	2:B:138:ASP:HB3	1.60	1.02
2:B:484:LEU:HD21	2:B:531:LYS:O	1.59	1.02
2:E:143:LYS:HE2	2:E:286:GLU:HG2	1.05	1.02
2:D:134:GLU:O	2:D:138:ASP:HB3	1.59	1.02
2:D:406:PRO:HG2	2:D:526:PRO:HG2	1.40	1.02
1:I:41:SER:O	1:I:45:SER:HB3	1.61	1.01
2:C:406:PRO:HG2	2:C:526:PRO:HG2	1.40	1.01
2:D:438:SER:CB	2:D:444:LEU:O	2.07	1.01
2:E:530:PRO:HD3	2:E:531:LYS:NZ	1.75	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:PRO:HG2	2:B:526:PRO:HG2	1.40	1.01
2:A:406:PRO:HG2	2:A:526:PRO:HG2	1.40	1.01
2:B:127:GLN:HB3	2:B:171:GLN:HA	1.40	1.00
2:B:530:PRO:HD3	2:B:531:LYS:HZ3	1.24	1.00
1:J:93:PHE:HE2	1:J:100:LEU:HD23	1.25	1.00
2:C:309:MET:SD	2:C:310:PRO:HD2	2.01	1.00
2:D:480:LEU:HD11	2:D:484:LEU:CD1	1.91	1.00
1:J:41:SER:O	1:J:45:SER:HB3	1.61	1.00
2:D:368:PRO:HB2	4:D:602:ATP:O3'	1.61	1.00
2:E:134:GLU:O	2:E:138:ASP:HB3	1.59	1.00
2:F:211:LEU:CD1	2:F:239:LEU:CD2	2.40	1.00
1:H:41:SER:O	1:H:45:SER:HB3	1.61	1.00
2:C:211:LEU:CD1	2:C:239:LEU:CD2	2.40	1.00
2:A:397:VAL:HG22	2:A:464:LEU:CB	1.91	1.00
2:E:159:GLY:H	2:E:165:LYS:HD3	1.22	1.00
1:K:41:SER:O	1:K:45:SER:HB3	1.62	1.00
1:L:41:SER:O	1:L:45:SER:HB3	1.62	1.00
2:E:211:LEU:CD1	2:E:239:LEU:CD2	2.40	1.00
2:B:400:PRO:CG	2:B:405:ILE:HG21	1.91	1.00
2:D:184:TYR:CE2	2:D:246:LEU:CD1	2.45	1.00
2:D:530:PRO:HD3	2:D:531:LYS:NZ	1.74	1.00
2:A:483:ARG:HA	2:A:483:ARG:CZ	1.92	0.99
2:B:156:PHE:CZ	2:B:278:SER:HB2	1.97	0.99
2:C:309:MET:SD	2:C:310:PRO:CD	2.49	0.99
1:I:93:PHE:HE2	1:I:100:LEU:HD23	1.24	0.99
2:B:211:LEU:CD1	2:B:239:LEU:CD2	2.40	0.99
2:E:335:MET:CE	2:E:373:SER:CA	2.41	0.99
2:B:128:MET:HA	2:B:128:MET:HE3	1.43	0.99
2:E:184:TYR:CE2	2:E:246:LEU:CD1	2.45	0.99
2:B:131:TYR:HD2	2:B:301:PHE:HD1	0.99	0.99
2:G:211:LEU:CD1	2:G:239:LEU:CD2	2.40	0.99
2:B:530:PRO:CD	2:B:531:LYS:HZ3	1.68	0.99
2:D:211:LEU:CD1	2:D:239:LEU:CD2	2.40	0.99
2:A:211:LEU:CD1	2:A:239:LEU:CD2	2.40	0.99
2:C:530:PRO:HD2	2:C:531:LYS:HZ2	1.12	0.99
2:D:366:ILE:HG23	2:E:279:ASN:HB2	1.44	0.99
1:M:41:SER:O	1:M:45:SER:HB3	1.62	0.99
2:D:227:THR:OG1	2:D:230:VAL:HG23	1.63	0.99
2:D:184:TYR:CD2	2:D:246:LEU:CD1	2.46	0.98
2:A:367:THR:OG1	2:A:368:PRO:HD3	1.63	0.98
2:C:530:PRO:HD3	2:C:531:LYS:HZ3	1.27	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:480:LEU:CD1	2:D:484:LEU:CD1	2.42	0.98
2:E:131:TYR:HD2	2:E:301:PHE:HD1	0.99	0.98
1:H:93:PHE:HE2	1:H:100:LEU:HD23	1.24	0.98
2:B:400:PRO:HG2	2:B:405:ILE:HG21	1.43	0.98
2:E:184:TYR:CD2	2:E:246:LEU:CD1	2.46	0.97
2:C:305:TYR:CB	2:C:337:PHE:CE2	2.47	0.97
2:A:131:TYR:HD2	2:A:301:PHE:HD1	0.99	0.97
2:D:530:PRO:HD2	2:D:531:LYS:HZ2	1.09	0.97
2:G:332:THR:HG23	2:G:374:LEU:HG	1.45	0.97
2:D:131:TYR:HD2	2:D:301:PHE:HD1	0.99	0.97
2:D:480:LEU:HD11	2:D:484:LEU:HD13	1.41	0.97
2:B:530:PRO:HD2	2:B:531:LYS:HZ2	1.17	0.97
2:B:533:MET:CE	2:B:533:MET:HA	1.95	0.97
2:A:305:TYR:OH	4:A:602:ATP:H2	1.48	0.96
2:C:401:PRO:HA	2:C:456:ILE:HG22	1.45	0.96
2:B:302:LEU:HD13	2:B:307:MET:SD	2.05	0.96
2:A:463:PHE:O	2:A:467:VAL:HG12	1.66	0.96
2:C:161:ALA:CB	2:C:273:ARG:HD3	1.96	0.96
2:D:528:ASP:C	2:D:531:LYS:HZ3	1.69	0.96
2:C:128:MET:HA	2:C:128:MET:HE3	1.45	0.96
2:E:528:ASP:C	2:E:531:LYS:HZ3	1.69	0.96
2:A:397:VAL:HG22	2:A:464:LEU:HB3	1.45	0.96
2:D:127:GLN:HG2	2:D:174:SER:CB	1.96	0.96
2:E:524:ILE:HG13	2:E:535:LEU:HD12	1.48	0.95
2:B:211:LEU:CD2	2:B:242:ARG:HG3	1.97	0.95
2:B:401:PRO:HA	2:B:456:ILE:HG22	1.49	0.95
2:C:211:LEU:CD2	2:C:242:ARG:HG3	1.97	0.95
2:D:355:LEU:CD1	2:D:462:MET:CE	2.44	0.95
2:E:335:MET:HE1	2:E:373:SER:CA	1.96	0.95
2:A:393:LEU:CD2	2:A:464:LEU:HD21	1.97	0.95
2:G:392:ALA:HB2	2:G:433:ARG:HD3	1.49	0.95
2:A:393:LEU:HD23	2:A:464:LEU:HD11	1.50	0.94
2:D:186:SER:HG	2:D:245:THR:HG23	1.23	0.94
2:E:530:PRO:HD3	2:E:531:LYS:HZ3	1.29	0.94
2:A:530:PRO:HD3	2:A:531:LYS:NZ	1.75	0.94
2:D:129:THR:HA	2:D:132:ILE:HD11	1.50	0.94
2:C:530:PRO:HD3	2:C:531:LYS:NZ	1.75	0.94
1:I:8:ARG:HG2	1:I:8:ARG:HH11	1.33	0.94
2:A:464:LEU:O	2:A:468:VAL:HG23	1.67	0.94
2:B:530:PRO:HD3	2:B:531:LYS:NZ	1.75	0.94
2:D:334:MET:HE2	2:D:334:MET:HA	1.49	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:8:ARG:HG2	1:J:8:ARG:HH11	1.33	0.93
2:C:528:ASP:C	2:C:531:LYS:HZ3	1.71	0.93
2:C:366:ILE:HG22	2:D:279:ASN:HB2	1.50	0.93
2:E:256:GLU:OE1	2:E:260:TRP:CD1	2.21	0.93
2:A:382:VAL:HG23	2:A:393:LEU:CD1	1.99	0.93
2:D:127:GLN:CD	2:D:174:SER:HB3	1.89	0.93
2:E:406:PRO:HG2	2:E:526:PRO:HG3	1.51	0.93
2:F:308:PRO:HB2	2:F:345:PHE:CE1	2.03	0.93
2:F:140:VAL:HG23	2:F:288:ILE:HD12	1.48	0.92
2:A:397:VAL:HG21	2:A:468:VAL:HG21	1.51	0.92
2:D:355:LEU:CD1	2:D:462:MET:HE1	1.98	0.92
2:D:533:MET:CB	2:D:540:TYR:CE2	2.11	0.92
2:C:127:GLN:CG	2:C:174:SER:CB	2.47	0.92
2:D:438:SER:HB2	2:D:444:LEU:O	1.69	0.92
2:F:143:LYS:HE2	2:F:286:GLU:HG2	1.52	0.92
2:D:406:PRO:HG2	2:D:526:PRO:HG3	1.51	0.92
2:E:334:MET:HE2	2:E:334:MET:HA	1.52	0.92
2:F:397:VAL:CG2	2:F:464:LEU:HB3	1.98	0.92
2:G:232:LYS:CE	2:G:260:TRP:CD2	2.53	0.92
1:L:8:ARG:HG2	1:L:8:ARG:HH11	1.35	0.91
2:F:185:ASP:HB2	2:F:244:ASN:HB2	1.52	0.91
2:A:406:PRO:HG2	2:A:526:PRO:HG3	1.51	0.91
2:D:484:LEU:HD21	2:D:533:MET:HB2	1.52	0.91
2:E:184:TYR:CZ	2:E:246:LEU:HD11	2.05	0.91
2:D:184:TYR:CZ	2:D:246:LEU:HD11	2.05	0.91
2:A:340:CYS:O	2:A:340:CYS:SG	2.29	0.91
2:B:258:ILE:CD1	2:B:277:ILE:CD1	2.38	0.91
2:D:530:PRO:CD	2:D:531:LYS:HZ3	1.76	0.90
2:D:530:PRO:HD3	2:D:531:LYS:HZ3	1.29	0.90
2:G:334:MET:HG2	4:G:602:ATP:O2'	1.72	0.90
1:K:8:ARG:HG2	1:K:8:ARG:HH11	1.35	0.90
2:B:533:MET:HB3	2:B:540:TYR:HE2	1.27	0.90
2:C:406:PRO:HG2	2:C:526:PRO:HG3	1.51	0.90
2:D:160:ARG:O	2:D:163:SER:HB3	1.71	0.90
2:A:158:HIS:CE1	2:A:289:GLU:HB2	2.07	0.89
2:B:528:ASP:C	2:B:531:LYS:HZ3	1.76	0.89
2:D:127:GLN:CG	2:D:174:SER:CB	2.50	0.89
1:H:8:ARG:HG2	1:H:8:ARG:HH11	1.33	0.89
2:F:140:VAL:CG2	2:F:288:ILE:CD1	2.47	0.89
2:F:140:VAL:HG22	2:F:288:ILE:HD12	1.53	0.89
1:M:8:ARG:HG2	1:M:8:ARG:HH11	1.35	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:HIS:CE1	2:B:289:GLU:HB2	2.07	0.89
2:B:406:PRO:HG2	2:B:526:PRO:HG3	1.51	0.89
1:I:47:MET:HB2	1:I:53:ARG:HG3	1.55	0.89
2:C:533:MET:HB3	2:C:540:TYR:HE2	1.36	0.89
2:D:158:HIS:HE1	2:D:289:GLU:HB2	1.38	0.89
2:D:184:TYR:CD1	2:D:246:LEU:HD13	2.08	0.89
2:E:530:PRO:CD	2:E:531:LYS:HZ3	1.76	0.89
2:A:158:HIS:HE1	2:A:289:GLU:HB2	1.38	0.89
2:G:373:SER:HB3	2:G:376:MET:HG2	1.54	0.89
2:A:530:PRO:CD	2:A:531:LYS:HZ2	1.73	0.89
2:C:161:ALA:CA	2:C:273:ARG:HD3	2.02	0.89
2:G:334:MET:HA	2:G:334:MET:HE2	1.54	0.88
2:B:367:THR:OG1	2:B:368:PRO:HD2	1.72	0.88
2:B:158:HIS:HE1	2:B:289:GLU:HB2	1.38	0.88
2:D:158:HIS:CE1	2:D:289:GLU:HB2	2.08	0.88
2:F:406:PRO:HG2	2:F:526:PRO:HG2	1.53	0.88
2:B:141:ILE:HG12	2:B:172:ALA:HB1	1.55	0.88
2:B:533:MET:CB	2:B:540:TYR:HE2	1.87	0.88
2:E:184:TYR:CD1	2:E:246:LEU:HD13	2.08	0.88
2:E:211:LEU:HD22	2:E:242:ARG:HG3	1.53	0.88
2:B:143:LYS:HE2	2:B:286:GLU:HG2	1.54	0.88
2:B:302:LEU:CD1	2:B:307:MET:CG	2.49	0.88
2:B:397:VAL:HG21	2:B:468:VAL:HG21	1.55	0.88
2:G:392:ALA:HB1	2:G:433:ARG:HD3	1.53	0.88
2:C:305:TYR:HB3	2:C:337:PHE:HZ	1.34	0.88
2:A:463:PHE:CE1	2:A:467:VAL:HG21	2.09	0.88
2:D:152:SER:HA	2:D:266:LEU:O	1.74	0.88
1:I:7:CYS:SG	1:I:62:ARG:HD3	2.14	0.88
1:J:7:CYS:SG	1:J:62:ARG:HD3	2.14	0.88
2:A:326:SER:O	2:A:459:ILE:HG12	1.74	0.88
2:D:438:SER:HA	2:D:444:LEU:H	1.39	0.88
1:L:47:MET:HB2	1:L:53:ARG:HG3	1.56	0.88
2:A:382:VAL:CG2	2:A:393:LEU:CD1	2.50	0.88
2:A:443:LEU:HD23	2:A:460:ILE:HD11	1.56	0.88
1:J:47:MET:HB2	1:J:53:ARG:HG3	1.55	0.87
1:J:93:PHE:CE2	1:J:100:LEU:HD23	2.07	0.87
2:D:305:TYR:OH	4:D:602:ATP:H2	1.57	0.87
2:D:533:MET:HB3	2:D:540:TYR:CD2	2.09	0.87
1:H:47:MET:HB2	1:H:53:ARG:HG3	1.55	0.87
1:I:93:PHE:CE2	1:I:100:LEU:HD23	2.07	0.87
1:H:93:PHE:CE2	1:H:100:LEU:HD23	2.07	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:102:ARG:HG3	1:K:103:PRO:HD2	1.55	0.87
1:L:102:ARG:HG3	1:L:103:PRO:HD2	1.55	0.87
2:G:232:LYS:HE2	2:G:260:TRP:CD2	2.08	0.87
2:C:211:LEU:HD11	2:C:239:LEU:HD22	1.55	0.87
2:E:401:PRO:HG3	2:E:461:HIS:CG	2.10	0.87
2:G:412:CYS:HB3	2:G:480:LEU:HA	1.57	0.87
1:H:7:CYS:SG	1:H:62:ARG:HD3	2.14	0.87
2:C:530:PRO:CD	2:C:531:LYS:HZ3	1.73	0.87
2:E:211:LEU:CD1	2:E:239:LEU:HD23	2.05	0.87
2:A:355:LEU:HD12	2:A:462:MET:HE1	1.57	0.87
2:A:366:ILE:HG12	2:A:372:LYS:HE2	1.55	0.87
2:E:211:LEU:HD11	2:E:239:LEU:HD22	1.55	0.87
2:F:211:LEU:HD11	2:F:239:LEU:HD22	1.55	0.87
2:G:366:ILE:HG12	2:G:372:LYS:HE2	1.57	0.87
2:B:425:GLN:O	2:B:425:GLN:NE2	2.08	0.87
2:D:211:LEU:CD1	2:D:239:LEU:HD23	2.05	0.87
2:B:393:LEU:HB2	2:B:437:LEU:HD11	1.57	0.86
2:D:184:TYR:CZ	2:D:246:LEU:CD1	2.57	0.86
2:E:314:LYS:O	2:E:318:VAL:HG23	1.75	0.86
1:M:102:ARG:HG3	1:M:103:PRO:HD2	1.55	0.86
2:A:211:LEU:HD11	2:A:239:LEU:HD22	1.56	0.86
2:B:484:LEU:CD2	2:B:531:LYS:O	2.23	0.86
2:F:211:LEU:CD1	2:F:239:LEU:HD23	2.05	0.86
2:A:314:LYS:O	2:A:318:VAL:HG23	1.76	0.86
2:F:402:GLY:HA3	2:F:458:HIS:CE1	2.11	0.86
2:B:211:LEU:HD11	2:B:239:LEU:HD22	1.56	0.86
2:C:309:MET:SD	2:C:310:PRO:HD3	2.15	0.86
2:G:314:LYS:O	2:G:318:VAL:HG23	1.75	0.86
2:C:403:VAL:HG12	2:C:405:ILE:HG22	1.58	0.86
2:D:211:LEU:HD11	2:D:239:LEU:HD22	1.55	0.86
2:C:143:LYS:HE2	2:C:286:GLU:CG	2.01	0.86
1:K:47:MET:HB2	1:K:53:ARG:HG3	1.56	0.85
2:A:366:ILE:HD13	2:A:372:LYS:HG2	1.58	0.85
2:E:184:TYR:CZ	2:E:246:LEU:CD1	2.57	0.85
1:L:7:CYS:SG	1:L:62:ARG:HD3	2.16	0.85
2:G:211:LEU:HD11	2:G:239:LEU:HD22	1.55	0.85
1:M:47:MET:HB2	1:M:53:ARG:HG3	1.56	0.85
2:A:393:LEU:HD21	2:A:464:LEU:HD21	1.56	0.85
2:B:293:LEU:H	2:B:328:GLY:HA3	1.41	0.85
1:K:7:CYS:SG	1:K:62:ARG:HD3	2.16	0.85
2:G:211:LEU:CD1	2:G:239:LEU:HD23	2.05	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:397:VAL:HG22	2:F:464:LEU:CB	1.99	0.85
2:B:360:LEU:HD11	2:B:462:MET:HE2	1.59	0.85
2:C:211:LEU:CD1	2:C:239:LEU:HD23	2.05	0.85
2:G:335:MET:HE1	2:G:374:LEU:N	1.92	0.85
2:G:393:LEU:HG	2:G:437:LEU:HD11	0.90	0.85
2:E:129:THR:O	2:E:132:ILE:HD11	1.77	0.84
2:B:211:LEU:CD1	2:B:239:LEU:HD23	2.05	0.84
2:D:483:ARG:CZ	2:D:483:ARG:HA	2.07	0.84
2:A:339:SER:HB2	2:A:365:CYS:SG	2.17	0.84
2:C:128:MET:HB2	2:C:171:GLN:NE2	1.92	0.84
2:C:448:ARG:HH21	2:C:452:LEU:HB2	1.42	0.84
2:C:524:ILE:HG23	2:C:526:PRO:HD3	1.59	0.84
2:D:524:ILE:HG23	2:D:526:PRO:HD3	1.59	0.84
1:H:97:GLU:HG3	1:K:51:LEU:HD11	1.58	0.84
1:M:7:CYS:SG	1:M:62:ARG:HD3	2.16	0.84
2:A:143:LYS:HE2	2:A:286:GLU:CG	2.01	0.84
2:D:186:SER:OG	2:D:245:THR:CG2	2.23	0.84
2:A:524:ILE:HG23	2:A:526:PRO:HD3	1.59	0.84
2:B:524:ILE:HG23	2:B:526:PRO:HD3	1.59	0.84
2:C:161:ALA:HA	2:C:273:ARG:HD3	1.60	0.84
2:C:538:LYS:HB2	2:C:538:LYS:NZ	1.93	0.84
2:E:524:ILE:HG23	2:E:526:PRO:HD3	1.59	0.84
1:H:75:PHE:HB2	1:H:84:ALA:HB2	1.60	0.84
2:G:392:ALA:HB2	2:G:433:ARG:CD	2.08	0.84
1:L:75:PHE:HB2	1:L:84:ALA:HB2	1.60	0.83
2:C:366:ILE:HG22	2:D:279:ASN:CB	2.08	0.83
2:D:143:LYS:HE2	2:D:286:GLU:CG	2.01	0.83
2:D:533:MET:HG3	2:D:540:TYR:CZ	2.13	0.83
2:E:335:MET:HE3	2:E:373:SER:CA	2.07	0.83
2:A:537:GLN:HA	2:A:540:TYR:HB2	1.59	0.83
2:A:211:LEU:CD1	2:A:239:LEU:HD23	2.05	0.83
2:D:309:MET:SD	2:D:310:PRO:HD2	2.17	0.83
1:J:75:PHE:HB2	1:J:84:ALA:HB2	1.60	0.83
2:B:156:PHE:CD2	2:B:278:SER:HB2	2.14	0.83
2:F:402:GLY:HA3	2:F:458:HIS:HE1	1.43	0.83
2:C:309:MET:HA	2:C:309:MET:CE	2.07	0.83
1:I:75:PHE:HB2	1:I:84:ALA:HB2	1.60	0.83
2:A:337:PHE:CE1	2:A:343:LYS:HE3	2.13	0.83
2:D:538:LYS:HB2	2:D:538:LYS:NZ	1.93	0.83
2:A:406:PRO:CG	2:A:526:PRO:HG3	2.09	0.82
2:E:160:ARG:O	2:E:163:SER:CB	2.26	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:366:ILE:HG21	2:D:279:ASN:HB2	1.59	0.82
1:J:44:ILE:HD11	1:J:60:ILE:HD12	1.61	0.82
2:C:406:PRO:CG	2:C:526:PRO:HG3	2.09	0.82
2:D:406:PRO:CG	2:D:526:PRO:HG3	2.09	0.82
2:F:524:ILE:HG23	2:F:526:PRO:HD3	1.60	0.82
1:H:44:ILE:HD11	1:H:60:ILE:HD12	1.61	0.82
2:A:406:PRO:CG	2:A:526:PRO:CG	2.57	0.82
1:M:75:PHE:HB2	1:M:84:ALA:HB2	1.60	0.82
2:A:366:ILE:HD11	2:A:372:LYS:HG2	1.59	0.82
2:D:360:LEU:HD11	2:D:462:MET:HE2	1.62	0.82
1:I:44:ILE:O	1:I:53:ARG:HG2	1.80	0.82
2:B:403:VAL:HG12	2:B:405:ILE:HG22	1.61	0.82
2:D:480:LEU:O	2:D:480:LEU:HD22	1.78	0.82
2:G:197:PRO:HD2	2:G:198:LYS:HE2	1.62	0.82
1:K:75:PHE:HB2	1:K:84:ALA:HB2	1.60	0.82
2:E:406:PRO:CG	2:E:526:PRO:HG3	2.09	0.82
2:E:184:TYR:CG	2:E:246:LEU:CD1	2.63	0.81
1:I:44:ILE:HD11	1:I:60:ILE:HD12	1.61	0.81
1:J:44:ILE:O	1:J:53:ARG:HG2	1.80	0.81
2:A:197:PRO:HD2	2:A:198:LYS:HE2	1.62	0.81
2:A:314:LYS:NZ	2:A:314:LYS:HB3	1.95	0.81
2:A:355:LEU:HD12	2:A:462:MET:CE	2.10	0.81
2:B:293:LEU:N	2:B:328:GLY:HA3	1.94	0.81
2:C:406:PRO:CG	2:C:526:PRO:CG	2.57	0.81
2:E:314:LYS:NZ	2:E:314:LYS:HB3	1.95	0.81
2:B:406:PRO:CG	2:B:526:PRO:CG	2.57	0.81
2:B:406:PRO:CG	2:B:526:PRO:HG3	2.09	0.81
2:C:366:ILE:CG2	2:D:279:ASN:CB	2.58	0.81
2:D:334:MET:HE2	2:D:334:MET:CA	2.05	0.81
2:D:406:PRO:CG	2:D:526:PRO:CG	2.57	0.81
2:E:406:PRO:CG	2:E:526:PRO:CG	2.57	0.81
2:F:197:PRO:HD2	2:F:198:LYS:HE2	1.62	0.81
2:G:314:LYS:HB3	2:G:314:LYS:NZ	1.95	0.81
2:A:463:PHE:O	2:A:467:VAL:CG1	2.27	0.81
2:B:533:MET:O	2:B:540:TYR:CD2	2.32	0.81
2:B:355:LEU:HD12	2:B:462:MET:CE	2.10	0.81
2:B:393:LEU:HD21	2:B:464:LEU:HD22	1.62	0.81
2:A:360:LEU:HD11	2:A:462:MET:HE2	1.61	0.81
2:D:184:TYR:CG	2:D:246:LEU:CD1	2.63	0.81
2:A:337:PHE:CZ	2:A:343:LYS:HE3	2.15	0.81
2:B:197:PRO:HD2	2:B:198:LYS:HE2	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:LEU:HD12	2:B:462:MET:HE1	1.63	0.81
2:D:248:VAL:HG13	2:D:269:LEU:HB3	1.63	0.81
2:A:397:VAL:CG2	2:A:464:LEU:HB3	2.10	0.81
2:E:248:VAL:HG13	2:E:269:LEU:HB3	1.63	0.81
2:B:211:LEU:HD11	2:B:239:LEU:HD23	1.63	0.80
2:F:115:LEU:HD21	2:F:180:ILE:HB	1.63	0.80
2:C:197:PRO:HD2	2:C:198:LYS:HE2	1.62	0.80
2:F:295:ILE:HD12	2:F:323:ILE:HG21	1.64	0.80
2:A:528:ASP:C	2:A:531:LYS:HZ3	1.85	0.80
2:A:528:ASP:HA	2:A:531:LYS:HZ1	1.46	0.80
2:B:368:PRO:HB2	4:B:602:ATP:O3'	1.81	0.80
2:E:141:ILE:HG12	2:E:172:ALA:HB1	1.63	0.80
2:G:115:LEU:HD21	2:G:180:ILE:HB	1.63	0.80
2:A:248:VAL:HG13	2:A:269:LEU:HB3	1.63	0.80
2:F:248:VAL:HG13	2:F:269:LEU:HB3	1.63	0.80
1:H:44:ILE:O	1:H:53:ARG:HG2	1.80	0.80
2:A:366:ILE:HD11	2:A:372:LYS:CG	2.11	0.80
2:C:248:VAL:HG13	2:C:269:LEU:HB3	1.63	0.80
2:E:197:PRO:HD2	2:E:198:LYS:HE2	1.62	0.80
2:D:197:PRO:HD2	2:D:198:LYS:HE2	1.62	0.80
2:B:248:VAL:HG13	2:B:269:LEU:HB3	1.63	0.80
2:E:115:LEU:HD21	2:E:180:ILE:HB	1.63	0.80
2:A:400:PRO:HB3	2:A:536:HIS:HB3	1.61	0.79
2:D:305:TYR:OH	4:D:602:ATP:C2	2.34	0.79
2:G:385:LEU:CD1	2:G:393:LEU:HD12	2.13	0.79
2:E:530:PRO:HD2	2:E:531:LYS:CE	2.13	0.79
2:A:401:PRO:HB3	2:A:461:HIS:CD2	2.17	0.79
2:B:309:MET:HA	2:B:309:MET:CE	2.13	0.79
2:B:484:LEU:O	2:B:487:ILE:CG2	2.30	0.79
2:C:406:PRO:HA	2:C:453:THR:HG22	1.64	0.79
2:F:403:VAL:HG12	2:F:405:ILE:HG22	1.65	0.79
2:A:115:LEU:HD21	2:A:180:ILE:HB	1.63	0.79
2:B:533:MET:CB	2:B:540:TYR:CE2	2.62	0.79
2:C:410:TRP:CZ3	2:C:454:PHE:HB2	2.17	0.79
2:G:232:LYS:CE	2:G:260:TRP:CE2	2.66	0.79
2:A:403:VAL:HG12	2:A:405:ILE:HG22	1.65	0.79
2:B:128:MET:HA	2:B:128:MET:CE	2.13	0.79
2:B:147:MET:HG2	2:B:153:PHE:CG	2.17	0.79
2:C:530:PRO:HD2	2:C:531:LYS:CE	2.13	0.79
2:G:332:THR:HG23	2:G:374:LEU:CG	2.11	0.79
2:G:369:TYR:HB2	4:G:602:ATP:H4'	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:128:MET:HG3	2:E:167:VAL:HG22	1.64	0.79
2:G:232:LYS:HE2	2:G:260:TRP:CG	2.18	0.79
2:G:332:THR:CG2	2:G:374:LEU:HG	2.11	0.79
2:C:127:GLN:HG2	2:C:174:SER:HB3	1.60	0.79
2:C:127:GLN:HB3	2:C:171:GLN:HA	1.64	0.79
2:G:232:LYS:HE3	2:G:260:TRP:CE2	2.16	0.79
2:B:308:PRO:CB	2:B:345:PHE:CZ	2.59	0.78
2:D:309:MET:HA	2:D:309:MET:CE	2.10	0.78
2:E:143:LYS:HE2	2:E:286:GLU:CG	2.01	0.78
2:B:220:PHE:HE1	2:B:223:VAL:CG2	1.96	0.78
2:E:159:GLY:CA	2:E:165:LYS:HD3	2.13	0.78
2:A:250:ASP:HA	2:A:271:THR:OG1	1.83	0.78
2:D:115:LEU:HD21	2:D:180:ILE:HB	1.63	0.78
2:D:360:LEU:CD1	2:D:462:MET:CE	2.61	0.78
2:A:360:LEU:CD1	2:A:462:MET:CE	2.61	0.78
2:A:476:GLY:HA2	2:A:479:ILE:HD12	1.65	0.78
2:C:127:GLN:CG	2:C:174:SER:HB3	2.13	0.78
2:F:406:PRO:HB2	2:F:409:LEU:HD23	1.65	0.78
2:A:464:LEU:O	2:A:468:VAL:CG2	2.30	0.78
2:A:530:PRO:HD2	2:A:531:LYS:HZ2	1.27	0.78
2:B:360:LEU:CD1	2:B:462:MET:CE	2.61	0.78
2:D:531:LYS:HD2	2:D:531:LYS:N	1.98	0.78
2:F:250:ASP:HA	2:F:271:THR:OG1	1.84	0.78
2:A:393:LEU:CD2	2:A:464:LEU:CD2	2.62	0.78
2:G:250:ASP:HA	2:G:271:THR:OG1	1.84	0.78
2:A:393:LEU:HD23	2:A:464:LEU:CD1	2.14	0.78
2:B:127:GLN:HG2	2:B:174:SER:HB2	1.64	0.78
2:B:250:ASP:HA	2:B:271:THR:OG1	1.83	0.78
2:A:305:TYR:OH	4:A:602:ATP:C2	2.36	0.78
2:B:115:LEU:HD21	2:B:180:ILE:HB	1.63	0.78
2:B:531:LYS:HD2	2:B:531:LYS:N	1.98	0.78
2:D:530:PRO:HD2	2:D:531:LYS:CE	2.13	0.78
2:E:393:LEU:HD21	2:E:464:LEU:HD22	1.64	0.78
2:C:250:ASP:HA	2:C:271:THR:OG1	1.83	0.77
2:A:474:ALA:O	2:A:477:ILE:CG2	2.32	0.77
2:D:533:MET:CG	2:D:540:TYR:CE2	2.67	0.77
2:E:250:ASP:HA	2:E:271:THR:OG1	1.83	0.77
2:E:403:VAL:HG12	2:E:405:ILE:HG22	1.66	0.77
2:F:319:LEU:HD21	2:F:345:PHE:HE2	1.46	0.77
2:G:232:LYS:HE3	2:G:260:TRP:CD2	2.19	0.77
2:G:413:VAL:HG13	2:G:480:LEU:HB2	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:LEU:HD21	2:C:180:ILE:HB	1.63	0.77
2:A:528:ASP:C	2:A:531:LYS:NZ	2.38	0.77
2:E:531:LYS:HD2	2:E:531:LYS:N	1.98	0.77
2:G:302:LEU:HD13	2:G:307:MET:HG2	1.66	0.77
2:B:530:PRO:HD2	2:B:531:LYS:CE	2.13	0.77
2:C:128:MET:HA	2:C:128:MET:CE	2.15	0.77
2:E:211:LEU:HD11	2:E:239:LEU:HD21	1.66	0.77
2:E:473:ILE:HG22	2:E:543:LEU:HD11	1.66	0.77
2:B:438:SER:HA	2:B:444:LEU:H	1.48	0.77
2:A:530:PRO:HD2	2:A:531:LYS:CE	2.13	0.77
2:E:487:ILE:H	2:E:487:ILE:HD12	1.49	0.77
2:D:446:GLY:HA2	2:D:454:PHE:HA	1.65	0.77
2:F:452:LEU:H	2:F:452:LEU:HD23	1.50	0.77
2:G:393:LEU:HD12	2:G:437:LEU:HD21	1.67	0.77
2:A:355:LEU:CD1	2:A:462:MET:HE1	2.15	0.77
2:B:366:ILE:CG2	2:C:279:ASN:CB	2.53	0.77
2:E:134:GLU:O	2:E:138:ASP:CB	2.33	0.77
2:E:528:ASP:C	2:E:531:LYS:NZ	2.38	0.77
2:F:211:LEU:HD11	2:F:239:LEU:HD21	1.66	0.77
2:C:528:ASP:C	2:C:531:LYS:NZ	2.38	0.76
2:B:134:GLU:O	2:B:138:ASP:CB	2.33	0.76
2:B:480:LEU:HD11	2:B:533:MET:HG2	1.66	0.76
2:D:211:LEU:HD11	2:D:239:LEU:HD21	1.66	0.76
2:F:424:GLU:HG2	2:F:426:LEU:H	1.48	0.76
2:D:528:ASP:C	2:D:531:LYS:NZ	2.38	0.76
2:G:452:LEU:HD23	2:G:452:LEU:H	1.50	0.76
1:L:44:ILE:HD11	1:L:60:ILE:HD12	1.68	0.76
2:B:528:ASP:C	2:B:531:LYS:NZ	2.38	0.76
2:C:134:GLU:O	2:C:138:ASP:CB	2.33	0.76
2:D:250:ASP:HA	2:D:271:THR:OG1	1.83	0.76
2:B:452:LEU:HD23	2:B:452:LEU:H	1.50	0.76
2:F:302:LEU:HD21	2:F:333:LEU:HD21	1.67	0.76
2:C:401:PRO:HA	2:C:456:ILE:CG2	2.15	0.76
2:C:531:LYS:HD2	2:C:531:LYS:N	1.98	0.76
2:D:184:TYR:CG	2:D:246:LEU:HD13	2.21	0.76
1:I:90:TYR:HE2	1:I:106:ILE:HD11	1.51	0.76
2:B:484:LEU:CD1	2:B:530:PRO:O	2.31	0.76
2:E:302:LEU:HD13	2:E:307:MET:HG2	1.68	0.76
2:E:452:LEU:HD23	2:E:452:LEU:H	1.50	0.76
2:C:211:LEU:HD22	2:C:242:ARG:HG3	1.68	0.76
2:D:452:LEU:HD23	2:D:452:LEU:H	1.50	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:211:LEU:HD11	2:F:239:LEU:HD23	1.64	0.76
2:D:310:PRO:HB2	2:D:316:GLU:CD	2.06	0.76
2:C:161:ALA:HB2	2:C:273:ARG:HD3	1.53	0.75
2:F:319:LEU:HD21	2:F:345:PHE:CE2	2.20	0.75
1:M:44:ILE:O	1:M:53:ARG:HG2	1.86	0.75
2:E:184:TYR:CG	2:E:246:LEU:HD13	2.21	0.75
2:A:452:LEU:HD23	2:A:452:LEU:H	1.50	0.75
2:B:400:PRO:HG3	2:B:405:ILE:HG21	1.67	0.75
1:M:44:ILE:HD11	1:M:60:ILE:HD12	1.68	0.75
2:A:152:SER:HA	2:A:266:LEU:O	1.87	0.75
2:B:152:SER:HA	2:B:266:LEU:O	1.87	0.75
2:B:528:ASP:HA	2:B:531:LYS:HZ1	1.52	0.75
2:B:531:LYS:H	2:B:531:LYS:CD	1.96	0.75
2:A:477:ILE:HD12	2:A:477:ILE:O	1.86	0.75
2:G:211:LEU:HD11	2:G:239:LEU:HD23	1.63	0.75
2:B:211:LEU:HD22	2:B:242:ARG:HG3	1.68	0.75
2:F:393:LEU:O	2:F:464:LEU:HD11	1.86	0.75
1:H:90:TYR:HE2	1:H:106:ILE:HD11	1.51	0.75
2:E:211:LEU:HD11	2:E:239:LEU:HD23	1.64	0.75
2:G:211:LEU:HD11	2:G:239:LEU:HD21	1.66	0.75
1:J:90:TYR:HE2	1:J:106:ILE:HD11	1.51	0.75
2:B:364:GLU:CD	2:B:372:LYS:HB3	2.07	0.75
2:D:134:GLU:O	2:D:138:ASP:CB	2.33	0.75
2:E:406:PRO:HB2	2:E:409:LEU:HD23	1.69	0.75
1:K:44:ILE:O	1:K:53:ARG:HG2	1.86	0.74
2:B:526:PRO:O	2:B:530:PRO:HG3	1.87	0.74
2:B:537:GLN:HA	2:B:540:TYR:HB2	1.66	0.74
2:C:211:LEU:HD21	2:C:242:ARG:HG3	1.67	0.74
2:E:526:PRO:O	2:E:530:PRO:HG3	1.87	0.74
1:L:44:ILE:O	1:L:53:ARG:HG2	1.86	0.74
2:B:342:PRO:HG2	2:B:347:LYS:HG3	1.67	0.74
2:G:486:GLU:C	2:G:487:ILE:HD12	2.07	0.74
2:C:526:PRO:O	2:C:530:PRO:HG3	1.87	0.74
2:F:336:PHE:CZ	2:F:351:LEU:HB2	2.22	0.74
2:A:334:MET:HE2	2:A:334:MET:CA	1.99	0.74
2:A:415:PRO:O	2:A:416:VAL:HG23	1.88	0.74
2:B:258:ILE:HD13	2:B:277:ILE:HD12	0.82	0.74
2:E:437:LEU:HB3	2:E:444:LEU:HD22	1.69	0.74
2:C:211:LEU:HD11	2:C:239:LEU:HD21	1.66	0.74
1:K:44:ILE:HD11	1:K:60:ILE:HD12	1.68	0.74
2:C:415:PRO:O	2:C:416:VAL:HG23	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:438:SER:HB2	2:D:444:LEU:HB3	1.67	0.74
2:D:526:PRO:O	2:D:530:PRO:HG3	1.87	0.74
2:B:137:VAL:HG22	2:B:168:ILE:HG23	1.70	0.74
2:E:152:SER:HA	2:E:266:LEU:O	1.87	0.74
2:A:397:VAL:HG22	2:A:464:LEU:HB2	1.70	0.74
2:B:408:LYS:HE3	2:B:427:ASP:CB	2.18	0.74
2:C:342:PRO:HG2	2:C:347:LYS:HG3	1.69	0.74
2:F:360:LEU:HD13	2:F:360:LEU:N	2.03	0.74
2:G:525:ARG:HG2	2:G:527:GLU:HG2	1.70	0.74
2:A:526:PRO:O	2:A:530:PRO:HG3	1.87	0.74
2:B:360:LEU:HD13	2:B:360:LEU:N	2.03	0.74
2:D:401:PRO:HA	2:D:456:ILE:HG22	1.68	0.74
2:F:386:SER:HB3	2:F:389:ASP:HB2	1.70	0.74
2:B:211:LEU:HD21	2:B:242:ARG:HG3	1.67	0.73
2:A:283:GLN:HG2	2:A:284:THR:H	1.53	0.73
2:A:386:SER:HB3	2:A:389:ASP:HB2	1.70	0.73
2:A:528:ASP:CA	2:A:531:LYS:HZ1	2.02	0.73
2:B:310:PRO:HB3	2:B:316:GLU:HG3	1.69	0.73
2:B:401:PRO:HB3	2:B:461:HIS:CD2	2.23	0.73
2:C:152:SER:HA	2:C:266:LEU:O	1.88	0.73
2:D:406:PRO:HA	2:D:453:THR:HG22	1.71	0.73
2:D:537:GLN:HA	2:D:540:TYR:HB2	1.68	0.73
2:B:214:GLU:OE2	2:C:233:ARG:NH2	2.21	0.73
2:B:386:SER:HB3	2:B:389:ASP:HB2	1.70	0.73
2:B:406:PRO:HA	2:B:453:THR:HG22	1.70	0.73
2:D:393:LEU:HD23	2:D:464:LEU:HD11	1.71	0.73
2:D:360:LEU:HD13	2:D:360:LEU:N	2.03	0.73
2:A:366:ILE:CD1	2:A:372:LYS:HE2	2.18	0.73
2:B:211:LEU:HD11	2:B:239:LEU:HD21	1.66	0.73
2:B:366:ILE:HG21	2:C:279:ASN:HB2	1.66	0.73
2:C:255:GLU:HB3	2:C:277:ILE:HG22	1.71	0.73
2:C:321:LYS:HD2	2:C:325:LEU:HG	1.71	0.73
2:D:159:GLY:N	2:D:165:LYS:HD3	2.03	0.73
2:D:184:TYR:CE1	2:D:246:LEU:CD1	2.72	0.73
2:E:211:LEU:HD21	2:E:242:ARG:HG3	1.70	0.73
2:F:140:VAL:HG23	2:F:288:ILE:HD13	1.68	0.73
2:B:437:LEU:O	2:B:443:LEU:HB2	1.88	0.73
2:C:127:GLN:CD	2:C:174:SER:HB3	2.09	0.73
2:D:314:LYS:HB3	2:D:314:LYS:NZ	1.99	0.73
2:E:159:GLY:H	2:E:165:LYS:CD	2.02	0.73
1:H:97:GLU:HG3	1:K:51:LEU:CD1	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:40:HIS:ND1	1:K:60:ILE:HD13	2.04	0.73
1:M:40:HIS:ND1	1:M:60:ILE:HD13	2.04	0.73
2:B:360:LEU:CD1	2:B:462:MET:HE2	2.18	0.73
2:C:386:SER:HB3	2:C:389:ASP:HB2	1.70	0.73
2:D:129:THR:CA	2:D:132:ILE:HD11	2.18	0.73
2:D:386:SER:HB3	2:D:389:ASP:HB2	1.70	0.73
2:E:293:LEU:CD1	2:E:330:PRO:HG3	2.19	0.73
2:E:386:SER:HB3	2:E:389:ASP:HB2	1.70	0.73
2:A:159:GLY:N	2:A:165:LYS:HD3	2.04	0.73
2:A:406:PRO:HA	2:A:453:THR:HG22	1.70	0.73
2:B:159:GLY:N	2:B:165:LYS:HD3	2.04	0.73
2:E:184:TYR:CE1	2:E:246:LEU:CD1	2.72	0.73
2:E:406:PRO:HA	2:E:453:THR:HG22	1.70	0.73
2:E:415:PRO:O	2:E:416:VAL:HG23	1.87	0.73
2:G:334:MET:HA	2:G:334:MET:CE	2.19	0.73
2:B:401:PRO:HB3	2:B:461:HIS:HD2	1.54	0.73
2:B:415:PRO:O	2:B:416:VAL:HG23	1.88	0.73
2:D:211:LEU:HD11	2:D:239:LEU:HD23	1.63	0.73
2:E:334:MET:HA	2:E:334:MET:CE	2.19	0.73
1:L:40:HIS:ND1	1:L:60:ILE:HD13	2.04	0.72
2:A:360:LEU:HD13	2:A:360:LEU:N	2.03	0.72
2:E:360:LEU:HD13	2:E:360:LEU:N	2.03	0.72
2:B:530:PRO:HD2	2:B:531:LYS:HD2	1.70	0.72
2:D:415:PRO:O	2:D:416:VAL:HG23	1.88	0.72
2:E:115:LEU:HD11	2:E:177:ASP:HA	1.69	0.72
2:A:206:ASP:OD2	2:B:227:THR:HG21	1.89	0.72
2:A:220:PHE:HE1	2:A:223:VAL:HG22	1.55	0.72
2:B:220:PHE:CE1	2:B:223:VAL:HG22	2.24	0.72
2:C:530:PRO:HD2	2:C:531:LYS:HD2	1.71	0.72
2:F:415:PRO:O	2:F:416:VAL:HG23	1.88	0.72
2:A:211:LEU:HD11	2:A:239:LEU:HD23	1.63	0.72
2:B:533:MET:HG3	2:B:540:TYR:OH	1.89	0.72
2:B:427:ASP:O	2:B:430:VAL:HG23	1.90	0.72
2:E:530:PRO:HD2	2:E:531:LYS:HD2	1.70	0.72
2:E:398:VAL:CG2	2:E:477:ILE:HG12	2.19	0.72
2:E:529:PHE:N	2:E:530:PRO:HD3	2.04	0.72
2:G:153:PHE:H	2:G:267:ARG:HB3	1.54	0.72
2:B:127:GLN:CB	2:B:171:GLN:HA	2.17	0.72
2:C:443:LEU:HD23	2:C:443:LEU:H	1.54	0.72
2:E:424:GLU:HG3	2:E:426:LEU:HG	1.71	0.72
2:F:368:PRO:HD3	2:G:279:ASN:O	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:406:PRO:HA	2:G:453:THR:HG22	1.70	0.72
2:G:483:ARG:HH21	2:G:483:ARG:HA	1.55	0.72
2:A:293:LEU:CD1	2:A:330:PRO:HG3	2.19	0.72
2:D:232:LYS:HE2	2:D:260:TRP:CE2	2.23	0.72
2:D:255:GLU:HB3	2:D:277:ILE:HG22	1.72	0.72
2:F:406:PRO:HA	2:F:453:THR:HG22	1.70	0.72
2:A:211:LEU:HD11	2:A:239:LEU:HD21	1.66	0.72
2:D:334:MET:CE	2:D:334:MET:HA	2.19	0.72
2:G:127:GLN:HB2	2:G:171:GLN:HG2	1.70	0.72
2:G:342:PRO:HG2	2:G:347:LYS:HG3	1.72	0.72
2:G:385:LEU:HD11	2:G:437:LEU:HD21	1.72	0.72
2:G:415:PRO:O	2:G:416:VAL:HG23	1.88	0.72
2:G:456:ILE:HG12	2:G:461:HIS:HB2	1.72	0.72
2:A:233:ARG:NH2	2:G:214:GLU:OE2	2.23	0.72
2:A:366:ILE:CD1	2:A:372:LYS:CG	2.64	0.72
2:A:385:LEU:HD11	2:A:437:LEU:HD21	1.72	0.72
2:A:531:LYS:HD2	2:A:531:LYS:N	1.98	0.72
2:E:184:TYR:CD1	2:E:246:LEU:CD1	2.73	0.72
2:A:127:GLN:HE21	2:A:174:SER:HB3	1.55	0.71
2:A:214:GLU:OE2	2:B:233:ARG:NH2	2.22	0.71
2:A:393:LEU:HD22	2:A:464:LEU:CD2	2.20	0.71
2:D:530:PRO:HD2	2:D:531:LYS:HD2	1.70	0.71
2:G:310:PRO:HB3	2:G:319:LEU:HD23	1.72	0.71
2:A:366:ILE:HG12	2:A:372:LYS:CE	2.19	0.71
2:G:413:VAL:CG1	2:G:480:LEU:HB2	2.19	0.71
2:A:382:VAL:HG23	2:A:393:LEU:HD13	1.60	0.71
2:A:530:PRO:HD2	2:A:531:LYS:HD2	1.71	0.71
2:C:445:SER:O	2:C:454:PHE:HA	1.90	0.71
2:D:533:MET:CG	2:D:540:TYR:HE2	2.01	0.71
2:G:386:SER:HB3	2:G:389:ASP:HB2	1.71	0.71
2:D:313:GLU:OE1	2:D:313:GLU:N	2.23	0.71
2:B:533:MET:O	2:B:540:TYR:CE2	2.43	0.71
2:C:528:ASP:HA	2:C:531:LYS:HZ1	1.56	0.71
2:D:484:LEU:HD21	2:D:533:MET:HG2	1.72	0.71
2:F:385:LEU:HD11	2:F:437:LEU:HD21	1.72	0.71
2:B:302:LEU:HD12	2:B:307:MET:HG2	1.71	0.71
2:C:529:PHE:N	2:C:530:PRO:HD3	2.04	0.71
2:E:401:PRO:HA	2:E:456:ILE:HG22	1.70	0.71
1:K:102:ARG:HG3	1:K:103:PRO:CD	2.21	0.71
1:M:64:GLN:HA	1:M:64:GLN:HE21	1.56	0.71
2:B:355:LEU:CD1	2:B:462:MET:HE1	2.21	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:LEU:HD11	2:B:437:LEU:HD21	1.72	0.71
2:D:529:PHE:N	2:D:530:PRO:HD3	2.05	0.71
2:F:255:GLU:HA	2:F:258:ILE:HD13	1.73	0.71
2:A:293:LEU:HD12	2:A:330:PRO:HG3	1.73	0.71
2:A:529:PHE:N	2:A:530:PRO:HD3	2.04	0.71
2:F:214:GLU:OE2	2:G:233:ARG:NH2	2.24	0.71
2:C:385:LEU:HD11	2:C:437:LEU:HD21	1.72	0.70
2:D:184:TYR:CD1	2:D:246:LEU:CD1	2.73	0.70
2:E:533:MET:HG3	2:E:540:TYR:CZ	2.26	0.70
2:B:401:PRO:HA	2:B:456:ILE:CG2	2.19	0.70
2:C:211:LEU:HD11	2:C:239:LEU:HD23	1.63	0.70
2:C:214:GLU:OE2	2:D:233:ARG:NH2	2.23	0.70
2:D:214:GLU:OE2	2:E:233:ARG:NH2	2.24	0.70
2:D:399:MET:HG2	2:D:410:TRP:CE2	2.26	0.70
2:E:141:ILE:HD13	2:E:176:SER:HB2	1.73	0.70
2:E:406:PRO:CG	2:E:526:PRO:HG2	2.20	0.70
2:B:529:PHE:N	2:B:530:PRO:HD3	2.04	0.70
2:C:143:LYS:CE	2:C:286:GLU:CG	2.67	0.70
2:C:305:TYR:HB2	2:C:337:PHE:CE2	2.25	0.70
2:C:406:PRO:HB2	2:C:409:LEU:HD23	1.73	0.70
2:D:437:LEU:O	2:D:443:LEU:HB2	1.92	0.70
1:L:102:ARG:HG3	1:L:103:PRO:CD	2.21	0.70
2:A:396:ALA:HB1	2:A:456:ILE:HD12	1.74	0.70
2:B:137:VAL:O	2:B:141:ILE:HG13	1.92	0.70
2:A:474:ALA:O	2:A:477:ILE:HG22	1.92	0.70
2:D:311:VAL:N	2:D:315:GLU:OE1	2.23	0.70
1:K:64:GLN:HA	1:K:64:GLN:HE21	1.56	0.70
2:D:385:LEU:HD11	2:D:437:LEU:HD21	1.72	0.70
2:D:438:SER:OG	2:D:444:LEU:O	2.10	0.70
2:F:137:VAL:O	2:F:141:ILE:HG13	1.92	0.70
1:M:102:ARG:HG3	1:M:103:PRO:CD	2.21	0.70
2:B:446:GLY:CA	2:B:454:PHE:CD2	2.74	0.70
2:C:531:LYS:H	2:C:531:LYS:CD	1.96	0.70
2:E:483:ARG:HA	2:E:483:ARG:HH21	1.55	0.70
2:B:302:LEU:CD1	2:B:307:MET:SD	2.80	0.70
2:E:385:LEU:HD11	2:E:437:LEU:HD21	1.72	0.70
1:J:37:THR:OG1	1:J:40:HIS:HD2	1.75	0.69
2:D:484:LEU:HD21	2:D:533:MET:CB	2.19	0.69
2:G:406:PRO:HB2	2:G:409:LEU:HD23	1.73	0.69
1:I:40:HIS:ND1	1:I:60:ILE:HD13	2.07	0.69
1:J:64:GLN:HA	1:J:64:GLN:HE21	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:339:SER:CB	2:A:365:CYS:SG	2.80	0.69
2:B:307:MET:HG3	2:B:308:PRO:HD2	1.75	0.69
2:C:137:VAL:O	2:C:141:ILE:HG13	1.92	0.69
2:D:406:PRO:CG	2:D:526:PRO:HG2	2.20	0.69
2:E:214:GLU:OE2	2:F:233:ARG:NH2	2.25	0.69
1:H:40:HIS:ND1	1:H:60:ILE:HD13	2.07	0.69
1:I:37:THR:OG1	1:I:40:HIS:HD2	1.75	0.69
2:C:393:LEU:CD2	2:C:464:LEU:HD21	2.21	0.69
1:H:64:GLN:HA	1:H:64:GLN:HE21	1.58	0.69
1:K:4:GLU:O	1:K:8:ARG:HB2	1.93	0.69
2:C:233:ARG:HH11	2:C:233:ARG:HG3	1.58	0.69
2:D:327:SER:HB2	2:D:459:ILE:HD11	1.74	0.69
2:E:262:GLN:HG3	2:E:283:GLN:OE1	1.93	0.69
2:B:127:GLN:HB3	2:B:171:GLN:CA	2.20	0.69
2:D:127:GLN:CG	2:D:174:SER:HB3	2.18	0.69
2:E:137:VAL:O	2:E:141:ILE:HG13	1.92	0.69
1:L:64:GLN:HE21	1:L:64:GLN:HA	1.56	0.69
2:A:137:VAL:O	2:A:141:ILE:HG13	1.92	0.69
2:A:233:ARG:HG3	2:A:233:ARG:HH11	1.58	0.69
2:A:319:LEU:HD12	2:A:319:LEU:O	1.92	0.69
2:E:293:LEU:HD12	2:E:330:PRO:HG3	1.73	0.69
1:J:40:HIS:ND1	1:J:60:ILE:HD13	2.07	0.69
1:M:4:GLU:O	1:M:8:ARG:HB2	1.93	0.69
2:G:137:VAL:O	2:G:141:ILE:HG13	1.92	0.69
1:I:64:GLN:HE21	1:I:64:GLN:HA	1.57	0.69
2:D:137:VAL:O	2:D:141:ILE:HG13	1.92	0.69
2:D:233:ARG:HG3	2:D:233:ARG:HH11	1.58	0.69
2:D:319:LEU:HD12	2:D:319:LEU:O	1.92	0.69
2:E:319:LEU:HD12	2:E:319:LEU:O	1.92	0.69
2:E:528:ASP:HA	2:E:531:LYS:HZ1	1.58	0.69
2:G:392:ALA:HB2	2:G:433:ARG:NE	2.07	0.69
2:G:438:SER:HA	2:G:444:LEU:H	1.58	0.69
1:H:37:THR:OG1	1:H:40:HIS:HD2	1.75	0.69
2:A:366:ILE:HG13	2:A:372:LYS:HE2	1.71	0.69
2:A:406:PRO:CG	2:A:526:PRO:HG2	2.20	0.69
2:C:309:MET:CG	2:C:310:PRO:HD2	2.22	0.69
2:D:232:LYS:CD	2:D:263:GLU:OE1	2.30	0.69
2:D:528:ASP:HA	2:D:531:LYS:HZ1	1.58	0.69
2:F:150:LEU:HD12	2:F:153:PHE:HB3	1.74	0.69
2:G:319:LEU:HD12	2:G:319:LEU:O	1.92	0.69
2:A:393:LEU:CD2	2:A:464:LEU:HD11	2.23	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:463:PHE:C	2:A:467:VAL:HG12	2.13	0.69
2:G:483:ARG:O	2:G:486:GLU:HG2	1.92	0.69
2:C:319:LEU:O	2:C:319:LEU:HD12	1.92	0.68
2:D:227:THR:OG1	2:D:230:VAL:CG2	2.39	0.68
2:F:200:THR:HG21	2:F:256:GLU:HB3	1.74	0.68
1:L:4:GLU:O	1:L:8:ARG:HB2	1.93	0.68
2:A:360:LEU:CD1	2:A:462:MET:HE2	2.21	0.68
2:A:396:ALA:HB1	2:A:456:ILE:CD1	2.22	0.68
2:B:406:PRO:HB2	2:B:409:LEU:HD23	1.75	0.68
2:B:408:LYS:HE3	2:B:427:ASP:HB2	1.75	0.68
2:C:164:GLY:HA2	4:C:602:ATP:PA	2.32	0.68
2:F:335:MET:HE3	2:F:364:GLU:HA	1.76	0.68
2:G:443:LEU:O	2:G:460:ILE:HG12	1.94	0.68
2:B:233:ARG:HH11	2:B:233:ARG:HG3	1.58	0.68
2:D:360:LEU:CD1	2:D:462:MET:HE2	2.22	0.68
2:F:396:ALA:HB3	2:F:464:LEU:CD1	2.23	0.68
2:G:412:CYS:SG	2:G:483:ARG:HB2	2.32	0.68
2:E:401:PRO:HA	2:E:456:ILE:CG2	2.24	0.68
2:F:394:ALA:HA	2:F:464:LEU:HD21	1.74	0.68
2:B:364:GLU:OE1	2:B:372:LYS:HB3	1.94	0.68
2:E:399:MET:O	2:E:401:PRO:HD3	1.94	0.68
2:A:232:LYS:CD	2:A:263:GLU:OE1	2.30	0.68
2:E:446:GLY:HA2	2:E:454:PHE:HA	1.74	0.68
2:F:446:GLY:HA2	2:F:454:PHE:HA	1.73	0.68
2:A:299:TYR:CE2	2:A:310:PRO:CG	2.45	0.68
2:E:233:ARG:HH11	2:E:233:ARG:HG3	1.58	0.68
2:G:233:ARG:HH11	2:G:233:ARG:HG3	1.58	0.68
2:G:315:GLU:HG3	2:G:316:GLU:N	2.07	0.68
2:G:482:GLN:O	2:G:485:LEU:HG	1.92	0.68
2:A:446:GLY:HA2	2:A:454:PHE:HA	1.76	0.68
2:A:463:PHE:CD2	2:A:464:LEU:HD23	2.29	0.68
2:C:158:HIS:CD2	2:C:275:VAL:CG2	2.77	0.68
2:F:233:ARG:HH11	2:F:233:ARG:HG3	1.58	0.68
2:G:312:GLY:O	2:G:315:GLU:HG3	1.93	0.68
2:B:320:ASN:O	2:B:323:ILE:HG12	1.94	0.68
1:H:96:ASN:O	1:H:98:PRO:HD3	1.94	0.67
2:B:220:PHE:CE1	2:B:223:VAL:CG2	2.77	0.67
2:D:143:LYS:CE	2:D:286:GLU:CG	2.67	0.67
2:E:159:GLY:N	2:E:165:LYS:CD	2.52	0.67
2:E:401:PRO:HG3	2:E:461:HIS:CD2	2.28	0.67
2:C:334:MET:HE2	2:C:334:MET:CA	2.11	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:448:ARG:HA	2:C:452:LEU:HA	1.75	0.67
2:D:262:GLN:HG3	2:D:283:GLN:OE1	1.94	0.67
1:I:96:ASN:O	1:I:98:PRO:HD3	1.94	0.67
2:C:127:GLN:HB3	2:C:171:GLN:CA	2.25	0.67
2:E:336:PHE:HZ	2:E:348:MET:HG3	1.60	0.67
2:A:305:TYR:CE2	2:A:334:MET:HE1	2.29	0.67
2:B:336:PHE:HZ	2:B:348:MET:HG3	1.60	0.67
2:C:406:PRO:CG	2:C:526:PRO:HG2	2.20	0.67
1:I:97:GLU:HB2	1:L:51:LEU:CD1	2.24	0.67
2:C:302:LEU:N	2:C:302:LEU:HD23	2.10	0.67
2:G:385:LEU:CD1	2:G:393:LEU:CD1	2.72	0.67
1:K:42:GLU:O	1:K:46:LYS:HG3	1.95	0.67
2:B:156:PHE:CE2	2:B:278:SER:CB	2.66	0.67
2:B:367:THR:OG1	2:B:368:PRO:CD	2.41	0.67
2:G:392:ALA:CB	2:G:433:ARG:CD	2.66	0.67
1:J:96:ASN:O	1:J:98:PRO:HD3	1.94	0.67
1:M:42:GLU:O	1:M:46:LYS:HG3	1.95	0.67
2:B:484:LEU:CG	2:B:531:LYS:O	2.42	0.67
2:B:355:LEU:CD1	2:B:462:MET:CE	2.72	0.67
2:A:406:PRO:HB2	2:A:409:LEU:HD23	1.77	0.67
2:D:232:LYS:CE	2:D:260:TRP:NE1	2.57	0.67
2:G:360:LEU:H	2:G:360:LEU:HD22	1.59	0.67
2:G:318:VAL:CG1	2:G:349:ALA:HB2	2.24	0.66
2:B:274:ASP:OD1	2:B:276:GLU:HB2	1.95	0.66
2:F:211:LEU:CD1	2:F:239:LEU:HD22	2.19	0.66
2:G:258:ILE:H	2:G:258:ILE:HD12	1.59	0.66
2:D:388:GLU:OE1	2:D:433:ARG:CZ	2.44	0.66
2:D:406:PRO:HB2	2:D:409:LEU:HD23	1.76	0.66
2:F:128:MET:HB2	2:F:171:GLN:NE2	2.10	0.66
2:B:530:PRO:HD2	2:B:531:LYS:CD	2.26	0.66
2:C:313:GLU:N	2:C:313:GLU:OE1	2.28	0.66
2:C:388:GLU:OE1	2:C:433:ARG:CZ	2.44	0.66
2:C:530:PRO:HD2	2:C:531:LYS:CD	2.26	0.66
2:G:354:LYS:NZ	2:G:358:ARG:HD2	2.10	0.66
2:B:388:GLU:OE1	2:B:433:ARG:CZ	2.44	0.66
2:A:529:PHE:HB3	2:A:532:PHE:CE1	2.31	0.66
2:B:533:MET:HA	2:B:533:MET:HE3	1.76	0.66
2:A:355:LEU:CD1	2:A:462:MET:CE	2.72	0.66
2:C:533:MET:CB	2:C:540:TYR:HE2	2.09	0.66
2:D:232:LYS:HE2	2:D:260:TRP:CD2	2.31	0.66
1:H:8:ARG:HG2	1:H:8:ARG:NH1	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:ILE:HG21	1:K:88:GLU:HG3	1.78	0.66
2:B:307:MET:HA	2:B:307:MET:HE3	1.78	0.66
2:D:115:LEU:CD2	2:D:180:ILE:HB	2.26	0.66
2:D:232:LYS:NZ	2:D:260:TRP:NE1	2.44	0.66
2:D:305:TYR:CE2	2:D:334:MET:HE1	2.28	0.66
2:D:486:GLU:HA	2:D:486:GLU:OE2	1.94	0.66
2:D:530:PRO:HD2	2:D:531:LYS:CD	2.26	0.66
2:E:115:LEU:CD2	2:E:180:ILE:HB	2.25	0.66
2:E:388:GLU:OE1	2:E:433:ARG:CZ	2.44	0.66
2:F:388:GLU:OE1	2:F:433:ARG:CZ	2.44	0.66
2:F:396:ALA:HB3	2:F:464:LEU:HD11	1.77	0.66
2:A:150:LEU:HD12	2:A:153:PHE:HB3	1.77	0.66
2:G:305:TYR:HB3	2:G:337:PHE:CZ	2.31	0.66
2:B:156:PHE:CZ	2:B:278:SER:CB	2.77	0.66
2:B:164:GLY:HA2	4:B:602:ATP:O1A	1.96	0.66
2:D:131:TYR:CE2	2:D:301:PHE:HD1	2.13	0.66
2:D:259:ARG:HH11	2:D:259:ARG:HG3	1.61	0.66
2:G:255:GLU:HA	2:G:258:ILE:HD13	1.78	0.66
2:G:534:GLN:HA	2:G:537:GLN:HB2	1.78	0.66
2:B:211:LEU:CD1	2:B:239:LEU:HD22	2.19	0.65
2:C:115:LEU:CD2	2:C:180:ILE:HB	2.26	0.65
2:C:141:ILE:HD12	2:C:175:LYS:NZ	2.11	0.65
2:C:232:LYS:CD	2:C:263:GLU:OE1	2.30	0.65
2:E:393:LEU:HB2	2:E:437:LEU:HD11	1.77	0.65
2:F:115:LEU:CD2	2:F:180:ILE:HB	2.25	0.65
1:K:37:THR:OG1	1:K:40:HIS:HD2	1.79	0.65
2:A:293:LEU:HD23	2:A:297:GLU:HB3	1.78	0.65
2:A:388:GLU:OE1	2:A:433:ARG:CZ	2.44	0.65
2:C:403:VAL:O	2:C:405:ILE:HG22	1.97	0.65
1:L:42:GLU:O	1:L:46:LYS:HG3	1.95	0.65
2:A:308:PRO:HB2	2:A:345:PHE:CE2	2.30	0.65
2:A:347:LYS:O	2:A:347:LYS:HD3	1.96	0.65
2:B:115:LEU:CD2	2:B:180:ILE:HB	2.25	0.65
2:G:115:LEU:CD2	2:G:180:ILE:HB	2.26	0.65
1:L:37:THR:OG1	1:L:40:HIS:HD2	1.79	0.65
2:A:115:LEU:CD2	2:A:180:ILE:HB	2.26	0.65
2:B:528:ASP:CA	2:B:531:LYS:HZ1	2.10	0.65
2:D:437:LEU:HB3	2:D:444:LEU:HD23	1.78	0.65
2:G:232:LYS:HD3	2:G:263:GLU:OE1	1.96	0.65
2:G:478:SER:O	2:G:482:GLN:HG2	1.95	0.65
2:E:227:THR:OG1	2:E:230:VAL:HG23	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:318:VAL:HG11	2:G:349:ALA:HB2	1.78	0.65
1:M:72:ILE:HG21	1:M:88:GLU:HG3	1.78	0.65
2:A:112:ARG:NH1	2:A:115:LEU:HD12	2.12	0.65
2:B:232:LYS:CD	2:B:263:GLU:OE1	2.30	0.65
2:C:529:PHE:HB3	2:C:532:PHE:CE1	2.31	0.65
2:D:347:LYS:O	2:D:347:LYS:HD3	1.96	0.65
2:G:293:LEU:HD23	2:G:297:GLU:HB3	1.78	0.65
2:A:483:ARG:HA	2:A:483:ARG:NE	2.11	0.65
2:D:313:GLU:CD	2:D:313:GLU:H	1.96	0.65
2:E:129:THR:O	2:E:132:ILE:CD1	2.45	0.65
2:E:133:ARG:O	2:E:137:VAL:HG23	1.96	0.65
2:G:398:VAL:HG11	2:G:477:ILE:HA	1.77	0.65
2:B:112:ARG:NH1	2:B:115:LEU:HD12	2.12	0.65
2:B:411:SER:HB3	2:B:427:ASP:OD2	1.97	0.65
1:J:4:GLU:O	1:J:8:ARG:HB2	1.97	0.65
2:B:302:LEU:HD13	2:B:307:MET:CB	2.26	0.65
2:C:305:TYR:CZ	2:C:334:MET:HE1	2.16	0.65
2:C:334:MET:CE	2:C:334:MET:HA	2.19	0.65
2:C:481:GLU:O	2:C:485:LEU:HD13	1.97	0.65
2:C:538:LYS:HB2	2:C:538:LYS:HZ2	1.62	0.65
2:E:131:TYR:CE2	2:E:301:PHE:HD1	2.13	0.65
2:E:211:LEU:HD23	2:E:242:ARG:NE	2.11	0.65
2:E:347:LYS:O	2:E:347:LYS:HD3	1.96	0.65
2:A:530:PRO:HD2	2:A:531:LYS:CD	2.26	0.65
2:B:293:LEU:HD23	2:B:297:GLU:HB3	1.78	0.65
2:B:347:LYS:O	2:B:347:LYS:HD3	1.96	0.65
2:B:399:MET:CE	2:B:413:VAL:HG21	2.27	0.65
2:C:347:LYS:O	2:C:347:LYS:HD3	1.96	0.65
2:D:133:ARG:O	2:D:137:VAL:HG23	1.96	0.65
2:D:310:PRO:HA	2:D:315:GLU:OE1	1.96	0.65
2:F:293:LEU:HD23	2:F:297:GLU:HB3	1.78	0.65
1:L:72:ILE:HG21	1:L:88:GLU:HG3	1.78	0.64
2:C:112:ARG:NH1	2:C:115:LEU:HD12	2.12	0.64
2:C:158:HIS:CD2	2:C:275:VAL:HG21	2.31	0.64
2:D:211:LEU:CD1	2:D:239:LEU:HD22	2.19	0.64
2:G:524:ILE:HD12	2:G:526:PRO:HG3	1.77	0.64
1:K:10:LEU:HD22	1:K:58:LEU:HD21	1.79	0.64
2:B:406:PRO:CG	2:B:526:PRO:HG2	2.20	0.64
2:C:133:ARG:O	2:C:137:VAL:HG23	1.96	0.64
2:G:347:LYS:HE3	2:G:351:LEU:HD21	1.79	0.64
1:J:37:THR:OG1	1:J:40:HIS:CD2	2.51	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:37:THR:OG1	1:M:40:HIS:HD2	1.79	0.64
2:B:133:ARG:O	2:B:137:VAL:HG23	1.96	0.64
2:B:352:ASN:O	2:B:355:LEU:HB2	1.97	0.64
2:D:388:GLU:OE1	2:D:433:ARG:NE	2.31	0.64
2:G:112:ARG:NH1	2:G:115:LEU:HD12	2.12	0.64
2:D:112:ARG:NH1	2:D:115:LEU:HD12	2.12	0.64
2:F:158:HIS:NE2	2:F:287:PHE:HB3	2.11	0.64
2:F:340:CYS:O	2:F:343:LYS:N	2.26	0.64
2:A:366:ILE:HD11	2:A:372:LYS:HE2	1.80	0.64
2:A:388:GLU:OE1	2:A:433:ARG:NE	2.31	0.64
2:C:388:GLU:OE1	2:C:433:ARG:NE	2.31	0.64
2:E:388:GLU:OE1	2:E:433:ARG:NE	2.31	0.64
2:E:530:PRO:HD2	2:E:531:LYS:CD	2.26	0.64
2:A:474:ALA:O	2:A:477:ILE:HG23	1.98	0.64
2:B:538:LYS:HB2	2:B:538:LYS:NZ	2.12	0.64
2:F:302:LEU:HB3	2:F:307:MET:CB	2.28	0.64
2:G:211:LEU:CD1	2:G:239:LEU:HD22	2.19	0.64
2:A:143:LYS:CE	2:A:286:GLU:CG	2.67	0.64
2:C:393:LEU:HD23	2:C:464:LEU:HD11	1.78	0.64
2:D:533:MET:HG3	2:D:540:TYR:CE2	2.31	0.64
2:E:293:LEU:HD23	2:E:297:GLU:HB3	1.78	0.64
2:F:112:ARG:NH1	2:F:115:LEU:HD12	2.12	0.64
2:F:475:ASN:O	2:F:479:ILE:HG13	1.98	0.64
2:A:211:LEU:CD1	2:A:239:LEU:HD22	2.20	0.64
2:A:220:PHE:CE1	2:A:223:VAL:HG22	2.33	0.64
2:A:307:MET:SD	2:A:308:PRO:HD2	2.38	0.64
2:B:388:GLU:OE1	2:B:433:ARG:NE	2.31	0.64
2:C:393:LEU:HD11	2:C:443:LEU:HD12	1.80	0.64
1:M:10:LEU:HD22	1:M:58:LEU:HD21	1.80	0.64
2:C:293:LEU:HD23	2:C:297:GLU:HB3	1.78	0.64
2:D:293:LEU:HD23	2:D:297:GLU:HB3	1.78	0.64
2:D:305:TYR:HE2	2:D:334:MET:SD	2.21	0.64
2:E:143:LYS:CE	2:E:286:GLU:CG	2.67	0.64
2:G:128:MET:HB2	2:G:171:GLN:NE2	2.12	0.64
2:G:158:HIS:NE2	2:G:287:PHE:HB3	2.12	0.64
1:H:37:THR:OG1	1:H:40:HIS:CD2	2.51	0.64
1:M:77:TYR:CD1	1:M:77:TYR:C	2.71	0.64
2:D:259:ARG:HG3	2:D:259:ARG:NH1	2.10	0.64
1:I:4:GLU:O	1:I:8:ARG:HB2	1.97	0.63
2:A:293:LEU:HD12	2:A:330:PRO:HD3	1.80	0.63
2:B:327:SER:HB2	2:B:459:ILE:HD11	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:TYR:HD2	2:F:136:HIS:HD1	1.46	0.63
1:I:72:ILE:HG21	1:I:88:GLU:HG3	1.79	0.63
1:J:72:ILE:HG21	1:J:88:GLU:HG3	1.79	0.63
2:D:274:ASP:OD1	2:D:276:GLU:HB2	1.97	0.63
2:E:112:ARG:NH1	2:E:115:LEU:HD12	2.12	0.63
2:E:141:ILE:HG23	2:E:179:LEU:CD2	2.29	0.63
2:G:360:LEU:HA	2:G:363:VAL:HG12	1.79	0.63
1:K:77:TYR:C	1:K:77:TYR:CD1	2.71	0.63
2:A:382:VAL:HG22	2:A:393:LEU:HD13	1.77	0.63
2:B:131:TYR:CE2	2:B:301:PHE:HD1	2.13	0.63
2:B:164:GLY:HA2	4:B:602:ATP:PA	2.39	0.63
2:C:405:ILE:HG12	2:C:410:TRP:CZ3	2.34	0.63
2:F:388:GLU:OE1	2:F:433:ARG:NE	2.31	0.63
2:F:437:LEU:HB3	2:F:444:LEU:HD22	1.80	0.63
2:G:392:ALA:HB2	2:G:433:ARG:HE	1.62	0.63
1:L:77:TYR:CD1	1:L:77:TYR:C	2.71	0.63
2:B:293:LEU:H	2:B:328:GLY:CA	2.11	0.63
2:B:399:MET:CG	2:B:400:PRO:HD2	2.20	0.63
2:C:128:MET:HG2	2:C:167:VAL:HG22	1.79	0.63
2:D:141:ILE:HG23	2:D:179:LEU:CD2	2.29	0.63
2:G:405:ILE:HG12	2:G:410:TRP:CZ3	2.34	0.63
2:A:405:ILE:HG12	2:A:410:TRP:CZ3	2.34	0.63
2:A:462:MET:HG3	2:A:465:LYS:HZ1	1.64	0.63
2:C:141:ILE:HG23	2:C:179:LEU:CD2	2.28	0.63
2:C:413:VAL:CG1	2:C:480:LEU:HB2	2.29	0.63
1:H:72:ILE:HG21	1:H:88:GLU:HG3	1.80	0.63
2:A:128:MET:HG3	2:A:167:VAL:HG22	1.81	0.63
2:A:463:PHE:CZ	2:A:467:VAL:HG21	2.33	0.63
2:B:187:ILE:HD12	2:B:246:LEU:O	1.99	0.63
2:C:322:THR:HG21	2:C:336:PHE:CE1	2.34	0.63
2:D:531:LYS:H	2:D:531:LYS:CD	1.96	0.63
2:E:211:LEU:HD23	2:E:242:ARG:CZ	2.29	0.63
2:E:307:MET:HG3	2:E:308:PRO:HD2	1.81	0.63
2:G:141:ILE:HG23	2:G:179:LEU:CD2	2.29	0.63
2:B:141:ILE:HG23	2:B:179:LEU:CD2	2.29	0.63
2:B:411:SER:CB	2:B:427:ASP:OD2	2.47	0.63
2:C:164:GLY:HA2	4:C:602:ATP:O1A	1.99	0.63
2:D:335:MET:CE	2:D:373:SER:HA	2.28	0.63
2:E:293:LEU:HD12	2:E:330:PRO:HD3	1.80	0.63
1:L:47:MET:HB2	1:L:53:ARG:CG	2.29	0.62
2:A:131:TYR:CE2	2:A:301:PHE:HD1	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:474:ALA:HA	2:A:477:ILE:HG22	1.81	0.62
2:C:187:ILE:HD12	2:C:246:LEU:O	1.99	0.62
2:C:358:ARG:HH21	2:D:426:LEU:HD21	1.64	0.62
2:G:409:LEU:HD13	2:G:484:LEU:HD11	1.79	0.62
1:I:37:THR:OG1	1:I:40:HIS:CD2	2.51	0.62
2:A:275:VAL:O	2:A:275:VAL:HG13	2.00	0.62
2:B:351:LEU:HD21	2:B:363:VAL:HG23	1.80	0.62
2:B:364:GLU:OE2	2:B:372:LYS:HB3	1.98	0.62
2:B:405:ILE:HG12	2:B:410:TRP:CZ3	2.34	0.62
2:C:393:LEU:HD22	2:C:464:LEU:HD21	1.82	0.62
2:D:484:LEU:HD21	2:D:533:MET:CG	2.28	0.62
1:J:77:TYR:CD1	1:J:77:TYR:C	2.73	0.62
1:K:10:LEU:HD13	1:K:58:LEU:CD2	2.29	0.62
2:B:528:ASP:CA	2:B:531:LYS:NZ	2.63	0.62
2:E:405:ILE:HG12	2:E:410:TRP:CZ3	2.34	0.62
1:L:10:LEU:HD13	1:L:58:LEU:CD2	2.30	0.62
2:A:141:ILE:HG23	2:A:179:LEU:CD2	2.29	0.62
2:B:259:ARG:CG	2:B:259:ARG:HH11	2.13	0.62
2:F:394:ALA:HA	2:F:464:LEU:CD2	2.29	0.62
2:G:385:LEU:HD13	2:G:393:LEU:HD12	1.80	0.62
2:B:195:THR:O	2:B:254:GLN:NE2	2.32	0.62
2:D:232:LYS:CE	2:D:260:TRP:CD2	2.83	0.62
1:H:77:TYR:C	1:H:77:TYR:CD1	2.73	0.62
2:C:211:LEU:CD1	2:C:239:LEU:HD22	2.19	0.62
2:C:528:ASP:CA	2:C:531:LYS:NZ	2.63	0.62
2:E:528:ASP:CA	2:E:531:LYS:NZ	2.63	0.62
2:G:315:GLU:O	2:G:318:VAL:N	2.32	0.62
1:K:17:LEU:HD23	1:K:21:PHE:CD2	2.35	0.62
2:A:439:LYS:O	2:A:440:ARG:CG	2.43	0.62
2:B:484:LEU:HD11	2:B:531:LYS:C	2.20	0.62
2:D:360:LEU:HD13	2:D:462:MET:HE3	1.81	0.62
2:E:464:LEU:O	2:E:468:VAL:HG22	1.99	0.62
1:H:42:GLU:O	1:H:46:LYS:HG3	2.00	0.62
1:J:42:GLU:O	1:J:46:LYS:HG3	2.00	0.62
1:L:10:LEU:HD22	1:L:58:LEU:HD21	1.80	0.62
2:D:484:LEU:CD2	2:D:533:MET:HG2	2.30	0.62
2:E:413:VAL:CG1	2:E:480:LEU:HB2	2.30	0.62
2:F:335:MET:CE	2:F:364:GLU:HA	2.29	0.62
2:G:529:PHE:HB3	2:G:532:PHE:CE1	2.34	0.62
2:D:122:GLY:HA3	2:D:187:ILE:HG23	1.82	0.62
2:D:438:SER:HB2	2:D:444:LEU:C	2.19	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:122:GLY:HA3	2:E:187:ILE:HG23	1.82	0.62
2:F:258:ILE:CG2	2:F:281:ALA:HB2	2.29	0.62
2:G:530:PRO:HD2	2:G:531:LYS:HE3	1.81	0.62
2:A:474:ALA:HA	2:A:477:ILE:CG2	2.30	0.62
2:A:528:ASP:CA	2:A:531:LYS:NZ	2.63	0.62
2:B:239:LEU:O	2:B:239:LEU:HD13	2.00	0.62
2:B:275:VAL:HG13	2:B:275:VAL:O	2.00	0.62
2:C:533:MET:HB3	2:C:540:TYR:CE2	2.27	0.62
2:E:437:LEU:HD13	2:E:444:LEU:HD13	1.80	0.62
2:F:218:LEU:H	2:F:218:LEU:HD23	1.63	0.62
2:G:401:PRO:HB2	2:G:458:HIS:CD2	2.34	0.62
1:I:47:MET:HB2	1:I:53:ARG:CG	2.30	0.61
1:L:17:LEU:HD23	1:L:21:PHE:CD2	2.35	0.61
2:D:298:CYS:SG	2:D:323:ILE:HG12	2.40	0.61
2:D:528:ASP:CA	2:D:531:LYS:NZ	2.63	0.61
2:G:396:ALA:HB2	2:G:414:ILE:HD11	1.82	0.61
1:M:10:LEU:HD13	1:M:58:LEU:CD2	2.30	0.61
2:B:127:GLN:CG	2:B:174:SER:HB2	2.30	0.61
2:E:398:VAL:HG21	2:E:477:ILE:HG12	1.82	0.61
2:G:312:GLY:H	2:G:315:GLU:HG2	1.64	0.61
1:M:17:LEU:HD23	1:M:21:PHE:CD2	2.35	0.61
2:C:117:ARG:HH22	2:D:240:ILE:HG22	1.66	0.61
2:D:239:LEU:O	2:D:239:LEU:HD13	2.00	0.61
2:D:309:MET:SD	2:D:310:PRO:CD	2.88	0.61
2:E:128:MET:HG3	2:E:167:VAL:CG2	2.31	0.61
2:F:122:GLY:HA3	2:F:187:ILE:HG23	1.82	0.61
2:B:533:MET:O	2:B:540:TYR:HD2	1.81	0.61
2:C:122:GLY:HA3	2:C:187:ILE:HG23	1.82	0.61
2:C:403:VAL:O	2:C:405:ILE:CG2	2.48	0.61
2:E:256:GLU:HA	2:E:256:GLU:OE2	1.99	0.61
2:F:400:PRO:HG2	2:F:405:ILE:HG21	1.82	0.61
2:F:478:SER:O	2:F:482:GLN:HG2	2.00	0.61
2:A:128:MET:HG3	2:A:167:VAL:CG2	2.31	0.61
2:A:259:ARG:HH11	2:A:259:ARG:CG	2.13	0.61
2:D:275:VAL:O	2:D:275:VAL:HG13	2.00	0.61
2:F:239:LEU:O	2:F:239:LEU:HD13	2.01	0.61
2:C:443:LEU:HD23	2:C:443:LEU:N	2.16	0.61
2:F:158:HIS:CE1	2:F:289:GLU:HB2	2.35	0.61
2:F:347:LYS:HE3	2:F:351:LEU:HD21	1.81	0.61
1:I:42:GLU:O	1:I:46:LYS:HG3	2.00	0.61
2:A:401:PRO:HB3	2:A:461:HIS:HD2	1.63	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:ARG:HB2	2:C:442:ALA:HB3	1.83	0.61
2:C:211:LEU:CD2	2:C:242:ARG:CG	2.76	0.61
2:D:355:LEU:HD12	2:D:462:MET:SD	2.41	0.61
2:E:204:PHE:O	2:E:207:ILE:HG22	2.01	0.61
2:F:204:PHE:O	2:F:207:ILE:HG22	2.01	0.61
2:G:438:SER:O	2:G:442:ALA:HA	2.01	0.61
2:B:204:PHE:O	2:B:207:ILE:HG22	2.01	0.61
2:C:204:PHE:O	2:C:207:ILE:HG22	2.01	0.61
2:D:204:PHE:O	2:D:207:ILE:HG22	2.01	0.61
2:D:308:PRO:HD3	2:D:343:LYS:HB3	1.81	0.61
2:E:211:LEU:CD1	2:E:239:LEU:HD22	2.19	0.61
2:E:529:PHE:N	2:E:531:LYS:HZ3	1.99	0.61
2:G:355:LEU:C	2:G:357:SER:H	2.04	0.61
1:I:77:TYR:CD1	1:I:77:TYR:C	2.73	0.61
2:A:204:PHE:O	2:A:207:ILE:HG22	2.01	0.61
2:B:122:GLY:HA3	2:B:187:ILE:HG23	1.82	0.61
2:C:211:LEU:HD23	2:C:242:ARG:NE	2.16	0.61
2:D:529:PHE:N	2:D:531:LYS:HZ3	1.99	0.61
2:G:314:LYS:HB3	2:G:314:LYS:HZ3	1.63	0.61
2:A:360:LEU:HD13	2:A:462:MET:HE3	1.82	0.60
2:A:467:VAL:O	2:A:467:VAL:HG22	2.01	0.60
2:B:399:MET:HG2	2:B:410:TRP:NE1	2.16	0.60
2:C:239:LEU:HD13	2:C:239:LEU:O	2.00	0.60
2:C:327:SER:HB3	2:C:459:ILE:HD11	1.81	0.60
2:D:368:PRO:CB	4:D:602:ATP:O3'	2.43	0.60
2:E:259:ARG:HH11	2:E:259:ARG:CG	2.13	0.60
2:B:211:LEU:HD23	2:B:242:ARG:NE	2.16	0.60
2:B:307:MET:HG3	2:B:308:PRO:CD	2.31	0.60
2:D:302:LEU:HD13	2:D:307:MET:SD	2.41	0.60
2:E:239:LEU:O	2:E:239:LEU:HD13	2.01	0.60
2:F:141:ILE:HG23	2:F:179:LEU:HD11	1.82	0.60
2:G:204:PHE:O	2:G:207:ILE:HG22	2.01	0.60
2:G:247:PHE:HB2	2:G:268:CYS:SG	2.41	0.60
1:K:37:THR:OG1	1:K:40:HIS:CD2	2.54	0.60
2:A:259:ARG:HG3	2:A:259:ARG:NH1	2.17	0.60
2:B:207:ILE:HD11	2:B:247:PHE:CD2	2.37	0.60
2:D:473:ILE:HG22	2:D:543:LEU:HD12	1.82	0.60
2:F:540:TYR:HA	2:F:543:LEU:HD23	1.84	0.60
2:B:483:ARG:HA	2:B:483:ARG:NH2	2.16	0.60
2:B:484:LEU:CD1	2:B:531:LYS:HA	2.31	0.60
2:D:141:ILE:HD12	2:D:175:LYS:NZ	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:239:LEU:O	2:G:239:LEU:HD13	2.00	0.60
2:A:407:VAL:HG23	2:A:452:LEU:O	2.01	0.60
2:B:477:ILE:O	2:B:477:ILE:HD13	2.02	0.60
2:E:398:VAL:HG23	2:E:477:ILE:HG12	1.82	0.60
2:E:407:VAL:HG23	2:E:452:LEU:O	2.02	0.60
2:F:207:ILE:HD11	2:F:247:PHE:CD2	2.37	0.60
1:J:47:MET:HB2	1:J:53:ARG:CG	2.30	0.60
1:K:47:MET:HB2	1:K:53:ARG:CG	2.29	0.60
2:A:122:GLY:HA3	2:A:187:ILE:HG23	1.82	0.60
2:A:239:LEU:O	2:A:239:LEU:HD13	2.01	0.60
2:A:398:VAL:HG23	2:A:398:VAL:O	2.01	0.60
2:B:524:ILE:HD13	2:B:526:PRO:HD3	1.83	0.60
2:C:309:MET:HA	2:C:309:MET:HE1	1.84	0.60
2:C:339:SER:O	2:C:339:SER:OG	2.14	0.60
2:D:335:MET:HE1	2:D:373:SER:HA	1.83	0.60
2:E:176:SER:HB3	2:E:179:LEU:HD22	1.81	0.60
2:G:122:GLY:HA3	2:G:187:ILE:HG23	1.82	0.60
2:G:207:ILE:HD11	2:G:247:PHE:CD2	2.37	0.60
2:B:336:PHE:CZ	2:B:348:MET:HG3	2.37	0.60
2:B:407:VAL:HG23	2:B:452:LEU:O	2.01	0.60
2:C:190:LEU:HD13	2:C:203:LEU:CD2	2.32	0.60
2:C:275:VAL:O	2:C:275:VAL:HG13	1.99	0.60
2:C:524:ILE:HD13	2:C:526:PRO:HD3	1.83	0.60
2:C:529:PHE:N	2:C:531:LYS:HZ3	2.00	0.60
2:D:355:LEU:HD12	2:D:355:LEU:O	2.01	0.60
2:D:407:VAL:HG23	2:D:452:LEU:O	2.01	0.60
2:E:350:GLN:HB3	2:E:354:LYS:HE2	1.83	0.60
2:F:407:VAL:HG23	2:F:452:LEU:O	2.02	0.60
2:B:128:MET:HG2	2:B:167:VAL:HG22	1.83	0.60
2:B:129:THR:O	2:B:132:ILE:HD11	2.02	0.60
2:C:445:SER:HB3	2:C:455:LYS:HG3	1.82	0.60
2:D:355:LEU:HD11	2:D:462:MET:HE3	1.75	0.60
2:F:127:GLN:HB2	2:F:171:GLN:HG2	1.83	0.60
2:B:339:SER:O	2:B:351:LEU:HD12	2.02	0.60
2:D:424:GLU:OE1	2:D:426:LEU:HB2	2.02	0.60
2:G:321:LYS:HD3	2:G:352:ASN:HB3	1.83	0.60
1:I:104:VAL:HG11	1:L:52:GLU:OE2	2.02	0.60
2:C:211:LEU:HD21	2:C:242:ARG:CG	2.32	0.60
2:F:175:LYS:NZ	2:F:175:LYS:HB3	2.16	0.60
2:G:309:MET:HE2	2:G:309:MET:HA	1.83	0.60
2:A:244:ASN:HA	2:A:267:ARG:CZ	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:436:ARG:O	2:A:440:ARG:HG3	2.02	0.59
2:B:259:ARG:NH1	2:B:259:ARG:HG3	2.17	0.59
2:B:351:LEU:O	2:B:351:LEU:HD23	2.02	0.59
2:C:528:ASP:CA	2:C:531:LYS:HZ1	2.14	0.59
2:D:207:ILE:HD11	2:D:247:PHE:CD2	2.37	0.59
2:E:460:ILE:O	2:E:464:LEU:HG	2.02	0.59
2:F:160:ARG:HG2	2:F:161:ALA:H	1.67	0.59
1:H:10:LEU:HD22	1:H:58:LEU:HD21	1.84	0.59
1:M:37:THR:OG1	1:M:40:HIS:CD2	2.54	0.59
2:A:342:PRO:HG2	2:A:347:LYS:HG3	1.84	0.59
2:C:313:GLU:H	2:C:313:GLU:CD	2.05	0.59
2:D:477:ILE:O	2:D:477:ILE:HD13	2.02	0.59
2:E:158:HIS:HE1	2:E:289:GLU:HB2	1.67	0.59
2:E:324:GLU:HG3	2:E:458:HIS:CE1	2.38	0.59
2:F:190:LEU:HD13	2:F:203:LEU:CD2	2.32	0.59
2:F:242:ARG:HB3	2:F:245:THR:OG1	2.03	0.59
1:I:8:ARG:HH11	1:I:8:ARG:CG	2.11	0.59
2:A:524:ILE:HD13	2:A:526:PRO:HD3	1.84	0.59
2:B:190:LEU:HD13	2:B:203:LEU:CD2	2.32	0.59
2:B:211:LEU:HD21	2:B:242:ARG:CG	2.32	0.59
2:D:533:MET:O	2:D:540:TYR:CD2	2.55	0.59
2:E:137:VAL:HG22	2:E:168:ILE:HG23	1.84	0.59
2:E:232:LYS:CD	2:E:263:GLU:OE1	2.30	0.59
2:G:258:ILE:HG21	2:G:281:ALA:HB2	1.84	0.59
2:G:412:CYS:CB	2:G:480:LEU:HA	2.31	0.59
1:I:10:LEU:HD13	1:I:58:LEU:CD2	2.33	0.59
1:J:17:LEU:HD23	1:J:21:PHE:CD2	2.37	0.59
1:L:37:THR:OG1	1:L:40:HIS:CD2	2.54	0.59
2:A:464:LEU:HA	2:A:467:VAL:HG13	1.75	0.59
2:B:128:MET:HB2	2:B:171:GLN:HE21	1.68	0.59
2:B:211:LEU:CD2	2:B:242:ARG:CG	2.76	0.59
2:D:309:MET:HA	2:D:309:MET:HE1	1.81	0.59
2:D:524:ILE:HD13	2:D:526:PRO:HD3	1.83	0.59
2:E:475:ASN:O	2:E:479:ILE:HG13	2.03	0.59
2:G:332:THR:HG23	2:G:374:LEU:CD2	2.32	0.59
1:L:8:ARG:HG2	1:L:8:ARG:NH1	2.11	0.59
2:A:190:LEU:HD13	2:A:203:LEU:CD2	2.32	0.59
2:A:305:TYR:CE2	2:A:334:MET:CE	2.85	0.59
2:A:327:SER:OG	2:A:458:HIS:HB2	2.02	0.59
2:D:190:LEU:HD13	2:D:203:LEU:CD2	2.32	0.59
2:E:158:HIS:CE1	2:E:289:GLU:HB2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:207:ILE:HD11	2:E:247:PHE:CD2	2.37	0.59
2:F:537:GLN:HA	2:F:540:TYR:CD2	2.38	0.59
2:G:140:VAL:HG12	2:G:172:ALA:HB1	1.85	0.59
1:I:17:LEU:HD23	1:I:21:PHE:CD2	2.37	0.59
2:C:293:LEU:CD1	2:C:330:PRO:HG3	2.32	0.59
2:A:533:MET:HB3	2:A:540:TYR:CE2	2.37	0.59
2:B:147:MET:HE2	2:B:147:MET:HA	1.83	0.59
2:C:207:ILE:HD11	2:C:247:PHE:CD2	2.37	0.59
2:C:445:SER:O	2:C:454:PHE:CA	2.50	0.59
2:D:310:PRO:HB2	2:D:316:GLU:OE2	2.03	0.59
2:C:436:ARG:O	2:C:440:ARG:HG3	2.02	0.59
2:D:457:ASP:H	2:D:460:ILE:HG22	1.68	0.59
2:F:214:GLU:HG3	2:G:237:ASN:ND2	2.17	0.59
2:F:315:GLU:HG3	2:F:316:GLU:N	2.18	0.59
2:G:143:LYS:HE2	2:G:286:GLU:HG2	1.84	0.59
2:G:190:LEU:HD13	2:G:203:LEU:CD2	2.32	0.59
1:J:10:LEU:HD13	1:J:58:LEU:CD2	2.33	0.59
2:A:133:ARG:O	2:A:137:VAL:HG23	2.01	0.59
2:B:529:PHE:N	2:B:531:LYS:HZ3	2.01	0.59
2:G:329:ASN:HB3	2:G:332:THR:OG1	2.03	0.59
2:G:339:SER:O	2:G:351:LEU:HD11	2.03	0.59
1:H:10:LEU:HD13	1:H:58:LEU:CD2	2.33	0.59
1:H:17:LEU:HD23	1:H:21:PHE:CD2	2.37	0.59
1:K:8:ARG:HG2	1:K:8:ARG:NH1	2.11	0.59
1:M:50:ARG:HA	1:M:53:ARG:HE	1.68	0.59
2:B:457:ASP:H	2:B:460:ILE:HG22	1.68	0.59
2:C:164:GLY:HA2	4:C:602:ATP:O3A	2.03	0.59
2:F:347:LYS:O	2:F:351:LEU:HG	2.02	0.59
2:D:140:VAL:HG12	2:D:172:ALA:HB1	1.85	0.58
2:D:160:ARG:O	2:D:163:SER:CB	2.47	0.58
2:F:211:LEU:HD21	2:F:242:ARG:HD2	1.84	0.58
1:J:10:LEU:HD22	1:J:58:LEU:HD21	1.84	0.58
2:A:305:TYR:HH	4:A:602:ATP:H2	1.50	0.58
2:B:426:LEU:HD23	2:B:426:LEU:C	2.23	0.58
2:C:368:PRO:HB2	4:C:602:ATP:O3'	2.03	0.58
2:D:187:ILE:HD12	2:D:246:LEU:O	2.03	0.58
2:D:321:LYS:HD2	2:D:325:LEU:HG	1.85	0.58
2:E:369:TYR:HB2	4:E:602:ATP:H4'	1.84	0.58
2:E:524:ILE:HD13	2:E:526:PRO:HD3	1.83	0.58
2:G:327:SER:HB2	2:G:459:ILE:CG1	2.32	0.58
2:G:398:VAL:HB	2:G:413:VAL:HG11	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:393:LEU:HD22	2:A:464:LEU:HD21	1.79	0.58
2:C:128:MET:HB2	2:C:171:GLN:HE21	1.65	0.58
2:D:220:PHE:CE1	2:D:223:VAL:HG22	2.38	0.58
2:D:355:LEU:CD1	2:D:462:MET:HE3	2.32	0.58
2:E:190:LEU:HD13	2:E:203:LEU:CD2	2.32	0.58
2:E:403:VAL:HG11	2:E:536:HIS:HE1	1.68	0.58
1:K:50:ARG:HA	1:K:53:ARG:HE	1.68	0.58
2:B:331:ALA:O	2:B:335:MET:HG3	2.04	0.58
2:B:446:GLY:HA3	2:B:454:PHE:CD2	2.38	0.58
2:C:127:GLN:CB	2:C:171:GLN:HA	2.32	0.58
2:C:532:PHE:C	2:C:534:GLN:H	2.06	0.58
2:D:533:MET:CG	2:D:540:TYR:OH	2.35	0.58
2:F:368:PRO:HB2	4:F:602:ATP:O3'	2.03	0.58
2:G:407:VAL:HG23	2:G:452:LEU:O	2.02	0.58
4:G:602:ATP:O2G	4:G:602:ATP:O1B	2.21	0.58
4:A:602:ATP:O1B	4:A:602:ATP:O2G	2.21	0.58
2:C:426:LEU:C	2:C:428:ASP:H	2.07	0.58
2:D:397:VAL:HG22	2:D:464:LEU:HD13	1.83	0.58
2:E:128:MET:HB2	2:E:171:GLN:HE21	1.67	0.58
1:M:23:PRO:HG2	1:M:53:ARG:C	2.24	0.58
2:A:140:VAL:HG12	2:A:172:ALA:HB1	1.85	0.58
2:A:338:LYS:HD2	2:A:367:THR:HB	1.85	0.58
2:C:129:THR:O	2:C:132:ILE:HD11	2.03	0.58
2:D:399:MET:HG2	2:D:410:TRP:NE1	2.18	0.58
2:D:404:ASP:HA	2:D:454:PHE:O	2.04	0.58
4:D:602:ATP:O1B	4:D:602:ATP:O2G	2.21	0.58
2:E:259:ARG:HG3	2:E:259:ARG:NH1	2.17	0.58
2:E:293:LEU:HD12	2:E:330:PRO:CG	2.34	0.58
2:G:310:PRO:HB2	2:G:316:GLU:OE2	2.02	0.58
2:C:439:LYS:C	2:C:440:ARG:HG2	2.23	0.58
2:D:405:ILE:HG12	2:D:410:TRP:CE3	2.39	0.58
1:H:68:LEU:O	1:H:68:LEU:HD13	2.04	0.58
1:K:23:PRO:HG2	1:K:53:ARG:C	2.24	0.58
1:M:47:MET:HB2	1:M:53:ARG:CG	2.29	0.58
2:A:523:VAL:O	2:A:523:VAL:HG12	2.04	0.58
2:C:158:HIS:CD2	2:C:275:VAL:HG23	2.39	0.58
2:C:457:ASP:H	2:C:460:ILE:HG22	1.68	0.58
2:F:211:LEU:CD2	2:F:242:ARG:HD2	2.33	0.58
2:G:386:SER:HB3	2:G:389:ASP:CB	2.33	0.58
2:G:486:GLU:O	2:G:487:ILE:HD12	2.02	0.58
1:H:25:ASP:HB3	1:H:78:ASN:HD21	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:10:LEU:HD22	1:I:58:LEU:HD21	1.84	0.58
1:L:50:ARG:HA	1:L:53:ARG:HE	1.68	0.58
2:B:314:LYS:O	2:B:318:VAL:HG23	2.04	0.58
2:C:140:VAL:HG12	2:C:172:ALA:HB1	1.85	0.58
2:C:439:LYS:O	2:C:440:ARG:CG	2.42	0.58
2:C:483:ARG:HH21	2:C:483:ARG:HA	1.69	0.58
2:D:523:VAL:O	2:D:523:VAL:HG12	2.04	0.58
2:E:255:GLU:HB3	2:E:277:ILE:HB	1.86	0.58
2:E:483:ARG:HA	2:E:483:ARG:NH2	2.18	0.58
2:F:115:LEU:HD11	2:F:177:ASP:HA	1.86	0.58
2:G:386:SER:O	2:G:390:ARG:N	2.37	0.58
2:G:398:VAL:CG1	2:G:477:ILE:HG12	2.33	0.58
2:G:523:VAL:O	2:G:523:VAL:HG12	2.04	0.58
1:L:23:PRO:HG2	1:L:53:ARG:C	2.24	0.58
2:C:341:GLU:O	2:C:343:LYS:N	2.37	0.58
2:F:403:VAL:HG11	2:F:536:HIS:CE1	2.39	0.58
4:F:602:ATP:O1B	4:F:602:ATP:O2G	2.21	0.58
1:I:25:ASP:HB3	1:I:78:ASN:HD21	1.69	0.57
1:J:50:ARG:HA	1:J:53:ARG:HE	1.68	0.57
2:A:439:LYS:C	2:A:440:ARG:HG2	2.23	0.57
2:B:482:GLN:O	2:B:485:LEU:HG	2.04	0.57
2:G:474:ALA:O	2:G:477:ILE:HG22	2.04	0.57
1:I:68:LEU:HD13	1:I:68:LEU:O	2.04	0.57
2:A:227:THR:HB	2:A:229:VAL:HG12	1.86	0.57
2:A:457:ASP:H	2:A:460:ILE:HG22	1.68	0.57
2:B:397:VAL:HG21	2:B:468:VAL:HG11	1.85	0.57
4:C:602:ATP:O1B	4:C:602:ATP:O2G	2.21	0.57
2:D:360:LEU:CD1	2:D:462:MET:HE3	2.34	0.57
2:E:355:LEU:HD21	2:E:363:VAL:HG21	1.86	0.57
2:E:528:ASP:CA	2:E:531:LYS:HZ1	2.17	0.57
4:E:602:ATP:O1B	4:E:602:ATP:O2G	2.21	0.57
2:F:316:GLU:O	2:F:319:LEU:HB2	2.04	0.57
2:A:474:ALA:C	2:A:477:ILE:HG22	2.23	0.57
2:F:523:VAL:O	2:F:523:VAL:HG12	2.04	0.57
1:H:50:ARG:HA	1:H:53:ARG:HE	1.68	0.57
1:K:49:THR:HG22	1:K:50:ARG:N	2.20	0.57
2:B:523:VAL:O	2:B:523:VAL:HG12	2.04	0.57
2:D:484:LEU:CG	2:D:533:MET:HG2	2.33	0.57
2:E:187:ILE:HD12	2:E:246:LEU:O	2.03	0.57
1:J:23:PRO:HG2	1:J:53:ARG:C	2.24	0.57
2:A:293:LEU:HD12	2:A:330:PRO:CG	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:483:ARG:HA	2:A:483:ARG:NH2	2.18	0.57
2:B:480:LEU:HD11	2:B:533:MET:CG	2.32	0.57
2:F:437:LEU:HD13	2:F:444:LEU:HD13	1.85	0.57
1:I:50:ARG:HA	1:I:53:ARG:HE	1.68	0.57
1:J:8:ARG:HG2	1:J:8:ARG:NH1	2.10	0.57
1:J:8:ARG:HH11	1:J:8:ARG:CG	2.11	0.57
2:D:438:SER:HB2	2:D:444:LEU:CB	2.35	0.57
1:H:47:MET:HB2	1:H:53:ARG:CG	2.30	0.57
1:K:68:LEU:O	1:K:68:LEU:HD13	2.05	0.57
2:B:233:ARG:HH11	2:B:233:ARG:CG	2.18	0.57
4:B:602:ATP:O1B	4:B:602:ATP:O2G	2.21	0.57
2:C:293:LEU:HD12	2:C:330:PRO:HG3	1.85	0.57
2:C:523:VAL:O	2:C:523:VAL:HG12	2.04	0.57
2:D:528:ASP:CA	2:D:531:LYS:HZ1	2.17	0.57
2:E:523:VAL:O	2:E:523:VAL:HG12	2.04	0.57
2:E:532:PHE:HB2	2:E:534:GLN:OE1	2.04	0.57
1:L:8:ARG:HH11	1:L:8:ARG:CG	2.14	0.57
2:A:536:HIS:HB2	2:A:540:TYR:CE2	2.39	0.57
2:B:156:PHE:CZ	2:B:278:SER:HA	2.39	0.57
2:C:214:GLU:HG3	2:D:237:ASN:ND2	2.19	0.57
2:F:302:LEU:HB3	2:F:307:MET:HB2	1.87	0.57
2:G:233:ARG:HH11	2:G:233:ARG:CG	2.17	0.57
2:G:437:LEU:HD13	2:G:444:LEU:HD13	1.87	0.57
1:I:23:PRO:HG2	1:I:53:ARG:C	2.24	0.57
2:C:341:GLU:HA	2:C:343:LYS:HZ1	1.69	0.57
2:D:214:GLU:HG3	2:E:237:ASN:ND2	2.19	0.57
2:G:302:LEU:CD1	2:G:307:MET:HG2	2.34	0.57
1:J:68:LEU:O	1:J:68:LEU:HD13	2.04	0.57
2:A:327:SER:HB2	2:A:459:ILE:HD11	1.87	0.57
2:D:470:ALA:HA	2:D:473:ILE:HD12	1.87	0.57
1:H:23:PRO:HG2	1:H:53:ARG:C	2.24	0.56
2:F:240:ILE:HG13	2:F:241:ASP:N	2.20	0.56
2:G:345:PHE:HA	2:G:348:MET:CE	2.35	0.56
2:G:483:ARG:HA	2:G:483:ARG:NH2	2.18	0.56
1:H:1:MET:CE	2:B:240:ILE:HB	2.35	0.56
1:M:49:THR:HG22	1:M:50:ARG:N	2.20	0.56
1:M:68:LEU:O	1:M:68:LEU:HD13	2.05	0.56
2:C:533:MET:O	2:C:540:TYR:CD2	2.58	0.56
2:F:233:ARG:HH11	2:F:233:ARG:CG	2.18	0.56
2:F:486:GLU:HB3	2:F:531:LYS:CG	2.36	0.56
1:J:25:ASP:HB3	1:J:78:ASN:HD21	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:THR:HG22	1:L:50:ARG:N	2.20	0.56
1:M:18:ILE:O	1:M:50:ARG:NH2	2.37	0.56
1:M:25:ASP:HB3	1:M:78:ASN:HD21	1.70	0.56
2:A:233:ARG:HH11	2:A:233:ARG:CG	2.17	0.56
2:B:240:ILE:HG13	2:B:241:ASP:N	2.21	0.56
2:B:484:LEU:HD11	2:B:530:PRO:C	2.22	0.56
2:B:533:MET:HA	2:B:533:MET:HE2	1.84	0.56
2:C:233:ARG:HH11	2:C:233:ARG:CG	2.17	0.56
2:C:322:THR:HG21	2:C:336:PHE:CZ	2.40	0.56
2:E:141:ILE:HD13	2:E:176:SER:CB	2.35	0.56
2:E:200:THR:HG21	2:E:256:GLU:HG3	1.87	0.56
2:F:160:ARG:HG2	2:F:161:ALA:N	2.20	0.56
2:F:314:LYS:O	2:F:317:ASP:HB2	2.05	0.56
2:F:539:PHE:CZ	2:F:543:LEU:HD21	2.40	0.56
2:G:435:LYS:O	2:G:439:LYS:HD3	2.04	0.56
2:B:360:LEU:HD13	2:B:462:MET:HE3	1.85	0.56
2:C:203:LEU:O	2:C:203:LEU:HD22	2.06	0.56
2:D:258:ILE:CD1	2:D:277:ILE:HD12	2.35	0.56
2:D:438:SER:HA	2:D:444:LEU:N	2.15	0.56
2:E:211:LEU:CD2	2:E:242:ARG:CG	2.76	0.56
2:E:233:ARG:HH11	2:E:233:ARG:CG	2.18	0.56
2:F:312:GLY:O	2:F:315:GLU:HG3	2.05	0.56
2:G:336:PHE:CZ	2:G:351:LEU:HB2	2.40	0.56
2:G:524:ILE:HD11	2:G:535:LEU:HD11	1.87	0.56
2:A:470:ALA:HA	2:A:473:ILE:HD12	1.87	0.56
2:C:444:LEU:HD12	2:C:445:SER:H	1.70	0.56
2:C:470:ALA:HA	2:C:473:ILE:HD12	1.87	0.56
2:D:203:LEU:O	2:D:203:LEU:HD22	2.06	0.56
2:D:473:ILE:CG2	2:D:543:LEU:HD12	2.36	0.56
2:B:484:LEU:HD11	2:B:531:LYS:CA	2.34	0.56
2:B:526:PRO:C	2:B:530:PRO:HG3	2.26	0.56
2:C:305:TYR:HD2	2:C:337:PHE:CG	2.23	0.56
2:E:240:ILE:HG13	2:E:241:ASP:N	2.21	0.56
2:F:253:VAL:HG11	2:F:380:ARG:NH1	2.20	0.56
1:L:25:ASP:HB3	1:L:78:ASN:HD21	1.70	0.56
2:A:369:TYR:C	2:A:371:TYR:H	2.08	0.56
2:A:457:ASP:O	2:A:460:ILE:HG22	2.06	0.56
2:C:335:MET:HE3	2:C:364:GLU:HA	1.88	0.56
2:D:480:LEU:HD11	2:D:484:LEU:HD11	1.85	0.56
2:E:526:PRO:C	2:E:530:PRO:HG3	2.26	0.56
2:A:338:LYS:HZ2	2:A:368:PRO:HD3	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:398:VAL:CG1	2:B:473:ILE:HG23	2.36	0.56
2:C:240:ILE:HG13	2:C:241:ASP:N	2.20	0.56
2:D:127:GLN:HB3	2:D:171:GLN:HG2	1.88	0.56
2:D:233:ARG:HH11	2:D:233:ARG:CG	2.17	0.56
1:I:98:PRO:O	1:I:99:ASP:HB2	2.06	0.56
1:L:68:LEU:O	1:L:68:LEU:HD13	2.05	0.56
2:F:353:ASN:O	2:F:356:GLU:HG3	2.05	0.56
1:H:18:ILE:O	1:H:50:ARG:NH2	2.38	0.56
2:C:526:PRO:C	2:C:530:PRO:HG3	2.26	0.56
2:E:203:LEU:O	2:E:203:LEU:HD22	2.06	0.56
1:J:93:PHE:HD2	1:J:100:LEU:HB3	1.70	0.55
2:A:136:HIS:HB3	2:A:168:ILE:HD13	1.87	0.55
2:B:480:LEU:CD1	2:B:533:MET:HG2	2.37	0.55
2:F:150:LEU:CD1	2:F:153:PHE:HB3	2.35	0.55
2:F:226:VAL:HG13	2:F:230:VAL:HB	1.88	0.55
1:K:18:ILE:O	1:K:50:ARG:NH2	2.37	0.55
1:K:25:ASP:HB3	1:K:78:ASN:HD21	1.70	0.55
2:A:305:TYR:CD2	2:A:334:MET:HE1	2.40	0.55
2:A:360:LEU:CD1	2:A:462:MET:HE3	2.34	0.55
2:A:526:PRO:C	2:A:530:PRO:HG3	2.26	0.55
2:B:397:VAL:HG21	2:B:468:VAL:CG2	2.32	0.55
2:C:217:LEU:O	2:C:220:PHE:HB3	2.06	0.55
2:D:136:HIS:HB3	2:D:168:ILE:HD13	1.87	0.55
2:D:256:GLU:HA	2:D:256:GLU:OE2	2.06	0.55
2:G:328:GLY:O	2:G:330:PRO:HD3	2.05	0.55
1:H:93:PHE:HD2	1:H:100:LEU:HB3	1.70	0.55
2:A:382:VAL:HG21	2:A:393:LEU:HD13	1.77	0.55
2:A:529:PHE:N	2:A:531:LYS:HZ3	2.05	0.55
2:B:321:LYS:HE2	2:B:321:LYS:HA	1.88	0.55
2:C:125:PRO:CD	2:C:189:TRP:CE2	2.89	0.55
2:C:293:LEU:N	2:C:328:GLY:HA3	2.21	0.55
2:D:206:ASP:OD1	2:E:227:THR:HG21	2.06	0.55
2:E:127:GLN:HB2	2:E:171:GLN:HA	1.88	0.55
2:E:221:PRO:HD2	2:E:223:VAL:HG13	1.88	0.55
2:E:368:PRO:HB2	4:E:602:ATP:O3'	2.06	0.55
2:B:214:GLU:HG3	2:C:237:ASN:ND2	2.22	0.55
2:B:457:ASP:O	2:B:460:ILE:HG22	2.06	0.55
2:C:165:LYS:NZ	4:C:602:ATP:O1G	2.40	0.55
2:D:399:MET:HG3	2:D:400:PRO:HD2	1.87	0.55
2:E:355:LEU:HD21	2:E:363:VAL:CG2	2.36	0.55
2:E:538:LYS:HZ3	2:E:539:PHE:H	1.52	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:203:LEU:O	2:G:203:LEU:HD22	2.05	0.55
1:H:98:PRO:O	1:H:99:ASP:HB2	2.06	0.55
1:J:97:GLU:HG2	1:J:100:LEU:HD22	1.89	0.55
2:A:203:LEU:O	2:A:203:LEU:HD22	2.05	0.55
2:A:214:GLU:HG3	2:B:237:ASN:ND2	2.21	0.55
2:A:368:PRO:HB2	4:A:602:ATP:O3'	2.06	0.55
2:G:354:LYS:HZ3	2:G:358:ARG:HD2	1.72	0.55
2:A:393:LEU:O	2:A:464:LEU:HD13	2.05	0.55
2:B:203:LEU:O	2:B:203:LEU:HD22	2.06	0.55
2:C:175:LYS:HZ2	2:C:175:LYS:HB3	1.70	0.55
2:D:182:ILE:N	2:D:182:ILE:HD12	2.22	0.55
2:D:480:LEU:O	2:D:484:LEU:HB2	2.06	0.55
2:D:487:ILE:HG23	2:D:487:ILE:O	2.05	0.55
2:E:217:LEU:O	2:E:220:PHE:HB3	2.06	0.55
2:F:385:LEU:CD1	2:F:393:LEU:HD12	2.37	0.55
2:G:182:ILE:N	2:G:182:ILE:HD12	2.22	0.55
2:A:338:LYS:HZ2	2:A:367:THR:HA	1.72	0.55
2:A:341:GLU:HB2	2:A:342:PRO:HD3	1.89	0.55
2:A:393:LEU:CD2	2:A:464:LEU:CD1	2.82	0.55
2:B:182:ILE:N	2:B:182:ILE:HD12	2.22	0.55
2:D:184:TYR:CE1	2:D:246:LEU:HD11	2.41	0.55
2:D:385:LEU:CD1	2:D:393:LEU:HD12	2.37	0.55
2:D:457:ASP:O	2:D:460:ILE:HG22	2.06	0.55
2:G:315:GLU:HG3	2:G:316:GLU:H	1.71	0.55
2:G:524:ILE:HG23	2:G:526:PRO:HD3	1.88	0.55
1:M:77:TYR:O	1:M:77:TYR:HD1	1.90	0.55
2:C:439:LYS:C	2:C:440:ARG:CG	2.76	0.55
2:D:533:MET:HG3	2:D:540:TYR:HH	1.63	0.55
2:E:182:ILE:HD12	2:E:182:ILE:N	2.22	0.55
2:F:397:VAL:HG11	2:F:465:LYS:HA	1.88	0.55
1:I:93:PHE:HD2	1:I:100:LEU:HB3	1.71	0.55
2:A:157:LEU:HD11	2:A:168:ILE:CG2	2.37	0.55
2:C:283:GLN:HG2	2:C:284:THR:H	1.71	0.55
2:C:305:TYR:HD2	2:C:337:PHE:CD2	2.25	0.55
2:C:385:LEU:CD1	2:C:393:LEU:HD12	2.37	0.55
2:D:526:PRO:C	2:D:530:PRO:HG3	2.26	0.55
2:E:214:GLU:HG3	2:F:237:ASN:ND2	2.22	0.55
2:E:335:MET:HE3	2:E:372:LYS:O	2.06	0.55
2:G:315:GLU:CG	2:G:316:GLU:N	2.70	0.55
2:A:182:ILE:HD12	2:A:182:ILE:N	2.22	0.55
2:C:182:ILE:HD12	2:C:182:ILE:N	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:457:ASP:O	2:C:460:ILE:HG22	2.06	0.55
2:D:330:PRO:HB2	4:D:602:ATP:C8	2.42	0.55
2:F:203:LEU:O	2:F:203:LEU:HD22	2.06	0.55
2:F:323:ILE:O	2:F:327:SER:N	2.40	0.55
2:F:336:PHE:CE1	2:F:351:LEU:HD12	2.42	0.55
2:F:425:GLN:HE21	2:F:426:LEU:HD23	1.72	0.55
2:G:302:LEU:HD13	2:G:307:MET:CG	2.37	0.55
1:J:101:LEU:HD12	1:J:105:VAL:HB	1.90	0.54
1:K:77:TYR:O	1:K:77:TYR:HD1	1.90	0.54
2:A:159:GLY:H	2:A:165:LYS:HD3	1.71	0.54
2:B:399:MET:HG2	2:B:410:TRP:CE2	2.41	0.54
2:C:136:HIS:HB3	2:C:168:ILE:HD13	1.87	0.54
2:D:165:LYS:NZ	4:D:602:ATP:O1G	2.40	0.54
2:D:321:LYS:HG3	2:D:352:ASN:OD1	2.06	0.54
2:D:355:LEU:HD12	2:D:462:MET:CE	2.36	0.54
2:F:456:ILE:HG13	2:F:460:ILE:HG23	1.89	0.54
2:F:487:ILE:H	2:F:487:ILE:HD12	1.71	0.54
2:A:463:PHE:O	2:A:467:VAL:CB	2.56	0.54
2:B:147:MET:HG3	2:B:150:LEU:HB3	1.88	0.54
2:C:314:LYS:HZ3	2:C:314:LYS:HB3	1.73	0.54
2:D:399:MET:CE	2:D:413:VAL:HG21	2.37	0.54
2:D:538:LYS:HB2	2:D:538:LYS:HZ3	1.67	0.54
2:F:182:ILE:HD12	2:F:182:ILE:N	2.22	0.54
1:K:29:TYR:CZ	1:K:33:LYS:HD2	2.43	0.54
2:A:276:GLU:OE1	2:A:276:GLU:HA	2.08	0.54
2:B:293:LEU:CD1	2:B:330:PRO:HG3	2.37	0.54
2:C:443:LEU:HA	2:C:460:ILE:HG12	1.88	0.54
2:D:220:PHE:HE1	2:D:223:VAL:HG22	1.73	0.54
2:D:259:ARG:HH11	2:D:259:ARG:CG	2.20	0.54
2:D:365:CYS:O	2:D:367:THR:HG22	2.08	0.54
2:E:184:TYR:CE1	2:E:246:LEU:HD11	2.41	0.54
2:F:232:LYS:HB3	2:F:264:LEU:HD21	1.88	0.54
2:F:355:LEU:HD21	2:F:363:VAL:HB	1.88	0.54
1:J:98:PRO:O	1:J:99:ASP:HB2	2.06	0.54
2:C:130:CYS:O	2:C:304:ALA:HB1	2.07	0.54
2:E:165:LYS:NZ	4:E:602:ATP:O1G	2.40	0.54
2:E:446:GLY:HA3	2:E:454:PHE:CD2	2.42	0.54
2:G:301:PHE:CZ	2:G:334:MET:CE	2.91	0.54
2:G:366:ILE:CG1	2:G:372:LYS:HE2	2.34	0.54
1:I:101:LEU:HD12	1:I:105:VAL:HB	1.90	0.54
1:M:8:ARG:HG2	1:M:8:ARG:NH1	2.11	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:240:ILE:HG13	2:A:241:ASP:N	2.21	0.54
2:C:157:LEU:HD11	2:C:168:ILE:CG2	2.37	0.54
2:C:240:ILE:HG13	2:C:241:ASP:OD1	2.08	0.54
2:C:535:LEU:O	2:C:535:LEU:HD23	2.08	0.54
2:D:175:LYS:HZ2	2:D:175:LYS:HB3	1.72	0.54
2:E:478:SER:O	2:E:482:GLN:HG2	2.07	0.54
2:F:165:LYS:NZ	4:F:602:ATP:O1G	2.40	0.54
2:G:540:TYR:HA	2:G:543:LEU:HD23	1.89	0.54
1:H:105:VAL:O	1:H:105:VAL:HG12	2.08	0.54
2:B:240:ILE:HG13	2:B:241:ASP:OD1	2.08	0.54
2:E:273:ARG:NH1	2:E:380:ARG:HH21	2.05	0.54
2:F:140:VAL:O	2:F:144:LEU:HD12	2.08	0.54
2:F:456:ILE:HG12	2:F:461:HIS:HB2	1.89	0.54
2:A:140:VAL:O	2:A:144:LEU:HD12	2.08	0.54
2:A:177:ASP:O	2:A:182:ILE:HD13	2.08	0.54
2:B:140:VAL:O	2:B:144:LEU:HD12	2.08	0.54
2:B:147:MET:HG2	2:B:153:PHE:CD2	2.43	0.54
2:C:399:MET:HG2	2:C:410:TRP:NE1	2.23	0.54
2:D:157:LEU:HD11	2:D:168:ILE:CG2	2.37	0.54
2:E:240:ILE:HG13	2:E:241:ASP:OD1	2.08	0.54
2:E:302:LEU:CD1	2:E:307:MET:HG2	2.36	0.54
2:E:342:PRO:HG2	2:E:347:LYS:HG3	1.90	0.54
2:F:456:ILE:HD11	2:F:461:HIS:HA	1.89	0.54
2:G:140:VAL:O	2:G:144:LEU:HD12	2.08	0.54
2:G:269:LEU:HD13	2:G:270:VAL:N	2.22	0.54
1:I:105:VAL:O	1:I:105:VAL:HG12	2.08	0.54
2:A:439:LYS:C	2:A:440:ARG:CG	2.76	0.54
2:E:297:GLU:O	2:E:298:CYS:C	2.47	0.54
2:F:314:LYS:NZ	2:F:314:LYS:HB3	2.23	0.54
1:M:29:TYR:CZ	1:M:33:LYS:HD2	2.43	0.54
2:A:443:LEU:HD23	2:A:460:ILE:CD1	2.35	0.54
2:A:474:ALA:CA	2:A:477:ILE:HG22	2.38	0.54
2:A:530:PRO:CD	2:A:531:LYS:HD2	2.37	0.54
2:B:276:GLU:OE1	2:B:276:GLU:HA	2.08	0.54
2:B:484:LEU:CD1	2:B:531:LYS:CA	2.86	0.54
2:C:478:SER:O	2:C:482:GLN:HG2	2.08	0.54
2:D:373:SER:OG	2:D:376:MET:HG2	2.07	0.54
2:E:530:PRO:CD	2:E:531:LYS:HD2	2.37	0.54
1:L:29:TYR:CZ	1:L:33:LYS:HD2	2.43	0.54
1:L:77:TYR:O	1:L:77:TYR:HD1	1.90	0.54
1:M:10:LEU:HD13	1:M:58:LEU:HD22	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:395:PHE:CD1	2:A:413:VAL:HB	2.43	0.54
2:B:483:ARG:HA	2:B:483:ARG:HH21	1.71	0.54
2:D:222:SER:O	2:D:222:SER:OG	2.17	0.54
2:D:276:GLU:OE1	2:D:276:GLU:HA	2.08	0.54
2:E:140:VAL:O	2:E:144:LEU:HD12	2.08	0.54
2:F:128:MET:HB2	2:F:171:GLN:HE21	1.71	0.54
2:F:308:PRO:O	2:F:345:PHE:CZ	2.61	0.54
2:F:405:ILE:HG12	2:F:410:TRP:CZ3	2.43	0.54
2:A:464:LEU:N	2:A:467:VAL:HG12	2.23	0.53
2:B:159:GLY:H	2:B:165:LYS:HD3	1.71	0.53
2:D:140:VAL:O	2:D:144:LEU:HD12	2.08	0.53
2:F:315:GLU:OE1	2:F:345:PHE:CE1	2.62	0.53
2:G:297:GLU:O	2:G:298:CYS:C	2.47	0.53
2:G:398:VAL:HG22	2:G:473:ILE:HG23	1.90	0.53
1:I:23:PRO:HG2	1:I:53:ARG:HB3	1.89	0.53
2:A:393:LEU:HD22	2:A:464:LEU:HD22	1.88	0.53
2:C:140:VAL:O	2:C:144:LEU:HD12	2.08	0.53
2:G:426:LEU:C	2:G:428:ASP:H	2.11	0.53
1:J:23:PRO:HG2	1:J:53:ARG:HB3	1.89	0.53
1:J:105:VAL:O	1:J:105:VAL:HG12	2.08	0.53
1:K:26:ALA:HA	1:K:74:PHE:CE2	2.44	0.53
2:B:309:MET:CE	2:B:309:MET:CA	2.86	0.53
2:C:297:GLU:O	2:C:298:CYS:C	2.47	0.53
2:D:170:SER:O	2:D:174:SER:HB2	2.09	0.53
2:D:321:LYS:HG3	2:D:352:ASN:CG	2.29	0.53
1:H:23:PRO:HG2	1:H:53:ARG:HB3	1.89	0.53
1:K:9:ALA:HB2	1:K:90:TYR:CE1	2.44	0.53
2:B:258:ILE:CD1	2:B:277:ILE:HD11	2.35	0.53
2:B:339:SER:O	2:B:351:LEU:CD1	2.57	0.53
2:C:141:ILE:HD12	2:C:175:LYS:HZ1	1.73	0.53
2:C:355:LEU:HD11	2:C:462:MET:HE1	1.90	0.53
2:D:341:GLU:N	2:D:342:PRO:HD2	2.23	0.53
2:E:256:GLU:OE1	2:E:260:TRP:NE1	2.41	0.53
2:F:240:ILE:HG13	2:F:241:ASP:OD1	2.08	0.53
2:F:297:GLU:O	2:F:298:CYS:C	2.47	0.53
2:F:446:GLY:HA3	2:F:454:PHE:CD2	2.43	0.53
1:H:8:ARG:HH11	1:H:8:ARG:CG	2.11	0.53
1:L:26:ALA:HA	1:L:74:PHE:CE2	2.44	0.53
2:A:248:VAL:CG1	2:A:269:LEU:HD12	2.39	0.53
2:B:200:THR:OG1	2:B:256:GLU:HB2	2.08	0.53
2:B:309:MET:SD	2:B:310:PRO:CD	2.97	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:484:LEU:HG	2:B:531:LYS:O	2.07	0.53
2:F:310:PRO:HA	2:F:315:GLU:CD	2.29	0.53
2:F:341:GLU:HB2	2:F:342:PRO:HD3	1.90	0.53
1:H:1:MET:HE3	2:B:240:ILE:HB	1.91	0.53
1:H:9:ALA:HB2	1:H:90:TYR:CE1	2.44	0.53
1:I:18:ILE:O	1:I:50:ARG:NH2	2.37	0.53
1:M:26:ALA:HA	1:M:74:PHE:CE2	2.44	0.53
2:B:248:VAL:CG1	2:B:269:LEU:HD12	2.39	0.53
2:C:161:ALA:CB	2:C:273:ARG:NE	2.72	0.53
2:C:539:PHE:O	2:C:542:SER:OG	2.25	0.53
2:F:248:VAL:CG1	2:F:269:LEU:HD12	2.39	0.53
1:H:101:LEU:HD12	1:H:105:VAL:HB	1.90	0.53
2:C:341:GLU:C	2:C:343:LYS:N	2.62	0.53
2:G:160:ARG:HG2	2:G:161:ALA:H	1.73	0.53
2:G:443:LEU:HD22	2:G:460:ILE:HD11	1.90	0.53
2:G:535:LEU:HD22	2:G:536:HIS:NE2	2.23	0.53
1:H:77:TYR:O	1:H:77:TYR:HD1	1.91	0.53
1:L:9:ALA:HB2	1:L:90:TYR:CE1	2.44	0.53
1:M:9:ALA:HB2	1:M:90:TYR:CE1	2.44	0.53
2:B:147:MET:HE2	2:B:147:MET:CA	2.38	0.53
2:G:184:TYR:HD2	2:G:267:ARG:HH22	1.56	0.53
2:G:248:VAL:HG13	2:G:269:LEU:HB3	1.90	0.53
1:J:77:TYR:O	1:J:77:TYR:HD1	1.91	0.53
2:A:446:GLY:HA3	2:A:454:PHE:CD2	2.44	0.53
2:B:530:PRO:CD	2:B:531:LYS:HD2	2.37	0.53
2:C:255:GLU:CB	2:C:277:ILE:HG22	2.39	0.53
2:C:484:LEU:O	2:C:486:GLU:N	2.41	0.53
2:E:531:LYS:H	2:E:531:LYS:CD	1.96	0.53
2:F:129:THR:HA	2:F:132:ILE:HD11	1.91	0.53
1:L:10:LEU:HD13	1:L:58:LEU:HD22	1.90	0.53
1:L:18:ILE:O	1:L:50:ARG:NH2	2.37	0.53
2:A:141:ILE:HD12	2:A:175:LYS:NZ	2.23	0.53
2:A:219:ASN:O	2:A:220:PHE:C	2.47	0.53
2:B:293:LEU:HD12	2:B:330:PRO:HG3	1.90	0.53
2:C:248:VAL:CG1	2:C:269:LEU:HD12	2.39	0.53
2:C:276:GLU:OE1	2:C:276:GLU:HA	2.08	0.53
2:C:530:PRO:CD	2:C:531:LYS:HD2	2.37	0.53
2:D:297:GLU:O	2:D:298:CYS:C	2.47	0.53
2:E:259:ARG:HH11	2:E:259:ARG:HG3	1.72	0.53
2:E:463:PHE:CD2	2:E:464:LEU:HD23	2.43	0.53
2:G:128:MET:HB2	2:G:171:GLN:HE21	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:387:ASP:O	2:G:390:ARG:HB3	2.09	0.53
1:H:21:PHE:CD1	1:H:75:PHE:HE1	2.27	0.52
1:I:77:TYR:HD1	1:I:77:TYR:O	1.91	0.52
2:A:237:ASN:ND2	2:G:214:GLU:HG3	2.24	0.52
2:A:406:PRO:CD	2:A:526:PRO:HG3	2.39	0.52
2:C:259:ARG:HG3	2:C:259:ARG:NH1	2.24	0.52
2:D:127:GLN:CG	2:D:174:SER:HB2	2.13	0.52
2:D:157:LEU:HD11	2:D:168:ILE:HG22	1.91	0.52
2:E:315:GLU:HA	2:E:318:VAL:HB	1.91	0.52
2:F:413:VAL:CG1	2:F:480:LEU:HB2	2.39	0.52
2:G:133:ARG:O	2:G:137:VAL:HG23	2.09	0.52
1:I:9:ALA:HB2	1:I:90:TYR:CE1	2.44	0.52
1:J:21:PHE:CD1	1:J:75:PHE:HE1	2.27	0.52
2:A:220:PHE:HE1	2:A:223:VAL:CG2	2.22	0.52
2:A:259:ARG:HH11	2:A:259:ARG:HG3	1.72	0.52
2:B:297:GLU:O	2:B:298:CYS:C	2.47	0.52
2:B:314:LYS:NZ	2:B:314:LYS:HB3	2.24	0.52
2:B:342:PRO:C	2:B:344:THR:N	2.63	0.52
2:B:484:LEU:C	2:B:487:ILE:HG22	2.29	0.52
2:C:112:ARG:HH11	2:C:115:LEU:HD12	1.75	0.52
2:C:283:GLN:HG2	2:C:284:THR:N	2.24	0.52
2:B:112:ARG:HH11	2:B:115:LEU:HD12	1.75	0.52
2:C:170:SER:O	2:C:174:SER:HB2	2.09	0.52
2:E:310:PRO:HB2	2:E:316:GLU:OE2	2.09	0.52
2:F:308:PRO:HB2	2:F:345:PHE:CD1	2.42	0.52
2:G:232:LYS:HE3	2:G:260:TRP:CZ2	2.44	0.52
2:D:184:TYR:CE2	2:D:246:LEU:HD11	2.31	0.52
2:D:219:ASN:O	2:D:220:PHE:C	2.47	0.52
2:D:227:THR:O	2:D:230:VAL:HB	2.09	0.52
2:F:412:CYS:HB3	2:F:483:ARG:HB2	1.92	0.52
2:B:252:VAL:HG11	2:B:258:ILE:HD12	1.91	0.52
2:B:259:ARG:HH11	2:B:259:ARG:HG3	1.72	0.52
2:B:406:PRO:CD	2:B:526:PRO:HG3	2.39	0.52
2:E:248:VAL:CG1	2:E:269:LEU:HD12	2.39	0.52
2:E:252:VAL:HG11	2:E:258:ILE:CD1	2.38	0.52
2:E:293:LEU:HD12	2:E:330:PRO:CD	2.40	0.52
2:A:297:GLU:O	2:A:298:CYS:C	2.47	0.52
2:B:446:GLY:HA3	2:B:454:PHE:CE2	2.44	0.52
2:C:157:LEU:HD11	2:C:168:ILE:HG22	1.91	0.52
2:C:269:LEU:HD22	2:C:270:VAL:H	1.75	0.52
2:D:112:ARG:HH11	2:D:115:LEU:HD12	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:317:ASP:HA	2:D:320:ASN:ND2	2.24	0.52
2:E:142:LYS:HE2	2:E:146:GLU:OE2	2.10	0.52
2:G:307:MET:O	2:G:308:PRO:C	2.48	0.52
1:K:10:LEU:HD13	1:K:58:LEU:HD22	1.90	0.52
2:A:529:PHE:N	2:A:530:PRO:CD	2.73	0.52
2:A:532:PHE:C	2:A:534:GLN:H	2.13	0.52
2:B:259:ARG:CG	2:B:259:ARG:NH1	2.73	0.52
2:C:406:PRO:CD	2:C:526:PRO:HG3	2.39	0.52
2:D:359:GLY:N	2:D:466:HIS:NE2	2.58	0.52
2:E:463:PHE:HD2	2:E:464:LEU:HD23	1.75	0.52
2:G:160:ARG:HH11	2:G:460:ILE:HD13	1.75	0.52
2:G:416:VAL:CG2	2:G:429:GLU:HG2	2.40	0.52
2:A:142:LYS:HE2	2:A:146:GLU:OE2	2.10	0.52
2:A:157:LEU:HD11	2:A:168:ILE:HG22	1.91	0.52
2:A:351:LEU:O	2:A:352:ASN:C	2.47	0.52
2:C:127:GLN:HB2	2:C:171:GLN:HG2	1.92	0.52
2:C:142:LYS:HE2	2:C:146:GLU:OE2	2.10	0.52
2:C:309:MET:CE	2:C:309:MET:CA	2.86	0.52
2:F:464:LEU:O	2:F:468:VAL:HG22	2.09	0.52
2:G:160:ARG:HG2	2:G:161:ALA:N	2.24	0.52
2:G:385:LEU:HD11	2:G:393:LEU:HD12	1.88	0.52
2:G:529:PHE:HB3	2:G:532:PHE:CZ	2.44	0.52
1:I:21:PHE:CD1	1:I:75:PHE:HE1	2.27	0.52
1:I:97:GLU:HG2	1:I:100:LEU:HD22	1.91	0.52
1:J:9:ALA:HB2	1:J:90:TYR:CE1	2.44	0.52
2:A:112:ARG:HH11	2:A:115:LEU:HD12	1.75	0.52
2:A:149:ASP:OD1	2:A:149:ASP:N	2.26	0.52
2:A:315:GLU:HA	2:A:318:VAL:HB	1.91	0.52
2:B:309:MET:SD	2:B:310:PRO:HD3	2.50	0.52
2:C:302:LEU:N	2:C:302:LEU:CD2	2.73	0.52
2:C:327:SER:H	2:C:459:ILE:HG12	1.74	0.52
2:B:416:VAL:CG2	2:B:429:GLU:HG2	2.40	0.52
2:D:228:SER:HB3	2:D:260:TRP:CZ2	2.45	0.52
2:D:248:VAL:CG1	2:D:269:LEU:HD12	2.39	0.52
2:E:200:THR:CB	2:E:256:GLU:HG3	2.40	0.52
2:E:327:SER:O	2:E:328:GLY:C	2.47	0.52
2:E:406:PRO:CD	2:E:526:PRO:HG3	2.39	0.52
2:G:327:SER:HB2	2:G:459:ILE:HD11	1.91	0.52
2:G:400:PRO:HB2	2:G:403:VAL:HG21	1.91	0.52
2:A:165:LYS:NZ	4:A:602:ATP:O1G	2.39	0.51
2:A:416:VAL:CG2	2:A:429:GLU:HG2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:GLU:HA	2:B:343:LYS:HZ1	1.75	0.51
2:D:255:GLU:CB	2:D:277:ILE:HG22	2.40	0.51
2:D:530:PRO:CD	2:D:531:LYS:HD2	2.37	0.51
2:F:152:SER:HA	2:F:266:LEU:O	2.10	0.51
2:A:293:LEU:HD12	2:A:330:PRO:CD	2.40	0.51
2:A:534:GLN:HA	2:A:537:GLN:CB	2.26	0.51
2:B:155:LEU:HD23	2:B:286:GLU:O	2.10	0.51
2:B:529:PHE:N	2:B:530:PRO:CD	2.73	0.51
2:C:158:HIS:O	2:C:289:GLU:HA	2.10	0.51
2:F:338:LYS:HB2	2:F:365:CYS:SG	2.50	0.51
2:G:315:GLU:OE2	2:G:316:GLU:HA	2.10	0.51
2:G:393:LEU:CD1	2:G:437:LEU:HD11	2.38	0.51
2:A:335:MET:HG2	2:A:365:CYS:H	1.75	0.51
2:C:132:ILE:N	2:C:132:ILE:HD12	2.25	0.51
2:C:210:MET:HE3	2:C:210:MET:CA	2.40	0.51
2:C:327:SER:H	2:C:459:ILE:CG1	2.24	0.51
2:E:132:ILE:HD12	2:E:132:ILE:N	2.26	0.51
2:F:142:LYS:HE2	2:F:146:GLU:OE2	2.10	0.51
2:F:398:VAL:HG11	2:F:477:ILE:N	2.26	0.51
2:G:155:LEU:HB3	2:G:269:LEU:CD2	2.40	0.51
2:G:298:CYS:O	2:G:299:TYR:C	2.49	0.51
2:G:329:ASN:HD22	2:G:330:PRO:HD2	1.75	0.51
2:A:141:ILE:HD12	2:A:175:LYS:HZ2	1.76	0.51
2:B:125:PRO:CD	2:B:189:TRP:CE2	2.93	0.51
2:C:364:GLU:HB2	2:C:372:LYS:O	2.11	0.51
2:D:258:ILE:HG21	2:D:280:ALA:HB3	1.92	0.51
2:E:258:ILE:HD13	2:E:277:ILE:HD12	1.91	0.51
2:F:486:GLU:N	2:F:531:LYS:HB3	2.26	0.51
2:G:351:LEU:O	2:G:355:LEU:HD23	2.11	0.51
1:K:21:PHE:CD1	1:K:75:PHE:HE1	2.29	0.51
2:C:341:GLU:HB2	2:C:342:PRO:HD3	1.92	0.51
2:C:529:PHE:N	2:C:530:PRO:CD	2.73	0.51
2:D:142:LYS:HE2	2:D:146:GLU:OE2	2.10	0.51
2:E:192:ASP:HB3	2:E:251:ASP:O	2.11	0.51
2:E:374:LEU:O	2:E:377:ALA:HB3	2.09	0.51
2:F:326:SER:O	2:F:327:SER:C	2.49	0.51
2:G:416:VAL:HG22	2:G:429:GLU:HG2	1.92	0.51
1:L:23:PRO:HG2	1:L:53:ARG:HB3	1.93	0.51
2:C:335:MET:HB3	2:C:363:VAL:HG12	1.90	0.51
2:D:307:MET:HE2	2:D:343:LYS:HG3	1.91	0.51
2:D:398:VAL:HG21	2:D:413:VAL:HG11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:PRO:CD	2:D:526:PRO:HG3	2.39	0.51
2:E:141:ILE:HG23	2:E:179:LEU:HD22	1.93	0.51
2:E:533:MET:HB2	2:E:536:HIS:HD2	1.75	0.51
2:F:209:LEU:HD21	2:F:220:PHE:CE1	2.46	0.51
2:G:307:MET:HE2	2:G:348:MET:SD	2.51	0.51
2:G:321:LYS:CD	2:G:352:ASN:HB3	2.40	0.51
2:A:326:SER:C	2:A:459:ILE:HG12	2.31	0.51
2:B:192:ASP:HB3	2:B:251:ASP:O	2.11	0.51
2:B:484:LEU:HG	2:B:531:LYS:HA	1.93	0.51
2:C:192:ASP:HB3	2:C:251:ASP:O	2.11	0.51
2:C:382:VAL:O	2:C:382:VAL:HG13	2.11	0.51
2:D:156:PHE:HB2	2:D:287:PHE:CD1	2.46	0.51
2:D:184:TYR:CE1	2:D:246:LEU:HD13	2.39	0.51
2:E:269:LEU:HD22	2:E:270:VAL:H	1.75	0.51
2:F:295:ILE:CD1	2:F:323:ILE:HG21	2.39	0.51
2:F:319:LEU:CD2	2:F:345:PHE:HE2	2.17	0.51
1:K:23:PRO:HG2	1:K:53:ARG:HB3	1.93	0.51
1:L:77:TYR:CD1	1:L:77:TYR:O	2.64	0.51
2:A:269:LEU:HD22	2:A:270:VAL:H	1.75	0.51
2:B:332:THR:HG21	2:B:459:ILE:HG21	1.92	0.51
2:B:382:VAL:O	2:B:382:VAL:HG13	2.11	0.51
2:C:226:VAL:HG13	2:C:230:VAL:HB	1.93	0.51
2:C:342:PRO:C	2:C:344:THR:N	2.63	0.51
2:D:141:ILE:HG23	2:D:179:LEU:HD22	1.93	0.51
2:D:309:MET:CE	2:D:309:MET:CA	2.86	0.51
2:E:298:CYS:O	2:E:299:TYR:C	2.49	0.51
2:G:142:LYS:HE2	2:G:146:GLU:OE2	2.10	0.51
1:I:24:ARG:NH2	1:I:53:ARG:HH11	2.09	0.51
1:J:24:ARG:NH2	1:J:53:ARG:HH11	2.09	0.51
1:K:77:TYR:CD1	1:K:77:TYR:O	2.64	0.51
1:M:21:PHE:CD1	1:M:75:PHE:HE1	2.29	0.51
2:A:309:MET:HB3	2:A:310:PRO:HD2	1.91	0.51
2:B:142:LYS:HE2	2:B:146:GLU:OE2	2.10	0.51
2:B:446:GLY:HA2	2:B:454:PHE:CD2	2.46	0.51
2:B:461:HIS:C	2:B:461:HIS:HD1	2.15	0.51
2:C:461:HIS:HD1	2:C:461:HIS:C	2.15	0.51
2:F:190:LEU:HD13	2:F:203:LEU:HD21	1.92	0.51
2:F:192:ASP:HB3	2:F:251:ASP:O	2.11	0.51
2:G:437:LEU:HB3	2:G:444:LEU:HD22	1.92	0.51
2:B:269:LEU:HD22	2:B:270:VAL:H	1.75	0.51
2:B:399:MET:HE3	2:B:413:VAL:HG21	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:399:MET:HG2	2:C:410:TRP:CE2	2.46	0.51
2:D:382:VAL:HG13	2:D:382:VAL:O	2.11	0.51
2:E:233:ARG:HA	2:E:236:CYS:SG	2.51	0.51
2:F:233:ARG:HA	2:F:236:CYS:SG	2.51	0.51
2:F:360:LEU:N	2:F:360:LEU:CD1	2.74	0.51
2:F:440:ARG:O	2:F:443:LEU:HG	2.11	0.51
2:G:535:LEU:HD22	2:G:536:HIS:CE1	2.45	0.51
1:M:49:THR:HG22	1:M:50:ARG:H	1.76	0.50
2:A:192:ASP:HB3	2:A:251:ASP:O	2.11	0.50
2:A:452:LEU:H	2:A:452:LEU:CD2	2.23	0.50
2:B:165:LYS:NZ	4:B:602:ATP:O1G	2.40	0.50
2:B:309:MET:HA	2:B:309:MET:HE1	1.92	0.50
2:C:210:MET:HE3	2:C:210:MET:HA	1.94	0.50
2:C:256:GLU:HA	2:C:256:GLU:OE2	2.11	0.50
2:C:537:GLN:HA	2:C:540:TYR:HB2	1.92	0.50
2:E:156:PHE:HB2	2:E:287:PHE:CD1	2.46	0.50
2:G:136:HIS:HB3	2:G:168:ILE:HD13	1.91	0.50
2:G:244:ASN:HA	2:G:267:ARG:HH21	1.76	0.50
2:G:335:MET:HE1	2:G:374:LEU:H	1.75	0.50
2:G:368:PRO:HB2	4:G:602:ATP:O3'	2.11	0.50
1:K:32:GLY:C	1:K:34:ASN:H	2.15	0.50
1:K:49:THR:HG22	1:K:50:ARG:H	1.76	0.50
1:M:23:PRO:HG2	1:M:53:ARG:HB3	1.93	0.50
2:A:231:LEU:O	2:A:235:ILE:HG13	2.12	0.50
2:A:247:PHE:CE1	2:A:266:LEU:HD22	2.46	0.50
2:A:337:PHE:C	2:A:339:SER:H	2.15	0.50
2:A:367:THR:CB	2:A:368:PRO:CD	2.83	0.50
2:A:416:VAL:HG22	2:A:429:GLU:HG2	1.92	0.50
2:A:535:LEU:HD22	2:A:536:HIS:CE1	2.46	0.50
2:B:252:VAL:HG11	2:B:258:ILE:CD1	2.41	0.50
2:C:156:PHE:HB2	2:C:287:PHE:CD1	2.46	0.50
2:C:276:GLU:HG2	2:C:439:LYS:O	2.11	0.50
2:D:192:ASP:HB3	2:D:251:ASP:O	2.11	0.50
2:D:405:ILE:HG23	2:D:410:TRP:CH2	2.47	0.50
2:D:438:SER:CA	2:D:444:LEU:O	2.59	0.50
2:D:452:LEU:H	2:D:452:LEU:CD2	2.23	0.50
2:E:190:LEU:HD13	2:E:203:LEU:HD21	1.92	0.50
2:E:533:MET:HG3	2:E:540:TYR:CE2	2.46	0.50
2:F:269:LEU:HD22	2:F:270:VAL:H	1.75	0.50
2:G:112:ARG:HH11	2:G:115:LEU:HD12	1.75	0.50
2:G:232:LYS:HE3	2:G:260:TRP:CE3	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:ARG:CG	1:I:8:ARG:NH1	2.74	0.50
2:A:276:GLU:HG2	2:A:439:LYS:O	2.11	0.50
2:B:156:PHE:HB2	2:B:287:PHE:CD1	2.46	0.50
2:B:219:ASN:O	2:B:220:PHE:C	2.47	0.50
2:B:298:CYS:O	2:B:299:TYR:C	2.49	0.50
2:B:329:ASN:HB3	2:B:332:THR:OG1	2.11	0.50
2:B:337:PHE:O	2:B:338:LYS:C	2.50	0.50
2:B:416:VAL:HG22	2:B:429:GLU:HG2	1.92	0.50
2:C:141:ILE:HG23	2:C:179:LEU:HD22	1.93	0.50
2:D:233:ARG:HA	2:D:236:CYS:SG	2.51	0.50
2:G:165:LYS:NZ	4:G:602:ATP:O1G	2.40	0.50
2:G:233:ARG:HA	2:G:236:CYS:SG	2.51	0.50
2:G:310:PRO:HA	2:G:315:GLU:OE1	2.12	0.50
2:G:485:LEU:HA	2:G:531:LYS:HB3	1.92	0.50
1:J:18:ILE:O	1:J:50:ARG:NH2	2.38	0.50
1:L:32:GLY:C	1:L:34:ASN:H	2.15	0.50
2:B:190:LEU:HD13	2:B:203:LEU:HD21	1.92	0.50
2:C:399:MET:CE	2:C:413:VAL:HG21	2.42	0.50
2:D:276:GLU:HG2	2:D:439:LYS:O	2.11	0.50
2:D:461:HIS:HD1	2:D:461:HIS:C	2.15	0.50
2:E:536:HIS:HB2	2:E:540:TYR:CE1	2.45	0.50
2:F:298:CYS:O	2:F:299:TYR:C	2.49	0.50
2:G:354:LYS:NZ	2:G:362:GLY:HA3	2.27	0.50
2:G:524:ILE:HD13	2:G:525:ARG:H	1.75	0.50
2:A:298:CYS:O	2:A:299:TYR:C	2.49	0.50
2:A:382:VAL:HG13	2:A:382:VAL:O	2.11	0.50
2:B:233:ARG:HA	2:B:236:CYS:SG	2.51	0.50
2:B:276:GLU:HG2	2:B:439:LYS:O	2.11	0.50
2:B:538:LYS:NZ	2:B:538:LYS:CB	2.73	0.50
2:C:214:GLU:HB3	2:D:237:ASN:HD21	1.76	0.50
2:D:231:LEU:O	2:D:235:ILE:HG13	2.12	0.50
2:D:397:VAL:HG21	2:D:468:VAL:HG21	1.94	0.50
2:E:231:LEU:O	2:E:235:ILE:HG13	2.12	0.50
2:E:539:PHE:CE1	2:E:543:LEU:HD23	2.47	0.50
2:F:274:ASP:C	2:F:274:ASP:OD1	2.48	0.50
2:F:319:LEU:CD2	2:F:345:PHE:CE2	2.90	0.50
2:G:150:LEU:CD1	2:G:153:PHE:HB3	2.42	0.50
1:I:8:ARG:HG2	1:I:8:ARG:NH1	2.10	0.50
1:I:104:VAL:CG1	1:L:52:GLU:OE2	2.59	0.50
2:A:233:ARG:HA	2:A:236:CYS:SG	2.51	0.50
2:B:195:THR:C	2:B:254:GLN:NE2	2.65	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:THR:HG23	2:C:257:THR:HA	1.93	0.50
2:C:233:ARG:HA	2:C:236:CYS:SG	2.51	0.50
2:C:321:LYS:CD	2:C:325:LEU:HG	2.40	0.50
2:D:132:ILE:HD12	2:D:132:ILE:N	2.26	0.50
2:D:141:ILE:HG23	2:D:179:LEU:HD21	1.94	0.50
2:D:269:LEU:HD22	2:D:270:VAL:H	1.75	0.50
2:E:141:ILE:CG1	2:E:172:ALA:HB1	2.40	0.50
2:F:218:LEU:HG	2:F:219:ASN:ND2	2.27	0.50
1:K:35:ILE:O	1:K:35:ILE:CG2	2.60	0.50
2:A:150:LEU:CD1	2:A:153:PHE:HB3	2.40	0.50
2:A:463:PHE:O	2:A:467:VAL:HB	2.12	0.50
2:D:220:PHE:HE1	2:D:223:VAL:CG2	2.25	0.50
2:E:184:TYR:CE1	2:E:246:LEU:HD13	2.39	0.50
2:E:201:PHE:CD1	2:E:201:PHE:C	2.85	0.50
2:G:190:LEU:HD13	2:G:203:LEU:HD21	1.92	0.50
1:J:97:GLU:HB2	1:M:51:LEU:CD1	2.42	0.50
1:M:32:GLY:C	1:M:34:ASN:H	2.15	0.50
2:B:341:GLU:HB2	2:B:342:PRO:HD3	1.92	0.50
2:C:141:ILE:HG23	2:C:179:LEU:HD21	1.94	0.50
2:C:533:MET:O	2:C:540:TYR:HD2	1.94	0.50
2:D:200:THR:OG1	2:D:256:GLU:HB3	2.12	0.50
2:D:258:ILE:HD13	2:D:277:ILE:HD12	1.94	0.50
2:D:337:PHE:CZ	2:D:343:LYS:HE2	2.46	0.50
2:D:539:PHE:CD1	2:D:539:PHE:C	2.86	0.50
2:E:336:PHE:CD1	2:E:336:PHE:C	2.85	0.50
2:F:321:LYS:HE2	2:F:321:LYS:HA	1.92	0.50
2:G:231:LEU:O	2:G:235:ILE:HG13	2.12	0.50
2:G:406:PRO:HG2	2:G:526:PRO:HG2	1.93	0.50
1:H:10:LEU:HD13	1:H:58:LEU:HD22	1.94	0.50
1:I:26:ALA:HA	1:I:74:PHE:CE2	2.47	0.50
1:M:77:TYR:CD1	1:M:77:TYR:O	2.64	0.50
2:C:190:LEU:HD13	2:C:203:LEU:HD21	1.92	0.50
2:C:298:CYS:O	2:C:299:TYR:C	2.49	0.50
2:C:300:ASP:OD1	2:C:300:ASP:N	2.45	0.50
2:C:539:PHE:CD1	2:C:539:PHE:C	2.85	0.50
2:D:155:LEU:HB3	2:D:269:LEU:HD23	1.94	0.50
2:D:360:LEU:CD1	2:D:360:LEU:N	2.74	0.50
2:E:155:LEU:HB3	2:E:269:LEU:HD23	1.94	0.50
2:E:391:SER:O	2:E:394:ALA:N	2.45	0.50
2:E:529:PHE:N	2:E:530:PRO:CD	2.73	0.50
2:F:300:ASP:OD1	2:F:300:ASP:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:49:THR:HG22	1:L:50:ARG:H	1.76	0.49
2:A:190:LEU:HD13	2:A:203:LEU:HD21	1.92	0.49
2:D:201:PHE:C	2:D:201:PHE:CD1	2.85	0.49
2:D:529:PHE:N	2:D:530:PRO:CD	2.73	0.49
2:E:382:VAL:O	2:E:382:VAL:HG13	2.11	0.49
2:F:155:LEU:HB3	2:F:269:LEU:HD23	1.94	0.49
2:F:340:CYS:O	2:F:341:GLU:C	2.49	0.49
2:G:170:SER:O	2:G:174:SER:HB2	2.12	0.49
2:B:231:LEU:O	2:B:235:ILE:HG13	2.12	0.49
2:C:201:PHE:CD1	2:C:201:PHE:C	2.85	0.49
2:C:293:LEU:H	2:C:328:GLY:HA3	1.77	0.49
2:D:342:PRO:C	2:D:344:THR:H	2.15	0.49
2:D:369:TYR:CE2	2:D:371:TYR:HD2	2.30	0.49
2:E:335:MET:HE1	2:E:374:LEU:N	2.26	0.49
2:F:201:PHE:CD1	2:F:201:PHE:C	2.85	0.49
2:F:214:GLU:HG3	2:G:237:ASN:HD21	1.77	0.49
2:F:299:TYR:HE2	2:F:310:PRO:HG3	1.77	0.49
2:F:311:VAL:HG13	2:F:312:GLY:H	1.76	0.49
2:G:115:LEU:HD11	2:G:177:ASP:HA	1.93	0.49
2:G:461:HIS:HD1	2:G:461:HIS:C	2.15	0.49
1:H:24:ARG:NH2	1:H:53:ARG:HH11	2.09	0.49
1:H:26:ALA:HA	1:H:74:PHE:CE2	2.47	0.49
1:L:21:PHE:CD1	1:L:75:PHE:HE1	2.29	0.49
2:A:409:LEU:HG	2:A:533:MET:HE2	1.93	0.49
2:B:127:GLN:HG2	2:B:174:SER:CB	2.38	0.49
2:B:214:GLU:HB3	2:C:237:ASN:HD21	1.77	0.49
2:B:426:LEU:HG	2:B:426:LEU:O	2.12	0.49
2:C:427:ASP:C	2:C:429:GLU:N	2.66	0.49
2:E:229:VAL:O	2:E:229:VAL:HG22	2.13	0.49
2:E:308:PRO:HG3	2:E:343:LYS:O	2.13	0.49
2:E:391:SER:O	2:E:392:ALA:C	2.51	0.49
2:G:315:GLU:C	2:G:318:VAL:H	2.16	0.49
1:I:97:GLU:HG3	1:I:100:LEU:HB2	1.95	0.49
2:A:170:SER:O	2:A:174:SER:HB2	2.12	0.49
2:B:143:LYS:NZ	2:B:286:GLU:HG3	2.25	0.49
2:B:147:MET:HG2	2:B:153:PHE:CD1	2.47	0.49
2:B:364:GLU:HG3	2:B:364:GLU:O	2.12	0.49
2:C:161:ALA:HB1	2:C:273:ARG:CZ	2.42	0.49
2:D:190:LEU:HD13	2:D:203:LEU:HD21	1.92	0.49
2:E:141:ILE:HG23	2:E:179:LEU:HD21	1.94	0.49
2:E:305:TYR:O	2:E:337:PHE:HZ	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:452:LEU:H	2:F:452:LEU:CD2	2.23	0.49
2:G:141:ILE:HG23	2:G:179:LEU:HD22	1.93	0.49
2:G:192:ASP:HB3	2:G:251:ASP:O	2.11	0.49
1:L:35:ILE:CG2	1:L:35:ILE:O	2.60	0.49
1:M:37:THR:H	1:M:40:HIS:HB2	1.77	0.49
2:B:128:MET:HG2	2:B:167:VAL:CG2	2.43	0.49
2:B:178:GLN:HG2	2:B:182:ILE:HG21	1.94	0.49
2:B:360:LEU:CD1	2:B:462:MET:HE3	2.38	0.49
2:B:452:LEU:H	2:B:452:LEU:CD2	2.23	0.49
2:D:210:MET:HA	2:D:210:MET:HE3	1.95	0.49
2:D:314:LYS:HB3	2:D:314:LYS:HZ3	1.76	0.49
2:F:152:SER:HA	2:F:266:LEU:C	2.33	0.49
2:F:220:PHE:CE1	2:F:223:VAL:HG13	2.48	0.49
2:G:153:PHE:CD1	2:G:267:ARG:HB3	2.47	0.49
2:G:246:LEU:HD23	2:G:247:PHE:N	2.28	0.49
1:H:58:LEU:O	1:H:62:ARG:HG3	2.12	0.49
1:I:37:THR:H	1:I:40:HIS:HB2	1.78	0.49
1:K:37:THR:O	1:K:40:HIS:HB2	2.13	0.49
2:A:229:VAL:HG22	2:A:229:VAL:O	2.13	0.49
2:A:300:ASP:OD1	2:A:300:ASP:N	2.45	0.49
2:A:337:PHE:C	2:A:337:PHE:CD1	2.86	0.49
2:A:461:HIS:HD1	2:A:461:HIS:C	2.15	0.49
2:B:141:ILE:HG23	2:B:179:LEU:HD21	1.94	0.49
2:B:537:GLN:HE22	2:B:541:ASP:HB3	1.78	0.49
2:C:155:LEU:HB3	2:C:269:LEU:HD23	1.94	0.49
2:C:405:ILE:HG12	2:C:410:TRP:CE3	2.48	0.49
2:C:426:LEU:O	2:C:427:ASP:HB3	2.13	0.49
2:D:298:CYS:O	2:D:299:TYR:C	2.49	0.49
2:D:446:GLY:HA3	2:D:454:PHE:CD2	2.47	0.49
2:D:462:MET:HA	2:D:465:LYS:HB2	1.93	0.49
2:D:529:PHE:HA	2:D:532:PHE:CE2	2.47	0.49
2:E:200:THR:HG23	2:E:257:THR:HA	1.95	0.49
2:E:533:MET:HG3	2:E:540:TYR:CE1	2.47	0.49
2:F:231:LEU:O	2:F:235:ILE:HG13	2.12	0.49
2:F:253:VAL:HG11	2:F:380:ARG:CZ	2.42	0.49
2:G:464:LEU:O	2:G:468:VAL:HG22	2.13	0.49
2:A:156:PHE:HB2	2:A:287:PHE:CD1	2.46	0.49
2:A:208:LEU:O	2:A:208:LEU:HD22	2.13	0.49
2:A:327:SER:HG	2:A:458:HIS:HB2	1.77	0.49
2:B:201:PHE:C	2:B:201:PHE:CD1	2.85	0.49
2:C:341:GLU:C	2:C:343:LYS:H	2.16	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:229:VAL:O	2:D:229:VAL:HG22	2.13	0.49
2:F:382:VAL:CG2	2:F:393:LEU:HD13	2.43	0.49
2:F:438:SER:HA	2:F:444:LEU:H	1.78	0.49
2:G:155:LEU:HB3	2:G:269:LEU:HD23	1.94	0.49
2:G:382:VAL:HG13	2:G:382:VAL:O	2.11	0.49
1:J:26:ALA:HA	1:J:74:PHE:CE2	2.47	0.49
2:B:300:ASP:N	2:B:300:ASP:OD1	2.45	0.49
2:B:311:VAL:HG13	2:B:312:GLY:H	1.78	0.49
2:C:382:VAL:CG2	2:C:393:LEU:HD13	2.43	0.49
2:D:127:GLN:CB	2:D:171:GLN:HG2	2.42	0.49
2:D:214:GLU:HB3	2:E:237:ASN:HD21	1.78	0.49
2:D:382:VAL:CG2	2:D:393:LEU:HD13	2.43	0.49
2:E:127:GLN:HG2	2:E:174:SER:CB	2.43	0.49
2:E:148:CYS:SG	2:E:149:ASP:N	2.85	0.49
2:E:315:GLU:O	2:E:319:LEU:N	2.41	0.49
2:E:364:GLU:CB	2:E:373:SER:HB3	2.43	0.49
2:E:405:ILE:HG12	2:E:410:TRP:CE3	2.48	0.49
2:F:486:GLU:HB3	2:F:531:LYS:HG2	1.94	0.49
2:G:201:PHE:C	2:G:201:PHE:CD1	2.85	0.49
2:G:389:ASP:OD2	2:G:436:ARG:NE	2.46	0.49
2:A:155:LEU:HB3	2:A:269:LEU:HD23	1.94	0.49
2:B:405:ILE:HG12	2:B:410:TRP:CE3	2.48	0.49
2:E:397:VAL:O	2:E:461:HIS:NE2	2.46	0.49
2:F:112:ARG:HH11	2:F:115:LEU:HD12	1.75	0.49
4:F:602:ATP:H2'	4:F:602:ATP:N3	2.28	0.49
1:H:29:TYR:CZ	1:H:33:LYS:HD2	2.48	0.49
1:M:35:ILE:CG2	1:M:35:ILE:O	2.60	0.49
2:A:201:PHE:CD1	2:A:201:PHE:C	2.85	0.49
2:A:315:GLU:O	2:A:319:LEU:N	2.40	0.49
2:A:405:ILE:HG12	2:A:410:TRP:CE3	2.48	0.49
4:A:602:ATP:H2'	4:A:602:ATP:N3	2.28	0.49
2:B:132:ILE:HD12	2:B:132:ILE:N	2.27	0.49
2:B:229:VAL:O	2:B:229:VAL:HG22	2.12	0.49
2:D:227:THR:HG1	2:D:230:VAL:HG23	1.73	0.49
2:D:337:PHE:CE1	2:D:343:LYS:HE2	2.48	0.49
2:G:156:PHE:HE1	2:G:277:ILE:HD11	1.78	0.49
1:J:32:GLY:C	1:J:34:ASN:H	2.17	0.48
1:M:24:ARG:NH2	1:M:53:ARG:HH11	2.11	0.48
2:A:336:PHE:CD1	2:A:336:PHE:C	2.85	0.48
2:B:208:LEU:O	2:B:208:LEU:HD22	2.13	0.48
2:C:231:LEU:O	2:C:235:ILE:HG13	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:258:ILE:HD13	2:C:277:ILE:HD12	1.95	0.48
2:E:133:ARG:HD3	2:E:136:HIS:CG	2.48	0.48
2:E:302:LEU:HD13	2:E:307:MET:CG	2.41	0.48
2:E:398:VAL:O	2:E:398:VAL:HG22	2.13	0.48
2:F:170:SER:O	2:F:174:SER:HB2	2.13	0.48
2:F:354:LYS:O	2:F:358:ARG:N	2.46	0.48
2:G:300:ASP:N	2:G:300:ASP:OD1	2.45	0.48
1:I:58:LEU:O	1:I:62:ARG:HG3	2.13	0.48
1:J:29:TYR:CZ	1:J:33:LYS:HD2	2.48	0.48
1:L:24:ARG:NH2	1:L:53:ARG:HH11	2.11	0.48
2:B:133:ARG:HD3	2:B:136:HIS:CG	2.48	0.48
2:B:392:ALA:HB2	2:B:433:ARG:HD3	1.96	0.48
2:D:127:GLN:HG2	2:D:171:GLN:HA	1.95	0.48
2:D:127:GLN:HB3	2:D:171:GLN:CG	2.43	0.48
2:D:397:VAL:HG22	2:D:464:LEU:HB3	1.94	0.48
2:D:401:PRO:HA	2:D:456:ILE:CG2	2.41	0.48
2:E:321:LYS:O	2:E:324:GLU:HB3	2.12	0.48
2:E:403:VAL:HG11	2:E:536:HIS:CE1	2.47	0.48
2:G:141:ILE:HG23	2:G:179:LEU:HD21	1.94	0.48
2:G:229:VAL:O	2:G:229:VAL:HG22	2.12	0.48
1:J:10:LEU:HD13	1:J:58:LEU:HD22	1.94	0.48
1:M:37:THR:O	1:M:40:HIS:HB2	2.13	0.48
2:A:214:GLU:HB3	2:B:237:ASN:HD21	1.78	0.48
2:B:141:ILE:HG23	2:B:179:LEU:HD22	1.93	0.48
2:B:155:LEU:HB3	2:B:269:LEU:HD23	1.94	0.48
2:B:329:ASN:OD1	2:B:332:THR:HG23	2.13	0.48
2:C:128:MET:HG2	2:C:167:VAL:CG2	2.42	0.48
2:C:133:ARG:HD3	2:C:136:HIS:CG	2.48	0.48
2:C:314:LYS:NZ	2:C:314:LYS:CB	2.75	0.48
2:C:378:LEU:O	2:C:379:GLN:C	2.52	0.48
2:E:486:GLU:O	2:E:487:ILE:C	2.52	0.48
2:F:382:VAL:O	2:F:382:VAL:HG13	2.11	0.48
2:G:208:LEU:O	2:G:208:LEU:HD22	2.13	0.48
1:I:77:TYR:CD1	1:I:77:TYR:O	2.67	0.48
1:K:88:GLU:O	1:K:91:ILE:HG22	2.14	0.48
2:A:141:ILE:HG23	2:A:179:LEU:HD22	1.93	0.48
2:B:147:MET:CA	2:B:147:MET:CE	2.91	0.48
2:D:206:ASP:OD1	2:E:227:THR:OG1	2.25	0.48
2:D:300:ASP:N	2:D:300:ASP:OD1	2.45	0.48
2:E:300:ASP:N	2:E:300:ASP:OD1	2.45	0.48
2:E:350:GLN:O	2:E:354:LYS:HG3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:208:LEU:O	2:F:208:LEU:HD22	2.13	0.48
2:G:341:GLU:HB3	2:G:342:PRO:HD3	1.94	0.48
2:G:397:VAL:HG11	2:G:465:LYS:HA	1.95	0.48
1:I:10:LEU:HD13	1:I:58:LEU:HD22	1.94	0.48
1:I:29:TYR:CZ	1:I:33:LYS:HD2	2.48	0.48
1:I:76:ASN:HA	1:I:81:SER:OG	2.14	0.48
1:K:37:THR:H	1:K:40:HIS:HB2	1.78	0.48
1:M:88:GLU:O	1:M:91:ILE:HG22	2.14	0.48
2:A:237:ASN:HD21	2:G:214:GLU:HB3	1.79	0.48
2:A:326:SER:O	2:A:459:ILE:CG1	2.54	0.48
2:B:334:MET:HG2	2:B:367:THR:OG1	2.13	0.48
2:D:208:LEU:O	2:D:208:LEU:HD22	2.13	0.48
2:D:399:MET:HG2	2:D:410:TRP:CZ2	2.48	0.48
2:E:326:SER:HA	2:E:459:ILE:HG23	1.95	0.48
2:E:360:LEU:N	2:E:360:LEU:CD1	2.74	0.48
2:F:531:LYS:H	2:F:531:LYS:HD2	1.78	0.48
2:F:536:HIS:HB2	2:F:540:TYR:CZ	2.48	0.48
2:G:405:ILE:HG12	2:G:410:TRP:CE3	2.48	0.48
1:J:76:ASN:HA	1:J:81:SER:OG	2.14	0.48
2:A:141:ILE:HG23	2:A:179:LEU:HD21	1.94	0.48
2:A:400:PRO:HD3	2:A:540:TYR:CZ	2.49	0.48
2:A:401:PRO:HA	2:A:456:ILE:HG22	1.95	0.48
2:B:308:PRO:HB3	2:B:345:PHE:CE2	2.42	0.48
2:B:319:LEU:O	2:B:323:ILE:HG23	2.13	0.48
2:B:378:LEU:O	2:B:379:GLN:C	2.52	0.48
2:C:208:LEU:O	2:C:208:LEU:HD22	2.13	0.48
2:C:335:MET:HE3	2:C:373:SER:HA	1.96	0.48
2:D:133:ARG:HD3	2:D:136:HIS:CG	2.49	0.48
2:D:327:SER:H	2:D:459:ILE:HG12	1.78	0.48
2:D:378:LEU:O	2:D:379:GLN:C	2.52	0.48
2:E:259:ARG:CG	2:E:259:ARG:NH1	2.73	0.48
2:F:140:VAL:HG22	2:F:288:ILE:CD1	2.28	0.48
2:F:529:PHE:HD1	2:F:532:PHE:CZ	2.31	0.48
2:G:227:THR:OG1	2:G:230:VAL:HG23	2.12	0.48
1:H:49:THR:HG22	1:H:50:ARG:N	2.29	0.48
1:K:58:LEU:O	1:K:62:ARG:HG3	2.14	0.48
2:A:283:GLN:HG2	2:A:284:THR:N	2.26	0.48
2:A:369:TYR:C	2:A:371:TYR:N	2.67	0.48
2:C:149:ASP:N	2:C:149:ASP:OD1	2.44	0.48
2:C:412:CYS:HB3	2:C:483:ARG:HB2	1.94	0.48
2:D:127:GLN:HB3	2:D:171:GLN:HA	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:208:LEU:O	2:E:208:LEU:HD22	2.13	0.48
2:E:210:MET:HE3	2:E:210:MET:HA	1.96	0.48
2:G:345:PHE:HA	2:G:348:MET:HE2	1.95	0.48
1:H:37:THR:H	1:H:40:HIS:HB2	1.78	0.48
1:I:102:ARG:HA	1:I:106:ILE:HB	1.96	0.48
1:J:58:LEU:O	1:J:62:ARG:HG3	2.13	0.48
1:L:37:THR:O	1:L:40:HIS:HB2	2.13	0.48
2:A:465:LYS:HB2	2:A:465:LYS:HE2	1.65	0.48
2:B:341:GLU:C	2:B:343:LYS:N	2.66	0.48
2:C:127:GLN:HB3	2:C:171:GLN:N	2.29	0.48
2:C:200:THR:OG1	2:C:256:GLU:HB3	2.14	0.48
4:C:602:ATP:H2'	4:C:602:ATP:N3	2.28	0.48
4:G:602:ATP:H2'	4:G:602:ATP:N3	2.28	0.48
1:H:21:PHE:CD1	1:H:75:PHE:CE1	3.02	0.48
1:I:21:PHE:CD1	1:I:75:PHE:CE1	3.02	0.48
1:I:32:GLY:C	1:I:34:ASN:H	2.17	0.48
1:I:97:GLU:CB	1:L:51:LEU:CD1	2.89	0.48
1:J:8:ARG:NH1	1:J:8:ARG:CG	2.74	0.48
1:J:37:THR:H	1:J:40:HIS:HB2	1.78	0.48
1:M:58:LEU:O	1:M:62:ARG:HG3	2.14	0.48
2:B:533:MET:HG3	2:B:540:TYR:CZ	2.48	0.48
4:B:602:ATP:N3	4:B:602:ATP:H2'	2.28	0.48
2:D:358:ARG:C	2:D:466:HIS:NE2	2.66	0.48
2:D:399:MET:HB2	2:D:399:MET:HE2	1.81	0.48
2:G:249:PHE:HE2	2:G:268:CYS:SG	2.37	0.48
1:I:49:THR:HG22	1:I:50:ARG:N	2.29	0.48
1:L:58:LEU:O	1:L:62:ARG:HG3	2.14	0.48
2:A:443:LEU:HA	2:A:460:ILE:HG12	1.96	0.48
2:B:306:GLY:O	2:B:337:PHE:HE1	1.96	0.48
2:E:112:ARG:HH11	2:E:115:LEU:HD12	1.75	0.48
2:E:307:MET:CG	2:E:308:PRO:HD2	2.44	0.48
2:F:336:PHE:CE1	2:F:348:MET:HA	2.48	0.48
2:G:426:LEU:C	2:G:428:ASP:N	2.67	0.48
1:I:88:GLU:O	1:I:91:ILE:HG22	2.14	0.47
1:K:24:ARG:NH2	1:K:53:ARG:HH11	2.11	0.47
1:L:22:GLU:OE2	1:L:24:ARG:HG3	2.15	0.47
2:A:445:SER:O	2:A:455:LYS:HG3	2.14	0.47
2:D:158:HIS:ND1	2:D:158:HIS:O	2.47	0.47
2:D:274:ASP:OD1	2:D:440:ARG:HD2	2.13	0.47
2:D:399:MET:HE1	2:D:413:VAL:HG21	1.95	0.47
4:D:602:ATP:H2'	4:D:602:ATP:N3	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:469:ASP:HB3	2:E:472:THR:OG1	2.13	0.47
2:G:532:PHE:HB3	2:G:535:LEU:HB2	1.96	0.47
1:I:4:GLU:HG3	1:I:5:ILE:N	2.29	0.47
1:J:77:TYR:CD1	1:J:77:TYR:O	2.67	0.47
1:L:37:THR:H	1:L:40:HIS:HB2	1.78	0.47
2:A:359:GLY:N	2:A:466:HIS:NE2	2.61	0.47
2:A:380:ARG:O	2:A:380:ARG:HD2	2.15	0.47
2:B:163:SER:O	2:B:330:PRO:HG2	2.14	0.47
2:B:537:GLN:NE2	2:B:541:ASP:HB3	2.29	0.47
2:C:214:GLU:CB	2:D:237:ASN:HD21	2.27	0.47
2:D:159:GLY:H	2:D:165:LYS:HD3	1.75	0.47
2:E:135:TYR:O	2:E:139:ARG:HB2	2.15	0.47
2:E:366:ILE:HG23	2:F:279:ASN:HB2	1.96	0.47
2:F:214:GLU:CG	2:G:237:ASN:HD21	2.27	0.47
2:F:321:LYS:O	2:F:325:LEU:HG	2.15	0.47
2:F:529:PHE:HB3	2:F:532:PHE:CE2	2.48	0.47
2:G:156:PHE:HB2	2:G:287:PHE:CD1	2.48	0.47
1:H:67:GLU:HG2	1:H:69:GLY:H	1.79	0.47
1:J:102:ARG:HA	1:J:106:ILE:HB	1.96	0.47
1:M:8:ARG:NH1	1:M:8:ARG:CG	2.75	0.47
1:M:22:GLU:OE2	1:M:24:ARG:HG3	2.14	0.47
2:A:335:MET:HE1	2:A:373:SER:HA	1.96	0.47
2:A:400:PRO:CB	2:A:536:HIS:HB3	2.37	0.47
2:B:158:HIS:ND1	2:B:158:HIS:O	2.47	0.47
2:C:393:LEU:HD11	2:C:443:LEU:CD1	2.44	0.47
2:D:335:MET:HA	2:D:365:CYS:SG	2.55	0.47
2:F:393:LEU:CB	2:F:437:LEU:HD11	2.45	0.47
2:G:355:LEU:O	2:G:357:SER:N	2.47	0.47
1:H:77:TYR:CD1	1:H:77:TYR:O	2.66	0.47
2:A:252:VAL:HG11	2:A:258:ILE:CD1	2.44	0.47
2:A:353:ASN:HA	2:A:356:GLU:CD	2.35	0.47
2:A:382:VAL:HG23	2:A:393:LEU:HD11	1.91	0.47
2:A:531:LYS:H	2:A:531:LYS:CD	1.96	0.47
2:C:484:LEU:HD11	2:C:530:PRO:O	2.14	0.47
2:D:393:LEU:CB	2:D:437:LEU:HD11	2.45	0.47
2:D:393:LEU:CD2	2:D:464:LEU:HD11	2.43	0.47
2:E:131:TYR:OH	2:E:297:GLU:HG2	2.15	0.47
2:E:378:LEU:O	2:E:379:GLN:C	2.52	0.47
2:E:452:LEU:H	2:E:452:LEU:CD2	2.23	0.47
2:F:134:GLU:O	2:F:135:TYR:C	2.52	0.47
2:F:255:GLU:OE2	2:F:259:ARG:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:314:LYS:HG2	2:G:315:GLU:N	2.30	0.47
1:J:67:GLU:HG2	1:J:69:GLY:H	1.79	0.47
2:B:332:THR:HG21	2:B:459:ILE:CG2	2.44	0.47
2:B:470:ALA:O	2:B:473:ILE:HB	2.15	0.47
2:D:226:VAL:HG12	2:D:230:VAL:HB	1.95	0.47
2:E:184:TYR:CE2	2:E:246:LEU:HD11	2.30	0.47
2:F:308:PRO:HD2	2:F:348:MET:CE	2.44	0.47
2:F:378:LEU:O	2:F:379:GLN:C	2.52	0.47
2:G:131:TYR:CD1	2:G:301:PHE:HD1	2.33	0.47
2:G:162:GLY:C	2:G:164:GLY:H	2.16	0.47
1:H:76:ASN:HA	1:H:81:SER:OG	2.14	0.47
1:I:67:GLU:HG2	1:I:69:GLY:H	1.79	0.47
1:J:4:GLU:HG3	1:J:5:ILE:N	2.29	0.47
1:L:88:GLU:O	1:L:91:ILE:HG22	2.14	0.47
2:A:158:HIS:ND1	2:A:158:HIS:O	2.47	0.47
2:A:378:LEU:O	2:A:379:GLN:C	2.52	0.47
2:B:164:GLY:HA2	4:B:602:ATP:O3A	2.15	0.47
2:B:354:LYS:O	2:B:358:ARG:HB2	2.13	0.47
2:C:259:ARG:HH11	2:C:259:ARG:CG	2.27	0.47
2:C:274:ASP:OD1	2:C:276:GLU:HB2	2.15	0.47
2:C:335:MET:O	2:C:365:CYS:SG	2.72	0.47
2:C:437:LEU:HD23	2:C:437:LEU:HA	1.69	0.47
2:E:214:GLU:HB3	2:F:237:ASN:HD21	1.79	0.47
2:F:380:ARG:HD2	2:F:380:ARG:O	2.15	0.47
2:G:127:GLN:CB	2:G:171:GLN:HA	2.45	0.47
2:G:301:PHE:CE2	2:G:334:MET:CE	2.97	0.47
2:G:309:MET:HA	2:G:309:MET:CE	2.45	0.47
2:G:413:VAL:HG12	2:G:476:GLY:O	2.14	0.47
1:J:21:PHE:CD1	1:J:75:PHE:CE1	3.02	0.47
1:J:49:THR:HG22	1:J:50:ARG:N	2.29	0.47
1:J:97:GLU:HG3	1:J:100:LEU:HB2	1.95	0.47
1:K:4:GLU:HG3	1:K:5:ILE:N	2.30	0.47
2:A:131:TYR:OH	2:A:297:GLU:HG2	2.15	0.47
2:A:187:ILE:HD11	2:A:248:VAL:CG2	2.45	0.47
2:A:229:VAL:HG11	2:G:206:ASP:CG	2.34	0.47
2:A:241:ASP:O	2:A:243:PRO:HD3	2.13	0.47
2:B:178:GLN:O	2:B:182:ILE:HB	2.13	0.47
2:B:187:ILE:HD11	2:B:248:VAL:CG2	2.45	0.47
2:B:459:ILE:H	2:B:459:ILE:HG13	1.41	0.47
2:C:206:ASP:CG	2:D:229:VAL:HG11	2.34	0.47
2:C:258:ILE:CD1	2:C:277:ILE:HD12	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:355:LEU:HD13	2:C:363:VAL:HG23	1.96	0.47
2:C:380:ARG:HD2	2:C:380:ARG:O	2.15	0.47
2:C:393:LEU:HB2	2:C:437:LEU:HD11	1.97	0.47
2:D:135:TYR:O	2:D:139:ARG:HB2	2.15	0.47
2:D:210:MET:HE3	2:D:210:MET:CA	2.43	0.47
2:D:240:ILE:H	2:D:240:ILE:HG13	1.57	0.47
2:D:274:ASP:CG	2:D:440:ARG:HD2	2.35	0.47
2:D:393:LEU:HB2	2:D:437:LEU:HD11	1.97	0.47
2:E:210:MET:HE3	2:E:210:MET:CA	2.45	0.47
2:E:412:CYS:HB3	2:E:483:ARG:HB2	1.96	0.47
2:E:524:ILE:HG13	2:E:535:LEU:CD1	2.34	0.47
4:E:602:ATP:N3	4:E:602:ATP:H2'	2.28	0.47
2:F:135:TYR:CZ	2:F:139:ARG:HD2	2.50	0.47
2:F:165:LYS:HG3	4:F:602:ATP:O2B	2.15	0.47
2:F:214:GLU:HB3	2:G:237:ASN:HD21	1.80	0.47
2:F:399:MET:HG3	2:F:400:PRO:HD2	1.95	0.47
2:F:455:LYS:NZ	2:F:457:ASP:HA	2.29	0.47
2:G:378:LEU:O	2:G:379:GLN:C	2.52	0.47
2:G:402:GLY:HA3	2:G:458:HIS:CE1	2.50	0.47
2:G:452:LEU:H	2:G:452:LEU:CD2	2.23	0.47
1:J:2:LEU:O	1:J:3:CYS:HB3	2.15	0.47
1:J:88:GLU:O	1:J:91:ILE:HG22	2.15	0.47
1:L:35:ILE:HG22	1:L:36:PHE:HD1	1.80	0.47
1:M:21:PHE:CD1	1:M:75:PHE:CE1	3.03	0.47
2:A:274:ASP:OD1	2:A:276:GLU:HB2	2.15	0.47
2:A:363:VAL:O	2:A:365:CYS:SG	2.59	0.47
2:A:366:ILE:HG12	2:A:372:LYS:NZ	2.29	0.47
2:A:460:ILE:HD12	2:A:460:ILE:HA	1.80	0.47
2:C:128:MET:CE	2:C:128:MET:CA	2.86	0.47
2:D:133:ARG:HD3	2:D:136:HIS:HB2	1.95	0.47
2:D:141:ILE:HD12	2:D:175:LYS:HZ1	1.79	0.47
2:E:350:GLN:HE22	2:F:426:LEU:CD2	2.27	0.47
2:F:156:PHE:HB2	2:F:287:PHE:CD1	2.50	0.47
2:F:397:VAL:O	2:F:461:HIS:NE2	2.48	0.47
2:G:345:PHE:HA	2:G:348:MET:HE3	1.96	0.47
2:G:485:LEU:O	2:G:487:ILE:N	2.47	0.47
2:G:536:HIS:HB2	2:G:540:TYR:CE2	2.50	0.47
1:K:22:GLU:OE2	1:K:24:ARG:HG3	2.14	0.47
1:M:35:ILE:HG22	1:M:36:PHE:HD1	1.80	0.47
2:B:131:TYR:OH	2:B:297:GLU:HG2	2.15	0.47
2:C:127:GLN:HB3	2:C:170:SER:C	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:314:LYS:HB3	2:C:314:LYS:NZ	2.29	0.47
2:C:393:LEU:CB	2:C:437:LEU:HD11	2.45	0.47
2:C:475:ASN:O	2:C:479:ILE:HG13	2.14	0.47
2:D:150:LEU:HD22	2:D:150:LEU:HA	1.76	0.47
2:G:201:PHE:HZ	2:G:224:GLU:HA	1.79	0.47
2:G:336:PHE:HE1	2:G:348:MET:HG2	1.80	0.47
2:A:295:ILE:HD13	2:A:295:ILE:N	2.30	0.47
2:A:320:ASN:O	2:A:321:LYS:C	2.53	0.47
2:C:165:LYS:HG3	4:C:602:ATP:O2B	2.15	0.47
2:E:308:PRO:HB2	2:E:345:PHE:CE1	2.50	0.47
2:E:380:ARG:HD2	2:E:380:ARG:O	2.15	0.47
2:F:295:ILE:HD13	2:F:295:ILE:N	2.31	0.47
2:F:543:LEU:H	2:F:543:LEU:HD22	1.80	0.47
2:G:158:HIS:CE1	2:G:289:GLU:HB2	2.50	0.47
2:G:258:ILE:HD12	2:G:258:ILE:N	2.26	0.47
2:G:315:GLU:O	2:G:319:LEU:N	2.39	0.47
1:H:2:LEU:O	1:H:3:CYS:HB3	2.15	0.46
1:H:32:GLY:C	1:H:34:ASN:H	2.16	0.46
2:A:165:LYS:HG2	2:A:290:VAL:HG21	1.97	0.46
2:B:135:TYR:O	2:B:139:ARG:HB2	2.15	0.46
2:C:135:TYR:O	2:C:139:ARG:HB2	2.15	0.46
2:C:413:VAL:HG13	2:C:480:LEU:HB2	1.96	0.46
2:D:388:GLU:OE1	2:D:433:ARG:NH2	2.49	0.46
2:E:295:ILE:N	2:E:295:ILE:HD13	2.31	0.46
2:E:537:GLN:O	2:E:538:LYS:C	2.54	0.46
2:F:393:LEU:HB2	2:F:437:LEU:HD11	1.97	0.46
2:G:210:MET:HA	2:G:210:MET:HE3	1.96	0.46
2:G:301:PHE:CZ	2:G:334:MET:HE1	2.49	0.46
2:G:318:VAL:HG13	2:G:349:ALA:HB2	1.96	0.46
2:G:342:PRO:CG	2:G:347:LYS:HG3	2.43	0.46
2:B:165:LYS:HG2	2:B:290:VAL:HG21	1.97	0.46
2:B:295:ILE:HD13	2:B:295:ILE:N	2.30	0.46
2:C:187:ILE:HD11	2:C:248:VAL:CG2	2.45	0.46
2:D:187:ILE:HD11	2:D:248:VAL:CG2	2.45	0.46
2:D:380:ARG:O	2:D:380:ARG:HD2	2.15	0.46
2:F:187:ILE:HD11	2:F:248:VAL:CG2	2.45	0.46
2:G:187:ILE:HD11	2:G:248:VAL:CG2	2.45	0.46
2:G:295:ILE:HD13	2:G:295:ILE:N	2.31	0.46
1:L:4:GLU:HG3	1:L:5:ILE:N	2.30	0.46
2:A:140:VAL:HG12	2:A:172:ALA:CB	2.46	0.46
2:B:208:LEU:HD22	2:B:208:LEU:C	2.36	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:131:TYR:OH	2:C:297:GLU:HG2	2.15	0.46
2:C:140:VAL:HG12	2:C:172:ALA:CB	2.46	0.46
2:D:305:TYR:HE2	2:D:334:MET:HE3	1.35	0.46
2:D:335:MET:HE1	2:D:374:LEU:H	1.80	0.46
2:G:398:VAL:H	2:G:399:MET:HE1	1.80	0.46
1:H:88:GLU:O	1:H:91:ILE:HG22	2.15	0.46
1:L:72:ILE:C	1:L:74:PHE:H	2.18	0.46
2:A:351:LEU:C	2:A:353:ASN:N	2.66	0.46
2:C:427:ASP:O	2:C:429:GLU:N	2.49	0.46
2:D:208:LEU:HD22	2:D:208:LEU:C	2.36	0.46
2:D:214:GLU:HG3	2:E:237:ASN:HD21	1.80	0.46
2:D:393:LEU:CD2	2:D:464:LEU:HD21	2.45	0.46
2:F:159:GLY:O	2:F:273:ARG:HA	2.15	0.46
2:F:210:MET:HA	2:F:210:MET:HE3	1.97	0.46
2:G:209:LEU:HD21	2:G:220:PHE:CD1	2.51	0.46
1:H:102:ARG:HA	1:H:106:ILE:HB	1.96	0.46
1:J:22:GLU:HG3	1:J:24:ARG:H	1.80	0.46
2:A:208:LEU:HD22	2:A:208:LEU:C	2.36	0.46
2:B:341:GLU:O	2:B:343:LYS:N	2.48	0.46
2:B:343:LYS:HD3	2:B:343:LYS:HA	1.63	0.46
2:B:388:GLU:OE1	2:B:433:ARG:NH2	2.49	0.46
2:C:165:LYS:HG2	2:C:290:VAL:HG21	1.97	0.46
2:D:140:VAL:HG12	2:D:172:ALA:CB	2.46	0.46
2:D:305:TYR:CD2	2:D:334:MET:HE1	2.51	0.46
2:D:471:GLN:HG2	2:D:475:ASN:OD1	2.16	0.46
2:E:133:ARG:HD3	2:E:136:HIS:HB2	1.97	0.46
2:E:165:LYS:HG3	4:E:602:ATP:O2B	2.15	0.46
2:E:371:TYR:O	2:E:372:LYS:C	2.52	0.46
2:G:140:VAL:HG12	2:G:172:ALA:CB	2.45	0.46
2:G:165:LYS:HG2	2:G:290:VAL:HG21	1.97	0.46
2:G:292:SER:HB3	2:G:327:SER:O	2.15	0.46
2:G:524:ILE:HD13	2:G:525:ARG:N	2.30	0.46
1:M:72:ILE:C	1:M:74:PHE:H	2.18	0.46
2:A:188:VAL:O	2:A:248:VAL:N	2.45	0.46
2:A:299:TYR:HE2	2:A:310:PRO:HG3	0.59	0.46
2:A:471:GLN:HG2	2:A:475:ASN:OD1	2.16	0.46
2:B:255:GLU:HB3	2:B:277:ILE:HB	1.98	0.46
2:B:380:ARG:HD2	2:B:380:ARG:O	2.15	0.46
2:C:351:LEU:HA	2:C:354:LYS:HB3	1.98	0.46
2:C:388:GLU:OE1	2:C:433:ARG:NH2	2.49	0.46
2:D:130:CYS:O	2:D:304:ALA:HB1	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:LYS:HG2	2:D:290:VAL:HG21	1.97	0.46
2:D:295:ILE:HD13	2:D:295:ILE:N	2.31	0.46
2:D:369:TYR:HD1	4:D:602:ATP:H5'1	1.81	0.46
2:D:374:LEU:HD22	2:D:374:LEU:HA	1.83	0.46
2:E:211:LEU:HA	2:E:242:ARG:NH2	2.30	0.46
2:F:209:LEU:HD21	2:F:220:PHE:CD1	2.50	0.46
2:G:132:ILE:HB	2:G:134:GLU:OE2	2.15	0.46
2:G:210:MET:HE3	2:G:210:MET:CA	2.46	0.46
2:G:307:MET:HG3	2:G:308:PRO:HD2	1.98	0.46
2:G:355:LEU:C	2:G:357:SER:N	2.69	0.46
1:I:9:ALA:HB2	1:I:90:TYR:CD1	2.51	0.46
1:K:21:PHE:CD1	1:K:75:PHE:CE1	3.03	0.46
1:K:35:ILE:HG22	1:K:36:PHE:HD1	1.80	0.46
1:K:72:ILE:C	1:K:74:PHE:H	2.18	0.46
2:A:388:GLU:OE1	2:A:433:ARG:NH2	2.49	0.46
2:A:459:ILE:H	2:A:459:ILE:HG13	1.41	0.46
2:B:116:ASP:OD1	2:B:116:ASP:N	2.49	0.46
2:B:133:ARG:HD3	2:B:136:HIS:HB2	1.97	0.46
2:B:165:LYS:HG3	4:B:602:ATP:O2B	2.15	0.46
2:B:214:GLU:CB	2:C:237:ASN:HD21	2.29	0.46
2:C:208:LEU:HD22	2:C:208:LEU:C	2.36	0.46
2:C:227:THR:OG1	2:C:230:VAL:HG23	2.16	0.46
2:C:335:MET:CE	2:C:364:GLU:HA	2.46	0.46
2:C:427:ASP:C	2:C:429:GLU:H	2.19	0.46
2:D:131:TYR:OH	2:D:297:GLU:HG2	2.15	0.46
2:D:165:LYS:HG3	4:D:602:ATP:O2B	2.15	0.46
2:E:187:ILE:HD11	2:E:248:VAL:CG2	2.45	0.46
2:F:388:GLU:OE1	2:F:433:ARG:NH2	2.49	0.46
2:G:165:LYS:HG3	4:G:602:ATP:O2B	2.15	0.46
2:G:380:ARG:O	2:G:380:ARG:HD2	2.15	0.46
2:G:403:VAL:HG11	2:G:536:HIS:CE1	2.51	0.46
2:G:437:LEU:CD2	2:G:443:LEU:HD12	2.46	0.46
2:G:541:ASP:OD1	2:G:542:SER:N	2.49	0.46
1:I:22:GLU:OE2	1:I:24:ARG:HG3	2.16	0.46
1:L:21:PHE:CD1	1:L:75:PHE:CE1	3.03	0.46
1:M:4:GLU:HG3	1:M:5:ILE:N	2.30	0.46
2:B:448:ARG:HD3	2:B:448:ARG:HA	1.77	0.46
2:C:406:PRO:CA	2:C:453:THR:HG22	2.42	0.46
2:D:474:ALA:O	2:D:478:SER:OG	2.34	0.46
2:G:344:THR:HG22	2:G:346:GLU:H	1.81	0.46
1:I:22:GLU:HG3	1:I:24:ARG:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:314:LYS:HB3	2:A:314:LYS:HZ3	1.77	0.46
2:A:323:ILE:O	2:A:327:SER:N	2.48	0.46
2:B:206:ASP:CG	2:C:229:VAL:HG11	2.36	0.46
2:B:240:ILE:C	2:B:242:ARG:H	2.19	0.46
2:C:148:CYS:SG	2:C:149:ASP:N	2.89	0.46
2:C:259:ARG:HG3	2:C:259:ARG:HH11	1.80	0.46
2:E:124:VAL:HA	2:E:125:PRO:HD3	1.68	0.46
2:E:398:VAL:HG13	2:E:413:VAL:HG11	1.98	0.46
2:G:484:LEU:HG	2:G:530:PRO:O	2.16	0.46
2:G:527:GLU:HG3	2:G:528:ASP:N	2.30	0.46
1:K:92:ASP:C	1:K:94:ALA:H	2.19	0.46
2:A:293:LEU:HD11	2:A:330:PRO:HG3	1.96	0.46
2:B:128:MET:HB2	2:B:171:GLN:NE2	2.30	0.46
2:D:214:GLU:CB	2:E:237:ASN:HD21	2.28	0.46
2:E:165:LYS:HG2	2:E:290:VAL:HG21	1.97	0.46
2:E:208:LEU:HD22	2:E:208:LEU:C	2.36	0.46
2:E:308:PRO:HB2	2:E:345:PHE:CZ	2.51	0.46
2:F:232:LYS:O	2:F:236:CYS:SG	2.63	0.46
2:F:315:GLU:HG3	2:F:316:GLU:OE2	2.16	0.46
2:F:399:MET:CE	2:F:413:VAL:HG21	2.46	0.46
1:H:9:ALA:HB2	1:H:90:TYR:CD1	2.51	0.45
1:I:2:LEU:O	1:I:3:CYS:HB3	2.15	0.45
2:A:116:ASP:OD1	2:A:116:ASP:N	2.49	0.45
2:A:165:LYS:HG3	4:A:602:ATP:O2B	2.15	0.45
2:B:538:LYS:HB2	2:B:538:LYS:HZ2	1.80	0.45
2:C:240:ILE:C	2:C:242:ARG:H	2.19	0.45
2:C:344:THR:HG22	2:C:346:GLU:HB3	1.97	0.45
2:C:438:SER:HB2	2:C:444:LEU:HB3	1.98	0.45
2:E:369:TYR:CE2	2:E:371:TYR:HD1	2.33	0.45
2:E:405:ILE:HA	2:E:406:PRO:HD3	1.82	0.45
2:F:208:LEU:HD22	2:F:208:LEU:C	2.36	0.45
2:G:132:ILE:CG2	2:G:137:VAL:HG21	2.46	0.45
2:G:208:LEU:HD22	2:G:208:LEU:C	2.36	0.45
1:H:71:LEU:O	1:H:71:LEU:HD13	2.16	0.45
1:I:71:LEU:O	1:I:71:LEU:HD13	2.16	0.45
1:J:22:GLU:OE2	1:J:24:ARG:HG3	2.16	0.45
1:J:71:LEU:HD13	1:J:71:LEU:O	2.16	0.45
2:B:305:TYR:OH	4:B:602:ATP:H2	1.99	0.45
2:B:400:PRO:HB2	2:B:403:VAL:HB	1.99	0.45
2:B:409:LEU:HD21	2:B:526:PRO:HB2	1.98	0.45
2:B:463:PHE:CD2	2:B:464:LEU:HD23	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:116:ASP:N	2:C:116:ASP:OD1	2.49	0.45
2:D:400:PRO:HB2	2:D:403:VAL:HG21	1.97	0.45
2:E:314:LYS:NZ	2:E:314:LYS:CB	2.73	0.45
2:E:326:SER:O	2:E:328:GLY:N	2.49	0.45
2:E:351:LEU:HA	2:E:354:LYS:HD2	1.99	0.45
2:F:141:ILE:HG23	2:F:179:LEU:CD1	2.47	0.45
2:G:249:PHE:HE2	2:G:268:CYS:HG	1.64	0.45
2:G:305:TYR:OH	4:G:602:ATP:H2	1.99	0.45
2:G:320:ASN:O	2:G:321:LYS:C	2.54	0.45
2:G:335:MET:CE	2:G:374:LEU:H	2.29	0.45
2:G:459:ILE:H	2:G:459:ILE:HG13	1.43	0.45
1:J:37:THR:O	1:J:40:HIS:HB2	2.17	0.45
1:L:92:ASP:C	1:L:94:ALA:H	2.20	0.45
2:B:533:MET:CA	2:B:540:TYR:HE2	2.29	0.45
2:D:206:ASP:CG	2:E:229:VAL:HG11	2.36	0.45
2:D:321:LYS:O	2:D:324:GLU:HB3	2.16	0.45
2:D:448:ARG:HD3	2:D:448:ARG:HA	1.77	0.45
2:E:178:GLN:HA	2:E:182:ILE:HD13	1.99	0.45
2:E:409:LEU:HD21	2:E:526:PRO:HB2	1.99	0.45
2:F:150:LEU:HD13	2:F:151:ASP:N	2.32	0.45
2:F:165:LYS:HG2	2:F:290:VAL:HG21	1.97	0.45
2:F:334:MET:O	2:F:338:LYS:HG2	2.16	0.45
2:F:402:GLY:CA	2:F:458:HIS:CE1	2.93	0.45
2:G:327:SER:HB2	2:G:459:ILE:HG12	1.98	0.45
1:J:9:ALA:HB2	1:J:90:TYR:CD1	2.51	0.45
1:M:92:ASP:C	1:M:94:ALA:H	2.20	0.45
2:C:125:PRO:HD3	2:C:189:TRP:CE2	2.52	0.45
2:C:305:TYR:CZ	2:C:334:MET:CE	2.86	0.45
2:D:359:GLY:N	2:D:466:HIS:CE1	2.84	0.45
2:E:437:LEU:HD23	2:E:437:LEU:HA	1.69	0.45
2:G:321:LYS:HB2	2:G:321:LYS:HE2	1.55	0.45
1:H:23:PRO:HG2	1:H:53:ARG:CB	2.46	0.45
1:I:23:PRO:HG2	1:I:53:ARG:CB	2.46	0.45
2:A:308:PRO:HB2	2:A:345:PHE:CZ	2.50	0.45
2:C:115:LEU:HA	2:C:115:LEU:HD23	1.53	0.45
2:C:160:ARG:HG3	2:C:441:GLY:O	2.16	0.45
2:C:342:PRO:C	2:C:344:THR:H	2.20	0.45
2:D:184:TYR:CG	2:D:246:LEU:HD12	2.25	0.45
2:E:116:ASP:N	2:E:116:ASP:OD1	2.49	0.45
2:E:344:THR:HG22	2:E:346:GLU:HB3	1.99	0.45
2:F:246:LEU:HD23	2:F:247:PHE:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:406:PRO:HD2	2:F:409:LEU:HG	1.98	0.45
2:G:206:ASP:O	2:G:210:MET:HG2	2.17	0.45
2:G:312:GLY:N	2:G:315:GLU:HG2	2.28	0.45
2:G:357:SER:O	2:G:466:HIS:HE1	1.99	0.45
1:H:22:GLU:HG3	1:H:24:ARG:H	1.80	0.45
2:B:115:LEU:HD23	2:B:115:LEU:HA	1.53	0.45
2:B:397:VAL:CG2	2:B:468:VAL:HG11	2.47	0.45
2:G:116:ASP:OD1	2:G:116:ASP:N	2.49	0.45
2:G:159:GLY:O	2:G:273:ARG:HA	2.17	0.45
2:G:399:MET:SD	2:G:413:VAL:HG21	2.57	0.45
2:G:437:LEU:HD23	2:G:437:LEU:HA	1.69	0.45
1:L:9:ALA:HB2	1:L:90:TYR:CD1	2.52	0.45
2:A:338:LYS:NZ	2:A:368:PRO:HD3	2.31	0.45
2:A:457:ASP:H	2:A:460:ILE:CG2	2.30	0.45
2:B:210:MET:HA	2:B:210:MET:HE3	1.98	0.45
2:B:341:GLU:C	2:B:343:LYS:H	2.20	0.45
2:C:211:LEU:CD2	2:C:242:ARG:CD	2.94	0.45
2:C:295:ILE:HD13	2:C:295:ILE:N	2.31	0.45
2:D:177:ASP:N	2:D:177:ASP:OD1	2.50	0.45
2:D:206:ASP:O	2:D:210:MET:HG2	2.17	0.45
2:F:161:ALA:C	2:F:163:SER:H	2.19	0.45
2:F:214:GLU:CB	2:G:237:ASN:HD21	2.30	0.45
2:F:298:CYS:O	2:F:301:PHE:N	2.50	0.45
2:G:234:MET:HE3	2:G:234:MET:HB2	1.73	0.45
1:H:4:GLU:HG3	1:H:5:ILE:N	2.32	0.45
1:H:22:GLU:OE2	1:H:24:ARG:HG3	2.16	0.45
1:H:37:THR:O	1:H:40:HIS:HB2	2.17	0.45
2:A:208:LEU:C	2:A:208:LEU:CD2	2.86	0.45
2:A:214:GLU:CB	2:B:237:ASN:HD21	2.29	0.45
2:A:264:LEU:O	2:A:265:ARG:C	2.56	0.45
2:B:211:LEU:CD2	2:B:242:ARG:CD	2.94	0.45
2:B:396:ALA:HA	2:B:399:MET:CE	2.47	0.45
2:C:161:ALA:HB1	2:C:273:ARG:NE	2.31	0.45
2:C:177:ASP:OD1	2:C:177:ASP:N	2.49	0.45
2:C:399:MET:N	2:C:399:MET:SD	2.90	0.45
2:D:129:THR:O	2:D:132:ILE:HD11	2.17	0.45
2:D:533:MET:CG	2:D:540:TYR:CZ	2.88	0.45
2:E:469:ASP:O	2:E:472:THR:N	2.50	0.45
2:F:144:LEU:HD23	2:F:153:PHE:CE2	2.51	0.45
2:F:210:MET:HE3	2:F:210:MET:CA	2.47	0.45
2:G:247:PHE:O	2:G:268:CYS:HB3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:301:PHE:CZ	2:G:334:MET:HE3	2.51	0.45
2:G:307:MET:SD	2:G:308:PRO:HD2	2.57	0.45
2:G:350:GLN:HE22	2:G:351:LEU:HD23	1.80	0.45
2:G:393:LEU:CD1	2:G:437:LEU:HD21	2.44	0.45
2:A:126:LYS:HD2	2:A:126:LYS:HA	1.43	0.45
2:A:336:PHE:CD1	2:A:336:PHE:O	2.70	0.45
2:A:538:LYS:NZ	2:A:538:LYS:HB3	2.31	0.45
2:B:298:CYS:O	2:B:301:PHE:N	2.50	0.45
2:C:410:TRP:CH2	2:C:454:PHE:C	2.91	0.45
2:E:388:GLU:OE1	2:E:433:ARG:NH2	2.49	0.45
2:E:448:ARG:HD3	2:E:448:ARG:HA	1.77	0.45
2:F:116:ASP:N	2:F:116:ASP:OD1	2.49	0.45
2:F:208:LEU:C	2:F:208:LEU:CD2	2.85	0.45
2:F:240:ILE:C	2:F:242:ARG:H	2.20	0.45
2:G:232:LYS:NZ	2:G:260:TRP:CE2	2.84	0.45
2:G:398:VAL:HG11	2:G:477:ILE:CA	2.46	0.45
2:G:399:MET:CE	2:G:413:VAL:HG21	2.47	0.45
2:A:206:ASP:O	2:A:210:MET:HG2	2.17	0.45
2:B:190:LEU:HD23	2:B:190:LEU:HA	1.79	0.45
2:B:264:LEU:O	2:B:265:ARG:C	2.56	0.45
2:C:206:ASP:O	2:C:210:MET:HG2	2.17	0.45
2:C:214:GLU:HG3	2:D:237:ASN:HD21	1.81	0.45
2:C:335:MET:HE3	2:C:372:LYS:O	2.18	0.45
2:D:374:LEU:O	2:D:377:ALA:HB3	2.17	0.45
2:E:208:LEU:C	2:E:208:LEU:CD2	2.86	0.45
2:E:298:CYS:O	2:E:301:PHE:N	2.50	0.45
2:E:386:SER:H	2:E:440:ARG:HH22	1.64	0.45
2:E:426:LEU:HA	2:E:429:GLU:HB2	1.97	0.45
2:F:206:ASP:O	2:F:210:MET:HG2	2.17	0.45
2:F:227:THR:OG1	2:F:229:VAL:HG12	2.17	0.45
2:F:394:ALA:O	2:F:468:VAL:HG11	2.17	0.45
2:G:298:CYS:SG	2:G:333:LEU:CD1	2.84	0.45
2:G:321:LYS:HG3	2:G:322:THR:N	2.32	0.45
1:I:72:ILE:C	1:I:74:PHE:H	2.21	0.44
1:M:35:ILE:O	1:M:36:PHE:HD1	2.01	0.44
2:A:314:LYS:NZ	2:A:314:LYS:CB	2.73	0.44
2:A:336:PHE:O	2:A:336:PHE:CG	2.70	0.44
2:B:117:ARG:HD2	2:B:117:ARG:HA	1.74	0.44
2:B:234:MET:HB2	2:B:234:MET:HE3	1.73	0.44
2:C:355:LEU:O	2:C:359:GLY:N	2.50	0.44
2:D:116:ASP:OD1	2:D:116:ASP:N	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:ILE:HD11	2:D:247:PHE:CE2	2.53	0.44
2:D:393:LEU:HD22	2:D:464:LEU:HD21	1.99	0.44
2:F:393:LEU:O	2:F:464:LEU:CD1	2.61	0.44
2:F:393:LEU:O	2:F:464:LEU:HD21	2.17	0.44
1:H:4:GLU:O	1:H:8:ARG:HB2	2.18	0.44
1:H:72:ILE:C	1:H:74:PHE:H	2.21	0.44
2:A:206:ASP:CG	2:B:227:THR:HG21	2.36	0.44
2:A:206:ASP:CG	2:B:229:VAL:HG11	2.37	0.44
2:A:233:ARG:CG	2:A:233:ARG:NH1	2.80	0.44
2:A:298:CYS:O	2:A:301:PHE:N	2.50	0.44
2:C:214:GLU:CG	2:D:237:ASN:HD21	2.30	0.44
2:C:330:PRO:HA	2:C:333:LEU:HD12	1.98	0.44
2:C:539:PHE:O	2:C:539:PHE:CG	2.70	0.44
2:D:298:CYS:O	2:D:301:PHE:N	2.50	0.44
2:E:206:ASP:O	2:E:210:MET:HG2	2.17	0.44
2:E:346:GLU:O	2:E:346:GLU:HG2	2.17	0.44
2:E:364:GLU:OE2	2:E:372:LYS:HB3	2.18	0.44
2:E:413:VAL:HG12	2:E:476:GLY:O	2.17	0.44
2:F:117:ARG:HD2	2:F:117:ARG:HA	1.73	0.44
1:J:23:PRO:HG2	1:J:53:ARG:CB	2.46	0.44
2:C:208:LEU:C	2:C:208:LEU:CD2	2.85	0.44
2:C:409:LEU:HD21	2:C:526:PRO:HB2	1.99	0.44
2:D:258:ILE:HD11	2:D:277:ILE:HD12	1.98	0.44
2:D:335:MET:HE3	2:D:373:SER:HA	1.97	0.44
2:D:539:PHE:CD1	2:D:539:PHE:O	2.70	0.44
2:E:398:VAL:CG1	2:E:413:VAL:HG11	2.48	0.44
2:E:538:LYS:NZ	2:E:539:PHE:H	2.15	0.44
2:F:137:VAL:HG13	2:F:172:ALA:HB2	1.99	0.44
2:F:335:MET:HE2	2:F:363:VAL:HG13	1.98	0.44
2:F:344:THR:HG22	2:F:346:GLU:H	1.82	0.44
2:F:400:PRO:HB3	2:F:536:HIS:CG	2.51	0.44
2:G:298:CYS:O	2:G:301:PHE:N	2.50	0.44
2:G:301:PHE:HZ	2:G:334:MET:HE3	1.82	0.44
2:A:339:SER:HB3	2:A:365:CYS:SG	2.55	0.44
2:B:128:MET:CG	2:B:167:VAL:CG2	2.95	0.44
2:B:537:GLN:NE2	2:B:537:GLN:O	2.51	0.44
2:C:424:GLU:O	2:C:425:GLN:C	2.54	0.44
2:D:127:GLN:H	2:D:127:GLN:HG3	1.43	0.44
2:D:409:LEU:HD21	2:D:526:PRO:HB2	1.99	0.44
2:E:128:MET:HE2	2:E:128:MET:HB3	1.84	0.44
2:E:158:HIS:HA	2:E:272:THR:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:207:ILE:HD11	2:E:247:PHE:CE2	2.52	0.44
2:G:135:TYR:CZ	2:G:139:ARG:HD2	2.52	0.44
2:G:258:ILE:HD11	2:G:277:ILE:HD12	1.98	0.44
2:G:354:LYS:HZ2	2:G:362:GLY:HA3	1.82	0.44
2:G:457:ASP:O	2:G:461:HIS:N	2.50	0.44
2:G:484:LEU:O	2:G:485:LEU:C	2.54	0.44
1:J:72:ILE:C	1:J:74:PHE:H	2.21	0.44
1:K:2:LEU:O	1:K:3:CYS:HB3	2.17	0.44
1:M:72:ILE:HG21	1:M:88:GLU:CG	2.46	0.44
2:B:342:PRO:C	2:B:344:THR:H	2.19	0.44
2:B:360:LEU:HD13	2:B:462:MET:CE	2.41	0.44
2:B:469:ASP:OD2	2:B:471:GLN:HB3	2.18	0.44
2:C:128:MET:CG	2:C:167:VAL:CG2	2.95	0.44
2:C:203:LEU:HD22	2:C:203:LEU:C	2.38	0.44
2:C:264:LEU:O	2:C:265:ARG:C	2.55	0.44
2:C:463:PHE:CD2	2:C:464:LEU:HD23	2.52	0.44
2:C:539:PHE:O	2:C:539:PHE:CD1	2.70	0.44
2:C:543:LEU:HD13	2:C:543:LEU:HA	1.79	0.44
2:D:208:LEU:C	2:D:208:LEU:CD2	2.86	0.44
2:D:214:GLU:CG	2:E:237:ASN:HD21	2.30	0.44
2:D:367:THR:OG1	2:D:368:PRO:HD2	2.18	0.44
2:E:275:VAL:O	2:E:275:VAL:HG22	2.18	0.44
2:E:333:LEU:HD23	2:E:333:LEU:HA	1.65	0.44
2:E:535:LEU:HD22	2:E:536:HIS:ND1	2.32	0.44
2:G:207:ILE:HD11	2:G:247:PHE:CE2	2.53	0.44
2:G:314:LYS:NZ	2:G:314:LYS:CB	2.73	0.44
2:G:529:PHE:HA	2:G:531:LYS:NZ	2.32	0.44
1:K:72:ILE:HG21	1:K:88:GLU:CG	2.46	0.44
1:K:97:GLU:HA	1:K:98:PRO:HD3	1.73	0.44
1:M:29:TYR:OH	1:M:33:LYS:HD2	2.18	0.44
2:A:115:LEU:HD23	2:A:115:LEU:HA	1.53	0.44
2:A:175:LYS:NZ	2:A:175:LYS:HB3	2.33	0.44
2:A:321:LYS:HB2	2:A:321:LYS:HE2	1.58	0.44
2:B:208:LEU:C	2:B:208:LEU:CD2	2.86	0.44
2:D:305:TYR:HB3	2:D:337:PHE:CZ	2.53	0.44
2:D:314:LYS:NZ	2:D:314:LYS:CB	2.73	0.44
2:D:329:ASN:HB3	2:D:332:THR:OG1	2.18	0.44
2:E:211:LEU:HD21	2:E:242:ARG:CG	2.44	0.44
2:E:336:PHE:O	2:E:336:PHE:CG	2.70	0.44
2:F:155:LEU:HA	2:F:155:LEU:HD23	1.78	0.44
2:G:460:ILE:HA	2:G:460:ILE:HD12	1.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:487:ILE:HD12	2:G:487:ILE:N	2.33	0.44
1:H:67:GLU:HG2	1:H:68:LEU:N	2.33	0.44
1:K:9:ALA:HB2	1:K:90:TYR:CD1	2.52	0.44
2:A:400:PRO:HG3	2:A:536:HIS:ND1	2.32	0.44
2:B:207:ILE:HD11	2:B:247:PHE:CE2	2.52	0.44
2:B:444:LEU:HD13	2:B:444:LEU:HA	1.71	0.44
2:C:133:ARG:HD3	2:C:136:HIS:HB2	1.99	0.44
2:C:207:ILE:HD11	2:C:247:PHE:CE2	2.53	0.44
2:C:220:PHE:O	2:C:220:PHE:CG	2.70	0.44
2:C:457:ASP:H	2:C:460:ILE:CG2	2.30	0.44
2:D:127:GLN:OE1	2:D:174:SER:HB3	2.17	0.44
2:D:305:TYR:HH	4:D:602:ATP:H2	1.61	0.44
2:D:343:LYS:N	2:D:343:LYS:HD2	2.33	0.44
2:D:539:PHE:O	2:D:539:PHE:CG	2.70	0.44
2:E:352:ASN:O	2:E:356:GLU:HG3	2.17	0.44
2:E:533:MET:SD	2:E:533:MET:N	2.82	0.44
2:F:161:ALA:HA	2:F:273:ARG:HD3	1.99	0.44
2:F:227:THR:OG1	2:F:230:VAL:HG23	2.17	0.44
2:F:485:LEU:HD23	2:F:485:LEU:H	1.83	0.44
2:G:327:SER:HB2	2:G:459:ILE:CD1	2.48	0.44
2:G:401:PRO:O	2:G:403:VAL:HG23	2.17	0.44
1:I:37:THR:O	1:I:40:HIS:HB2	2.17	0.44
1:L:35:ILE:O	1:L:36:PHE:HD1	2.01	0.44
2:A:335:MET:CE	2:A:373:SER:HA	2.48	0.44
2:A:463:PHE:CD2	2:A:464:LEU:CD2	3.00	0.44
2:C:537:GLN:NE2	2:C:537:GLN:O	2.51	0.44
2:E:233:ARG:CG	2:E:233:ARG:NH1	2.80	0.44
2:E:350:GLN:HE22	2:F:426:LEU:HD21	1.83	0.44
2:E:353:ASN:HA	2:E:356:GLU:CD	2.39	0.44
2:F:397:VAL:N	2:F:464:LEU:HD13	2.33	0.44
2:G:369:TYR:HD1	4:G:602:ATP:H5'1	1.82	0.44
1:L:29:TYR:OH	1:L:33:LYS:HD2	2.18	0.44
1:M:2:LEU:O	1:M:3:CYS:HB3	2.17	0.44
2:A:337:PHE:C	2:A:339:SER:N	2.70	0.44
2:A:541:ASP:OD1	2:A:542:SER:N	2.51	0.44
2:B:233:ARG:CG	2:B:233:ARG:NH1	2.80	0.44
2:B:350:GLN:OE1	2:B:350:GLN:HA	2.18	0.44
2:D:165:LYS:HE3	2:D:272:THR:O	2.18	0.44
2:D:537:GLN:O	2:D:537:GLN:NE2	2.51	0.44
2:E:203:LEU:HD22	2:E:203:LEU:C	2.38	0.44
2:E:256:GLU:OE1	2:E:260:TRP:HD1	1.92	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:338:LYS:HD2	2:E:338:LYS:HA	1.75	0.44
2:E:465:LYS:HG3	2:E:473:ILE:HD13	1.99	0.44
2:F:131:TYR:CG	2:F:301:PHE:HD1	2.36	0.44
2:F:161:ALA:C	2:F:163:SER:N	2.70	0.44
2:F:178:GLN:HA	2:F:182:ILE:HD13	2.00	0.44
2:F:207:ILE:HD11	2:F:247:PHE:CE2	2.53	0.44
2:F:231:LEU:HD23	2:F:260:TRP:HZ3	1.83	0.44
2:F:530:PRO:HD2	2:F:531:LYS:HE3	1.99	0.44
2:G:208:LEU:C	2:G:208:LEU:CD2	2.85	0.44
2:G:301:PHE:HZ	2:G:334:MET:CE	2.30	0.44
1:I:72:ILE:HG21	1:I:88:GLU:CG	2.47	0.43
1:L:2:LEU:O	1:L:3:CYS:HB3	2.17	0.43
2:A:366:ILE:HD11	2:A:372:LYS:CE	2.47	0.43
2:A:400:PRO:HG3	2:A:536:HIS:CG	2.53	0.43
2:B:206:ASP:O	2:B:210:MET:HG2	2.17	0.43
2:B:309:MET:SD	2:B:310:PRO:HD2	2.58	0.43
2:B:311:VAL:N	2:B:316:GLU:OE2	2.51	0.43
2:B:355:LEU:CD1	2:B:462:MET:HE3	2.48	0.43
2:C:126:LYS:HB3	2:C:126:LYS:HE2	1.56	0.43
2:C:128:MET:CG	2:C:167:VAL:HG22	2.48	0.43
2:C:223:VAL:O	2:C:226:VAL:HB	2.18	0.43
2:C:443:LEU:N	2:C:443:LEU:CD2	2.80	0.43
2:D:346:GLU:HG2	2:D:346:GLU:O	2.17	0.43
2:F:455:LYS:HZ3	2:F:457:ASP:HA	1.83	0.43
2:F:537:GLN:HA	2:F:540:TYR:HD2	1.82	0.43
2:G:333:LEU:HD23	2:G:333:LEU:HA	1.65	0.43
1:M:9:ALA:HB2	1:M:90:TYR:CD1	2.52	0.43
2:A:325:LEU:HD23	2:A:325:LEU:HA	1.76	0.43
2:D:128:MET:HE3	2:D:128:MET:HB3	1.91	0.43
2:D:310:PRO:CB	2:D:316:GLU:OE2	2.65	0.43
2:D:400:PRO:HB2	2:D:403:VAL:CG2	2.48	0.43
2:D:480:LEU:O	2:D:484:LEU:N	2.50	0.43
2:E:200:THR:CG2	2:E:256:GLU:HG3	2.47	0.43
2:E:214:GLU:HG3	2:F:237:ASN:HD21	1.83	0.43
2:E:214:GLU:CB	2:F:237:ASN:HD21	2.31	0.43
2:E:336:PHE:CD1	2:E:336:PHE:O	2.70	0.43
2:F:307:MET:O	2:F:308:PRO:C	2.55	0.43
2:F:480:LEU:O	2:F:484:LEU:HB2	2.18	0.43
2:G:347:LYS:O	2:G:351:LEU:HG	2.18	0.43
1:H:72:ILE:HG21	1:H:88:GLU:CG	2.47	0.43
2:A:463:PHE:CE1	2:A:467:VAL:CG2	2.93	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:529:PHE:HA	2:B:532:PHE:CE2	2.53	0.43
2:C:448:ARG:NH2	2:C:452:LEU:HB2	2.21	0.43
2:D:427:ASP:O	2:D:430:VAL:HG23	2.17	0.43
2:D:457:ASP:H	2:D:460:ILE:CG2	2.30	0.43
2:E:220:PHE:O	2:E:220:PHE:CG	2.70	0.43
2:F:343:LYS:HD3	2:F:343:LYS:HA	1.90	0.43
2:F:367:THR:OG1	2:F:368:PRO:HD2	2.19	0.43
2:B:274:ASP:CG	2:B:440:ARG:HD2	2.39	0.43
2:B:320:ASN:OD1	2:B:320:ASN:N	2.51	0.43
2:D:115:LEU:HD23	2:D:115:LEU:HA	1.53	0.43
2:E:211:LEU:CD2	2:E:242:ARG:NE	2.78	0.43
2:F:334:MET:HE2	2:F:334:MET:HB2	1.60	0.43
2:G:334:MET:HE3	2:G:334:MET:HB2	1.71	0.43
1:J:67:GLU:HG2	1:J:68:LEU:N	2.33	0.43
1:K:35:ILE:O	1:K:36:PHE:HD1	2.01	0.43
2:A:127:GLN:HE21	2:A:174:SER:CB	2.26	0.43
2:A:237:ASN:HD21	2:G:214:GLU:CB	2.31	0.43
2:B:325:LEU:O	2:B:458:HIS:HB2	2.18	0.43
2:B:344:THR:HG22	2:B:346:GLU:HB3	2.00	0.43
2:C:341:GLU:O	2:C:342:PRO:C	2.57	0.43
2:D:203:LEU:HD22	2:D:203:LEU:C	2.38	0.43
2:D:538:LYS:HB2	2:D:538:LYS:HZ2	1.80	0.43
2:E:337:PHE:O	2:E:337:PHE:CD1	2.70	0.43
2:E:398:VAL:HG21	2:E:477:ILE:HA	2.00	0.43
2:F:301:PHE:O	2:F:305:TYR:HD1	2.01	0.43
2:G:315:GLU:O	2:G:316:GLU:C	2.56	0.43
1:H:24:ARG:NH2	1:H:53:ARG:NH1	2.67	0.43
1:L:8:ARG:NH1	1:L:8:ARG:CG	2.76	0.43
1:L:35:ILE:HG22	1:L:36:PHE:CD1	2.54	0.43
2:A:214:GLU:HG3	2:B:237:ASN:HD21	1.82	0.43
2:B:126:LYS:HB3	2:B:126:LYS:HE2	1.54	0.43
2:C:353:ASN:HA	2:C:356:GLU:HG3	2.01	0.43
2:C:426:LEU:C	2:C:428:ASP:N	2.72	0.43
2:D:234:MET:HB2	2:D:234:MET:HE3	1.73	0.43
2:D:264:LEU:O	2:D:265:ARG:C	2.56	0.43
2:D:461:HIS:O	2:D:461:HIS:ND1	2.49	0.43
2:G:117:ARG:HD2	2:G:117:ARG:HA	1.74	0.43
2:G:190:LEU:HD23	2:G:190:LEU:HA	1.79	0.43
2:G:455:LYS:HE2	2:G:455:LYS:HB3	1.83	0.43
2:C:178:GLN:O	2:C:182:ILE:HB	2.19	0.43
2:C:446:GLY:HA2	2:C:454:PHE:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:437:LEU:HD13	2:D:444:LEU:HD22	2.01	0.43
2:E:293:LEU:HD11	2:E:330:PRO:HG3	1.96	0.43
2:F:161:ALA:O	2:F:163:SER:N	2.52	0.43
2:F:165:LYS:HE3	2:F:272:THR:O	2.19	0.43
2:F:315:GLU:OE1	2:F:345:PHE:CD1	2.72	0.43
2:G:295:ILE:HD12	2:G:295:ILE:HA	1.82	0.43
2:G:298:CYS:HG	2:G:333:LEU:HD11	1.75	0.43
2:G:447:LYS:HE3	2:G:449:MET:O	2.19	0.43
1:J:35:ILE:HG22	1:J:36:PHE:HD1	1.83	0.43
1:K:29:TYR:OH	1:K:33:LYS:HD2	2.18	0.43
1:L:97:GLU:HA	1:L:98:PRO:HD3	1.73	0.43
2:A:214:GLU:CG	2:B:237:ASN:HD21	2.31	0.43
2:A:315:GLU:C	2:A:318:VAL:H	2.22	0.43
2:B:228:SER:C	2:B:230:VAL:N	2.71	0.43
2:B:332:THR:CG2	2:B:374:LEU:HG	2.48	0.43
2:B:408:LYS:HE3	2:B:427:ASP:HB3	1.98	0.43
2:B:540:TYR:HD1	2:B:540:TYR:HA	1.76	0.43
2:C:165:LYS:HE3	2:C:272:THR:O	2.19	0.43
2:D:204:PHE:HA	2:D:207:ILE:HG22	2.01	0.43
2:D:260:TRP:O	2:D:263:GLU:HB3	2.18	0.43
2:F:126:LYS:NZ	2:G:283:GLN:HG2	2.34	0.43
1:I:24:ARG:NH2	1:I:53:ARG:NH1	2.67	0.43
1:I:35:ILE:HG22	1:I:36:PHE:HD1	1.84	0.43
1:K:21:PHE:CG	1:K:22:GLU:N	2.87	0.43
1:L:21:PHE:CG	1:L:22:GLU:N	2.87	0.43
1:L:72:ILE:HG21	1:L:88:GLU:CG	2.46	0.43
2:A:165:LYS:HE3	2:A:272:THR:O	2.19	0.43
2:A:210:MET:HA	2:A:210:MET:HE3	1.99	0.43
2:B:128:MET:CG	2:B:167:VAL:HG22	2.49	0.43
2:B:346:GLU:HG2	2:B:346:GLU:O	2.17	0.43
2:B:457:ASP:H	2:B:460:ILE:CG2	2.30	0.43
2:C:444:LEU:HD13	2:C:444:LEU:HA	1.82	0.43
2:E:127:GLN:HG2	2:E:174:SER:OG	2.19	0.43
2:E:190:LEU:HA	2:E:190:LEU:HD23	1.79	0.43
2:E:438:SER:HA	2:E:444:LEU:H	1.84	0.43
2:F:220:PHE:HE1	2:F:223:VAL:HG13	1.82	0.43
2:F:258:ILE:N	2:F:258:ILE:HD12	2.34	0.43
2:F:315:GLU:CG	2:F:316:GLU:N	2.82	0.43
2:G:115:LEU:HD23	2:G:115:LEU:HA	1.53	0.43
2:G:203:LEU:HD22	2:G:203:LEU:C	2.38	0.43
2:G:233:ARG:CG	2:G:233:ARG:NH1	2.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:35:ILE:HG22	1:H:36:PHE:HD1	1.84	0.43
2:A:203:LEU:HD22	2:A:203:LEU:C	2.38	0.43
2:A:525:ARG:HH11	2:A:527:GLU:HG2	1.84	0.43
2:B:338:LYS:HD2	2:B:338:LYS:HA	1.85	0.43
2:E:200:THR:HG21	2:E:256:GLU:CG	2.48	0.43
2:E:204:PHE:HA	2:E:207:ILE:HG22	2.01	0.43
2:E:264:LEU:O	2:E:265:ARG:C	2.56	0.43
2:E:328:GLY:O	2:E:330:PRO:HD3	2.19	0.43
2:F:203:LEU:HD22	2:F:203:LEU:C	2.38	0.43
2:F:347:LYS:HD2	2:F:351:LEU:HD11	2.01	0.43
2:G:165:LYS:HE3	2:G:272:THR:O	2.19	0.43
2:G:315:GLU:HA	2:G:318:VAL:HB	2.00	0.43
1:H:1:MET:HE1	2:B:240:ILE:HB	2.01	0.42
1:I:67:GLU:HG2	1:I:68:LEU:N	2.33	0.42
1:M:35:ILE:HG22	1:M:36:PHE:CD1	2.54	0.42
2:A:346:GLU:O	2:A:346:GLU:HG2	2.17	0.42
2:B:165:LYS:HE3	2:B:272:THR:O	2.19	0.42
2:B:525:ARG:HH11	2:B:527:GLU:HG2	1.84	0.42
2:D:161:ALA:HA	2:D:273:ARG:HD3	2.01	0.42
2:D:233:ARG:CG	2:D:233:ARG:NH1	2.80	0.42
2:D:461:HIS:C	2:D:461:HIS:ND1	2.73	0.42
2:E:538:LYS:H	2:E:538:LYS:HG3	1.60	0.42
2:F:120:LEU:HD21	2:G:236:CYS:HB2	2.01	0.42
2:F:539:PHE:CE2	2:F:543:LEU:HD21	2.54	0.42
2:G:405:ILE:HA	2:G:406:PRO:HD3	1.82	0.42
2:G:525:ARG:NH2	2:G:529:PHE:HE2	2.17	0.42
2:A:117:ARG:HD2	2:A:117:ARG:HA	1.73	0.42
2:B:438:SER:HA	2:B:444:LEU:N	2.25	0.42
2:B:452:LEU:HD23	2:B:452:LEU:N	2.28	0.42
2:C:460:ILE:HD12	2:C:460:ILE:HA	1.80	0.42
2:C:525:ARG:HH11	2:C:527:GLU:HG2	1.84	0.42
2:D:482:GLN:N	2:D:482:GLN:CD	2.73	0.42
2:E:123:ASN:HD22	2:E:123:ASN:HA	1.63	0.42
2:E:479:ILE:O	2:E:483:ARG:HG2	2.19	0.42
2:F:359:GLY:CA	2:F:466:HIS:NE2	2.82	0.42
2:F:385:LEU:CD1	2:F:437:LEU:HD21	2.46	0.42
2:F:399:MET:HG2	2:F:410:TRP:CE2	2.54	0.42
2:G:437:LEU:HD22	2:G:443:LEU:HD12	2.02	0.42
1:J:72:ILE:HG21	1:J:88:GLU:CG	2.47	0.42
2:A:361:VAL:O	2:A:364:GLU:HG2	2.19	0.42
2:B:203:LEU:HD22	2:B:203:LEU:C	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:MET:HE3	2:B:210:MET:CA	2.49	0.42
2:B:214:GLU:CG	2:C:237:ASN:HD21	2.32	0.42
2:B:252:VAL:CG1	2:B:277:ILE:HD11	2.49	0.42
2:B:437:LEU:HD23	2:B:437:LEU:HA	1.69	0.42
2:C:127:GLN:H	2:C:127:GLN:HG3	1.38	0.42
2:C:346:GLU:O	2:C:346:GLU:HG2	2.17	0.42
2:E:351:LEU:HD23	2:E:354:LYS:HD2	2.01	0.42
2:E:525:ARG:HH11	2:E:527:GLU:HG2	1.84	0.42
2:G:355:LEU:HD21	2:G:363:VAL:HB	2.01	0.42
1:H:8:ARG:NH1	1:H:8:ARG:CG	2.74	0.42
1:M:21:PHE:CG	1:M:22:GLU:N	2.87	0.42
2:A:152:SER:O	2:A:283:GLN:OE1	2.38	0.42
2:A:310:PRO:HD3	2:A:319:LEU:HD23	1.99	0.42
2:A:351:LEU:O	2:A:354:LYS:N	2.52	0.42
2:C:131:TYR:CD2	2:C:301:PHE:CD1	3.08	0.42
2:C:204:PHE:HA	2:C:207:ILE:HG22	2.01	0.42
2:D:424:GLU:C	2:D:426:LEU:H	2.22	0.42
2:E:239:LEU:HD22	2:E:239:LEU:HA	1.91	0.42
2:E:351:LEU:O	2:E:355:LEU:HD23	2.20	0.42
2:F:131:TYR:OH	2:F:297:GLU:HG2	2.19	0.42
2:F:133:ARG:HD3	2:F:168:ILE:HD11	2.01	0.42
2:A:178:GLN:O	2:A:182:ILE:HB	2.19	0.42
2:A:452:LEU:HD23	2:A:452:LEU:N	2.28	0.42
2:B:147:MET:HB2	2:B:147:MET:HE3	1.80	0.42
2:D:437:LEU:HD23	2:D:437:LEU:HA	1.69	0.42
2:E:273:ARG:CZ	2:E:380:ARG:HH21	2.32	0.42
2:E:315:GLU:C	2:E:318:VAL:H	2.23	0.42
2:E:329:ASN:O	2:E:333:LEU:HB2	2.19	0.42
2:F:128:MET:HA	2:F:128:MET:CE	2.50	0.42
2:G:159:GLY:N	2:G:165:LYS:HD3	2.34	0.42
2:A:152:SER:O	2:A:283:GLN:CD	2.58	0.42
2:A:366:ILE:CG1	2:A:372:LYS:HG2	2.46	0.42
2:A:366:ILE:HD11	2:A:372:LYS:CD	2.50	0.42
2:B:115:LEU:HD11	2:B:177:ASP:HA	2.01	0.42
2:B:269:LEU:HD22	2:B:270:VAL:N	2.34	0.42
2:B:397:VAL:HG22	2:B:464:LEU:HB3	2.02	0.42
2:B:461:HIS:C	2:B:461:HIS:ND1	2.73	0.42
2:C:302:LEU:HD23	2:C:302:LEU:H	1.81	0.42
2:C:340:CYS:O	2:C:343:LYS:N	2.36	0.42
2:C:528:ASP:HA	2:C:531:LYS:NZ	2.28	0.42
2:D:483:ARG:HA	2:D:483:ARG:NH2	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:525:ARG:HH11	2:D:527:GLU:HG2	1.84	0.42
2:D:540:TYR:HD1	2:D:540:TYR:HA	1.71	0.42
2:E:364:GLU:HB3	2:E:373:SER:HB3	2.01	0.42
2:E:397:VAL:HG22	2:E:464:LEU:HB3	2.00	0.42
2:F:240:ILE:CG1	2:F:241:ASP:OD1	2.68	0.42
2:F:455:LYS:HE2	2:F:455:LYS:HB2	1.79	0.42
2:G:406:PRO:CA	2:G:453:THR:HG22	2.47	0.42
2:G:456:ILE:HG23	2:G:456:ILE:O	2.19	0.42
1:H:35:ILE:O	1:H:35:ILE:CG2	2.68	0.42
2:A:321:LYS:HG3	2:A:322:THR:N	2.33	0.42
2:A:406:PRO:CA	2:A:453:THR:HG22	2.47	0.42
2:B:297:GLU:O	2:B:300:ASP:N	2.53	0.42
2:B:461:HIS:ND1	2:B:461:HIS:O	2.49	0.42
2:C:297:GLU:O	2:C:300:ASP:N	2.53	0.42
2:C:461:HIS:C	2:C:461:HIS:ND1	2.72	0.42
2:D:152:SER:O	2:D:152:SER:OG	2.34	0.42
2:E:115:LEU:HD23	2:E:115:LEU:HA	1.53	0.42
2:E:172:ALA:HA	2:E:175:LYS:HB3	2.02	0.42
2:E:220:PHE:CZ	2:F:225:HIS:HB3	2.55	0.42
2:E:240:ILE:CG1	2:E:241:ASP:OD1	2.68	0.42
2:E:334:MET:HE3	2:E:334:MET:HB2	1.72	0.42
2:E:536:HIS:HB2	2:E:540:TYR:CD1	2.54	0.42
2:F:158:HIS:O	2:F:289:GLU:HA	2.20	0.42
2:F:204:PHE:HA	2:F:207:ILE:HG22	2.01	0.42
1:I:35:ILE:O	1:I:35:ILE:CG2	2.68	0.42
2:B:200:THR:HG21	2:B:256:GLU:CB	2.50	0.42
2:B:407:VAL:HG21	2:B:452:LEU:HD12	2.02	0.42
2:B:474:ALA:O	2:B:477:ILE:HG22	2.20	0.42
2:D:344:THR:HG22	2:D:346:GLU:HB3	2.01	0.42
2:D:396:ALA:HA	2:D:399:MET:CE	2.50	0.42
2:F:407:VAL:HG21	2:F:452:LEU:HD12	2.02	0.42
2:F:471:GLN:HG2	2:F:475:ASN:HD21	1.85	0.42
2:G:232:LYS:CE	2:G:260:TRP:CE3	3.02	0.42
2:A:396:ALA:O	2:A:399:MET:HB2	2.20	0.42
2:E:407:VAL:HG21	2:E:452:LEU:HD12	2.02	0.42
2:F:115:LEU:HD23	2:F:115:LEU:HA	1.53	0.42
2:G:264:LEU:O	2:G:265:ARG:C	2.56	0.42
1:I:24:ARG:CZ	1:I:53:ARG:HH11	2.33	0.42
1:K:35:ILE:HG22	1:K:36:PHE:CD1	2.54	0.42
2:A:329:ASN:O	2:A:333:LEU:HB2	2.19	0.42
2:B:227:THR:O	2:B:230:VAL:HB	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:ILE:CG1	2:B:241:ASP:OD1	2.68	0.42
2:C:399:MET:SD	2:C:413:VAL:HG21	2.60	0.42
2:C:461:HIS:ND1	2:C:461:HIS:O	2.49	0.42
2:D:178:GLN:O	2:D:182:ILE:HB	2.19	0.42
2:F:226:VAL:HG13	2:F:230:VAL:CG1	2.50	0.42
2:G:307:MET:CG	2:G:308:PRO:HD2	2.50	0.42
2:A:250:ASP:HA	2:A:271:THR:HG1	1.81	0.41
2:A:484:LEU:HG	2:A:531:LYS:O	2.20	0.41
2:B:437:LEU:HD22	2:B:443:LEU:HD12	2.03	0.41
2:C:240:ILE:CG1	2:C:241:ASP:OD1	2.68	0.41
2:C:481:GLU:O	2:C:484:LEU:HB3	2.20	0.41
2:D:297:GLU:O	2:D:300:ASP:N	2.53	0.41
2:E:227:THR:HB	2:E:229:VAL:HG12	2.02	0.41
2:E:369:TYR:N	4:E:602:ATP:HO3'	2.18	0.41
2:F:248:VAL:HG13	2:F:269:LEU:HD12	2.02	0.41
2:F:297:GLU:O	2:F:300:ASP:N	2.53	0.41
2:G:152:SER:H	2:G:267:ARG:CG	2.33	0.41
2:G:389:ASP:OD1	2:G:433:ARG:HG2	2.20	0.41
2:G:412:CYS:SG	2:G:484:LEU:HD12	2.59	0.41
2:G:461:HIS:O	2:G:461:HIS:ND1	2.49	0.41
1:J:35:ILE:O	1:J:35:ILE:CG2	2.68	0.41
1:M:30:LEU:C	1:M:32:GLY:N	2.73	0.41
1:M:35:ILE:O	1:M:36:PHE:CD1	2.73	0.41
2:A:463:PHE:C	2:A:467:VAL:CG1	2.82	0.41
2:A:481:GLU:O	2:A:484:LEU:HB3	2.20	0.41
2:B:156:PHE:CZ	2:B:278:SER:CA	3.03	0.41
2:B:214:GLU:HG3	2:C:237:ASN:HD21	1.84	0.41
2:B:406:PRO:CA	2:B:453:THR:HG22	2.47	0.41
2:D:355:LEU:HD13	2:D:355:LEU:HA	1.86	0.41
2:D:385:LEU:HD11	2:D:393:LEU:HD12	2.02	0.41
2:E:338:LYS:HB2	2:E:365:CYS:SG	2.59	0.41
2:F:175:LYS:HB3	2:F:175:LYS:HZ2	1.84	0.41
2:F:354:LYS:HD3	2:F:362:GLY:CA	2.50	0.41
2:F:412:CYS:O	2:F:479:ILE:HG22	2.19	0.41
2:F:529:PHE:N	2:F:530:PRO:CD	2.83	0.41
2:G:127:GLN:HB2	2:G:171:GLN:HA	2.02	0.41
1:J:24:ARG:NH2	1:J:53:ARG:NH1	2.67	0.41
1:K:35:ILE:O	1:K:36:PHE:CD1	2.73	0.41
1:K:67:GLU:HG2	1:K:69:GLY:H	1.85	0.41
2:A:448:ARG:HD3	2:A:448:ARG:HA	1.77	0.41
2:B:130:CYS:O	2:B:304:ALA:HB1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:PHE:HA	2:B:207:ILE:HG22	2.01	0.41
2:B:222:SER:O	2:B:222:SER:OG	2.34	0.41
2:C:484:LEU:HD21	2:C:530:PRO:O	2.21	0.41
2:D:269:LEU:HD22	2:D:270:VAL:N	2.35	0.41
2:D:385:LEU:HD23	2:D:385:LEU:HA	1.85	0.41
2:E:155:LEU:HD23	2:E:155:LEU:HA	1.78	0.41
2:F:302:LEU:HB3	2:F:307:MET:HB3	2.02	0.41
2:F:355:LEU:HD13	2:F:359:GLY:O	2.20	0.41
2:G:531:LYS:HZ2	2:G:532:PHE:HE1	1.68	0.41
1:L:35:ILE:O	1:L:36:PHE:CD1	2.73	0.41
2:A:333:LEU:HD23	2:A:333:LEU:HA	1.65	0.41
2:C:211:LEU:HD21	2:C:242:ARG:CD	2.50	0.41
2:C:269:LEU:HD22	2:C:270:VAL:N	2.34	0.41
2:C:305:TYR:HD2	2:C:337:PHE:CD1	2.39	0.41
2:C:402:GLY:N	2:C:456:ILE:O	2.40	0.41
2:C:446:GLY:HA2	2:C:453:THR:O	2.20	0.41
2:D:149:ASP:OD1	2:D:149:ASP:N	2.43	0.41
2:D:369:TYR:CE2	2:D:371:TYR:HB2	2.55	0.41
2:D:534:GLN:CD	2:D:534:GLN:N	2.73	0.41
2:E:169:ALA:O	2:E:173:LEU:HG	2.21	0.41
1:I:67:GLU:HG2	1:I:69:GLY:N	2.36	0.41
1:L:30:LEU:C	1:L:32:GLY:N	2.73	0.41
1:L:67:GLU:HG2	1:L:69:GLY:H	1.85	0.41
2:A:297:GLU:O	2:A:300:ASP:N	2.53	0.41
2:B:302:LEU:HD13	2:B:307:MET:HB2	1.99	0.41
2:C:141:ILE:HD12	2:C:175:LYS:HZ2	1.84	0.41
2:C:233:ARG:CG	2:C:233:ARG:NH1	2.80	0.41
2:C:369:TYR:C	2:C:371:TYR:H	2.24	0.41
2:D:125:PRO:CD	2:D:189:TRP:CE2	3.03	0.41
2:D:273:ARG:O	2:D:441:GLY:HA2	2.20	0.41
2:D:407:VAL:HG21	2:D:452:LEU:HD12	2.02	0.41
2:D:460:ILE:HD12	2:D:460:ILE:HA	1.80	0.41
2:E:234:MET:HB2	2:E:234:MET:HE3	1.73	0.41
2:E:248:VAL:HG13	2:E:269:LEU:HD12	2.03	0.41
2:E:397:VAL:HG21	2:E:468:VAL:HG21	2.01	0.41
2:F:127:GLN:CD	2:F:174:SER:HB3	2.41	0.41
2:F:143:LYS:HZ3	2:F:143:LYS:HG3	1.80	0.41
2:F:359:GLY:N	2:F:466:HIS:NE2	2.68	0.41
2:F:367:THR:O	2:F:369:TYR:N	2.54	0.41
2:F:386:SER:H	2:F:440:ARG:NH2	2.18	0.41
2:F:405:ILE:HA	2:F:406:PRO:HD3	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:334:MET:CG	4:G:602:ATP:O2'	2.56	0.41
1:H:24:ARG:CZ	1:H:53:ARG:HH11	2.33	0.41
1:H:72:ILE:HG23	1:H:84:ALA:HB1	2.02	0.41
1:J:100:LEU:HG	1:J:104:VAL:HG21	2.02	0.41
1:K:67:GLU:HG2	1:K:68:LEU:N	2.36	0.41
2:A:140:VAL:CG1	2:A:172:ALA:CB	2.99	0.41
2:A:395:PHE:CE2	2:A:415:PRO:HD3	2.56	0.41
2:A:409:LEU:HD21	2:A:526:PRO:HB2	2.01	0.41
2:A:461:HIS:C	2:A:461:HIS:ND1	2.73	0.41
2:A:533:MET:HB3	2:A:540:TYR:HE2	1.83	0.41
2:B:340:CYS:O	2:B:343:LYS:N	2.37	0.41
2:C:125:PRO:HG2	2:C:189:TRP:CZ2	2.56	0.41
2:C:160:ARG:CB	2:C:442:ALA:HB3	2.50	0.41
2:C:324:GLU:C	2:C:326:SER:N	2.74	0.41
2:C:334:MET:CE	2:C:334:MET:CA	2.86	0.41
2:C:385:LEU:HD11	2:C:393:LEU:HD12	2.02	0.41
2:E:214:GLU:CG	2:F:237:ASN:HD21	2.33	0.41
2:E:309:MET:HA	2:E:309:MET:CE	2.50	0.41
2:E:310:PRO:CB	2:E:319:LEU:HD23	2.29	0.41
2:E:325:LEU:O	2:E:459:ILE:HG23	2.21	0.41
2:A:124:VAL:HA	2:A:125:PRO:HD3	1.68	0.41
2:A:248:VAL:HG13	2:A:269:LEU:HD12	2.03	0.41
2:A:305:TYR:HE2	2:A:334:MET:CE	2.32	0.41
2:A:314:LYS:HG2	2:A:315:GLU:N	2.35	0.41
2:A:407:VAL:HG21	2:A:452:LEU:HD12	2.02	0.41
2:B:125:PRO:HD3	2:B:189:TRP:CE2	2.55	0.41
2:C:140:VAL:CG1	2:C:172:ALA:CB	2.99	0.41
2:C:355:LEU:HD11	2:C:462:MET:CE	2.50	0.41
2:D:342:PRO:C	2:D:344:THR:N	2.74	0.41
2:D:404:ASP:HA	2:D:455:LYS:HB3	2.02	0.41
2:E:240:ILE:CG1	2:E:241:ASP:N	2.83	0.41
2:E:297:GLU:O	2:E:300:ASP:N	2.53	0.41
2:E:386:SER:H	2:E:440:ARG:NH2	2.18	0.41
2:E:529:PHE:HB3	2:E:532:PHE:CZ	2.56	0.41
2:F:263:GLU:O	2:F:265:ARG:NH1	2.42	0.41
2:F:406:PRO:CA	2:F:453:THR:HG22	2.47	0.41
2:G:297:GLU:O	2:G:300:ASP:N	2.53	0.41
2:G:407:VAL:HG21	2:G:452:LEU:HD12	2.02	0.41
2:G:426:LEU:HD12	2:G:426:LEU:HA	1.84	0.41
1:H:100:LEU:HG	1:H:104:VAL:HG21	2.02	0.41
1:K:8:ARG:NH1	1:K:8:ARG:CG	2.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:22:GLU:OE1	1:K:50:ARG:HD2	2.21	0.41
1:K:72:ILE:HG23	1:K:84:ALA:HB1	2.03	0.41
1:M:23:PRO:HG2	1:M:53:ARG:CB	2.51	0.41
1:M:24:ARG:NH2	1:M:53:ARG:NH1	2.69	0.41
2:A:234:MET:HB2	2:A:234:MET:HE3	1.73	0.41
2:A:295:ILE:HD12	2:A:295:ILE:HA	1.83	0.41
2:C:399:MET:HG3	2:C:405:ILE:CD1	2.51	0.41
2:D:342:PRO:O	2:D:343:LYS:HB2	2.20	0.41
2:F:220:PHE:CD1	2:F:221:PRO:HD2	2.56	0.41
2:F:269:LEU:HD22	2:F:270:VAL:N	2.34	0.41
2:F:311:VAL:N	2:F:316:GLU:OE2	2.53	0.41
2:G:204:PHE:HA	2:G:207:ILE:HG22	2.01	0.41
2:G:409:LEU:HD13	2:G:484:LEU:CD1	2.50	0.41
1:I:100:LEU:HG	1:I:104:VAL:HG21	2.02	0.41
1:J:72:ILE:HG23	1:J:84:ALA:HB1	2.02	0.41
2:A:182:ILE:N	2:A:182:ILE:CD1	2.84	0.41
2:A:204:PHE:HA	2:A:207:ILE:HG22	2.01	0.41
2:A:337:PHE:O	2:A:339:SER:N	2.54	0.41
2:A:385:LEU:CD1	2:A:437:LEU:HD21	2.46	0.41
2:B:182:ILE:N	2:B:182:ILE:CD1	2.84	0.41
2:B:248:VAL:HG13	2:B:269:LEU:HD12	2.03	0.41
2:B:437:LEU:HD22	2:B:443:LEU:CD1	2.51	0.41
2:C:141:ILE:CD1	2:C:175:LYS:HZ2	2.33	0.41
2:C:295:ILE:HD12	2:C:295:ILE:HA	1.82	0.41
2:C:301:PHE:CE2	2:C:305:TYR:CE2	3.09	0.41
2:C:329:ASN:O	2:C:333:LEU:HG	2.20	0.41
2:C:385:LEU:HA	2:C:385:LEU:HD23	1.85	0.41
2:C:452:LEU:N	2:C:452:LEU:HD23	2.36	0.41
2:D:182:ILE:N	2:D:182:ILE:CD1	2.84	0.41
2:D:206:ASP:OD1	2:E:227:THR:CB	2.69	0.41
2:D:533:MET:O	2:D:540:TYR:CE2	2.74	0.41
2:E:160:ARG:O	2:E:163:SER:N	2.50	0.41
2:E:269:LEU:HD22	2:E:270:VAL:N	2.35	0.41
2:E:385:LEU:CD1	2:E:437:LEU:HD21	2.46	0.41
2:F:255:GLU:O	2:F:258:ILE:N	2.54	0.41
2:F:323:ILE:O	2:F:324:GLU:C	2.58	0.41
2:F:452:LEU:HD23	2:F:452:LEU:N	2.28	0.41
2:F:474:ALA:O	2:F:477:ILE:HG22	2.20	0.41
2:G:127:GLN:HB2	2:G:171:GLN:CG	2.46	0.41
2:G:140:VAL:CG1	2:G:172:ALA:CB	2.99	0.41
2:G:264:LEU:HB3	2:G:266:LEU:HG	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:24:ARG:NH2	1:K:53:ARG:NH1	2.69	0.41
2:A:128:MET:HG3	2:A:167:VAL:HG21	2.03	0.41
2:A:302:LEU:O	2:A:303:GLU:C	2.60	0.41
2:A:369:TYR:O	2:A:371:TYR:N	2.54	0.41
2:A:369:TYR:OH	4:A:602:ATP:O3G	2.35	0.41
2:C:117:ARG:HD2	2:C:117:ARG:HA	1.73	0.41
2:C:298:CYS:O	2:C:301:PHE:N	2.53	0.41
2:D:134:GLU:N	2:D:134:GLU:OE1	2.54	0.41
2:D:140:VAL:CG1	2:D:172:ALA:CB	2.99	0.41
2:D:248:VAL:HG13	2:D:269:LEU:HD12	2.03	0.41
2:E:150:LEU:HD23	2:E:150:LEU:HA	1.91	0.41
2:E:302:LEU:O	2:E:303:GLU:C	2.60	0.41
2:E:385:LEU:HA	2:E:385:LEU:HD23	1.85	0.41
2:F:484:LEU:HD21	2:F:534:GLN:OE1	2.21	0.41
2:G:200:THR:HG21	2:G:256:GLU:HB3	2.02	0.41
2:G:469:ASP:O	2:G:473:ILE:HG13	2.21	0.41
1:H:67:GLU:HG2	1:H:69:GLY:N	2.36	0.40
1:J:24:ARG:CZ	1:J:53:ARG:HH11	2.33	0.40
1:M:67:GLU:HG2	1:M:68:LEU:N	2.36	0.40
2:A:405:ILE:HA	2:A:406:PRO:HD3	1.82	0.40
2:B:308:PRO:HG2	2:B:345:PHE:CD1	2.56	0.40
2:B:312:GLY:O	2:B:313:GLU:C	2.59	0.40
2:C:203:LEU:CD2	2:C:203:LEU:C	2.89	0.40
2:C:234:MET:HB2	2:C:234:MET:HE3	1.74	0.40
2:C:248:VAL:HG13	2:C:269:LEU:HD12	2.03	0.40
2:E:283:GLN:HE21	2:E:283:GLN:HB3	1.52	0.40
2:E:369:TYR:HD1	4:E:602:ATP:H5'1	1.87	0.40
2:E:473:ILE:HG22	2:E:543:LEU:CD1	2.44	0.40
2:E:528:ASP:HA	2:E:531:LYS:NZ	2.27	0.40
2:F:167:VAL:HG12	2:F:168:ILE:N	2.36	0.40
2:F:369:TYR:C	2:F:371:TYR:H	2.24	0.40
2:F:396:ALA:HB1	2:F:456:ILE:HD12	2.03	0.40
2:F:448:ARG:HA	2:F:448:ARG:HD3	1.77	0.40
2:G:385:LEU:CD1	2:G:437:LEU:HD21	2.46	0.40
1:L:67:GLU:HG2	1:L:68:LEU:N	2.36	0.40
2:A:210:MET:HE3	2:A:210:MET:CA	2.52	0.40
2:A:239:LEU:HD22	2:A:239:LEU:HA	1.91	0.40
2:A:244:ASN:HA	2:A:267:ARG:NE	2.36	0.40
2:B:198:LYS:N	2:B:198:LYS:HD3	2.37	0.40
2:B:211:LEU:HD21	2:B:242:ARG:CD	2.50	0.40
2:B:355:LEU:C	2:B:357:SER:H	2.25	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:PRO:HB3	2:C:461:HIS:CD2	2.55	0.40
2:D:232:LYS:HE2	2:D:260:TRP:CG	2.55	0.40
2:D:412:CYS:HB3	2:D:480:LEU:HD23	2.04	0.40
2:D:483:ARG:HA	2:D:483:ARG:NE	2.33	0.40
2:F:267:ARG:O	2:F:268:CYS:SG	2.78	0.40
2:F:314:LYS:HA	2:F:317:ASP:OD2	2.21	0.40
2:G:182:ILE:N	2:G:182:ILE:CD1	2.84	0.40
2:G:335:MET:CE	2:G:374:LEU:N	2.72	0.40
2:G:360:LEU:O	2:G:363:VAL:HG12	2.21	0.40
1:I:72:ILE:HG23	1:I:84:ALA:HB1	2.02	0.40
1:L:24:ARG:CZ	1:L:53:ARG:HH11	2.35	0.40
1:M:43:LEU:HD13	1:M:43:LEU:HA	1.96	0.40
1:M:67:GLU:HG2	1:M:69:GLY:H	1.85	0.40
2:A:255:GLU:OE2	2:A:256:GLU:N	2.54	0.40
2:B:337:PHE:O	2:B:339:SER:N	2.54	0.40
2:C:190:LEU:HA	2:C:190:LEU:HD23	1.79	0.40
2:D:367:THR:O	2:D:368:PRO:C	2.58	0.40
2:E:130:CYS:O	2:E:304:ALA:HB1	2.21	0.40
2:E:364:GLU:HB2	2:E:373:SER:HB3	2.02	0.40
2:E:366:ILE:HD11	2:F:280:ALA:HB2	2.03	0.40
2:F:240:ILE:CG1	2:F:241:ASP:N	2.83	0.40
2:F:313:GLU:O	2:F:317:ASP:N	2.54	0.40
2:F:457:ASP:O	2:F:460:ILE:HG22	2.21	0.40
2:G:367:THR:OG1	2:G:368:PRO:HD2	2.21	0.40
2:A:339:SER:O	2:A:339:SER:OG	2.35	0.40
2:A:385:LEU:HD23	2:A:385:LEU:HA	1.85	0.40
2:A:480:LEU:O	2:A:484:LEU:HB2	2.21	0.40
2:A:534:GLN:C	2:A:537:GLN:H	2.25	0.40
2:B:399:MET:HB2	2:B:399:MET:HE2	1.72	0.40
2:C:198:LYS:N	2:C:198:LYS:HD3	2.37	0.40
2:C:393:LEU:CD1	2:C:443:LEU:HD12	2.49	0.40
2:D:321:LYS:O	2:D:322:THR:C	2.60	0.40
2:E:335:MET:HE1	2:E:374:LEU:H	1.86	0.40
2:F:182:ILE:N	2:F:182:ILE:CD1	2.84	0.40
2:F:393:LEU:HD23	2:F:464:LEU:HD11	2.03	0.40
2:F:455:LYS:HD3	2:F:455:LYS:O	2.21	0.40
2:F:456:ILE:HG23	2:F:456:ILE:O	2.20	0.40
2:G:427:ASP:O	2:G:430:VAL:HG23	2.21	0.40
2:G:452:LEU:HD23	2:G:452:LEU:N	2.28	0.40
2:G:461:HIS:C	2:G:461:HIS:ND1	2.73	0.40
1:H:58:LEU:HD23	1:H:58:LEU:HA	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:67:GLU:HG2	1:J:69:GLY:N	2.36	0.40
1:K:30:LEU:C	1:K:32:GLY:N	2.73	0.40
1:L:23:PRO:HG2	1:L:53:ARG:CB	2.51	0.40
1:M:22:GLU:OE1	1:M:50:ARG:HD2	2.21	0.40
2:A:130:CYS:O	2:A:304:ALA:HB1	2.21	0.40
2:A:203:LEU:CD2	2:A:203:LEU:C	2.90	0.40
2:A:395:PHE:CD2	2:A:415:PRO:HD3	2.56	0.40
2:B:177:ASP:OD1	2:B:177:ASP:N	2.55	0.40
2:B:369:TYR:C	2:B:371:TYR:H	2.24	0.40
2:C:230:VAL:O	2:C:234:MET:CB	2.70	0.40
2:C:232:LYS:O	2:C:236:CYS:SG	2.63	0.40
2:D:371:TYR:CE1	2:D:377:ALA:HA	2.57	0.40
2:E:242:ARG:N	2:E:243:PRO:HD3	2.36	0.40
2:E:343:LYS:HD3	2:E:343:LYS:HA	1.91	0.40
2:F:203:LEU:CD2	2:F:203:LEU:C	2.89	0.40
2:F:206:ASP:CG	2:G:229:VAL:HG11	2.42	0.40
2:F:230:VAL:O	2:F:234:MET:CB	2.70	0.40
2:F:293:LEU:N	2:F:328:GLY:HA3	2.37	0.40
2:F:437:LEU:HD23	2:F:437:LEU:HA	1.69	0.40
2:G:248:VAL:CG1	2:G:269:LEU:HD12	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	H	108/110 (98%)	85 (79%)	18 (17%)	5 (5%)	2	23
1	I	108/110 (98%)	85 (79%)	18 (17%)	5 (5%)	2	23
1	J	108/110 (98%)	85 (79%)	18 (17%)	5 (5%)	2	23
1	K	103/110 (94%)	79 (77%)	18 (18%)	6 (6%)	1	18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	103/110 (94%)	78 (76%)	19 (18%)	6 (6%)	1	18
1	M	103/110 (94%)	79 (77%)	18 (18%)	6 (6%)	1	18
2	A	385/549 (70%)	320 (83%)	65 (17%)	0	100	100
2	B	385/549 (70%)	328 (85%)	56 (14%)	1 (0%)	41	75
2	C	385/549 (70%)	334 (87%)	48 (12%)	3 (1%)	19	59
2	D	385/549 (70%)	336 (87%)	48 (12%)	1 (0%)	41	75
2	E	385/549 (70%)	331 (86%)	50 (13%)	4 (1%)	15	55
2	F	385/549 (70%)	348 (90%)	36 (9%)	1 (0%)	41	75
2	G	385/549 (70%)	337 (88%)	47 (12%)	1 (0%)	41	75
All	All	3328/4503 (74%)	2825 (85%)	459 (14%)	44 (1%)	16	50

