Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:33 am BST

PDB ID	:	3B8E
Title	:	Crystal structure of the sodium-potassium pump
Authors	:	Morth, J.P.; Pedersen, P.B.; Toustrup-Jensen, M.S.; Soerensen, T.L.M.; Petersen, J.; Andersen, J.P.; Vilsen, B.; Nissen, P.
Deposited on	:	2007-11-01
Resolution	:	3.50 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:

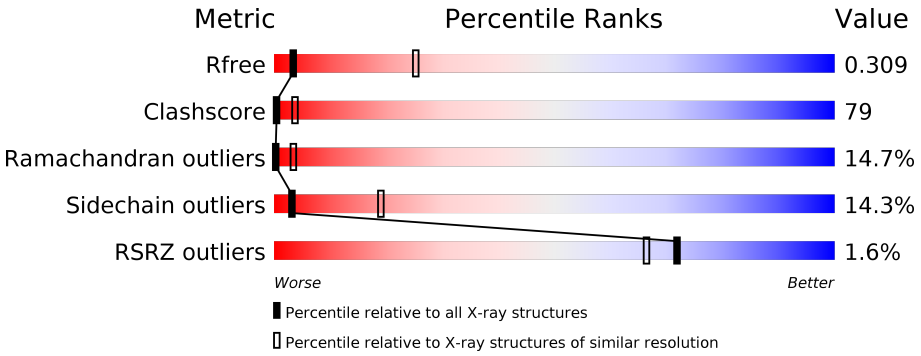
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	998	% 22% 58% 18% .
1	C	998	% 22% 57% 19% .
2	B	46	20% 57% 15% 9%
2	D	46	15% 52% 28% .
3	G	29	34% 41% 48% 10%
3	H	29	24% 45% 52% .

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16718 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	998	Total	C	N	O	S	0	0	0
			7740	4931	1304	1458	47			
1	C	998	Total	C	N	O	S	0	0	0
			7740	4931	1304	1458	47			

- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	46	Total	C	N	O	S	0	0	0
			370	252	54	62	2			
2	D	46	Total	C	N	O	S	0	0	0
			370	252	54	62	2			

- Molecule 3 is a protein called Na+/K+ ATPase gamma subunit transcript variant a.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	29	Total	C	N	O	0	0	0
			228	152	40	36			
3	H	29	Total	C	N	O	0	0	0
			228	152	40	36			

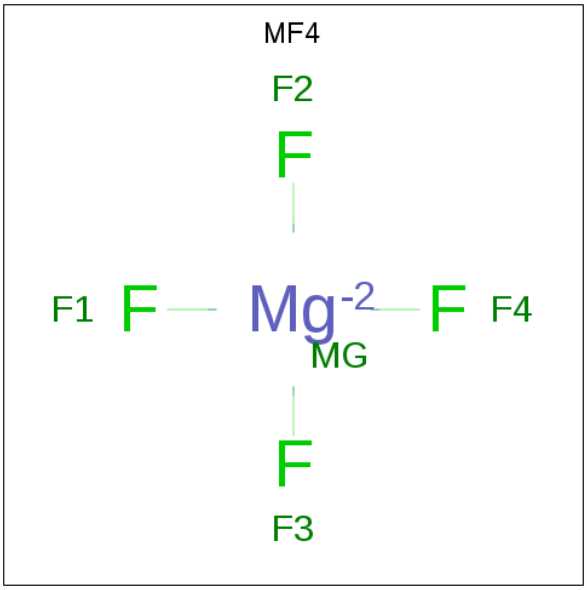
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is RUBIDIUM ION (three-letter code: RB) (formula: Rb).

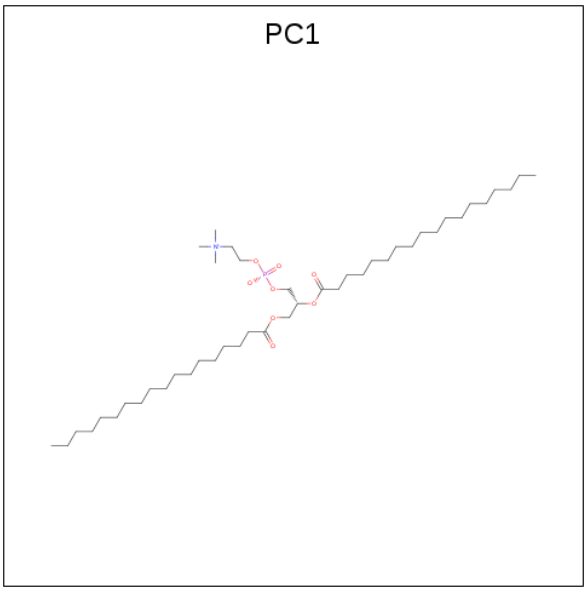
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Rb 3 3	0	0
5	C	3	Total Rb 3 3	0	0

- Molecule 6 is TETRAFLUOROMAGNESATE(2-) (three-letter code: MF4) (formula: F_4Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total F Mg 5 4 1	0	0
6	C	1	Total F Mg 5 4 1	0	0

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).

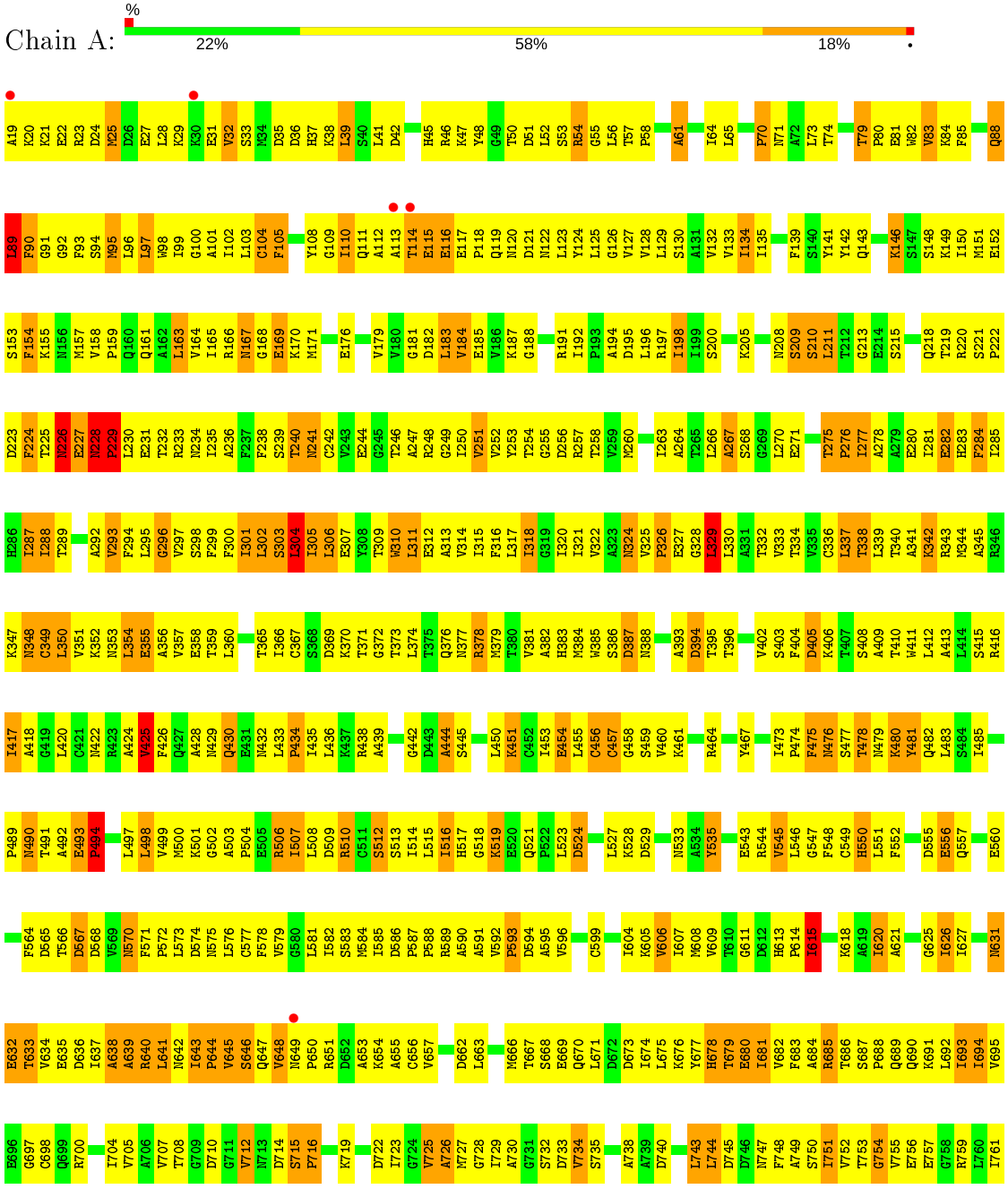


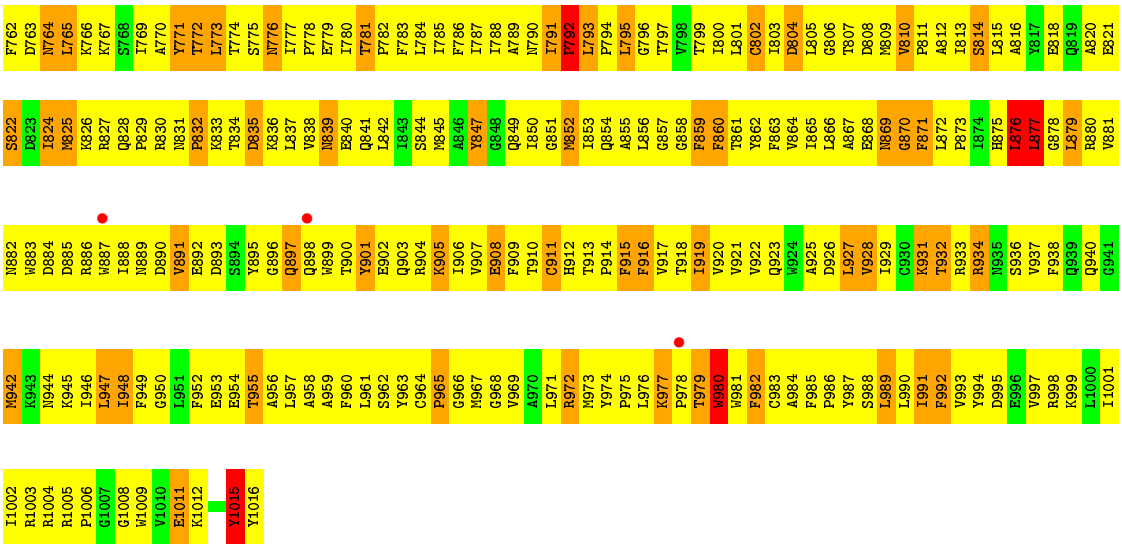
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			12	6	1	4	1		
7	C	1	Total	C	N	O	P	0	0
			12	6	1	4	1		

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.

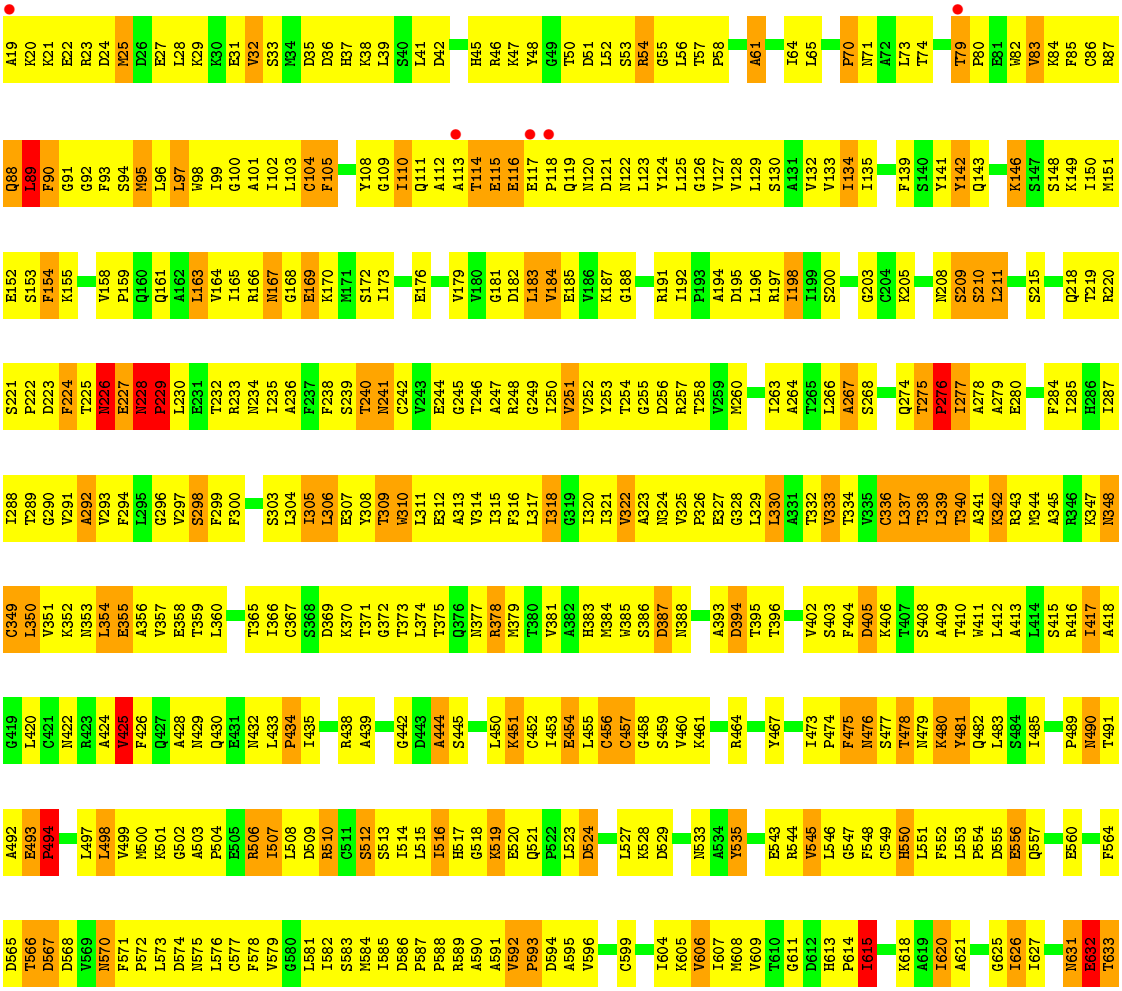
- Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

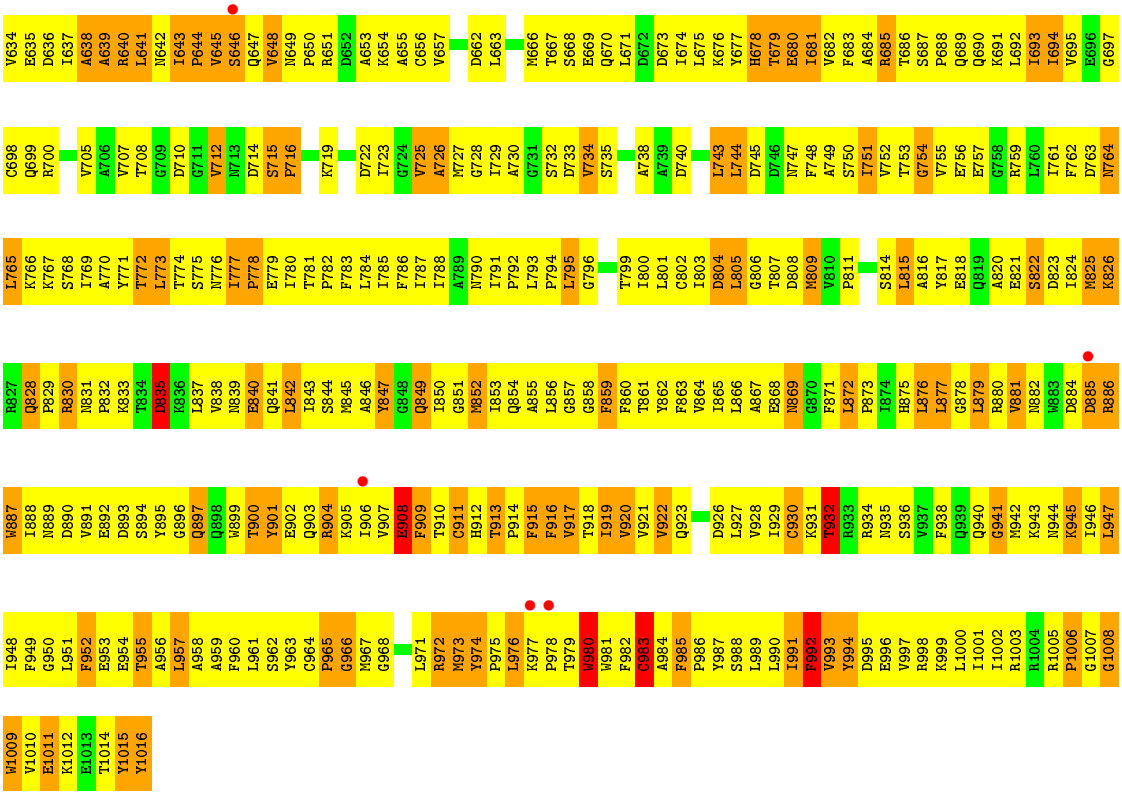




• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

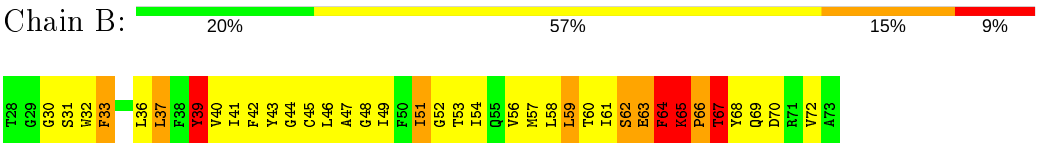
Chain C:





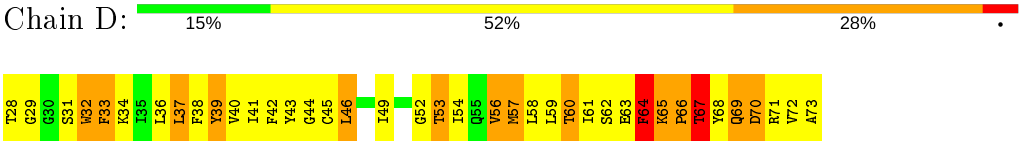
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain B:



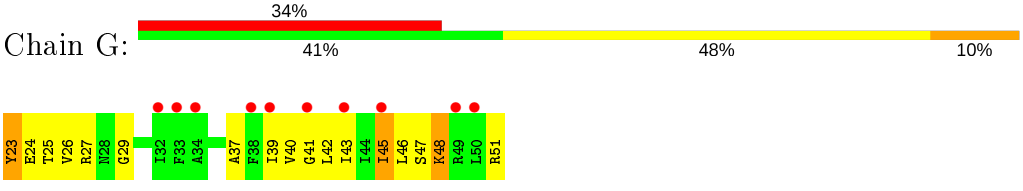
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

Chain D:



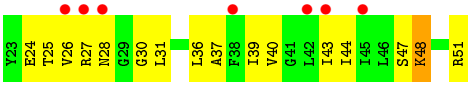
• Molecule 3: Na+/K+ ATPase gamma subunit transcript variant a

Chain G:



• Molecule 3: Na+/K+ ATPase gamma subunit transcript variant a

Chain H:


Y23
E24
T25
V26
R27
N28
G29
G30
L31
L36
A37
F38
I39
V40
G41
L42
I43
I44
I45
L46
S47
K48
R51

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.93Å 261.50Å 334.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 48.03 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.50) 99.6 (48.03-3.50)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	0.26	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.277 , 0.313 0.272 , 0.309	Depositor DCC
R_{free} test set	1550 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	89.0	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 70.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	16718	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PC1, MF4, RB

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	0.42	0/7890	0.71	1/10706 (0.0%)
1	C	0.41	0/7890	0.71	1/10706 (0.0%)
2	B	0.54	0/380	0.78	0/513
2	D	0.49	0/380	0.78	0/513
3	G	0.42	0/230	0.65	0/307
3	H	0.40	0/230	0.67	0/307
All	All	0.42	0/17000	0.71	2/23052 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	901	TYR	N-CA-C	-6.21	94.23	111.00
1	C	901	TYR	N-CA-C	-5.44	96.32	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	39	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7740	0	7796	1284	0
1	C	7740	0	7796	1222	0
2	B	370	0	378	76	0
2	D	370	0	378	87	0
3	G	228	0	254	30	0
3	H	228	0	254	32	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	3	0	0	0	0
5	C	3	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
7	B	12	0	13	1	0
7	C	12	0	13	0	0
All	All	16718	0	16882	2657	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 79.

