



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:55 am BST

PDB ID : 2X0B
Title : Crystal structure of human angiotensinogen complexed with renin
Authors : Zhou, A.; Wei, Z.; Yan, Y.; Carrell, R.W.; Read, R.J.
Deposited on : 2009-12-08
Resolution : 4.33 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

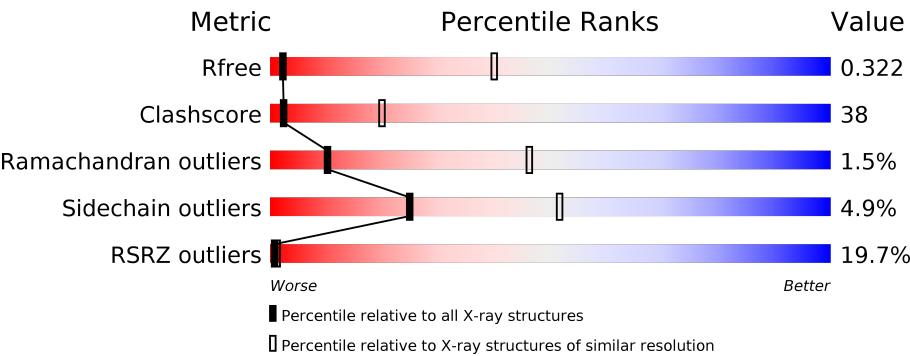
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.33 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1018 (4.84-3.80)
Clashscore	141614	1081 (4.84-3.80)
Ramachandran outliers	138981	1033 (4.84-3.80)
Sidechain outliers	138945	1016 (4.84-3.80)
RSRZ outliers	127900	1078 (4.92-3.70)

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

Mol	Chain	Length	Quality of chain
1	A	383	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>55%</div><div>29%</div><div>•</div><div>14%</div></div>
1	C	383	<div><div>14%</div><div><div></div><div></div><div></div><div></div></div><div>55%</div><div>30%</div><div>•</div><div>14%</div></div>
1	E	383	<div><div>13%</div><div><div></div><div></div><div></div><div></div></div><div>56%</div><div>28%</div><div>•</div><div>14%</div></div>
1	G	383	<div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>54%</div><div>30%</div><div>•</div><div>14%</div></div>
2	B	452	<div><div>17%</div><div><div></div><div></div><div></div><div></div></div><div>52%</div><div>37%</div><div>•</div><div>6%</div></div>
2	D	452	<div><div>29%</div><div><div></div><div></div><div></div><div></div></div><div>53%</div><div>36%</div><div>•</div><div>6%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	452	<div><div></div><div>17%</div><div>52%</div><div>38%</div><div>• 6%</div></div>
2	H	452	<div><div></div><div>29%</div><div>53%</div><div>36%</div><div>• 6%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23244 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RENIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			
1	C	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			
1	E	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			
1	G	330	Total	C	N	O	S	0	0	1
			2540	1625	411	490	14			

- Molecule 2 is a protein called ANGIOTENSINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			
2	D	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			
2	F	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			
2	H	423	Total	C	N	O	S	0	0	0
			3271	2106	546	605	14			

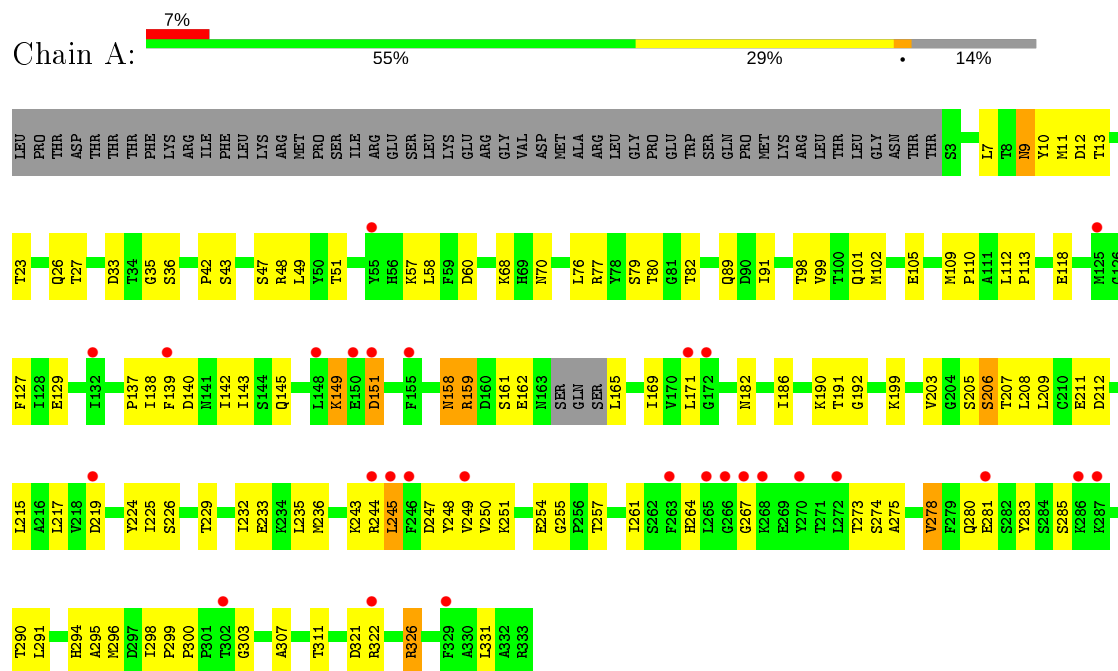
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	47	ASN	ASP	conflict	UNP P01019
D	47	ASN	ASP	conflict	UNP P01019
F	47	ASN	ASP	conflict	UNP P01019
H	47	ASN	ASP	conflict	UNP P01019

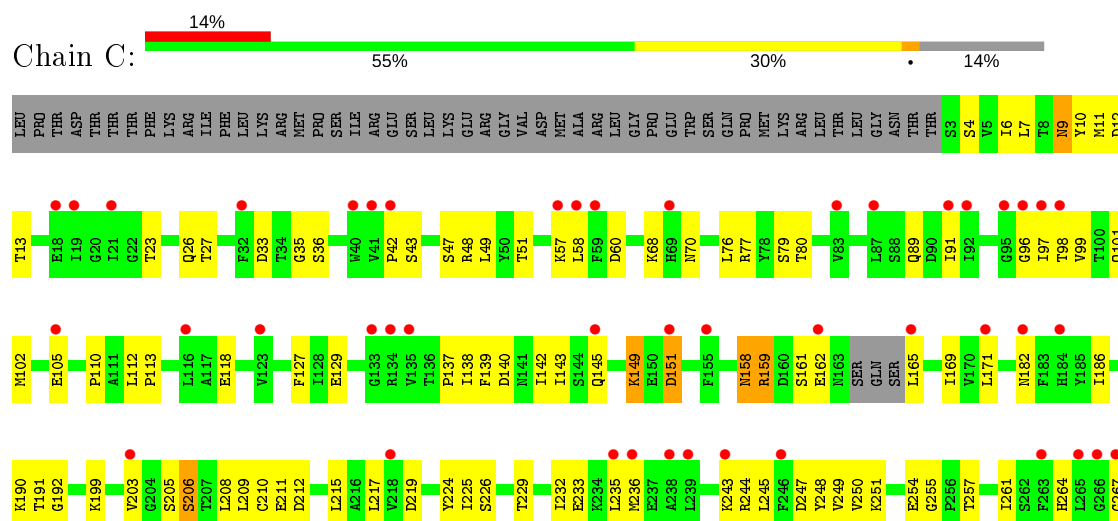
3 Residue-property plots [i](#)

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

• Molecule 1: RENIN

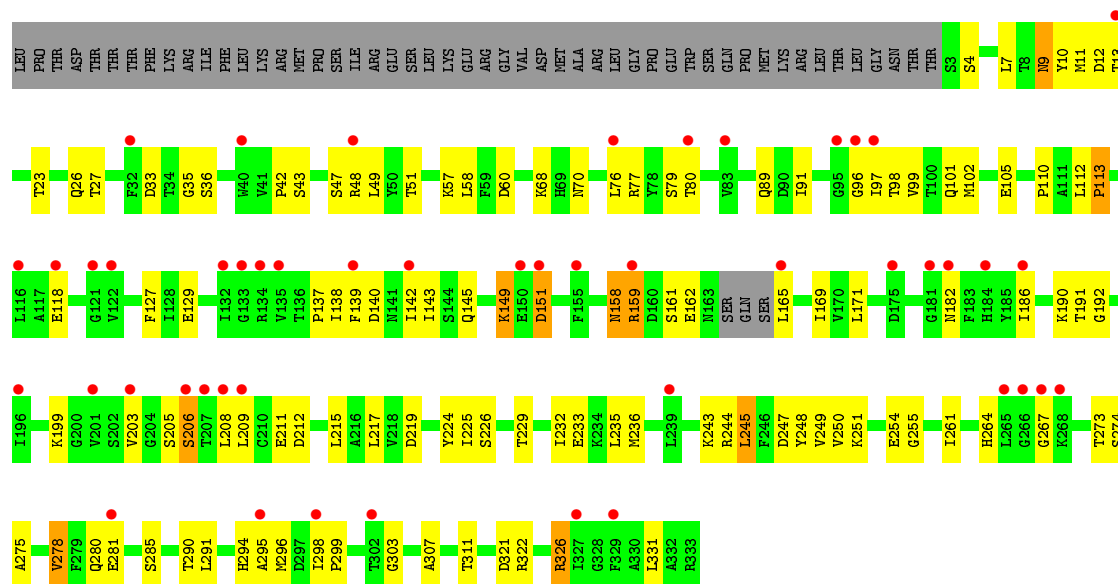


• Molecule 1: RENIN

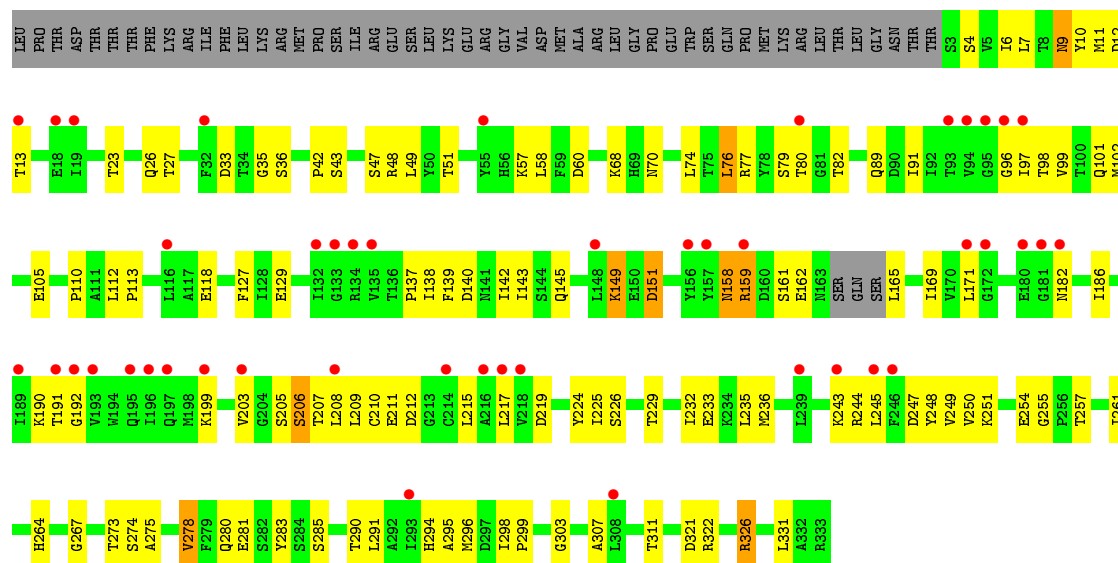




• Molecule 1: RENIN



• Molecule 1: RENIN



• Molecule 2: ANGIOTENSINOGEN







4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	212.47Å 212.47Å 474.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.52 – 4.33 48.52 – 4.34	Depositor EDS
% Data completeness (in resolution range)	96.3 (48.52-4.33) 84.2 (48.52-4.34)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 4.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_249)	Depositor
R, R_{free}	0.309 , 0.334 0.293 , 0.322	Depositor DCC
R_{free} test set	2253 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	200.1	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 381.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23244	wwPDB-VP
Average B, all atoms (Å ²)	325.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/2599	0.67	0/3523
1	C	0.35	0/2599	0.67	0/3523
1	E	0.35	0/2599	0.67	0/3523
1	G	0.35	0/2599	0.67	0/3523
2	B	0.31	0/3345	0.51	5/4557 (0.1%)
2	D	0.31	0/3345	0.51	5/4557 (0.1%)
2	F	0.31	0/3345	0.51	5/4557 (0.1%)
2	H	0.31	0/3345	0.51	5/4557 (0.1%)
All	All	0.33	0/23776	0.59	20/32320 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	8	PHE	CZ-CE2-CD2	6.16	127.50	120.10
2	F	8	PHE	CZ-CE2-CD2	6.13	127.45	120.10
2	B	8	PHE	CZ-CE2-CD2	6.12	127.44	120.10
2	D	8	PHE	CZ-CE2-CD2	6.08	127.39	120.10
2	H	8	PHE	CG-CD1-CE1	5.27	126.60	120.80
2	B	8	PHE	CG-CD1-CE1	5.26	126.58	120.80
2	F	135	ASP	CB-CG-OD2	5.26	123.03	118.30
2	H	6	HIS	CA-CB-CG	-5.22	104.72	113.60
2	F	8	PHE	CG-CD1-CE1	5.20	126.53	120.80
2	D	8	PHE	CG-CD1-CE1	5.20	126.52	120.80
2	H	135	ASP	CB-CG-OD2	5.20	122.98	118.30
2	B	6	HIS	CA-CB-CG	-5.19	104.77	113.60
2	F	6	HIS	CA-CB-CG	-5.19	104.78	113.60
2	F	143	ASP	CB-CG-OD2	5.18	122.96	118.30
2	B	135	ASP	CB-CG-OD2	5.17	122.95	118.30
2	D	6	HIS	CA-CB-CG	-5.17	104.81	113.60
2	D	135	ASP	CB-CG-OD2	5.16	122.95	118.30
2	D	143	ASP	CB-CG-OD2	5.16	122.94	118.30
2	H	143	ASP	CB-CG-OD2	5.14	122.93	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	143	ASP	CB-CG-OD2	5.11	122.90	118.30

There are no chirality outliers.

There are no planarity outliers.

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	A	2540	0	2471	198	3
1	C	2540	0	2471	232	2
1	E	2540	0	2470	199	0
1	G	2540	0	2472	227	0
2	B	3271	0	3268	331	28
2	D	3271	0	3268	348	0
2	F	3271	0	3268	360	27
2	H	3271	0	3267	365	0
All	All	23244	0	22955	1748	30

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 38.

All (1748) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:THR:CB	2:D:83:ARG:HH11	1.23	1.49
2:D:142:LEU:CD1	2:D:146:LYS:HE3	1.47	1.45
2:H:142:LEU:CD1	2:H:146:LYS:HE3	1.47	1.43
2:B:142:LEU:CD1	2:B:146:LYS:HE3	1.47	1.42
2:F:142:LEU:CD1	2:F:146:LYS:HE3	1.47	1.42
1:C:98:THR:N	2:F:449:LEU:HD21	1.35	1.35
2:D:131:VAL:HG13	2:D:132:PRO:CA	1.57	1.34
2:F:142:LEU:HD12	2:F:146:LYS:CE	1.56	1.34
2:F:131:VAL:HG13	2:F:132:PRO:CA	1.57	1.33
2:D:142:LEU:HD12	2:D:146:LYS:CE	1.57	1.33
2:B:142:LEU:HD12	2:B:146:LYS:CE	1.56	1.33