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	175	LYS
2	E	282	SER
2	C	485	LEU
2	G	356	GLU
1	H	2	LEU
1	H	73	ASP
1	I	2	LEU
1	I	73	ASP
1	J	2	LEU
1	J	73	ASP
1	K	2	LEU
1	K	73	ASP
1	K	104	VAL
1	L	2	LEU
1	L	73	ASP
1	L	104	VAL
1	M	2	LEU
1	M	73	ASP
1	M	104	VAL
2	C	428	ASP
2	E	221	PRO
2	E	372	LYS
1	K	35	ILE
1	L	35	ILE
1	M	35	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	102	ARG
1	L	102	ARG
1	M	102	ARG
2	D	364	GLU
2	F	368	PRO
1	H	70	PRO
1	I	35	ILE
1	I	70	PRO
1	J	70	PRO
1	K	70	PRO
1	L	70	PRO
1	M	70	PRO
2	C	342	PRO
1	H	35	ILE
1	J	35	ILE
1	H	108	PRO
1	I	108	PRO
1	J	108	PRO
2	E	366	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	H	100/100 (100%)	88 (88%)	12 (12%)	5	27
1	I	100/100 (100%)	87 (87%)	13 (13%)	4	24
1	J	100/100 (100%)	87 (87%)	13 (13%)	4	24
1	K	96/100 (96%)	82 (85%)	14 (15%)	3	20
1	L	96/100 (96%)	82 (85%)	14 (15%)	3	20
1	M	96/100 (96%)	82 (85%)	14 (15%)	3	20
2	A	356/501 (71%)	235 (66%)	121 (34%)	0	1
2	B	356/501 (71%)	234 (66%)	122 (34%)	0	1
2	C	356/501 (71%)	244 (68%)	112 (32%)	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	356/501 (71%)	232 (65%)	124 (35%)	0	1
2	E	356/501 (71%)	262 (74%)	94 (26%)	0	4
2	F	356/501 (71%)	283 (80%)	73 (20%)	1	7
2	G	356/501 (71%)	291 (82%)	65 (18%)	1	10
All	All	3080/4107 (75%)	2289 (74%)	791 (26%)	2	4