All (2657) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:VAL:HA	1:A:911:CYS:HB2	1.23	1.20
1:C:909:PHE:HB3	1:C:973:MET:HB2	1.31	1.13
1:A:867:ALA:HA	1:A:871:PHE:HB2	1.16	1.12
1:A:971:LEU:HD23	1:A:972:ARG:H	1.11	1.12
1:A:792:PRO:HG2	1:A:880:ARG:HH21	1.14	1.12
1:A:913:THR:OG1	1:A:972:ARG:HB3	1.47	1.11
1:C:872:LEU:HB3	1:C:875:HIS:HB2	1.25	1.11
1:C:889:ASN:HD22	1:C:895:TYR:N	1.48	1.10
1:A:54:ARG:HB3	1:A:54:ARG:HH11	1.16	1.09
1:A:899:TRP:HA	1:A:902:GLU:HB3	1.26	1.09
1:A:895:TYR:HA	1:A:899:TRP:HB2	1.30	1.07
1:C:918:THR:HG22	1:C:984:ALA:HB2	1.32	1.05
1:C:777:ILE:HB	1:C:778:PRO:HD3	1.37	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ALA:HA	1:A:871:PHE:CB	1.86	1.05
1:C:329:LEU:HD21	1:C:769:ILE:HG13	1.37	1.04
1:A:643:ILE:HB	1:A:644:PRO:HD3	1.41	1.02
1:C:643:ILE:HB	1:C:644:PRO:HD3	1.41	1.02
1:A:514:ILE:HG22	1:A:578:PHE:HB3	1.41	1.02
1:C:907:VAL:HA	1:C:911:CYS:HB2	1.39	1.02
1:A:810:VAL:HG23	1:A:811:PRO:HD3	1.38	1.02
1:C:54:ARG:HH11	1:C:54:ARG:HB3	1.17	1.02
1:A:715:SER:HB2	1:A:716:PRO:HD3	1.41	1.02
1:C:514:ILE:HG22	1:C:578:PHE:HB3	1.40	1.02
1:A:902:GLU:HA	1:A:905:LYS:HG2	1.38	1.02
1:C:41:LEU:H	1:C:41:LEU:HD12	1.24	1.01
1:A:947:LEU:HG	1:A:948:ILE:HD12	1.41	1.01
1:A:913:THR:HB	1:A:914:PRO:HD3	1.40	1.01
1:A:275:THR:HG21	1:A:355:GLU:HG3	1.41	1.01
1:C:103:LEU:HD21	1:C:314:VAL:HB	1.41	1.00
1:C:971:LEU:HD23	1:C:972:ARG:H	1.21	1.00
1:A:631:ASN:HD22	1:A:632:GLU:N	1.60	0.99
1:C:715:SER:HB2	1:C:716:PRO:HD3	1.40	0.99
1:A:365:THR:HB	1:A:705:VAL:HG12	1.43	0.99
1:C:365:THR:HB	1:C:705:VAL:HG12	1.43	0.98
1:C:656:CYS:H	1:C:680:GLU:HB2	1.26	0.98
1:A:904:ARG:HH11	1:A:907:VAL:HG11	1.29	0.98
1:C:631:ASN:HD22	1:C:632:GLU:N	1.61	0.98
1:A:909:PHE:CD1	1:A:973:MET:HB2	1.98	0.98
1:A:41:LEU:HD12	1:A:41:LEU:H	1.29	0.97
1:C:565:ASP:H	1:C:570:ASN:HD22	1.12	0.97
1:A:367:CYS:HB2	1:A:707:VAL:HG22	1.46	0.97
1:C:886:ARG:HA	1:C:896:GLY:HA3	1.47	0.96
2:B:58:LEU:HA	2:B:61:ILE:HG12	1.45	0.96
1:C:228:ASN:HD22	1:C:228:ASN:H	1.07	0.96
1:A:97:LEU:HD21	1:A:325:VAL:HG21	1.47	0.96
1:C:485:ILE:HG12	1:C:498:LEU:HB2	1.48	0.95
1:A:485:ILE:HG12	1:A:498:LEU:HB2	1.49	0.95
1:A:565:ASP:H	1:A:570:ASN:HD22	1.13	0.95
1:C:913:THR:OG1	1:C:972:ARG:HB2	1.64	0.95
1:A:329:LEU:HD23	1:A:772:THR:HG21	1.48	0.95
1:A:861:THR:O	1:A:865:ILE:HG12	1.65	0.95
1:A:770:ALA:HB2	1:A:1016:TYR:OH	1.67	0.95
1:A:88:GLN:HA	1:A:91:GLY:HA3	1.49	0.95
1:C:866:LEU:CB	1:C:871:PHE:HB2	1.96	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HB	1:A:183:LEU:HD21	1.48	0.95
1:C:165:ILE:HB	1:C:183:LEU:HD21	1.47	0.95
1:C:367:CYS:HB2	1:C:707:VAL:HG22	1.46	0.94
1:A:777:ILE:HB	1:A:778:PRO:HD3	1.47	0.94
1:A:889:ASN:HD21	1:A:895:TYR:HD1	1.14	0.94
1:C:867:ALA:HA	1:C:871:PHE:HB3	1.49	0.94
1:C:899:TRP:HA	1:C:902:GLU:HB3	1.50	0.93
1:A:656:CYS:H	1:A:680:GLU:HB2	1.28	0.93
1:C:516:ILE:HG21	1:C:521:GLN:HE21	1.33	0.93
1:C:514:ILE:HD11	1:C:527:LEU:HD23	1.49	0.93
1:A:228:ASN:HD22	1:A:228:ASN:H	1.07	0.93
1:A:95:MET:HG2	1:A:96:LEU:HD12	1.51	0.93
1:C:842:LEU:HD12	1:C:843:ILE:HD13	1.51	0.93
1:C:839:ASN:HD22	1:C:841:GLN:HB2	1.34	0.93
1:C:181:GLY:H	1:C:251:VAL:HG23	1.35	0.92
1:C:961:LEU:HA	1:C:964:CYS:SG	2.08	0.92
1:C:872:LEU:HD12	1:C:876:LEU:N	1.85	0.92
1:A:872:LEU:HB2	1:A:876:LEU:HD22	1.52	0.92
1:A:929:ILE:HD12	1:A:999:LYS:HZ2	1.35	0.92
1:A:973:MET:HG3	1:A:974:TYR:H	1.33	0.91
1:C:879:LEU:HD12	1:C:880:ARG:H	1.33	0.91
1:C:879:LEU:HD12	1:C:880:ARG:N	1.86	0.91
1:C:785:ILE:HD13	1:C:788:ILE:HD12	1.51	0.91
1:C:908:GLU:O	1:C:972:ARG:HG3	1.71	0.91
1:A:170:LYS:HD3	1:C:169:GLU:HG3	1.50	0.91
1:A:831:ASN:ND2	1:A:834:THR:H	1.68	0.91
1:A:872:LEU:HB3	1:A:875:HIS:HB2	1.51	0.90
1:C:95:MET:HG2	1:C:96:LEU:HD12	1.51	0.90
1:A:872:LEU:HD12	1:A:876:LEU:HD13	1.52	0.90
1:C:867:ALA:CA	1:C:871:PHE:HB3	2.01	0.90
1:C:354:LEU:O	1:C:357:VAL:HG23	1.72	0.90
1:C:679:THR:HG22	1:C:681:ILE:HD11	1.54	0.90
1:A:516:ILE:HG21	1:A:521:GLN:HE21	1.33	0.90
1:A:898:GLN:OE1	2:B:72:VAL:HG22	1.72	0.89
1:A:909:PHE:HD1	1:A:973:MET:HB2	1.31	0.89
1:A:679:THR:HG22	1:A:681:ILE:HD11	1.53	0.89
1:A:827:ARG:HD3	1:A:828:GLN:H	1.38	0.89
1:A:680:GLU:HG2	1:A:682:VAL:H	1.38	0.89
1:C:902:GLU:HA	1:C:905:LYS:HB2	1.55	0.89
1:A:181:GLY:H	1:A:251:VAL:HG23	1.36	0.89
1:A:861:THR:OG1	1:A:918:THR:HG21	1.72	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:803:ILE:HA	1:C:807:THR:HG22	1.52	0.89
1:C:764:ASN:HD21	1:C:818:GLU:CB	1.86	0.88
1:A:514:ILE:HD11	1:A:527:LEU:HD23	1.52	0.88
1:C:304:LEU:HD21	1:C:310:TRP:HZ3	1.36	0.88
1:A:631:ASN:HD22	1:A:632:GLU:H	1.17	0.88
1:A:633:THR:HA	1:A:636:ASP:OD2	1.74	0.88
1:A:902:GLU:HA	1:A:905:LYS:CG	2.02	0.88
1:A:971:LEU:CD2	1:A:972:ARG:H	1.85	0.88
2:D:33:PHE:H	2:D:33:PHE:HD2	1.21	0.88
1:C:680:GLU:HG2	1:C:682:VAL:H	1.38	0.87
1:A:103:LEU:HD13	1:A:317:LEU:HD12	1.57	0.87
1:A:493:GLU:HB2	1:A:494:PRO:HD2	1.56	0.87
1:C:633:THR:HA	1:C:636:ASP:OD2	1.72	0.87
1:A:304:LEU:HD11	1:A:310:TRP:HZ3	1.40	0.87
1:A:360:LEU:HD13	1:A:723:ILE:HD13	1.57	0.87
1:C:631:ASN:HD22	1:C:632:GLU:H	1.20	0.86
1:A:19:ALA:N	1:A:20:LYS:HZ3	1.73	0.86
1:A:932:THR:HG23	1:A:999:LYS:HZ3	1.36	0.86
1:C:19:ALA:N	1:C:20:LYS:HZ3	1.73	0.86
3:G:48:LYS:HZ1	3:G:51:ARG:HH21	1.23	0.86
1:A:228:ASN:H	1:A:228:ASN:ND2	1.73	0.86
1:C:493:GLU:HB2	1:C:494:PRO:HD2	1.56	0.86
1:C:830:ARG:HH21	1:C:832:PRO:HA	1.40	0.86
1:C:999:LYS:O	1:C:1003:ARG:HG3	1.76	0.86
1:A:373:THR:HA	1:A:727:MET:HE3	1.57	0.86
1:A:226:ASN:O	1:A:228:ASN:N	2.07	0.86
1:A:889:ASN:HD22	1:A:895:TYR:N	1.74	0.86
1:C:611:GLY:HA2	1:C:686:THR:H	1.39	0.86
1:A:867:ALA:CA	1:A:871:PHE:HB2	2.06	0.85
1:A:300:PHE:O	1:A:304:LEU:HB3	1.76	0.85
1:A:611:GLY:HA2	1:A:686:THR:H	1.39	0.85
1:C:226:ASN:O	1:C:228:ASN:N	2.08	0.85
1:C:952:PHE:CD1	3:H:40:VAL:HG21	2.12	0.85
1:C:917:VAL:O	1:C:921:VAL:HG23	1.76	0.85
1:C:993:VAL:O	1:C:997:VAL:HG23	1.76	0.85
1:C:952:PHE:HD1	3:H:40:VAL:HG21	1.40	0.85
1:C:516:ILE:HD13	1:C:521:GLN:HE21	1.43	0.84
1:C:867:ALA:N	1:C:871:PHE:HB3	1.92	0.84
1:A:28:LEU:C	1:A:29:LYS:HD3	1.98	0.84
1:A:792:PRO:HG2	1:A:880:ARG:NH2	1.92	0.84
1:A:96:LEU:HD21	1:A:292:ALA:HB1	1.59	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LEU:O	1:A:357:VAL:HG23	1.75	0.84
1:A:606:VAL:O	1:A:681:ILE:HG23	1.77	0.84
1:C:606:VAL:O	1:C:681:ILE:HG23	1.77	0.84
1:A:769:ILE:O	1:A:772:THR:HG22	1.77	0.84
1:C:360:LEU:HD13	1:C:723:ILE:HD13	1.60	0.84
1:A:329:LEU:HD21	1:A:769:ILE:HG13	1.59	0.84
1:A:111:GLN:HB2	1:A:115:GLU:OE2	1.79	0.83
1:A:58:PRO:HD3	1:A:167:ASN:HB2	1.58	0.83
1:A:889:ASN:ND2	1:A:895:TYR:H	1.75	0.83
1:C:655:ALA:HB1	1:C:680:GLU:HA	1.60	0.83
1:A:332:THR:HG23	1:A:813:ILE:HD13	1.59	0.83
1:C:902:GLU:HA	1:C:905:LYS:CB	2.08	0.83
1:A:973:MET:HE2	1:A:974:TYR:H	1.41	0.83
1:A:516:ILE:HD13	1:A:521:GLN:HE21	1.44	0.83
1:C:228:ASN:H	1:C:228:ASN:ND2	1.74	0.83
1:A:605:LYS:HE3	1:A:679:THR:HG23	1.61	0.83
1:C:111:GLN:HB2	1:C:115:GLU:OE2	1.79	0.83
1:C:648:VAL:HG23	1:C:649:ASN:H	1.44	0.83
1:A:589:ARG:HB2	1:A:592:VAL:HG23	1.60	0.83
1:C:605:LYS:HE3	1:C:679:THR:HG23	1.59	0.83
2:D:34:LYS:HA	2:D:37:LEU:HG	1.61	0.83
1:C:277:ILE:HD13	1:C:278:ALA:N	1.93	0.83
1:A:299:PHE:CE1	1:A:784:LEU:HG	2.14	0.82
1:A:565:ASP:H	1:A:570:ASN:ND2	1.77	0.82
1:A:648:VAL:HG23	1:A:649:ASN:H	1.43	0.82
1:C:58:PRO:HD3	1:C:167:ASN:HB2	1.58	0.82
1:C:379:MET:HG3	1:C:444:ALA:HB1	1.61	0.82
1:A:952:PHE:HB3	3:G:37:ALA:HB1	1.58	0.82
1:C:514:ILE:HD11	1:C:527:LEU:CD2	2.09	0.82
1:A:900:THR:HA	1:A:903:GLN:HG2	1.60	0.82
1:C:381:VAL:HG21	1:C:452:CYS:HB2	1.59	0.82
1:C:889:ASN:HD22	1:C:895:TYR:H	1.26	0.82
1:C:857:GLY:HA2	1:C:987:TYR:CD2	2.15	0.82
1:A:655:ALA:HB1	1:A:680:GLU:HA	1.59	0.81
1:A:827:ARG:HD3	1:A:828:GLN:N	1.94	0.81
2:D:60:THR:HG22	2:D:61:ILE:H	1.45	0.81
1:A:791:ILE:HD11	1:A:862:TYR:HE1	1.43	0.81
1:A:929:ILE:HG12	1:A:995:ASP:HB3	1.62	0.81
1:C:769:ILE:HG23	1:C:770:ALA:N	1.96	0.81
1:A:282:GLU:O	1:A:285:ILE:HG22	1.79	0.81
1:A:931:LYS:NZ	1:A:931:LYS:HB3	1.96	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LEU:C	1:C:29:LYS:HD3	2.01	0.81
1:C:304:LEU:HD21	1:C:310:TRP:CZ3	2.15	0.81
1:A:773:LEU:O	1:A:776:ASN:HB2	1.81	0.81
1:A:785:ILE:HD13	1:A:788:ILE:HD12	1.60	0.81
1:C:565:ASP:H	1:C:570:ASN:ND2	1.77	0.81
1:A:983:CYS:O	1:A:986:PRO:HD2	1.81	0.80
1:C:103:LEU:HD22	1:C:318:ILE:HG22	1.62	0.80
1:C:976:LEU:HG	1:C:978:PRO:HD2	1.63	0.80
1:A:975:PRO:HB2	1:A:980:TRP:HB3	1.63	0.80
1:C:842:LEU:HD23	1:C:1016:TYR:HE1	1.46	0.80
1:A:775:SER:O	1:A:779:GLU:HG3	1.81	0.80
1:C:866:LEU:HB3	1:C:871:PHE:HB2	1.64	0.80
1:C:971:LEU:CD2	1:C:972:ARG:H	1.95	0.80
1:A:973:MET:HG3	1:A:974:TYR:N	1.96	0.80
1:C:516:ILE:HD13	1:C:521:GLN:NE2	1.97	0.80
1:A:771:TYR:HD2	1:A:772:THR:N	1.80	0.79
1:A:879:LEU:HD11	1:A:881:VAL:HG23	1.64	0.79
1:A:889:ASN:OD1	1:A:893:ASP:HB2	1.82	0.79
1:C:649:ASN:HB2	1:C:650:PRO:HD3	1.65	0.79
1:C:839:ASN:ND2	1:C:841:GLN:HB2	1.97	0.79
1:A:857:GLY:HA2	1:A:987:TYR:CD2	2.17	0.79
1:A:54:ARG:NH1	1:A:54:ARG:HB3	1.98	0.79
1:A:971:LEU:HD23	1:A:972:ARG:N	1.94	0.79
1:A:129:LEU:CD2	1:A:801:LEU:HD11	2.13	0.79
1:A:683:PHE:CG	1:A:694:ILE:HD11	2.17	0.79
1:C:373:THR:HA	1:C:727:MET:HE3	1.65	0.79
1:C:943:LYS:HA	1:C:948:ILE:HD11	1.63	0.79
1:C:683:PHE:CG	1:C:694:ILE:HD11	2.17	0.79
1:C:872:LEU:HG	1:C:876:LEU:HB2	1.62	0.79
1:A:514:ILE:HD11	1:A:527:LEU:CD2	2.13	0.79
1:C:889:ASN:ND2	1:C:895:TYR:N	2.29	0.78
1:C:901:TYR:O	1:C:905:LYS:HB2	1.83	0.78
2:D:60:THR:HG22	2:D:61:ILE:N	1.98	0.78
1:A:129:LEU:HD23	1:A:801:LEU:HD11	1.63	0.78
1:C:913:THR:O	1:C:916:PHE:HB3	1.83	0.78
1:A:227:GLU:OE1	1:A:229:PRO:HD2	1.83	0.78
1:A:516:ILE:HD13	1:A:521:GLN:NE2	1.98	0.78
1:A:743:LEU:H	1:A:743:LEU:HD23	1.48	0.78
1:A:771:TYR:HE1	1:A:927:LEU:HB2	1.48	0.78
1:C:435:ILE:HA	1:C:438:ARG:HD2	1.65	0.78
1:A:889:ASN:ND2	1:A:895:TYR:N	2.31	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ILE:HA	1:A:438:ARG:HD2	1.66	0.78
1:A:606:VAL:C	1:A:681:ILE:HG23	2.04	0.78
1:A:649:ASN:HB2	1:A:650:PRO:HD3	1.64	0.78
1:C:101:ALA:O	1:C:105:PHE:HB2	1.84	0.78
1:C:615:ILE:H	1:C:615:ILE:HD13	1.49	0.78
1:C:759:ARG:HD2	1:C:825:MET:HE1	1.66	0.78
3:H:39:ILE:O	3:H:43:ILE:HB	1.84	0.78
1:A:886:ARG:O	1:A:888:ILE:N	2.15	0.78
1:A:989:LEU:O	1:A:993:VAL:HG13	1.83	0.78
1:A:406:LYS:HZ2	1:A:411:TRP:HE1	1.32	0.78
1:C:205:LYS:HG2	1:C:219:THR:HG22	1.65	0.78
1:A:871:PHE:CD2	1:A:873:PRO:HG3	2.18	0.77
1:C:885:ASP:OD1	1:C:897:GLN:HB3	1.84	0.77
1:A:103:LEU:HD22	1:A:318:ILE:HG22	1.65	0.77
1:C:564:PHE:HA	1:C:570:ASN:HD21	1.49	0.77
1:C:92:GLY:HA2	1:C:285:ILE:HD13	1.67	0.77
1:A:615:ILE:H	1:A:615:ILE:HD13	1.47	0.77
1:C:310:TRP:HA	1:C:310:TRP:CE3	2.19	0.77
1:A:917:VAL:O	1:A:921:VAL:HG23	1.84	0.77
1:A:771:TYR:CE1	1:A:927:LEU:HB2	2.19	0.77
1:C:866:LEU:HB2	1:C:871:PHE:HB2	1.64	0.77
2:D:40:VAL:HG23	2:D:41:ILE:HD13	1.65	0.77
1:A:101:ALA:O	1:A:105:PHE:HB2	1.84	0.77
2:D:66:PRO:O	2:D:67:THR:HB	1.81	0.77
1:A:564:PHE:HA	1:A:570:ASN:HD21	1.49	0.76
1:C:892:GLU:OE1	2:D:65:LYS:HG2	1.85	0.76
2:D:33:PHE:O	2:D:37:LEU:N	2.18	0.76
1:C:280:GLU:HA	1:C:280:GLU:OE2	1.85	0.76
3:G:23:TYR:O	3:G:27:ARG:HG2	1.84	0.76
1:A:435:ILE:HA	1:A:438:ARG:CD	2.15	0.76
1:C:435:ILE:HA	1:C:438:ARG:CD	2.15	0.76
1:A:779:GLU:HB3	1:A:800:ILE:HD12	1.67	0.76
1:A:28:LEU:O	1:A:29:LYS:HD3	1.85	0.76
1:A:910:THR:O	1:A:912:HIS:N	2.19	0.76
1:A:205:LYS:HG2	1:A:219:THR:HG22	1.67	0.76
1:A:301:ILE:HG22	1:A:302:LEU:N	1.98	0.76
1:C:28:LEU:O	1:C:29:LYS:HD3	1.86	0.76
1:C:976:LEU:HD23	1:C:979:THR:H	1.51	0.76
1:A:839:ASN:N	1:A:839:ASN:HD22	1.82	0.76
1:C:381:VAL:CG2	1:C:452:CYS:HB2	2.15	0.76
1:C:831:ASN:HD21	1:C:833:LYS:HB2	1.50	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ILE:HG12	2:B:46:LEU:HD21	1.68	0.76
1:A:304:LEU:HD23	1:A:313:ALA:HB2	1.66	0.75
1:C:770:ALA:HB2	1:C:842:LEU:HD21	1.68	0.75
1:A:181:GLY:N	1:A:251:VAL:HG23	2.02	0.75
1:A:990:LEU:O	1:A:993:VAL:HG22	1.84	0.75
1:A:929:ILE:HD12	1:A:999:LYS:NZ	1.99	0.75
1:A:875:HIS:O	1:A:876:LEU:HB2	1.83	0.75
1:C:197:ARG:HH11	1:C:197:ARG:HG2	1.51	0.75
1:C:860:PHE:CE1	2:D:53:THR:HB	2.21	0.75
1:A:973:MET:HE2	1:A:974:TYR:N	2.01	0.75
1:C:606:VAL:C	1:C:681:ILE:HG23	2.05	0.75
1:C:654:LYS:O	1:C:678:HIS:HB2	1.86	0.75
1:C:687:SER:OG	1:C:690:GLN:HG3	1.87	0.75
1:A:154:PHE:CE2	1:A:264:ALA:HA	2.22	0.75
2:D:33:PHE:HB2	2:D:37:LEU:HD23	1.69	0.75
1:A:626:ILE:HG23	1:A:681:ILE:CG2	2.17	0.75
1:C:285:ILE:HD11	1:C:330:LEU:HD11	1.67	0.75
2:D:34:LYS:NZ	2:D:37:LEU:HD21	2.02	0.75
1:C:626:ILE:HG23	1:C:681:ILE:CG2	2.17	0.75
2:B:65:LYS:HE3	2:B:67:THR:OG1	1.87	0.74
1:C:853:ILE:HG22	2:D:46:LEU:HD21	1.69	0.74
1:A:197:ARG:HG2	1:A:197:ARG:HH11	1.50	0.74
1:A:821:GLU:O	1:A:822:SER:HB2	1.86	0.74
2:B:40:VAL:HG23	2:B:41:ILE:HD13	1.69	0.74
1:A:516:ILE:HG21	1:A:521:GLN:NE2	2.03	0.74
1:C:743:LEU:H	1:C:743:LEU:HD23	1.50	0.74
2:B:63:GLU:CD	2:B:63:GLU:H	1.91	0.74
1:C:150:ILE:HG21	1:C:267:ALA:O	1.87	0.74
1:C:181:GLY:N	1:C:251:VAL:HG23	2.01	0.74
1:C:854:GLN:HG2	1:C:991:ILE:HD11	1.68	0.74
1:A:92:GLY:O	1:A:285:ILE:HD11	1.86	0.74
1:C:931:LYS:HD2	1:C:947:LEU:CD1	2.18	0.74
1:C:929:ILE:HD12	1:C:999:LYS:HZ2	1.53	0.74
1:A:654:LYS:O	1:A:678:HIS:HB2	1.87	0.74
1:C:154:PHE:CE2	1:C:264:ALA:HA	2.22	0.74
1:C:227:GLU:OE1	1:C:229:PRO:HD2	1.87	0.74
1:C:103:LEU:CD2	1:C:314:VAL:HB	2.17	0.74
1:C:369:ASP:O	1:C:373:THR:HB	1.87	0.74
1:C:815:LEU:O	1:C:818:GLU:HB2	1.87	0.74
1:C:889:ASN:OD1	1:C:890:ASP:N	2.21	0.74
1:A:476:ASN:HD22	1:A:480:LYS:HA	1.53	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:SER:OG	1:A:690:GLN:HG3	1.87	0.74
1:A:280:GLU:HG2	1:A:837:LEU:HB2	1.70	0.74
1:A:895:TYR:CD2	1:A:899:TRP:HB3	2.22	0.74
1:C:406:LYS:HZ2	1:C:411:TRP:HE1	1.34	0.74
1:C:477:SER:O	1:C:478:THR:HG22	1.88	0.74
1:C:516:ILE:HG21	1:C:521:GLN:NE2	2.03	0.74
1:C:803:ILE:HA	1:C:807:THR:CG2	2.18	0.74
1:A:564:PHE:HA	1:A:570:ASN:ND2	2.03	0.73
1:A:372:GLY:HA3	1:A:710:ASP:OD1	1.88	0.73
1:C:897:GLN:C	1:C:899:TRP:H	1.89	0.73
1:C:564:PHE:HA	1:C:570:ASN:ND2	2.03	0.73
1:A:200:SER:HA	1:A:222:PRO:HB3	1.70	0.73
1:A:888:ILE:HG22	1:A:889:ASN:N	2.03	0.73
1:C:803:ILE:O	1:C:808:ASP:HB2	1.88	0.73
1:A:304:LEU:HD11	1:A:310:TRP:CZ3	2.23	0.73
1:C:96:LEU:HA	1:C:99:ILE:HG22	1.71	0.73
1:C:995:ASP:OD2	1:C:998:ARG:HD3	1.88	0.73
1:C:873:PRO:HB3	2:D:58:LEU:HD11	1.69	0.73
1:C:96:LEU:HD21	1:C:292:ALA:HB1	1.69	0.73
1:A:477:SER:O	1:A:478:THR:HG22	1.89	0.73
1:A:973:MET:CG	1:A:974:TYR:H	2.02	0.73
1:A:929:ILE:CG1	1:A:995:ASP:HB3	2.17	0.73
1:C:515:LEU:O	1:C:516:ILE:HG23	1.87	0.73
1:A:37:HIS:HA	1:A:197:ARG:HD2	1.71	0.73
1:C:888:ILE:HG22	1:C:889:ASN:N	2.04	0.73
1:C:320:ILE:HA	1:C:323:ALA:HB3	1.69	0.73
1:C:372:GLY:HA3	1:C:710:ASP:OD1	1.89	0.73
1:A:515:LEU:O	1:A:516:ILE:HG23	1.88	0.72
1:A:289:THR:HA	1:A:292:ALA:HB2	1.70	0.72
1:C:200:SER:HA	1:C:222:PRO:HB3	1.70	0.72
1:C:872:LEU:HD12	1:C:876:LEU:CA	2.20	0.72
2:B:64:PHE:O	2:B:65:LYS:HB3	1.88	0.72
1:A:631:ASN:ND2	1:A:632:GLU:N	2.35	0.72
1:C:476:ASN:HD22	1:C:480:LYS:HA	1.54	0.72
1:C:872:LEU:HD23	1:C:872:LEU:N	2.04	0.72
1:A:904:ARG:HH11	1:A:907:VAL:CG1	2.02	0.72
1:C:886:ARG:CA	1:C:896:GLY:HA3	2.19	0.72
2:D:31:SER:HA	2:D:33:PHE:HE2	1.55	0.72
1:A:103:LEU:HD22	1:A:318:ILE:CG2	2.19	0.72
1:C:255:GLY:O	1:C:258:THR:HG23	1.89	0.72
1:A:904:ARG:NH1	1:A:907:VAL:HG11	2.03	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:VAL:HG21	1:C:452:CYS:CB	2.18	0.72
1:C:872:LEU:HB3	1:C:875:HIS:CB	2.12	0.72
1:A:483:LEU:HB3	1:A:500:MET:HB3	1.72	0.72
1:C:867:ALA:N	1:C:871:PHE:CB	2.52	0.72
1:C:976:LEU:HD21	1:C:978:PRO:HB2	1.71	0.72
1:C:732:SER:C	1:C:734:VAL:H	1.93	0.71
1:A:227:GLU:CD	1:A:229:PRO:HD2	2.10	0.71