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:VAL:HG13	2:B:132:PRO:CA	1.57	1.32
2:H:131:VAL:HG13	2:H:132:PRO:CA	1.58	1.32
2:D:272:SER:O	1:G:6:ILE:HG13	1.24	1.32
1:G:51:THR:OG1	2:H:83:ARG:CD	1.77	1.32
2:H:142:LEU:HD12	2:H:146:LYS:CE	1.56	1.32
1:G:51:THR:OG1	2:H:83:ARG:HD3	1.21	1.31
1:E:98:THR:N	2:H:449:LEU:HD21	1.44	1.29
1:E:4:SER:OG	2:H:274:SER:OG	1.52	1.27
2:D:3:VAL:HB	2:D:4:TYR:CD2	1.69	1.26
1:E:51:THR:CB	2:F:83:ARG:HH11	1.47	1.26
2:B:3:VAL:HB	2:B:4:TYR:CD2	1.69	1.26
2:F:3:VAL:HB	2:F:4:TYR:CD2	1.69	1.26
2:H:3:VAL:HB	2:H:4:TYR:CD2	1.69	1.25
2:D:449:LEU:HD21	1:G:98:THR:N	1.51	1.24
1:G:51:THR:CB	2:H:83:ARG:HH11	1.49	1.24
1:C:96:GLY:O	2:F:449:LEU:HD22	1.10	1.24
1:E:51:THR:CG2	2:F:83:ARG:CG	2.14	1.22
1:E:35:GLY:O	2:F:12:ILE:HG22	1.39	1.21
1:C:51:THR:CB	2:D:83:ARG:NH1	1.98	1.21
1:C:97:ILE:C	2:F:449:LEU:HD21	1.60	1.21
1:C:35:GLY:O	2:D:12:ILE:HG22	1.39	1.20
1:A:35:GLY:O	2:B:12:ILE:HG22	1.39	1.20
1:E:23:THR:CG2	2:H:95:VAL:HG21	1.72	1.20
1:C:51:THR:CG2	2:D:83:ARG:HG3	1.71	1.19
1:C:51:THR:HG23	2:D:83:ARG:CG	1.69	1.19
1:E:51:THR:CG2	2:F:83:ARG:HG3	1.72	1.18
1:G:51:THR:CB	2:H:83:ARG:HD3	1.73	1.18
1:A:51:THR:CG2	2:B:83:ARG:CG	2.20	1.17
1:G:35:GLY:O	2:H:12:ILE:HG22	1.39	1.16
1:C:51:THR:CG2	2:D:83:ARG:CG	2.21	1.16
2:F:131:VAL:HG13	2:F:132:PRO:CB	1.75	1.15
2:B:131:VAL:HG13	2:B:132:PRO:CB	1.75	1.15
2:D:131:VAL:HG13	2:D:132:PRO:CB	1.75	1.15
1:A:51:THR:HG21	2:B:83:ARG:HG3	1.16	1.15
1:C:110:PRO:HB3	2:D:132:PRO:HD2	1.26	1.15
1:C:23:THR:HG23	2:F:95:VAL:HG21	1.20	1.15
2:F:126:GLN:CA	2:F:131:VAL:HG21	1.78	1.14
2:B:126:GLN:CA	2:B:131:VAL:HG21	1.78	1.14
2:H:131:VAL:HG13	2:H:132:PRO:CB	1.75	1.14
2:D:131:VAL:HG13	2:D:132:PRO:HA	1.22	1.13
1:C:97:ILE:HA	2:F:449:LEU:CD1	1.79	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:126:GLN:CA	2:D:131:VAL:HG21	1.78	1.12
2:H:126:GLN:CA	2:H:131:VAL:HG21	1.78	1.12
1:E:112:LEU:HD22	2:F:76:LEU:HD21	1.28	1.12
2:B:131:VAL:HG13	2:B:132:PRO:HA	1.22	1.12
1:E:49:LEU:HD13	2:F:367:GLU:HG3	1.11	1.11
1:E:51:THR:HG23	2:F:83:ARG:HG2	1.30	1.10
1:C:51:THR:HG21	2:D:83:ARG:HG3	1.22	1.10
2:F:131:VAL:HG13	2:F:132:PRO:HA	1.22	1.10
1:E:51:THR:HG23	2:F:83:ARG:CG	1.75	1.10
2:B:126:GLN:O	2:B:131:VAL:HG23	1.51	1.10
1:A:110:PRO:HB3	2:B:132:PRO:HD2	1.15	1.10
2:D:126:GLN:HA	2:D:131:VAL:HG21	1.32	1.10
1:C:23:THR:HG23	2:F:95:VAL:CG2	1.81	1.10
1:G:110:PRO:CB	2:H:135:ASP:OD1	2.00	1.10
2:F:126:GLN:O	2:F:131:VAL:HG23	1.51	1.09
2:H:131:VAL:CG1	2:H:132:PRO:CA	2.30	1.09
2:B:126:GLN:HA	2:B:131:VAL:HG21	1.32	1.09
2:F:131:VAL:CG1	2:F:132:PRO:CA	2.30	1.09
2:B:131:VAL:CG1	2:B:132:PRO:CA	2.30	1.09
1:C:49:LEU:HD13	2:D:367:GLU:HG3	1.28	1.08
1:G:51:THR:OG1	2:H:83:ARG:CZ	2.01	1.08
1:A:112:LEU:HD22	2:B:76:LEU:CD2	1.82	1.08
2:D:131:VAL:CG1	2:D:132:PRO:CA	2.30	1.08
2:H:131:VAL:HG13	2:H:132:PRO:HA	1.22	1.08
2:D:95:VAL:HG21	1:G:23:THR:HG23	1.36	1.07
2:D:126:GLN:O	2:D:131:VAL:HG23	1.51	1.07
1:E:51:THR:HG21	2:F:83:ARG:HG3	1.10	1.07
1:G:51:THR:OG1	2:H:83:ARG:NE	1.86	1.07
2:H:126:GLN:O	2:H:131:VAL:HG23	1.51	1.07
1:C:51:THR:HB	2:D:83:ARG:HH11	1.13	1.07
2:H:131:VAL:CG1	2:H:132:PRO:HB3	1.85	1.07
2:F:131:VAL:CG1	2:F:132:PRO:HB3	1.85	1.07
1:E:23:THR:HG23	2:H:95:VAL:HG21	1.08	1.07
2:B:131:VAL:CG1	2:B:132:PRO:HB3	1.85	1.06
1:G:51:THR:CB	2:H:83:ARG:NH1	2.17	1.06
1:E:13:THR:HG21	2:F:5:ILE:CG2	1.85	1.06
1:C:13:THR:HG21	2:D:5:ILE:CG2	1.85	1.06
2:F:126:GLN:HA	2:F:131:VAL:HG21	1.32	1.06
2:H:126:GLN:HA	2:H:131:VAL:HG21	1.32	1.06
1:A:13:THR:HG21	2:B:5:ILE:CG2	1.85	1.06
1:G:13:THR:HG21	2:H:5:ILE:CG2	1.85	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:HG21	2:B:83:ARG:CG	1.81	1.06
1:C:96:GLY:O	2:F:449:LEU:CD2	2.02	1.06
1:E:51:THR:HB	2:F:83:ARG:HH11	1.18	1.06
1:G:110:PRO:HB3	2:H:132:PRO:CD	1.86	1.05
2:D:272:SER:O	1:G:6:ILE:CG1	2.04	1.05
2:H:132:PRO:HG2	2:H:135:ASP:CA	1.87	1.05
1:E:23:THR:CG2	2:H:95:VAL:CG2	2.35	1.05
2:D:131:VAL:CG1	2:D:132:PRO:HB3	1.85	1.05
2:F:126:GLN:O	2:F:131:VAL:CG2	2.05	1.05
1:G:112:LEU:HD22	2:H:76:LEU:HD21	1.36	1.05
1:C:110:PRO:CB	2:D:135:ASP:OD1	2.05	1.05
2:B:132:PRO:HG2	2:B:135:ASP:CA	1.87	1.04
2:B:122:ALA:O	2:B:126:GLN:HG3	1.57	1.04
2:B:126:GLN:O	2:B:131:VAL:CG2	2.05	1.04
1:A:112:LEU:HD22	2:B:76:LEU:HD21	1.10	1.04
1:C:49:LEU:O	2:D:127:ALA:O	1.76	1.04
2:D:126:GLN:O	2:D:131:VAL:CG2	2.05	1.04
2:D:449:LEU:HD21	1:G:98:THR:H	1.03	1.04
2:F:132:PRO:HG2	2:F:135:ASP:CA	1.86	1.04
1:G:51:THR:HG21	2:H:83:ARG:HG3	1.39	1.04
2:F:122:ALA:O	2:F:126:GLN:HG3	1.57	1.03
2:H:126:GLN:O	2:H:131:VAL:CG2	2.05	1.03
2:D:132:PRO:HG2	2:D:135:ASP:CA	1.87	1.03
2:H:122:ALA:O	2:H:126:GLN:HG3	1.57	1.02
1:A:49:LEU:HD13	2:B:367:GLU:HG3	1.38	1.02
2:D:122:ALA:O	2:D:126:GLN:HG3	1.57	1.02
1:A:112:LEU:CD2	2:B:76:LEU:HD21	1.90	1.02
2:B:142:LEU:HD11	2:B:146:LYS:HE3	1.42	1.01
2:D:142:LEU:HD11	2:D:146:LYS:HE3	1.42	1.01
1:A:51:THR:CB	2:B:83:ARG:HH11	1.71	1.01
1:A:51:THR:HG23	2:B:83:ARG:HG2	1.42	1.01
2:B:131:VAL:CG1	2:B:132:PRO:CB	2.39	1.01
1:G:110:PRO:CB	2:H:132:PRO:HD2	1.90	1.00
2:B:131:VAL:HG13	2:B:132:PRO:HB3	1.43	1.00
1:C:6:ILE:HG13	2:F:272:SER:O	1.61	1.00
2:D:131:VAL:CG1	2:D:132:PRO:CB	2.39	0.99
1:C:51:THR:OG1	2:D:83:ARG:NH1	1.78	0.99
1:G:110:PRO:HB2	2:H:135:ASP:OD1	1.63	0.99
2:F:142:LEU:HD11	2:F:146:LYS:HE3	1.42	0.99
2:H:126:GLN:HA	2:H:131:VAL:CG2	1.93	0.99
1:E:112:LEU:HD22	2:F:76:LEU:CD2	1.91	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:PRO:HB3	2:B:132:PRO:CD	1.93	0.98
1:C:112:LEU:HD22	2:D:76:LEU:HD21	1.45	0.98
2:B:126:GLN:HA	2:B:131:VAL:CG2	1.93	0.98
2:D:274:SER:OG	1:G:4:SER:OG	1.80	0.98
1:E:98:THR:H	2:H:449:LEU:CD2	1.76	0.98
2:F:131:VAL:CG1	2:F:132:PRO:CB	2.39	0.98
1:G:51:THR:CG2	2:H:83:ARG:CG	2.40	0.98
2:F:126:GLN:HA	2:F:131:VAL:CG2	1.93	0.98
2:H:131:VAL:HG13	2:H:132:PRO:HB3	1.43	0.98
1:G:110:PRO:CG	2:H:135:ASP:OD1	2.12	0.98
2:D:142:LEU:HD12	2:D:146:LYS:HE3	0.98	0.98
1:G:51:THR:HG23	2:H:83:ARG:CG	1.93	0.98
2:B:142:LEU:HD12	2:B:146:LYS:HE3	0.98	0.97
1:A:112:LEU:CD2	2:B:76:LEU:CD2	2.40	0.97
1:A:51:THR:HG23	2:B:83:ARG:CG	1.90	0.97
1:E:110:PRO:HB3	2:F:132:PRO:HD2	1.41	0.97
2:D:126:GLN:HA	2:D:131:VAL:CG2	1.93	0.97
1:G:51:THR:CG2	2:H:83:ARG:HD3	1.94	0.97
2:H:131:VAL:CG1	2:H:132:PRO:CB	2.39	0.97
1:C:110:PRO:CG	2:D:135:ASP:OD1	2.13	0.97
1:E:51:THR:CB	2:F:83:ARG:NH1	2.25	0.97
1:G:13:THR:HG21	2:H:5:ILE:HG21	1.47	0.97
1:E:13:THR:HG21	2:F:5:ILE:HG21	1.47	0.97
1:G:49:LEU:O	2:H:127:ALA:O	1.83	0.96
1:C:98:THR:N	2:F:449:LEU:CD2	2.27	0.96
2:B:16:SER:O	2:B:17:THR:HG23	1.65	0.96
2:F:142:LEU:HD12	2:F:146:LYS:HE3	0.98	0.96
2:F:16:SER:O	2:F:17:THR:HG23	1.65	0.96
2:H:16:SER:O	2:H:17:THR:HG23	1.65	0.96
2:H:142:LEU:HD12	2:H:146:LYS:HE3	0.98	0.96
2:H:142:LEU:HD11	2:H:146:LYS:HE3	1.42	0.95
1:E:98:THR:N	2:H:449:LEU:CD2	2.27	0.95
1:G:110:PRO:HB3	2:H:132:PRO:HD2	0.95	0.95
1:E:23:THR:HG23	2:H:95:VAL:CG2	1.96	0.95
2:D:449:LEU:HD22	1:G:96:GLY:O	1.65	0.95
1:C:23:THR:CG2	2:F:95:VAL:CG2	2.44	0.95
1:G:77:ARG:HH21	2:H:16:SER:N	1.65	0.95
1:C:112:LEU:CD2	2:D:72:MET:HG3	1.97	0.95
1:E:98:THR:H	2:H:449:LEU:HD21	0.80	0.95
1:A:77:ARG:HH21	2:B:16:SER:N	1.65	0.94
2:D:16:SER:O	2:D:17:THR:HG23	1.65	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ILE:HA	2:F:449:LEU:HD11	1.45	0.94
1:C:13:THR:HG21	2:D:5:ILE:HG21	1.47	0.94
1:C:51:THR:HG23	2:D:83:ARG:HG2	1.44	0.94
1:C:23:THR:HG21	2:F:95:VAL:HB	1.47	0.94
1:G:51:THR:CG2	2:H:83:ARG:HH11	1.78	0.94
1:G:112:LEU:CD2	2:H:76:LEU:HD21	1.97	0.94
1:E:77:ARG:HH21	2:F:16:SER:N	1.65	0.94
1:C:96:GLY:C	2:F:449:LEU:HD22	1.88	0.94
1:C:77:ARG:HH21	2:D:16:SER:N	1.65	0.94
1:G:51:THR:OG1	2:H:83:ARG:NH1	2.00	0.94
2:D:126:GLN:CA	2:D:131:VAL:CG2	2.47	0.93
1:A:13:THR:HG21	2:B:5:ILE:HG21	1.47	0.93
1:C:51:THR:HB	2:D:83:ARG:NH1	1.71	0.93
1:E:49:LEU:HD13	2:F:367:GLU:CG	1.96	0.93
2:F:132:PRO:HG2	2:F:135:ASP:HA	1.50	0.93
1:G:112:LEU:CD2	2:H:72:MET:HG3	1.98	0.93
1:C:112:LEU:HD23	2:D:72:MET:HG3	1.51	0.92
2:F:126:GLN:CA	2:F:131:VAL:CG2	2.47	0.92
2:B:132:PRO:HG2	2:B:135:ASP:HA	1.50	0.92
2:D:131:VAL:HG13	2:D:132:PRO:HB3	1.43	0.92
1:E:26:GLN:HE22	1:E:60:ASP:H	1.17	0.92
1:G:51:THR:CG2	2:H:83:ARG:HG3	1.99	0.92
1:A:26:GLN:HE22	1:A:60:ASP:H	1.17	0.92
1:G:49:LEU:HD13	2:H:367:GLU:HG3	1.51	0.92
2:H:133:TRP:CZ3	2:H:142:LEU:HD23	2.05	0.92
2:H:132:PRO:HG2	2:H:135:ASP:HA	1.50	0.92
1:G:79:SER:OG	2:H:9:HIS:ND1	2.02	0.92
2:B:131:VAL:CG1	2:B:132:PRO:HA	1.97	0.92
1:A:79:SER:OG	2:B:9:HIS:ND1	2.02	0.92
2:D:133:TRP:CZ3	2:D:142:LEU:HD23	2.05	0.92
1:C:51:THR:CG2	2:D:83:ARG:HH11	1.83	0.92
1:C:97:ILE:CA	2:F:449:LEU:HD21	2.00	0.92
1:C:112:LEU:CD1	2:D:76:LEU:HD22	2.00	0.91
2:F:115:LEU:HD23	2:F:144:ALA:HB1	1.51	0.91
2:D:115:LEU:HD23	2:D:144:ALA:HB1	1.51	0.91
2:H:126:GLN:CA	2:H:131:VAL:CG2	2.47	0.91
2:B:126:GLN:CA	2:B:131:VAL:CG2	2.47	0.91
2:B:133:TRP:CZ3	2:B:142:LEU:HD23	2.05	0.90
1:E:79:SER:OG	2:F:9:HIS:ND1	2.02	0.90
1:C:79:SER:OG	2:D:9:HIS:ND1	2.02	0.90
2:F:142:LEU:CD1	2:F:146:LYS:CE	2.32	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:115:LEU:HD23	2:H:144:ALA:HB1	1.51	0.90
2:B:115:LEU:HD23	2:B:144:ALA:HB1	1.51	0.90
1:G:112:LEU:CD1	2:H:76:LEU:CD2	2.50	0.90
2:H:131:VAL:CG1	2:H:132:PRO:HA	1.97	0.90
2:H:142:LEU:CD1	2:H:146:LYS:CE	2.32	0.90
2:B:257:GLY:HA2	1:G:257:THR:HG21	1.52	0.90
1:A:257:THR:HG21	2:H:257:GLY:HA2	1.53	0.90
1:C:112:LEU:HD13	2:D:76:LEU:CD2	2.01	0.90
2:D:131:VAL:CG1	2:D:132:PRO:HA	1.97	0.90
2:F:133:TRP:CZ3	2:F:142:LEU:HD23	2.05	0.90
2:D:132:PRO:HG2	2:D:135:ASP:HA	1.50	0.90
2:D:272:SER:C	1:G:6:ILE:HG13	1.92	0.90
1:A:77:ARG:HD3	2:B:136:LYS:HZ1	1.36	0.89
1:G:112:LEU:HD23	2:H:72:MET:HG3	1.52	0.89
1:A:51:THR:HB	2:B:83:ARG:HH11	1.36	0.89
1:G:26:GLN:HE22	1:G:60:ASP:H	1.17	0.89
1:C:26:GLN:HE22	1:C:60:ASP:H	1.17	0.89
2:F:131:VAL:CG1	2:F:132:PRO:HA	1.96	0.89
1:E:79:SER:HB2	2:F:9:HIS:HB3	1.54	0.88
1:G:79:SER:HB2	2:H:9:HIS:HB3	1.54	0.88
1:A:79:SER:HB2	2:B:9:HIS:HB3	1.54	0.88
1:E:49:LEU:CD1	2:F:367:GLU:HG3	2.01	0.88
1:C:110:PRO:HG3	2:D:135:ASP:CG	1.93	0.88
1:G:51:THR:CG2	2:H:83:ARG:CD	2.51	0.88
1:G:112:LEU:HD13	2:H:76:LEU:CD2	2.04	0.87
1:C:294:HIS:CE1	2:D:7:PRO:HG3	2.09	0.87
1:E:219:ASP:OD1	2:F:11:VAL:HG22	1.74	0.87
1:G:294:HIS:CE1	2:H:7:PRO:HG3	2.10	0.87
1:E:23:THR:HG21	2:H:95:VAL:CG2	2.03	0.87
1:A:77:ARG:NH2	2:B:15:GLU:HB3	1.90	0.87
1:C:77:ARG:NH2	2:D:15:GLU:HB3	1.90	0.87
1:A:219:ASP:OD1	2:B:11:VAL:HG22	1.75	0.86
1:C:98:THR:H	2:F:449:LEU:HD21	1.35	0.86
1:E:294:HIS:CE1	2:F:7:PRO:HG3	2.10	0.86
1:C:97:ILE:HA	2:F:449:LEU:CD2	2.05	0.86
1:C:219:ASP:OD1	2:D:11:VAL:HG22	1.75	0.86
1:E:224:TYR:CE2	1:E:294:HIS:NE2	2.44	0.86
2:F:126:GLN:O	2:F:131:VAL:CB	2.23	0.86
1:G:112:LEU:HD11	2:H:76:LEU:HD22	1.54	0.86
1:G:112:LEU:CD1	2:H:76:LEU:HD22	2.04	0.86
1:G:224:TYR:CE2	1:G:294:HIS:NE2	2.44	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:ASP:OD1	2:H:11:VAL:HG22	1.75	0.86
2:B:126:GLN:O	2:B:131:VAL:CB	2.23	0.86
1:A:294:HIS:CE1	2:B:7:PRO:HG3	2.10	0.86
1:A:224:TYR:CE2	1:A:294:HIS:NE2	2.44	0.86
2:H:126:GLN:O	2:H:131:VAL:CB	2.23	0.86
1:G:77:ARG:NH2	2:H:15:GLU:HB3	1.90	0.86
1:C:79:SER:HB2	2:D:9:HIS:HB3	1.55	0.85
1:A:51:THR:CG2	2:B:83:ARG:HG3	1.92	0.85
1:G:51:THR:HG1	2:H:83:ARG:HD3	1.36	0.85
1:C:224:TYR:CE2	1:C:294:HIS:NE2	2.44	0.85
1:C:97:ILE:CA	2:F:449:LEU:CD2	2.53	0.85
1:E:158:ASN:ND2	1:E:159:ARG:H	1.75	0.85
2:D:126:GLN:O	2:D:131:VAL:CB	2.23	0.85
1:G:112:LEU:CD2	2:H:76:LEU:CD2	2.53	0.85
2:F:132:PRO:CG	2:F:135:ASP:HA	2.07	0.85
1:E:77:ARG:NH2	2:F:15:GLU:HB3	1.90	0.85
2:B:132:PRO:CG	2:B:135:ASP:HA	2.07	0.85
1:E:112:LEU:CD2	2:F:76:LEU:CD2	2.54	0.85
1:C:112:LEU:HD22	2:D:76:LEU:CD2	2.07	0.85
1:G:49:LEU:HB3	2:H:127:ALA:HB3	1.58	0.85
2:H:132:PRO:CG	2:H:135:ASP:HA	2.07	0.85
1:G:51:THR:HB	2:H:83:ARG:NH1	1.90	0.85
1:E:51:THR:HB	2:F:83:ARG:NH1	1.87	0.84
2:D:132:PRO:HG2	2:D:135:ASP:N	1.91	0.84
2:D:95:VAL:HG21	1:G:23:THR:CG2	2.06	0.84
1:A:158:ASN:ND2	1:A:159:ARG:H	1.75	0.84
1:C:110:PRO:HG3	2:D:135:ASP:OD1	1.74	0.84
2:D:285:THR:HG22	2:D:343:THR:HG22	1.60	0.84
2:D:3:VAL:HA	2:D:4:TYR:CB	2.07	0.84
2:D:3:VAL:HA	2:D:4:TYR:HB3	1.60	0.84
2:F:3:VAL:HA	2:F:4:TYR:HB3	1.60	0.84
1:G:110:PRO:HG3	2:H:135:ASP:CG	1.97	0.84
2:B:132:PRO:HG2	2:B:135:ASP:N	1.91	0.84
2:D:132:PRO:CG	2:D:135:ASP:HA	2.07	0.84
2:D:142:LEU:CD1	2:D:146:LYS:CE	2.32	0.84
2:H:132:PRO:HG2	2:H:135:ASP:N	1.91	0.84
2:B:285:THR:HG22	2:B:343:THR:HG22	1.60	0.83
1:C:158:ASN:ND2	1:C:159:ARG:H	1.75	0.83
1:G:158:ASN:ND2	1:G:159:ARG:H	1.75	0.83
2:F:132:PRO:HG2	2:F:135:ASP:N	1.91	0.83
1:E:51:THR:OG1	2:F:83:ARG:NH1	2.02	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:VAL:HA	2:F:4:TYR:CB	2.07	0.83
2:H:285:THR:HG22	2:H:343:THR:HG22	1.60	0.83
2:H:3:VAL:HA	2:H:4:TYR:CB	2.07	0.82
2:F:285:THR:HG22	2:F:343:THR:HG22	1.60	0.82
1:C:97:ILE:C	2:F:449:LEU:CD2	2.47	0.82
2:B:3:VAL:HA	2:B:4:TYR:CB	2.07	0.82
1:C:149:LYS:HA	1:C:149:LYS:HE3	1.61	0.82
2:F:131:VAL:HG13	2:F:132:PRO:HB3	1.43	0.81
1:E:149:LYS:HE3	1:E:149:LYS:HA	1.61	0.81
1:A:77:ARG:HD3	2:B:136:LYS:NZ	1.94	0.81
1:E:112:LEU:CD2	2:F:76:LEU:HD21	2.10	0.81
2:H:3:VAL:HA	2:H:4:TYR:HB3	1.60	0.81
2:B:3:VAL:HA	2:B:4:TYR:HB3	1.60	0.81
1:G:51:THR:HB	2:H:83:ARG:HH11	1.40	0.81
1:A:80:THR:HG23	2:B:9:HIS:HB3	1.63	0.81
1:E:158:ASN:HD22	1:E:159:ARG:H	1.27	0.81
1:G:149:LYS:HE3	1:G:149:LYS:HA	1.61	0.81
2:H:115:LEU:CD2	2:H:144:ALA:HB1	2.11	0.81
2:D:115:LEU:CD2	2:D:144:ALA:HB1	2.11	0.81
1:C:80:THR:HG23	2:D:9:HIS:HB3	1.63	0.81
1:A:51:THR:CB	2:B:83:ARG:NH1	2.43	0.81
2:B:115:LEU:CD2	2:B:144:ALA:HB1	2.11	0.80
2:F:126:GLN:C	2:F:131:VAL:CG2	2.49	0.80
1:G:224:TYR:CD2	1:G:294:HIS:CD2	2.69	0.80
1:C:224:TYR:CD2	1:C:294:HIS:CD2	2.69	0.80
2:F:115:LEU:CD2	2:F:144:ALA:HB1	2.11	0.80
1:G:79:SER:CB	2:H:9:HIS:ND1	2.45	0.80
1:A:149:LYS:HE3	1:A:149:LYS:HA	1.61	0.80
2:B:126:GLN:C	2:B:131:VAL:CG2	2.49	0.80
1:A:79:SER:CB	2:B:9:HIS:ND1	2.45	0.80
1:E:224:TYR:CD2	1:E:294:HIS:CD2	2.69	0.80
2:B:126:GLN:CB	2:B:131:VAL:HG21	2.12	0.80
1:E:79:SER:CB	2:F:9:HIS:ND1	2.45	0.80
2:H:126:GLN:C	2:H:131:VAL:CG2	2.49	0.80
2:D:126:GLN:C	2:D:131:VAL:CG2	2.49	0.80
1:C:79:SER:CB	2:D:9:HIS:ND1	2.45	0.80
1:E:80:THR:HG23	2:F:9:HIS:HB3	1.63	0.80
1:G:49:LEU:HB3	2:H:127:ALA:CB	2.12	0.80
2:H:126:GLN:CB	2:H:131:VAL:HG21	2.12	0.80
2:F:126:GLN:CB	2:F:131:VAL:HG21	2.12	0.80
1:G:112:LEU:HD22	2:H:76:LEU:CD2	2.09	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:449:LEU:CD2	1:G:98:THR:N	2.42	0.79
1:A:9:ASN:HD21	1:A:12:ASP:H	1.30	0.79
2:B:142:LEU:CD1	2:B:146:LYS:CE	2.32	0.79
1:G:80:THR:HG23	2:H:9:HIS:HB3	1.63	0.79
1:C:158:ASN:HD22	1:C:159:ARG:H	1.28	0.79
1:C:112:LEU:CD1	2:D:76:LEU:CD2	2.59	0.79
1:C:23:THR:CG2	2:F:95:VAL:HB	2.12	0.79
1:A:224:TYR:CD2	1:A:294:HIS:CD2	2.69	0.79
2:D:126:GLN:O	2:D:131:VAL:HB	1.83	0.79
1:A:77:ARG:HD2	2:B:15:GLU:HA	1.66	0.78
1:C:9:ASN:HD21	1:C:12:ASP:H	1.30	0.78
2:D:126:GLN:CB	2:D:131:VAL:HG21	2.12	0.78
1:E:9:ASN:HD21	1:E:12:ASP:H	1.30	0.78
1:E:274:SER:O	1:E:278:VAL:HG13	1.84	0.78
1:A:158:ASN:HD22	1:A:159:ARG:H	1.28	0.78
1:A:274:SER:O	1:A:278:VAL:HG13	1.84	0.78
2:F:126:GLN:O	2:F:131:VAL:HB	1.84	0.78
1:G:112:LEU:HD13	2:H:76:LEU:HD21	1.65	0.78
1:G:77:ARG:NH2	2:H:16:SER:N	2.32	0.78
1:G:158:ASN:HD22	1:G:159:ARG:H	1.27	0.78
2:B:126:GLN:O	2:B:131:VAL:HB	1.84	0.77
1:G:274:SER:O	1:G:278:VAL:HG13	1.84	0.77
1:C:77:ARG:NH2	2:D:16:SER:N	2.32	0.77
1:C:274:SER:O	1:C:278:VAL:HG13	1.84	0.77
2:D:5:ILE:HG22	2:D:6:HIS:N	2.00	0.77
1:E:13:THR:CG2	2:F:5:ILE:HG21	2.15	0.77
1:G:224:TYR:CD2	1:G:294:HIS:NE2	2.53	0.77
1:E:224:TYR:CD2	1:E:294:HIS:NE2	2.53	0.76
1:C:13:THR:CG2	2:D:5:ILE:HG21	2.15	0.76
1:E:96:GLY:O	2:H:447:ASN:ND2	2.18	0.76
1:G:49:LEU:CB	2:H:127:ALA:HB3	2.16	0.76
1:A:49:LEU:O	2:B:127:ALA:O	2.03	0.76
1:A:77:ARG:NH2	2:B:16:SER:N	2.32	0.76
1:C:112:LEU:HD11	2:D:76:LEU:HD22	1.68	0.76
1:G:77:ARG:HD2	2:H:15:GLU:HA	1.65	0.76
1:C:112:LEU:CD2	2:D:76:LEU:CD2	2.63	0.76
1:G:9:ASN:HD21	1:G:12:ASP:H	1.30	0.76
2:H:5:ILE:HG22	2:H:6:HIS:N	2.00	0.76
1:C:110:PRO:HB2	2:D:135:ASP:OD1	1.84	0.76
2:H:126:GLN:O	2:H:131:VAL:HB	1.84	0.76
2:B:320:LEU:HD11	2:B:426:PRO:HB2	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:TYR:CD2	1:C:294:HIS:NE2	2.53	0.76
1:E:77:ARG:NH2	2:F:16:SER:N	2.32	0.76
2:F:320:LEU:HD11	2:F:426:PRO:HB2	1.68	0.76
2:H:320:LEU:HD11	2:H:426:PRO:HB2	1.68	0.76
1:A:224:TYR:CD2	1:A:294:HIS:NE2	2.53	0.76
1:E:49:LEU:O	2:F:127:ALA:O	2.03	0.76
2:F:5:ILE:HG22	2:F:6:HIS:N	2.00	0.76
1:A:51:THR:HB	2:B:83:ARG:NH1	2.01	0.76
1:C:77:ARG:HD2	2:D:15:GLU:HA	1.66	0.75
1:A:13:THR:CG2	2:B:5:ILE:HG21	2.15	0.75
1:E:77:ARG:HD2	2:F:15:GLU:HA	1.66	0.75
2:D:320:LEU:HD11	2:D:426:PRO:HB2	1.68	0.75
1:G:13:THR:CG2	2:H:5:ILE:HG21	2.15	0.75
1:A:296:MET:HG2	2:B:9:HIS:NE2	2.02	0.75
2:D:142:LEU:O	2:D:146:LYS:HB2	1.87	0.75
1:G:51:THR:HG21	2:H:83:ARG:HH11	1.49	0.75
1:A:245:LEU:CD1	2:B:68:LEU:CD2	2.26	0.74
1:E:296:MET:HG2	2:F:9:HIS:NE2	2.02	0.74
1:E:96:GLY:O	2:H:449:LEU:HD22	1.87	0.74
1:A:110:PRO:CB	2:B:132:PRO:HD2	2.07	0.74
1:C:296:MET:HG2	2:D:9:HIS:NE2	2.02	0.74
2:H:3:VAL:O	2:H:3:VAL:HG23	1.88	0.74
1:G:51:THR:HG23	2:H:83:ARG:CD	2.16	0.74
2:B:5:ILE:HG22	2:B:6:HIS:N	2.00	0.74
2:F:5:ILE:HG22	2:F:6:HIS:H	1.53	0.74
1:G:296:MET:HG2	2:H:9:HIS:NE2	2.02	0.74
2:F:142:LEU:O	2:F:146:LYS:HB2	1.87	0.73
2:F:3:VAL:HG23	2:F:3:VAL:O	1.88	0.73
1:A:77:ARG:HH21	2:B:16:SER:H	1.36	0.73
2:D:3:VAL:CB	2:D:4:TYR:CD2	2.62	0.73
2:D:5:ILE:HG22	2:D:6:HIS:H	1.53	0.73
1:G:80:THR:HG23	2:H:9:HIS:CB	2.19	0.73
2:B:176:VAL:HG23	2:B:198:THR:HG21	1.71	0.73
2:D:161:GLN:CB	2:D:168:ALA:HB2	2.19	0.73
1:E:112:LEU:CD1	2:F:76:LEU:HD22	2.19	0.73
2:F:161:GLN:CB	2:F:168:ALA:HB2	2.18	0.73
1:G:51:THR:HG23	2:H:83:ARG:HG2	1.67	0.73
2:H:123:ASP:HA	2:H:126:GLN:OE1	1.89	0.73
1:E:77:ARG:HH21	2:F:16:SER:H	1.36	0.73
1:A:80:THR:HG23	2:B:9:HIS:CB	2.19	0.73
2:F:123:ASP:HA	2:F:126:GLN:OE1	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LEU:O	2:B:146:LYS:HB2	1.87	0.72
2:H:142:LEU:O	2:H:146:LYS:HB2	1.87	0.72
2:B:123:ASP:HA	2:B:126:GLN:OE1	1.89	0.72
2:B:3:VAL:O	2:B:3:VAL:HG23	1.88	0.72
1:E:110:PRO:CB	2:F:135:ASP:OD1	2.37	0.72
2:H:5:ILE:HG22	2:H:6:HIS:H	1.53	0.72
1:C:80:THR:HG23	2:D:9:HIS:CB	2.19	0.72
2:F:132:PRO:HG2	2:F:135:ASP:H	1.54	0.72
1:G:51:THR:HG23	2:H:83:ARG:HD3	1.70	0.72
1:C:49:LEU:HB3	2:D:127:ALA:CB	2.20	0.72
2:D:176:VAL:HG23	2:D:198:THR:HG21	1.71	0.72
1:E:80:THR:HG23	2:F:9:HIS:CB	2.19	0.72
2:F:16:SER:O	2:F:17:THR:CG2	2.37	0.72
2:F:176:VAL:HG23	2:F:198:THR:HG21	1.71	0.72
1:C:23:THR:CG2	2:F:95:VAL:CB	2.68	0.72
2:H:69:ARG:HG3	2:H:133:TRP:HZ2	1.55	0.72
2:B:143:ASP:O	2:B:144:ALA:HB3	1.89	0.72
2:B:161:GLN:CB	2:B:168:ALA:HB2	2.19	0.72
1:G:112:LEU:CD1	2:H:76:LEU:HD21	2.18	0.72
2:H:132:PRO:HG2	2:H:135:ASP:H	1.54	0.71
2:H:176:VAL:HG23	2:H:198:THR:HG21	1.71	0.71
2:D:69:ARG:HG3	2:D:133:TRP:HZ2	1.55	0.71
2:H:161:GLN:CB	2:H:168:ALA:HB2	2.19	0.71
2:B:3:VAL:CB	2:B:4:TYR:CD2	2.63	0.71
2:D:3:VAL:O	2:D:3:VAL:HG23	1.88	0.71
1:E:70:ASN:HB2	1:E:102:MET:HE1	1.73	0.71
1:E:77:ARG:HD3	2:F:136:LYS:HZ1	1.54	0.71
2:D:123:ASP:HA	2:D:126:GLN:OE1	1.89	0.71
1:C:77:ARG:HD3	2:D:136:LYS:HZ1	1.56	0.71
1:C:77:ARG:HH21	2:D:16:SER:H	1.36	0.71
2:F:69:ARG:HG3	2:F:133:TRP:HZ2	1.55	0.71
2:D:142:LEU:HD12	2:D:146:LYS:HE2	1.70	0.71
2:H:143:ASP:O	2:H:144:ALA:HB3	1.89	0.71
2:B:285:THR:HG23	1:G:283:TYR:HB2	1.73	0.71
2:F:142:LEU:HD12	2:F:146:LYS:HE2	1.70	0.71
2:B:5:ILE:HG22	2:B:6:HIS:H	1.53	0.71
2:B:16:SER:O	2:B:17:THR:CG2	2.37	0.71
2:B:69:ARG:HG3	2:B:133:TRP:HZ2	1.55	0.71
1:G:49:LEU:C	2:H:127:ALA:HB1	2.11	0.70
2:H:16:SER:O	2:H:17:THR:CG2	2.37	0.70
1:A:49:LEU:HD13	2:B:367:GLU:CG	2.18	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:LEU:HD21	2:D:379:GLN:CG	2.21	0.70
2:F:118:LEU:HD21	2:F:379:GLN:CG	2.22	0.70
2:F:3:VAL:CB	2:F:4:TYR:CD2	2.63	0.70
2:D:95:VAL:CG2	1:G:23:THR:CG2	2.68	0.70
1:C:49:LEU:HD13	2:D:367:GLU:CG	2.13	0.70
2:F:143:ASP:O	2:F:144:ALA:HB3	1.89	0.70
1:G:244:ARG:HD3	1:G:247:ASP:OD2	1.92	0.70
1:A:77:ARG:CD	2:B:136:LYS:HZ1	2.05	0.70
2:B:118:LEU:HD21	2:B:379:GLN:CG	2.21	0.70
2:H:118:LEU:HD21	2:H:379:GLN:CG	2.21	0.70
2:B:132:PRO:HG2	2:B:135:ASP:H	1.54	0.70
1:E:244:ARG:HD3	1:E:247:ASP:OD2	1.92	0.70
2:B:142:LEU:HD12	2:B:146:LYS:HE2	1.70	0.70
2:D:143:ASP:O	2:D:144:ALA:HB3	1.89	0.70
1:G:51:THR:HG21	2:H:83:ARG:CG	2.12	0.70
1:G:77:ARG:HH21	2:H:16:SER:H	1.36	0.70
1:A:110:PRO:CB	2:B:135:ASP:OD1	2.40	0.69
2:H:3:VAL:CB	2:H:4:TYR:CD2	2.62	0.69
2:B:132:PRO:O	2:B:134:LYS:N	2.24	0.69
1:C:244:ARG:HD3	1:C:247:ASP:OD2	1.92	0.69
1:G:70:ASN:HB2	1:G:102:MET:HE1	1.75	0.69
1:A:70:ASN:HB2	1:A:102:MET:HE1	1.75	0.69
1:C:97:ILE:HA	2:F:449:LEU:HD13	1.74	0.69
2:D:16:SER:O	2:D:17:THR:CG2	2.37	0.69
1:G:112:LEU:CD2	2:H:72:MET:CG	2.71	0.69
2:D:329:GLN:N	2:D:333:LEU:HD21	2.08	0.69
2:F:329:GLN:N	2:F:333:LEU:HD21	2.08	0.69
1:G:296:MET:HG2	2:H:9:HIS:CE1	2.28	0.69
1:A:244:ARG:HD3	1:A:247:ASP:OD2	1.92	0.69
1:A:296:MET:HG2	2:B:9:HIS:CE1	2.28	0.69
1:E:9:ASN:C	1:E:9:ASN:HD22	1.96	0.69
2:B:329:GLN:N	2:B:333:LEU:HD21	2.08	0.69
2:B:135:ASP:O	2:B:136:LYS:HG3	1.93	0.69
1:C:70:ASN:HB2	1:C:102:MET:HE1	1.74	0.69
2:D:132:PRO:HG2	2:D:135:ASP:H	1.54	0.69
1:A:77:ARG:HD2	2:B:15:GLU:HG2	1.75	0.68
1:G:82:THR:OG1	2:H:136:LYS:HE3	1.93	0.68
2:H:135:ASP:O	2:H:136:LYS:HG3	1.93	0.68
2:B:69:ARG:NH1	2:B:133:TRP:CH2	2.62	0.68
1:E:77:ARG:HD2	2:F:15:GLU:HG2	1.75	0.68
2:H:132:PRO:CG	2:H:135:ASP:CA	2.68	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:PRO:HG3	2:H:135:ASP:OD1	1.88	0.68
1:G:9:ASN:HD22	1:G:9:ASN:C	1.96	0.68
2:H:69:ARG:NH1	2:H:133:TRP:CH2	2.62	0.68
1:A:9:ASN:C	1:A:9:ASN:HD22	1.96	0.68
2:D:135:ASP:O	2:D:136:LYS:HG3	1.93	0.68
1:C:296:MET:HG2	2:D:9:HIS:CE1	2.28	0.68
1:E:296:MET:HG2	2:F:9:HIS:CE1	2.28	0.68
2:F:132:PRO:O	2:F:134:LYS:N	2.24	0.68
2:F:69:ARG:NH1	2:F:133:TRP:CH2	2.62	0.68
2:B:134:LYS:O	2:B:135:ASP:HB2	1.93	0.68
1:A:224:TYR:CE2	2:B:7:PRO:HB3	2.29	0.68
1:C:77:ARG:HD2	2:D:15:GLU:HG2	1.75	0.68
2:D:69:ARG:NH1	2:D:133:TRP:CH2	2.62	0.68
2:H:132:PRO:O	2:H:134:LYS:N	2.24	0.68
1:A:77:ARG:CD	2:B:136:LYS:NZ	2.57	0.68
1:C:79:SER:HB2	2:D:9:HIS:CB	2.24	0.68
2:H:329:GLN:N	2:H:333:LEU:HD21	2.08	0.68
1:G:79:SER:HB2	2:H:9:HIS:CB	2.24	0.68
1:C:23:THR:CG2	2:F:95:VAL:HG21	2.06	0.67
1:A:257:THR:OG1	2:H:403:GLU:O	2.09	0.67
1:C:224:TYR:CE2	2:D:7:PRO:HB3	2.29	0.67
2:F:134:LYS:O	2:F:135:ASP:HB2	1.93	0.67
2:H:134:LYS:O	2:H:135:ASP:HB2	1.93	0.67
1:C:49:LEU:CB	2:D:127:ALA:HB3	2.25	0.67
2:D:134:LYS:O	2:D:135:ASP:HB2	1.93	0.67
1:E:79:SER:HB2	2:F:9:HIS:CB	2.24	0.67
1:G:224:TYR:CE2	2:H:7:PRO:HB3	2.29	0.67
1:C:112:LEU:HD13	2:D:76:LEU:HD21	1.74	0.67
1:C:112:LEU:CD2	2:D:76:LEU:HD21	2.18	0.67
1:G:49:LEU:CB	2:H:127:ALA:CB	2.73	0.67
2:B:84:ILE:HG21	2:B:362:LEU:HD11	1.77	0.67
1:C:9:ASN:HD22	1:C:9:ASN:C	1.96	0.67
1:E:110:PRO:CG	2:F:135:ASP:OD1	2.43	0.67
1:G:77:ARG:HD2	2:H:15:GLU:HG2	1.75	0.67
1:A:110:PRO:CG	2:B:135:ASP:OD1	2.42	0.67
1:E:224:TYR:CE2	2:F:7:PRO:HB3	2.29	0.67
1:A:112:LEU:CD1	2:B:76:LEU:HD22	2.24	0.67
2:F:135:ASP:O	2:F:136:LYS:HG3	1.93	0.67
2:H:84:ILE:HG21	2:H:362:LEU:HD11	1.77	0.67
2:H:141:ARG:O	2:H:146:LYS:HG2	1.90	0.66
1:A:9:ASN:HD22	1:A:10:TYR:N	1.93	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:LEU:HD21	2:B:379:GLN:CD	2.16	0.66
1:A:36:SER:HA	2:B:12:ILE:CG2	2.25	0.66
1:C:77:ARG:CD	2:D:136:LYS:HZ1	2.08	0.66
2:F:106:VAL:HG13	2:F:359:LEU:HD11	1.77	0.66
1:G:110:PRO:CG	2:H:135:ASP:CG	2.59	0.66
1:G:9:ASN:HD22	1:G:10:TYR:N	1.93	0.66
1:G:36:SER:HA	2:H:12:ILE:CG2	2.25	0.66
2:F:84:ILE:HG21	2:F:362:LEU:HD11	1.77	0.66
2:D:118:LEU:HD21	2:D:379:GLN:CD	2.16	0.66
2:D:14:ASN:HD22	2:D:14:ASN:N	1.94	0.66
1:E:229:THR:O	1:E:233:GLU:HG2	1.96	0.66
1:C:49:LEU:HB3	2:D:127:ALA:HB3	1.76	0.66
1:A:79:SER:HB2	2:B:9:HIS:CB	2.24	0.66
1:C:229:THR:O	1:C:233:GLU:HG2	1.96	0.66
2:D:84:ILE:HG21	2:D:362:LEU:HD11	1.77	0.66
1:E:9:ASN:HD22	1:E:10:TYR:N	1.93	0.66
2:H:118:LEU:HD21	2:H:379:GLN:CD	2.16	0.66
2:H:3:VAL:HB	2:H:4:TYR:CE2	2.30	0.66
2:F:128:ILE:HG23	2:F:367:GLU:HG2	1.78	0.66
2:H:14:ASN:N	2:H:14:ASN:HD22	1.94	0.66
1:A:112:LEU:HD13	2:B:76:LEU:CD1	2.26	0.65
1:C:110:PRO:HB3	2:D:132:PRO:CD	2.16	0.65
2:D:3:VAL:O	2:D:3:VAL:CG2	2.44	0.65
2:F:3:VAL:HB	2:F:4:TYR:CE2	2.30	0.65
1:A:229:THR:O	1:A:233:GLU:HG2	1.96	0.65
2:D:132:PRO:O	2:D:134:LYS:N	2.24	0.65
2:F:14:ASN:HD22	2:F:14:ASN:N	1.94	0.65
1:G:229:THR:O	1:G:233:GLU:HG2	1.96	0.65
2:B:3:VAL:HB	2:B:4:TYR:CE2	2.31	0.65
1:C:36:SER:HA	2:D:12:ILE:CG2	2.25	0.65
2:F:118:LEU:HD21	2:F:379:GLN:CD	2.16	0.65
2:H:3:VAL:CG2	2:H:3:VAL:O	2.44	0.65
2:B:128:ILE:HG23	2:B:367:GLU:HG2	1.78	0.65
2:B:4:TYR:CD1	2:B:5:ILE:HD12	2.32	0.65
2:B:106:VAL:HG13	2:B:359:LEU:HD11	1.77	0.65
2:B:249:VAL:CG1	2:B:395:ILE:HG22	2.27	0.65
1:A:245:LEU:H	2:B:68:LEU:HD21	1.60	0.65
2:D:106:VAL:HG13	2:D:359:LEU:HD11	1.77	0.65
2:D:3:VAL:HB	2:D:4:TYR:CE2	2.30	0.65
2:H:249:VAL:CG1	2:H:395:ILE:HG22	2.27	0.65
2:B:14:ASN:N	2:B:14:ASN:HD22	1.94	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:THR:HG21	2:F:95:VAL:CB	2.25	0.65
2:D:128:ILE:HG23	2:D:367:GLU:HG2	1.78	0.65
2:H:106:VAL:HG13	2:H:359:LEU:HD11	1.77	0.65
1:G:49:LEU:O	2:H:127:ALA:C	2.33	0.65
2:H:128:ILE:HG23	2:H:367:GLU:HG2	1.78	0.65
1:A:208:LEU:HD12	1:A:209:LEU:HG	1.79	0.65
1:C:9:ASN:HD22	1:C:10:TYR:N	1.93	0.65