All (791) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	1	MET
1	H	15	THR
1	H	17	LEU
1	H	45	SER
1	H	46	LYS
1	H	51	LEU
1	H	52	GLU
1	H	64	GLN
1	H	67	GLU
1	H	68	LEU
1	H	77	TYR
1	H	95	ILE
1	I	1	MET
1	I	4	GLU
1	I	15	THR
1	I	17	LEU
1	I	45	SER
1	I	46	LYS
1	I	51	LEU
1	I	52	GLU
1	I	64	GLN
1	I	67	GLU
1	I	68	LEU
1	I	77	TYR
1	I	95	ILE
1	J	1	MET
1	J	4	GLU
1	J	15	THR
1	J	17	LEU
1	J	45	SER
1	J	46	LYS
1	J	51	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	52	GLU
1	J	64	GLN
1	J	67	GLU
1	J	68	LEU
1	J	77	TYR
1	J	95	ILE
1	K	1	MET
1	K	4	GLU
1	K	15	THR
1	K	17	LEU
1	K	45	SER
1	K	46	LYS
1	K	52	GLU
1	K	64	GLN
1	K	67	GLU
1	K	68	LEU
1	K	77	TYR
1	K	97	GLU
1	K	99	ASP
1	K	104	VAL
1	L	1	MET
1	L	4	GLU
1	L	15	THR
1	L	17	LEU
1	L	45	SER
1	L	46	LYS
1	L	52	GLU
1	L	64	GLN
1	L	67	GLU
1	L	68	LEU
1	L	77	TYR
1	L	97	GLU
1	L	99	ASP
1	L	104	VAL
1	M	1	MET
1	M	4	GLU
1	M	15	THR
1	M	17	LEU
1	M	45	SER
1	M	46	LYS
1	M	52	GLU
1	M	64	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	67	GLU
1	M	68	LEU
1	M	77	TYR
1	M	97	GLU
1	M	99	ASP
1	M	104	VAL
2	A	113	GLN
2	A	115	LEU
2	A	116	ASP
2	A	117	ARG
2	A	126	LYS
2	A	127	GLN
2	A	128	MET
2	A	130	CYS
2	A	136	HIS
2	A	139	ARG
2	A	143	LYS
2	A	149	ASP
2	A	155	LEU
2	A	157	LEU
2	A	174	SER
2	A	175	LYS
2	A	179	LEU
2	A	180	ILE
2	A	185	ASP
2	A	189	TRP
2	A	198	LYS
2	A	201	PHE
2	A	203	LEU
2	A	205	THR
2	A	207	ILE
2	A	208	LEU
2	A	212	LYS
2	A	217	LEU
2	A	218	LEU
2	A	220	PHE
2	A	224	GLU
2	A	226	VAL
2	A	227	THR
2	A	233	ARG
2	A	239	LEU
2	A	244	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	248	VAL
2	A	253	VAL
2	A	255	GLU
2	A	256	GLU
2	A	257	THR
2	A	259	ARG
2	A	262	GLN
2	A	269	LEU
2	A	277	ILE
2	A	278	SER
2	A	286	GLU
2	A	293	LEU
2	A	295	ILE
2	A	296	ASP
2	A	297	GLU
2	A	298	CYS
2	A	300	ASP
2	A	302	LEU
2	A	314	LYS
2	A	319	LEU
2	A	321	LYS
2	A	327	SER
2	A	332	THR
2	A	333	LEU
2	A	334	MET
2	A	335	MET
2	A	336	PHE
2	A	339	SER
2	A	340	CYS
2	A	341	GLU
2	A	343	LYS
2	A	345	PHE
2	A	346	GLU
2	A	350	GLN
2	A	351	LEU
2	A	355	LEU
2	A	356	GLU
2	A	360	LEU
2	A	363	VAL
2	A	369	TYR
2	A	373	SER
2	A	374	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	381	CYS
2	A	382	VAL
2	A	387	ASP
2	A	388	GLU
2	A	391	SER
2	A	393	LEU
2	A	399	MET
2	A	405	ILE
2	A	408	LYS
2	A	410	TRP
2	A	424	GLU
2	A	425	GLN
2	A	426	LEU
2	A	427	ASP
2	A	435	LYS
2	A	437	LEU
2	A	439	LYS
2	A	447	LYS
2	A	448	ARG
2	A	449	MET
2	A	451	VAL
2	A	452	LEU
2	A	455	LYS
2	A	456	ILE
2	A	459	ILE
2	A	465	LYS
2	A	468	VAL
2	A	475	ASN
2	A	477	ILE
2	A	478	SER
2	A	480	LEU
2	A	482	GLN
2	A	483	ARG
2	A	486	GLU
2	A	487	ILE
2	A	522	THR
2	A	524	ILE
2	A	527	GLU
2	A	531	LYS
2	A	533	MET
2	A	534	GLN
2	A	538	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	539	PHE
2	B	113	GLN
2	B	115	LEU
2	B	116	ASP
2	B	117	ARG
2	B	126	LYS
2	B	127	GLN
2	B	130	CYS
2	B	134	GLU
2	B	136	HIS
2	B	139	ARG
2	B	143	LYS
2	B	147	MET
2	B	148	CYS
2	B	150	LEU
2	B	155	LEU
2	B	157	LEU
2	B	176	SER
2	B	177	ASP
2	B	178	GLN
2	B	179	LEU
2	B	180	ILE
2	B	185	ASP
2	B	189	TRP
2	B	198	LYS
2	B	201	PHE
2	B	203	LEU
2	B	205	THR
2	B	207	ILE
2	B	208	LEU
2	B	212	LYS
2	B	217	LEU
2	B	218	LEU
2	B	220	PHE
2	B	222	SER
2	B	223	VAL
2	B	224	GLU
2	B	226	VAL
2	B	228	SER
2	B	233	ARG
2	B	239	LEU
2	B	241	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	244	ASN
2	B	248	VAL
2	B	253	VAL
2	B	255	GLU
2	B	258	ILE
2	B	259	ARG
2	B	262	GLN
2	B	269	LEU
2	B	277	ILE
2	B	278	SER
2	B	279	ASN
2	B	283	GLN
2	B	285	CYS
2	B	286	GLU
2	B	293	LEU
2	B	295	ILE
2	B	296	ASP
2	B	297	GLU
2	B	298	CYS
2	B	300	ASP
2	B	302	LEU
2	B	307	MET
2	B	309	MET
2	B	311	VAL
2	B	314	LYS
2	B	316	GLU
2	B	320	ASN
2	B	321	LYS
2	B	334	MET
2	B	343	LYS
2	B	345	PHE
2	B	346	GLU
2	B	350	GLN
2	B	355	LEU
2	B	356	GLU
2	B	360	LEU
2	B	363	VAL
2	B	364	GLU
2	B	366	ILE
2	B	367	THR
2	B	369	TYR
2	B	373	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	374	LEU
2	B	381	CYS
2	B	382	VAL
2	B	387	ASP
2	B	405	ILE
2	B	408	LYS
2	B	410	TRP
2	B	424	GLU
2	B	425	GLN
2	B	426	LEU
2	B	427	ASP
2	B	428	ASP
2	B	435	LYS
2	B	437	LEU
2	B	439	LYS
2	B	444	LEU
2	B	445	SER
2	B	448	ARG
2	B	449	MET
2	B	451	VAL
2	B	452	LEU
2	B	455	LYS
2	B	456	ILE
2	B	459	ILE
2	B	475	ASN
2	B	477	ILE
2	B	478	SER
2	B	522	THR
2	B	524	ILE
2	B	527	GLU
2	B	531	LYS
2	B	533	MET
2	B	534	GLN
2	B	537	GLN
2	B	538	LYS
2	B	539	PHE
2	B	540	TYR
2	B	542	SER
2	B	543	LEU
2	C	113	GLN
2	C	115	LEU
2	C	116	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	117	ARG
2	C	126	LYS
2	C	127	GLN
2	C	130	CYS
2	C	134	GLU
2	C	136	HIS
2	C	139	ARG
2	C	143	LYS
2	C	150	LEU
2	C	155	LEU
2	C	157	LEU
2	C	160	ARG
2	C	174	SER
2	C	175	LYS
2	C	177	ASP
2	C	179	LEU
2	C	180	ILE
2	C	185	ASP
2	C	189	TRP
2	C	198	LYS
2	C	201	PHE
2	C	203	LEU
2	C	205	THR
2	C	207	ILE
2	C	208	LEU
2	C	212	LYS
2	C	217	LEU
2	C	218	LEU
2	C	220	PHE
2	C	224	GLU
2	C	233	ARG
2	C	239	LEU
2	C	241	ASP
2	C	244	ASN
2	C	248	VAL
2	C	253	VAL
2	C	255	GLU
2	C	256	GLU
2	C	259	ARG
2	C	262	GLN
2	C	269	LEU
2	C	278	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	285	CYS
2	C	286	GLU
2	C	293	LEU
2	C	295	ILE
2	C	296	ASP
2	C	297	GLU
2	C	298	CYS
2	C	300	ASP
2	C	302	LEU
2	C	309	MET
2	C	311	VAL
2	C	313	GLU
2	C	314	LYS
2	C	315	GLU
2	C	316	GLU
2	C	317	ASP
2	C	319	LEU
2	C	323	ILE
2	C	334	MET
2	C	335	MET
2	C	336	PHE
2	C	343	LYS
2	C	345	PHE
2	C	346	GLU
2	C	350	GLN
2	C	366	ILE
2	C	369	TYR
2	C	373	SER
2	C	374	LEU
2	C	381	CYS
2	C	382	VAL
2	C	387	ASP
2	C	388	GLU
2	C	405	ILE
2	C	408	LYS
2	C	410	TRP
2	C	426	LEU
2	C	435	LYS
2	C	437	LEU
2	C	439	LYS
2	C	443	LEU
2	C	444	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	445	SER
2	C	447	LYS
2	C	449	MET
2	C	455	LYS
2	C	456	ILE
2	C	459	ILE
2	C	464	LEU
2	C	465	LYS
2	C	467	VAL
2	C	477	ILE
2	C	485	LEU
2	C	486	GLU
2	C	487	ILE
2	C	522	THR
2	C	524	ILE
2	C	527	GLU
2	C	531	LYS
2	C	533	MET
2	C	534	GLN
2	C	536	HIS
2	C	537	GLN
2	C	538	LYS
2	C	540	TYR
2	C	542	SER
2	C	543	LEU
2	D	113	GLN
2	D	115	LEU
2	D	116	ASP
2	D	117	ARG
2	D	127	GLN
2	D	128	MET
2	D	130	CYS
2	D	134	GLU
2	D	136	HIS
2	D	139	ARG
2	D	143	LYS
2	D	150	LEU
2	D	151	ASP
2	D	155	LEU
2	D	157	LEU
2	D	160	ARG
2	D	174	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	175	LYS
2	D	177	ASP
2	D	179	LEU
2	D	180	ILE
2	D	185	ASP
2	D	189	TRP
2	D	198	LYS
2	D	201	PHE
2	D	203	LEU
2	D	205	THR
2	D	207	ILE
2	D	208	LEU
2	D	212	LYS
2	D	217	LEU
2	D	218	LEU
2	D	220	PHE
2	D	223	VAL
2	D	224	GLU
2	D	228	SER
2	D	233	ARG
2	D	239	LEU
2	D	240	ILE
2	D	242	ARG
2	D	245	THR
2	D	246	LEU
2	D	248	VAL
2	D	253	VAL
2	D	255	GLU
2	D	256	GLU
2	D	259	ARG
2	D	260	TRP
2	D	262	GLN
2	D	269	LEU
2	D	278	SER
2	D	285	CYS
2	D	286	GLU
2	D	293	LEU
2	D	295	ILE
2	D	296	ASP
2	D	297	GLU
2	D	298	CYS
2	D	300	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	302	LEU
2	D	307	MET
2	D	309	MET
2	D	311	VAL
2	D	313	GLU
2	D	314	LYS
2	D	315	GLU
2	D	316	GLU
2	D	317	ASP
2	D	319	LEU
2	D	334	MET
2	D	335	MET
2	D	338	LYS
2	D	345	PHE
2	D	346	GLU
2	D	348	MET
2	D	350	GLN
2	D	351	LEU
2	D	355	LEU
2	D	356	GLU
2	D	360	LEU
2	D	363	VAL
2	D	367	THR
2	D	374	LEU
2	D	381	CYS
2	D	382	VAL
2	D	387	ASP
2	D	388	GLU
2	D	405	ILE
2	D	408	LYS
2	D	410	TRP
2	D	424	GLU
2	D	435	LYS
2	D	437	LEU
2	D	439	LYS
2	D	444	LEU
2	D	447	LYS
2	D	448	ARG
2	D	449	MET
2	D	451	VAL
2	D	452	LEU
2	D	455	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	456	ILE
2	D	459	ILE
2	D	465	LYS
2	D	467	VAL
2	D	475	ASN
2	D	477	ILE
2	D	478	SER
2	D	480	LEU
2	D	483	ARG
2	D	486	GLU
2	D	487	ILE
2	D	522	THR
2	D	524	ILE
2	D	527	GLU
2	D	531	LYS
2	D	532	PHE
2	D	533	MET
2	D	535	LEU
2	D	537	GLN
2	D	538	LYS
2	D	540	TYR
2	D	542	SER
2	D	543	LEU
2	E	113	GLN
2	E	115	LEU
2	E	116	ASP
2	E	117	ARG
2	E	126	LYS
2	E	128	MET
2	E	130	CYS
2	E	134	GLU
2	E	136	HIS
2	E	139	ARG
2	E	143	LYS
2	E	150	LEU
2	E	155	LEU
2	E	157	LEU
2	E	179	LEU
2	E	180	ILE
2	E	185	ASP
2	E	189	TRP
2	E	198	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	201	PHE
2	E	203	LEU
2	E	205	THR
2	E	207	ILE
2	E	208	LEU
2	E	212	LYS
2	E	217	LEU
2	E	218	LEU
2	E	220	PHE
2	E	226	VAL
2	E	233	ARG
2	E	239	LEU
2	E	241	ASP
2	E	244	ASN
2	E	246	LEU
2	E	248	VAL
2	E	253	VAL
2	E	255	GLU
2	E	256	GLU
2	E	259	ARG
2	E	262	GLN
2	E	269	LEU
2	E	283	GLN
2	E	285	CYS
2	E	286	GLU
2	E	293	LEU
2	E	295	ILE
2	E	296	ASP
2	E	297	GLU
2	E	298	CYS
2	E	300	ASP
2	E	302	LEU
2	E	314	LYS
2	E	319	LEU
2	E	323	ILE
2	E	332	THR
2	E	333	LEU
2	E	334	MET
2	E	335	MET
2	E	336	PHE
2	E	338	LYS
2	E	339	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	345	PHE
2	E	346	GLU
2	E	360	LEU
2	E	363	VAL
2	E	374	LEU
2	E	381	CYS
2	E	382	VAL
2	E	387	ASP
2	E	388	GLU
2	E	405	ILE
2	E	408	LYS
2	E	410	TRP
2	E	435	LYS
2	E	437	LEU
2	E	439	LYS
2	E	447	LYS
2	E	448	ARG
2	E	449	MET
2	E	451	VAL
2	E	452	LEU
2	E	455	LYS
2	E	456	ILE
2	E	459	ILE
2	E	477	ILE
2	E	522	THR
2	E	524	ILE
2	E	527	GLU
2	E	531	LYS
2	E	533	MET
2	E	534	GLN
2	E	536	HIS
2	E	538	LYS
2	E	543	LEU
2	F	113	GLN
2	F	115	LEU
2	F	116	ASP
2	F	117	ARG
2	F	136	HIS
2	F	139	ARG
2	F	143	LYS
2	F	155	LEU
2	F	174	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	179	LEU
2	F	180	ILE
2	F	185	ASP
2	F	189	TRP
2	F	198	LYS
2	F	201	PHE
2	F	203	LEU
2	F	205	THR
2	F	207	ILE
2	F	208	LEU
2	F	212	LYS
2	F	217	LEU
2	F	233	ARG
2	F	239	LEU
2	F	241	ASP
2	F	248	VAL
2	F	256	GLU
2	F	269	LEU
2	F	293	LEU
2	F	295	ILE
2	F	296	ASP
2	F	297	GLU
2	F	298	CYS
2	F	300	ASP
2	F	314	LYS
2	F	315	GLU
2	F	316	GLU
2	F	321	LYS
2	F	329	ASN
2	F	332	THR
2	F	333	LEU
2	F	343	LYS
2	F	346	GLU
2	F	350	GLN
2	F	355	LEU
2	F	360	LEU
2	F	369	TYR
2	F	373	SER
2	F	374	LEU
2	F	381	CYS
2	F	382	VAL
2	F	387	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	388	GLU
2	F	405	ILE
2	F	408	LYS
2	F	410	TRP
2	F	424	GLU
2	F	426	LEU
2	F	435	LYS
2	F	437	LEU
2	F	439	LYS
2	F	447	LYS
2	F	448	ARG
2	F	449	MET
2	F	451	VAL
2	F	452	LEU
2	F	455	LYS
2	F	457	ASP
2	F	459	ILE
2	F	477	ILE
2	F	522	THR
2	F	524	ILE
2	F	531	LYS
2	F	533	MET
2	G	113	GLN
2	G	115	LEU
2	G	116	ASP
2	G	117	ARG
2	G	139	ARG
2	G	143	LYS
2	G	155	LEU
2	G	174	SER
2	G	179	LEU
2	G	180	ILE
2	G	185	ASP
2	G	189	TRP
2	G	198	LYS
2	G	201	PHE
2	G	203	LEU
2	G	205	THR
2	G	207	ILE
2	G	208	LEU
2	G	212	LYS
2	G	217	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	218	LEU
2	G	226	VAL
2	G	233	ARG
2	G	239	LEU
2	G	248	VAL
2	G	253	VAL
2	G	262	GLN
2	G	267	ARG
2	G	293	LEU
2	G	295	ILE
2	G	296	ASP
2	G	297	GLU
2	G	298	CYS
2	G	300	ASP
2	G	302	LEU
2	G	314	LYS
2	G	315	GLU
2	G	316	GLU
2	G	319	LEU
2	G	321	LYS
2	G	332	THR
2	G	333	LEU
2	G	334	MET
2	G	335	MET
2	G	350	GLN
2	G	356	GLU
2	G	374	LEU
2	G	381	CYS
2	G	382	VAL
2	G	405	ILE
2	G	408	LYS
2	G	409	LEU
2	G	410	TRP
2	G	424	GLU
2	G	435	LYS
2	G	437	LEU
2	G	448	ARG
2	G	449	MET
2	G	451	VAL
2	G	452	LEU
2	G	459	ILE
2	G	477	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	522	THR
2	G	524	ILE
2	G	531	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	34	ASN
1	H	40	HIS
1	H	78	ASN
1	I	34	ASN
1	I	40	HIS
1	I	78	ASN
1	J	34	ASN
1	J	40	HIS
1	J	78	ASN
1	K	34	ASN
1	K	40	HIS
1	K	78	ASN
1	L	34	ASN
1	L	40	HIS
1	L	78	ASN
1	M	34	ASN
1	M	40	HIS
1	M	78	ASN
2	A	123	ASN
2	A	127	GLN
2	A	219	ASN
2	A	244	ASN
2	A	458	HIS
2	A	471	GLN
2	B	123	ASN
2	B	219	ASN
2	B	244	ASN
2	B	254	GLN
2	B	425	GLN
2	B	471	GLN
2	B	482	GLN
2	B	537	GLN
2	C	123	ASN
2	C	171	GLN
2	C	219	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	244	ASN
2	C	320	ASN
2	C	350	GLN
2	C	471	GLN
2	C	482	GLN
2	C	537	GLN
2	D	123	ASN
2	D	219	ASN
2	D	244	ASN
2	D	320	ASN
2	D	458	HIS
2	D	471	GLN
2	D	482	GLN
2	D	537	GLN
2	E	123	ASN
2	E	171	GLN
2	E	219	ASN
2	E	244	ASN
2	E	320	ASN
2	E	350	GLN
2	E	471	GLN
2	E	482	GLN
2	E	536	HIS
2	F	123	ASN
2	F	171	GLN
2	F	219	ASN
2	F	244	ASN
2	F	262	GLN
2	F	425	GLN
2	F	458	HIS
2	F	471	GLN
2	F	482	GLN
2	F	536	HIS
2	G	123	ASN
2	G	171	GLN
2	G	219	ASN
2	G	244	ASN
2	G	283	GLN
2	G	329	ASN
2	G	350	GLN
2	G	458	HIS
2	G	466	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	471	GLN
2	G	475	ASN
2	G	482	GLN