1:C:807:THR:HG23	1:C:808:ASP:H	1.55	0.71
1:A:1015:TYR:O	1:A:1016:TYR:HB2	1.89	0.71
1:A:96:LEU:HA	1:A:99:ILE:HG22	1.71	0.71
1:C:198:ILE:H	1:C:198:ILE:HD13	1.54	0.71
1:C:350:LEU:H	1:C:744:LEU:HD11	1.56	0.71
1:C:807:THR:HG23	1:C:808:ASP:N	2.05	0.71
1:A:369:ASP:O	1:A:373:THR:HB	1.90	0.71
1:A:896:GLY:O	1:A:900:THR:N	2.24	0.71
2:B:58:LEU:C	2:B:60:THR:H	1.92	0.71
1:C:483:LEU:HB3	1:C:500:MET:HB3	1.72	0.71
1:C:872:LEU:HD22	1:C:891:VAL:CG1	2.20	0.71
1:A:732:SER:C	1:A:734:VAL:H	1.93	0.71
1:C:314:VAL:O	1:C:318:ILE:HG23	1.91	0.71
1:A:88:GLN:C	1:A:90:PHE:H	1.92	0.71
2:B:49:ILE:O	2:B:53:THR:HG23	1.91	0.71
1:C:493:GLU:CD	1:C:493:GLU:H	1.93	0.71
1:A:840:GLU:HG2	1:A:841:GLN:H	1.54	0.71
1:A:667:THR:OG1	1:A:670:GLN:HG3	1.91	0.71
2:D:33:PHE:N	2:D:33:PHE:HD2	1.87	0.71
1:A:195:ASP:OD2	1:A:258:THR:HB	1.91	0.70
1:C:1009:TRP:O	1:C:1011:GLU:N	2.23	0.70
1:C:821:GLU:OE1	1:C:932:THR:HA	1.91	0.70
1:C:899:TRP:CZ2	2:D:70:ASP:HB3	2.26	0.70
1:C:776:ASN:O	1:C:779:GLU:HG2	1.91	0.70
1:A:255:GLY:O	1:A:258:THR:HG23	1.90	0.70
1:A:881:VAL:HG12	1:A:882:ASN:N	2.06	0.70
1:A:950:GLY:HA2	1:A:953:GLU:HB2	1.73	0.70
1:C:683:PHE:CD2	1:C:694:ILE:HD11	2.27	0.70
1:A:48:TYR:OH	1:A:252:VAL:HG13	1.91	0.70
1:C:1011:GLU:OE2	1:C:1012:LYS:N	2.24	0.70
1:C:92:GLY:HA2	1:C:285:ILE:CD1	2.21	0.70
1:C:631:ASN:ND2	1:C:632:GLU:N	2.37	0.70
1:C:774:THR:OG1	1:C:846:ALA:HB1	1.92	0.70
1:A:493:GLU:CD	1:A:493:GLU:H	1.93	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ALA:CB	1:A:680:GLU:HA	2.22	0.70
1:A:936:SER:H	1:A:1003:ARG:NH2	1.90	0.70
1:C:585:ILE:HG12	1:C:586:ASP:H	1.54	0.70
1:C:647:GLN:O	1:C:650:PRO:HD2	1.92	0.70
1:C:966:GLY:C	1:C:968:GLY:H	1.93	0.70
1:C:853:ILE:CG2	2:D:46:LEU:HD21	2.22	0.70
1:C:227:GLU:CD	1:C:229:PRO:HD2	2.12	0.70
1:A:227:GLU:O	1:A:229:PRO:N	2.24	0.70
1:A:79:THR:H	1:A:80:PRO:HD3	1.57	0.70
1:A:198:ILE:HD13	1:A:198:ILE:H	1.56	0.70
1:A:789:ALA:O	1:A:791:ILE:N	2.24	0.70
1:C:227:GLU:O	1:C:229:PRO:N	2.24	0.70
1:A:585:ILE:HG12	1:A:586:ASP:H	1.56	0.69
1:A:794:PRO:O	1:A:912:HIS:HD2	1.75	0.69
1:A:865:ILE:HG13	1:A:914:PRO:HB2	1.74	0.69
1:C:37:HIS:HA	1:C:197:ARG:HD2	1.73	0.69
1:C:764:ASN:HD21	1:C:818:GLU:HB3	1.57	0.69
1:C:325:VAL:HG23	1:C:325:VAL:O	1.92	0.69
1:A:309:THR:OG1	1:A:312:GLU:HG3	1.92	0.69
1:A:325:VAL:O	1:A:325:VAL:HG23	1.91	0.69
1:A:889:ASN:ND2	1:A:895:TYR:HD1	1.90	0.69
1:C:48:TYR:OH	1:C:252:VAL:HG13	1.92	0.69
2:D:54:ILE:O	2:D:57:MET:HG3	1.91	0.69
1:A:867:ALA:HB2	2:B:57:MET:HE1	1.75	0.69
1:A:647:GLN:O	1:A:650:PRO:HD2	1.92	0.69
1:C:481:TYR:HD2	1:C:481:TYR:C	1.96	0.69
1:C:515:LEU:HD23	1:C:519:LYS:O	1.91	0.69
1:C:764:ASN:HD21	1:C:818:GLU:HB2	1.55	0.69
1:A:350:LEU:H	1:A:744:LEU:HD11	1.57	0.69
1:C:694:ILE:HG22	1:C:695:VAL:N	2.07	0.69
1:C:872:LEU:HD13	1:C:890:ASP:OD2	1.93	0.69
1:A:37:HIS:CE1	1:A:228:ASN:O	2.46	0.69
1:C:899:TRP:CA	1:C:902:GLU:HB3	2.22	0.69
1:A:54:ARG:HH11	1:A:54:ARG:CB	2.00	0.69
1:A:831:ASN:HD22	1:A:834:THR:H	1.39	0.69
1:A:791:ILE:HD11	1:A:862:TYR:CE1	2.25	0.69
1:A:885:ASP:OD1	1:A:897:GLN:HB2	1.93	0.69
1:A:944:ASN:O	1:A:948:ILE:HD13	1.93	0.69
1:C:54:ARG:NH1	1:C:54:ARG:HB3	1.99	0.69
1:A:515:LEU:HD23	1:A:519:LYS:O	1.92	0.69
1:C:828:GLN:HE21	1:C:828:GLN:N	1.90	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:TYR:CA	1:A:899:TRP:HB2	2.18	0.69
1:C:1006:PRO:O	1:C:1012:LYS:HD2	1.93	0.69
1:C:655:ALA:CB	1:C:680:GLU:HA	2.23	0.69
3:G:48:LYS:NZ	3:G:51:ARG:HH21	1.91	0.69
1:A:918:THR:HB	1:A:984:ALA:HB2	1.75	0.68
1:C:310:TRP:HE3	1:C:310:TRP:HA	1.56	0.68
1:C:37:HIS:CE1	1:C:228:ASN:O	2.46	0.68
1:A:494:PRO:HG2	1:A:552:PHE:HB3	1.76	0.68
1:A:909:PHE:HB3	1:A:973:MET:CB	2.23	0.68
2:B:53:THR:O	2:B:57:MET:HB2	1.92	0.68
1:A:301:ILE:O	1:A:303:SER:N	2.25	0.68
1:A:304:LEU:HD22	1:A:304:LEU:O	1.92	0.68
1:A:871:PHE:CE2	1:A:873:PRO:HG3	2.27	0.68
1:A:973:MET:O	1:A:975:PRO:HD3	1.93	0.68
1:C:164:VAL:HG12	1:C:184:VAL:HB	1.75	0.68
1:A:311:LEU:O	1:A:315:ILE:HG12	1.94	0.68
1:C:481:TYR:C	1:C:481:TYR:CD2	2.67	0.68
1:A:150:ILE:HG21	1:A:267:ALA:O	1.92	0.68
1:A:694:ILE:HG22	1:A:695:VAL:N	2.07	0.68
1:A:767:LYS:HE2	1:A:933:ARG:HG3	1.74	0.68
1:A:982:PHE:O	1:A:986:PRO:HD3	1.94	0.68
1:A:997:VAL:O	1:A:1001:ILE:HG12	1.92	0.68
1:C:897:GLN:O	1:C:897:GLN:HG3	1.93	0.68
1:C:95:MET:HG2	1:C:96:LEU:H	1.59	0.68
1:A:856:LEU:HD11	2:B:46:LEU:HD22	1.74	0.68
1:C:318:ILE:O	1:C:322:VAL:HG23	1.93	0.68
1:C:432:ASN:OD1	1:C:434:PRO:HD2	1.93	0.68
1:C:79:THR:H	1:C:80:PRO:HD3	1.58	0.68
1:C:280:GLU:HG3	1:C:837:LEU:HB3	1.75	0.68
2:D:37:LEU:O	2:D:37:LEU:HD12	1.94	0.68
1:A:164:VAL:HG12	1:A:184:VAL:HB	1.74	0.68
1:A:481:TYR:C	1:A:481:TYR:HD2	1.96	0.68
1:A:263:ILE:HD11	1:A:689:GLN:OE1	1.94	0.68
1:C:715:SER:HB2	1:C:716:PRO:CD	2.22	0.68
1:C:982:PHE:O	1:C:986:PRO:HD3	1.94	0.68
2:D:31:SER:HA	2:D:33:PHE:CE2	2.29	0.68
1:A:453:ILE:O	1:A:454:GLU:HG2	1.94	0.68
1:A:693:ILE:O	1:A:693:ILE:HD13	1.94	0.68
1:C:656:CYS:N	1:C:680:GLU:HB2	2.06	0.68
1:C:872:LEU:HB2	1:C:875:HIS:C	2.13	0.68
1:C:494:PRO:HG2	1:C:552:PHE:HB3	1.74	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:815:LEU:HD11	1:C:930:CYS:O	1.94	0.67
1:C:909:PHE:HB3	1:C:973:MET:CB	2.19	0.67
1:A:523:LEU:HD23	1:A:524:ASP:N	2.09	0.67
1:A:779:GLU:OE2	1:A:800:ILE:HG23	1.93	0.67
1:A:944:ASN:CG	1:A:947:LEU:HB3	2.14	0.67
1:A:304:LEU:HD13	1:A:304:LEU:O	1.95	0.67
1:A:889:ASN:CG	1:A:893:ASP:HB2	2.13	0.67
1:C:523:LEU:HD23	1:C:524:ASP:N	2.10	0.67
3:H:44:ILE:HA	3:H:47:SER:HB2	1.76	0.67
1:A:314:VAL:O	1:A:318:ILE:HG23	1.93	0.67
1:C:824:ILE:C	1:C:826:LYS:H	1.97	0.67
1:C:910:THR:HG22	1:C:911:CYS:N	2.10	0.67
1:A:998:ARG:HA	1:A:1001:ILE:HB	1.77	0.67
1:C:589:ARG:HG3	1:C:589:ARG:HH11	1.60	0.67
1:C:769:ILE:CG2	1:C:770:ALA:N	2.58	0.67
1:C:769:ILE:HG23	1:C:770:ALA:H	1.59	0.67
1:C:384:MET:HG2	1:C:582:ILE:HG12	1.76	0.67
1:C:667:THR:OG1	1:C:670:GLN:HG3	1.94	0.67
1:A:481:TYR:CD2	1:A:481:TYR:C	2.68	0.67
1:A:932:THR:HG23	1:A:999:LYS:NZ	2.09	0.67
1:C:618:LYS:HD3	1:C:657:VAL:HG21	1.76	0.67
1:A:464:ARG:HG3	1:A:464:ARG:HH11	1.59	0.67
1:C:339:LEU:O	1:C:343:ARG:HB2	1.94	0.67
1:C:693:ILE:O	1:C:693:ILE:HD13	1.94	0.67
1:C:802:CYS:O	1:C:807:THR:HG22	1.95	0.67
1:A:296:GLY:HA2	1:A:320:ILE:HD13	1.77	0.67
1:A:373:THR:O	1:A:589:ARG:NH1	2.28	0.67
1:C:41:LEU:H	1:C:41:LEU:CD1	2.03	0.67
1:A:50:THR:O	1:A:52:LEU:HD12	1.95	0.66
1:C:54:ARG:CB	1:C:54:ARG:HH11	2.01	0.66
1:C:971:LEU:HD23	1:C:972:ARG:N	2.02	0.66
2:B:37:LEU:C	2:B:37:LEU:HD12	2.15	0.66
1:C:228:ASN:HD22	1:C:228:ASN:N	1.79	0.66
1:C:606:VAL:O	1:C:681:ILE:HD12	1.95	0.66
1:C:871:PHE:CZ	1:C:873:PRO:HA	2.29	0.66
1:C:936:SER:HB3	1:C:1003:ARG:HH22	1.61	0.66
1:C:329:LEU:O	1:C:332:THR:HB	1.94	0.66
1:C:591:ALA:C	1:C:593:PRO:HD2	2.16	0.66
1:C:910:THR:HG22	1:C:911:CYS:H	1.59	0.66
1:A:618:LYS:HD3	1:A:657:VAL:HG21	1.77	0.66
1:A:611:GLY:O	1:A:685:ARG:HD2	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TRP:O	1:A:85:PHE:N	2.29	0.66
1:A:888:ILE:HG22	1:A:889:ASN:H	1.58	0.66
1:A:384:MET:HG2	1:A:582:ILE:HG12	1.76	0.66
1:A:929:ILE:CD1	1:A:995:ASP:HB3	2.26	0.66
1:C:841:GLN:HG2	1:C:1014:THR:HA	1.78	0.66
1:C:370:LYS:HG3	1:C:620:ILE:HG21	1.78	0.66
1:A:432:ASN:OD1	1:A:434:PRO:HD2	1.95	0.66
1:A:771:TYR:CD2	1:A:772:THR:N	2.62	0.66
1:A:781:THR:OG1	1:A:782:PRO:HD3	1.96	0.66
1:A:879:LEU:HD11	1:A:881:VAL:CG2	2.25	0.66
1:A:900:THR:HA	1:A:903:GLN:CG	2.26	0.66
3:G:45:ILE:O	3:G:48:LYS:HG2	1.95	0.66
1:A:651:ARG:C	1:A:653:ALA:H	1.99	0.66
1:A:872:LEU:HB3	1:A:875:HIS:CB	2.24	0.66
1:A:913:THR:O	1:A:916:PHE:HB3	1.96	0.66
1:C:23:ARG:HA	1:C:27:GLU:HG3	1.78	0.66
1:C:769:ILE:CG2	1:C:770:ALA:H	2.08	0.66
1:A:789:ALA:O	1:A:791:ILE:HG22	1.95	0.66
1:C:50:THR:O	1:C:52:LEU:HD12	1.96	0.66
1:A:606:VAL:O	1:A:681:ILE:HD12	1.96	0.66
1:A:773:LEU:HD12	1:A:774:THR:N	2.11	0.66
1:C:453:ILE:O	1:C:454:GLU:HG2	1.95	0.66
1:A:565:ASP:OD2	1:A:568:ASP:HB3	1.96	0.65
1:A:744:LEU:H	1:A:744:LEU:HD12	1.60	0.65
1:A:802:CYS:SG	1:A:961:LEU:HD21	2.36	0.65
1:A:959:ALA:HA	1:A:962:SER:OG	1.96	0.65
1:C:350:LEU:HG	1:C:351:VAL:N	2.10	0.65
1:A:23:ARG:HA	1:A:27:GLU:HG3	1.77	0.65
1:A:333:VAL:O	1:A:337:LEU:HD22	1.95	0.65
1:C:360:LEU:O	1:C:755:VAL:HG23	1.97	0.65
1:A:636:ASP:OD1	1:A:643:ILE:HA	1.96	0.65
1:A:683:PHE:CD2	1:A:694:ILE:HD11	2.30	0.65
1:C:828:GLN:H	1:C:828:GLN:HE21	1.44	0.65
1:C:886:ARG:O	1:C:888:ILE:N	2.28	0.65
2:D:34:LYS:HD3	2:D:37:LEU:HD21	1.79	0.65
2:D:60:THR:CG2	2:D:61:ILE:H	2.08	0.65
1:C:565:ASP:OD2	1:C:568:ASP:HB3	1.96	0.65
1:A:350:LEU:HG	1:A:351:VAL:N	2.12	0.65
1:C:656:CYS:H	1:C:680:GLU:CB	2.06	0.65
2:D:33:PHE:CD2	2:D:33:PHE:N	2.59	0.65
1:A:643:ILE:HB	1:A:644:PRO:CD	2.24	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ARG:HA	1:A:896:GLY:CA	2.27	0.65
1:C:464:ARG:HH11	1:C:464:ARG:HG3	1.61	0.65
1:C:777:ILE:HB	1:C:778:PRO:CD	2.20	0.65
1:A:715:SER:HB2	1:A:716:PRO:CD	2.23	0.65
1:A:254:THR:HG23	1:A:257:ARG:HH21	1.60	0.65
1:A:759:ARG:HH21	1:A:829:PRO:HA	1.58	0.65
1:A:955:THR:O	1:A:958:ALA:HB3	1.97	0.65
1:C:103:LEU:HD13	1:C:317:LEU:HD12	1.77	0.65
1:C:254:THR:HG23	1:C:257:ARG:HH21	1.60	0.65
1:C:263:ILE:HD11	1:C:689:GLN:OE1	1.97	0.65
1:A:95:MET:HG2	1:A:96:LEU:H	1.60	0.65
1:A:995:ASP:O	1:A:998:ARG:HG2	1.95	0.65
1:C:195:ASP:OD2	1:C:258:THR:HB	1.97	0.65
1:A:656:CYS:O	1:A:680:GLU:HB2	1.97	0.64
1:C:111:GLN:CB	1:C:115:GLU:HG3	2.27	0.64
1:C:636:ASP:OD1	1:C:643:ILE:HA	1.97	0.64
1:C:284:PHE:CD1	1:C:838:VAL:HG21	2.32	0.64
1:A:764:ASN:ND2	1:A:818:GLU:O	2.30	0.64
1:A:807:THR:HG23	1:A:954:GLU:HG3	1.79	0.64
1:C:344:MET:CE	1:C:357:VAL:HG13	2.27	0.64
1:A:228:ASN:N	1:A:228:ASN:HD22	1.79	0.64
1:A:591:ALA:C	1:A:593:PRO:HD2	2.18	0.64
1:A:898:GLN:HG3	1:A:899:TRP:H	1.62	0.64
1:C:305:ILE:HB	1:C:307:GLU:OE1	1.97	0.64
1:C:197:ARG:HG2	1:C:197:ARG:NH1	2.11	0.64
1:C:205:LYS:HG2	1:C:219:THR:CG2	2.27	0.64
1:A:810:VAL:CG2	1:A:811:PRO:HD3	2.23	0.64
1:C:777:ILE:HD13	1:C:780:ILE:CD1	2.27	0.64
1:C:872:LEU:HD22	1:C:891:VAL:HG13	1.80	0.64
1:A:881:VAL:CG1	1:A:882:ASN:N	2.60	0.64
1:A:892:GLU:OE1	2:B:65:LYS:HG2	1.97	0.64
1:C:417:ILE:HG22	1:C:548:PHE:HD2	1.63	0.64
1:C:965:PRO:HG3	3:H:31:LEU:HD21	1.78	0.64
1:A:944:ASN:HB3	1:A:947:LEU:HD23	1.78	0.64
2:D:28:THR:HB	2:D:32:TRP:HE1	1.63	0.64
1:A:111:GLN:CB	1:A:115:GLU:HG3	2.28	0.64
1:A:589:ARG:HG3	1:A:589:ARG:HH11	1.62	0.64
1:A:900:THR:CA	1:A:903:GLN:HG2	2.28	0.64
1:C:651:ARG:C	1:C:653:ALA:H	1.99	0.64
1:C:656:CYS:O	1:C:680:GLU:HB2	1.97	0.64
2:D:52:GLY:O	2:D:56:VAL:HG22	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:47:SER:O	3:G:48:LYS:HD2	1.97	0.64
1:A:82:TRP:O	1:A:84:LYS:N	2.30	0.64
1:C:366:ILE:HB	1:C:606:VAL:HG12	1.80	0.64
1:A:670:GLN:O	1:A:674:ILE:HD13	1.98	0.64
1:A:982:PHE:HD2	1:A:982:PHE:H	1.46	0.64
1:A:366:ILE:HB	1:A:606:VAL:HG12	1.80	0.63
1:A:909:PHE:HB3	1:A:973:MET:HB3	1.80	0.63
1:A:865:ILE:HG21	1:A:911:CYS:H	1.62	0.63
1:C:871:PHE:O	1:C:873:PRO:HD3	1.98	0.63
1:A:370:LYS:HG3	1:A:620:ILE:HG21	1.78	0.63
1:C:881:VAL:HG12	1:C:882:ASN:N	2.14	0.63
1:C:889:ASN:ND2	1:C:893:ASP:HB3	2.13	0.63
1:C:88:GLN:HA	1:C:91:GLY:HA3	1.80	0.63
1:C:900:THR:HA	1:C:903:GLN:HG2	1.80	0.63
1:C:914:PRO:HA	1:C:917:VAL:HG23	1.80	0.63
3:H:37:ALA:HA	3:H:40:VAL:HG22	1.81	0.63
1:A:111:GLN:HG3	1:A:115:GLU:HG3	1.80	0.63
1:C:296:GLY:HA2	1:C:320:ILE:HD13	1.81	0.63
1:C:911:CYS:C	1:C:914:PRO:HD2	2.18	0.63
1:A:782:PRO:HG2	1:A:795:LEU:HD12	1.80	0.63
1:C:744:LEU:HD12	1:C:744:LEU:H	1.64	0.63
1:A:490:ASN:O	1:A:492:ALA:N	2.32	0.63
1:A:732:SER:O	1:A:734:VAL:N	2.32	0.63
1:A:170:LYS:CD	1:C:169:GLU:HG3	2.25	0.63
1:C:51:ASP:CG	1:C:54:ARG:HB2	2.19	0.63
1:A:341:ALA:C	1:A:343:ARG:H	2.00	0.63
1:A:656:CYS:H	1:A:680:GLU:CB	2.07	0.63
1:A:170:LYS:O	1:C:169:GLU:HB3	1.98	0.63
1:C:589:ARG:HB2	1:C:592:VAL:HG23	1.81	0.63
1:C:777:ILE:HD13	1:C:780:ILE:HD11	1.81	0.63
1:C:910:THR:O	1:C:912:HIS:N	2.32	0.63
3:H:43:ILE:HG22	3:H:43:ILE:O	1.98	0.63
1:A:412:LEU:O	1:A:415:SER:HB3	1.98	0.62
1:C:111:GLN:HG3	1:C:115:GLU:HG3	1.80	0.62
1:A:205:LYS:HG2	1:A:219:THR:CG2	2.29	0.62
1:A:344:MET:CE	1:A:357:VAL:HG13	2.29	0.62
1:A:824:ILE:C	1:A:826:LYS:H	2.02	0.62
1:A:759:ARG:NH2	1:A:829:PRO:HA	2.14	0.62
1:C:103:LEU:HD22	1:C:318:ILE:CG2	2.29	0.62
1:C:670:GLN:O	1:C:674:ILE:HD13	1.99	0.62
1:C:915:PHE:O	1:C:919:ILE:HG12	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:976:LEU:O	1:C:976:LEU:HD23	1.99	0.62
1:A:310:TRP:CE3	1:A:310:TRP:HA	2.34	0.62
1:A:329:LEU:O	1:A:332:THR:HB	1.99	0.62
2:B:37:LEU:C	2:B:39:TYR:H	2.03	0.62
1:C:412:LEU:O	1:C:415:SER:HB3	1.99	0.62
1:C:929:ILE:HG12	1:C:995:ASP:HB3	1.80	0.62
1:C:979:THR:O	1:C:981:TRP:N	2.32	0.62
1:A:995:ASP:HA	1:A:998:ARG:HG2	1.80	0.62
1:A:860:PHE:HD1	2:B:53:THR:HG1	1.46	0.62
1:C:450:LEU:HD23	1:C:450:LEU:C	2.20	0.62
1:A:572:PRO:O	1:A:573:LEU:HD23	1.99	0.62
1:A:634:VAL:HG23	1:A:635:GLU:N	2.14	0.62
1:A:763:ASP:O	1:A:765:LEU:N	2.31	0.62
1:C:753:THR:HG22	1:C:753:THR:O	1.99	0.62
1:C:853:ILE:HG22	2:D:46:LEU:CD2	2.29	0.62
1:C:417:ILE:CG2	1:C:548:PHE:HD2	2.11	0.62
1:C:856:LEU:HD11	2:D:46:LEU:HD13	1.80	0.62
1:A:743:LEU:CD2	1:A:743:LEU:N	2.62	0.62
1:A:771:TYR:O	1:A:773:LEU:N	2.32	0.62
1:A:791:ILE:HG12	1:A:791:ILE:O	1.98	0.62
2:B:63:GLU:HG2	2:B:64:PHE:CE2	2.35	0.62
1:A:1011:GLU:CD	1:A:1011:GLU:H	2.01	0.62
1:A:267:ALA:HB2	1:A:716:PRO:HG3	1.82	0.62
1:C:680:GLU:CD	1:C:681:ILE:N	2.53	0.62
1:C:267:ALA:HB2	1:C:716:PRO:HG3	1.82	0.62
1:C:872:LEU:HD12	1:C:876:LEU:HA	1.82	0.62
1:A:163:LEU:HD21	1:A:170:LYS:HB2	1.82	0.62
1:A:413:ALA:O	1:A:416:ARG:HG2	1.98	0.62
1:A:417:ILE:HG22	1:A:548:PHE:HD2	1.63	0.62
1:A:872:LEU:CB	1:A:875:HIS:HB2	2.27	0.62
1:C:907:VAL:HG13	1:C:908:GLU:H	1.63	0.62
1:C:854:GLN:HE22	1:C:923:GLN:NE2	1.98	0.62
1:A:753:THR:HG22	1:A:753:THR:O	1.99	0.61
1:C:634:VAL:HG23	1:C:635:GLU:N	2.14	0.61
1:C:82:TRP:O	1:C:85:PHE:N	2.32	0.61
1:A:179:VAL:O	1:A:251:VAL:HG21	1.99	0.61
1:A:371:THR:CG2	1:A:377:ASN:HD22	2.13	0.61
1:A:433:LEU:O	1:A:435:ILE:N	2.34	0.61
1:A:980:TRP:HA	1:A:980:TRP:CE3	2.35	0.61
2:B:45:CYS:O	2:B:49:ILE:HG12	2.00	0.61
2:B:58:LEU:HD23	2:B:61:ILE:HG13	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:C	2:B:65:LYS:HD2	2.21	0.61
1:C:643:ILE:O	1:C:647:GLN:HB3	2.00	0.61
1:C:949:PHE:O	1:C:953:GLU:OE2	2.17	0.61
1:C:974:TYR:CD2	1:C:974:TYR:N	2.67	0.61
1:A:417:ILE:CG2	1:A:548:PHE:HD2	2.12	0.61
1:A:643:ILE:O	1:A:647:GLN:HB3	2.01	0.61
1:C:185:GLU:OE1	1:C:248:ARG:NH1	2.33	0.61
1:C:565:ASP:N	1:C:570:ASN:HD22	1.91	0.61
1:C:764:ASN:ND2	1:C:818:GLU:HB2	2.16	0.61
1:C:821:GLU:O	1:C:822:SER:HB2	2.00	0.61
1:C:916:PHE:HD2	1:C:916:PHE:C	2.03	0.61
3:H:48:LYS:HA	3:H:48:LYS:NZ	2.15	0.61
1:A:280:GLU:C	1:A:282:GLU:H	2.02	0.61
1:A:743:LEU:CD2	1:A:743:LEU:H	2.13	0.61
1:A:777:ILE:HB	1:A:778:PRO:CD	2.27	0.61
1:C:163:LEU:HD21	1:C:170:LYS:HB2	1.81	0.61
1:C:223:ASP:O	1:C:224:PHE:HB3	2.00	0.61
1:C:860:PHE:HE1	2:D:53:THR:HB	1.60	0.61
1:A:631:ASN:O	1:A:634:VAL:HG22	1.99	0.61
1:A:785:ILE:HG21	1:A:859:PHE:HZ	1.65	0.61
1:C:631:ASN:O	1:C:634:VAL:HG22	2.00	0.61
1:C:643:ILE:HB	1:C:644:PRO:CD	2.24	0.61
1:C:892:GLU:HB2	2:D:65:LYS:NZ	2.16	0.61
1:C:889:ASN:OD1	1:C:893:ASP:HB2	2.01	0.61
1:C:916:PHE:CD2	1:C:916:PHE:C	2.74	0.61
1:C:974:TYR:N	1:C:974:TYR:HD2	1.99	0.61
1:A:197:ARG:NH1	1:A:197:ARG:HG2	2.11	0.61
1:A:555:ASP:C	1:A:557:GLN:H	2.03	0.61
1:A:867:ALA:HA	1:A:871:PHE:CG	2.36	0.61
1:C:413:ALA:O	1:C:416:ARG:HG2	2.00	0.61
1:C:931:LYS:HD2	1:C:947:LEU:HD11	1.83	0.61
1:A:51:ASP:CG	1:A:54:ARG:HB2	2.20	0.61
1:A:589:ARG:HB2	1:A:592:VAL:CG2	2.31	0.61
1:A:680:GLU:CD	1:A:681:ILE:N	2.54	0.61
1:C:918:THR:CG2	1:C:984:ALA:HB2	2.20	0.61
3:H:48:LYS:HZ3	3:H:48:LYS:HA	1.66	0.61