1:E:36:SER:HA	2:F:12:ILE:CG2	2.25	0.65
1:E:112:LEU:HD13	2:F:76:LEU:CD2	2.26	0.65
2:H:4:TYR:CD1	2:H:5:ILE:HD12	2.32	0.65
2:B:3:VAL:CG2	2:B:3:VAL:O	2.44	0.65
1:C:208:LEU:HD12	1:C:209:LEU:HG	1.79	0.65
2:D:4:TYR:CD1	2:D:5:ILE:HD12	2.32	0.65
1:E:110:PRO:HG3	2:F:135:ASP:OD1	1.97	0.65
2:F:3:VAL:CG2	2:F:3:VAL:O	2.44	0.64
2:B:144:ALA:O	2:B:148:LEU:HG	1.97	0.64
1:C:49:LEU:CB	2:D:127:ALA:CB	2.75	0.64
2:D:249:VAL:CG1	2:D:395:ILE:HG22	2.27	0.64
1:C:273:THR:HG22	1:C:275:ALA:H	1.63	0.64
1:C:6:ILE:CG1	2:F:272:SER:O	2.44	0.64
1:E:208:LEU:HD12	1:E:209:LEU:HG	1.79	0.64
1:A:273:THR:HG22	1:A:275:ALA:H	1.63	0.64
2:F:249:VAL:CG1	2:F:395:ILE:HG22	2.27	0.64
2:H:142:LEU:HD12	2:H:146:LYS:HE2	1.70	0.64
1:C:36:SER:HA	2:D:12:ILE:HG21	1.80	0.64
2:B:142:LEU:HD12	2:B:146:LYS:CD	2.27	0.64
1:E:273:THR:HG22	1:E:275:ALA:H	1.63	0.64
2:F:133:TRP:CH2	2:F:142:LEU:HD23	2.33	0.64
2:B:133:TRP:CH2	2:B:142:LEU:HD23	2.33	0.64
1:E:219:ASP:OD1	2:F:11:VAL:CG2	2.45	0.64
2:F:4:TYR:CD1	2:F:5:ILE:HD12	2.32	0.64
1:G:273:THR:HG22	1:G:275:ALA:H	1.63	0.64
2:H:144:ALA:O	2:H:148:LEU:HG	1.97	0.63
1:C:96:GLY:HA2	2:F:447:ASN:ND2	2.14	0.63
2:F:142:LEU:HD12	2:F:146:LYS:CD	2.27	0.63
2:F:144:ALA:O	2:F:148:LEU:HG	1.97	0.63
1:A:36:SER:HA	2:B:12:ILE:HG21	1.80	0.63
1:G:219:ASP:OD1	2:H:11:VAL:CG2	2.46	0.63
1:C:23:THR:HG23	2:F:95:VAL:CB	2.29	0.63
2:D:144:ALA:O	2:D:148:LEU:HG	1.97	0.63
2:D:133:TRP:CH2	2:D:142:LEU:HD23	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:SER:HA	2:F:12:ILE:HG21	1.80	0.63
1:G:208:LEU:HD12	1:G:209:LEU:HG	1.79	0.63
1:G:77:ARG:NE	2:H:136:LYS:HZ3	1.96	0.63
1:C:219:ASP:OD1	2:D:11:VAL:CG2	2.46	0.63
2:H:133:TRP:CH2	2:H:142:LEU:HD23	2.33	0.63
2:F:131:VAL:CG1	2:F:132:PRO:N	2.58	0.63
1:A:158:ASN:ND2	1:A:159:ARG:N	2.47	0.62
1:E:112:LEU:HD23	2:F:72:MET:HG3	1.81	0.62
1:G:36:SER:HA	2:H:12:ILE:HG21	1.80	0.62
1:A:112:LEU:HD21	2:B:76:LEU:CD2	2.30	0.62
1:E:158:ASN:ND2	1:E:159:ARG:N	2.47	0.62
1:G:77:ARG:HD3	2:H:136:LYS:NZ	2.14	0.62
1:A:158:ASN:HD22	1:A:159:ARG:N	1.97	0.62
1:A:219:ASP:OD1	2:B:11:VAL:CG2	2.46	0.62
2:F:142:LEU:HD12	2:F:146:LYS:CG	2.30	0.62
1:G:158:ASN:HD22	1:G:159:ARG:N	1.97	0.62
2:H:131:VAL:CG1	2:H:132:PRO:N	2.58	0.62
2:B:118:LEU:HD11	2:B:379:GLN:HG3	1.82	0.62
1:G:158:ASN:ND2	1:G:159:ARG:N	2.47	0.62
2:F:131:VAL:HG12	2:F:132:PRO:CD	2.30	0.62
1:G:51:THR:HG1	2:H:83:ARG:CD	1.96	0.62
1:E:13:THR:CG2	2:F:5:ILE:CG2	2.72	0.61
2:D:118:LEU:HD11	2:D:379:GLN:HG3	1.82	0.61
1:E:158:ASN:HD22	1:E:159:ARG:N	1.97	0.61
1:C:77:ARG:CD	2:D:15:GLU:HG2	2.31	0.61
2:D:131:VAL:HG12	2:D:132:PRO:CD	2.30	0.61
1:G:99:VAL:HG12	1:G:145:GLN:OE1	2.01	0.61
1:A:77:ARG:CD	2:B:15:GLU:HG2	2.31	0.61
1:C:6:ILE:HG13	2:F:272:SER:C	2.20	0.61
1:C:9:ASN:HD21	1:C:12:ASP:N	1.99	0.61
1:E:99:VAL:HG12	1:E:145:GLN:OE1	2.01	0.61
1:E:77:ARG:CZ	2:F:15:GLU:HB3	2.30	0.61
1:G:217:LEU:HD13	1:G:219:ASP:HB2	1.83	0.61
1:E:23:THR:CG2	2:H:95:VAL:HG23	2.27	0.61
1:C:77:ARG:CZ	2:D:15:GLU:HB3	2.30	0.61
2:H:131:VAL:HG12	2:H:132:PRO:CD	2.30	0.61
1:G:77:ARG:CD	2:H:15:GLU:HG2	2.31	0.61
1:A:257:THR:CB	2:H:403:GLU:O	2.47	0.61
2:D:142:LEU:HD12	2:D:146:LYS:CG	2.30	0.61
1:A:77:ARG:NH2	2:B:16:SER:O	2.34	0.61
2:B:403:GLU:O	1:G:257:THR:HB	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:MET:HG2	2:D:9:HIS:CD2	2.36	0.61
1:G:77:ARG:NH2	2:H:16:SER:O	2.34	0.61
2:H:142:LEU:HD12	2:H:146:LYS:CG	2.30	0.61
1:C:158:ASN:ND2	1:C:159:ARG:N	2.47	0.61
1:A:296:MET:HG2	2:B:9:HIS:CD2	2.36	0.60
2:B:142:LEU:CD1	2:B:146:LYS:CG	2.77	0.60
1:A:51:THR:OG1	2:B:83:ARG:NH1	2.28	0.60
2:F:132:PRO:CG	2:F:135:ASP:CA	2.67	0.60
1:G:77:ARG:CZ	2:H:15:GLU:HB3	2.30	0.60
1:C:217:LEU:HD13	1:C:219:ASP:HB2	1.83	0.60
2:F:118:LEU:HD11	2:F:379:GLN:HG3	1.82	0.60
1:E:77:ARG:NH2	2:F:16:SER:O	2.34	0.60
2:H:118:LEU:HD11	2:H:379:GLN:HG3	1.82	0.60
2:H:142:LEU:HD12	2:H:146:LYS:CD	2.28	0.60
1:A:217:LEU:HD13	1:A:219:ASP:HB2	1.83	0.60
1:A:99:VAL:HG12	1:A:145:GLN:OE1	2.01	0.60
2:B:131:VAL:CG1	2:B:132:PRO:N	2.58	0.60
1:E:296:MET:HG2	2:F:9:HIS:CD2	2.36	0.60
1:E:9:ASN:HD21	1:E:12:ASP:N	1.99	0.60
1:G:112:LEU:HD13	2:H:76:LEU:CD1	2.30	0.60
1:C:99:VAL:HG12	1:C:145:GLN:OE1	2.01	0.60
1:C:4:SER:OG	2:F:274:SER:OG	2.20	0.60
2:B:131:VAL:HG12	2:B:132:PRO:CD	2.30	0.60
2:D:131:VAL:CG1	2:D:132:PRO:N	2.58	0.60
1:E:112:LEU:CD2	2:F:72:MET:HG3	2.31	0.60
1:G:9:ASN:HD21	1:G:12:ASP:N	1.99	0.60
1:C:77:ARG:NH2	2:D:16:SER:O	2.34	0.60
2:B:142:LEU:HD12	2:B:146:LYS:CG	2.30	0.60
1:E:77:ARG:CD	2:F:15:GLU:HG2	2.31	0.60
2:H:431:VAL:HG22	2:H:441:PHE:HB2	1.83	0.60
2:B:431:VAL:HG22	2:B:441:PHE:HB2	1.83	0.60
2:D:142:LEU:HD12	2:D:146:LYS:CD	2.28	0.60
1:A:77:ARG:CZ	2:B:15:GLU:HB3	2.30	0.60
1:E:217:LEU:HD13	1:E:219:ASP:HB2	1.83	0.60
2:F:431:VAL:HG22	2:F:441:PHE:HB2	1.84	0.60
2:D:381:LEU:HD22	2:D:386:ILE:HD11	1.84	0.59
1:A:112:LEU:CD1	2:B:76:LEU:CD2	2.80	0.59
1:E:51:THR:CG2	2:F:83:ARG:HH11	2.15	0.59
1:C:190:LYS:HG3	1:C:191:THR:O	2.02	0.59
2:D:431:VAL:HG22	2:D:441:PHE:HB2	1.84	0.59
1:C:13:THR:CG2	2:D:5:ILE:CG2	2.72	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:LYS:HG3	1:E:191:THR:O	2.02	0.59
1:E:97:ILE:HA	2:H:449:LEU:CD2	2.31	0.59
1:A:190:LYS:HG3	1:A:191:THR:O	2.02	0.59
2:B:381:LEU:HD22	2:B:386:ILE:HD11	1.84	0.59
2:B:382:SER:HB3	2:B:386:ILE:HD12	1.85	0.59
1:G:296:MET:HG2	2:H:9:HIS:CD2	2.36	0.59
1:A:112:LEU:HD13	2:B:76:LEU:CD2	2.33	0.59
2:B:352:VAL:HG12	2:B:398:GLU:HG3	1.84	0.59
1:C:112:LEU:CD2	2:D:72:MET:CG	2.78	0.59
2:H:382:SER:HB3	2:H:386:ILE:HD12	1.85	0.59
1:C:49:LEU:HB3	2:D:128:ILE:N	2.17	0.59
1:G:9:ASN:ND2	1:G:12:ASP:H	2.01	0.59
2:H:141:ARG:O	2:H:145:HIS:HB2	2.03	0.59
2:B:141:ARG:O	2:B:145:HIS:HB2	2.03	0.59
2:D:131:VAL:HG12	2:D:132:PRO:CB	2.32	0.59
2:D:141:ARG:O	2:D:145:HIS:HB2	2.03	0.59
2:F:141:ARG:O	2:F:145:HIS:HB2	2.02	0.59
1:C:97:ILE:HA	2:F:449:LEU:CG	2.32	0.58
2:D:131:VAL:HG12	2:D:132:PRO:N	2.18	0.58
2:D:382:SER:HB3	2:D:386:ILE:HD12	1.85	0.58
2:F:352:VAL:HG12	2:F:398:GLU:HG3	1.84	0.58
1:C:49:LEU:O	2:D:127:ALA:C	2.42	0.58
1:E:110:PRO:HB3	2:F:132:PRO:CD	2.24	0.58
1:A:257:THR:HB	2:H:403:GLU:O	2.03	0.58
2:F:381:LEU:HD22	2:F:386:ILE:HD11	1.84	0.58
2:D:5:ILE:CG2	2:D:6:HIS:H	2.16	0.58
1:G:298:ILE:HD13	2:H:11:VAL:HG11	1.86	0.58
1:C:298:ILE:HD13	2:D:11:VAL:HG11	1.86	0.58
2:F:382:SER:HB3	2:F:386:ILE:HD12	1.85	0.58
1:A:110:PRO:HG3	2:B:135:ASP:OD1	2.03	0.58
1:C:9:ASN:ND2	1:C:12:ASP:H	2.01	0.58
1:C:101:GLN:NE2	1:C:138:ILE:HA	2.18	0.58
1:C:158:ASN:HD22	1:C:159:ARG:N	1.97	0.58
1:C:321:ASP:OD1	1:C:326:ARG:HD2	2.04	0.58
1:E:79:SER:HB2	2:F:9:HIS:CG	2.39	0.58
2:F:5:ILE:CG2	2:F:6:HIS:H	2.16	0.58
1:G:79:SER:HB2	2:H:9:HIS:CG	2.39	0.58
2:H:381:LEU:HD22	2:H:386:ILE:HD11	1.84	0.58
1:C:79:SER:HB2	2:D:9:HIS:CG	2.39	0.58
1:G:321:ASP:OD1	1:G:326:ARG:HD2	2.04	0.58
2:B:126:GLN:C	2:B:131:VAL:HG23	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:LEU:O	2:B:154:VAL:HG22	2.04	0.58
1:E:321:ASP:OD1	1:E:326:ARG:HD2	2.04	0.58
1:E:79:SER:HG	2:F:9:HIS:CE1	2.19	0.58
1:G:190:LYS:HG3	1:G:191:THR:O	2.02	0.58
2:F:151:LEU:O	2:F:154:VAL:HG22	2.04	0.58
1:A:13:THR:CG2	2:B:5:ILE:CG2	2.72	0.58
1:A:79:SER:HB2	2:B:9:HIS:CG	2.39	0.58
2:D:115:LEU:HD23	2:D:144:ALA:CB	2.31	0.58
1:E:101:GLN:NE2	1:E:138:ILE:HA	2.19	0.58
1:E:77:ARG:HD2	2:F:15:GLU:CA	2.34	0.58
1:E:97:ILE:HA	2:H:449:LEU:HD22	1.86	0.58
2:H:151:LEU:O	2:H:154:VAL:HG22	2.04	0.58
2:H:352:VAL:HG12	2:H:398:GLU:HG3	1.84	0.58
1:A:110:PRO:HB2	2:B:135:ASP:OD1	2.04	0.57
2:B:5:ILE:CG2	2:B:6:HIS:N	2.67	0.57
2:H:5:ILE:CG2	2:H:6:HIS:H	2.16	0.57
2:D:352:VAL:HG12	2:D:398:GLU:HG3	1.84	0.57
2:D:3:VAL:CA	2:D:4:TYR:CB	2.82	0.57
2:D:5:ILE:CG2	2:D:6:HIS:N	2.67	0.57
1:E:298:ILE:HD13	2:F:11:VAL:HG11	1.86	0.57
1:G:77:ARG:HD2	2:H:15:GLU:CA	2.34	0.57
2:D:351:LEU:HD12	2:D:399:LEU:HD12	1.87	0.57
2:D:69:ARG:HG3	2:D:133:TRP:CZ2	2.39	0.57
1:G:77:ARG:CD	2:H:136:LYS:NZ	2.68	0.57
2:B:131:VAL:HG12	2:B:132:PRO:N	2.18	0.57
2:D:126:GLN:HB3	2:D:131:VAL:HG21	1.86	0.57
1:G:101:GLN:NE2	1:G:138:ILE:HA	2.19	0.57
2:H:143:ASP:O	2:H:144:ALA:CB	2.52	0.57
1:A:245:LEU:HD12	2:B:68:LEU:HD23	1.84	0.57
1:A:321:ASP:OD1	1:A:326:ARG:HD2	2.03	0.57
1:A:9:ASN:HD21	1:A:12:ASP:N	1.99	0.57
2:B:132:PRO:CG	2:B:135:ASP:CA	2.67	0.57
2:F:131:VAL:HG12	2:F:132:PRO:N	2.18	0.57
1:A:112:LEU:CD2	2:B:76:LEU:HD22	2.33	0.57
2:B:143:ASP:O	2:B:144:ALA:CB	2.52	0.57
1:A:49:LEU:CD1	2:B:367:GLU:HG3	2.25	0.57
2:B:351:LEU:HD12	2:B:399:LEU:HD12	1.86	0.57
2:D:132:PRO:CG	2:D:135:ASP:CA	2.68	0.57
1:C:97:ILE:CA	2:F:449:LEU:HD11	2.27	0.57
1:A:9:ASN:ND2	1:A:12:ASP:H	2.01	0.57
1:A:101:GLN:NE2	1:A:138:ILE:HA	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:LEU:O	2:D:154:VAL:HG22	2.04	0.57
1:E:112:LEU:CD1	2:F:76:LEU:CD2	2.81	0.57
2:F:126:GLN:HB3	2:F:131:VAL:HG21	1.86	0.57
2:F:351:LEU:HD12	2:F:399:LEU:HD12	1.87	0.57
2:D:141:ARG:O	2:D:146:LYS:HG2	1.90	0.57
2:F:126:GLN:C	2:F:131:VAL:HG23	2.18	0.57
2:F:5:ILE:CG2	2:F:6:HIS:N	2.67	0.57
2:H:131:VAL:HG12	2:H:132:PRO:N	2.18	0.57
2:H:351:LEU:HD12	2:H:399:LEU:HD12	1.86	0.57
2:B:16:SER:O	2:B:17:THR:CB	2.53	0.57
2:F:143:ASP:O	2:F:144:ALA:CB	2.52	0.57
1:G:79:SER:HG	2:H:9:HIS:CE1	2.20	0.57
2:H:16:SER:O	2:H:17:THR:CB	2.53	0.57
1:A:281:GLU:OE1	2:B:4:TYR:CE2	2.58	0.56
1:E:281:GLU:OE1	2:F:4:TYR:CE2	2.58	0.56
1:G:281:GLU:OE1	2:H:4:TYR:CE2	2.58	0.56
2:H:5:ILE:CG2	2:H:6:HIS:N	2.67	0.56
1:A:298:ILE:HD13	2:B:11:VAL:HG11	1.86	0.56
2:B:5:ILE:CG2	2:B:6:HIS:H	2.16	0.56
2:H:126:GLN:C	2:H:131:VAL:HG23	2.18	0.56
2:H:131:VAL:HG12	2:H:132:PRO:CB	2.33	0.56
1:A:36:SER:HB3	2:B:12:ILE:HB	1.88	0.56
2:B:69:ARG:HG3	2:B:133:TRP:CZ2	2.39	0.56
1:C:251:LYS:NZ	1:C:285:SER:HB2	2.21	0.56
2:F:16:SER:O	2:F:17:THR:CB	2.53	0.56
1:C:77:ARG:NE	2:D:136:LYS:NZ	2.54	0.56
1:A:251:LYS:NZ	1:A:285:SER:HB2	2.21	0.56
1:A:77:ARG:HD2	2:B:15:GLU:CA	2.34	0.56
1:C:6:ILE:CG1	2:F:273:THR:HA	2.36	0.56
2:F:346:LEU:HD23	2:F:347:THR:N	2.21	0.56
2:B:346:LEU:HD23	2:B:347:THR:N	2.21	0.56
2:D:16:SER:O	2:D:17:THR:CB	2.53	0.56
1:E:110:PRO:HG3	2:F:135:ASP:CG	2.25	0.56
1:E:9:ASN:ND2	1:E:12:ASP:H	2.01	0.56
1:E:251:LYS:NZ	1:E:285:SER:HB2	2.21	0.56
1:G:35:GLY:O	2:H:12:ILE:CG2	2.33	0.56
2:F:141:ARG:O	2:F:146:LYS:HG2	1.91	0.56
2:F:69:ARG:HG3	2:F:133:TRP:CZ2	2.39	0.56
2:H:132:PRO:C	2:H:134:LYS:H	2.10	0.56
1:C:110:PRO:CG	2:D:135:ASP:CG	2.67	0.56
2:D:215:ALA:O	2:D:218:ILE:HG22	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:3:VAL:CA	2:F:4:TYR:CB	2.82	0.56
1:A:211:GLU:H	1:A:211:GLU:CD	2.10	0.55
1:A:43:SER:HB2	1:A:105:GLU:HB3	1.88	0.55
1:C:101:GLN:HE22	1:C:138:ILE:HA	1.71	0.55
1:C:281:GLU:OE1	2:D:4:TYR:CE2	2.58	0.55
1:E:112:LEU:HD13	2:F:76:LEU:HD22	1.88	0.55
2:H:126:GLN:HB3	2:H:131:VAL:HG21	1.86	0.55
2:H:215:ALA:O	2:H:218:ILE:HG22	2.06	0.55
2:H:439:LEU:HD22	2:H:442:LEU:HD11	1.88	0.55
1:C:211:GLU:CD	1:C:211:GLU:H	2.10	0.55
2:D:132:PRO:C	2:D:134:LYS:H	2.09	0.55
1:E:43:SER:HB2	1:E:105:GLU:HB3	1.88	0.55
1:E:211:GLU:H	1:E:211:GLU:CD	2.10	0.55
1:E:77:ARG:HD3	2:F:136:LYS:NZ	2.21	0.55
1:C:36:SER:HB3	2:D:12:ILE:HB	1.88	0.55
2:D:118:LEU:HD21	2:D:379:GLN:OE1	2.07	0.55
2:F:215:ALA:O	2:F:218:ILE:HG22	2.06	0.55
1:G:36:SER:HB3	2:H:12:ILE:HB	1.88	0.55
2:B:153:ALA:O	2:B:157:LEU:HD13	2.07	0.55
2:B:215:ALA:O	2:B:218:ILE:HG22	2.06	0.55
1:C:298:ILE:O	1:C:303:GLY:HA3	2.07	0.55
2:D:84:ILE:HD13	2:D:362:LEU:HD11	1.89	0.55
1:G:101:GLN:HE22	1:G:138:ILE:HA	1.71	0.55
2:H:153:ALA:O	2:H:157:LEU:HD13	2.07	0.55
2:H:118:LEU:HD21	2:H:379:GLN:OE1	2.07	0.55
1:A:298:ILE:O	1:A:303:GLY:HA3	2.07	0.55
2:F:131:VAL:HG12	2:F:132:PRO:CB	2.32	0.55
1:A:143:ILE:HD13	1:A:151:ASP:OD2	2.07	0.55
2:F:84:ILE:HD13	2:F:362:LEU:HD11	1.89	0.55
1:G:211:GLU:CD	1:G:211:GLU:H	2.10	0.55
1:G:251:LYS:NZ	1:G:285:SER:HB2	2.21	0.55
2:H:346:LEU:HD23	2:H:347:THR:N	2.21	0.55
1:A:51:THR:CG2	2:B:83:ARG:HH11	2.18	0.55
2:D:346:LEU:HD23	2:D:347:THR:N	2.21	0.55
2:D:118:LEU:HD21	2:D:379:GLN:HG3	1.89	0.55
2:F:153:ALA:O	2:F:157:LEU:HD13	2.07	0.55
1:G:51:THR:HG21	2:H:83:ARG:NH1	2.20	0.55
2:H:84:ILE:HD13	2:H:362:LEU:HD11	1.89	0.55
1:A:225:ILE:HG13	1:A:311:THR:HB	1.89	0.55
2:D:153:ALA:O	2:D:157:LEU:HD13	2.07	0.55
1:E:273:THR:HG22	1:E:274:SER:N	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:LEU:HD21	2:F:379:GLN:OE1	2.07	0.55
2:F:439:LEU:HD22	2:F:442:LEU:HD11	1.88	0.55
1:A:255:GLY:HA3	1:A:280:GLN:HE22	1.72	0.55
1:C:225:ILE:HG13	1:C:311:THR:HB	1.89	0.55
1:C:6:ILE:HG13	2:F:273:THR:HA	1.89	0.55
1:A:112:LEU:HD11	2:B:76:LEU:HD22	1.88	0.55
1:C:143:ILE:HD13	1:C:151:ASP:OD2	2.07	0.55
1:E:298:ILE:O	1:E:303:GLY:HA3	2.07	0.54
2:F:118:LEU:HD21	2:F:379:GLN:HG3	1.89	0.54
1:G:255:GLY:HA3	1:G:280:GLN:HE22	1.72	0.54
2:H:277:VAL:HG13	2:H:278:PRO:HD2	1.89	0.54
1:C:255:GLY:HA3	1:C:280:GLN:HE22	1.72	0.54
1:E:251:LYS:HZ1	1:E:285:SER:HB2	1.72	0.54
1:E:36:SER:HB3	2:F:12:ILE:HB	1.88	0.54
1:G:298:ILE:O	1:G:303:GLY:HA3	2.07	0.54
2:H:142:LEU:CD1	2:H:146:LYS:CG	2.77	0.54
2:H:4:TYR:N	2:H:4:TYR:CD1	2.75	0.54
2:B:126:GLN:HB3	2:B:131:VAL:HG21	1.86	0.54
2:B:118:LEU:HD21	2:B:379:GLN:OE1	2.07	0.54
1:C:77:ARG:HD2	2:D:15:GLU:CA	2.34	0.54
2:D:4:TYR:N	2:D:4:TYR:CD1	2.75	0.54
1:E:143:ILE:HD13	1:E:151:ASP:OD2	2.07	0.54
1:G:43:SER:HB2	1:G:105:GLU:HB3	1.88	0.54
2:B:126:GLN:HA	2:B:131:VAL:HG23	1.87	0.54
2:B:243:LEU:HD11	2:B:245:PHE:HB2	1.90	0.54
2:B:439:LEU:HD22	2:B:442:LEU:HD11	1.88	0.54
1:C:43:SER:HB2	1:C:105:GLU:HB3	1.88	0.54
2:D:143:ASP:O	2:D:144:ALA:CB	2.52	0.54
2:F:115:LEU:HD23	2:F:144:ALA:CB	2.31	0.54
1:A:215:LEU:N	1:A:215:LEU:HD12	2.23	0.54
1:A:9:ASN:ND2	1:A:9:ASN:C	2.61	0.54
1:C:215:LEU:N	1:C:215:LEU:HD12	2.23	0.54
1:E:255:GLY:HA3	1:E:280:GLN:HE22	1.72	0.54
1:A:226:SER:OG	1:A:307:ALA:HB3	2.08	0.54
2:B:333:LEU:N	2:B:333:LEU:HD13	2.23	0.54
2:F:243:LEU:HD11	2:F:245:PHE:HB2	1.90	0.54
1:E:244:ARG:HD2	1:E:249:VAL:HG13	1.90	0.54
1:E:9:ASN:C	1:E:9:ASN:ND2	2.61	0.54
2:F:277:VAL:HG13	2:F:278:PRO:HD2	1.89	0.54
1:A:211:GLU:O	1:A:212:ASP:HB2	2.08	0.54
2:B:131:VAL:HG12	2:B:132:PRO:CB	2.33	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:TYR:N	2:B:4:TYR:CD1	2.75	0.54
1:C:211:GLU:O	1:C:212:ASP:HB2	2.08	0.54
2:H:115:LEU:HD23	2:H:144:ALA:CB	2.31	0.54
1:G:13:THR:CG2	2:H:5:ILE:CG2	2.72	0.54
1:A:244:ARG:HD2	1:A:249:VAL:HG13	1.90	0.54
1:C:226:SER:OG	1:C:307:ALA:HB3	2.08	0.54
1:C:244:ARG:HD2	1:C:249:VAL:HG13	1.90	0.54
2:D:126:GLN:C	2:D:131:VAL:HG23	2.18	0.54
2:D:439:LEU:HD22	2:D:442:LEU:HD11	1.88	0.54
2:D:449:LEU:CD2	1:G:97:ILE:HA	2.38	0.54
1:C:51:THR:HG21	2:D:83:ARG:HH11	1.72	0.54
2:F:126:GLN:C	2:F:131:VAL:HB	2.28	0.54
2:F:132:PRO:C	2:F:134:LYS:H	2.09	0.54
2:H:243:LEU:HD11	2:H:245:PHE:HB2	1.90	0.54
2:B:126:GLN:C	2:B:131:VAL:HB	2.28	0.54
1:E:211:GLU:O	1:E:212:ASP:HB2	2.08	0.54
2:F:441:PHE:C	2:F:442:LEU:HD12	2.29	0.54
1:G:99:VAL:HG11	1:G:142:ILE:HG12	1.90	0.54
1:A:101:GLN:HE22	1:A:138:ILE:HA	1.71	0.53
2:B:277:VAL:HG13	2:B:278:PRO:HD2	1.89	0.53
2:D:126:GLN:C	2:D:131:VAL:HB	2.28	0.53
2:F:135:ASP:O	2:F:136:LYS:CG	2.57	0.53
2:H:126:GLN:C	2:H:131:VAL:HB	2.28	0.53
2:B:132:PRO:C	2:B:134:LYS:H	2.10	0.53
1:E:215:LEU:N	1:E:215:LEU:HD12	2.23	0.53
1:E:99:VAL:HG11	1:E:142:ILE:HG12	1.90	0.53
2:B:135:ASP:O	2:B:136:LYS:CG	2.57	0.53
2:B:441:PHE:C	2:B:442:LEU:HD12	2.29	0.53
2:D:277:VAL:HG13	2:D:278:PRO:HD2	1.89	0.53
2:D:333:LEU:N	2:D:333:LEU:HD13	2.23	0.53
2:D:441:PHE:C	2:D:442:LEU:HD12	2.29	0.53
1:G:273:THR:HG22	1:G:274:SER:N	2.22	0.53
2:H:118:LEU:HD21	2:H:379:GLN:HG3	1.89	0.53
1:A:112:LEU:HD23	2:B:72:MET:HG3	1.89	0.53
1:C:77:ARG:NE	2:D:136:LYS:HZ3	2.07	0.53
2:F:3:VAL:HB	2:F:4:TYR:HD2	1.62	0.53
1:C:98:THR:OG1	2:F:449:LEU:HD23	2.08	0.53
1:G:211:GLU:O	1:G:212:ASP:HB2	2.08	0.53
1:G:226:SER:OG	1:G:307:ALA:HB3	2.08	0.53
2:B:9:HIS:CE1	2:B:11:VAL:CG2	2.92	0.53
2:D:243:LEU:HD11	2:D:245:PHE:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:ILE:HG13	1:E:311:THR:HB	1.89	0.53
1:G:143:ILE:HD13	1:G:151:ASP:OD2	2.07	0.53
1:G:215:LEU:N	1:G:215:LEU:HD12	2.23	0.53
1:E:226:SER:OG	1:E:307:ALA:HB3	2.08	0.53
2:H:69:ARG:HG3	2:H:133:TRP:CZ2	2.39	0.53
1:A:99:VAL:HG11	1:A:142:ILE:HG12	1.90	0.53
1:C:273:THR:HG22	1:C:274:SER:N	2.22	0.53
1:E:77:ARG:CZ	2:F:136:LYS:HZ3	2.21	0.53
2:H:441:PHE:C	2:H:442:LEU:HD12	2.29	0.53
2:B:118:LEU:HD21	2:B:379:GLN:HG3	1.89	0.53
1:C:251:LYS:HZ1	1:C:285:SER:HB2	1.72	0.53
1:G:225:ILE:HG13	1:G:311:THR:HB	1.89	0.53
2:B:84:ILE:HD13	2:B:362:LEU:HD11	1.89	0.53
2:F:333:LEU:HD13	2:F:333:LEU:N	2.23	0.53
1:G:9:ASN:ND2	1:G:9:ASN:C	2.61	0.53
2:H:126:GLN:HA	2:H:131:VAL:HG23	1.87	0.53
1:C:27:THR:O	1:C:57:LYS:HG2	2.09	0.53
1:C:99:VAL:HG11	1:C:142:ILE:HG12	1.90	0.53
2:D:298:VAL:HG22	2:D:312:ILE:HA	1.91	0.53
2:H:333:LEU:HD13	2:H:333:LEU:N	2.23	0.53
2:B:141:ARG:O	2:B:146:LYS:HG2	1.91	0.52
2:F:84:ILE:O	2:F:91:LEU:HD21	2.09	0.52
1:G:77:ARG:CD	2:H:136:LYS:HZ3	2.22	0.52
1:A:49:LEU:HB3	2:B:127:ALA:HB3	1.91	0.52
1:E:101:GLN:HE22	1:E:138:ILE:HA	1.71	0.52
1:G:244:ARG:HD2	1:G:249:VAL:HG13	1.90	0.52
2:H:298:VAL:HG22	2:H:312:ILE:HA	1.92	0.52
2:B:298:VAL:HG22	2:B:312:ILE:HA	1.91	0.52
1:C:161:SER:OG	1:C:162:GLU:N	2.42	0.52
2:D:84:ILE:O	2:D:91:LEU:HD21	2.09	0.52
2:D:9:HIS:CE1	2:D:11:VAL:CG2	2.92	0.52
2:F:4:TYR:CD1	2:F:4:TYR:N	2.75	0.52
1:A:273:THR:HG22	1:A:274:SER:N	2.22	0.52
2:D:125:LEU:O	2:D:129:LEU:HG	2.09	0.52
1:C:77:ARG:CZ	2:D:136:LYS:HZ3	2.22	0.52
2:F:125:LEU:O	2:F:129:LEU:HG	2.09	0.52
2:F:74:GLY:HA3	2:F:438:ALA:HB2	1.92	0.52
2:H:74:GLY:HA3	2:H:438:ALA:HB2	1.91	0.52
2:H:84:ILE:O	2:H:91:LEU:HD21	2.09	0.52
1:A:251:LYS:HZ1	1:A:285:SER:HB2	1.74	0.52
1:A:27:THR:O	1:A:57:LYS:HG2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:GLY:HA3	2:D:438:ALA:HB2	1.92	0.52
2:H:9:HIS:CE1	2:H:11:VAL:CG2	2.92	0.52
2:H:3:VAL:CA	2:H:4:TYR:CB	2.82	0.52
1:A:245:LEU:HD12	2:B:68:LEU:CD2	2.12	0.52
2:F:298:VAL:HG22	2:F:312:ILE:HA	1.91	0.52
2:F:9:HIS:CE1	2:F:11:VAL:CG2	2.92	0.52
1:A:79:SER:HG	2:B:9:HIS:CE1	2.22	0.52
1:G:27:THR:O	1:G:57:LYS:HG2	2.09	0.52
2:D:135:ASP:O	2:D:136:LYS:CG	2.57	0.52
2:B:115:LEU:HD23	2:B:144:ALA:CB	2.31	0.51
1:A:51:THR:CG2	2:B:83:ARG:HG2	2.07	0.51
1:C:49:LEU:HB3	2:D:127:ALA:C	2.30	0.51
2:D:142:LEU:CD1	2:D:146:LYS:CG	2.77	0.51
1:C:49:LEU:CD1	2:D:367:GLU:HG3	2.19	0.51
1:G:206:SER:O	1:G:208:LEU:HG	2.11	0.51
2:D:272:SER:O	1:G:6:ILE:CD1	2.57	0.51
2:H:125:LEU:O	2:H:129:LEU:HG	2.09	0.51
1:C:206:SER:O	1:C:208:LEU:HG	2.11	0.51
1:C:23:THR:CG2	2:F:95:VAL:HG23	2.38	0.51
2:H:135:ASP:O	2:H:136:LYS:CG	2.57	0.51
2:H:142:LEU:CD1	2:H:146:LYS:CD	2.88	0.51
1:A:79:SER:HB2	2:B:9:HIS:ND1	2.24	0.51
2:D:69:ARG:NH1	2:D:133:TRP:CZ2	2.79	0.51
1:G:112:LEU:HD21	2:H:76:LEU:CD2	2.36	0.51
1:A:206:SER:O	1:A:208:LEU:HG	2.11	0.51
1:C:10:TYR:CG	1:C:118:GLU:HG3	2.46	0.51
1:E:27:THR:O	1:E:57:LYS:HG2	2.09	0.51
2:B:125:LEU:O	2:B:129:LEU:HG	2.09	0.51
2:B:74:GLY:CA	2:B:438:ALA:HB2	2.41	0.51
1:E:77:ARG:CD	2:F:136:LYS:HZ1	2.22	0.51
1:G:251:LYS:O	1:G:254:GLU:HG3	2.11	0.51
2:B:403:GLU:O	1:G:257:THR:CB	2.58	0.51
2:H:114:TYR:HB2	2:H:129:LEU:HD11	1.93	0.51
1:A:161:SER:OG	1:A:162:GLU:N	2.42	0.51
1:A:251:LYS:O	1:A:254:GLU:HG3	2.11	0.51
2:B:3:VAL:CA	2:B:4:TYR:CB	2.82	0.51
2:B:69:ARG:NH1	2:B:133:TRP:CZ2	2.79	0.51
2:B:84:ILE:O	2:B:91:LEU:HD21	2.09	0.51
2:D:144:ALA:O	2:D:148:LEU:CG	2.59	0.51
1:A:10:TYR:CG	1:A:118:GLU:HG3	2.46	0.51
1:G:161:SER:OG	1:G:162:GLU:N	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:GLY:CA	2:H:438:ALA:HB2	2.41	0.51
2:B:142:LEU:CD1	2:B:146:LYS:CD	2.88	0.51
2:B:82:PHE:CZ	2:B:333:LEU:HD23	2.46	0.51
1:C:251:LYS:O	1:C:254:GLU:HG3	2.11	0.51
2:B:123:ASP:HA	2:B:126:GLN:CD	2.31	0.51
2:B:74:GLY:HA3	2:B:438:ALA:HB2	1.92	0.51
2:D:74:GLY:CA	2:D:438:ALA:HB2	2.41	0.51
1:E:161:SER:OG	1:E:162:GLU:N	2.42	0.51
1:E:224:TYR:CD2	2:F:7:PRO:HB3	2.46	0.51
2:F:114:TYR:HB2	2:F:129:LEU:HD11	1.93	0.51
2:F:142:LEU:CD1	2:F:146:LYS:CD	2.87	0.51
1:G:273:THR:CG2	1:G:274:SER:N	2.74	0.51
2:H:377:ASN:C	2:H:378:LEU:HD22	2.32	0.51
1:C:273:THR:CG2	1:C:274:SER:N	2.74	0.51
2:D:82:PHE:CZ	2:D:333:LEU:HD23	2.46	0.51
2:B:114:TYR:HB2	2:B:129:LEU:HD11	1.93	0.50
2:B:144:ALA:O	2:B:148:LEU:CG	2.59	0.50
2:B:377:ASN:C	2:B:378:LEU:HD22	2.32	0.50
1:C:79:SER:HB2	2:D:9:HIS:ND1	2.24	0.50
1:C:79:SER:HG	2:D:9:HIS:CE1	2.25	0.50
1:C:9:ASN:C	1:C:9:ASN:ND2	2.61	0.50
2:D:142:LEU:CD1	2:D:146:LYS:CD	2.88	0.50
1:C:79:SER:CB	2:D:9:HIS:CG	2.94	0.50
1:E:206:SER:O	1:E:208:LEU:HG	2.11	0.50
1:G:77:ARG:HD3	2:H:136:LYS:HZ1	1.75	0.50
2:H:314:PRO:HG3	2:H:320:LEU:HD22	1.93	0.50
1:G:79:SER:HB2	2:H:9:HIS:ND1	2.24	0.50
1:A:273:THR:CG2	1:A:274:SER:N	2.74	0.50
1:C:77:ARG:CD	2:D:136:LYS:NZ	2.74	0.50
1:E:10:TYR:CG	1:E:118:GLU:HG3	2.46	0.50
1:G:10:TYR:CG	1:G:118:GLU:HG3	2.46	0.50
1:A:224:TYR:CD2	2:B:7:PRO:HB3	2.46	0.50
2:D:114:TYR:HB2	2:D:129:LEU:HD11	1.93	0.50
1:A:79:SER:CB	2:B:9:HIS:CG	2.94	0.50
1:C:49:LEU:HB2	2:D:127:ALA:HB3	1.94	0.50
1:E:79:SER:HB2	2:F:9:HIS:ND1	2.24	0.50
2:F:82:PHE:CZ	2:F:333:LEU:HD23	2.46	0.50
2:F:74:GLY:CA	2:F:438:ALA:HB2	2.41	0.50
1:G:79:SER:CB	2:H:9:HIS:CG	2.94	0.50
2:D:449:LEU:HD21	1:G:97:ILE:C	2.25	0.50
1:E:273:THR:CG2	1:E:274:SER:N	2.74	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:TYR:CD2	2:H:7:PRO:HB3	2.46	0.50
1:G:264:HIS:HE1	1:G:267:GLY:HA2	1.77	0.50
2:H:123:ASP:HA	2:H:126:GLN:CD	2.31	0.50
1:A:77:ARG:NE	2:B:136:LYS:HZ3	2.10	0.50
2:B:157:LEU:HD23	2:B:436:ALA:HB2	1.94	0.50
1:C:224:TYR:CD2	2:D:7:PRO:HB3	2.46	0.50
1:C:35:GLY:O	2:D:12:ILE:CG2	2.34	0.50
2:D:171:LEU:HD23	2:D:172:LEU:N	2.27	0.50
2:F:157:LEU:HD23	2:F:436:ALA:HB2	1.93	0.50
2:B:171:LEU:HD23	2:B:172:LEU:N	2.27	0.50
2:D:123:ASP:HA	2:D:126:GLN:CD	2.31	0.50
2:D:377:ASN:C	2:D:378:LEU:HD22	2.32	0.50
1:E:251:LYS:O	1:E:254:GLU:HG3	2.11	0.50
2:F:243:LEU:HD13	2:F:244:ALA:N	2.27	0.50
1:A:205:SER:O	1:A:206:SER:HB3	2.12	0.50
1:A:264:HIS:HE1	1:A:267:GLY:HA2	1.77	0.50
1:C:10:TYR:CD1	1:C:118:GLU:HG3	2.47	0.50
2:D:243:LEU:HD13	2:D:244:ALA:N	2.27	0.50
1:E:205:SER:O	1:E:206:SER:HB3	2.12	0.50
2:F:144:ALA:O	2:F:148:LEU:CG	2.59	0.50
2:H:157:LEU:HD23	2:H:436:ALA:HB2	1.93	0.50
2:H:82:PHE:CZ	2:H:333:LEU:HD23	2.46	0.50
1:A:49:LEU:O	2:B:127:ALA:C	2.49	0.50
2:B:243:LEU:HD13	2:B:244:ALA:N	2.27	0.50
2:D:14:ASN:O	2:D:15:GLU:O	2.30	0.50
2:D:314:PRO:HG3	2:D:320:LEU:HD22	1.93	0.50
1:E:264:HIS:HE1	1:E:267:GLY:HA2	1.77	0.50
2:F:69:ARG:NH1	2:F:133:TRP:CZ2	2.79	0.50
2:F:314:PRO:HG3	2:F:320:LEU:HD22	1.93	0.50
1:G:10:TYR:CD1	1:G:118:GLU:HG3	2.47	0.50
1:G:77:ARG:HD2	2:H:15:GLU:CG	2.42	0.50
1:G:112:LEU:CG	2:H:76:LEU:HD21	2.42	0.50
1:A:110:PRO:HG3	2:B:135:ASP:CG	2.32	0.49
2:B:14:ASN:O	2:B:15:GLU:O	2.30	0.49
1:C:112:LEU:HD13	2:D:76:LEU:HD22	1.70	0.49
1:E:79:SER:CB	2:F:9:HIS:CG	2.94	0.49
1:G:205:SER:O	1:G:206:SER:HB3	2.12	0.49
1:A:10:TYR:CD1	1:A:118:GLU:HG3	2.47	0.49
2:B:314:PRO:HG3	2:B:320:LEU:HD22	1.93	0.49
1:A:112:LEU:CD2	2:B:72:MET:HG3	2.43	0.49
1:C:205:SER:O	1:C:206:SER:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ARG:HD2	2:D:15:GLU:CG	2.42	0.49
2:D:175:VAL:CG1	2:D:200:VAL:HG11	2.42	0.49
2:D:258:PHE:O	2:D:401:ALA:HB1	2.13	0.49
2:F:123:ASP:HA	2:F:126:GLN:CD	2.31	0.49
2:F:377:ASN:C	2:F:378:LEU:HD22	2.32	0.49
1:G:77:ARG:HH21	2:H:15:GLU:C	2.16	0.49
2:B:258:PHE:O	2:B:401:ALA:HB1	2.13	0.49
2:H:175:VAL:CG1	2:H:200:VAL:HG11	2.42	0.49
2:H:243:LEU:HD13	2:H:244:ALA:N	2.27	0.49
2:H:258:PHE:O	2:H:401:ALA:HB1	2.13	0.49
2:F:171:LEU:HD23	2:F:172:LEU:N	2.27	0.49
2:D:157:LEU:HD23	2:D:436:ALA:HB2	1.93	0.49
2:F:175:VAL:CG1	2:F:200:VAL:HG11	2.42	0.49
2:H:14:ASN:O	2:H:15:GLU:O	2.30	0.49
2:H:39:ILE:HD11	2:H:217:LYS:HB3	1.95	0.49
2:B:175:VAL:CG1	2:B:200:VAL:HG11	2.42	0.49
2:B:9:HIS:CE1	2:B:11:VAL:HG21	2.48	0.49
2:D:9:HIS:CE1	2:D:11:VAL:HG21	2.48	0.49
1:E:112:LEU:HD11	2:F:76:LEU:HD22	1.90	0.49
2:H:144:ALA:O	2:H:148:LEU:CG	2.59	0.49
2:H:171:LEU:HD23	2:H:172:LEU:N	2.27	0.49
2:H:82:PHE:CE1	2:H:333:LEU:HD23	2.48	0.49
2:B:110:LEU:HB3	2:B:129:LEU:HD22	1.55	0.49
1:C:77:ARG:HD3	2:D:136:LYS:NZ	2.26	0.49
1:E:10:TYR:CD1	1:E:118:GLU:HG3	2.47	0.49
2:F:126:GLN:HA	2:F:131:VAL:HG23	1.87	0.49
2:F:39:ILE:HD11	2:F:217:LYS:HB3	1.95	0.49
2:D:39:ILE:HD11	2:D:217:LYS:HB3	1.95	0.49
2:D:303:PHE:HB2	2:D:307:ALA:HB3	1.95	0.49
2:D:392:LEU:HD23	2:D:393:ASN:N	2.28	0.49
2:F:329:GLN:H	2:F:333:LEU:HD11	1.78	0.49
2:B:329:GLN:H	2:B:333:LEU:HD11	1.78	0.48
2:F:14:ASN:O	2:F:15:GLU:O	2.30	0.48
2:F:82:PHE:CE1	2:F:333:LEU:HD23	2.48	0.48
1:G:112:LEU:HD23	2:H:72:MET:CG	2.30	0.48
1:G:232:ILE:HG13	1:G:295:ALA:HA	1.95	0.48
2:F:392:LEU:HD23	2:F:393:ASN:N	2.28	0.48
2:H:392:LEU:HD23	2:H:393:ASN:N	2.28	0.48
1:A:77:ARG:HH21	2:B:15:GLU:C	2.16	0.48
1:A:112:LEU:HD13	2:B:76:LEU:HD13	1.95	0.48
2:H:275:VAL:HG12	2:H:277:VAL:HG23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:PHE:CE1	2:B:333:LEU:HD23	2.48	0.48
2:D:275:VAL:HG12	2:D:277:VAL:HG23	1.96	0.48
2:D:329:GLN:H	2:D:333:LEU:HD11	1.78	0.48
2:D:82:PHE:CE1	2:D:333:LEU:HD23	2.48	0.48
1:G:47:SER:OG	1:G:49:LEU:HD23	2.13	0.48
2:F:159:VAL:HA	2:F:170:LEU:HD21	1.96	0.48
2:F:258:PHE:O	2:F:401:ALA:HB1	2.13	0.48
2:H:329:GLN:H	2:H:333:LEU:HD11	1.78	0.48
1:A:47:SER:OG	1:A:49:LEU:HD23	2.13	0.48
1:C:186:ILE:HD12	1:C:186:ILE:N	2.29	0.48
1:C:264:HIS:HE1	1:C:267:GLY:HA2	1.77	0.48
1:E:232:ILE:HG13	1:E:295:ALA:HA	1.95	0.48
1:E:281:GLU:OE1	2:F:4:TYR:CZ	2.67	0.48
2:H:161:GLN:CB	2:H:164:ALA:HB3	2.44	0.48