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 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	D	602	3	26,33,33	1.10	2 (7%)	31,52,52	1.90	10 (32%)
4	ATP	A	602	3	26,33,33	1.11	3 (11%)	31,52,52	1.91	10 (32%)
4	ATP	G	602	3	26,33,33	1.11	2 (7%)	31,52,52	1.92	10 (32%)
4	ATP	E	602	3	26,33,33	1.11	3 (11%)	31,52,52	1.92	10 (32%)
4	ATP	B	602	3	26,33,33	1.11	2 (7%)	31,52,52	1.91	10 (32%)
4	ATP	C	602	3	26,33,33	1.11	2 (7%)	31,52,52	1.92	10 (32%)
4	ATP	F	602	3	26,33,33	1.11	2 (7%)	31,52,52	1.91	10 (32%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	D	602	3	-	5/18/38/38	0/3/3/3
4	ATP	A	602	3	-	5/18/38/38	0/3/3/3
4	ATP	G	602	3	-	5/18/38/38	0/3/3/3
4	ATP	E	602	3	-	5/18/38/38	0/3/3/3
4	ATP	B	602	3	-	5/18/38/38	0/3/3/3
4	ATP	C	602	3	-	5/18/38/38	0/3/3/3
4	ATP	F	602	3	-	5/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	602	ATP	C5-C4	3.01	1.48	1.40
4	G	602	ATP	C5-C4	3.00	1.48	1.40
4	B	602	ATP	C5-C4	2.98	1.48	1.40
4	C	602	ATP	C5-C4	2.97	1.48	1.40
4	A	602	ATP	C5-C4	2.96	1.48	1.40
4	F	602	ATP	C5-C4	2.93	1.48	1.40
4	D	602	ATP	C5-C4	2.92	1.48	1.40
4	F	602	ATP	O4'-C1'	2.89	1.45	1.41
4	C	602	ATP	O4'-C1'	2.86	1.45	1.41
4	B	602	ATP	O4'-C1'	2.86	1.45	1.41
4	E	602	ATP	O4'-C1'	2.86	1.45	1.41
4	G	602	ATP	O4'-C1'	2.84	1.45	1.41
4	D	602	ATP	O4'-C1'	2.82	1.45	1.41
4	A	602	ATP	O4'-C1'	2.77	1.44	1.41
4	E	602	ATP	C2-N3	2.01	1.35	1.32
4	A	602	ATP	C2-N3	2.00	1.35	1.32