1:A:385:TRP:HB3	1:A:581:LEU:HB2	1.82	0.61
1:C:179:VAL:O	1:C:251:VAL:HG21	2.00	0.61
1:C:615:ILE:CD1	1:C:615:ILE:H	2.08	0.61
1:C:929:ILE:HD12	1:C:999:LYS:NZ	2.15	0.61
2:D:58:LEU:O	2:D:60:THR:N	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:THR:N	1:C:80:PRO:CD	2.64	0.61
1:A:796:GLY:O	1:A:799:THR:HB	2.00	0.61
1:C:183:LEU:HD23	1:C:183:LEU:O	2.00	0.61
1:C:635:GLU:CB	1:C:647:GLN:HE22	2.14	0.61
1:C:639:ALA:O	1:C:641:LEU:N	2.31	0.61
1:C:96:LEU:CD2	1:C:292:ALA:HB1	2.31	0.61
1:C:982:PHE:H	1:C:982:PHE:HD2	1.47	0.61
1:A:450:LEU:HD23	1:A:450:LEU:C	2.22	0.60
1:A:865:ILE:CG2	1:A:910:THR:HG22	2.30	0.60
1:A:888:ILE:CG2	1:A:889:ASN:H	2.13	0.60
2:B:63:GLU:HG2	2:B:64:PHE:CD2	2.36	0.60
1:C:590:ALA:O	1:C:593:PRO:HD2	2.01	0.60
1:C:889:ASN:ND2	1:C:895:TYR:H	1.96	0.60
1:A:872:LEU:HB3	1:A:875:HIS:C	2.20	0.60
1:C:490:ASN:O	1:C:492:ALA:N	2.34	0.60
1:C:556:GLU:CD	1:C:556:GLU:H	2.02	0.60
1:C:732:SER:O	1:C:734:VAL:N	2.32	0.60
1:A:79:THR:N	1:A:80:PRO:CD	2.65	0.60
1:A:918:THR:CB	1:A:984:ALA:HB2	2.30	0.60
1:C:22:GLU:OE1	1:C:22:GLU:HA	2.01	0.60
1:C:111:GLN:OE1	1:C:311:LEU:HD11	2.01	0.60
1:C:371:THR:CG2	1:C:377:ASN:HD22	2.13	0.60
1:C:499:VAL:HG12	1:C:550:HIS:CB	2.31	0.60
1:C:767:LYS:NZ	1:C:821:GLU:OE1	2.29	0.60
1:C:931:LYS:HD2	1:C:947:LEU:HD13	1.84	0.60
1:A:22:GLU:C	1:A:24:ASP:H	2.03	0.60
1:A:499:VAL:HG12	1:A:550:HIS:CB	2.31	0.60
1:A:913:THR:HB	1:A:914:PRO:CD	2.22	0.60
1:A:976:LEU:H	1:A:980:TRP:HD1	1.46	0.60
1:A:990:LEU:HA	1:A:993:VAL:HG22	1.83	0.60
1:C:110:ILE:O	1:C:311:LEU:HD21	2.02	0.60
1:C:341:ALA:C	1:C:343:ARG:H	2.04	0.60
1:C:743:LEU:CD2	1:C:743:LEU:N	2.64	0.60
1:C:959:ALA:HB2	1:C:981:TRP:CH2	2.37	0.60
1:A:556:GLU:H	1:A:556:GLU:CD	2.05	0.60
1:C:852:MET:O	1:C:855:ALA:HB3	2.02	0.60
1:C:888:ILE:HG22	1:C:889:ASN:H	1.66	0.60
1:A:303:SER:C	1:A:305:ILE:H	2.05	0.60
1:A:889:ASN:OD1	1:A:890:ASP:N	2.24	0.60
1:C:551:LEU:HD22	1:C:576:LEU:HD23	1.83	0.60
1:C:784:LEU:CD2	1:C:788:ILE:HD11	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:872:LEU:CG	1:C:876:LEU:HB2	2.31	0.60
1:A:320:ILE:O	1:A:324:ASN:HB2	2.00	0.60
1:C:831:ASN:HD21	1:C:833:LYS:CB	2.14	0.60
1:C:22:GLU:C	1:C:24:ASP:H	2.04	0.60
1:C:406:LYS:NZ	1:C:411:TRP:HE1	2.00	0.60
1:C:385:TRP:HB3	1:C:581:LEU:HB2	1.83	0.60
1:C:611:GLY:O	1:C:685:ARG:HD2	2.01	0.60
2:D:63:GLU:N	2:D:63:GLU:OE1	2.35	0.60
3:G:39:ILE:O	3:G:43:ILE:HB	2.01	0.60
3:G:41:GLY:O	3:G:45:ILE:HG22	2.02	0.60
3:H:40:VAL:O	3:H:44:ILE:HD12	2.02	0.60
1:A:852:MET:O	1:A:855:ALA:HB3	2.02	0.60
1:C:433:LEU:O	1:C:435:ILE:N	2.34	0.60
1:C:763:ASP:O	1:C:765:LEU:N	2.35	0.60
1:A:284:PHE:C	1:A:284:PHE:CD1	2.74	0.59
1:A:860:PHE:CE1	2:B:53:THR:HB	2.36	0.59
1:A:691:LYS:HE2	1:A:714:ASP:OD1	2.02	0.59
1:A:889:ASN:ND2	1:A:895:TYR:HB2	2.17	0.59
1:C:759:ARG:HD2	1:C:825:MET:CE	2.31	0.59
1:C:952:PHE:HB3	3:H:37:ALA:HB1	1.82	0.59
1:A:205:LYS:HA	1:A:218:GLN:O	2.02	0.59
1:A:96:LEU:H	1:A:96:LEU:HD12	1.66	0.59
1:C:857:GLY:HA2	1:C:987:TYR:CE2	2.37	0.59
1:C:872:LEU:HD12	1:C:876:LEU:H	1.64	0.59
3:G:47:SER:C	3:G:48:LYS:HD2	2.22	0.59
1:A:1005:ARG:HD3	1:A:1009:TRP:HE1	1.67	0.59
1:A:347:LYS:CD	1:A:753:THR:HG21	2.32	0.59
1:C:354:LEU:HD12	1:C:354:LEU:H	1.68	0.59
1:C:691:LYS:HE2	1:C:714:ASP:OD1	2.02	0.59
1:A:895:TYR:HA	1:A:899:TRP:CB	2.19	0.59
1:A:896:GLY:O	1:A:899:TRP:N	2.36	0.59
1:A:990:LEU:HD12	1:A:993:VAL:CG2	2.32	0.59
1:C:649:ASN:O	1:C:651:ARG:HG3	2.02	0.59
1:C:743:LEU:H	1:C:743:LEU:CD2	2.16	0.59
1:C:889:ASN:HB2	1:C:895:TYR:H	1.67	0.59
1:A:183:LEU:O	1:A:183:LEU:HD23	2.03	0.59
1:A:22:GLU:OE1	1:A:22:GLU:HA	2.02	0.59
1:A:565:ASP:N	1:A:570:ASN:HD22	1.91	0.59
1:A:635:GLU:CB	1:A:647:GLN:HE22	2.14	0.59
1:A:683:PHE:CD1	1:A:694:ILE:HD11	2.37	0.59
1:A:863:PHE:HD2	2:B:54:ILE:HD11	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:745:ASP:OD1	1:C:747:ASN:HB3	2.03	0.59
3:G:42:LEU:HA	3:G:46:LEU:HD22	1.84	0.59
1:A:310:TRP:HE3	1:A:310:TRP:HA	1.67	0.59
1:A:406:LYS:NZ	1:A:411:TRP:HE1	1.98	0.59
1:A:360:LEU:O	1:A:755:VAL:HG23	2.02	0.59
1:A:763:ASP:C	1:A:765:LEU:H	2.05	0.59
1:A:864:VAL:HG22	2:B:57:MET:HE2	1.84	0.59
1:C:303:SER:C	1:C:305:ILE:H	2.06	0.59
1:A:635:GLU:HB3	1:A:647:GLN:HE22	1.68	0.59
1:C:98:TRP:CD1	1:C:133:VAL:HG11	2.38	0.59
1:C:929:ILE:CD1	1:C:995:ASP:HB3	2.31	0.59
1:A:224:PHE:CG	1:A:225:THR:N	2.71	0.59
1:A:551:LEU:HD22	1:A:576:LEU:HD23	1.84	0.59
1:A:608:MET:N	1:A:681:ILE:O	2.36	0.59
1:C:842:LEU:CD2	1:C:1016:TYR:HE1	2.13	0.59
1:C:383:HIS:O	1:C:384:MET:HG3	2.03	0.59
1:C:876:LEU:O	1:C:878:GLY:N	2.35	0.59
2:D:60:THR:CG2	2:D:61:ILE:N	2.66	0.59
1:A:648:VAL:HG23	1:A:649:ASN:N	2.17	0.58
1:A:671:LEU:CD2	1:A:675:LEU:HB2	2.32	0.58
1:A:745:ASP:OD1	1:A:747:ASN:HB3	2.03	0.58
1:A:771:TYR:CD2	1:A:771:TYR:C	2.76	0.58
1:C:191:ARG:HA	1:C:241:ASN:HB3	1.85	0.58
1:C:303:SER:O	1:C:308:TYR:HD2	1.85	0.58
1:C:347:LYS:CD	1:C:753:THR:HG21	2.33	0.58
1:A:839:ASN:N	1:A:839:ASN:ND2	2.52	0.58
1:A:979:THR:C	1:A:981:TRP:H	2.04	0.58
1:C:154:PHE:CD2	1:C:264:ALA:HA	2.37	0.58
1:C:336:CYS:O	1:C:339:LEU:HB2	2.03	0.58
1:C:555:ASP:C	1:C:557:GLN:H	2.04	0.58
1:C:671:LEU:CD2	1:C:675:LEU:HB2	2.33	0.58
1:C:770:ALA:HB2	1:C:842:LEU:CD2	2.33	0.58
1:C:773:LEU:HD11	1:C:842:LEU:HD11	1.84	0.58
1:C:926:ASP:O	1:C:929:ILE:HG22	2.03	0.58
1:A:1001:ILE:CG2	1:A:1011:GLU:HG2	2.33	0.58
1:A:514:ILE:CG2	1:A:578:PHE:HB3	2.27	0.58
1:C:275:THR:OG1	1:C:278:ALA:HB3	2.04	0.58
1:C:493:GLU:HB2	1:C:494:PRO:CD	2.31	0.58
1:C:572:PRO:O	1:C:573:LEU:HD23	2.02	0.58
1:C:210:SER:HA	1:C:712:VAL:HG13	1.85	0.58
1:A:313:ALA:O	1:A:316:PHE:HB3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:SER:HA	1:A:712:VAL:HG13	1.85	0.58
1:A:854:GLN:HE21	1:A:922:VAL:HG23	1.68	0.58
1:C:111:GLN:HB2	1:C:115:GLU:HG3	1.86	0.58
1:C:96:LEU:H	1:C:96:LEU:HD12	1.67	0.58
1:A:125:LEU:HD22	1:A:318:ILE:HD13	1.84	0.58
1:C:224:PHE:CG	1:C:225:THR:N	2.71	0.58
1:C:648:VAL:HG23	1:C:649:ASN:N	2.18	0.58
1:C:777:ILE:C	1:C:779:GLU:H	2.07	0.58
1:C:871:PHE:C	1:C:872:LEU:HD23	2.22	0.58
1:C:875:HIS:O	1:C:876:LEU:HB3	2.04	0.58
1:A:1015:TYR:O	1:A:1016:TYR:CB	2.52	0.58
1:A:111:GLN:HB2	1:A:115:GLU:HG3	1.86	0.58
1:A:931:LYS:HZ2	1:A:931:LYS:HB3	1.68	0.58
1:A:98:TRP:CD1	1:A:133:VAL:HG11	2.38	0.58
1:C:284:PHE:CE1	1:C:769:ILE:HD11	2.38	0.58
1:A:141:TYR:C	1:A:143:GLN:H	2.07	0.58
1:A:277:ILE:HG13	1:A:358:GLU:OE1	2.03	0.58
1:A:639:ALA:O	1:A:641:LEU:N	2.31	0.58
1:A:769:ILE:HA	1:A:772:THR:HG22	1.85	0.58
2:B:52:GLY:O	2:B:56:VAL:HG22	2.02	0.58
1:C:417:ILE:HG22	1:C:418:ALA:N	2.19	0.58
1:A:374:LEU:O	1:A:592:VAL:HG21	2.03	0.58
1:A:656:CYS:N	1:A:680:GLU:HB2	2.08	0.58
1:A:626:ILE:HG23	1:A:681:ILE:HG21	1.85	0.58
1:A:859:PHE:O	1:A:862:TYR:HB3	2.03	0.58
1:A:976:LEU:HD23	1:A:976:LEU:O	2.04	0.58
1:A:980:TRP:HA	1:A:980:TRP:HE3	1.69	0.58
1:A:929:ILE:HD11	1:A:995:ASP:HB3	1.85	0.58
1:C:747:ASN:OD1	1:C:749:ALA:HB3	2.04	0.58
1:C:777:ILE:O	1:C:779:GLU:N	2.37	0.58
1:A:208:ASN:OD1	1:A:240:THR:HG21	2.04	0.58
1:A:37:HIS:CD2	1:A:232:THR:HG21	2.39	0.58
1:A:743:LEU:HD23	1:A:743:LEU:N	2.19	0.58
1:A:888:ILE:CG2	1:A:889:ASN:N	2.67	0.58
1:A:949:PHE:HE1	3:G:40:VAL:HB	1.69	0.58
2:B:66:PRO:HG2	2:B:68:TYR:HE2	1.69	0.58
1:C:374:LEU:O	1:C:592:VAL:HG21	2.03	0.58
1:C:985:PHE:N	1:C:986:PRO:CD	2.67	0.58
1:C:984:ALA:C	1:C:986:PRO:HD2	2.24	0.58
2:D:66:PRO:HG2	2:D:68:TYR:HE2	1.68	0.58
3:H:44:ILE:HG22	3:H:48:LYS:HD3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:CD2	1:A:318:ILE:HD13	2.33	0.58
1:A:223:ASP:O	1:A:224:PHE:HB3	2.03	0.58
1:C:141:TYR:C	1:C:143:GLN:H	2.08	0.58
1:C:420:LEU:HD12	1:C:420:LEU:N	2.19	0.58
1:C:631:ASN:HB3	1:C:634:VAL:CG2	2.34	0.58
1:A:383:HIS:O	1:A:384:MET:HG3	2.04	0.57
1:A:476:ASN:ND2	1:A:480:LYS:HA	2.17	0.57
1:A:773:LEU:HD12	1:A:773:LEU:C	2.25	0.57
1:A:88:GLN:HA	1:A:91:GLY:CA	2.30	0.57
1:A:936:SER:C	1:A:938:PHE:N	2.58	0.57
1:C:666:MET:HA	1:C:670:GLN:NE2	2.18	0.57
1:C:97:LEU:HD21	1:C:325:VAL:HG21	1.86	0.57
1:A:649:ASN:O	1:A:651:ARG:HG3	2.04	0.57
1:A:863:PHE:HD2	2:B:54:ILE:CD1	2.17	0.57
1:C:1001:ILE:O	1:C:1005:ARG:HB2	2.03	0.57
1:C:1002:ILE:O	1:C:1005:ARG:O	2.22	0.57
1:C:683:PHE:CD1	1:C:694:ILE:HD11	2.38	0.57
1:C:962:SER:O	1:C:974:TYR:HA	2.04	0.57
1:C:899:TRP:HZ2	2:D:70:ASP:C	2.08	0.57
1:A:96:LEU:CD2	1:A:292:ALA:HB1	2.31	0.57
1:A:840:GLU:O	1:A:841:GLN:C	2.43	0.57
1:A:875:HIS:O	1:A:876:LEU:CB	2.52	0.57
1:A:944:ASN:OD1	1:A:947:LEU:N	2.32	0.57
2:B:58:LEU:O	2:B:60:THR:N	2.37	0.57
1:C:188:GLY:HA2	1:C:242:CYS:SG	2.44	0.57
1:C:608:MET:N	1:C:681:ILE:O	2.38	0.57
2:D:63:GLU:HG2	2:D:64:PHE:CD1	2.39	0.57
3:H:37:ALA:O	3:H:40:VAL:HG22	2.04	0.57
1:A:631:ASN:HB3	1:A:634:VAL:CG2	2.34	0.57
1:A:840:GLU:HG2	1:A:841:GLN:N	2.19	0.57
1:A:977:LYS:HB3	1:A:978:PRO:HD3	1.86	0.57
1:C:37:HIS:CD2	1:C:232:THR:HG21	2.39	0.57
1:C:379:MET:CG	1:C:444:ALA:HB1	2.32	0.57
1:C:635:GLU:HB3	1:C:647:GLN:HE22	1.69	0.57
1:C:626:ILE:HD12	1:C:681:ILE:HG21	1.86	0.57
1:C:929:ILE:CD1	1:C:999:LYS:HZ2	2.17	0.57
1:A:123:LEU:C	1:A:123:LEU:HD13	2.25	0.57
1:A:420:LEU:HD12	1:A:420:LEU:N	2.20	0.57
1:A:863:PHE:HB3	1:A:871:PHE:CZ	2.39	0.57
1:A:866:LEU:HD23	1:A:906:ILE:HG21	1.85	0.57
1:A:971:LEU:HD23	1:A:972:ARG:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:LEU:HD23	1:C:450:LEU:O	2.04	0.57
1:C:476:ASN:ND2	1:C:480:LYS:HA	2.18	0.57
1:C:79:THR:H	1:C:80:PRO:CD	2.17	0.57
1:C:983:CYS:O	1:C:986:PRO:HD2	2.05	0.57
1:A:154:PHE:CD2	1:A:264:ALA:HA	2.39	0.57
1:A:493:GLU:HB2	1:A:494:PRO:CD	2.31	0.57
1:A:814:SER:OG	1:A:947:LEU:HB2	2.04	0.57
2:B:33:PHE:CD1	2:B:33:PHE:C	2.78	0.57
1:C:514:ILE:CG2	1:C:578:PHE:HB3	2.26	0.57
1:C:763:ASP:C	1:C:765:LEU:H	2.08	0.57
1:A:435:ILE:HA	1:A:438:ARG:HD3	1.86	0.57
1:A:687:SER:H	1:A:690:GLN:HE21	1.51	0.57
1:A:872:LEU:HB2	1:A:876:LEU:CD2	2.31	0.57
1:A:854:GLN:HG2	1:A:922:VAL:HB	1.86	0.57
1:A:936:SER:H	1:A:1003:ARG:HH22	1.52	0.57
1:C:585:ILE:HG12	1:C:586:ASP:N	2.19	0.57
1:C:861:THR:CB	1:C:918:THR:HG21	2.35	0.57
1:A:185:GLU:OE1	1:A:248:ARG:NH1	2.37	0.57
1:A:432:ASN:C	1:A:434:PRO:HD2	2.25	0.57
1:A:904:ARG:C	1:A:906:ILE:H	2.08	0.57
1:C:881:VAL:HG12	1:C:882:ASN:H	1.69	0.57
1:C:889:ASN:CG	1:C:893:ASP:HB2	2.24	0.57
1:C:973:MET:CE	1:C:973:MET:HA	2.35	0.57
2:D:36:LEU:C	2:D:38:PHE:H	2.08	0.57
1:A:284:PHE:HB2	1:A:838:VAL:HG11	1.85	0.57
1:A:354:LEU:H	1:A:354:LEU:HD12	1.70	0.57
1:A:507:ILE:O	1:A:510:ARG:HG2	2.05	0.57
1:A:777:ILE:HD11	1:A:847:TYR:CD1	2.40	0.57
1:A:910:THR:HG22	1:A:911:CYS:H	1.70	0.57
1:A:913:THR:OG1	1:A:972:ARG:CB	2.37	0.57
1:A:867:ALA:HB1	2:B:61:ILE:CD1	2.35	0.57
1:C:759:ARG:HH21	1:C:829:PRO:HA	1.70	0.57
1:C:854:GLN:CG	1:C:991:ILE:HD11	2.35	0.57
1:A:294:PHE:O	1:A:298:SER:HB2	2.05	0.56
1:A:37:HIS:NE2	1:A:228:ASN:O	2.38	0.56
1:A:497:LEU:HD12	1:A:551:LEU:O	2.05	0.56
1:A:585:ILE:HG12	1:A:586:ASP:N	2.19	0.56
1:A:767:LYS:CB	1:A:815:LEU:HD12	2.35	0.56
1:A:927:LEU:HG	1:A:927:LEU:O	2.05	0.56
1:C:55:GLY:HA2	1:C:183:LEU:HD22	1.87	0.56
1:C:37:HIS:NE2	1:C:228:ASN:O	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:LYS:HD2	1:C:753:THR:HG21	1.87	0.56
1:A:432:ASN:CB	1:A:434:PRO:HD2	2.35	0.56
1:A:483:LEU:HD23	1:A:500:MET:CE	2.34	0.56
1:A:948:ILE:HD12	1:A:948:ILE:H	1.69	0.56
1:C:354:LEU:O	1:C:356:ALA:N	2.38	0.56
1:C:432:ASN:CB	1:C:434:PRO:HD2	2.35	0.56
1:C:432:ASN:C	1:C:434:PRO:HD2	2.25	0.56
1:C:507:ILE:O	1:C:510:ARG:HG2	2.05	0.56
1:C:863:PHE:HD2	2:D:54:ILE:HD11	1.68	0.56
1:C:205:LYS:HA	1:C:218:GLN:O	2.05	0.56
1:C:223:ASP:O	1:C:234:ASN:HB3	2.06	0.56
1:C:826:LYS:HD3	1:C:826:LYS:O	2.04	0.56
1:C:792:PRO:HD2	1:C:862:TYR:OH	2.06	0.56
1:A:103:LEU:HD21	1:A:314:VAL:HB	1.88	0.56
1:A:191:ARG:HA	1:A:241:ASN:HB3	1.86	0.56
1:A:23:ARG:C	1:A:27:GLU:HB2	2.25	0.56
1:A:988:SER:O	1:A:991:ILE:HB	2.06	0.56
1:C:888:ILE:CG2	1:C:889:ASN:N	2.68	0.56
1:C:889:ASN:HD22	1:C:894:SER:C	2.06	0.56
1:C:955:THR:O	1:C:958:ALA:HB3	2.05	0.56
1:A:92:GLY:C	1:A:285:ILE:HD11	2.25	0.56
1:A:332:THR:HG21	1:A:812:ALA:HB1	1.88	0.56
1:A:355:GLU:OE1	1:A:355:GLU:N	2.37	0.56
1:A:417:ILE:HG22	1:A:418:ALA:N	2.19	0.56
1:C:435:ILE:HA	1:C:438:ARG:HD3	1.86	0.56
1:C:885:ASP:O	1:C:886:ARG:HB3	2.05	0.56
1:C:88:GLN:NE2	1:C:89:LEU:N	2.54	0.56
1:A:945:LYS:HE2	3:G:51:ARG:NH2	2.20	0.56
1:A:97:LEU:CD2	1:A:325:VAL:HG21	2.29	0.56
1:A:378:ARG:HH11	1:A:378:ARG:HG3	1.71	0.56
1:A:432:ASN:O	1:A:438:ARG:NH1	2.39	0.56
2:B:58:LEU:C	2:B:60:THR:N	2.56	0.56
1:C:23:ARG:C	1:C:27:GLU:HB2	2.26	0.56
1:C:355:GLU:N	1:C:355:GLU:OE1	2.38	0.56
1:C:636:ASP:OD1	1:C:647:GLN:HG2	2.05	0.56
1:C:687:SER:H	1:C:690:GLN:HE21	1.52	0.56
1:C:771:TYR:O	1:C:774:THR:HG22	2.06	0.56
1:A:354:LEU:O	1:A:356:ALA:N	2.38	0.56
1:A:605:LYS:HE3	1:A:679:THR:CG2	2.33	0.56
1:C:294:PHE:O	1:C:298:SER:HB2	2.06	0.56
1:C:626:ILE:HD12	1:C:681:ILE:CG2	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:902:GLU:HA	1:C:905:LYS:HB3	1.85	0.56
1:A:344:MET:HE1	1:A:357:VAL:HG13	1.88	0.56
1:A:680:GLU:CD	1:A:681:ILE:H	2.08	0.56
1:A:79:THR:H	1:A:80:PRO:CD	2.18	0.56
2:B:47:ALA:O	2:B:51:ILE:HG12	2.06	0.56
1:C:123:LEU:C	1:C:123:LEU:HD13	2.26	0.56
1:C:710:ASP:HB2	1:C:730:ALA:O	2.06	0.56
1:A:223:ASP:O	1:A:234:ASN:HB3	2.06	0.56
2:B:40:VAL:O	2:B:44:GLY:N	2.39	0.56
1:C:906:ILE:C	1:C:910:THR:HB	2.26	0.56
1:C:973:MET:HE2	1:C:973:MET:HA	1.87	0.56
1:C:868:GLU:HA	2:D:68:TYR:CE2	2.39	0.56
1:A:50:THR:OG1	1:A:56:LEU:HD13	2.06	0.56
1:A:901:TYR:O	1:A:905:LYS:HE2	2.05	0.56
1:A:947:LEU:HG	1:A:948:ILE:N	2.21	0.56
1:C:481:TYR:HA	1:C:502:GLY:HA3	1.88	0.56
1:A:289:THR:HA	1:A:292:ALA:CB	2.36	0.55
1:A:900:THR:HG23	1:A:903:GLN:HE21	1.69	0.55
1:C:1015:TYR:CD2	1:C:1015:TYR:C	2.80	0.55
1:C:93:PHE:CE2	1:C:288:ILE:HG21	2.42	0.55
1:C:506:ARG:HG2	1:C:506:ARG:HH11	1.71	0.55
1:C:694:ILE:CG2	1:C:695:VAL:N	2.69	0.55
1:C:966:GLY:O	1:C:968:GLY:N	2.37	0.55
1:A:909:PHE:CB	1:A:973:MET:HB2	2.36	0.55
1:A:811:PRO:HB3	1:A:927:LEU:HD13	1.88	0.55
1:C:589:ARG:HG3	1:C:589:ARG:NH1	2.21	0.55
1:C:626:ILE:HG23	1:C:681:ILE:HG21	1.86	0.55
1:C:913:THR:HG21	1:C:975:PRO:HD3	1.87	0.55
1:C:974:TYR:CE1	3:H:27:ARG:HD2	2.40	0.55
1:A:666:MET:HA	1:A:670:GLN:NE2	2.20	0.55
1:A:886:ARG:HB2	1:A:896:GLY:HA3	1.88	0.55
1:C:770:ALA:CB	1:C:1016:TYR:OH	2.55	0.55
1:C:888:ILE:CG2	1:C:889:ASN:H	2.20	0.55
1:C:922:VAL:HA	1:C:988:SER:OG	2.05	0.55
1:A:1006:PRO:O	1:A:1012:LYS:HD2	2.06	0.55
1:A:504:PRO:HG3	1:A:535:TYR:CE1	2.40	0.55
1:A:692:LEU:HD23	1:A:693:ILE:N	2.22	0.55
1:A:710:ASP:HB2	1:A:730:ALA:O	2.06	0.55
1:A:784:LEU:O	1:A:788:ILE:HG13	2.06	0.55
1:C:324:ASN:O	1:C:326:PRO:HD3	2.07	0.55
2:D:66:PRO:HG2	2:D:68:TYR:CE2	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:OG1	1:A:761:ILE:HG13	2.06	0.55
1:A:347:LYS:HD2	1:A:753:THR:HG21	1.87	0.55
1:A:420:LEU:HD21	1:A:467:TYR:HB2	1.89	0.55
1:A:433:LEU:N	1:A:434:PRO:CD	2.70	0.55
1:A:636:ASP:OD1	1:A:647:GLN:HG2	2.05	0.55
2:B:66:PRO:HG2	2:B:68:TYR:CE2	2.42	0.55
1:C:208:ASN:OD1	1:C:240:THR:HG21	2.06	0.55
1:C:344:MET:HE2	1:C:357:VAL:HG13	1.87	0.55
1:C:483:LEU:HD23	1:C:500:MET:CE	2.36	0.55
1:C:680:GLU:CD	1:C:681:ILE:H	2.08	0.55
1:C:88:GLN:NE2	1:C:89:LEU:HB2	2.22	0.55
1:C:908:GLU:HB3	1:C:909:PHE:HD2	1.71	0.55
1:A:747:ASN:OD1	1:A:749:ALA:HB3	2.05	0.55
1:A:884:ASP:O	1:A:885:ASP:HB3	2.07	0.55
1:A:88:GLN:O	1:A:94:SER:HB2	2.07	0.55
1:C:300:PHE:O	1:C:304:LEU:N	2.40	0.55
1:C:369:ASP:OD1	1:C:710:ASP:OD2	2.25	0.55
1:C:840:GLU:HA	1:C:843:ILE:HG12	1.89	0.55
1:C:866:LEU:O	1:C:869:ASN:N	2.40	0.55
1:C:909:PHE:N	1:C:909:PHE:CD2	2.73	0.55
1:A:110:ILE:HB	1:A:311:LEU:HD23	1.88	0.55
1:A:309:THR:O	1:A:312:GLU:HB2	2.06	0.55
1:A:480:LYS:CE	1:A:503:ALA:HB2	2.36	0.55