2:H:356:SER:HB3	2:H:392:LEU:HD21	1.96	0.48
1:G:281:GLU:OE1	2:H:4:TYR:CZ	2.67	0.48
1:A:232:ILE:HG13	1:A:295:ALA:HA	1.96	0.48
2:B:392:LEU:HD23	2:B:393:ASN:N	2.28	0.48
1:E:127:PHE:CB	1:E:192:GLY:HA2	2.44	0.48
1:E:49:LEU:CD1	2:F:367:GLU:CG	2.74	0.48
2:F:175:VAL:HG12	2:F:200:VAL:HG11	1.96	0.48
1:E:112:LEU:HD13	2:F:76:LEU:CD1	2.44	0.48
1:G:112:LEU:HD13	2:H:76:LEU:HD11	1.95	0.48
2:B:159:VAL:HA	2:B:170:LEU:HD21	1.96	0.48
2:B:285:THR:CG2	2:B:343:THR:HG22	2.39	0.48
2:D:181:ALA:HB2	2:D:242:THR:HA	1.96	0.48
1:E:110:PRO:HB2	2:F:135:ASP:OD1	2.11	0.48
1:G:127:PHE:CB	1:G:192:GLY:HA2	2.44	0.48
2:H:3:VAL:HB	2:H:4:TYR:HD2	1.62	0.48
1:A:186:ILE:N	1:A:186:ILE:HD12	2.29	0.48
1:A:281:GLU:OE1	2:B:4:TYR:CZ	2.67	0.48
1:C:47:SER:OG	1:C:49:LEU:HD23	2.13	0.48
1:G:127:PHE:HB2	1:G:192:GLY:HA2	1.96	0.48
2:H:175:VAL:HG12	2:H:200:VAL:HG11	1.96	0.48
1:A:127:PHE:CB	1:A:192:GLY:HA2	2.44	0.48
2:B:181:ALA:HB2	2:B:242:THR:HA	1.96	0.48
1:C:281:GLU:OE1	2:D:4:TYR:CZ	2.67	0.48
1:E:186:ILE:HD12	1:E:186:ILE:N	2.29	0.48
2:H:9:HIS:CE1	2:H:11:VAL:HG21	2.48	0.48
2:H:69:ARG:NH1	2:H:133:TRP:CZ2	2.79	0.48
2:B:175:VAL:HG12	2:B:200:VAL:HG11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ILE:HD11	2:B:217:LYS:HB3	1.95	0.47
2:B:356:SER:HB3	2:B:392:LEU:HD21	1.96	0.47
1:C:77:ARG:HH21	2:D:15:GLU:C	2.16	0.47
2:F:161:GLN:CB	2:F:164:ALA:HB3	2.44	0.47
2:F:303:PHE:HB2	2:F:307:ALA:HB3	1.95	0.47
2:B:303:PHE:HB2	2:B:307:ALA:HB3	1.95	0.47
1:E:159:ARG:HH11	1:E:159:ARG:HG2	1.79	0.47
2:F:356:SER:HB3	2:F:392:LEU:HD21	1.96	0.47
1:G:77:ARG:O	2:H:13:HIS:CE1	2.67	0.47
1:A:159:ARG:HG2	1:A:159:ARG:HH11	1.79	0.47
2:B:441:PHE:O	2:B:442:LEU:HD12	2.14	0.47
1:E:35:GLY:O	2:F:12:ILE:CG2	2.33	0.47
2:F:158:LEU:HD12	2:F:440:HIS:CD2	2.49	0.47
2:H:288:HIS:HB2	2:H:299:THR:HG22	1.96	0.47
2:H:303:PHE:HB2	2:H:307:ALA:HB3	1.95	0.47
1:C:232:ILE:HG13	1:C:295:ALA:HA	1.96	0.47
2:D:159:VAL:HA	2:D:170:LEU:HD21	1.96	0.47
2:D:277:VAL:HG21	2:D:448:PRO:HD2	1.97	0.47
1:E:47:SER:OG	1:E:49:LEU:HD23	2.14	0.47
1:E:77:ARG:HD2	2:F:15:GLU:CG	2.42	0.47
1:E:77:ARG:NE	2:F:136:LYS:HZ3	2.13	0.47
2:H:181:ALA:HB2	2:H:242:THR:HA	1.96	0.47
2:B:161:GLN:CB	2:B:164:ALA:HB3	2.44	0.47
2:B:288:HIS:HB2	2:B:299:THR:HG22	1.96	0.47
1:C:77:ARG:O	2:D:13:HIS:CE1	2.67	0.47
2:D:110:LEU:HB3	2:D:129:LEU:HD22	1.55	0.47
1:E:77:ARG:O	2:F:13:HIS:CE1	2.67	0.47
2:F:9:HIS:CE1	2:F:11:VAL:HG21	2.48	0.47
2:F:288:HIS:HB2	2:F:299:THR:HG22	1.96	0.47
2:F:43:THR:OG1	2:F:204:ARG:NH1	2.48	0.47
1:G:186:ILE:N	1:G:186:ILE:HD12	2.29	0.47
2:H:441:PHE:O	2:H:442:LEU:HD12	2.15	0.47
1:A:127:PHE:HB2	1:A:192:GLY:HA2	1.96	0.47
2:B:275:VAL:HG12	2:B:277:VAL:HG23	1.95	0.47
2:D:158:LEU:HD12	2:D:440:HIS:CD2	2.49	0.47
2:D:161:GLN:CB	2:D:164:ALA:HB3	2.44	0.47
2:D:288:HIS:HB2	2:D:299:THR:HG22	1.96	0.47
2:D:43:THR:OG1	2:D:204:ARG:NH1	2.48	0.47
1:G:110:PRO:HG3	2:H:135:ASP:CB	2.45	0.47
2:B:158:LEU:HD12	2:B:440:HIS:CD2	2.49	0.47
2:B:43:THR:OG1	2:B:204:ARG:NH1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ARG:HH11	1:C:159:ARG:HG2	1.79	0.47
1:C:203:VAL:HG22	1:C:261:ILE:HD12	1.97	0.47
2:D:175:VAL:HG12	2:D:200:VAL:HG11	1.96	0.47
1:E:203:VAL:HG22	1:E:261:ILE:HD12	1.97	0.47
2:F:179:PHE:CG	2:F:218:ILE:HD11	2.50	0.47
2:F:441:PHE:O	2:F:442:LEU:HD12	2.15	0.47
2:H:159:VAL:HA	2:H:170:LEU:HD21	1.96	0.47
2:H:158:LEU:HD12	2:H:440:HIS:CD2	2.49	0.47
2:B:255:MET:HE1	2:B:399:LEU:HD13	1.96	0.47
2:D:356:SER:HB3	2:D:392:LEU:HD21	1.96	0.47
2:F:181:ALA:HB2	2:F:242:THR:HA	1.96	0.47
2:H:277:VAL:HG21	2:H:448:PRO:HD2	1.97	0.47
1:A:203:VAL:HG22	1:A:261:ILE:HD12	1.97	0.47
2:D:441:PHE:O	2:D:442:LEU:HD12	2.15	0.47
2:F:277:VAL:HG21	2:F:448:PRO:HD2	1.97	0.47
2:D:447:ASN:ND2	1:G:96:GLY:O	2.48	0.47
1:E:23:THR:HG21	2:H:95:VAL:HG23	1.89	0.47
1:E:199:LYS:HD2	1:E:264:HIS:CE1	2.50	0.47
2:F:275:VAL:HG12	2:F:277:VAL:HG23	1.96	0.47
1:G:203:VAL:HG22	1:G:261:ILE:HD12	1.97	0.47
1:A:77:ARG:O	2:B:13:HIS:CE1	2.67	0.47
1:C:127:PHE:CB	1:C:192:GLY:HA2	2.44	0.47
1:E:68:LYS:HB2	1:E:89:GLN:HB3	1.97	0.47
2:F:3:VAL:CA	2:F:4:TYR:CG	2.98	0.47
1:G:68:LYS:HB2	1:G:89:GLN:HB3	1.97	0.47
2:H:36:PRO:HB2	2:H:204:ARG:HA	1.98	0.47
1:A:68:LYS:HB2	1:A:89:GLN:HB3	1.97	0.46
2:B:179:PHE:CG	2:B:218:ILE:HD11	2.50	0.46
1:C:49:LEU:C	2:D:127:ALA:HB1	2.36	0.46
2:D:95:VAL:HB	1:G:23:THR:HG21	1.98	0.46
1:E:127:PHE:HB2	1:E:192:GLY:HA2	1.96	0.46
2:B:137:ASN:OD1	2:B:143:ASP:OD2	2.34	0.46
2:B:277:VAL:HG21	2:B:448:PRO:HD2	1.97	0.46
2:B:304:THR:O	2:B:306:SER:N	2.48	0.46
2:D:111:ALA:HA	2:D:129:LEU:HD13	1.97	0.46
2:D:36:PRO:HB2	2:D:204:ARG:HA	1.98	0.46
2:H:255:MET:HE2	2:H:399:LEU:HD22	1.97	0.46
2:B:111:ALA:HA	2:B:129:LEU:HD13	1.97	0.46
2:B:3:VAL:CA	2:B:4:TYR:CG	2.98	0.46
2:D:159:VAL:O	2:D:159:VAL:HG13	2.16	0.46
2:F:69:ARG:NH1	2:F:133:TRP:HH2	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:LEU:H	2:F:68:LEU:HD21	1.78	0.46
1:A:35:GLY:O	2:B:12:ILE:CG2	2.33	0.46
1:C:68:LYS:HB2	1:C:89:GLN:HB3	1.97	0.46
2:D:179:PHE:CG	2:D:218:ILE:HD11	2.50	0.46
2:H:43:THR:OG1	2:H:204:ARG:NH1	2.48	0.46
1:E:77:ARG:CD	2:F:136:LYS:NZ	2.79	0.46
2:F:17:THR:HG23	2:F:136:LYS:NZ	2.31	0.46
2:F:137:ASN:OD1	2:F:143:ASP:OD2	2.34	0.46
1:G:48:ARG:HD3	1:G:48:ARG:HA	1.76	0.46
2:B:159:VAL:O	2:B:159:VAL:HG13	2.16	0.46
2:D:3:VAL:CA	2:D:4:TYR:CG	2.98	0.46
1:E:49:LEU:HB3	2:F:127:ALA:CB	2.46	0.46
1:G:159:ARG:HG2	1:G:159:ARG:HH11	1.79	0.46
2:H:159:VAL:O	2:H:159:VAL:HG13	2.16	0.46
1:A:77:ARG:HD2	2:B:15:GLU:CG	2.42	0.46
1:C:23:THR:OG1	1:C:91:ILE:HD11	2.16	0.46
2:D:16:SER:O	2:D:17:THR:OG1	2.34	0.46
2:D:181:ALA:HB1	2:D:182:PRO:CD	2.46	0.46
2:F:255:MET:HE2	2:F:399:LEU:HD22	1.98	0.46
1:G:235:LEU:HD23	1:G:235:LEU:C	2.36	0.46
2:H:179:PHE:CG	2:H:218:ILE:HD11	2.50	0.46
2:H:351:LEU:HD12	2:H:399:LEU:CD1	2.46	0.46
2:H:3:VAL:CA	2:H:4:TYR:CG	2.98	0.46
1:A:235:LEU:HD23	1:A:235:LEU:C	2.36	0.46
1:C:49:LEU:HB2	2:D:127:ALA:CB	2.45	0.46
1:E:112:LEU:CD2	2:F:76:LEU:HD22	2.42	0.46
1:E:290:THR:HG22	1:E:291:LEU:N	2.31	0.46
2:F:111:ALA:HA	2:F:129:LEU:HD13	1.97	0.46
1:C:97:ILE:HA	2:F:449:LEU:HD21	1.75	0.46
2:H:137:ASN:OD1	2:H:143:ASP:OD2	2.34	0.46
1:A:245:LEU:CD1	2:B:68:LEU:HD22	2.18	0.46
2:D:17:THR:O	2:D:18:CYS:C	2.54	0.46
1:E:235:LEU:HD23	1:E:235:LEU:C	2.36	0.46
1:E:77:ARG:HD2	2:F:15:GLU:CB	2.46	0.46
1:G:23:THR:OG1	1:G:91:ILE:HD11	2.16	0.46
1:A:199:LYS:HD2	1:A:264:HIS:CE1	2.50	0.45
1:C:199:LYS:HD2	1:C:264:HIS:CE1	2.50	0.45
2:D:158:LEU:HD23	2:D:159:VAL:N	2.31	0.45
1:E:36:SER:CB	2:F:12:ILE:HB	2.46	0.45
2:F:230:THR:HG21	2:F:248:TYR:CD1	2.51	0.45
1:G:49:LEU:HB2	2:H:127:ALA:HB3	1.96	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:14:ASN:O	2:H:15:GLU:C	2.54	0.45
1:A:290:THR:HG22	1:A:291:LEU:N	2.31	0.45
1:A:77:ARG:HD2	2:B:15:GLU:CB	2.46	0.45
2:B:17:THR:O	2:B:18:CYS:C	2.54	0.45
1:C:235:LEU:HD23	1:C:235:LEU:C	2.37	0.45
2:D:230:THR:HG21	2:D:248:TYR:CD1	2.51	0.45
2:D:230:THR:HG21	2:D:248:TYR:HD1	1.82	0.45
1:G:199:LYS:HD2	1:G:264:HIS:CE1	2.50	0.45
2:H:16:SER:O	2:H:17:THR:OG1	2.34	0.45
2:B:181:ALA:HB1	2:B:182:PRO:CD	2.46	0.45
2:B:36:PRO:HB2	2:B:204:ARG:HA	1.97	0.45
2:D:131:VAL:HG12	2:D:132:PRO:HB3	1.91	0.45
2:F:159:VAL:HG13	2:F:159:VAL:O	2.16	0.45
2:F:158:LEU:HD23	2:F:159:VAL:N	2.31	0.45
2:H:111:ALA:HA	2:H:129:LEU:HD13	1.98	0.45
2:H:230:THR:HG21	2:H:248:TYR:HD1	1.82	0.45
1:A:36:SER:CB	2:B:12:ILE:HB	2.46	0.45
2:D:151:LEU:HD12	2:D:154:VAL:HG21	1.98	0.45
1:E:11:MET:O	1:E:12:ASP:HB2	2.17	0.45
2:F:131:VAL:HG12	2:F:132:PRO:HD3	1.99	0.45
2:F:36:PRO:HB2	2:F:204:ARG:HA	1.98	0.45
2:H:230:THR:HG21	2:H:248:TYR:CD1	2.51	0.45
1:A:137:PRO:HD2	1:A:140:ASP:OD2	2.17	0.45
2:B:14:ASN:O	2:B:15:GLU:C	2.54	0.45
2:B:351:LEU:HD12	2:B:399:LEU:CD1	2.46	0.45
2:D:292:ILE:HD12	2:D:293:GLN:N	2.32	0.45
2:D:367:GLU:C	2:D:368:LEU:HD23	2.37	0.45
2:D:255:MET:HE2	2:D:399:LEU:HD22	1.97	0.45
1:G:190:LYS:HD2	1:G:191:THR:H	1.82	0.45
2:B:158:LEU:HD23	2:B:159:VAL:N	2.31	0.45
2:B:230:THR:HG21	2:B:248:TYR:CD1	2.51	0.45
1:C:190:LYS:HD2	1:C:191:THR:H	1.82	0.45
1:E:77:ARG:HH21	2:F:15:GLU:C	2.16	0.45
2:F:151:LEU:HD12	2:F:154:VAL:HG21	1.98	0.45
2:F:181:ALA:HB1	2:F:182:PRO:CD	2.46	0.45
2:F:326:LEU:O	2:F:333:LEU:HD12	2.17	0.45
2:F:395:ILE:HD12	2:F:395:ILE:C	2.37	0.45
1:G:137:PRO:HD2	1:G:140:ASP:OD2	2.17	0.45
1:G:290:THR:HG22	1:G:291:LEU:N	2.31	0.45
1:G:77:ARG:HD2	2:H:15:GLU:CB	2.46	0.45
1:G:36:SER:CB	2:H:12:ILE:HB	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:VAL:CB	2:H:132:PRO:HA	2.36	0.45
2:H:158:LEU:HD23	2:H:159:VAL:N	2.31	0.45
1:A:245:LEU:C	2:B:68:LEU:HD13	2.36	0.45
1:C:127:PHE:HB2	1:C:192:GLY:HA2	1.97	0.45
1:C:98:THR:H	2:F:449:LEU:CD2	2.12	0.45
2:D:351:LEU:HD12	2:D:399:LEU:CD1	2.46	0.45
1:E:23:THR:OG1	1:E:91:ILE:HD11	2.16	0.45
1:A:49:LEU:C	2:B:127:ALA:HB1	2.37	0.45
1:A:7:LEU:HD11	1:A:169:ILE:HG13	1.99	0.45
1:A:23:THR:OG1	1:A:91:ILE:HD11	2.16	0.45
1:C:137:PRO:HD2	1:C:140:ASP:OD2	2.17	0.45
2:D:131:VAL:HG12	2:D:132:PRO:HD3	1.99	0.45
2:D:304:THR:O	2:D:306:SER:N	2.48	0.45
2:D:381:LEU:HD23	2:D:381:LEU:C	2.37	0.45
1:E:23:THR:HG21	2:H:95:VAL:CB	2.46	0.45
2:F:324:GLU:HG3	2:F:428:LEU:HD11	1.99	0.45
2:H:14:ASN:ND2	2:H:14:ASN:N	2.64	0.45
2:B:151:LEU:HD12	2:B:154:VAL:HG21	1.98	0.45
2:B:292:ILE:HD12	2:B:293:GLN:N	2.32	0.45
2:B:395:ILE:C	2:B:395:ILE:HD12	2.37	0.45
1:C:77:ARG:HD2	2:D:15:GLU:CB	2.46	0.45
2:D:14:ASN:O	2:D:15:GLU:C	2.54	0.45
2:D:37:ALA:HB1	2:D:38:PRO:HD2	1.98	0.45
1:C:112:LEU:HD13	2:D:76:LEU:CD1	2.47	0.45
1:E:190:LYS:HD2	1:E:191:THR:H	1.82	0.45
2:H:110:LEU:HB3	2:H:129:LEU:HD22	1.55	0.45
2:H:132:PRO:CD	2:H:135:ASP:HA	2.47	0.45
2:H:181:ALA:HB1	2:H:182:PRO:CD	2.46	0.45
2:H:176:VAL:CG2	2:H:198:THR:HG21	2.46	0.45
2:H:381:LEU:HD23	2:H:381:LEU:C	2.37	0.45
1:C:290:THR:HG22	1:C:291:LEU:N	2.31	0.45
2:D:126:GLN:HA	2:D:131:VAL:HG23	1.87	0.45
2:D:395:ILE:C	2:D:395:ILE:HD12	2.37	0.45
1:E:137:PRO:HD2	1:E:140:ASP:OD2	2.17	0.45
2:F:17:THR:CG2	2:F:136:LYS:HD3	2.47	0.45
2:F:175:VAL:HG12	2:F:200:VAL:CB	2.47	0.45
2:B:230:THR:HG21	2:B:248:TYR:HD1	1.82	0.44
2:D:326:LEU:O	2:D:333:LEU:HD12	2.17	0.44
2:F:14:ASN:O	2:F:15:GLU:C	2.54	0.44
1:G:7:LEU:HD11	1:G:169:ILE:HG13	1.99	0.44
2:H:292:ILE:HD12	2:H:293:GLN:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:MET:O	1:A:12:ASP:HB2	2.17	0.44
1:A:82:THR:OG1	2:B:136:LYS:HE3	2.18	0.44
2:B:312:ILE:HG21	2:B:327:THR:HG21	1.99	0.44
2:B:326:LEU:O	2:B:333:LEU:CD1	2.66	0.44
1:C:36:SER:CB	2:D:12:ILE:HB	2.46	0.44
2:D:95:VAL:CG2	1:G:23:THR:HG21	2.47	0.44
2:F:367:GLU:C	2:F:368:LEU:HD23	2.37	0.44
2:H:255:MET:HE3	2:H:399:LEU:HB3	1.99	0.44
1:A:190:LYS:HD2	1:A:191:THR:H	1.82	0.44
2:B:121:THR:HA	2:B:372:LEU:HD11	2.00	0.44
2:B:175:VAL:HG12	2:B:200:VAL:CB	2.47	0.44
2:B:326:LEU:O	2:B:333:LEU:HD12	2.17	0.44
2:D:137:ASN:OD1	2:D:143:ASP:OD2	2.34	0.44
2:D:285:THR:CG2	2:D:343:THR:HG22	2.39	0.44
1:E:7:LEU:HD11	1:E:169:ILE:HG13	1.99	0.44
2:F:17:THR:O	2:F:18:CYS:C	2.54	0.44
2:F:255:MET:HE3	2:F:399:LEU:HB3	1.99	0.44
1:G:151:ASP:O	1:G:322:ARG:HB2	2.18	0.44
2:H:17:THR:O	2:H:18:CYS:C	2.54	0.44
2:H:367:GLU:C	2:H:368:LEU:HD23	2.37	0.44
2:H:428:LEU:HD13	2:H:444:ARG:HA	1.99	0.44
2:B:132:PRO:CD	2:B:135:ASP:HA	2.47	0.44
2:B:367:GLU:C	2:B:368:LEU:HD23	2.37	0.44
2:B:37:ALA:HB1	2:B:38:PRO:HD2	1.99	0.44
2:B:324:GLU:HG3	2:B:428:LEU:HD11	1.99	0.44
2:D:132:PRO:C	2:D:134:LYS:N	2.70	0.44
2:F:285:THR:CG2	2:F:343:THR:HG22	2.39	0.44
1:G:244:ARG:HD2	1:G:249:VAL:CG1	2.48	0.44
1:A:109:MET:HA	1:A:110:PRO:HD2	1.86	0.44
2:B:381:LEU:HD23	2:B:381:LEU:C	2.37	0.44
1:C:299:PRO:HA	1:C:300:PRO:HD3	1.84	0.44
1:C:110:PRO:HB3	2:D:135:ASP:OD1	2.07	0.44
2:D:121:THR:HA	2:D:372:LEU:HD11	2.00	0.44
2:F:16:SER:O	2:F:17:THR:OG1	2.34	0.44
2:F:351:LEU:HD12	2:F:399:LEU:CD1	2.46	0.44
2:H:175:VAL:HG12	2:H:200:VAL:CB	2.47	0.44
1:C:7:LEU:HD11	1:C:169:ILE:HG13	1.99	0.44
2:D:131:VAL:CB	2:D:132:PRO:HA	2.36	0.44
2:D:175:VAL:HG12	2:D:200:VAL:CB	2.47	0.44
2:F:381:LEU:HD23	2:F:381:LEU:C	2.37	0.44
2:F:37:ALA:HB1	2:F:38:PRO:HD2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:326:LEU:O	2:H:333:LEU:HD12	2.17	0.44
2:H:37:ALA:HB1	2:H:38:PRO:HD2	1.99	0.44
2:D:4:TYR:HD1	2:D:5:ILE:H	1.66	0.44
1:C:112:LEU:CD1	2:D:76:LEU:HD21	2.38	0.44
1:E:151:ASP:O	1:E:322:ARG:HB2	2.18	0.44
2:F:132:PRO:CD	2:F:135:ASP:HA	2.47	0.44
2:F:17:THR:HG21	2:F:136:LYS:HD3	1.99	0.44
2:F:180:THR:HB	2:F:184:LEU:HD13	2.00	0.44
2:F:292:ILE:HD12	2:F:293:GLN:N	2.32	0.44
2:F:312:ILE:HG21	2:F:327:THR:HG21	2.00	0.44
1:C:97:ILE:CA	2:F:449:LEU:HD22	2.38	0.44
1:G:243:LYS:HB2	1:G:248:TYR:CE2	2.53	0.44
2:H:324:GLU:HG3	2:H:428:LEU:HD11	1.99	0.44
2:B:124:ARG:HD3	2:B:372:LEU:HD13	2.00	0.44
2:D:134:LYS:O	2:D:135:ASP:CB	2.65	0.44
2:D:326:LEU:O	2:D:333:LEU:CD1	2.66	0.44
2:F:132:PRO:C	2:F:134:LYS:N	2.70	0.44
2:F:131:VAL:CB	2:F:132:PRO:HA	2.36	0.44
2:F:230:THR:HG21	2:F:248:TYR:HD1	1.82	0.44
2:F:326:LEU:O	2:F:333:LEU:CD1	2.66	0.44
2:F:249:VAL:HG11	2:F:395:ILE:HG22	2.00	0.44
1:G:129:GLU:N	1:G:129:GLU:OE1	2.51	0.44
1:G:11:MET:O	1:G:12:ASP:HB2	2.17	0.44
1:G:224:TYR:CE2	1:G:294:HIS:CE1	3.06	0.44
2:H:110:LEU:HD21	2:H:125:LEU:HD22	2.00	0.44
2:H:312:ILE:HG21	2:H:327:THR:HG21	1.99	0.44
2:H:326:LEU:O	2:H:333:LEU:CD1	2.66	0.44
2:H:395:ILE:HD12	2:H:395:ILE:C	2.37	0.44
1:A:49:LEU:CB	2:B:127:ALA:HB3	2.48	0.44
1:C:243:LYS:HB2	1:C:248:TYR:CE2	2.53	0.44
1:E:77:ARG:NE	2:F:136:LYS:NZ	2.66	0.44
2:F:106:VAL:HG13	2:F:359:LEU:CD1	2.48	0.44
2:F:428:LEU:HD13	2:F:444:ARG:HA	1.99	0.44
1:E:245:LEU:HA	2:F:68:LEU:HD11	0.87	0.44
1:E:42:PRO:HB2	1:E:58:LEU:HD23	2.00	0.43
1:G:42:PRO:HB2	1:G:58:LEU:HD23	2.00	0.43
2:H:249:VAL:HG11	2:H:395:ILE:HG22	2.00	0.43
1:A:299:PRO:HA	1:A:300:PRO:HD3	1.84	0.43
1:A:49:LEU:HB3	2:B:127:ALA:CB	2.48	0.43
2:B:110:LEU:HD21	2:B:125:LEU:HD22	2.00	0.43
1:C:321:ASP:HB3	1:C:326:ARG:HG3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ARG:HD2	1:E:249:VAL:CG1	2.48	0.43
1:G:139:PHE:CE1	1:G:143:ILE:HD11	2.53	0.43
2:H:151:LEU:HD12	2:H:154:VAL:HG21	1.98	0.43
1:A:151:ASP:O	1:A:322:ARG:HB2	2.18	0.43
1:A:42:PRO:HB2	1:A:58:LEU:HD23	2.00	0.43
2:H:221:PHE:O	2:H:225:VAL:HG23	2.19	0.43
2:H:285:THR:CG2	2:H:343:THR:HG22	2.39	0.43
1:A:206:SER:O	1:A:208:LEU:N	2.50	0.43
1:A:217:LEU:CD1	1:A:219:ASP:HB2	2.48	0.43
1:C:244:ARG:HD2	1:C:249:VAL:CG1	2.48	0.43
2:D:255:MET:HE3	2:D:399:LEU:HB3	1.99	0.43
2:D:428:LEU:HD13	2:D:444:ARG:HA	1.99	0.43
1:E:139:PHE:CE1	1:E:143:ILE:HD11	2.53	0.43
1:E:243:LYS:HB2	1:E:248:TYR:CE2	2.53	0.43
1:A:139:PHE:CE1	1:A:143:ILE:HD11	2.53	0.43
1:A:244:ARG:HD2	1:A:249:VAL:CG1	2.47	0.43
2:B:279:MET:HB3	2:B:279:MET:HE3	1.90	0.43
1:C:49:LEU:CB	2:D:127:ALA:HB1	2.47	0.43
1:C:299:PRO:HG2	2:D:13:HIS:HB2	2.01	0.43
2:D:180:THR:HB	2:D:184:LEU:HD13	2.00	0.43
2:D:221:PHE:O	2:D:225:VAL:HG23	2.19	0.43
2:D:124:ARG:HD3	2:D:372:LEU:HD13	2.00	0.43
1:E:112:LEU:HA	1:E:113:PRO:HA	1.80	0.43
1:E:236:MET:HG3	1:E:248:TYR:CD2	2.54	0.43
1:E:321:ASP:HB3	1:E:326:ARG:HG3	2.01	0.43
2:F:304:THR:O	2:F:306:SER:N	2.48	0.43
2:B:16:SER:O	2:B:17:THR:OG1	2.34	0.43
2:B:180:THR:HB	2:B:184:LEU:HD13	2.00	0.43
2:D:201:VAL:HG12	2:D:203:PRO:HD3	2.01	0.43
1:E:48:ARG:HA	1:E:48:ARG:HD3	1.76	0.43
1:E:49:LEU:HB3	2:F:127:ALA:HB3	2.00	0.43
2:F:124:ARG:O	2:F:128:ILE:HG13	2.19	0.43
2:F:4:TYR:HD1	2:F:5:ILE:H	1.66	0.43
1:A:236:MET:HG3	1:A:248:TYR:CD2	2.54	0.43
1:A:243:LYS:HB2	1:A:248:TYR:CE2	2.53	0.43
2:B:142:LEU:O	2:B:146:LYS:CB	2.64	0.43
2:B:175:VAL:HG12	2:B:200:VAL:HB	2.01	0.43
2:B:428:LEU:HD13	2:B:444:ARG:HA	1.99	0.43
2:D:249:VAL:HG11	2:D:395:ILE:HG22	2.00	0.43
2:D:324:GLU:HG3	2:D:428:LEU:HD11	1.99	0.43
1:C:6:ILE:HG12	2:F:273:THR:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:124:ARG:O	2:H:128:ILE:HG13	2.19	0.43
2:H:148:LEU:HD22	2:H:197:TYR:HB2	2.01	0.43
2:B:102:SER:HB3	2:B:105:ALA:HB3	2.01	0.43
2:B:3:VAL:C	2:B:4:TYR:CG	2.92	0.43
2:B:4:TYR:HD1	2:B:5:ILE:H	1.66	0.43
1:C:191:THR:HG22	1:C:192:GLY:N	2.34	0.43
2:D:14:ASN:ND2	2:D:14:ASN:N	2.65	0.43
2:D:179:PHE:CD2	2:D:218:ILE:HD11	2.54	0.43
2:D:3:VAL:C	2:D:4:TYR:CG	2.92	0.43
1:E:224:TYR:CE2	1:E:294:HIS:CE1	3.06	0.43
2:F:124:ARG:HD3	2:F:372:LEU:HD13	2.00	0.43
2:F:72:MET:O	2:F:76:LEU:HD23	2.19	0.43
2:H:102:SER:HB3	2:H:105:ALA:HB3	2.01	0.43
2:H:304:THR:O	2:H:306:SER:N	2.48	0.43
1:A:321:ASP:HB3	1:A:326:ARG:HG3	2.01	0.43
2:B:131:VAL:CB	2:B:132:PRO:HA	2.36	0.43
2:B:179:PHE:CD2	2:B:218:ILE:HD11	2.54	0.43
1:C:11:MET:O	1:C:12:ASP:HB2	2.17	0.43
1:C:139:PHE:CE1	1:C:143:ILE:HD11	2.53	0.43
1:C:151:ASP:O	1:C:322:ARG:HB2	2.18	0.43
1:C:42:PRO:HB2	1:C:58:LEU:HD23	2.00	0.43
2:D:312:ILE:HG21	2:D:327:THR:HG21	1.99	0.43
1:E:129:GLU:N	1:E:129:GLU:OE1	2.51	0.43
2:F:121:THR:HA	2:F:372:LEU:HD11	2.00	0.43
2:F:14:ASN:ND2	2:F:14:ASN:N	2.65	0.43
2:F:255:MET:HE1	2:F:399:LEU:HD13	2.01	0.43
1:A:112:LEU:HD13	2:B:76:LEU:HD11	2.00	0.43
1:A:129:GLU:N	1:A:129:GLU:OE1	2.51	0.43
2:D:148:LEU:HD22	2:D:197:TYR:HB2	2.01	0.43
1:G:191:THR:HG22	1:G:192:GLY:N	2.34	0.43
2:H:69:ARG:NH1	2:H:133:TRP:HH2	2.13	0.43
2:B:87:MET:SD	2:B:91:LEU:HD23	2.59	0.42
1:C:236:MET:HG3	1:C:248:TYR:CD2	2.54	0.42
2:D:132:PRO:CD	2:D:135:ASP:HA	2.47	0.42
1:E:294:HIS:HE1	2:F:7:PRO:HG3	1.77	0.42
1:G:70:ASN:ND2	1:G:102:MET:HE3	2.34	0.42
2:H:180:THR:HB	2:H:184:LEU:HD13	2.00	0.42
2:D:124:ARG:O	2:D:128:ILE:HG13	2.19	0.42
2:D:87:MET:SD	2:D:91:LEU:HD23	2.59	0.42
1:E:191:THR:HG22	1:E:192:GLY:N	2.34	0.42
2:H:106:VAL:HG13	2:H:359:LEU:CD1	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:MET:O	2:H:76:LEU:HD23	2.19	0.42
2:B:134:LYS:O	2:B:135:ASP:CB	2.65	0.42
1:A:77:ARG:NE	2:B:136:LYS:NZ	2.67	0.42
2:B:201:VAL:HG12	2:B:203:PRO:HD3	2.01	0.42
1:C:217:LEU:CD1	1:C:219:ASP:HB2	2.47	0.42
2:D:102:SER:HB3	2:D:105:ALA:HB3	2.01	0.42
2:D:54:GLN:O	2:D:58:VAL:HG23	2.20	0.42
1:E:33:ASP:OD1	2:F:10:LEU:HB3	2.20	0.42
2:F:142:LEU:O	2:F:146:LYS:CB	2.64	0.42
2:F:3:VAL:C	2:F:4:TYR:CG	2.92	0.42
2:H:121:THR:HA	2:H:372:LEU:HD11	2.00	0.42
1:A:70:ASN:ND2	1:A:102:MET:HE3	2.34	0.42
2:B:124:ARG:O	2:B:128:ILE:HG13	2.19	0.42
1:E:217:LEU:CD1	1:E:219:ASP:HB2	2.47	0.42
2:F:48:GLU:HG2	2:F:171:LEU:HD11	2.01	0.42
2:H:179:PHE:CD2	2:H:218:ILE:HD11	2.54	0.42
2:H:201:VAL:HG12	2:H:203:PRO:HD3	2.01	0.42
2:H:124:ARG:HD3	2:H:372:LEU:HD13	2.00	0.42
1:G:236:MET:HG3	1:G:248:TYR:CE2	2.55	0.42
2:H:16:SER:C	2:H:17:THR:OG1	2.58	0.42
2:H:48:GLU:HG2	2:H:171:LEU:HD11	2.01	0.42
2:H:4:TYR:HD1	2:H:5:ILE:H	1.66	0.42
1:A:191:THR:HG22	1:A:192:GLY:N	2.34	0.42
1:A:33:ASP:OD1	2:B:10:LEU:HB3	2.20	0.42
2:B:249:VAL:HG11	2:B:395:ILE:HG22	2.00	0.42
1:C:129:GLU:N	1:C:129:GLU:OE1	2.51	0.42
1:C:33:ASP:OD1	2:D:10:LEU:HB3	2.20	0.42
2:D:106:VAL:O	2:D:109:THR:HG22	2.20	0.42
1:E:236:MET:HG3	1:E:248:TYR:CE2	2.55	0.42
2:F:110:LEU:HD21	2:F:125:LEU:HD22	2.00	0.42
1:C:96:GLY:CA	2:F:447:ASN:ND2	2.81	0.42
2:F:87:MET:SD	2:F:91:LEU:HD23	2.59	0.42
1:G:236:MET:HG3	1:G:248:TYR:CD2	2.54	0.42
1:G:321:ASP:HB3	1:G:326:ARG:HG3	2.01	0.42
2:H:106:VAL:O	2:H:109:THR:HG22	2.20	0.42
2:H:54:GLN:O	2:H:58:VAL:HG23	2.20	0.42
2:B:144:ALA:O	2:B:148:LEU:HD12	2.19	0.42
2:B:54:GLN:O	2:B:58:VAL:HG23	2.20	0.42
1:C:48:ARG:HA	1:C:48:ARG:HD3	1.76	0.42
2:D:255:MET:HE1	2:D:399:LEU:HD13	2.01	0.42
2:F:179:PHE:CD2	2:F:218:ILE:HD11	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:4:TYR:CE1	2:F:5:ILE:HD12	2.55	0.42
2:H:131:VAL:HG12	2:H:132:PRO:HD3	1.99	0.42
1:G:299:PRO:HG2	2:H:13:HIS:HB2	2.01	0.42
2:H:144:ALA:O	2:H:148:LEU:HD12	2.19	0.42
2:H:34:PHE:CZ	2:H:191:VAL:HG21	2.55	0.42
1:A:283:TYR:HB2	2:H:285:THR:HG23	2.02	0.42
2:H:301:VAL:O	2:H:301:VAL:HG13	2.20	0.42
1:G:294:HIS:HE1	2:H:7:PRO:HG3	1.77	0.42
1:A:236:MET:HG3	1:A:248:TYR:CE2	2.55	0.42
2:B:16:SER:C	2:B:17:THR:OG1	2.58	0.42
2:B:221:PHE:O	2:B:225:VAL:HG23	2.19	0.42
2:B:72:MET:O	2:B:76:LEU:HD23	2.19	0.42
1:A:112:LEU:HD21	2:B:76:LEU:HD22	1.99	0.42
2:F:102:SER:HB3	2:F:105:ALA:HB3	2.01	0.42
2:F:34:PHE:CZ	2:F:191:VAL:HG21	2.55	0.42
2:H:175:VAL:HG12	2:H:200:VAL:HB	2.01	0.42
2:B:106:VAL:HG13	2:B:359:LEU:CD1	2.48	0.42
1:A:299:PRO:HG2	2:B:13:HIS:HB2	2.01	0.42
2:B:255:MET:CE	2:B:399:LEU:HD13	2.50	0.42
2:B:288:HIS:CG	2:B:299:THR:HG22	2.55	0.42
1:C:236:MET:HG3	1:C:248:TYR:CE2	2.55	0.42
1:C:278:VAL:HG21	1:C:280:GLN:NE2	2.35	0.42
2:D:110:LEU:HD21	2:D:125:LEU:HD22	2.00	0.42
2:D:175:VAL:HG12	2:D:200:VAL:HB	2.01	0.42
2:F:144:ALA:O	2:F:148:LEU:HD12	2.19	0.42
2:F:255:MET:CE	2:F:399:LEU:HD13	2.50	0.42
2:H:87:MET:SD	2:H:91:LEU:HD23	2.59	0.42
2:F:148:LEU:HD22	2:F:197:TYR:HB2	2.01	0.42
2:F:221:PHE:O	2:F:225:VAL:HG23	2.19	0.42
2:F:54:GLN:O	2:F:58:VAL:HG23	2.20	0.42
1:G:161:SER:O	1:G:162:GLU:CB	2.68	0.42
2:H:132:PRO:C	2:H:134:LYS:N	2.70	0.42
2:H:288:HIS:CG	2:H:299:THR:HG22	2.55	0.42
2:H:255:MET:HE1	2:H:399:LEU:HD13	2.01	0.42
2:B:106:VAL:O	2:B:109:THR:HG22	2.20	0.41
2:B:301:VAL:HG13	2:B:301:VAL:O	2.20	0.41
2:D:133:TRP:CE3	2:D:134:LYS:HB2	2.55	0.41
2:D:34:PHE:CZ	2:D:191:VAL:HG21	2.55	0.41
2:B:148:LEU:HD22	2:B:197:TYR:HB2	2.01	0.41
2:B:34:PHE:CZ	2:B:191:VAL:HG21	2.55	0.41
2:B:255:MET:HE3	2:B:399:LEU:HB3	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:ALA:O	2:D:148:LEU:HD12	2.19	0.41
2:D:16:SER:C	2:D:17:THR:OG1	2.58	0.41
2:D:288:HIS:CG	2:D:299:THR:HG22	2.55	0.41
1:E:13:THR:HG21	2:F:5:ILE:HG22	1.92	0.41
1:E:299:PRO:HG2	2:F:13:HIS:HB2	2.01	0.41
2:F:131:VAL:HG12	2:F:132:PRO:HB3	1.91	0.41
1:G:217:LEU:CD1	1:G:219:ASP:HB2	2.47	0.41
2:H:3:VAL:C	2:H:4:TYR:CG	2.92	0.41
2:B:131:VAL:HG12	2:B:132:PRO:HD3	1.99	0.41
1:C:70:ASN:ND2	1:C:102:MET:HE3	2.34	0.41
1:C:51:THR:CG2	2:D:83:ARG:NH1	2.65	0.41
2:D:135:ASP:C	2:D:136:LYS:HG3	2.40	0.41
2:D:305:GLU:O	2:D:306:SER:C	2.59	0.41
2:D:72:MET:O	2:D:76:LEU:HD23	2.19	0.41
1:E:165:LEU:HD23	1:E:165:LEU:N	2.35	0.41
2:F:175:VAL:HG12	2:F:200:VAL:HB	2.01	0.41
2:F:201:VAL:HG12	2:F:203:PRO:HD3	2.01	0.41
2:F:206:LEU:HD21	2:F:214:ALA:HB1	2.03	0.41
2:F:288:HIS:CG	2:F:299:THR:HG22	2.55	0.41
2:H:255:MET:CE	2:H:399:LEU:HD13	2.50	0.41
2:B:14:ASN:ND2	2:B:14:ASN:N	2.65	0.41
1:C:161:SER:O	1:C:162:GLU:CB	2.68	0.41
2:D:34:PHE:CZ	2:D:186:LEU:HD11	2.56	0.41
2:D:93:GLY:O	2:D:95:VAL:HG23	2.21	0.41
1:E:161:SER:O	1:E:162:GLU:CB	2.68	0.41
2:F:133:TRP:CE3	2:F:134:LYS:HB2	2.55	0.41
2:B:48:GLU:HG2	2:B:171:LEU:HD11	2.01	0.41
2:B:206:LEU:HD21	2:B:214:ALA:HB1	2.03	0.41
2:B:305:GLU:O	2:B:306:SER:C	2.59	0.41
2:D:142:LEU:O	2:D:146:LYS:CB	2.64	0.41
2:D:206:LEU:HD21	2:D:214:ALA:HB1	2.03	0.41
2:F:144:ALA:O	2:F:148:LEU:CD1	2.69	0.41
1:G:110:PRO:HA	2:H:131:VAL:O	2.19	0.41
2:B:144:ALA:O	2:B:148:LEU:CD1	2.69	0.41
2:B:93:GLY:O	2:B:95:VAL:HG23	2.21	0.41
1:C:224:TYR:CE2	1:C:294:HIS:CE1	3.06	0.41
2:D:17:THR:HB	2:D:18:CYS:H	1.75	0.41
2:D:4:TYR:CE1	2:D:5:ILE:HD12	2.55	0.41
2:F:16:SER:C	2:F:17:THR:OG1	2.58	0.41
2:F:34:PHE:CZ	2:F:186:LEU:HD11	2.56	0.41
1:G:165:LEU:N	1:G:165:LEU:HD23	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:133:TRP:CE3	2:H:134:LYS:HB2	2.55	0.41
2:D:301:VAL:HG13	2:D:301:VAL:O	2.20	0.41
1:E:278:VAL:HG21	1:E:280:GLN:NE2	2.35	0.41
2:F:301:VAL:HG13	2:F:301:VAL:O	2.20	0.41
1:G:278:VAL:HG21	1:G:280:GLN:NE2	2.35	0.41
2:H:144:ALA:O	2:H:148:LEU:CD1	2.69	0.41
1:A:161:SER:O	1:A:162:GLU:CB	2.68	0.41
1:A:224:TYR:CE2	1:A:294:HIS:CE1	3.06	0.41
1:A:278:VAL:HG21	1:A:280:GLN:NE2	2.35	0.41
1:C:165:LEU:N	1:C:165:LEU:HD23	2.35	0.41
2:F:135:ASP:C	2:F:136:LYS:HG3	2.40	0.41
2:F:279:MET:HB3	2:F:279:MET:HE3	1.90	0.41
2:H:135:ASP:C	2:H:136:LYS:HG3	2.40	0.41
1:E:97:ILE:CA	2:H:449:LEU:HD22	2.50	0.41
2:F:98:ALA:HB2	2:F:353:LEU:HB3	2.03	0.41
1:G:74:LEU:HD12	1:G:76:LEU:HD11	2.03	0.41
2:H:4:TYR:CE1	2:H:5:ILE:HD12	2.55	0.41
2:B:133:TRP:CE3	2:B:134:LYS:HB2	2.55	0.41
1:C:210:CYS:O	1:C:210:CYS:SG	2.79	0.41
2:D:69:ARG:NH1	2:D:133:TRP:HH2	2.13	0.41
2:D:98:ALA:HB2	2:D:353:LEU:HB3	2.03	0.41
2:H:93:GLY:O	2:H:95:VAL:HG23	2.21	0.41
2:D:48:GLU:HG2	2:D:171:LEU:HD11	2.01	0.41
2:D:255:MET:CE	2:D:399:LEU:HD13	2.50	0.41
1:G:210:CYS:O	1:G:210:CYS:SG	2.79	0.41
1:G:33:ASP:OD1	2:H:10:LEU:HB3	2.20	0.41
1:G:49:LEU:CB	2:H:127:ALA:HB1	2.48	0.41
2:H:305:GLU:O	2:H:306:SER:C	2.59	0.41
1:A:165:LEU:HD23	1:A:165:LEU:N	2.35	0.40
2:B:135:ASP:C	2:B:136:LYS:HG3	2.40	0.40
2:F:176:VAL:CG2	2:F:198:THR:HG21	2.46	0.40
2:F:113:LEU:HD11	2:F:391:VAL:HG21	2.04	0.40
2:H:132:PRO:HG2	2:H:135:ASP:C	2.40	0.40
2:H:34:PHE:CZ	2:H:186:LEU:HD11	2.56	0.40
1:A:207:THR:O	1:A:207:THR:HG22	2.21	0.40
1:C:51:THR:HG21	2:D:83:ARG:NH1	2.34	0.40
1:E:49:LEU:HB3	2:F:128:ILE:N	2.36	0.40
2:H:142:LEU:O	2:H:146:LYS:CB	2.64	0.40
2:H:3:VAL:HB	2:H:4:TYR:CG	2.43	0.40
1:E:97:ILE:CA	2:H:449:LEU:CD2	2.97	0.40
2:B:98:ALA:HB2	2:B:353:LEU:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:106:VAL:HG13	2:D:359:LEU:CD1	2.48	0.40
2:D:144:ALA:O	2:D:148:LEU:CD1	2.69	0.40
2:F:106:VAL:O	2:F:109:THR:HG22	2.20	0.40
2:H:98:ALA:HB2	2:H:353:LEU:HB3	2.03	0.40
2:B:4:TYR:CE1	2:B:5:ILE:HD12	2.55	0.40
2:D:137:ASN:C	2:D:139:THR:H	2.25	0.40
1:G:206:SER:O	1:G:208:LEU:N	2.50	0.40
1:G:224:TYR:HD2	1:G:294:HIS:CD2	2.33	0.40
1:A:48:ARG:HA	1:A:48:ARG:HD3	1.76	0.40
2:B:34:PHE:CZ	2:B:186:LEU:HD11	2.56	0.40
2:B:255:MET:CE	2:B:399:LEU:HD22	2.52	0.40
2:B:69:ARG:NH1	2:B:133:TRP:HH2	2.13	0.40
1:C:206:SER:O	1:C:208:LEU:N	2.50	0.40
1:G:207:THR:HG22	1:G:207:THR:O	2.21	0.40
1:G:251:LYS:HZ1	1:G:285:SER:HB2	1.83	0.40