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	602	ATP	PB-O3B-PG	-5.44	114.14	132.83
4	B	602	ATP	PB-O3B-PG	-5.43	114.18	132.83
4	F	602	ATP	PB-O3B-PG	-5.43	114.20	132.83
4	D	602	ATP	PB-O3B-PG	-5.42	114.21	132.83
4	A	602	ATP	PB-O3B-PG	-5.42	114.23	132.83
4	G	602	ATP	PB-O3B-PG	-5.42	114.24	132.83
4	C	602	ATP	PB-O3B-PG	-5.41	114.25	132.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	602	ATP	C3'-C2'-C1'	3.76	106.64	100.98
4	F	602	ATP	C3'-C2'-C1'	3.75	106.62	100.98
4	E	602	ATP	C3'-C2'-C1'	3.75	106.62	100.98
4	B	602	ATP	C3'-C2'-C1'	3.72	106.59	100.98
4	A	602	ATP	C3'-C2'-C1'	3.72	106.57	100.98
4	D	602	ATP	C3'-C2'-C1'	3.70	106.55	100.98
4	G	602	ATP	C3'-C2'-C1'	3.70	106.55	100.98
4	A	602	ATP	PA-O3A-PB	-3.26	121.62	132.83
4	C	602	ATP	PA-O3A-PB	-3.26	121.64	132.83
4	B	602	ATP	PA-O3A-PB	-3.26	121.64	132.83
4	E	602	ATP	PA-O3A-PB	-3.25	121.67	132.83
4	G	602	ATP	PA-O3A-PB	-3.24	121.69	132.83
4	F	602	ATP	PA-O3A-PB	-3.24	121.72	132.83
4	D	602	ATP	PA-O3A-PB	-3.23	121.73	132.83
4	C	602	ATP	O3G-PG-O2G	2.71	118.00	107.64
4	D	602	ATP	O3G-PG-O2G	2.70	117.95	107.64
4	A	602	ATP	O3G-PG-O2G	2.70	117.94	107.64
4	E	602	ATP	O3G-PG-O2G	2.70	117.94	107.64
4	G	602	ATP	O3G-PG-O2G	2.69	117.90	107.64
4	B	602	ATP	O3G-PG-O2G	2.68	117.88	107.64
4	F	602	ATP	O3G-PG-O2G	2.67	117.84	107.64
4	G	602	ATP	N3-C2-N1	-2.59	124.62	128.68
4	B	602	ATP	N3-C2-N1	-2.57	124.66	128.68
4	F	602	ATP	N3-C2-N1	-2.57	124.67	128.68
4	A	602	ATP	N3-C2-N1	-2.55	124.69	128.68
4	E	602	ATP	N3-C2-N1	-2.54	124.70	128.68
4	C	602	ATP	N3-C2-N1	-2.54	124.71	128.68
4	D	602	ATP	N3-C2-N1	-2.50	124.78	128.68
4	G	602	ATP	O2B-PB-O1B	2.45	124.35	112.24
4	A	602	ATP	O2B-PB-O1B	2.45	124.34	112.24
4	B	602	ATP	O2B-PB-O1B	2.45	124.33	112.24
4	D	602	ATP	O2B-PB-O1B	2.44	124.32	112.24
4	E	602	ATP	O2B-PB-O1B	2.44	124.32	112.24
4	F	602	ATP	O2B-PB-O1B	2.44	124.29	112.24
4	C	602	ATP	O2B-PB-O1B	2.43	124.28	112.24
4	E	602	ATP	O3G-PG-O3B	-2.34	96.79	104.64
4	D	602	ATP	O3G-PG-O3B	-2.33	96.82	104.64
4	G	602	ATP	O3G-PG-O3B	-2.33	96.83	104.64
4	C	602	ATP	O3G-PG-O3B	-2.33	96.84	104.64
4	A	602	ATP	O3G-PG-O3B	-2.32	96.85	104.64
4	F	602	ATP	O3G-PG-O3B	-2.32	96.86	104.64
4	B	602	ATP	O3G-PG-O3B	-2.32	96.86	104.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	602	ATP	C4-C5-N7	-2.22	107.09	109.40
4	G	602	ATP	C4-C5-N7	-2.16	107.15	109.40
4	C	602	ATP	C4-C5-N7	-2.11	107.20	109.40
4	B	602	ATP	C4-C5-N7	-2.10	107.21	109.40
4	F	602	ATP	C4-C5-N7	-2.09	107.22	109.40
4	A	602	ATP	C4-C5-N7	-2.08	107.23	109.40
4	F	602	ATP	O2'-C2'-C3'	-2.07	105.14	111.82
4	D	602	ATP	C4-C5-N7	-2.05	107.26	109.40
4	D	602	ATP	O2'-C2'-C3'	-2.05	105.19	111.82
4	C	602	ATP	O2'-C2'-C3'	-2.04	105.21	111.82
4	B	602	ATP	O5'-C5'-C4'	-2.04	101.98	108.99
4	A	602	ATP	O2'-C2'-C3'	-2.04	105.23	111.82
4	G	602	ATP	O2'-C2'-C3'	-2.03	105.26	111.82
4	G	602	ATP	O5'-C5'-C4'	-2.03	102.01	108.99
4	E	602	ATP	O5'-C5'-C4'	-2.03	102.02	108.99
4	B	602	ATP	O2'-C2'-C3'	-2.03	105.27	111.82
4	A	602	ATP	O5'-C5'-C4'	-2.02	102.03	108.99
4	C	602	ATP	O5'-C5'-C4'	-2.02	102.03	108.99
4	E	602	ATP	O2'-C2'-C3'	-2.02	105.29	111.82
4	D	602	ATP	O5'-C5'-C4'	-2.02	102.05	108.99
4	F	602	ATP	O5'-C5'-C4'	-2.01	102.06	108.99