1:A:626:ILE:HD12	1:A:681:ILE:HG21	1.88	0.55
1:A:367:CYS:CB	1:A:707:VAL:HG22	2.31	0.55
1:A:911:CYS:C	1:A:914:PRO:HD2	2.27	0.55
1:C:752:VAL:C	1:C:754:GLY:H	2.10	0.55
1:C:831:ASN:ND2	1:C:833:LYS:HB2	2.20	0.55
2:D:60:THR:O	2:D:61:ILE:HB	2.07	0.55
1:A:815:LEU:O	1:A:818:GLU:HB2	2.07	0.55
1:A:866:LEU:HD23	1:A:906:ILE:CG2	2.35	0.55
1:A:936:SER:C	1:A:938:PHE:H	2.09	0.55
1:C:291:VAL:HG23	1:C:324:ASN:OD1	2.07	0.55
1:A:289:THR:O	1:A:289:THR:HG22	2.07	0.55
1:A:515:LEU:HD12	1:A:579:VAL:HG13	1.88	0.55
1:A:680:GLU:CG	1:A:682:VAL:H	2.15	0.55
1:A:842:LEU:HD13	1:A:1016:TYR:CE1	2.42	0.55
1:A:881:VAL:CG1	1:A:882:ASN:H	2.20	0.55
1:A:891:VAL:O	1:A:891:VAL:HG23	2.06	0.55
1:C:304:LEU:HD23	1:C:313:ALA:HB1	1.88	0.55
1:C:651:ARG:C	1:C:653:ALA:N	2.60	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:804:ASP:O	1:C:809:MET:HG2	2.07	0.55
1:A:29:LYS:HG3	1:A:266:LEU:HD22	1.89	0.55
1:A:450:LEU:HD23	1:A:450:LEU:O	2.07	0.55
1:A:475:PHE:O	1:A:476:ASN:C	2.45	0.55
1:A:483:LEU:C	1:A:483:LEU:HD12	2.27	0.55
1:A:592:VAL:O	1:A:596:VAL:HG23	2.06	0.55
1:A:769:ILE:HG23	1:A:770:ALA:N	2.21	0.55
1:A:299:PHE:HE1	1:A:784:LEU:HG	1.71	0.55
1:A:886:ARG:CA	1:A:896:GLY:HA3	2.37	0.55
1:A:976:LEU:N	1:A:980:TRP:HB2	2.22	0.55
1:C:208:ASN:HA	1:C:240:THR:CG2	2.37	0.55
2:D:29:GLY:O	2:D:32:TRP:HD1	1.90	0.55
1:A:56:LEU:HD22	1:A:182:ASP:HB3	1.88	0.54
1:A:354:LEU:HD12	1:A:354:LEU:N	2.22	0.54
1:A:752:VAL:C	1:A:754:GLY:H	2.11	0.54
1:A:803:ILE:HA	1:A:807:THR:HB	1.89	0.54
1:A:830:ARG:HH21	1:A:832:PRO:HA	1.72	0.54
1:A:931:LYS:HZ3	1:A:931:LYS:HB3	1.69	0.54
1:C:1007:GLY:HA2	1:C:1012:LYS:HD3	1.88	0.54
1:C:405:ASP:O	1:C:406:LYS:HB3	2.07	0.54
1:C:592:VAL:O	1:C:596:VAL:HG23	2.06	0.54
1:C:605:LYS:HE3	1:C:679:THR:CG2	2.32	0.54
1:C:825:MET:CE	1:C:825:MET:HA	2.36	0.54
2:D:66:PRO:HG2	2:D:67:THR:H	1.71	0.54
1:A:1011:GLU:OE2	1:A:1012:LYS:N	2.36	0.54
1:A:378:ARG:CZ	1:A:436:LEU:HD22	2.37	0.54
1:A:481:TYR:HA	1:A:502:GLY:HA3	1.89	0.54
1:A:606:VAL:HG23	1:A:681:ILE:HG21	1.88	0.54
1:A:886:ARG:HA	1:A:896:GLY:HA2	1.89	0.54
1:C:354:LEU:HD12	1:C:354:LEU:N	2.21	0.54
1:C:432:ASN:O	1:C:438:ARG:NH1	2.41	0.54
1:C:504:PRO:HG3	1:C:535:TYR:CE1	2.42	0.54
1:C:690:GLN:O	1:C:693:ILE:HG22	2.07	0.54
1:A:305:ILE:HB	1:A:307:GLU:OE1	2.07	0.54
1:A:946:ILE:HG22	1:A:947:LEU:N	2.22	0.54
1:C:852:MET:O	1:C:855:ALA:N	2.40	0.54
1:C:889:ASN:HD21	1:C:893:ASP:HB3	1.72	0.54
1:C:896:GLY:O	1:C:899:TRP:HB2	2.07	0.54
1:C:932:THR:HG21	1:C:935:ASN:O	2.08	0.54
1:C:966:GLY:C	1:C:968:GLY:N	2.61	0.54
1:A:126:GLY:O	1:A:130:SER:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:PHE:O	1:A:303:SER:OG	2.15	0.54
1:A:779:GLU:HB3	1:A:800:ILE:CD1	2.36	0.54
1:A:898:GLN:CD	2:B:72:VAL:HG22	2.27	0.54
1:C:475:PHE:O	1:C:476:ASN:C	2.44	0.54
1:C:500:MET:HG3	1:C:549:CYS:SG	2.47	0.54
1:C:499:VAL:HG12	1:C:550:HIS:HB3	1.90	0.54
1:C:871:PHE:CE2	1:C:873:PRO:HA	2.42	0.54
1:C:98:TRP:NE1	1:C:133:VAL:HG11	2.23	0.54
2:D:58:LEU:O	2:D:60:THR:O	2.26	0.54
1:A:651:ARG:C	1:A:653:ALA:N	2.60	0.54
1:A:694:ILE:CG2	1:A:695:VAL:N	2.70	0.54
1:C:433:LEU:N	1:C:434:PRO:CD	2.71	0.54
1:C:909:PHE:N	1:C:909:PHE:HD2	2.04	0.54
1:A:770:ALA:CB	1:A:1016:TYR:OH	2.49	0.54
1:A:114:THR:O	1:A:116:GLU:N	2.41	0.54
1:A:208:ASN:HA	1:A:240:THR:CG2	2.38	0.54
1:A:188:GLY:HA2	1:A:242:CYS:SG	2.48	0.54
1:A:767:LYS:HB3	1:A:815:LEU:HD12	1.88	0.54
1:A:783:PHE:H	1:A:783:PHE:HD2	1.56	0.54
1:A:904:ARG:HD3	1:A:907:VAL:CG1	2.38	0.54
1:A:97:LEU:HD21	1:A:325:VAL:CG2	2.32	0.54
1:C:252:VAL:O	1:C:253:TYR:CD1	2.61	0.54
1:C:606:VAL:HG23	1:C:681:ILE:HG21	1.89	0.54
1:C:891:VAL:C	1:C:892:GLU:CD	2.66	0.54
1:C:974:TYR:H	1:C:974:TYR:HD2	1.52	0.54
1:C:995:ASP:HA	1:C:998:ARG:CD	2.38	0.54
2:D:40:VAL:O	2:D:44:GLY:N	2.41	0.54
1:A:1005:ARG:HD3	1:A:1009:TRP:NE1	2.22	0.54
1:A:349:CYS:HA	1:A:743:LEU:HA	1.90	0.54
1:A:409:ALA:O	1:A:412:LEU:HB3	2.08	0.54
1:A:589:ARG:NH1	1:A:589:ARG:HG3	2.23	0.54
1:A:786:PHE:CD1	1:A:786:PHE:O	2.61	0.54
1:C:515:LEU:HD12	1:C:579:VAL:HG13	1.90	0.54
1:C:725:VAL:CG1	1:C:743:LEU:HD21	2.38	0.54
1:C:849:GLN:HG3	2:D:42:PHE:CZ	2.42	0.54
2:D:40:VAL:HG23	2:D:41:ILE:CD1	2.38	0.54
1:A:281:ILE:HG22	1:A:281:ILE:O	2.08	0.54
1:A:150:ILE:HD11	1:A:738:ALA:HA	1.88	0.54
1:C:1015:TYR:HD2	1:C:1015:TYR:C	2.11	0.54
1:C:450:LEU:CD2	1:C:450:LEU:C	2.76	0.54
1:A:506:ARG:HG2	1:A:506:ARG:HH11	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:824:ILE:O	1:A:826:LYS:N	2.40	0.54
1:C:725:VAL:HG12	1:C:743:LEU:CD2	2.38	0.54
3:H:44:ILE:O	3:H:48:LYS:HG2	2.08	0.54
1:A:626:ILE:HD12	1:A:681:ILE:CG2	2.38	0.54
1:A:755:VAL:O	1:A:759:ARG:HG3	2.07	0.54
1:A:98:TRP:NE1	1:A:133:VAL:HG11	2.23	0.54
1:C:104:CYS:SG	1:C:125:LEU:HD23	2.48	0.54
1:C:50:THR:OG1	1:C:56:LEU:HD13	2.08	0.54
1:C:929:ILE:CG1	1:C:995:ASP:HB3	2.38	0.54
1:A:405:ASP:O	1:A:406:LYS:HB3	2.07	0.53
1:A:493:GLU:O	1:A:494:PRO:O	2.26	0.53
1:A:654:LYS:HA	1:A:654:LYS:HE2	1.90	0.53
1:A:926:ASP:HA	1:A:929:ILE:HG22	1.90	0.53
1:A:92:GLY:HA2	1:A:285:ILE:HD11	1.90	0.53
1:A:163:LEU:HG	1:C:169:GLU:HG2	1.91	0.53
1:C:626:ILE:HG23	1:C:681:ILE:HB	1.89	0.53
1:C:944:ASN:O	1:C:946:ILE:N	2.41	0.53
1:A:198:ILE:HA	1:A:249:GLY:CA	2.39	0.53
1:A:504:PRO:HG3	1:A:535:TYR:HE1	1.73	0.53
1:A:779:GLU:OE2	1:A:800:ILE:HD12	2.08	0.53
1:A:865:ILE:HG21	1:A:911:CYS:N	2.23	0.53
1:C:208:ASN:HA	1:C:240:THR:HG22	1.90	0.53
1:C:640:ARG:O	1:C:642:ASN:N	2.41	0.53
1:C:743:LEU:HD23	1:C:743:LEU:N	2.21	0.53
1:C:950:GLY:HA2	1:C:953:GLU:HB2	1.90	0.53
1:A:907:VAL:CA	1:A:911:CYS:HB2	2.17	0.53
1:C:485:ILE:HA	1:C:498:LEU:HA	1.91	0.53
1:A:150:ILE:HD11	1:A:738:ALA:CA	2.38	0.53
1:A:386:SER:O	1:A:387:ASP:HB2	2.08	0.53
1:A:513:SER:O	1:A:577:CYS:HA	2.08	0.53
1:A:725:VAL:CG1	1:A:743:LEU:HD21	2.38	0.53
1:A:92:GLY:CA	1:A:285:ILE:HD11	2.38	0.53
1:C:198:ILE:HA	1:C:249:GLY:CA	2.39	0.53
1:C:786:PHE:HD1	1:C:787:ILE:HD13	1.73	0.53
1:C:851:GLY:O	1:C:855:ALA:HB2	2.08	0.53
1:C:976:LEU:CD2	1:C:978:PRO:HB2	2.37	0.53
1:A:55:GLY:HA2	1:A:183:LEU:HD22	1.88	0.53
1:A:680:GLU:OE2	1:A:681:ILE:N	2.42	0.53
1:A:725:VAL:HG12	1:A:743:LEU:CD2	2.39	0.53
1:A:744:LEU:N	1:A:744:LEU:HD12	2.24	0.53
1:C:117:GLU:C	1:C:119:GLN:H	2.12	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:LEU:O	1:C:315:ILE:HG12	2.09	0.53
1:C:692:LEU:HD23	1:C:693:ILE:N	2.23	0.53
1:C:842:LEU:HD13	1:C:842:LEU:C	2.29	0.53
1:C:899:TRP:HA	1:C:902:GLU:CB	2.33	0.53
1:C:919:ILE:O	1:C:922:VAL:HG23	2.09	0.53
1:C:963:TYR:HD2	3:H:30:GLY:H	1.54	0.53
1:A:197:ARG:HA	1:A:235:ILE:HD13	1.91	0.53
1:A:644:PRO:HA	1:A:648:VAL:HG22	1.91	0.53
1:A:705:VAL:N	1:A:722:ASP:OD2	2.42	0.53
1:A:732:SER:C	1:A:734:VAL:N	2.61	0.53
1:A:886:ARG:HA	1:A:896:GLY:HA3	1.90	0.53
1:A:971:LEU:C	1:A:972:ARG:NE	2.62	0.53
1:C:56:LEU:HD22	1:C:182:ASP:HB3	1.90	0.53
1:C:183:LEU:HA	1:C:249:GLY:O	2.09	0.53
1:C:480:LYS:CE	1:C:503:ALA:HB2	2.38	0.53
1:C:615:ILE:N	1:C:615:ILE:HD13	2.21	0.53
1:C:680:GLU:CG	1:C:682:VAL:H	2.15	0.53
2:D:40:VAL:HG23	2:D:41:ILE:N	2.23	0.53
1:A:208:ASN:HA	1:A:240:THR:HG22	1.89	0.53
1:A:183:LEU:HA	1:A:249:GLY:O	2.08	0.53
1:A:834:THR:HG22	1:A:835:ASP:N	2.22	0.53
1:C:114:THR:O	1:C:116:GLU:N	2.41	0.53
1:C:606:VAL:O	1:C:607:ILE:HG13	2.09	0.53
1:C:961:LEU:HD11	1:C:971:LEU:HD13	1.91	0.53
1:A:117:GLU:C	1:A:119:GLN:H	2.12	0.53
1:A:303:SER:OG	1:A:304:LEU:N	2.42	0.53
1:A:318:ILE:O	1:A:318:ILE:HD12	2.08	0.53
1:A:615:ILE:N	1:A:615:ILE:HD13	2.19	0.53
1:A:876:LEU:O	1:A:878:GLY:N	2.42	0.53
1:C:103:LEU:CD1	1:C:317:LEU:HD12	2.39	0.53
1:C:105:PHE:HD1	1:C:126:GLY:HA3	1.74	0.53
1:C:409:ALA:O	1:C:412:LEU:HB3	2.08	0.53
1:C:680:GLU:OE2	1:C:681:ILE:N	2.41	0.53
1:C:897:GLN:C	1:C:899:TRP:N	2.57	0.53
1:A:117:GLU:N	1:A:118:PRO:CD	2.72	0.53
1:A:104:CYS:SG	1:A:125:LEU:HD23	2.49	0.53
1:A:715:SER:CB	1:A:716:PRO:HD3	2.28	0.53
1:A:885:ASP:CG	1:A:897:GLN:HB2	2.29	0.53
1:A:993:VAL:O	1:A:997:VAL:HG23	2.09	0.53
1:C:417:ILE:HG21	1:C:548:PHE:HB3	1.90	0.53
1:C:914:PRO:HA	1:C:917:VAL:CG2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:PHE:HD1	1:A:126:GLY:HA3	1.74	0.53
1:A:338:THR:O	1:A:342:LYS:HG2	2.09	0.53
1:A:500:MET:HG3	1:A:549:CYS:SG	2.48	0.53
1:A:921:VAL:O	1:A:988:SER:OG	2.18	0.53
1:A:949:PHE:O	1:A:953:GLU:OE1	2.26	0.53
2:B:66:PRO:CG	2:B:68:TYR:CE2	2.92	0.53
1:C:1015:TYR:CD2	1:C:1016:TYR:N	2.77	0.53
1:C:150:ILE:HD11	1:C:738:ALA:CA	2.39	0.53
1:C:963:TYR:HA	1:C:974:TYR:CD2	2.44	0.53
1:A:777:ILE:HG13	1:A:851:GLY:HA3	1.91	0.52
1:A:973:MET:CG	1:A:974:TYR:N	2.64	0.52
1:C:1015:TYR:O	1:C:1016:TYR:HB2	2.08	0.52
1:C:952:PHE:N	1:C:952:PHE:CD2	2.77	0.52
1:A:499:VAL:HG12	1:A:550:HIS:HB3	1.91	0.52
1:C:408:SER:OG	1:C:517:HIS:HA	2.09	0.52
1:C:507:ILE:HG22	1:C:508:LEU:N	2.25	0.52
1:C:288:ILE:HD11	1:C:773:LEU:HD22	1.91	0.52
1:C:995:ASP:O	1:C:999:LYS:HG3	2.09	0.52
1:C:892:GLU:OE1	2:D:65:LYS:CG	2.56	0.52
1:A:347:LYS:HB2	1:A:347:LYS:NZ	2.24	0.52
1:A:690:GLN:O	1:A:693:ILE:HG22	2.09	0.52
1:A:861:THR:CB	1:A:918:THR:HG21	2.39	0.52
1:A:867:ALA:HB1	2:B:61:ILE:HD12	1.92	0.52
1:C:158:VAL:CG2	1:C:159:PRO:HD2	2.39	0.52
1:C:473:ILE:HD12	1:C:483:LEU:HD11	1.92	0.52
1:C:88:GLN:C	1:C:90:PHE:H	2.11	0.52
1:C:94:SER:HB3	1:C:133:VAL:HG13	1.91	0.52
1:A:141:TYR:C	1:A:143:GLN:N	2.63	0.52
1:A:304:LEU:HD21	1:A:310:TRP:CE3	2.43	0.52
1:A:450:LEU:CD2	1:A:450:LEU:C	2.77	0.52
1:A:516:ILE:HD13	1:A:521:GLN:HG2	1.92	0.52
1:A:860:PHE:CD2	1:A:860:PHE:C	2.82	0.52
1:A:918:THR:CG2	1:A:984:ALA:HB2	2.38	0.52
1:A:280:GLU:C	1:A:282:GLU:N	2.62	0.52
1:A:424:ALA:CB	1:A:450:LEU:HD12	2.38	0.52
1:A:555:ASP:C	1:A:557:GLN:N	2.63	0.52
1:A:571:PHE:HB2	1:A:572:PRO:HD2	1.91	0.52
1:A:369:ASP:OD1	1:A:710:ASP:OD2	2.27	0.52
1:C:96:LEU:O	1:C:100:GLY:N	2.43	0.52
1:C:338:THR:O	1:C:342:LYS:HG2	2.09	0.52
1:C:344:MET:HE1	1:C:357:VAL:HG13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ALA:HA	1:C:348:ASN:O	2.09	0.52
1:C:644:PRO:HA	1:C:648:VAL:HG22	1.90	0.52
1:C:755:VAL:O	1:C:759:ARG:HG3	2.10	0.52
1:C:963:TYR:CD2	3:H:30:GLY:N	2.75	0.52
3:H:44:ILE:HG22	3:H:44:ILE:O	2.08	0.52
1:A:998:ARG:O	1:A:1001:ILE:HB	2.10	0.52
1:A:275:THR:CG2	1:A:355:GLU:HG3	2.29	0.52
1:C:126:GLY:O	1:C:130:SER:HB2	2.10	0.52
1:C:424:ALA:CB	1:C:450:LEU:HD12	2.39	0.52
1:A:606:VAL:O	1:A:607:ILE:HG13	2.09	0.52
1:C:111:GLN:CG	1:C:115:GLU:HG3	2.39	0.52
1:C:336:CYS:SG	1:C:816:ALA:HB2	2.50	0.52
1:C:58:PRO:O	1:C:61:ALA:HB3	2.10	0.52
1:C:654:LYS:HA	1:C:654:LYS:HE2	1.90	0.52
1:A:103:LEU:HD23	1:A:103:LEU:O	2.09	0.52
1:A:304:LEU:CD2	1:A:313:ALA:HB2	2.37	0.52
1:A:408:SER:OG	1:A:517:HIS:HA	2.10	0.52
1:A:336:CYS:CB	1:A:765:LEU:HD21	2.40	0.52
1:A:79:THR:N	1:A:80:PRO:HD3	2.22	0.52
1:C:103:LEU:HD23	1:C:103:LEU:O	2.08	0.52
1:C:504:PRO:HD3	1:C:545:VAL:O	2.09	0.52
1:C:900:THR:C	1:C:902:GLU:N	2.63	0.52
1:C:998:ARG:O	1:C:1001:ILE:N	2.42	0.52
1:C:999:LYS:O	1:C:1002:ILE:HB	2.10	0.52
1:A:111:GLN:CG	1:A:115:GLU:HG3	2.40	0.52
1:A:454:GLU:OE1	1:A:459:SER:HA	2.09	0.52
1:A:510:ARG:O	1:A:510:ARG:HG3	2.10	0.52
1:A:791:ILE:CD1	1:A:862:TYR:HE1	2.19	0.52
1:A:871:PHE:O	1:A:872:LEU:HD23	2.10	0.52
1:C:386:SER:O	1:C:387:ASP:HB2	2.10	0.52
1:C:406:LYS:O	1:C:406:LYS:HG3	2.10	0.52
1:C:516:ILE:C	1:C:518:GLY:H	2.13	0.52
1:C:555:ASP:C	1:C:557:GLN:N	2.64	0.52
1:C:606:VAL:C	1:C:607:ILE:HG13	2.30	0.52
1:C:705:VAL:N	1:C:722:ASP:OD2	2.42	0.52
1:C:316:PHE:CZ	1:C:787:ILE:HG13	2.44	0.52
1:C:791:ILE:HG13	1:C:792:PRO:N	2.25	0.52
1:C:807:THR:CG2	1:C:808:ASP:N	2.73	0.52
1:C:830:ARG:HH21	1:C:832:PRO:CA	2.18	0.52
1:A:379:MET:HG3	1:A:444:ALA:HB1	1.92	0.52
1:A:590:ALA:O	1:A:593:PRO:HD2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:ILE:O	1:A:765:LEU:HB2	2.10	0.52
1:A:766:LYS:HA	1:A:769:ILE:HG22	1.91	0.52
1:A:329:LEU:CD2	1:A:769:ILE:HG13	2.35	0.52
1:A:811:PRO:HB3	1:A:927:LEU:CD1	2.40	0.52
1:A:842:LEU:C	1:A:842:LEU:HD12	2.30	0.52
1:A:88:GLN:O	1:A:90:PHE:N	2.42	0.52
1:C:445:SER:HA	1:C:584:MET:SD	2.50	0.52
1:C:784:LEU:HD22	1:C:788:ILE:HD11	1.92	0.52
1:C:778:PRO:HG2	1:C:854:GLN:HB3	1.91	0.52
1:C:865:ILE:HG21	1:C:911:CYS:HA	1.92	0.52
1:C:929:ILE:HD11	1:C:995:ASP:HB3	1.92	0.52
2:D:33:PHE:CE1	2:D:34:LYS:HE2	2.45	0.52
2:D:34:LYS:CD	2:D:37:LEU:HD21	2.40	0.52
2:D:34:LYS:HD3	2:D:37:LEU:CD2	2.40	0.52
2:D:34:LYS:HZ2	2:D:37:LEU:HD21	1.75	0.52
1:A:158:VAL:CG2	1:A:159:PRO:HD2	2.41	0.51
1:C:165:ILE:CD1	1:C:170:LYS:HB3	2.40	0.51
1:C:219:THR:O	1:C:220:ARG:NE	2.39	0.51
1:C:197:ARG:HA	1:C:235:ILE:HD13	1.92	0.51
1:C:513:SER:O	1:C:577:CYS:HA	2.10	0.51
1:C:715:SER:CB	1:C:716:PRO:HD3	2.27	0.51
1:C:340:THR:HG21	1:C:761:ILE:HG13	1.92	0.51
1:A:1015:TYR:CD2	1:A:1016:TYR:N	2.78	0.51
1:A:304:LEU:O	1:A:306:LEU:N	2.43	0.51
1:A:504:PRO:HD3	1:A:545:VAL:O	2.09	0.51
1:A:647:GLN:OE1	1:A:647:GLN:HA	2.09	0.51
1:A:626:ILE:HG23	1:A:681:ILE:HB	1.91	0.51
1:C:332:THR:O	1:C:333:VAL:C	2.49	0.51
1:C:497:LEU:HD12	1:C:551:LEU:O	2.09	0.51
1:C:959:ALA:HA	1:C:962:SER:OG	2.10	0.51
1:A:252:VAL:O	1:A:253:TYR:CD1	2.62	0.51
1:A:424:ALA:O	1:A:425:VAL:HG13	2.11	0.51
1:A:56:LEU:CD2	1:A:182:ASP:HB3	2.40	0.51
1:A:865:ILE:HG13	1:A:914:PRO:CB	2.40	0.51
1:C:117:GLU:N	1:C:118:PRO:CD	2.73	0.51
1:C:115:GLU:O	1:C:119:GLN:HB2	2.11	0.51
1:C:420:LEU:HD21	1:C:467:TYR:HB2	1.91	0.51
1:C:889:ASN:ND2	1:C:893:ASP:CB	2.73	0.51
1:A:516:ILE:C	1:A:518:GLY:H	2.13	0.51
1:A:417:ILE:HG21	1:A:548:PHE:HB3	1.92	0.51
1:A:886:ARG:CB	1:A:896:GLY:HA3	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:996:GLU:O	1:C:1000:LEU:HD13	2.09	0.51
1:C:454:GLU:OE1	1:C:459:SER:HA	2.11	0.51
1:C:899:TRP:O	1:C:903:GLN:N	2.44	0.51
3:G:37:ALA:O	3:G:40:VAL:HG22	2.10	0.51
1:A:483:LEU:HD23	1:A:500:MET:HE2	1.92	0.51
1:A:606:VAL:C	1:A:607:ILE:HG13	2.31	0.51
1:A:607:ILE:HA	1:A:681:ILE:HA	1.92	0.51
1:A:615:ILE:CD1	1:A:615:ILE:H	2.07	0.51
1:A:679:THR:O	1:A:681:ILE:HG12	2.10	0.51
1:C:349:CYS:HA	1:C:743:LEU:HA	1.91	0.51
1:C:79:THR:O	1:C:79:THR:HG22	2.10	0.51
1:C:982:PHE:O	1:C:985:PHE:HB3	2.11	0.51
1:A:485:ILE:HA	1:A:498:LEU:HA	1.92	0.51
1:C:1008:GLY:HA3	1:C:1012:LYS:HB2	1.93	0.51
1:C:266:LEU:O	1:C:268:SER:N	2.40	0.51
1:C:305:ILE:HB	1:C:307:GLU:CD	2.30	0.51
1:C:510:ARG:HG3	1:C:510:ARG:O	2.09	0.51
1:C:56:LEU:CD2	1:C:182:ASP:HB3	2.41	0.51
1:C:626:ILE:HG23	1:C:681:ILE:CB	2.40	0.51
1:C:905:LYS:C	1:C:907:VAL:H	2.12	0.51
1:A:997:VAL:O	1:A:1001:ILE:N	2.42	0.51
1:A:165:ILE:CD1	1:A:170:LYS:HB3	2.40	0.51
1:A:277:ILE:HD13	1:A:277:ILE:C	2.31	0.51
1:A:867:ALA:C	1:A:869:ASN:H	2.12	0.51
2:B:60:THR:O	2:B:61:ILE:C	2.49	0.51
1:C:347:LYS:HB2	1:C:347:LYS:NZ	2.26	0.51
1:C:483:LEU:C	1:C:483:LEU:HD12	2.31	0.51
1:C:761:ILE:O	1:C:765:LEU:HB2	2.10	0.51
1:C:807:THR:OG1	1:C:954:GLU:HG3	2.10	0.51
1:A:108:TYR:HE1	1:A:119:GLN:HG2	1.75	0.51
1:A:640:ARG:O	1:A:642:ASN:N	2.44	0.51
1:A:690:GLN:HA	1:A:693:ILE:HG22	1.93	0.51
1:C:785:ILE:HG13	1:C:859:PHE:CE2	2.46	0.51
1:A:370:LYS:CG	1:A:620:ILE:HG21	2.41	0.51
1:A:609:VAL:HG12	1:A:691:LYS:HG2	1.93	0.51
1:A:872:LEU:HB3	1:A:876:LEU:N	2.25	0.51
1:C:277:ILE:HG21	1:C:358:GLU:HB2	1.93	0.51
1:C:480:LYS:HE2	1:C:503:ALA:HB2	1.93	0.51
1:C:516:ILE:HD13	1:C:521:GLN:HG2	1.92	0.51
1:C:607:ILE:HA	1:C:681:ILE:HA	1.93	0.51
1:C:766:LYS:O	1:C:769:ILE:HG22	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:774:THR:CB	1:C:846:ALA:HB1	2.41	0.51
1:C:916:PHE:HD2	1:C:917:VAL:N	2.08	0.51
1:A:20:LYS:HD2	1:A:20:LYS:N	2.25	0.51
1:A:523:LEU:C	1:A:523:LEU:HD23	2.32	0.51
1:A:445:SER:HA	1:A:584:MET:SD	2.51	0.51
1:A:764:ASN:ND2	1:A:816:ALA:O	2.42	0.51
1:C:609:VAL:HG12	1:C:691:LYS:HG2	1.93	0.51
1:C:793:LEU:N	1:C:904:ARG:HH22	2.09	0.51
1:C:805:LEU:HD12	1:C:809:MET:CE	2.40	0.51
1:C:949:PHE:CE2	3:H:44:ILE:HG21	2.46	0.51