All (30) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLN:NE2	2:F:40:GLN:C[8_434]	0.58	1.62
2:B:40:GLN:C	2:F:40:GLN:NE2[8_434]	0.62	1.58
2:B:40:GLN:CA	2:F:40:GLN:NE2[8_434]	1.08	1.12
2:B:40:GLN:CD	2:F:40:GLN:C[8_434]	1.11	1.09
2:B:40:GLN:NE2	2:F:40:GLN:O[8_434]	1.14	1.06
2:B:40:GLN:C	2:F:40:GLN:CD[8_434]	1.15	1.05
2:B:40:GLN:NE2	2:F:40:GLN:CA[8_434]	1.29	0.91
2:B:40:GLN:O	2:F:40:GLN:NE2[8_434]	1.36	0.84
2:B:40:GLN:CG	2:F:40:GLN:CG[8_434]	1.37	0.83
2:B:40:GLN:OE1	2:F:41:ALA:N[8_434]	1.41	0.79
2:B:41:ALA:N	2:F:40:GLN:OE1[8_434]	1.44	0.76
1:A:23:THR:CG2	2:B:95:VAL:CG2[2_545]	1.51	0.69
1:C:257:THR:OG1	2:F:403:GLU:O[3_655]	1.59	0.61
2:B:40:GLN:CA	2:F:40:GLN:CD[8_434]	1.62	0.58
1:A:23:THR:CG2	2:B:95:VAL:CB[2_545]	1.62	0.58
2:B:40:GLN:CD	2:F:40:GLN:CA[8_434]	1.72	0.48
2:B:40:GLN:CD	2:F:40:GLN:O[8_434]	1.75	0.45
2:B:41:ALA:N	2:F:40:GLN:CD[8_434]	1.75	0.45
2:B:40:GLN:CB	2:F:40:GLN:CD[8_434]	1.78	0.42
2:B:40:GLN:CD	2:F:41:ALA:N[8_434]	1.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLN:OE1	2:F:40:GLN:C[8_434]	1.79	0.41
1:C:257:THR:CB	2:F:403:GLU:O[3_655]	1.86	0.34
2:B:40:GLN:C	2:F:40:GLN:OE1[8_434]	1.87	0.33
2:B:40:GLN:CB	2:F:40:GLN:CG[8_434]	1.88	0.32
2:B:40:GLN:CD	2:F:40:GLN:CB[8_434]	1.89	0.31
2:B:41:ALA:N	2:F:40:GLN:NE2[8_434]	1.89	0.31
2:B:40:GLN:NE2	2:F:41:ALA:N[8_434]	1.90	0.30
2:B:40:GLN:O	2:F:40:GLN:CD[8_434]	1.91	0.29
1:A:98:THR:N	2:B:449:LEU:CD2[2_545]	1.92	0.28
2:B:40:GLN:CG	2:F:40:GLN:CB[8_434]	2.00	0.20