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	ATP	C5'-O5'-PA-O3A
4	A	602	ATP	O4'-C4'-C5'-O5'
4	A	602	ATP	C3'-C4'-C5'-O5'
4	B	602	ATP	C5'-O5'-PA-O3A
4	B	602	ATP	O4'-C4'-C5'-O5'
4	B	602	ATP	C3'-C4'-C5'-O5'
4	C	602	ATP	C5'-O5'-PA-O3A
4	C	602	ATP	O4'-C4'-C5'-O5'
4	C	602	ATP	C3'-C4'-C5'-O5'
4	D	602	ATP	C5'-O5'-PA-O3A
4	D	602	ATP	O4'-C4'-C5'-O5'
4	D	602	ATP	C3'-C4'-C5'-O5'
4	E	602	ATP	C5'-O5'-PA-O3A
4	E	602	ATP	O4'-C4'-C5'-O5'
4	E	602	ATP	C3'-C4'-C5'-O5'
4	F	602	ATP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	F	602	ATP	O4'-C4'-C5'-O5'
4	F	602	ATP	C3'-C4'-C5'-O5'
4	G	602	ATP	C5'-O5'-PA-O3A
4	G	602	ATP	O4'-C4'-C5'-O5'
4	G	602	ATP	C3'-C4'-C5'-O5'
4	A	602	ATP	C5'-O5'-PA-O1A
4	B	602	ATP	C5'-O5'-PA-O1A
4	C	602	ATP	C5'-O5'-PA-O1A
4	D	602	ATP	C5'-O5'-PA-O1A
4	E	602	ATP	C5'-O5'-PA-O1A
4	F	602	ATP	C5'-O5'-PA-O1A
4	G	602	ATP	C5'-O5'-PA-O1A
4	A	602	ATP	PA-O3A-PB-O1B
4	B	602	ATP	PA-O3A-PB-O1B
4	C	602	ATP	PA-O3A-PB-O1B
4	D	602	ATP	PA-O3A-PB-O1B
4	E	602	ATP	PA-O3A-PB-O1B
4	F	602	ATP	PA-O3A-PB-O1B
4	G	602	ATP	PA-O3A-PB-O1B