1:C:853:ILE:HG23	2:D:46:LEU:HD11	1.93	0.51
1:A:288:ILE:HG22	1:A:289:THR:N	2.26	0.50
1:A:480:LYS:HE2	1:A:503:ALA:HB2	1.91	0.50
1:A:773:LEU:CD1	1:A:773:LEU:C	2.79	0.50
1:A:94:SER:HB3	1:A:133:VAL:HG13	1.92	0.50
1:C:166:ARG:O	1:C:167:ASN:C	2.48	0.50
1:C:297:VAL:O	1:C:300:PHE:HB3	2.12	0.50
1:C:350:LEU:HG	1:C:351:VAL:H	1.76	0.50
1:C:88:GLN:O	1:C:94:SER:HB2	2.11	0.50
1:C:913:THR:OG1	1:C:972:ARG:CB	2.50	0.50
1:C:944:ASN:HB3	1:C:947:LEU:HB3	1.93	0.50
2:D:66:PRO:HB2	2:D:68:TYR:CZ	2.46	0.50
3:G:48:LYS:HA	3:G:48:LYS:HZ2	1.75	0.50
1:A:166:ARG:O	1:A:167:ASN:C	2.49	0.50
1:A:50:THR:HG21	1:A:181:GLY:O	2.10	0.50
1:A:325:VAL:O	1:A:325:VAL:CG2	2.59	0.50
1:A:345:ALA:HA	1:A:348:ASN:O	2.10	0.50
1:A:674:ILE:O	1:A:678:HIS:CE1	2.64	0.50
1:A:725:VAL:HG11	1:A:751:ILE:HD11	1.93	0.50
1:A:783:PHE:HA	1:A:786:PHE:HB3	1.93	0.50
1:A:79:THR:HG22	1:A:79:THR:O	2.11	0.50
1:C:208:ASN:O	1:C:209:SER:C	2.49	0.50
1:C:50:THR:CB	1:C:56:LEU:HD13	2.42	0.50
1:A:626:ILE:HG23	1:A:681:ILE:CB	2.41	0.50
1:C:1011:GLU:O	1:C:1014:THR:C	2.49	0.50
1:C:633:THR:O	1:C:636:ASP:HB2	2.12	0.50
1:C:679:THR:O	1:C:681:ILE:HG12	2.11	0.50
1:C:743:LEU:CD1	1:C:750:SER:HB2	2.41	0.50
1:C:89:LEU:HD23	1:C:89:LEU:O	2.11	0.50
1:C:998:ARG:HG3	1:C:999:LYS:N	2.27	0.50
3:H:36:LEU:O	3:H:40:VAL:HG13	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:LEU:O	1:A:805:LEU:HD12	2.12	0.50
1:A:909:PHE:CG	1:A:973:MET:HB2	2.44	0.50
1:C:166:ARG:O	1:C:168:GLY:N	2.45	0.50
1:C:481:TYR:HD2	1:C:481:TYR:O	1.94	0.50
1:C:483:LEU:HD23	1:C:500:MET:HE2	1.92	0.50
1:C:571:PHE:HB2	1:C:572:PRO:HD2	1.93	0.50
1:C:776:ASN:O	1:C:779:GLU:N	2.44	0.50
1:A:295:LEU:HB2	1:A:320:ILE:HD11	1.92	0.50
1:A:889:ASN:ND2	1:A:895:TYR:CD1	2.70	0.50
1:A:904:ARG:HD3	1:A:907:VAL:HG11	1.94	0.50
2:B:56:VAL:HA	2:B:59:LEU:HD12	1.93	0.50
1:C:499:VAL:HG12	1:C:550:HIS:HB2	1.94	0.50
1:C:651:ARG:NH1	1:C:677:TYR:CE2	2.80	0.50
1:C:150:ILE:HD11	1:C:738:ALA:HA	1.94	0.50
1:A:108:TYR:CE1	1:A:119:GLN:HA	2.47	0.50
1:A:284:PHE:HZ	1:A:329:LEU:HD11	1.77	0.50
1:A:651:ARG:NH1	1:A:677:TYR:CE2	2.80	0.50
1:A:327:GLU:HG2	1:A:801:LEU:HD22	1.94	0.50
1:C:378:ARG:HG3	1:C:378:ARG:HH11	1.77	0.50
1:C:916:PHE:O	1:C:919:ILE:HB	2.12	0.50
1:C:944:ASN:O	1:C:945:LYS:C	2.49	0.50
1:A:109:GLY:O	1:A:111:GLN:N	2.44	0.50
1:A:227:GLU:OE2	1:A:229:PRO:HD2	2.12	0.50
1:A:275:THR:O	1:A:278:ALA:N	2.44	0.50
1:A:50:THR:CB	1:A:56:LEU:HD13	2.42	0.50
1:A:637:ILE:C	1:A:639:ALA:H	2.15	0.50
1:A:840:GLU:H	1:A:840:GLU:CD	2.14	0.50
1:A:918:THR:HG22	1:A:984:ALA:HB2	1.94	0.50
1:C:512:SER:HB3	1:C:575:ASN:HA	1.93	0.50
1:C:637:ILE:C	1:C:639:ALA:H	2.15	0.50
1:C:867:ALA:HB2	1:C:871:PHE:HD2	1.77	0.50
1:C:895:TYR:HD2	1:C:899:TRP:HE3	1.58	0.50
1:A:936:SER:N	1:A:1003:ARG:NH2	2.57	0.50
1:A:115:GLU:O	1:A:119:GLN:HB2	2.11	0.50
1:A:45:HIS:HB2	1:A:52:LEU:HD13	1.94	0.50
1:A:499:VAL:HG12	1:A:550:HIS:HB2	1.93	0.50
1:C:111:GLN:HE22	1:C:118:PRO:HB3	1.77	0.50
1:C:424:ALA:O	1:C:425:VAL:HG13	2.12	0.50
1:C:504:PRO:HG3	1:C:535:TYR:HE1	1.76	0.50
1:C:714:ASP:O	1:C:715:SER:C	2.49	0.50
1:C:762:PHE:CE2	1:C:830:ARG:HD2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:952:PHE:HD2	1:C:952:PHE:N	2.09	0.50
1:A:969:VAL:C	1:A:971:LEU:H	2.15	0.50
1:A:975:PRO:HA	1:A:980:TRP:HD1	1.77	0.50
1:A:992:PHE:CD1	1:A:992:PHE:C	2.85	0.50
1:C:842:LEU:CD2	1:C:1016:TYR:CE1	2.94	0.50
1:C:20:LYS:N	1:C:20:LYS:HD2	2.26	0.50
1:C:375:THR:HA	1:C:588:PRO:HA	1.93	0.50
1:C:493:GLU:O	1:C:494:PRO:O	2.29	0.50
1:C:807:THR:CG2	1:C:808:ASP:H	2.22	0.50
1:A:111:GLN:HE22	1:A:118:PRO:HB3	1.77	0.49
1:A:482:GLN:O	1:A:500:MET:HA	2.12	0.49
1:A:483:LEU:HB3	1:A:500:MET:CB	2.42	0.49
1:A:58:PRO:O	1:A:61:ALA:HB3	2.12	0.49
1:A:896:GLY:O	1:A:899:TRP:C	2.50	0.49
1:A:982:PHE:CD2	1:A:982:PHE:N	2.80	0.49
1:C:205:LYS:CG	1:C:219:THR:HG22	2.39	0.49
1:C:824:ILE:C	1:C:826:LYS:N	2.66	0.49
1:C:929:ILE:HG12	1:C:995:ASP:CB	2.42	0.49
1:C:931:LYS:C	1:C:932:THR:HG22	2.32	0.49
1:C:959:ALA:C	1:C:961:LEU:H	2.14	0.49
1:C:98:TRP:HE1	1:C:133:VAL:HG11	1.77	0.49
2:D:57:MET:HE2	2:D:57:MET:O	2.12	0.49
1:A:184:VAL:O	1:A:248:ARG:HA	2.12	0.49
1:A:406:LYS:HG3	1:A:406:LYS:O	2.12	0.49
1:A:779:GLU:HA	1:A:795:LEU:CD1	2.43	0.49
1:C:141:TYR:C	1:C:143:GLN:N	2.64	0.49
1:C:370:LYS:CG	1:C:620:ILE:HG21	2.42	0.49
1:C:508:LEU:HD13	1:C:508:LEU:C	2.33	0.49
1:C:82:TRP:O	1:C:84:LYS:N	2.45	0.49
1:A:344:MET:HE2	1:A:357:VAL:HG13	1.94	0.49
1:A:606:VAL:HG23	1:A:681:ILE:CG2	2.42	0.49
1:A:697:GLY:HA2	1:A:700:ARG:NH1	2.28	0.49
1:A:98:TRP:HE1	1:A:133:VAL:HG11	1.76	0.49
1:C:523:LEU:C	1:C:523:LEU:HD23	2.32	0.49
1:C:605:LYS:HZ2	1:C:676:LYS:HE2	1.77	0.49
1:C:88:GLN:O	1:C:90:PHE:N	2.39	0.49
1:C:976:LEU:CD2	1:C:979:THR:H	2.22	0.49
2:D:41:ILE:HD13	2:D:41:ILE:N	2.28	0.49
1:C:892:GLU:HB2	2:D:65:LYS:HZ3	1.76	0.49
1:A:341:ALA:O	1:A:343:ARG:N	2.45	0.49
1:A:501:LYS:HA	1:A:547:GLY:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:ASP:C	1:A:811:PRO:HD2	2.33	0.49
1:A:811:PRO:HA	1:A:814:SER:HB3	1.94	0.49
1:A:956:ALA:O	1:A:957:LEU:C	2.51	0.49
1:C:963:TYR:HD2	3:H:30:GLY:HA3	1.77	0.49
1:A:166:ARG:O	1:A:168:GLY:N	2.45	0.49
1:A:332:THR:HG23	1:A:813:ILE:CD1	2.36	0.49
1:A:96:LEU:O	1:A:100:GLY:N	2.45	0.49
2:B:61:ILE:HG22	2:B:66:PRO:HD3	1.94	0.49
1:C:111:GLN:NE2	1:C:118:PRO:CB	2.76	0.49
1:C:647:GLN:HA	1:C:647:GLN:OE1	2.11	0.49
1:C:918:THR:O	1:C:921:VAL:HB	2.12	0.49
1:C:964:CYS:O	1:C:966:GLY:N	2.46	0.49
2:D:57:MET:C	2:D:57:MET:SD	2.91	0.49
1:A:148:SER:O	1:A:149:LYS:HB2	2.12	0.49
1:A:182:ASP:O	1:A:251:VAL:HG22	2.13	0.49
1:A:209:SER:O	1:A:211:LEU:N	2.45	0.49
1:A:296:GLY:CA	1:A:320:ILE:HD13	2.43	0.49
1:A:871:PHE:CG	1:A:873:PRO:HG3	2.47	0.49
2:B:66:PRO:CG	2:B:68:TYR:HE2	2.24	0.49
1:C:184:VAL:O	1:C:248:ARG:HA	2.12	0.49
1:C:321:ILE:C	1:C:323:ALA:H	2.15	0.49
1:C:872:LEU:CD2	1:C:872:LEU:N	2.73	0.49
1:A:150:ILE:C	1:A:152:GLU:N	2.64	0.49
1:A:266:LEU:O	1:A:268:SER:N	2.42	0.49
1:A:329:LEU:HD22	1:A:329:LEU:O	2.12	0.49
1:A:51:ASP:OD2	1:A:54:ARG:HB2	2.13	0.49
1:A:714:ASP:O	1:A:715:SER:C	2.50	0.49
1:A:865:ILE:HG21	1:A:911:CYS:HA	1.95	0.49
1:A:916:PHE:CD2	1:A:916:PHE:C	2.86	0.49
1:A:960:PHE:O	1:A:964:CYS:HB3	2.12	0.49
1:C:108:TYR:CE1	1:C:119:GLN:HA	2.46	0.49
1:C:196:LEU:CD1	1:C:236:ALA:HB3	2.42	0.49
1:C:266:LEU:C	1:C:268:SER:H	2.16	0.49
1:C:880:ARG:NH1	1:C:903:GLN:O	2.45	0.49
1:C:889:ASN:ND2	1:C:895:TYR:CG	2.81	0.49
1:A:341:ALA:C	1:A:343:ARG:N	2.66	0.49
1:A:508:LEU:HD13	1:A:508:LEU:C	2.32	0.49
1:A:340:THR:HG21	1:A:761:ILE:HG13	1.94	0.49
1:A:779:GLU:HA	1:A:795:LEU:HD13	1.94	0.49
1:A:909:PHE:HB3	1:A:973:MET:HB2	1.90	0.49
1:A:860:PHE:HE1	2:B:53:THR:O	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:LYS:HG3	1:C:266:LEU:HD22	1.94	0.49
1:C:96:LEU:HB3	1:C:321:ILE:HD12	1.95	0.49
1:C:497:LEU:HD12	1:C:498:LEU:N	2.27	0.49
1:C:316:PHE:HE1	1:C:783:PHE:HB3	1.78	0.49
1:C:316:PHE:HD1	1:C:783:PHE:HD1	1.60	0.49
1:C:814:SER:OG	1:C:946:ILE:HG22	2.13	0.49
1:C:896:GLY:O	1:C:897:GLN:O	2.31	0.49
1:C:864:VAL:HG11	2:D:57:MET:HE3	1.95	0.49
3:H:44:ILE:CG2	3:H:48:LYS:HD3	2.43	0.49
1:A:327:GLU:HG2	1:A:801:LEU:CD2	2.43	0.49
1:A:365:THR:HB	1:A:705:VAL:CG1	2.31	0.49
1:A:689:GLN:N	1:A:689:GLN:OE1	2.41	0.49
1:A:950:GLY:HA2	1:A:953:GLU:CB	2.42	0.49
1:C:148:SER:O	1:C:149:LYS:HB2	2.12	0.49
1:C:689:GLN:N	1:C:689:GLN:OE1	2.40	0.49
1:C:779:GLU:HB2	1:C:800:ILE:CD1	2.43	0.49
2:D:60:THR:C	2:D:62:SER:H	2.16	0.49
1:A:150:ILE:O	1:A:152:GLU:N	2.46	0.49
1:A:208:ASN:O	1:A:209:SER:C	2.50	0.49
1:A:303:SER:O	1:A:305:ILE:N	2.46	0.49
1:A:304:LEU:HD21	1:A:310:TRP:CZ3	2.48	0.49
1:A:464:ARG:HG3	1:A:464:ARG:NH1	2.26	0.49
1:A:625:GLY:O	1:A:627:ILE:N	2.46	0.49
1:A:839:ASN:H	1:A:839:ASN:HD22	1.55	0.49
1:A:95:MET:HG2	1:A:96:LEU:N	2.28	0.49
2:B:31:SER:C	2:B:33:PHE:H	2.16	0.49
1:C:150:ILE:C	1:C:152:GLU:N	2.65	0.49
1:C:585:ILE:O	1:C:587:PRO:HD3	2.13	0.49
1:C:690:GLN:HA	1:C:693:ILE:HG22	1.93	0.49
1:C:79:THR:N	1:C:80:PRO:HD3	2.24	0.49
1:C:897:GLN:O	1:C:899:TRP:N	2.38	0.49
1:A:1011:GLU:N	1:A:1011:GLU:OE2	2.46	0.48
1:A:266:LEU:C	1:A:268:SER:H	2.16	0.48
1:A:339:LEU:C	1:A:341:ALA:H	2.17	0.48
1:A:786:PHE:HD2	1:A:793:LEU:HA	1.77	0.48
1:A:831:ASN:ND2	1:A:833:LYS:H	2.11	0.48
1:A:831:ASN:HD21	1:A:834:THR:H	1.53	0.48
1:A:850:ILE:HD12	1:A:850:ILE:N	2.28	0.48
1:A:88:GLN:C	1:A:90:PHE:N	2.64	0.48
2:B:62:SER:OG	2:B:66:PRO:HD3	2.12	0.48
1:C:108:TYR:HE1	1:C:119:GLN:HG2	1.77	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:SER:OG	1:C:734:VAL:HB	2.12	0.48
1:C:196:LEU:HD12	1:C:196:LEU:O	2.13	0.48
1:C:420:LEU:HD12	1:C:420:LEU:H	1.77	0.48
1:C:460:VAL:HG23	1:C:461:LYS:N	2.27	0.48
1:C:494:PRO:CG	1:C:552:PHE:HB3	2.42	0.48
1:C:606:VAL:HG23	1:C:681:ILE:CG2	2.43	0.48
1:A:196:LEU:CD1	1:A:236:ALA:HB3	2.43	0.48
1:A:305:ILE:O	1:A:307:GLU:N	2.46	0.48
1:A:948:ILE:CD1	1:A:948:ILE:H	2.26	0.48
1:C:158:VAL:HG23	1:C:159:PRO:HD2	1.95	0.48
1:C:187:LYS:HG3	1:C:188:GLY:N	2.28	0.48
1:C:483:LEU:HB3	1:C:500:MET:CB	2.42	0.48
1:C:875:HIS:O	1:C:876:LEU:CB	2.60	0.48
1:C:932:THR:HG23	1:C:999:LYS:HZ3	1.78	0.48
1:C:944:ASN:OD1	1:C:944:ASN:O	2.31	0.48
2:D:34:LYS:CE	2:D:37:LEU:HD21	2.42	0.48
1:A:473:ILE:HD12	1:A:483:LEU:HD11	1.95	0.48
1:A:856:LEU:CD1	2:B:46:LEU:HD22	2.42	0.48
1:A:898:GLN:HG3	1:A:899:TRP:N	2.28	0.48
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.95	0.48
1:A:93:PHE:O	1:A:97:LEU:HD23	2.12	0.48
1:C:501:LYS:HA	1:C:547:GLY:O	2.14	0.48
1:A:111:GLN:NE2	1:A:118:PRO:CB	2.76	0.48
1:A:644:PRO:HA	1:A:648:VAL:CG2	2.43	0.48
1:A:889:ASN:ND2	1:A:893:ASP:HB2	2.28	0.48
1:A:892:GLU:OE1	2:B:65:LYS:CG	2.59	0.48
1:A:896:GLY:O	1:A:898:GLN:N	2.46	0.48
1:C:1000:LEU:HD12	1:C:1000:LEU:N	2.29	0.48
1:C:549:CYS:HB2	1:C:577:CYS:O	2.13	0.48
1:C:884:ASP:OD1	1:C:887:TRP:HB2	2.13	0.48
1:C:908:GLU:HB3	1:C:909:PHE:CD2	2.48	0.48
1:A:71:ASN:O	1:A:176:GLU:HA	2.14	0.48
1:A:337:LEU:O	1:A:339:LEU:N	2.46	0.48
1:A:516:ILE:HG13	1:A:519:LYS:HB2	1.95	0.48
1:A:896:GLY:O	1:A:897:GLN:C	2.51	0.48
1:A:990:LEU:HA	1:A:993:VAL:CG2	2.44	0.48
1:C:42:ASP:OD2	1:C:46:ARG:NH2	2.47	0.48
1:C:636:ASP:N	1:C:647:GLN:HE21	2.11	0.48
1:C:901:TYR:O	1:C:905:LYS:HD2	2.13	0.48
1:C:814:SER:CB	1:C:946:ILE:HG22	2.43	0.48
1:C:961:LEU:HD12	1:C:964:CYS:SG	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:ILE:HG21	1:A:1011:GLU:HG2	1.95	0.48
1:A:432:ASN:C	1:A:434:PRO:CD	2.82	0.48
1:A:565:ASP:N	1:A:570:ASN:ND2	2.54	0.48
1:A:611:GLY:HA2	1:A:686:THR:N	2.20	0.48
1:A:766:LYS:O	1:A:769:ILE:HG22	2.12	0.48
1:A:895:TYR:HB3	1:A:899:TRP:O	2.13	0.48
1:C:121:ASP:O	1:C:123:LEU:N	2.47	0.48
1:C:192:ILE:HG22	1:C:194:ALA:O	2.13	0.48
1:C:227:GLU:OE2	1:C:229:PRO:HD2	2.13	0.48
1:C:371:THR:HG22	1:C:377:ASN:HD22	1.79	0.48
1:C:50:THR:HG21	1:C:181:GLY:O	2.14	0.48
1:C:523:LEU:HD21	1:C:528:LYS:NZ	2.28	0.48
1:C:794:PRO:O	1:C:912:HIS:HD2	1.97	0.48
1:C:792:PRO:HG2	1:C:880:ARG:HH21	1.78	0.48
1:C:959:ALA:C	1:C:961:LEU:N	2.67	0.48
1:C:93:PHE:HA	1:C:95:MET:SD	2.54	0.48
1:A:918:THR:O	1:A:922:VAL:HG22	2.14	0.48
1:C:434:PRO:O	1:C:438:ARG:HG3	2.14	0.48
1:C:51:ASP:OD2	1:C:54:ARG:HB2	2.13	0.48
1:C:626:ILE:HG22	1:C:627:ILE:HG13	1.96	0.48
1:C:644:PRO:HA	1:C:648:VAL:CG2	2.43	0.48
1:C:759:ARG:NH2	1:C:829:PRO:HA	2.29	0.48
1:C:889:ASN:ND2	1:C:894:SER:N	2.61	0.48
1:C:857:GLY:CA	1:C:987:TYR:CD2	2.94	0.48
1:C:864:VAL:CG1	2:D:57:MET:SD	3.02	0.48
1:A:205:LYS:HB2	1:A:244:GLU:HG3	1.96	0.48
1:A:782:PRO:HG2	1:A:795:LEU:HB2	1.96	0.48
1:A:831:ASN:OD1	1:A:832:PRO:HD2	2.14	0.48
2:B:62:SER:CB	2:B:66:PRO:HD3	2.44	0.48
1:C:274:GLN:HB3	1:C:279:ALA:HB2	1.94	0.48
1:C:734:VAL:HG22	1:C:735:SER:N	2.28	0.48
1:C:904:ARG:HA	1:C:907:VAL:CG1	2.44	0.48
1:A:567:ASP:OD2	1:A:567:ASP:N	2.45	0.48
1:A:549:CYS:HB2	1:A:577:CYS:O	2.13	0.48
1:C:111:GLN:NE2	1:C:118:PRO:HB3	2.29	0.48
1:C:432:ASN:C	1:C:434:PRO:CD	2.82	0.48
1:C:625:GLY:O	1:C:627:ILE:N	2.47	0.48
1:C:818:GLU:OE2	1:C:931:LYS:HE2	2.13	0.48
1:C:886:ARG:N	1:C:896:GLY:HA3	2.29	0.48
1:A:275:THR:OG1	1:A:355:GLU:HB2	2.14	0.48
1:A:512:SER:HB3	1:A:575:ASN:HA	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:ARG:CA	1:A:896:GLY:CA	2.92	0.48
1:A:904:ARG:C	1:A:906:ILE:N	2.67	0.48
1:A:946:ILE:HD13	3:G:45:ILE:HD11	1.95	0.48
2:B:63:GLU:N	2:B:63:GLU:CD	2.62	0.48
1:A:899:TRP:HZ2	2:B:70:ASP:O	1.97	0.48
1:C:350:LEU:H	1:C:744:LEU:CD1	2.26	0.48
1:C:387:ASP:O	1:C:388:ASN:HB3	2.14	0.48
1:C:65:LEU:HD23	1:C:65:LEU:C	2.35	0.48
1:C:777:ILE:CB	1:C:778:PRO:HD3	2.24	0.48
1:C:796:GLY:O	1:C:800:ILE:HG12	2.14	0.48
1:A:329:LEU:O	1:A:333:VAL:HG23	2.14	0.47
1:A:41:LEU:CD1	1:A:41:LEU:H	2.07	0.47
1:A:422:ASN:HB3	1:A:464:ARG:NH2	2.29	0.47
1:A:545:VAL:HG12	1:A:583:SER:HB3	1.96	0.47
1:A:633:THR:O	1:A:636:ASP:HB2	2.14	0.47
1:A:651:ARG:HH12	1:A:677:TYR:HE2	1.62	0.47
1:A:716:PRO:O	1:A:719:LYS:N	2.47	0.47
1:A:726:ALA:O	1:A:727:MET:HG2	2.14	0.47
1:A:743:LEU:CD1	1:A:750:SER:HB2	2.43	0.47
1:A:756:GLU:HA	1:A:825:MET:CE	2.44	0.47
1:A:900:THR:HA	1:A:903:GLN:HE21	1.78	0.47
1:A:911:CYS:CA	1:A:914:PRO:HD2	2.44	0.47
1:A:936:SER:O	1:A:938:PHE:N	2.47	0.47
1:A:995:ASP:HA	1:A:998:ARG:CD	2.43	0.47
1:C:117:GLU:C	1:C:119:GLN:N	2.67	0.47
1:C:516:ILE:HG13	1:C:519:LYS:HB2	1.95	0.47
1:C:626:ILE:CG2	1:C:681:ILE:HB	2.44	0.47
1:C:885:ASP:CG	1:C:897:GLN:HB3	2.34	0.47
1:C:955:THR:HG22	1:C:956:ALA:N	2.28	0.47
1:A:626:ILE:CG2	1:A:681:ILE:HB	2.44	0.47
1:A:756:GLU:HA	1:A:825:MET:HE3	1.96	0.47
1:A:966:GLY:O	1:A:969:VAL:HG23	2.14	0.47
1:A:990:LEU:CA	1:A:993:VAL:HG22	2.44	0.47
1:A:899:TRP:CZ2	2:B:70:ASP:C	2.88	0.47
1:C:348:ASN:O	1:C:349:CYS:C	2.51	0.47
1:C:45:HIS:HB2	1:C:52:LEU:HD13	1.95	0.47
1:C:482:GLN:O	1:C:500:MET:HA	2.12	0.47
1:C:516:ILE:O	1:C:516:ILE:HG13	2.14	0.47
1:C:872:LEU:HB2	1:C:875:HIS:O	2.13	0.47
1:A:507:ILE:HG22	1:A:508:LEU:N	2.27	0.47
1:A:555:ASP:O	1:A:557:GLN:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:HG21	1:A:761:ILE:CG1	2.44	0.47
1:A:765:LEU:O	1:A:769:ILE:N	2.47	0.47
1:A:889:ASN:ND2	1:A:895:TYR:CB	2.77	0.47
1:C:651:ARG:HH12	1:C:677:TYR:HE2	1.62	0.47
1:C:785:ILE:HG13	1:C:859:PHE:HE2	1.79	0.47
1:A:432:ASN:HB2	1:A:434:PRO:HD2	1.96	0.47
1:A:631:ASN:OD1	1:A:634:VAL:HG13	2.14	0.47
1:A:769:ILE:O	1:A:770:ALA:C	2.52	0.47
1:A:865:ILE:HG23	1:A:910:THR:HG22	1.97	0.47
1:A:963:TYR:O	1:A:965:PRO:HD3	2.14	0.47
1:C:71:ASN:O	1:C:176:GLU:HA	2.14	0.47
1:C:277:ILE:HD13	1:C:278:ALA:CA	2.45	0.47
1:C:340:THR:HG23	1:C:343:ARG:NH2	2.29	0.47
1:C:55:GLY:HA2	1:C:183:LEU:CD2	2.44	0.47
1:C:792:PRO:CG	1:C:880:ARG:HH21	2.27	0.47
1:A:348:ASN:O	1:A:349:CYS:C	2.52	0.47
1:A:460:VAL:HG23	1:A:461:LYS:N	2.29	0.47
1:A:523:LEU:HD21	1:A:528:LYS:NZ	2.29	0.47
1:A:879:LEU:CD1	1:A:881:VAL:HG23	2.39	0.47
1:A:906:ILE:O	1:A:910:THR:HB	2.15	0.47
1:C:432:ASN:HB2	1:C:434:PRO:HD2	1.96	0.47
1:C:744:LEU:HD12	1:C:744:LEU:N	2.27	0.47
1:C:914:PRO:C	1:C:916:PHE:N	2.67	0.47
2:D:39:TYR:O	2:D:43:TYR:HD1	1.96	0.47
3:G:39:ILE:O	3:G:39:ILE:HG22	2.15	0.47
1:A:229:PRO:HG2	1:A:230:LEU:H	1.79	0.47
1:A:516:ILE:HG13	1:A:516:ILE:O	2.14	0.47
1:A:494:PRO:CG	1:A:552:PHE:HB3	2.43	0.47
1:A:783:PHE:CD2	1:A:783:PHE:N	2.82	0.47
1:C:631:ASN:OD1	1:C:634:VAL:HG13	2.15	0.47
1:C:674:ILE:HD12	1:C:674:ILE:N	2.30	0.47
1:C:129:LEU:CD2	1:C:801:LEU:HD11	2.44	0.47
1:C:823:ASP:OD1	1:C:826:LYS:HB2	2.14	0.47
1:A:674:ILE:HD12	1:A:674:ILE:N	2.30	0.47
1:A:979:THR:C	1:A:981:TRP:N	2.67	0.47
1:C:134:ILE:HG22	1:C:135:ILE:N	2.30	0.47
1:C:150:ILE:O	1:C:152:GLU:N	2.48	0.47
1:C:674:ILE:O	1:C:678:HIS:CE1	2.68	0.47
1:C:340:THR:HG21	1:C:761:ILE:CG1	2.45	0.47
1:C:911:CYS:O	1:C:914:PRO:HD2	2.15	0.47