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	41	76
1	C	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	41	76
1	E	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	41	76
1	G	326/383 (85%)	314 (96%)	11 (3%)	1 (0%)	41	76
2	B	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	6	36
2	D	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	6	36
2	F	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	6	36
2	H	417/452 (92%)	359 (86%)	48 (12%)	10 (2%)	6	36
All	All	2972/3340 (89%)	2692 (91%)	236 (8%)	44 (2%)	10	46

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	SER
2	B	15	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	17	THR
1	C	206	SER
2	D	15	GLU
2	D	17	THR
1	E	206	SER
2	F	15	GLU
2	F	17	THR
1	G	206	SER
2	H	15	GLU
2	H	17	THR
2	B	4	TYR
2	B	139	THR
2	D	4	TYR
2	D	139	THR
2	F	4	TYR
2	F	139	THR
2	H	4	TYR
2	H	139	THR
2	B	144	ALA
2	B	379	GLN
2	D	144	ALA
2	D	379	GLN
2	F	144	ALA
2	F	379	GLN
2	H	144	ALA
2	H	379	GLN
2	B	295	ASN
2	B	437	THR
2	D	295	ASN
2	D	437	THR
2	F	295	ASN
2	F	437	THR
2	H	295	ASN
2	H	437	THR
2	B	336	MET
2	D	336	MET
2	F	336	MET
2	H	336	MET
2	B	352	VAL
2	D	352	VAL
2	F	352	VAL
2	H	352	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/330 (84%)	265 (95%)	14 (5%)	24	51
1	C	279/330 (84%)	265 (95%)	14 (5%)	24	51
1	E	279/330 (84%)	265 (95%)	14 (5%)	24	51
1	G	279/330 (84%)	265 (95%)	14 (5%)	24	51
2	B	358/385 (93%)	341 (95%)	17 (5%)	26	53
2	D	358/385 (93%)	341 (95%)	17 (5%)	26	53
2	F	358/385 (93%)	341 (95%)	17 (5%)	26	53
2	H	358/385 (93%)	341 (95%)	17 (5%)	26	53
All	All	2548/2860 (89%)	2424 (95%)	124 (5%)	25	51