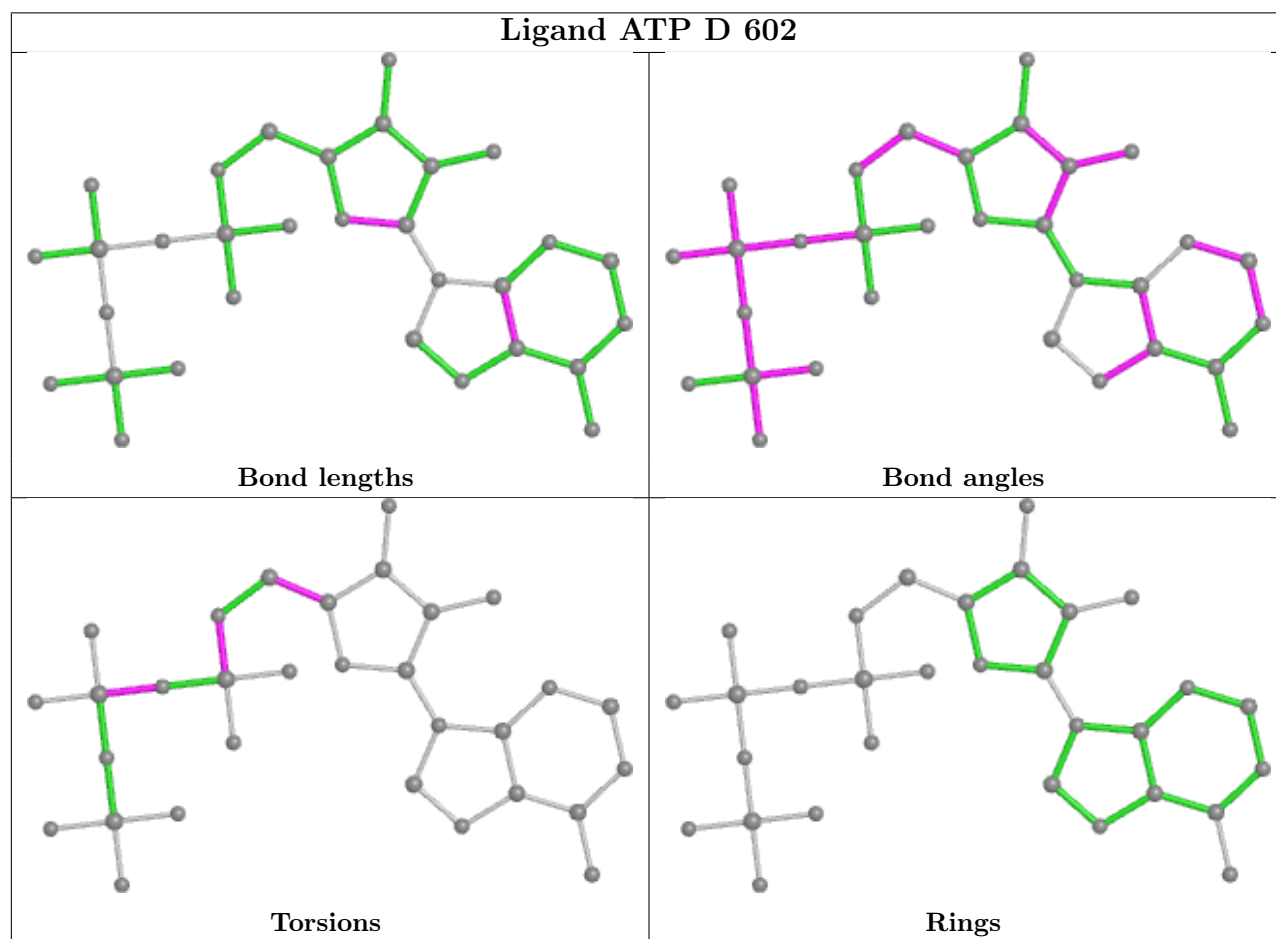
There are no ring outliers.

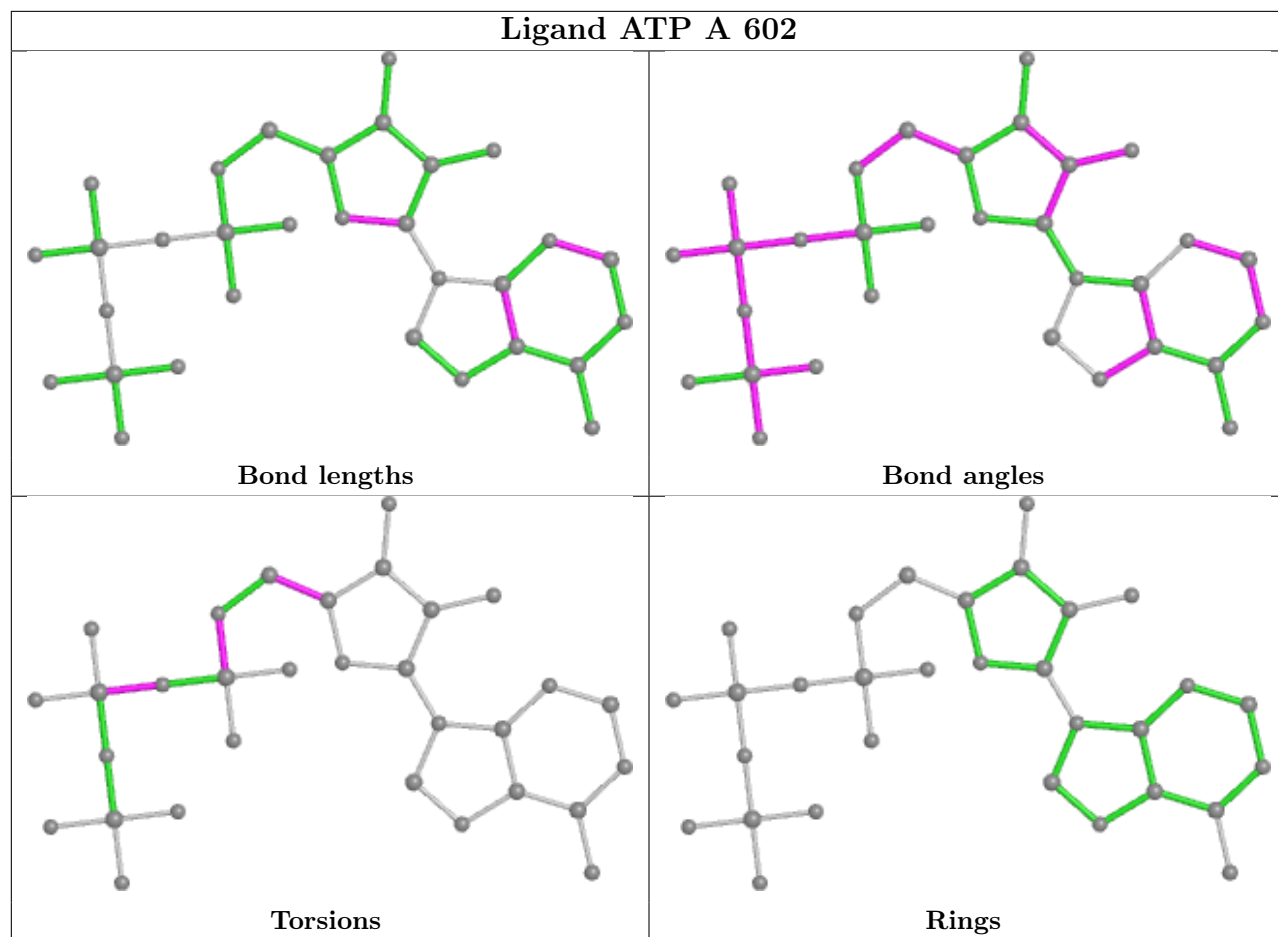
7 monomers are involved in 60 short contacts:

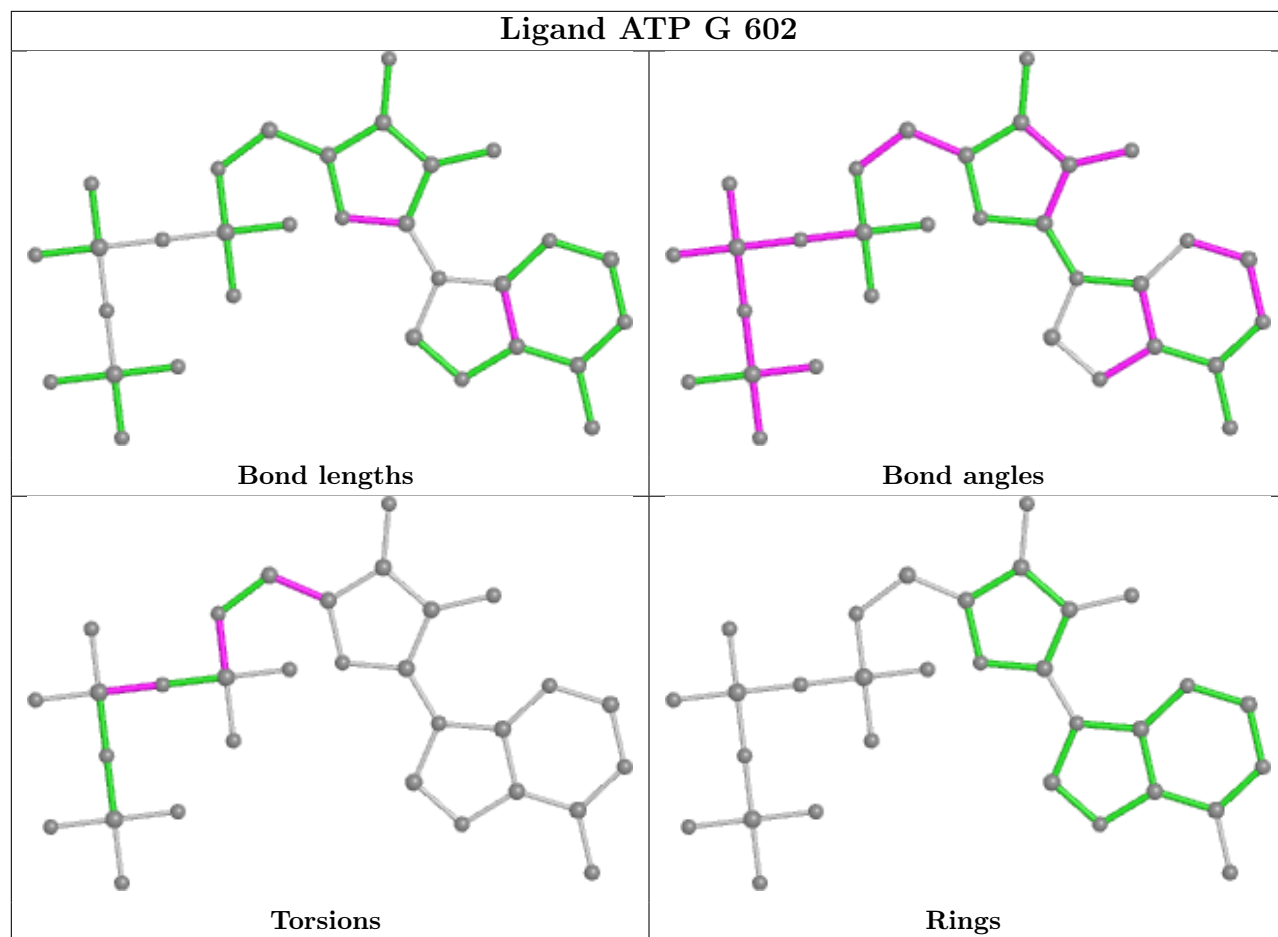
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	602	ATP	11	0
4	A	602	ATP	9	0
4	G	602	ATP	10	0
4	E	602	ATP	8	0
4	B	602	ATP	9	0
4	C	602	ATP	8	0
4	F	602	ATP	5	0

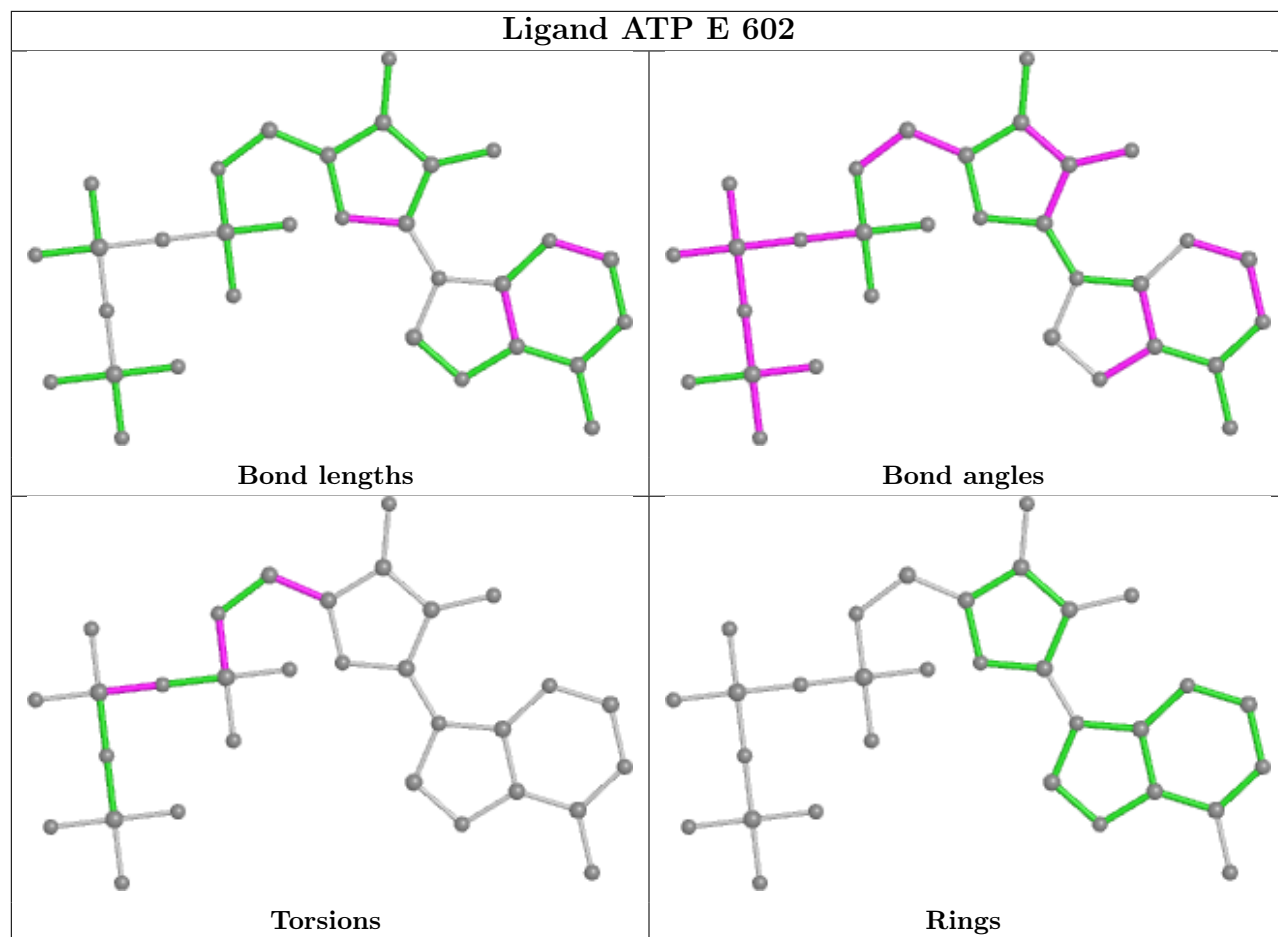
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

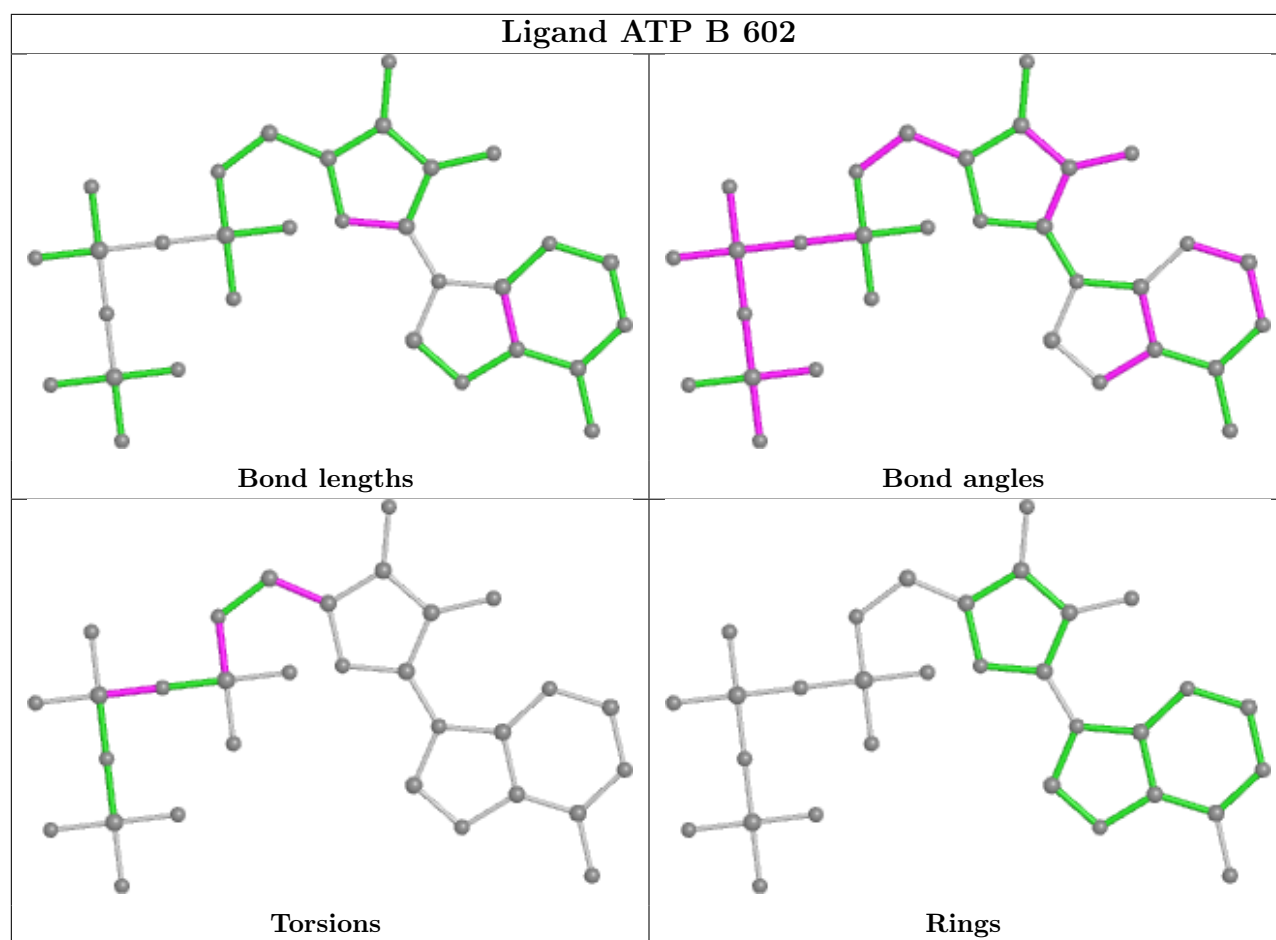
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

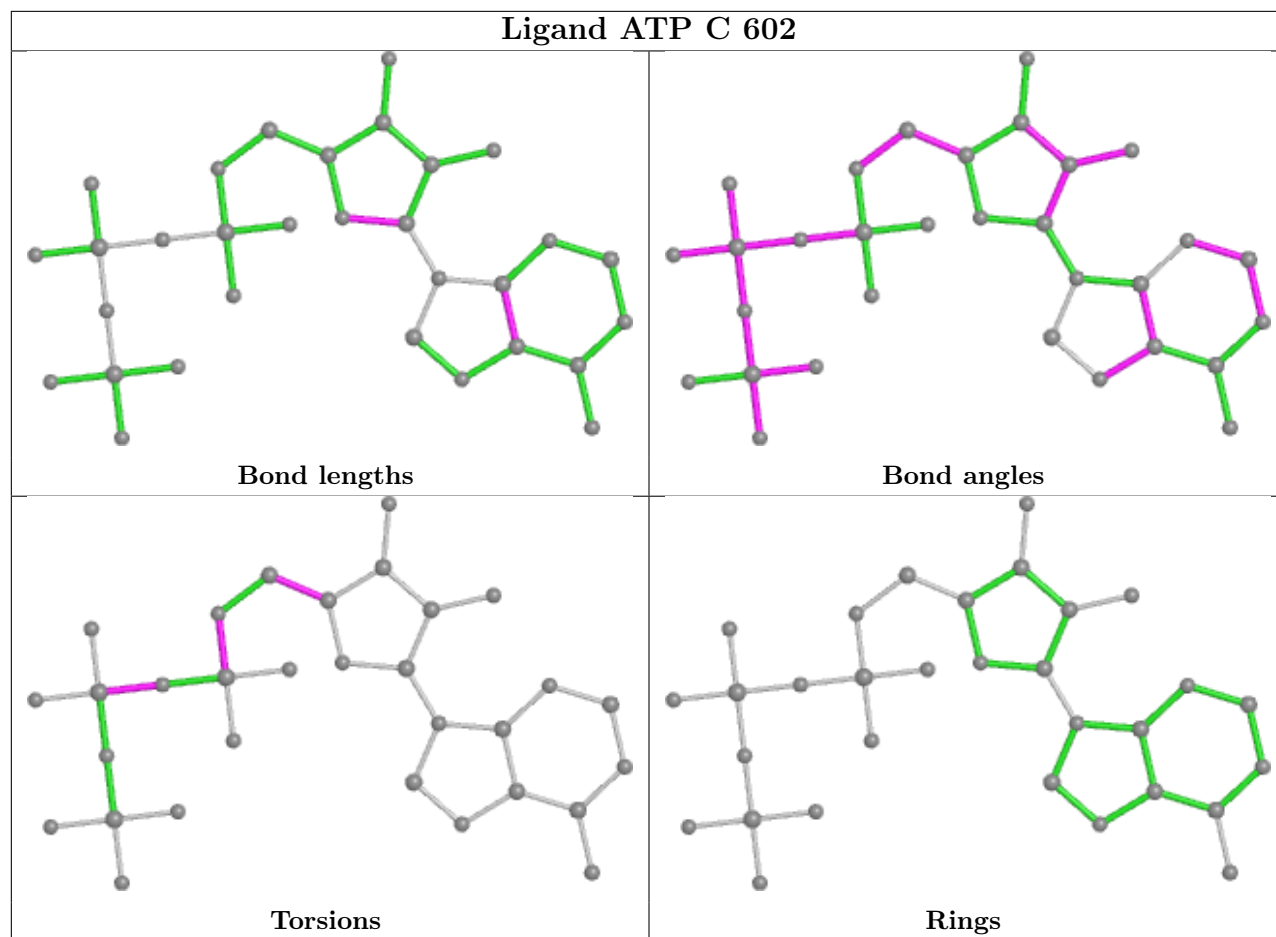


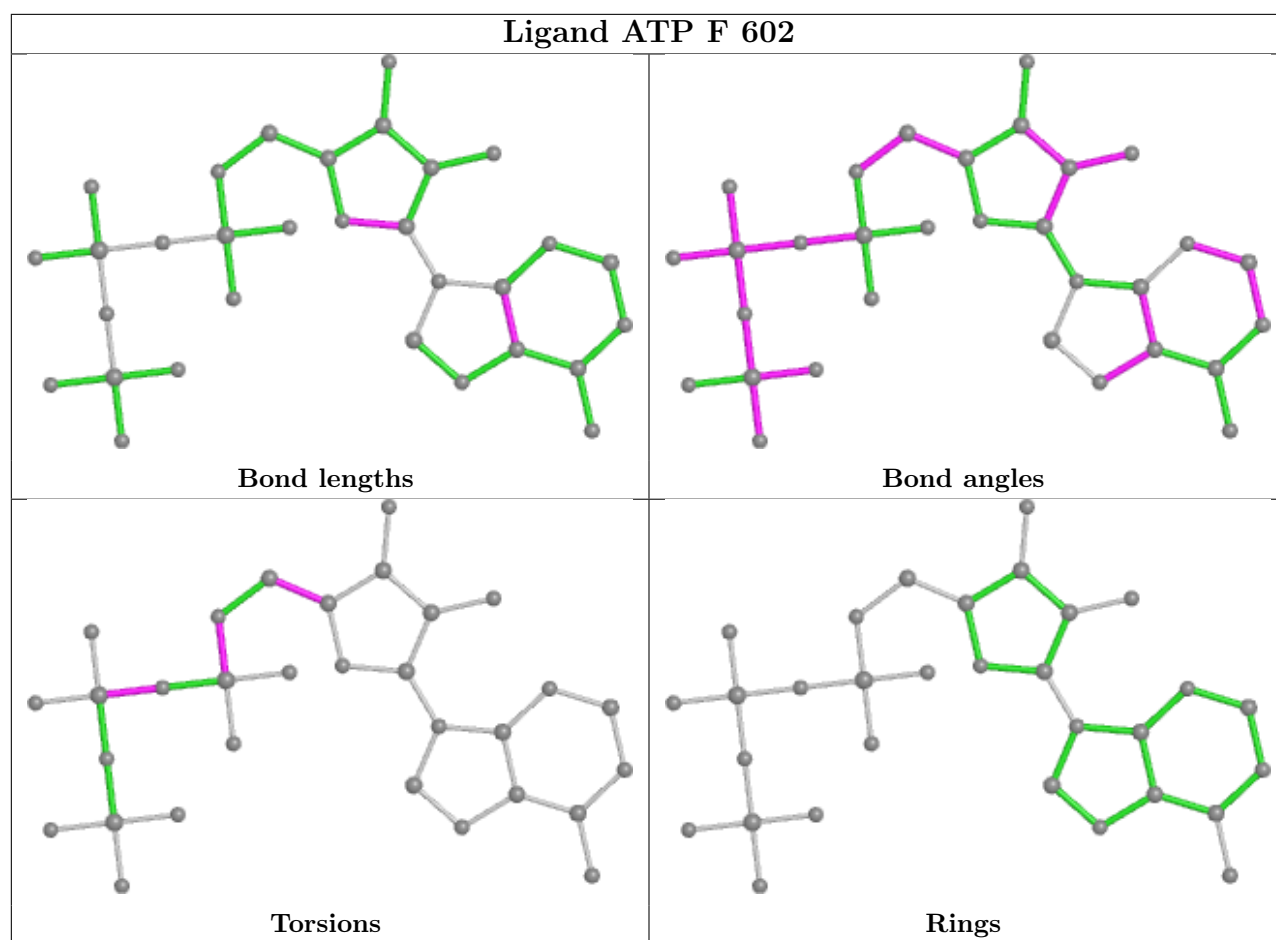












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

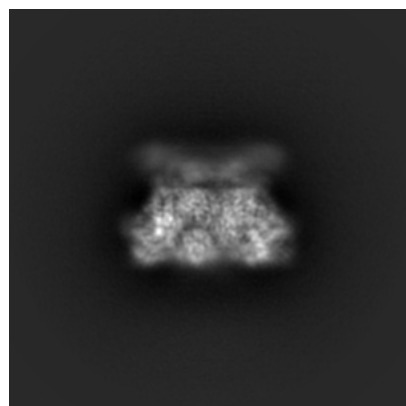
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36451. These allow visual inspection of the internal detail of the map and identification of artifacts.