1:C:914:PRO:C	1:C:916:PHE:H	2.17	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:45:ILE:C	3:G:47:SER:H	2.16	0.47
1:A:158:VAL:HG23	1:A:159:PRO:HD2	1.96	0.47
1:A:301:ILE:HG22	1:A:302:LEU:H	1.75	0.47
1:A:671:LEU:HD23	1:A:675:LEU:HB2	1.96	0.47
1:A:674:ILE:CD1	1:A:674:ILE:H	2.28	0.47
1:A:675:LEU:HD21	1:A:698:CYS:HA	1.96	0.47
1:A:88:GLN:NE2	1:A:89:LEU:N	2.62	0.47
1:A:947:LEU:HG	1:A:948:ILE:H	1.80	0.47
1:A:987:TYR:O	1:A:988:SER:C	2.53	0.47
1:C:29:LYS:HD3	1:C:29:LYS:N	2.25	0.47
1:C:723:ILE:HA	1:C:740:ASP:OD1	2.14	0.47
1:A:192:ILE:HG22	1:A:194:ALA:O	2.14	0.47
1:A:96:LEU:HD11	1:A:289:THR:HG23	1.97	0.47
1:A:337:LEU:HD11	1:A:358:GLU:OE1	2.15	0.47
1:A:350:LEU:HG	1:A:351:VAL:H	1.78	0.47
1:A:769:ILE:CG2	1:A:770:ALA:N	2.78	0.47
1:A:866:LEU:O	1:A:870:GLY:N	2.44	0.47
1:A:88:GLN:C	1:A:91:GLY:H	2.17	0.47
2:B:61:ILE:O	2:B:62:SER:HB3	2.15	0.47
1:C:198:ILE:HA	1:C:249:GLY:HA3	1.97	0.47
1:C:769:ILE:HD13	1:C:838:VAL:HG22	1.97	0.47
1:C:777:ILE:HA	1:C:780:ILE:HD12	1.97	0.47
1:C:781:THR:HA	1:C:784:LEU:CB	2.45	0.47
1:C:781:THR:HA	1:C:784:LEU:HB2	1.97	0.47
1:C:808:ASP:C	1:C:811:PRO:HD2	2.35	0.47
3:G:48:LYS:HA	3:G:48:LYS:NZ	2.30	0.47
1:A:589:ARG:O	1:A:593:PRO:HD3	2.15	0.47
1:A:649:ASN:HB2	1:A:650:PRO:CD	2.42	0.47
1:A:762:PHE:CE1	1:A:830:ARG:NH1	2.83	0.47
1:A:907:VAL:O	1:A:910:THR:O	2.32	0.47
2:B:37:LEU:O	2:B:39:TYR:N	2.43	0.47
2:B:48:GLY:HA2	2:B:51:ILE:CG1	2.45	0.47
1:A:899:TRP:CZ2	2:B:70:ASP:O	2.68	0.47
1:C:555:ASP:O	1:C:557:GLN:N	2.48	0.47
1:C:643:ILE:O	1:C:648:VAL:HG13	2.15	0.47
1:C:650:PRO:O	1:C:651:ARG:C	2.53	0.47
1:C:675:LEU:HD21	1:C:698:CYS:HA	1.96	0.47
1:C:795:LEU:HD22	1:C:800:ILE:CD1	2.45	0.47
1:C:92:GLY:HA2	1:C:330:LEU:HD11	1.96	0.47
3:G:45:ILE:O	3:G:45:ILE:HD13	2.15	0.47
1:A:55:GLY:HA2	1:A:183:LEU:CD2	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:SER:C	1:A:479:ASN:H	2.19	0.47
1:A:481:TYR:O	1:A:481:TYR:HD2	1.97	0.47
1:A:919:ILE:HD13	1:A:919:ILE:HA	1.78	0.47
1:A:926:ASP:C	1:A:928:VAL:H	2.17	0.47
1:A:992:PHE:HD1	1:A:992:PHE:C	2.18	0.47
2:B:31:SER:O	2:B:33:PHE:N	2.48	0.47
1:C:467:TYR:CD1	1:C:489:PRO:HD3	2.49	0.47
1:C:777:ILE:HA	1:C:780:ILE:CD1	2.45	0.47
1:C:906:ILE:HG22	1:C:906:ILE:O	2.15	0.47
1:A:111:GLN:NE2	1:A:118:PRO:HB3	2.30	0.46
1:A:141:TYR:O	1:A:143:GLN:N	2.48	0.46
1:A:358:GLU:OE2	1:A:761:ILE:HG22	2.15	0.46
1:A:434:PRO:O	1:A:438:ARG:HG3	2.15	0.46
1:A:811:PRO:HB3	1:A:927:LEU:CD2	2.45	0.46
2:B:66:PRO:O	2:B:67:THR:CB	2.63	0.46
1:C:205:LYS:HB2	1:C:244:GLU:HG3	1.96	0.46
1:C:298:SER:C	1:C:300:PHE:H	2.18	0.46
1:C:565:ASP:N	1:C:570:ASN:ND2	2.54	0.46
1:C:674:ILE:CD1	1:C:674:ILE:H	2.28	0.46
1:C:84:LYS:HG2	1:C:146:LYS:NZ	2.31	0.46
1:C:910:THR:O	1:C:911:CYS:C	2.54	0.46
1:C:931:LYS:HB3	1:C:931:LYS:NZ	2.30	0.46
1:C:93:PHE:O	1:C:97:LEU:HD23	2.16	0.46
1:C:985:PHE:CD1	1:C:985:PHE:C	2.89	0.46
1:A:387:ASP:O	1:A:388:ASN:HB3	2.15	0.46
1:A:643:ILE:O	1:A:648:VAL:HG13	2.15	0.46
1:A:723:ILE:HA	1:A:740:ASP:OD1	2.15	0.46
1:A:842:LEU:HD12	1:A:842:LEU:O	2.15	0.46
1:A:865:ILE:HG21	1:A:911:CYS:CA	2.45	0.46
1:A:867:ALA:O	1:A:869:ASN:N	2.42	0.46
1:A:976:LEU:N	1:A:980:TRP:CD1	2.69	0.46
1:A:865:ILE:HA	1:A:980:TRP:CH2	2.50	0.46
1:C:226:ASN:O	1:C:228:ASN:ND2	2.39	0.46
1:C:995:ASP:HA	1:C:998:ARG:HD3	1.97	0.46
1:A:117:GLU:C	1:A:119:GLN:N	2.67	0.46
1:A:325:VAL:O	1:A:327:GLU:N	2.48	0.46
1:A:755:VAL:HG13	1:A:825:MET:HE1	1.96	0.46
1:C:725:VAL:HG11	1:C:751:ILE:HD11	1.97	0.46
1:C:889:ASN:CG	1:C:890:ASP:H	2.10	0.46
1:C:928:VAL:HG12	1:C:928:VAL:O	2.16	0.46
1:A:1012:LYS:O	1:A:1015:TYR:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASP:O	1:A:123:LEU:N	2.48	0.46
1:A:774:THR:HG21	1:A:850:ILE:CG2	2.46	0.46
1:A:834:THR:O	1:A:836:LYS:HG2	2.15	0.46
1:A:852:MET:O	1:A:855:ALA:N	2.48	0.46
1:A:907:VAL:HG13	1:A:908:GLU:N	2.29	0.46
1:A:990:LEU:C	1:A:993:VAL:HG22	2.35	0.46
2:B:42:PHE:O	2:B:46:LEU:HB2	2.14	0.46
1:C:922:VAL:HG12	1:C:988:SER:HA	1.97	0.46
3:G:41:GLY:O	3:G:46:LEU:HD13	2.16	0.46
1:A:350:LEU:H	1:A:744:LEU:CD1	2.27	0.46
1:A:858:GLY:HA3	1:A:915:PHE:CE2	2.51	0.46
1:A:860:PHE:HE1	2:B:53:THR:HB	1.78	0.46
1:C:103:LEU:HD23	1:C:103:LEU:C	2.36	0.46
1:C:477:SER:C	1:C:479:ASN:H	2.19	0.46
1:C:861:THR:HB	1:C:918:THR:HG21	1.97	0.46
3:H:43:ILE:O	3:H:43:ILE:CG2	2.62	0.46
1:A:134:ILE:HG22	1:A:135:ILE:N	2.31	0.46
1:A:406:LYS:HD2	1:A:411:TRP:NE1	2.30	0.46
1:A:420:LEU:H	1:A:420:LEU:HD12	1.80	0.46
1:A:379:MET:CG	1:A:444:ALA:HB1	2.45	0.46
1:A:725:VAL:HG12	1:A:743:LEU:HD21	1.97	0.46
1:A:890:ASP:O	1:A:893:ASP:OD2	2.32	0.46
1:A:900:THR:N	1:A:903:GLN:H	2.13	0.46
1:C:182:ASP:O	1:C:251:VAL:HG22	2.16	0.46
1:A:139:PHE:C	1:A:141:TYR:H	2.18	0.46
1:A:22:GLU:OE1	1:A:25:MET:HB3	2.16	0.46
1:A:636:ASP:N	1:A:647:GLN:HE21	2.13	0.46
1:A:881:VAL:HG12	1:A:883:TRP:H	1.80	0.46
1:A:900:THR:C	1:A:902:GLU:N	2.66	0.46
1:A:906:ILE:HG22	1:A:906:ILE:O	2.16	0.46
1:C:497:LEU:HD11	1:C:550:HIS:HB2	1.98	0.46
2:D:71:ARG:HG3	2:D:71:ARG:HH11	1.80	0.46
1:A:759:ARG:HD2	1:A:825:MET:HE1	1.98	0.46
1:A:945:LYS:HB3	3:G:48:LYS:HE3	1.98	0.46
1:A:971:LEU:C	1:A:972:ARG:CZ	2.84	0.46
2:B:62:SER:HB3	2:B:66:PRO:HD3	1.97	0.46
1:C:102:ILE:HG23	1:C:103:LEU:N	2.31	0.46
1:C:316:PHE:CE2	1:C:787:ILE:HG13	2.51	0.46
1:C:36:ASP:HB2	1:C:47:LYS:HZ2	1.81	0.46
1:C:411:TRP:O	1:C:412:LEU:C	2.53	0.46
1:C:422:ASN:HB3	1:C:464:ARG:NH2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:ASP:N	1:C:567:ASP:OD2	2.46	0.46
1:C:129:LEU:HD23	1:C:801:LEU:HD11	1.98	0.46
1:C:992:PHE:HD1	1:C:993:VAL:N	2.14	0.46
2:D:53:THR:O	2:D:57:MET:HB3	2.16	0.46
2:D:72:VAL:HG12	2:D:73:ALA:N	2.31	0.46
1:A:187:LYS:HD2	1:A:188:GLY:H	1.81	0.46
1:A:187:LYS:HG3	1:A:188:GLY:N	2.30	0.46
1:A:287:ILE:HG22	1:A:288:ILE:N	2.30	0.46
1:A:467:TYR:CD1	1:A:489:PRO:HD3	2.51	0.46
1:A:626:ILE:HG22	1:A:627:ILE:HG13	1.98	0.46
1:A:771:TYR:CE2	1:A:808:ASP:HB3	2.51	0.46
1:A:877:LEU:N	1:A:877:LEU:HD12	2.30	0.46
1:A:944:ASN:O	1:A:945:LYS:C	2.54	0.46
1:A:947:LEU:CG	1:A:948:ILE:N	2.78	0.46
1:C:114:THR:O	1:C:115:GLU:C	2.54	0.46
1:C:294:PHE:C	1:C:296:GLY:H	2.18	0.46
1:C:349:CYS:O	1:C:349:CYS:SG	2.74	0.46
1:C:671:LEU:HD23	1:C:675:LEU:HB2	1.97	0.46
1:C:762:PHE:CE1	1:C:830:ARG:NH1	2.84	0.46
1:C:84:LYS:C	1:C:86:CYS:H	2.19	0.46
1:A:102:ILE:HG23	1:A:103:LEU:N	2.31	0.46
1:A:22:GLU:C	1:A:24:ASP:N	2.69	0.46
1:A:650:PRO:O	1:A:651:ARG:C	2.53	0.46
1:A:793:LEU:HB3	1:A:904:ARG:HH12	1.81	0.46
1:A:322:VAL:HG12	1:A:800:ILE:CG2	2.45	0.46
2:B:39:TYR:O	2:B:43:TYR:HD1	1.99	0.46
1:C:229:PRO:HG2	1:C:230:LEU:H	1.81	0.46
1:C:545:VAL:HG12	1:C:583:SER:HB3	1.98	0.46
1:C:634:VAL:CG2	1:C:635:GLU:N	2.79	0.46
1:C:692:LEU:C	1:C:692:LEU:HD23	2.35	0.46
1:C:708:THR:HG21	1:C:748:PHE:HE1	1.81	0.46
1:C:971:LEU:C	1:C:972:ARG:NE	2.70	0.46
1:A:224:PHE:HD2	1:A:233:ARG:H	1.56	0.45
1:A:504:PRO:CG	1:A:535:TYR:CE1	2.99	0.45
1:A:914:PRO:HA	1:A:917:VAL:HG22	1.98	0.45
1:A:93:PHE:HA	1:A:95:MET:SD	2.55	0.45
1:A:972:ARG:N	1:A:972:ARG:NE	2.64	0.45
1:A:998:ARG:O	1:A:1002:ILE:N	2.30	0.45
1:C:890:ASP:OD2	1:C:891:VAL:HG13	2.16	0.45
1:C:96:LEU:HA	1:C:99:ILE:CG2	2.44	0.45
1:C:962:SER:HB2	1:C:975:PRO:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LEU:CA	1:C:99:ILE:HG22	2.42	0.45
3:G:42:LEU:CA	3:G:46:LEU:HD22	2.46	0.45
1:A:29:LYS:CG	1:A:266:LEU:HD22	2.45	0.45
1:A:333:VAL:HG13	1:A:765:LEU:CD1	2.46	0.45
1:A:42:ASP:OD2	1:A:46:ARG:NH2	2.49	0.45
1:A:52:LEU:HG	1:A:250:ILE:HD11	1.96	0.45
1:A:801:LEU:O	1:A:802:CYS:HB2	2.15	0.45
1:A:991:ILE:O	1:A:994:TYR:N	2.49	0.45
2:B:48:GLY:HA2	2:B:51:ILE:HG12	1.98	0.45
1:C:139:PHE:C	1:C:141:TYR:H	2.19	0.45
1:C:187:LYS:HD2	1:C:188:GLY:H	1.81	0.45
1:C:287:ILE:CG2	1:C:288:ILE:N	2.78	0.45
1:C:289:THR:HA	1:C:292:ALA:HB3	1.98	0.45
1:C:591:ALA:O	1:C:592:VAL:C	2.55	0.45
1:C:866:LEU:O	1:C:867:ALA:C	2.54	0.45
1:C:910:THR:O	1:C:914:PRO:HD2	2.16	0.45
1:A:329:LEU:HD13	1:A:330:LEU:N	2.31	0.45
1:A:585:ILE:O	1:A:587:PRO:HD3	2.16	0.45
1:A:634:VAL:CG2	1:A:635:GLU:N	2.79	0.45
1:A:65:LEU:HD23	1:A:65:LEU:C	2.37	0.45
1:A:82:TRP:C	1:A:84:LYS:N	2.67	0.45
1:C:22:GLU:OE1	1:C:25:MET:HB3	2.17	0.45
1:C:304:LEU:O	1:C:306:LEU:N	2.48	0.45
1:C:634:VAL:HG23	1:C:635:GLU:H	1.81	0.45
1:C:991:ILE:O	1:C:992:PHE:C	2.53	0.45
1:A:454:GLU:HA	1:A:454:GLU:OE1	2.17	0.45
1:A:692:LEU:C	1:A:692:LEU:HD23	2.37	0.45
1:A:797:THR:C	1:A:799:THR:N	2.69	0.45
1:A:774:THR:HG21	1:A:850:ILE:HG22	1.99	0.45
1:C:609:VAL:HG11	1:C:691:LYS:HA	1.99	0.45
1:C:830:ARG:NH2	1:C:832:PRO:HA	2.19	0.45
1:C:854:GLN:HE21	1:C:922:VAL:HB	1.82	0.45
1:C:909:PHE:HA	1:C:972:ARG:HB3	1.97	0.45
1:A:196:LEU:HD12	1:A:196:LEU:O	2.17	0.45
1:A:371:THR:HG22	1:A:377:ASN:HD22	1.80	0.45
1:A:424:ALA:HB1	1:A:450:LEU:HD12	1.97	0.45
1:A:594:ASP:OD2	1:A:595:ALA:N	2.49	0.45
1:A:634:VAL:HG23	1:A:635:GLU:H	1.81	0.45
1:A:850:ILE:N	1:A:850:ILE:CD1	2.79	0.45
1:C:367:CYS:CB	1:C:707:VAL:HG22	2.31	0.45
1:C:73:LEU:HB2	1:C:155:LYS:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:767:LYS:HB3	1:C:815:LEU:CD1	2.46	0.45
1:C:842:LEU:HD23	1:C:1016:TYR:CE1	2.37	0.45
1:C:871:PHE:CD1	1:C:872:LEU:N	2.85	0.45
1:C:972:ARG:HD2	1:C:972:ARG:N	2.32	0.45
2:D:62:SER:HB3	2:D:66:PRO:HD3	1.99	0.45
3:H:51:ARG:C	3:H:51:ARG:HD2	2.37	0.45
1:A:393:ALA:O	1:A:395:THR:HG23	2.17	0.45
1:A:411:TRP:O	1:A:412:LEU:C	2.54	0.45
1:A:599:CYS:O	1:A:604:ILE:HB	2.17	0.45
1:A:824:ILE:C	1:A:826:LYS:N	2.70	0.45
1:A:856:LEU:O	1:A:859:PHE:N	2.48	0.45
1:C:164:VAL:HA	1:C:184:VAL:HA	1.99	0.45
1:C:330:LEU:O	1:C:333:VAL:CG2	2.65	0.45
1:C:394:ASP:C	1:C:396:THR:H	2.19	0.45
1:C:545:VAL:CG1	1:C:583:SER:HB3	2.47	0.45
1:C:716:PRO:O	1:C:719:LYS:N	2.50	0.45
1:C:732:SER:C	1:C:734:VAL:N	2.62	0.45
1:C:725:VAL:HG12	1:C:743:LEU:HD21	1.97	0.45
1:C:781:THR:N	1:C:782:PRO:CD	2.80	0.45
1:C:907:VAL:HG13	1:C:908:GLU:N	2.30	0.45
1:C:87:ARG:NH1	1:C:91:GLY:HA2	2.32	0.45
1:A:110:ILE:HG22	1:A:110:ILE:O	2.17	0.45
1:A:105:PHE:CD1	1:A:126:GLY:HA3	2.51	0.45
1:A:198:ILE:HA	1:A:249:GLY:HA3	1.99	0.45
1:A:303:SER:C	1:A:305:ILE:N	2.69	0.45
1:A:311:LEU:HD13	1:A:311:LEU:O	2.16	0.45
1:A:545:VAL:CG1	1:A:583:SER:HB3	2.46	0.45
1:A:920:VAL:O	1:A:923:GLN:HB2	2.16	0.45
1:A:925:ALA:HB1	1:A:992:PHE:HB2	1.99	0.45
1:C:22:GLU:C	1:C:24:ASP:N	2.70	0.45
1:C:284:PHE:CZ	1:C:329:LEU:HD11	2.52	0.45
1:C:611:GLY:HA2	1:C:686:THR:N	2.20	0.45
1:C:865:ILE:HG22	1:C:911:CYS:SG	2.57	0.45
1:C:929:ILE:CD1	1:C:999:LYS:NZ	2.79	0.45
3:H:26:VAL:C	3:H:28:ASN:N	2.69	0.45
1:A:1016:TYR:CD1	1:A:1016:TYR:O	2.70	0.45
1:A:164:VAL:HA	1:A:184:VAL:HA	1.97	0.45
1:A:275:THR:O	1:A:276:PRO:C	2.55	0.45
1:A:318:ILE:O	1:A:322:VAL:HG23	2.16	0.45
1:A:349:CYS:O	1:A:349:CYS:SG	2.74	0.45
1:A:38:LYS:HG3	1:A:38:LYS:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:O	1:A:422:ASN:N	2.49	0.45
1:C:311:LEU:O	1:C:314:VAL:HG22	2.17	0.45
1:C:435:ILE:O	1:C:451:LYS:HD2	2.17	0.45
1:C:464:ARG:HG3	1:C:464:ARG:NH1	2.28	0.45
1:C:527:LEU:C	1:C:529:ASP:N	2.71	0.45
1:C:800:ILE:C	1:C:802:CYS:H	2.19	0.45
1:C:814:SER:HB2	1:C:946:ILE:HG22	1.98	0.45
1:C:82:TRP:O	1:C:83:VAL:C	2.54	0.45
1:C:844:SER:C	1:C:846:ALA:H	2.20	0.45
1:C:88:GLN:HE21	1:C:89:LEU:N	2.14	0.45
1:C:940:GLN:O	1:C:941:GLY:C	2.55	0.45
1:C:964:CYS:C	1:C:966:GLY:H	2.19	0.45
1:C:971:LEU:O	1:C:972:ARG:CZ	2.65	0.45
1:A:223:ASP:O	1:A:224:PHE:CB	2.65	0.45
1:A:406:LYS:HD2	1:A:411:TRP:CD1	2.51	0.45
1:A:884:ASP:OD1	1:A:885:ASP:N	2.50	0.45
1:A:947:LEU:O	1:A:948:ILE:C	2.55	0.45
2:B:31:SER:OG	2:B:31:SER:O	2.28	0.45
1:A:867:ALA:CB	2:B:57:MET:HE1	2.46	0.45
1:C:289:THR:O	1:C:292:ALA:HB3	2.17	0.45
1:C:358:GLU:OE2	1:C:761:ILE:HG22	2.17	0.45
1:C:493:GLU:N	1:C:493:GLU:CD	2.66	0.45
1:C:697:GLY:HA2	1:C:700:ARG:NH1	2.32	0.45
1:C:826:LYS:HE2	1:C:826:LYS:HA	1.99	0.45
1:C:865:ILE:CG2	1:C:865:ILE:O	2.64	0.45
1:C:963:TYR:CD1	1:C:974:TYR:HB3	2.52	0.45
1:C:963:TYR:HD2	3:H:30:GLY:N	2.14	0.45
3:G:23:TYR:C	3:G:25:THR:H	2.19	0.45
1:A:128:VAL:O	1:A:132:VAL:HG23	2.17	0.45
1:A:185:GLU:HA	1:A:247:ALA:O	2.17	0.45
1:A:544:ARG:O	1:A:583:SER:HA	2.17	0.45
1:A:771:TYR:C	1:A:773:LEU:H	2.20	0.45
1:C:337:LEU:O	1:C:339:LEU:N	2.50	0.45
1:C:514:ILE:HD11	1:C:527:LEU:HD22	1.97	0.45
1:C:905:LYS:C	1:C:907:VAL:N	2.70	0.45
1:C:904:ARG:NH1	1:C:907:VAL:HG21	2.32	0.45
1:C:993:VAL:HG23	1:C:994:TYR:N	2.32	0.45
1:C:864:VAL:HG11	2:D:57:MET:CE	2.47	0.45
1:A:302:LEU:O	1:A:303:SER:HB3	2.16	0.44
1:A:762:PHE:CZ	1:A:830:ARG:NH1	2.85	0.44
1:A:860:PHE:CE2	1:A:864:VAL:HG21	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:ILE:HD11	1:A:995:ASP:CB	2.47	0.44
1:A:936:SER:O	1:A:940:GLN:HB3	2.17	0.44
1:C:1007:GLY:O	1:C:1008:GLY:C	2.55	0.44
1:C:141:TYR:O	1:C:143:GLN:N	2.49	0.44
1:C:223:ASP:O	1:C:224:PHE:CB	2.63	0.44
1:C:309:THR:HG23	1:C:312:GLU:OE1	2.16	0.44
1:C:613:HIS:NE2	1:C:685:ARG:NH1	2.65	0.44
1:C:780:ILE:N	1:C:782:PRO:HD2	2.32	0.44
1:C:95:MET:HG2	1:C:96:LEU:N	2.28	0.44
1:A:103:LEU:HD23	1:A:103:LEU:C	2.37	0.44
1:A:205:LYS:CG	1:A:219:THR:HG22	2.41	0.44
1:A:226:ASN:O	1:A:228:ASN:ND2	2.40	0.44
1:A:394:ASP:C	1:A:396:THR:H	2.20	0.44
1:A:497:LEU:HD11	1:A:550:HIS:HB2	1.99	0.44
1:A:680:GLU:OE2	1:A:682:VAL:N	2.51	0.44
1:A:929:ILE:HG12	1:A:995:ASP:CB	2.40	0.44
1:A:967:MET:C	1:A:969:VAL:N	2.71	0.44
1:A:995:ASP:CG	1:A:998:ARG:HD3	2.37	0.44
1:C:110:ILE:HG22	1:C:110:ILE:O	2.16	0.44
1:C:479:ASN:O	1:C:480:LYS:O	2.35	0.44
1:C:636:ASP:N	1:C:647:GLN:NE2	2.65	0.44
2:D:66:PRO:CG	2:D:68:TYR:CE2	3.01	0.44
3:G:23:TYR:N	3:G:23:TYR:CD1	2.84	0.44
1:A:114:THR:O	1:A:115:GLU:C	2.55	0.44
1:A:734:VAL:HG22	1:A:735:SER:N	2.31	0.44
1:A:328:GLY:HA3	1:A:804:ASP:O	2.17	0.44
1:A:82:TRP:O	1:A:83:VAL:C	2.55	0.44
1:C:209:SER:O	1:C:211:LEU:N	2.46	0.44
1:C:326:PRO:HA	1:C:804:ASP:OD2	2.17	0.44
1:C:347:LYS:O	1:C:348:ASN:HB2	2.17	0.44
1:C:454:GLU:OE1	1:C:454:GLU:HA	2.17	0.44
1:C:605:LYS:NZ	1:C:676:LYS:HE2	2.32	0.44
1:C:769:ILE:O	1:C:770:ALA:C	2.53	0.44
1:C:796:GLY:O	1:C:799:THR:HB	2.16	0.44
1:C:872:LEU:CD1	1:C:890:ASP:OD2	2.64	0.44
3:H:31:LEU:HD12	3:H:31:LEU:N	2.32	0.44
1:A:120:ASN:O	1:A:124:TYR:HB2	2.18	0.44
1:A:81:GLU:OE2	1:A:146:LYS:HE2	2.17	0.44
1:A:490:ASN:HB3	1:A:493:GLU:OE2	2.18	0.44
1:A:585:ILE:CG1	1:A:586:ASP:H	2.29	0.44
1:A:642:ASN:HB2	1:A:645:VAL:HG21	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ILE:CG2	1:A:179:VAL:HB	2.47	0.44
1:A:73:LEU:HB2	1:A:155:LYS:HB2	1.99	0.44
1:A:814:SER:O	1:A:815:LEU:C	2.55	0.44
1:A:815:LEU:HD21	1:A:927:LEU:HD12	2.00	0.44
1:A:885:ASP:OD2	1:A:897:GLN:HB2	2.16	0.44
2:B:37:LEU:C	2:B:39:TYR:N	2.70	0.44
1:A:171:MET:HA	1:C:170:LYS:O	2.17	0.44
1:C:223:ASP:CG	1:C:224:PHE:H	2.20	0.44
1:C:304:LEU:CD2	1:C:310:TRP:HZ3	2.20	0.44
1:C:814:SER:O	1:C:815:LEU:C	2.54	0.44
1:C:850:ILE:O	1:C:850:ILE:CG2	2.66	0.44
1:A:322:VAL:HG12	1:A:800:ILE:HG21	2.00	0.44
1:A:347:LYS:O	1:A:348:ASN:HB2	2.17	0.44
1:A:872:LEU:CB	1:A:876:LEU:HD22	2.37	0.44
1:A:917:VAL:HG23	1:A:918:THR:N	2.32	0.44
1:C:127:VAL:O	1:C:130:SER:HB3	2.18	0.44
1:C:299:PHE:CE1	1:C:784:LEU:HD21	2.53	0.44
1:C:594:ASP:OD2	1:C:595:ALA:N	2.50	0.44
1:C:640:ARG:O	1:C:641:LEU:C	2.56	0.44
1:C:642:ASN:HB2	1:C:645:VAL:HG21	1.99	0.44
1:C:756:GLU:HB2	1:C:825:MET:SD	2.57	0.44
1:A:219:THR:O	1:A:220:ARG:NE	2.44	0.44
1:A:280:GLU:HG2	1:A:837:LEU:CB	2.45	0.44
1:A:480:LYS:HG2	1:A:506:ARG:HG3	1.99	0.44
1:A:892:GLU:O	1:A:893:ASP:OD1	2.36	0.44
1:C:406:LYS:HD2	1:C:411:TRP:NE1	2.32	0.44
1:C:480:LYS:HG2	1:C:506:ARG:HG3	2.00	0.44
1:C:551:LEU:HB2	1:C:576:LEU:HD22	2.00	0.44
1:C:662:ASP:O	1:C:666:MET:HG3	2.17	0.44
1:C:866:LEU:HD23	1:C:906:ILE:HG22	1.99	0.44
1:A:688:PRO:HB2	1:A:689:GLN:OE1	2.18	0.44
1:A:708:THR:HG21	1:A:748:PHE:HE1	1.83	0.44