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	76	LEU
1	A	113	PRO
1	A	149	LYS
1	A	151	ASP
1	A	158	ASN
1	A	159	ARG
1	A	171	LEU
1	A	182	ASN
1	A	245	LEU
1	A	250	VAL
1	A	278	VAL
1	A	326	ARG
1	A	331	LEU
2	B	4	TYR
2	B	14	ASN
2	B	16	SER
2	B	17	THR
2	B	18	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	54	GLN
2	B	101	LEU
2	B	118	LEU
2	B	204	ARG
2	B	266	GLU
2	B	296	PHE
2	B	333	LEU
2	B	347	THR
2	B	354	GLN
2	B	386	ILE
2	B	417	GLU
2	B	439	LEU
1	C	9	ASN
1	C	76	LEU
1	C	113	PRO
1	C	149	LYS
1	C	151	ASP
1	C	158	ASN
1	C	159	ARG
1	C	171	LEU
1	C	182	ASN
1	C	245	LEU
1	C	250	VAL
1	C	278	VAL
1	C	326	ARG
1	C	331	LEU
2	D	4	TYR
2	D	14	ASN
2	D	16	SER
2	D	17	THR
2	D	18	CYS
2	D	54	GLN
2	D	101	LEU
2	D	118	LEU
2	D	204	ARG
2	D	266	GLU
2	D	296	PHE
2	D	333	LEU
2	D	347	THR
2	D	354	GLN
2	D	386	ILE
2	D	417	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	439	LEU
1	E	9	ASN
1	E	76	LEU
1	E	113	PRO
1	E	149	LYS
1	E	151	ASP
1	E	158	ASN
1	E	159	ARG
1	E	171	LEU
1	E	182	ASN
1	E	245	LEU
1	E	250	VAL
1	E	278	VAL
1	E	326	ARG
1	E	331	LEU
2	F	4	TYR
2	F	14	ASN
2	F	16	SER
2	F	17	THR
2	F	18	CYS
2	F	54	GLN
2	F	101	LEU
2	F	118	LEU
2	F	204	ARG
2	F	266	GLU
2	F	296	PHE
2	F	333	LEU
2	F	347	THR
2	F	354	GLN
2	F	386	ILE
2	F	417	GLU
2	F	439	LEU
1	G	9	ASN
1	G	76	LEU
1	G	113	PRO
1	G	149	LYS
1	G	151	ASP
1	G	158	ASN
1	G	159	ARG
1	G	171	LEU
1	G	182	ASN
1	G	245	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	250	VAL
1	G	278	VAL
1	G	326	ARG
1	G	331	LEU
2	H	4	TYR
2	H	14	ASN
2	H	16	SER
2	H	17	THR
2	H	18	CYS
2	H	54	GLN
2	H	101	LEU
2	H	118	LEU
2	H	204	ARG
2	H	266	GLU
2	H	296	PHE
2	H	333	LEU
2	H	347	THR
2	H	354	GLN
2	H	386	ILE
2	H	417	GLU
2	H	439	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	26	GLN
1	A	101	GLN
1	A	141	ASN
1	A	158	ASN
1	A	195	GLN
1	A	197	GLN
1	A	264	HIS
1	A	280	GLN
2	B	13	HIS
2	B	14	ASN
2	B	137	ASN
2	B	188	GLN
1	C	9	ASN
1	C	26	GLN
1	C	101	GLN
1	C	141	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	158	ASN
1	C	195	GLN
1	C	197	GLN
1	C	264	HIS
1	C	280	GLN
2	D	13	HIS
2	D	14	ASN
2	D	137	ASN
2	D	188	GLN
1	E	9	ASN
1	E	26	GLN
1	E	101	GLN
1	E	141	ASN
1	E	158	ASN
1	E	195	GLN
1	E	197	GLN
1	E	264	HIS
1	E	280	GLN
2	F	13	HIS
2	F	14	ASN
2	F	137	ASN
2	F	188	GLN
2	F	447	ASN
1	G	9	ASN
1	G	26	GLN
1	G	101	GLN
1	G	141	ASN
1	G	158	ASN
1	G	195	GLN
1	G	197	GLN
1	G	264	HIS
1	G	280	GLN
2	H	13	HIS
2	H	14	ASN
2	H	137	ASN
2	H	192	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/383 (86%)	0.59	28 (8%) 10 9	177, 273, 376, 684	0
1	C	330/383 (86%)	0.74	52 (15%) 2 2	200, 315, 406, 568	0
1	E	330/383 (86%)	0.73	48 (14%) 2 3	236, 314, 400, 518	0
1	G	330/383 (86%)	0.80	45 (13%) 3 3	240, 337, 443, 633	0
2	B	423/452 (93%)	1.12	78 (18%) 1 1	131, 273, 412, 537	1 (0%)
2	D	423/452 (93%)	1.56	133 (31%) 0 0	225, 360, 512, 725	1 (0%)
2	F	423/452 (93%)	1.14	78 (18%) 1 1	180, 285, 429, 757	1 (0%)
2	H	423/452 (93%)	1.62	131 (30%) 0 0	212, 357, 521, 686	1 (0%)
All	All	3012/3340 (90%)	1.08	593 (19%) 1 1	131, 317, 467, 757	4 (0%)