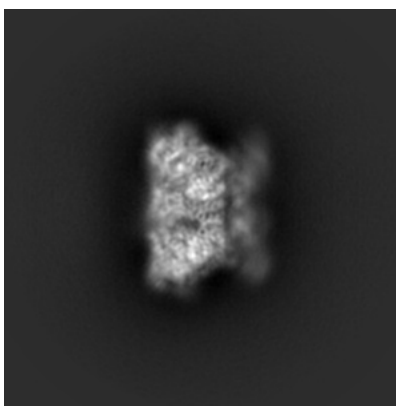
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

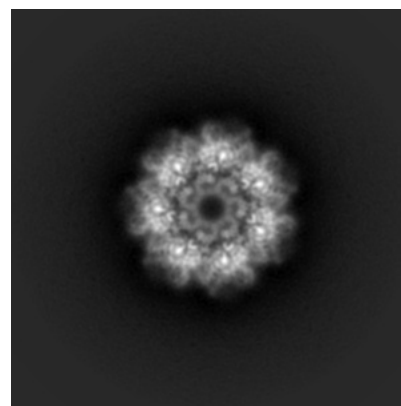
6.1.1 Primary map



X

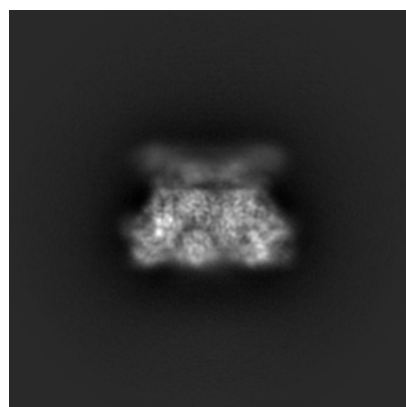


Y

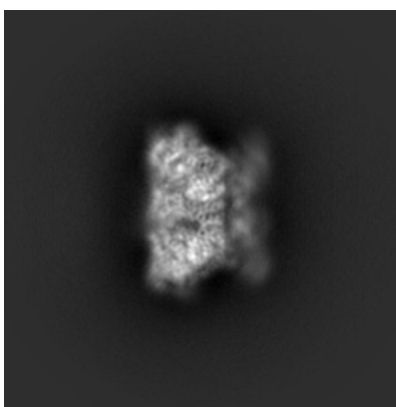


Z

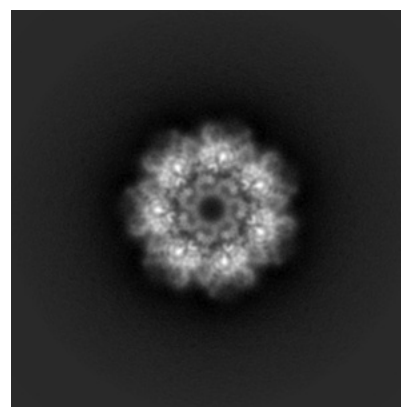
6.1.2 Raw map



X



Y

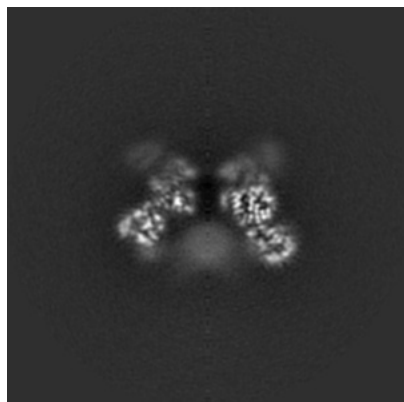


Z

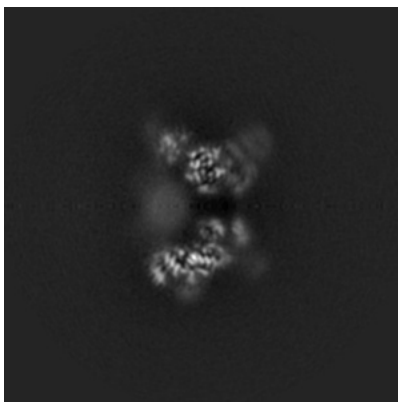
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

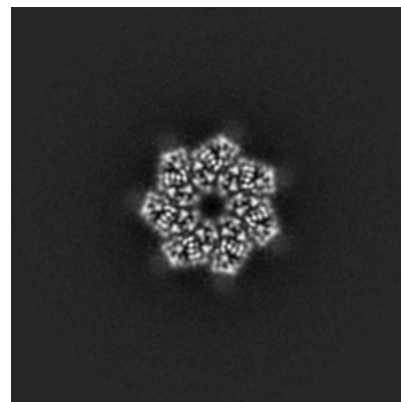
6.2.1 Primary map



X Index: 128

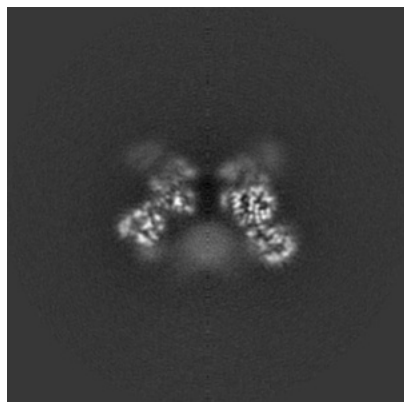


Y Index: 128

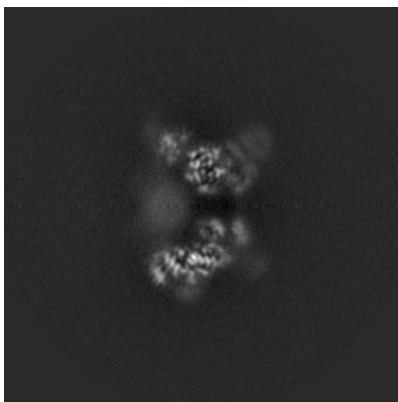


Z Index: 128

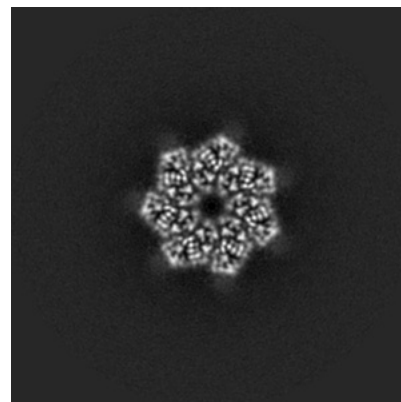
6.2.2 Raw map



X Index: 128



Y Index: 128

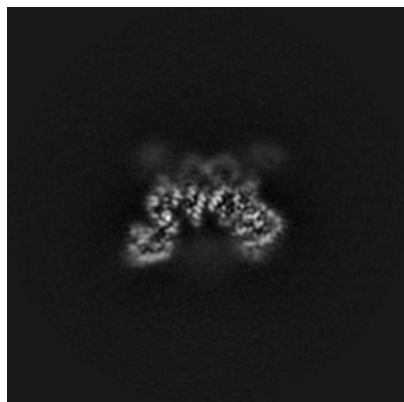


Z Index: 128

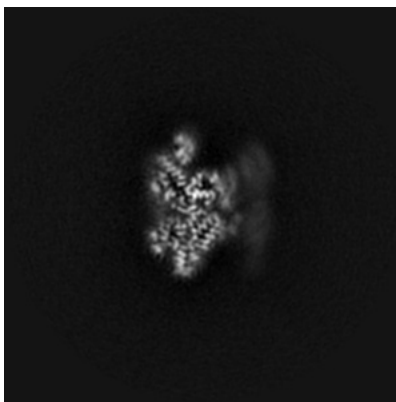
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

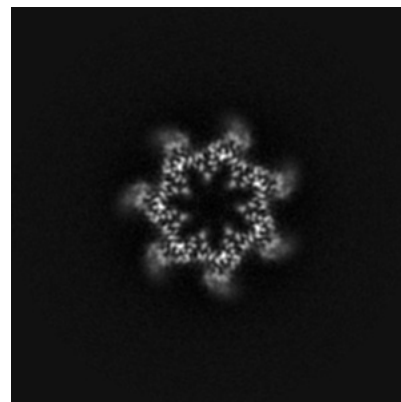
6.3.1 Primary map



X Index: 109

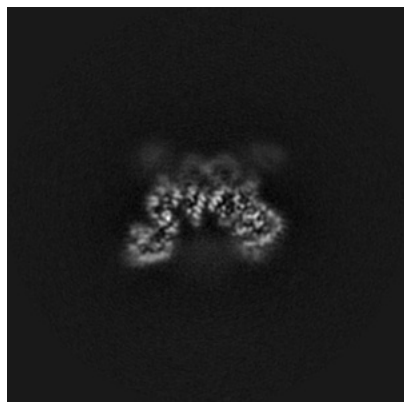


Y Index: 95

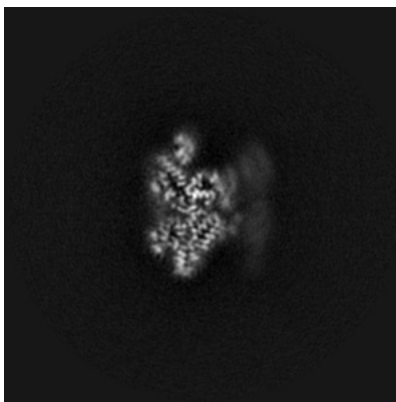


Z Index: 121

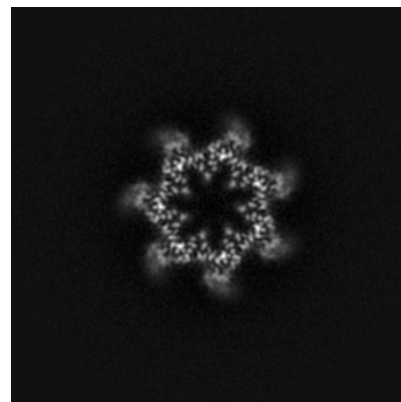
6.3.2 Raw map



X Index: 109



Y Index: 95

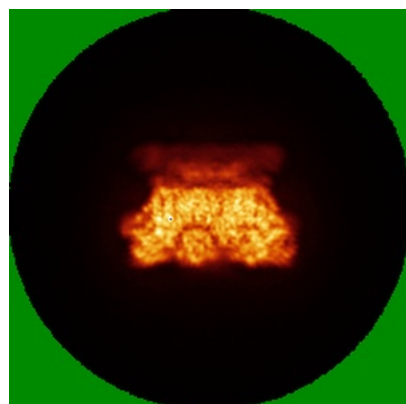


Z Index: 121

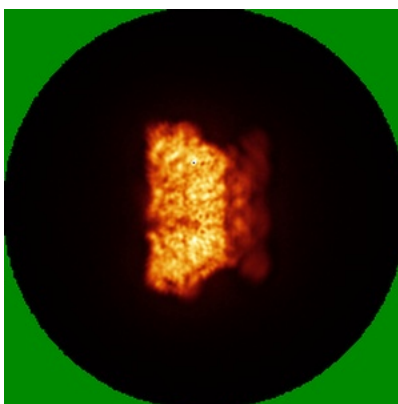
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

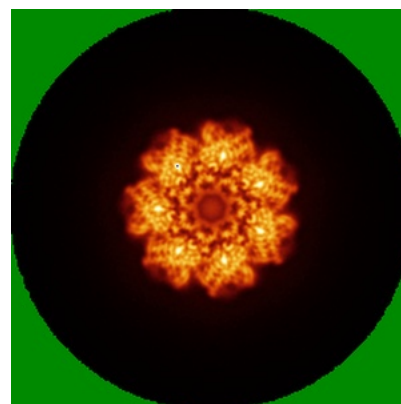
6.4.1 Primary map



X

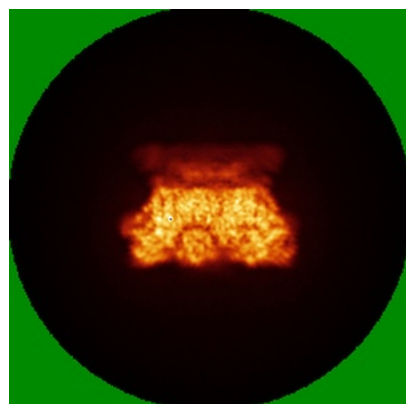


Y

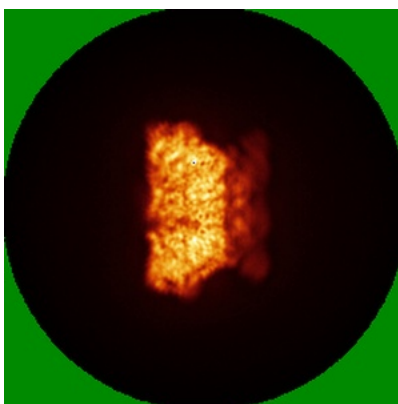


Z

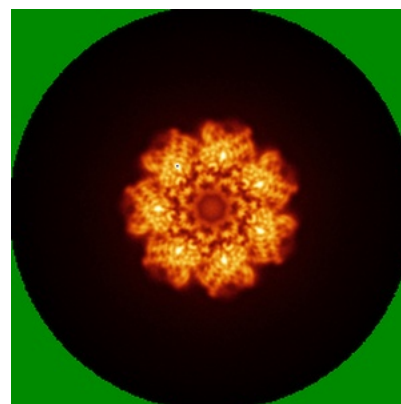
6.4.2 Raw map



X



Y

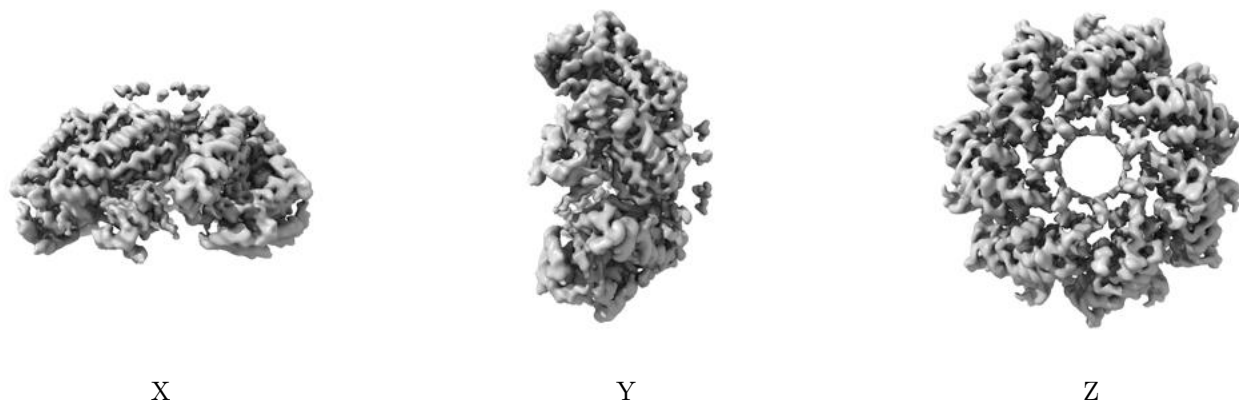


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

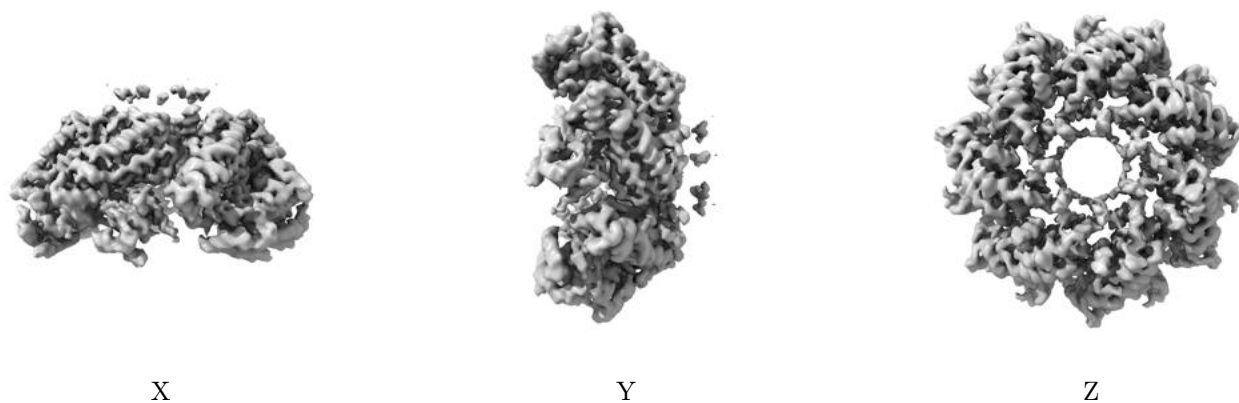
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

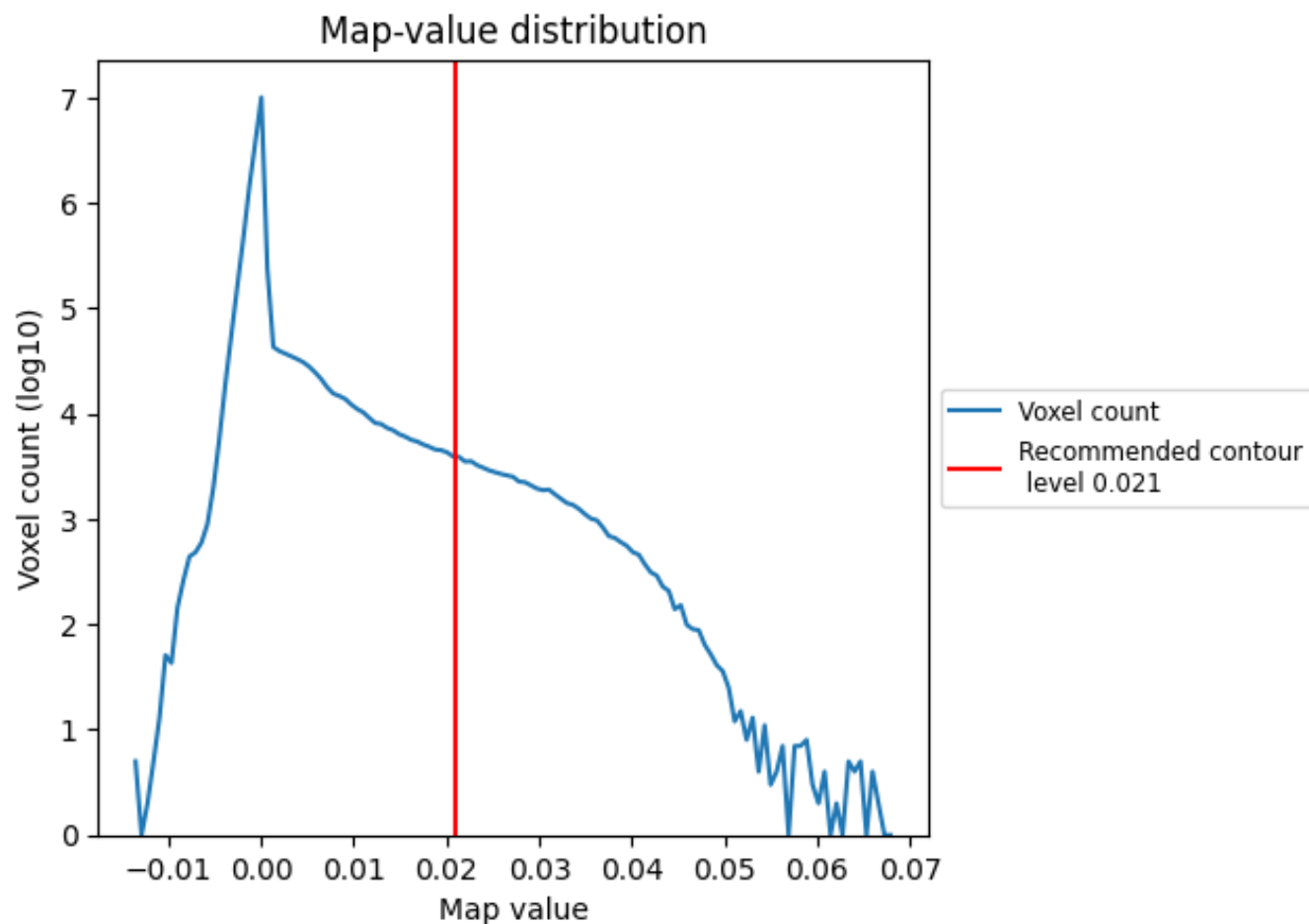
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

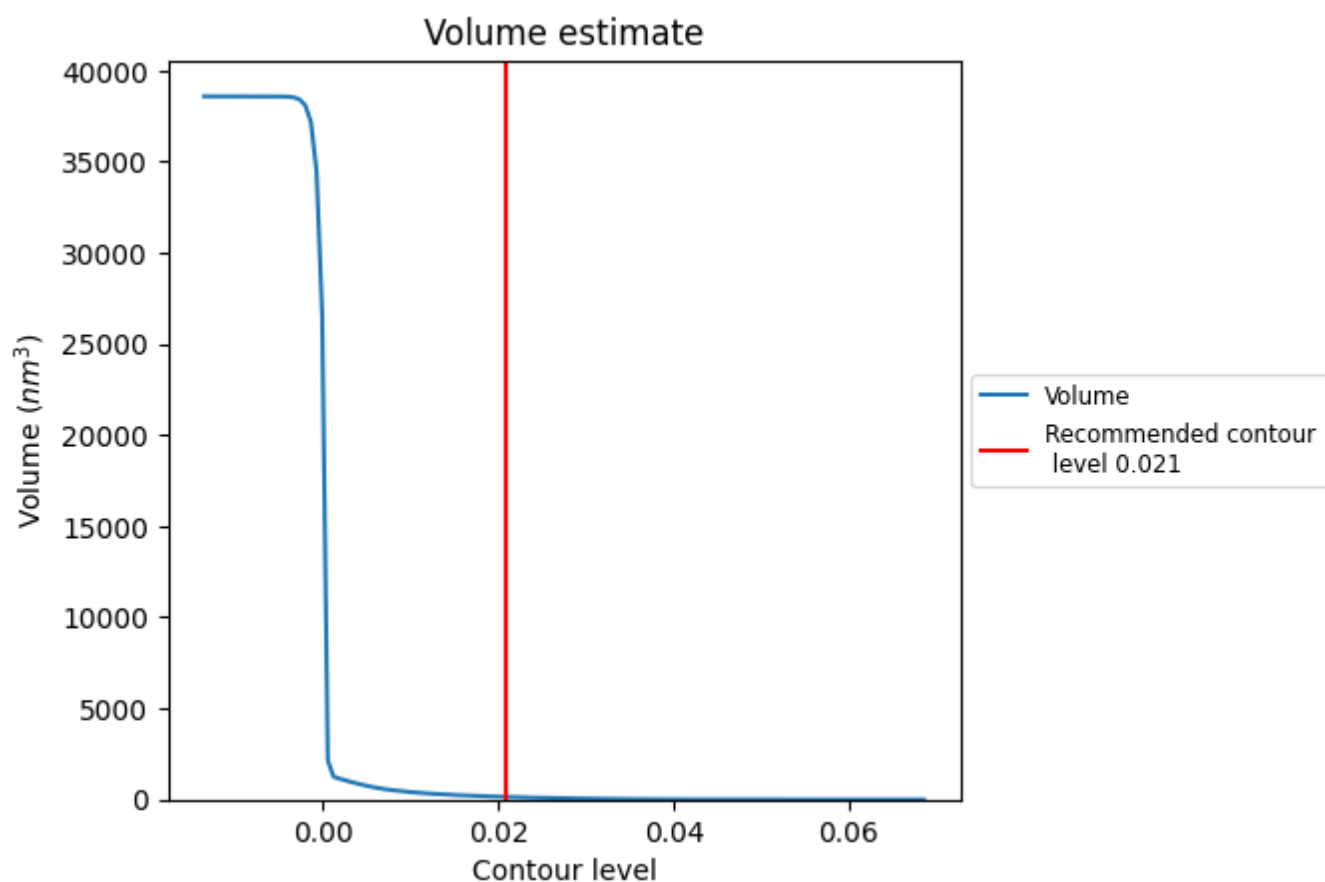
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

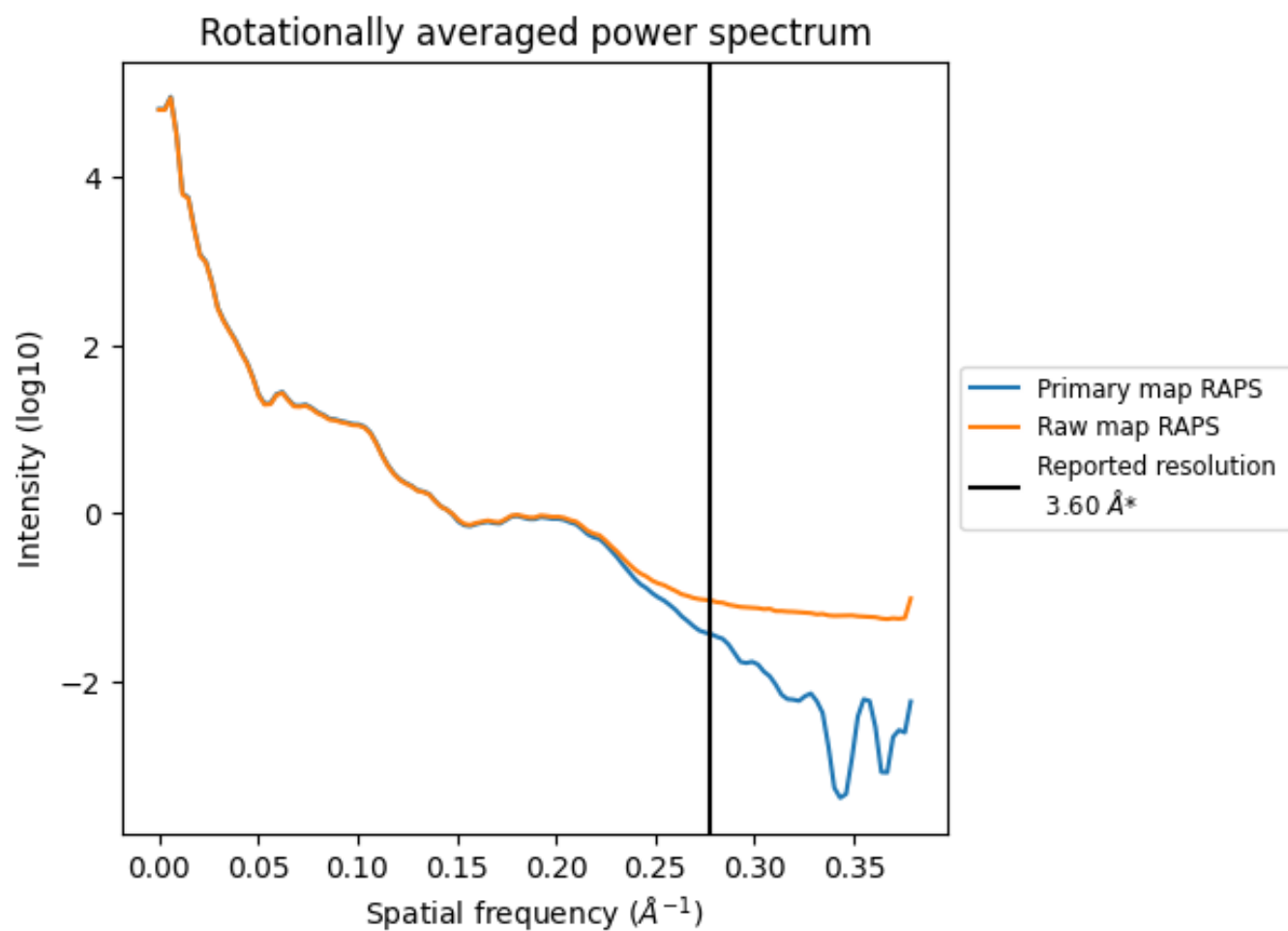
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 143 nm^3 ; this corresponds to an approximate mass of 129 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

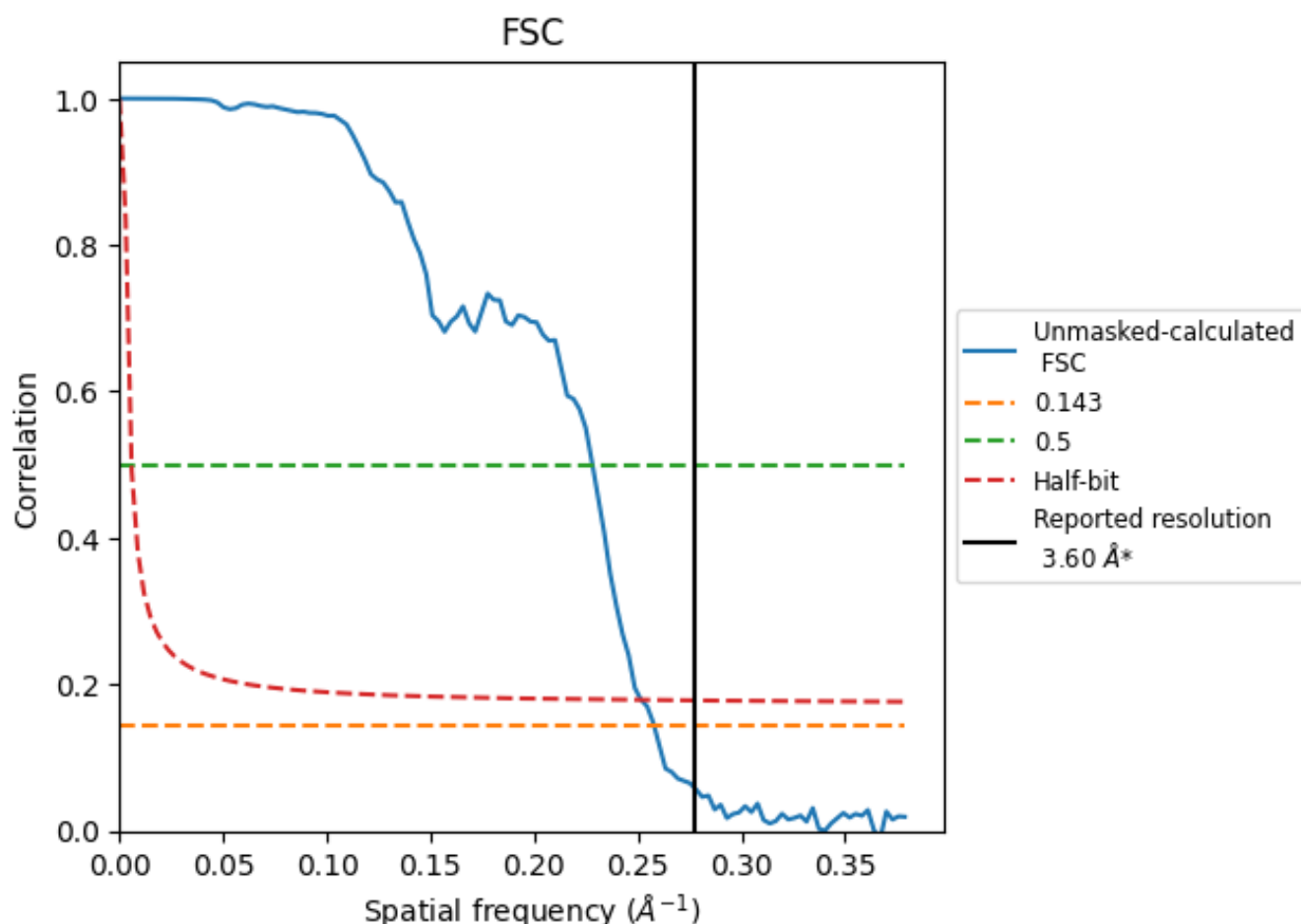


*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

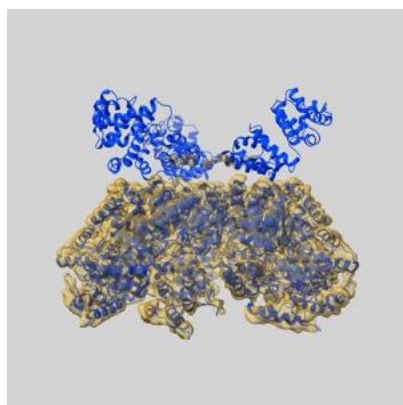
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	4.38	3.97

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

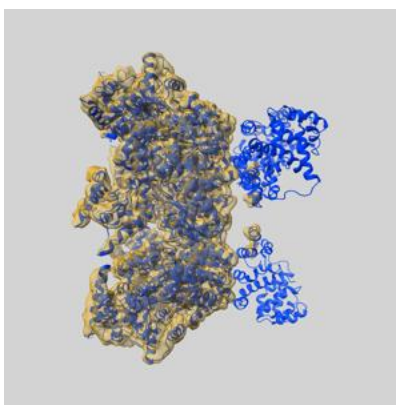
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36451 and PDB model 8JO0. Per-residue inclusion information can be found in section [3](#) on page [7](#).

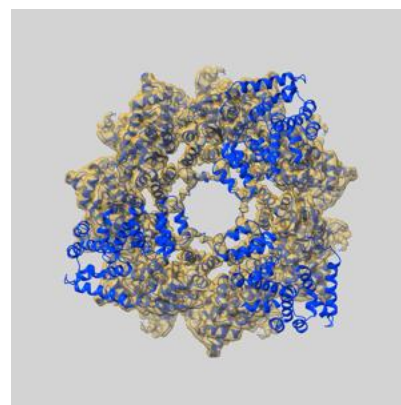
9.1 Map-model overlay [i](#)



X



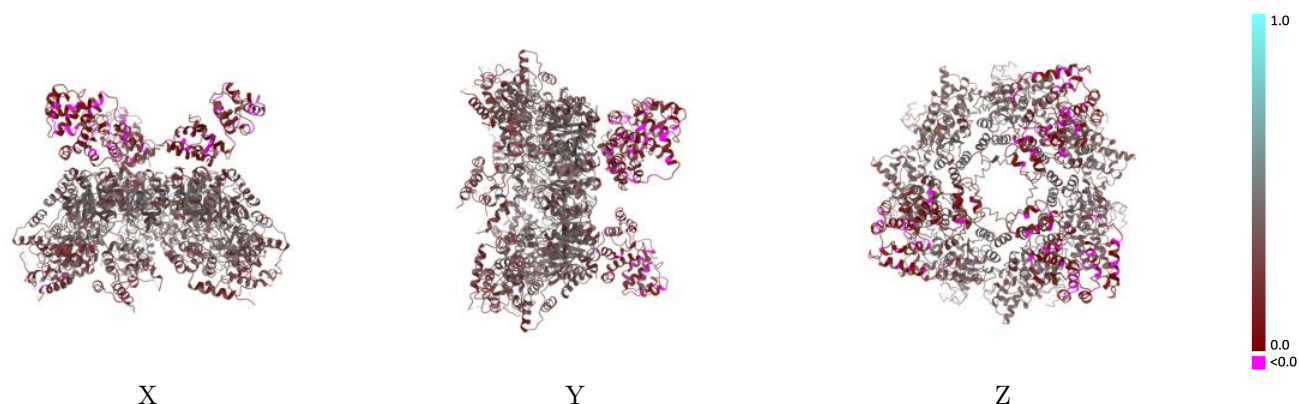
Y



Z

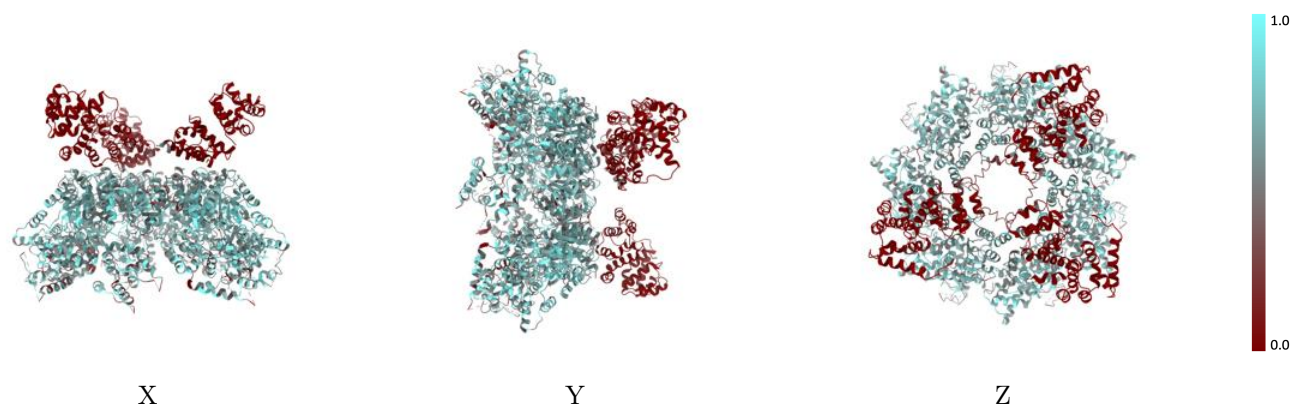
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



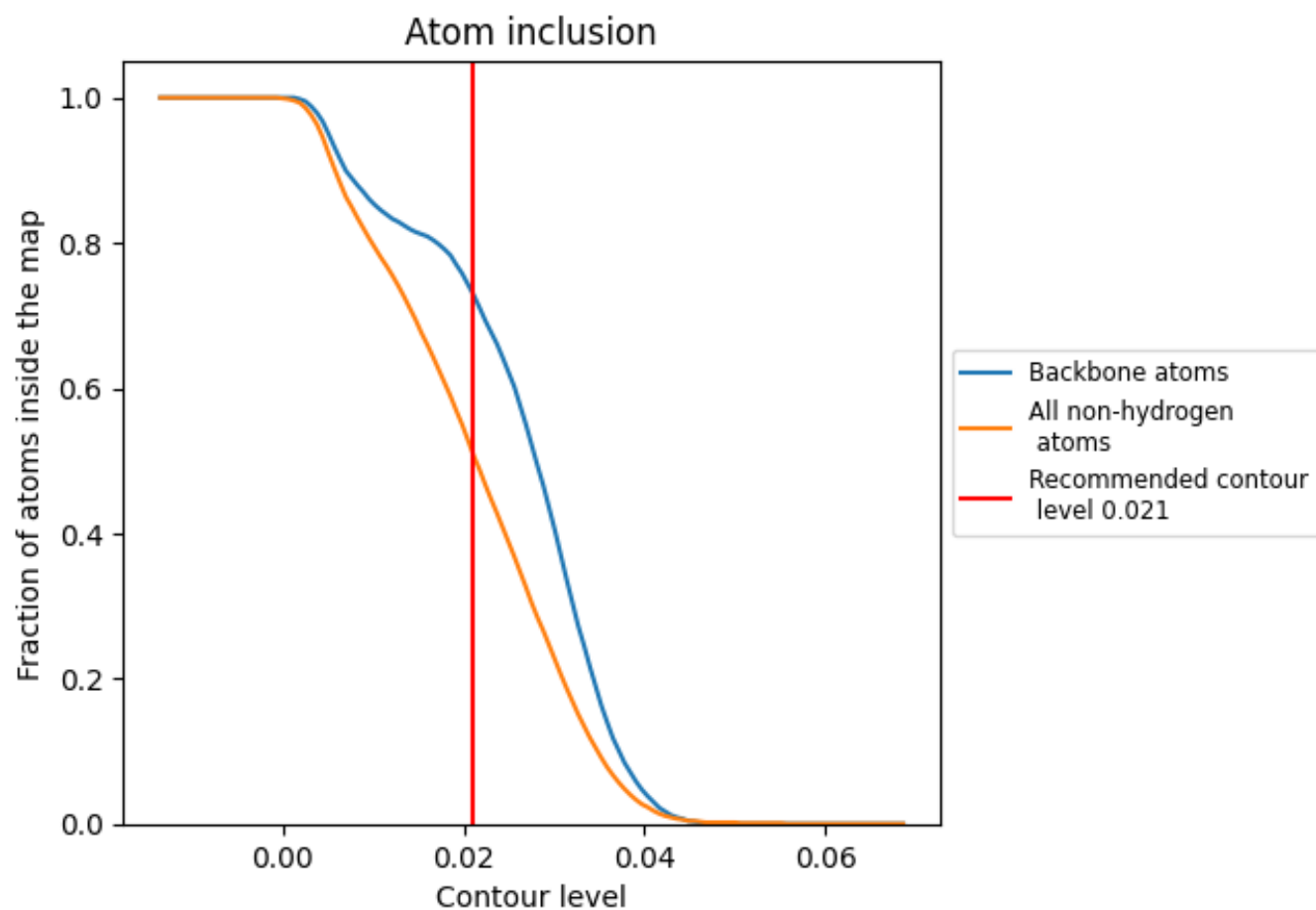
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.021).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5110	<div></div> 0.3030
A	<div></div> 0.6300	<div></div> 0.3560
B	<div></div> 0.6310	<div></div> 0.3530
C	<div></div> 0.6310	<div></div> 0.3540
D	<div></div> 0.6340	<div></div> 0.3580
E	<div></div> 0.6310	<div></div> 0.3520
F	<div></div> 0.6330	<div></div> 0.3410
G	<div></div> 0.6300	<div></div> 0.3450
H	<div></div> 0.0240	<div></div> 0.1310
I	<div></div> 0.0150	<div></div> 0.1020
J	<div></div> 0.0250	<div></div> 0.1190
K	<div></div> 0.0000	<div></div> 0.0900
L	<div></div> 0.0000	<div></div> 0.0720
M	<div></div> 0.0000	<div></div> 0.1070