All (593) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	416	PRO	13.9
2	H	416	PRO	13.2
2	D	231	GLY	13.1
2	D	133	TRP	13.0
2	H	221	PHE	12.4
2	F	168	ALA	11.9
2	F	167	GLN	11.8
2	F	166	SER	11.8
1	G	95	GLY	11.6
2	B	417	GLU	11.5
1	G	134	ARG	10.6
2	H	233	SER	10.0
2	H	133	TRP	10.0
2	H	166	SER	10.0
2	F	447	ASN	10.0
2	H	167	GLN	9.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	167	GLN	9.6
2	H	373	HIS	9.3
2	B	403	GLU	9.1
1	G	133	GLY	9.0
2	D	230	THR	9.0
1	G	96	GLY	9.0
2	D	337	LYS	8.9
2	D	132	PRO	8.9
2	H	168	ALA	8.5
2	D	134	LYS	8.2
2	H	417	GLU	8.1
2	F	337	LYS	7.9
2	B	133	TRP	7.9
2	H	370	ALA	7.8
2	H	447	ASN	7.8
2	F	449	LEU	7.8
2	D	44	SER	7.7
1	C	269	GLU	7.7
2	F	133	TRP	7.6
2	F	416	PRO	7.5
2	D	416	PRO	7.4
2	F	446	ALA	7.4
2	H	179	PHE	7.4
2	H	301	VAL	7.3
2	D	226	THR	7.3
2	H	218	ILE	7.1
2	F	334	ASN	6.9
2	B	140	SER	6.8
2	H	232	CYS	6.8
1	E	182	ASN	6.7
2	D	386	ILE	6.7
2	F	448	PRO	6.6
2	H	18	CYS	6.6
2	D	202	LEU	6.6
1	G	218	VAL	6.6
2	D	339	LEU	6.6
2	D	367	GLU	6.6
2	H	222	MET	6.5
2	D	203	PRO	6.5
2	D	334	ASN	6.5
1	C	268	LYS	6.5
2	H	339	LEU	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	167	GLN	6.4
2	D	43	THR	6.3
2	D	114	TYR	6.3
2	H	243	LEU	6.3
2	H	169	GLN	6.2
2	H	217	LYS	6.2
2	F	403	GLU	6.2
2	D	168	ALA	6.1
2	B	447	ASN	6.1
2	H	234	LEU	6.0
2	H	172	LEU	6.0
2	B	168	ALA	5.9
2	H	178	VAL	5.8
2	H	6	HIS	5.7
2	D	232	CYS	5.7
1	G	172	GLY	5.7
2	H	170	LEU	5.7
2	D	3	VAL	5.7
2	H	43	THR	5.7
2	B	374	THR	5.7
2	D	403	GLU	5.6
2	B	339	LEU	5.6
2	B	373	HIS	5.5
1	C	270	TYR	5.5
1	G	246	PHE	5.5
1	G	181	GLY	5.5
1	C	322	ARG	5.5
2	H	134	LYS	5.4
2	D	387	ARG	5.4
2	H	214	ALA	5.4
2	F	169	GLN	5.4
2	H	403	GLU	5.4
2	F	366	ALA	5.4
1	G	132	ILE	5.4
2	F	5	ILE	5.4
2	D	417	GLU	5.3
2	H	371	ILE	5.2
2	D	225	VAL	5.2
2	B	337	LYS	5.2
2	H	352	VAL	5.2
2	D	362	LEU	5.2
1	E	151	ASP	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	190	PHE	5.2
2	H	231	GLY	5.1
2	H	337	LYS	5.1
1	C	239	LEU	5.1
2	B	386	ILE	5.1
2	B	141	ARG	5.1
2	D	335	TRP	5.0
1	G	217	LEU	5.0
2	D	222	MET	5.0
1	G	55	TYR	5.0
1	E	266	GLY	4.9
2	F	367	GLU	4.9
2	D	447	ASN	4.9
2	H	386	ILE	4.8
2	D	172	LEU	4.8
2	H	174	THR	4.8
2	H	448	PRO	4.8
2	D	135	ASP	4.8
2	D	221	PHE	4.8
2	H	328	PHE	4.8
1	G	182	ASN	4.8
2	H	165	ASP	4.7
1	E	96	GLY	4.7
2	F	164	ALA	4.7
2	D	46	VAL	4.7
2	D	36	PRO	4.7
1	E	121	GLY	4.7
2	D	271	ASN	4.7
2	H	164	ALA	4.7
2	F	339	LEU	4.6
2	H	159	VAL	4.6
2	D	45	PRO	4.6
2	D	234	LEU	4.6
2	D	352	VAL	4.6
2	H	366	ALA	4.6
2	D	316	TYR	4.6
2	D	229	LYS	4.5
2	D	190	PHE	4.5
2	B	446	ALA	4.5
2	D	4	TYR	4.5
1	A	172	GLY	4.5
2	D	116	GLY	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	95	VAL	4.5
1	A	266	GLY	4.4
2	D	59	ALA	4.4
2	D	402	ASP	4.4
2	H	265	GLN	4.4
2	D	338	LYS	4.4
1	A	246	PHE	4.3
2	H	132	PRO	4.3
1	E	239	LEU	4.3
1	A	151	ASP	4.3
2	D	448	PRO	4.3
2	D	48	GLU	4.3
2	F	362	LEU	4.3
2	H	376	LEU	4.3
2	H	362	LEU	4.3
2	B	426	PRO	4.3
1	E	208	LEU	4.2
2	H	158	LEU	4.2
2	D	228	TRP	4.2
2	D	136	LYS	4.2
2	H	147	VAL	4.2
2	F	373	HIS	4.2
2	H	116	GLY	4.2
2	D	140	SER	4.2
2	D	446	ALA	4.2
2	D	113	LEU	4.2
2	D	254	LYS	4.2
1	A	281	GLU	4.1
1	C	95	GLY	4.1
1	E	281	GLU	4.1
2	B	207	ASP	4.1
2	H	135	ASP	4.1
1	E	80	THR	4.1
1	E	150	GLU	4.1
2	B	166	SER	4.1
2	H	225	VAL	4.1
2	B	4	TYR	4.0
2	D	179	PHE	4.0
2	D	426	PRO	4.0
1	E	118	GLU	4.0
2	H	5	ILE	4.0
2	D	204	ARG	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	196	ILE	3.9
2	F	417	GLU	3.9
2	H	155	GLN	3.9
2	D	245	PHE	3.9
1	G	135	VAL	3.9
2	B	402	ASP	3.9
2	H	264	PRO	3.9
2	D	285	THR	3.9
2	H	374	THR	3.9
2	D	303	PHE	3.8
2	H	209	THR	3.8
2	H	338	LYS	3.8
2	B	367	GLU	3.8
2	H	369	PRO	3.8
1	C	96	GLY	3.8
2	D	343	THR	3.8
2	H	334	ASN	3.8
1	C	203	VAL	3.8
1	C	58	LEU	3.8
2	D	353	LEU	3.8
2	D	5	ILE	3.7
2	B	427	PHE	3.7
1	C	21	ILE	3.7
2	H	312	ILE	3.7
1	E	327	ILE	3.7
1	G	208	LEU	3.7
1	G	94	VAL	3.7
2	D	186	LEU	3.7
2	D	365	GLN	3.6
1	G	308	LEU	3.6
2	H	256	LYS	3.6
2	H	139	THR	3.6
2	B	387	ARG	3.6
2	F	287	GLN	3.6
2	F	386	ILE	3.6
1	G	245	LEU	3.6
2	H	300	GLN	3.6
2	H	303	PHE	3.6
1	E	76	LEU	3.6
2	D	276	SER	3.6
2	D	180	THR	3.6
1	E	329	PHE	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	349	PRO	3.5
1	E	181	GLY	3.5
1	C	298	ILE	3.5
1	E	295	ALA	3.5
2	F	352	VAL	3.5
2	F	255	MET	3.5
1	A	302	THR	3.5
1	C	235	LEU	3.5
2	H	55	LEU	3.4
2	B	370	ALA	3.4
2	D	255	MET	3.4
1	G	116	LEU	3.4
2	H	211	LEU	3.4
1	A	286	LYS	3.4
2	H	160	ALA	3.4
2	H	351	LEU	3.4
1	E	268	LYS	3.4
1	A	270	TYR	3.4
2	D	92	TRP	3.4
2	H	399	LEU	3.4
1	E	134	ARG	3.4
2	H	152	GLN	3.3
1	E	267	GLY	3.3
1	E	206	SER	3.3
2	H	220	ARG	3.3
1	E	135	VAL	3.3
2	D	237	ALA	3.3
1	G	195	GLN	3.3
1	G	80	THR	3.3
1	C	246	PHE	3.3
2	B	352	VAL	3.3
2	F	350	GLN	3.3
2	B	425	ARG	3.3
2	F	374	THR	3.3
1	E	265	LEU	3.3
2	H	367	GLU	3.3
2	H	8	PHE	3.2
2	H	180	THR	3.2
2	H	194	LEU	3.2
1	C	155	PHE	3.2
2	H	202	LEU	3.2
2	H	363	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	256	LYS	3.2
2	F	159	VAL	3.2
1	C	271	THR	3.2
2	B	271	ASN	3.2
2	D	13	HIS	3.2
2	F	301	VAL	3.2
2	F	238	SER	3.2
1	C	92	ILE	3.2
2	D	301	VAL	3.2
1	C	267	GLY	3.2
2	D	284	GLY	3.2
2	H	299	THR	3.1
1	G	239	LEU	3.1
2	H	378	LEU	3.1
2	F	385	ARG	3.1
2	H	213	VAL	3.1
1	C	42	PRO	3.1
2	D	39	ILE	3.1
2	F	335	TRP	3.1
2	H	203	PRO	3.1
2	D	6	HIS	3.1
1	C	266	GLY	3.1
2	B	313	GLN	3.1
2	D	427	PHE	3.1
2	H	137	ASN	3.1
1	G	197	GLN	3.1
1	G	243	LYS	3.1
1	C	59	PHE	3.1
2	H	377	ASN	3.1
2	D	178	VAL	3.1
2	H	390	GLU	3.1
1	A	322	ARG	3.1
2	H	316	TYR	3.1
2	H	95	VAL	3.1
2	F	129	LEU	3.1
1	G	171	LEU	3.0
2	B	338	LYS	3.0
1	G	189	ILE	3.0
2	F	254	LYS	3.0
2	H	226	THR	3.0
2	D	233	SER	3.0
2	F	294	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	162	GLY	3.0
2	F	445	VAL	3.0
1	E	83	VAL	3.0
2	H	52	GLN	3.0
2	F	201	VAL	3.0
2	F	351	LEU	3.0
1	G	191	THR	3.0
2	B	362	LEU	3.0
2	B	312	ILE	3.0
1	C	57	LYS	3.0
1	G	193	VAL	3.0
1	A	132	ILE	3.0
2	D	397	PHE	3.0
2	F	444	ARG	3.0
2	B	444	ARG	2.9
1	G	203	VAL	2.9
1	C	182	ASN	2.9
2	D	166	SER	2.9
1	E	40	TRP	2.9
2	H	215	ALA	2.9
1	C	243	LYS	2.9
1	G	148	LEU	2.9
2	D	201	VAL	2.9
1	E	165	LEU	2.9
2	B	327	THR	2.9
1	E	207	THR	2.9
1	G	32	PHE	2.9
2	D	16	SER	2.9
1	A	150	GLU	2.9
2	F	286	PHE	2.9
2	F	178	VAL	2.9
2	D	381	LEU	2.9
2	D	206	LEU	2.9
2	D	261	LEU	2.9
1	C	32	PHE	2.9
2	B	83	ARG	2.9
1	C	184	HIS	2.9
2	H	242	THR	2.8
1	E	32	PHE	2.8
2	H	365	GLN	2.8
2	B	134	LYS	2.8
1	A	148	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	435	SER	2.8
2	D	171	LEU	2.8
1	C	162	GLU	2.8
2	F	91	LEU	2.8
2	D	277	VAL	2.8
2	H	92	TRP	2.8
2	H	173	SER	2.8
2	H	171	LEU	2.8
1	G	97	ILE	2.8
1	A	329	PHE	2.8
1	E	48	ARG	2.8
1	C	281	GLU	2.8
1	A	245	LEU	2.8
2	F	165	ASP	2.8
2	B	172	LEU	2.8
2	F	6	HIS	2.7
2	B	399	LEU	2.7
1	C	171	LEU	2.7
1	A	171	LEU	2.7
2	H	204	ARG	2.7
2	B	445	VAL	2.7
2	D	218	ILE	2.7
2	B	5	ILE	2.7
1	G	214	CYS	2.7
2	H	402	ASP	2.7
2	F	170	LEU	2.7
2	D	93	GLY	2.7
1	E	175	ASP	2.7
2	H	136	LYS	2.7
2	D	357	TYR	2.7
2	H	428	LEU	2.7
1	E	302	THR	2.7
2	B	211	LEU	2.7
1	E	97	ILE	2.6
2	D	344	ILE	2.6
1	C	263	PHE	2.6
2	B	43	THR	2.6
1	G	196	ILE	2.6
1	E	155	PHE	2.6
1	E	184	HIS	2.6
1	C	97	ILE	2.6
2	D	128	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	267	GLY	2.6
2	D	445	VAL	2.6
2	F	388	VAL	2.6
2	D	299	THR	2.6
1	G	13	THR	2.6
2	B	376	LEU	2.6
1	C	133	GLY	2.6
1	C	98	THR	2.6
2	D	336	MET	2.6
1	E	95	GLY	2.6
1	A	155	PHE	2.6
2	F	163	ARG	2.6
1	A	265	LEU	2.6
2	H	9	HIS	2.6
2	B	303	PHE	2.6
2	H	425	ARG	2.6
1	G	192	GLY	2.6
2	H	244	ALA	2.6
2	H	381	LEU	2.6
2	H	235	MET	2.5
2	D	269	VAL	2.5
1	E	298	ILE	2.5
2	B	351	LEU	2.5
1	E	133	GLY	2.5
1	A	263	PHE	2.5
2	D	296	PHE	2.5
2	D	354	GLN	2.5
2	D	170	LEU	2.5
2	H	372	LEU	2.5
2	F	67	LYS	2.5
2	D	143	ASP	2.5
2	D	52	GLN	2.5
1	C	40	TRP	2.5
2	F	338	LYS	2.5
1	C	91	ILE	2.5
1	A	219	ASP	2.5
2	H	186	LEU	2.5
1	A	287	LYS	2.5
2	F	402	ASP	2.5
2	H	67	LYS	2.5
2	H	388	VAL	2.5
2	B	87	MET	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	182	PRO	2.5
2	F	426	PRO	2.5
2	D	183	GLY	2.5
1	E	186	ILE	2.5
2	D	331	ASN	2.5
2	H	3	VAL	2.4
2	F	4	TYR	2.4
2	D	211	LEU	2.4
2	F	399	LEU	2.4
2	F	202	LEU	2.4
1	C	145	GLN	2.4
2	D	72	MET	2.4
2	F	176	VAL	2.4
2	B	202	LEU	2.4
2	F	52	GLN	2.4
2	B	371	ILE	2.4
2	D	34	PHE	2.4
2	B	158	LEU	2.4
2	D	243	LEU	2.4
2	F	312	ILE	2.4
2	H	62	LEU	2.4
2	F	84	ILE	2.4
2	B	3	VAL	2.4
2	D	84	ILE	2.4
2	H	255	MET	2.4
1	C	151	ASP	2.4
1	E	116	LEU	2.3
2	F	303	PHE	2.3
2	F	293	GLN	2.3
2	B	237	ALA	2.3
2	B	159	VAL	2.3
2	D	449	LEU	2.3
2	F	300	GLN	2.3
2	F	376	LEU	2.3
2	H	83	ARG	2.3
2	B	256	LYS	2.3
2	D	88	HIS	2.3
1	C	116	LEU	2.3
2	B	255	MET	2.3
1	E	201	VAL	2.3
2	B	251	PHE	2.3
1	E	139	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	142	ILE	2.3
1	G	156	TYR	2.3
2	B	448	PRO	2.3
2	F	136	LYS	2.3
2	D	368	LEU	2.3
1	C	69	HIS	2.3
2	H	296	PHE	2.3
1	G	159	ARG	2.3
1	A	125	MET	2.3
1	C	134	ARG	2.3
2	B	203	PRO	2.3
1	C	41	VAL	2.3
1	C	236	MET	2.3
1	G	199	LYS	2.3
1	G	19	ILE	2.3
2	B	170	LEU	2.3
2	D	235	MET	2.3
2	F	363	LEU	2.3
2	H	395	ILE	2.3
1	G	180	GLU	2.2
1	C	123	VAL	2.2
2	H	84	ILE	2.2
1	C	135	VAL	2.2
2	D	141	ARG	2.2
2	B	225	VAL	2.2
2	D	287	GLN	2.2
2	F	349	PRO	2.2
2	F	296	PHE	2.2
1	C	18	GLU	2.2
1	C	19	ILE	2.2
2	B	96	HIS	2.2
2	H	254	LYS	2.2
2	H	287	GLN	2.2
2	H	68	LEU	2.2
1	G	157	TYR	2.2
1	A	268	LYS	2.2
1	C	87	LEU	2.2
1	C	105	GLU	2.2
1	E	122	VAL	2.2
2	F	155	GLN	2.2
2	H	311	LEU	2.2
2	B	132	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	169	GLN	2.2
2	F	313	GLN	2.2
2	H	210	GLU	2.2
2	H	314	PRO	2.2
2	B	334	ASN	2.2
1	G	18	GLU	2.2
2	B	92	TRP	2.2
2	B	128	ILE	2.2
1	G	93	THR	2.2
2	D	117	ALA	2.2
2	F	113	LEU	2.2
2	F	387	ARG	2.2
2	B	143	ASP	2.2
2	H	110	LEU	2.2
2	D	356	SER	2.2
2	H	161	GLN	2.1
1	C	165	LEU	2.1
2	F	162	GLY	2.1
2	H	51	LEU	2.1
1	G	216	ALA	2.1
1	E	13	THR	2.1
2	D	175	VAL	2.1
2	B	231	GLY	2.1
1	A	272	LEU	2.1
1	E	132	ILE	2.1
2	B	265	GLN	2.1
2	D	283	MET	2.1
1	E	159	ARG	2.1
2	D	373	HIS	2.1
2	D	328	PHE	2.1
2	D	363	LEU	2.1
1	A	249	VAL	2.1
2	D	236	GLY	2.1
2	B	59	ALA	2.1
2	H	189	PRO	2.1
2	H	10	LEU	2.1
1	C	83	VAL	2.1
2	H	98	ALA	2.1
2	F	134	LYS	2.1
2	H	157	LEU	2.1
2	D	425	ARG	2.1
2	F	141	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	209	LEU	2.1
2	H	309	LEU	2.1
2	F	59	ALA	2.1
2	B	67	LYS	2.1
2	F	14	ASN	2.1
2	B	301	VAL	2.1
2	D	200	VAL	2.1
2	B	385	ARG	2.1
2	D	251	PHE	2.1
2	B	86	GLY	2.1
1	A	139	PHE	2.1
2	B	221	PHE	2.1
1	E	203	VAL	2.1
1	A	55	TYR	2.0
1	A	244	ARG	2.0
1	C	218	VAL	2.0
2	B	354	GLN	2.0
1	C	238	ALA	2.0
2	B	328	PHE	2.0
2	B	137	ASN	2.0
2	H	261	LEU	2.0
2	D	208	PHE	2.0
2	F	425	ARG	2.0
2	D	159	VAL	2.0
1	C	265	LEU	2.0
2	F	199	PRO	2.0
2	D	35	ILE	2.0
2	F	140	SER	2.0
2	D	419	LEU	2.0
1	G	293	ILE	2.0
2	B	266	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.