1:A:773:LEU:O	1:A:776:ASN:N	2.41	0.44
1:A:938:PHE:C	1:A:940:GLN:H	2.21	0.44
1:A:949:PHE:CE1	3:G:40:VAL:HB	2.51	0.44
1:A:115:GLU:O	1:A:116:GLU:O	2.35	0.44
1:A:117:GLU:O	1:A:119:GLN:N	2.50	0.44
1:A:127:VAL:O	1:A:130:SER:HB3	2.18	0.44
1:A:778:PRO:HG2	1:A:854:GLN:HB3	1.98	0.44
1:A:129:LEU:HD21	1:A:801:LEU:HD11	1.97	0.44
1:A:803:ILE:O	1:A:808:ASP:N	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:LYS:HB2	1:A:815:LEU:HD12	2.00	0.44
1:A:897:GLN:HG2	1:A:901:TYR:CE1	2.53	0.44
1:A:94:SER:HA	1:A:97:LEU:HB2	1.99	0.44
1:C:117:GLU:O	1:C:119:GLN:N	2.51	0.44
1:C:92:GLY:CA	1:C:285:ILE:HD13	2.42	0.44
1:C:329:LEU:C	1:C:329:LEU:HD13	2.38	0.44
1:C:770:ALA:CB	1:C:842:LEU:HD21	2.44	0.44
1:C:897:GLN:HA	1:C:900:THR:HB	1.99	0.44
1:A:225:THR:HG22	1:A:226:ASN:H	1.83	0.44
1:A:45:HIS:C	1:A:45:HIS:ND1	2.71	0.44
1:A:46:ARG:HG3	1:A:46:ARG:HH11	1.83	0.44
1:A:527:LEU:C	1:A:529:ASP:N	2.71	0.44
1:A:543:GLU:HB3	1:A:585:ILE:HB	1.99	0.44
1:A:900:THR:HA	1:A:903:GLN:NE2	2.33	0.44
1:A:873:PRO:CG	2:B:58:LEU:HD21	2.48	0.44
1:C:115:GLU:O	1:C:116:GLU:O	2.36	0.44
1:C:352:LYS:C	1:C:353:ASN:HD22	2.20	0.44
1:C:631:ASN:HB3	1:C:634:VAL:HG22	1.98	0.44
1:C:976:LEU:N	1:C:980:TRP:CD1	2.85	0.44
1:A:123:LEU:HD13	1:A:123:LEU:O	2.18	0.43
1:A:223:ASP:CG	1:A:224:PHE:H	2.20	0.43
1:A:29:LYS:HD3	1:A:29:LYS:N	2.22	0.43
1:A:854:GLN:HE21	1:A:922:VAL:CG2	2.29	0.43
1:A:948:ILE:HD12	1:A:948:ILE:N	2.33	0.43
1:A:973:MET:CE	1:A:974:TYR:H	2.22	0.43
1:C:187:LYS:CD	1:C:188:GLY:H	2.31	0.43
1:C:187:LYS:CG	1:C:188:GLY:N	2.80	0.43
1:C:384:MET:SD	1:C:411:TRP:HZ3	2.41	0.43
1:C:426:PHE:HA	1:C:439:ALA:O	2.18	0.43
1:C:591:ALA:C	1:C:593:PRO:CD	2.86	0.43
1:A:36:ASP:HB2	1:A:47:LYS:HZ2	1.83	0.43
1:A:516:ILE:HD13	1:A:521:GLN:CG	2.48	0.43
1:A:498:LEU:CD2	1:A:551:LEU:HB3	2.48	0.43
1:A:645:VAL:C	1:A:647:GLN:H	2.22	0.43
1:A:889:ASN:HD21	1:A:895:TYR:H	1.58	0.43
1:A:96:LEU:CA	1:A:99:ILE:HG22	2.43	0.43
1:C:456:CYS:C	1:C:457:CYS:SG	2.96	0.43
1:C:544:ARG:O	1:C:583:SER:HA	2.18	0.43
1:C:892:GLU:O	2:D:65:LYS:NZ	2.51	0.43
1:A:497:LEU:HD12	1:A:498:LEU:N	2.32	0.43
1:A:944:ASN:OD1	1:A:947:LEU:HB3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ALA:O	1:C:114:THR:N	2.52	0.43
1:C:226:ASN:C	1:C:228:ASN:N	2.71	0.43
1:C:374:LEU:HD22	1:C:592:VAL:HG13	1.99	0.43
1:C:734:VAL:O	1:C:735:SER:C	2.57	0.43
1:C:825:MET:HE2	1:C:825:MET:HA	1.99	0.43
1:C:896:GLY:O	1:C:899:TRP:CB	2.67	0.43
1:A:949:PHE:HD1	3:G:40:VAL:O	2.02	0.43
1:A:209:SER:O	1:A:213:GLY:N	2.46	0.43
1:A:209:SER:C	1:A:211:LEU:H	2.22	0.43
1:A:708:THR:HG22	1:A:725:VAL:HB	2.00	0.43
1:A:729:ILE:HG13	1:A:730:ALA:N	2.33	0.43
1:A:802:CYS:SG	1:A:961:LEU:CD2	3.06	0.43
1:A:759:ARG:HD2	1:A:825:MET:CE	2.48	0.43
1:A:927:LEU:O	1:A:928:VAL:HG23	2.19	0.43
1:A:944:ASN:C	1:A:948:ILE:HD13	2.39	0.43
1:A:985:PHE:HB3	1:A:986:PRO:HD3	1.99	0.43
1:C:105:PHE:CD1	1:C:126:GLY:HA3	2.51	0.43
1:C:225:THR:HG22	1:C:226:ASN:H	1.83	0.43
1:C:355:GLU:O	1:C:359:THR:HG23	2.18	0.43
1:C:483:LEU:CB	1:C:500:MET:HB3	2.45	0.43
1:C:635:GLU:HA	1:C:638:ALA:HB3	2.01	0.43
1:C:726:ALA:O	1:C:727:MET:HG2	2.18	0.43
1:C:963:TYR:HD2	3:H:30:GLY:CA	2.32	0.43
1:A:293:VAL:C	1:A:295:LEU:N	2.71	0.43
1:A:381:VAL:HG13	1:A:582:ILE:CG2	2.48	0.43
1:A:333:VAL:HG13	1:A:765:LEU:HD11	1.99	0.43
1:C:161:GLN:HA	1:C:161:GLN:OE1	2.19	0.43
1:C:225:THR:HG22	1:C:226:ASN:N	2.34	0.43
1:C:490:ASN:HB3	1:C:493:GLU:OE2	2.19	0.43
1:C:506:ARG:O	1:C:507:ILE:C	2.56	0.43
1:C:50:THR:HB	1:C:56:LEU:HD13	1.99	0.43
1:C:64:ILE:CG2	1:C:179:VAL:HB	2.48	0.43
1:C:684:ALA:O	1:C:685:ARG:C	2.57	0.43
1:C:729:ILE:HG13	1:C:730:ALA:N	2.33	0.43
1:C:322:VAL:CG1	1:C:801:LEU:HD21	2.49	0.43
1:C:982:PHE:O	1:C:985:PHE:N	2.50	0.43
1:A:293:VAL:O	1:A:297:VAL:HG22	2.18	0.43
1:A:352:LYS:C	1:A:353:ASN:HD22	2.21	0.43
1:A:631:ASN:HB3	1:A:634:VAL:HG22	1.98	0.43
1:A:646:SER:O	1:A:650:PRO:HG2	2.19	0.43
1:A:680:GLU:HG2	1:A:682:VAL:N	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:SER:O	1:A:690:GLN:N	2.52	0.43
1:A:765:LEU:HD23	1:A:765:LEU:HA	1.68	0.43
1:A:871:PHE:CD1	1:A:872:LEU:N	2.87	0.43
1:A:927:LEU:O	1:A:928:VAL:CG2	2.67	0.43
1:A:967:MET:C	1:A:969:VAL:H	2.20	0.43
1:A:974:TYR:CE1	3:G:27:ARG:HD2	2.53	0.43
1:C:504:PRO:CG	1:C:535:TYR:CE1	3.02	0.43
1:C:867:ALA:N	1:C:871:PHE:HB2	2.31	0.43
3:G:48:LYS:HZ2	3:G:48:LYS:CB	2.32	0.43
1:A:1001:ILE:HG22	1:A:1011:GLU:HG2	2.01	0.43
1:A:101:ALA:HA	1:A:104:CYS:SG	2.57	0.43
1:A:901:TYR:O	1:A:905:LYS:HG2	2.18	0.43
1:A:950:GLY:O	1:A:954:GLU:N	2.52	0.43
1:C:169:GLU:H	1:C:169:GLU:CD	2.21	0.43
1:A:169:GLU:HG2	1:C:170:LYS:HE3	2.01	0.43
1:C:209:SER:C	1:C:211:LEU:H	2.22	0.43
1:C:523:LEU:HD21	1:C:528:LYS:CE	2.49	0.43
1:C:585:ILE:CG1	1:C:586:ASP:H	2.28	0.43
1:C:65:LEU:HD23	1:C:65:LEU:O	2.19	0.43
1:C:680:GLU:OE2	1:C:682:VAL:N	2.51	0.43
1:C:732:SER:HB2	1:C:734:VAL:HG13	2.00	0.43
1:C:835:ASP:OD1	1:C:835:ASP:N	2.49	0.43
1:C:866:LEU:C	1:C:871:PHE:HB2	2.39	0.43
1:C:886:ARG:H	1:C:896:GLY:HA3	1.83	0.43
1:C:96:LEU:O	1:C:99:ILE:HG22	2.19	0.43
2:D:45:CYS:O	2:D:49:ILE:HG12	2.19	0.43
1:A:797:THR:C	1:A:799:THR:H	2.21	0.43
1:C:936:SER:CB	1:C:1003:ARG:HH22	2.31	0.43
1:C:775:SER:O	1:C:779:GLU:OE1	2.36	0.43
3:G:39:ILE:O	3:G:39:ILE:CG2	2.67	0.43
3:H:25:THR:O	3:H:25:THR:HG22	2.18	0.43
1:A:354:LEU:H	1:A:354:LEU:CD1	2.30	0.43
1:A:605:LYS:NZ	1:A:676:LYS:HE2	2.34	0.43
1:A:604:ILE:HD11	1:A:755:VAL:HG21	2.00	0.43
1:A:815:LEU:CD2	1:A:927:LEU:HD12	2.49	0.43
1:C:109:GLY:O	1:C:111:GLN:N	2.46	0.43
1:C:120:ASN:O	1:C:124:TYR:HB2	2.18	0.43
1:C:128:VAL:O	1:C:132:VAL:HG23	2.19	0.43
1:C:185:GLU:HA	1:C:247:ALA:O	2.18	0.43
1:C:52:LEU:HG	1:C:250:ILE:HD11	2.00	0.43
1:C:406:LYS:HD2	1:C:411:TRP:CD1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:872:LEU:HB2	1:C:876:LEU:HB2	1.99	0.43
1:C:910:THR:O	1:C:914:PRO:CD	2.67	0.43
2:D:62:SER:CB	2:D:66:PRO:HD3	2.49	0.43
1:A:56:LEU:H	1:A:166:ARG:HA	1.84	0.43
1:A:303:SER:HB2	1:A:787:ILE:HG21	2.01	0.43
1:A:635:GLU:HA	1:A:638:ALA:HB3	2.00	0.43
1:A:928:VAL:HA	1:A:931:LYS:HB2	2.00	0.43
1:C:354:LEU:CD1	1:C:354:LEU:H	2.29	0.43
1:C:467:TYR:HD1	1:C:489:PRO:HD3	1.83	0.43
1:C:589:ARG:O	1:C:593:PRO:HD3	2.18	0.43
1:C:607:ILE:HA	1:C:681:ILE:CG2	2.49	0.43
1:C:828:GLN:H	1:C:828:GLN:NE2	2.14	0.43
1:C:944:ASN:O	1:C:947:LEU:N	2.52	0.43
1:C:990:LEU:O	1:C:991:ILE:C	2.57	0.43
1:A:111:GLN:HB2	1:A:115:GLU:CG	2.49	0.42
1:A:170:LYS:HG3	1:C:169:GLU:HA	2.02	0.42
1:A:50:THR:HB	1:A:56:LEU:HD13	2.01	0.42
1:A:587:PRO:HA	1:A:588:PRO:HD3	1.73	0.42
1:A:636:ASP:N	1:A:647:GLN:NE2	2.67	0.42
1:A:910:THR:HG22	1:A:911:CYS:N	2.34	0.42
1:A:959:ALA:HB2	1:A:981:TRP:CH2	2.53	0.42
1:A:96:LEU:HA	1:A:99:ILE:CG2	2.45	0.42
1:C:1008:GLY:O	1:C:1012:LYS:HB3	2.18	0.42
1:C:111:GLN:HB2	1:C:115:GLU:CG	2.49	0.42
1:C:56:LEU:H	1:C:166:ARG:HA	1.83	0.42
1:C:224:PHE:HD2	1:C:233:ARG:H	1.61	0.42
1:C:294:PHE:O	1:C:298:SER:CB	2.66	0.42
1:C:520:GLU:HG2	1:C:520:GLU:O	2.19	0.42
1:C:688:PRO:HB2	1:C:689:GLN:OE1	2.18	0.42
1:C:765:LEU:HD23	1:C:765:LEU:HA	1.66	0.42
1:C:980:TRP:C	1:C:983:CYS:SG	2.97	0.42
1:A:1003:ARG:O	1:A:1004:ARG:C	2.56	0.42
1:A:435:ILE:O	1:A:451:LYS:HD2	2.19	0.42
1:A:607:ILE:HA	1:A:681:ILE:CG2	2.49	0.42
1:A:769:ILE:CA	1:A:772:THR:HG22	2.48	0.42
1:A:802:CYS:C	1:A:803:ILE:HD13	2.40	0.42
1:C:424:ALA:HB1	1:C:450:LEU:HD12	2.00	0.42
1:C:543:GLU:HB3	1:C:585:ILE:HB	2.00	0.42
2:D:67:THR:C	2:D:68:TYR:CD2	2.92	0.42
2:D:68:TYR:N	2:D:68:TYR:CD2	2.87	0.42
1:A:280:GLU:HG3	1:A:837:LEU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:C	1:A:341:ALA:N	2.72	0.42
1:A:426:PHE:HA	1:A:439:ALA:O	2.19	0.42
1:A:479:ASN:O	1:A:480:LYS:O	2.37	0.42
1:A:640:ARG:O	1:A:641:LEU:C	2.58	0.42
1:A:682:VAL:HG13	1:A:682:VAL:O	2.20	0.42
1:A:734:VAL:O	1:A:735:SER:C	2.58	0.42
1:A:855:ALA:O	1:A:859:PHE:HB2	2.19	0.42
1:A:904:ARG:O	1:A:906:ILE:N	2.52	0.42
1:A:995:ASP:HA	1:A:998:ARG:CG	2.45	0.42
1:C:111:GLN:NE2	1:C:118:PRO:HB2	2.34	0.42
1:C:205:LYS:HA	1:C:219:THR:HA	2.00	0.42
1:C:277:ILE:O	1:C:280:GLU:N	2.44	0.42
1:C:682:VAL:HG13	1:C:682:VAL:O	2.20	0.42
1:C:808:ASP:O	1:C:811:PRO:HD2	2.19	0.42
1:C:828:GLN:NE2	1:C:828:GLN:N	2.64	0.42
1:C:794:PRO:HB2	1:C:915:PHE:HE1	1.84	0.42
1:C:954:GLU:O	1:C:957:LEU:N	2.52	0.42
1:C:968:GLY:HA3	1:C:973:MET:HE3	2.01	0.42
1:C:909:PHE:HA	1:C:972:ARG:CB	2.49	0.42
1:C:94:SER:HA	1:C:97:LEU:HB2	2.01	0.42
1:C:995:ASP:O	1:C:998:ARG:HG2	2.20	0.42
1:A:112:ALA:O	1:A:114:THR:N	2.52	0.42
1:A:506:ARG:O	1:A:507:ILE:C	2.57	0.42
1:C:599:CYS:O	1:C:604:ILE:HB	2.19	0.42
1:C:621:ALA:HB1	1:C:627:ILE:HG13	2.02	0.42
1:C:604:ILE:HD11	1:C:755:VAL:HG21	2.01	0.42
1:C:777:ILE:HD13	1:C:780:ILE:HD12	1.98	0.42
1:C:865:ILE:CG2	1:C:911:CYS:SG	3.07	0.42
1:C:961:LEU:HD21	1:C:971:LEU:CD1	2.49	0.42
2:D:40:VAL:HG23	2:D:41:ILE:H	1.85	0.42
1:A:609:VAL:HG11	1:A:691:LYS:HA	2.02	0.42
1:A:793:LEU:O	1:A:907:VAL:HG21	2.19	0.42
1:C:291:VAL:O	1:C:293:VAL:N	2.52	0.42
1:C:651:ARG:O	1:C:653:ALA:N	2.53	0.42
1:A:169:GLU:H	1:A:169:GLU:CD	2.23	0.42
1:A:226:ASN:HB3	1:A:227:GLU:H	1.70	0.42
1:A:276:PRO:HD2	1:A:359:THR:HG22	2.02	0.42
1:A:606:VAL:HG21	1:A:626:ILE:HD13	2.01	0.42
1:A:667:THR:O	1:A:668:SER:C	2.58	0.42
1:C:41:LEU:N	1:C:41:LEU:HD12	2.09	0.42
1:C:516:ILE:HD13	1:C:521:GLN:CG	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:645:VAL:C	1:C:647:GLN:H	2.21	0.42
1:C:689:GLN:CD	1:C:689:GLN:H	2.22	0.42
1:C:826:LYS:HE2	1:C:826:LYS:CA	2.50	0.42
1:C:872:LEU:CB	1:C:875:HIS:C	2.84	0.42
1:C:908:GLU:C	1:C:910:THR:H	2.21	0.42
1:C:913:THR:HB	1:C:914:PRO:HD3	2.01	0.42
1:C:972:ARG:CD	1:C:972:ARG:N	2.82	0.42
1:A:36:ASP:HB3	1:A:39:LEU:HD21	2.01	0.42
1:A:393:ALA:O	1:A:395:THR:N	2.53	0.42
1:A:416:ARG:O	1:A:417:ILE:C	2.57	0.42
1:A:551:LEU:HB2	1:A:576:LEU:HD22	2.01	0.42
1:A:385:TRP:CB	1:A:581:LEU:HB2	2.48	0.42
1:A:370:LYS:HD2	1:A:620:ILE:HG21	2.01	0.42
1:A:671:LEU:O	1:A:671:LEU:HD23	2.20	0.42
1:A:911:CYS:N	1:A:914:PRO:HD2	2.35	0.42
2:B:40:VAL:HG23	2:B:41:ILE:N	2.34	0.42
1:C:276:PRO:HD2	1:C:359:THR:HG22	2.01	0.42
1:C:385:TRP:CB	1:C:581:LEU:HB2	2.49	0.42
1:C:589:ARG:HB2	1:C:592:VAL:CG2	2.47	0.42
1:C:605:LYS:NZ	1:C:676:LYS:CE	2.83	0.42
1:C:687:SER:O	1:C:690:GLN:N	2.53	0.42
1:C:916:PHE:CD2	1:C:917:VAL:N	2.88	0.42
1:C:984:ALA:C	1:C:986:PRO:CD	2.88	0.42
1:A:103:LEU:HD13	1:A:317:LEU:CD1	2.39	0.42
1:A:187:LYS:CG	1:A:188:GLY:N	2.82	0.42
1:A:284:PHE:HB2	1:A:838:VAL:CG1	2.47	0.42
1:A:293:VAL:O	1:A:295:LEU:N	2.53	0.42
1:A:771:TYR:C	1:A:773:LEU:N	2.73	0.42
1:A:906:ILE:C	1:A:910:THR:HB	2.40	0.42
1:A:937:VAL:CG1	1:A:942:MET:HG2	2.50	0.42
1:A:963:TYR:O	1:A:965:PRO:CD	2.68	0.42
1:A:988:SER:HA	1:A:991:ILE:HD12	2.01	0.42
2:B:48:GLY:O	2:B:51:ILE:HB	2.19	0.42
1:A:860:PHE:CE1	2:B:53:THR:O	2.72	0.42
1:C:651:ARG:NH1	1:C:677:TYR:HE2	2.18	0.42
1:C:150:ILE:CD1	1:C:738:ALA:HB2	2.49	0.42
1:C:850:ILE:O	1:C:850:ILE:HG22	2.20	0.42
1:C:794:PRO:HG2	1:C:859:PHE:HE1	1.85	0.42
1:C:936:SER:C	1:C:938:PHE:N	2.72	0.42
1:C:977:LYS:N	1:C:978:PRO:CD	2.83	0.42
1:A:194:ALA:HA	1:A:238:PHE:HD1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:PRO:HG3	1:A:704:ILE:HD12	2.01	0.42
1:A:350:LEU:CG	1:A:351:VAL:N	2.81	0.42
1:A:456:CYS:C	1:A:457:CYS:SG	2.98	0.42
1:A:786:PHE:CD2	1:A:793:LEU:HA	2.55	0.42
1:A:284:PHE:HB2	1:A:838:VAL:CB	2.49	0.42
2:B:31:SER:C	2:B:33:PHE:N	2.72	0.42
1:C:498:LEU:CD2	1:C:551:LEU:HB3	2.50	0.42
1:C:649:ASN:HB2	1:C:650:PRO:CD	2.43	0.42
1:C:891:VAL:O	1:C:891:VAL:HG23	2.20	0.42
1:C:856:LEU:CD1	2:D:46:LEU:HD13	2.48	0.42
3:G:48:LYS:HZ2	3:G:48:LYS:HB3	1.83	0.42
1:A:102:ILE:CG2	1:A:103:LEU:N	2.83	0.42
1:A:170:LYS:O	1:A:170:LYS:HG3	2.19	0.42
1:A:483:LEU:CB	1:A:500:MET:HB3	2.46	0.42
1:A:919:ILE:CG2	1:A:920:VAL:N	2.83	0.42
1:A:995:ASP:CA	1:A:998:ARG:HG2	2.47	0.42
1:C:102:ILE:CG2	1:C:103:LEU:N	2.83	0.42
1:C:239:SER:OG	1:C:260:MET:HG3	2.20	0.42
1:C:38:LYS:HG3	1:C:38:LYS:O	2.20	0.42
1:C:343:ARG:NH1	1:C:757:GLU:OE1	2.52	0.42
1:C:770:ALA:O	1:C:771:TYR:C	2.58	0.42
1:C:771:TYR:CD2	1:C:771:TYR:C	2.93	0.42
1:C:850:ILE:O	1:C:854:GLN:HG3	2.20	0.42
1:C:932:THR:HG1	1:C:935:ASN:H	1.59	0.42
2:D:34:LYS:C	2:D:36:LEU:N	2.70	0.42
1:A:317:LEU:O	1:A:321:ILE:HG12	2.20	0.41
1:A:444:ALA:O	1:A:445:SER:C	2.58	0.41
1:A:467:TYR:HD1	1:A:489:PRO:HD3	1.84	0.41
1:A:32:VAL:HG13	1:A:689:GLN:NE2	2.35	0.41
1:A:732:SER:CB	1:A:734:VAL:HG13	2.50	0.41
1:A:802:CYS:O	1:A:803:ILE:HD13	2.19	0.41
1:C:535:TYR:CE1	1:C:545:VAL:HG21	2.55	0.41
1:C:667:THR:O	1:C:668:SER:C	2.57	0.41
1:C:881:VAL:CG1	1:C:882:ASN:N	2.81	0.41
1:C:885:ASP:OD1	1:C:897:GLN:CB	2.61	0.41
1:A:198:ILE:HA	1:A:249:GLY:HA2	2.02	0.41
1:A:732:SER:HB2	1:A:734:VAL:HG13	2.01	0.41
1:A:896:GLY:HA2	1:A:900:THR:OG1	2.20	0.41
1:A:896:GLY:O	1:A:900:THR:HB	2.20	0.41
1:A:995:ASP:C	1:A:998:ARG:HG2	2.40	0.41
1:C:194:ALA:HA	1:C:238:PHE:HD1	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:GLU:HG3	1:C:837:LEU:CB	2.47	0.41
1:C:330:LEU:O	1:C:333:VAL:HG23	2.20	0.41
1:C:668:SER:OG	1:C:669:GLU:N	2.51	0.41
1:C:872:LEU:HD22	1:C:891:VAL:HG11	2.00	0.41
1:C:902:GLU:C	1:C:904:ARG:N	2.71	0.41
1:C:976:LEU:C	1:C:978:PRO:HD2	2.40	0.41
1:A:225:THR:HG22	1:A:226:ASN:N	2.36	0.41
1:A:235:ILE:HD13	1:A:235:ILE:HA	1.94	0.41
1:A:785:ILE:C	1:A:787:ILE:N	2.74	0.41
1:A:771:TYR:HE2	1:A:808:ASP:HB3	1.82	0.41
1:A:872:LEU:HD22	1:A:890:ASP:OD2	2.20	0.41
1:A:92:GLY:HA2	1:A:285:ILE:CD1	2.50	0.41
1:A:976:LEU:N	1:A:980:TRP:HD1	2.15	0.41
7:B:1:PC1:H143	7:B:1:PC1:H111	1.82	0.41
1:C:725:VAL:HG12	1:C:743:LEU:HD23	2.01	0.41
1:C:777:ILE:C	1:C:779:GLU:N	2.71	0.41
1:C:907:VAL:CA	1:C:911:CYS:HB2	2.29	0.41
1:A:134:ILE:HG22	1:A:135:ILE:HD13	2.02	0.41
1:A:227:GLU:HB3	1:A:231:GLU:HB2	2.03	0.41
1:A:239:SER:OG	1:A:260:MET:HG3	2.21	0.41
1:A:355:GLU:O	1:A:359:THR:HG23	2.20	0.41
1:A:384:MET:SD	1:A:411:TRP:HZ3	2.43	0.41
1:A:668:SER:OG	1:A:669:GLU:N	2.53	0.41
1:A:680:GLU:CG	1:A:681:ILE:N	2.83	0.41
1:A:777:ILE:C	1:A:779:GLU:N	2.74	0.41
1:A:867:ALA:C	1:A:869:ASN:N	2.74	0.41
1:A:163:LEU:CD2	1:C:169:GLU:HG2	2.50	0.41
1:C:183:LEU:CD2	1:C:183:LEU:H	2.33	0.41
1:C:393:ALA:O	1:C:395:THR:HG23	2.20	0.41
1:C:444:ALA:O	1:C:445:SER:C	2.59	0.41
1:C:45:HIS:C	1:C:45:HIS:ND1	2.73	0.41
1:C:587:PRO:HA	1:C:588:PRO:HD3	1.75	0.41
1:A:165:ILE:HD13	1:A:170:LYS:HA	2.03	0.41
1:A:187:LYS:CD	1:A:188:GLY:H	2.33	0.41
1:A:354:LEU:O	1:A:355:GLU:C	2.59	0.41
1:A:410:THR:HA	1:A:515:LEU:HD13	2.01	0.41
1:A:613:HIS:NE2	1:A:685:ARG:NH1	2.67	0.41
1:A:621:ALA:HB1	1:A:627:ILE:HG13	2.02	0.41
1:A:692:LEU:O	1:A:693:ILE:C	2.56	0.41
1:A:210:SER:CB	1:A:712:VAL:HG11	2.51	0.41
1:A:804:ASP:N	1:A:804:ASP:OD1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:LEU:HD12	1:A:947:LEU:C	2.41	0.41
1:A:989:LEU:O	1:A:990:LEU:C	2.59	0.41
2:B:36:LEU:O	2:B:39:TYR:CB	2.69	0.41
1:C:108:TYR:HE1	1:C:119:GLN:HA	1.83	0.41
1:C:305:ILE:O	1:C:306:LEU:C	2.58	0.41
1:C:32:VAL:HG13	1:C:689:GLN:NE2	2.35	0.41
1:C:606:VAL:HG21	1:C:626:ILE:HD13	2.02	0.41
1:C:646:SER:O	1:C:650:PRO:HG2	2.19	0.41
1:C:892:GLU:HB2	2:D:65:LYS:HZ2	1.86	0.41
3:H:37:ALA:CA	3:H:40:VAL:HG22	2.49	0.41
1:A:161:GLN:HA	1:A:161:GLN:OE1	2.19	0.41
1:A:103:LEU:CD1	1:A:317:LEU:HD12	2.41	0.41
1:A:324:ASN:O	1:A:326:PRO:HD3	2.20	0.41
1:A:591:ALA:C	1:A:593:PRO:CD	2.88	0.41
1:A:777:ILE:O	1:A:779:GLU:N	2.54	0.41
1:A:280:GLU:CG	1:A:837:LEU:HB2	2.48	0.41
1:A:885:ASP:OD1	1:A:897:GLN:CB	2.67	0.41
1:C:134:ILE:HG22	1:C:135:ILE:HD13	2.03	0.41
1:C:172:SER:O	1:C:173:ILE:HG23	2.20	0.41
1:C:29:LYS:C	1:C:31:GLU:H	2.21	0.41
1:C:651:ARG:NH1	1:C:677:TYR:CD2	2.89	0.41
1:C:680:GLU:OE2	1:C:681:ILE:CA	2.69	0.41
1:C:708:THR:HG22	1:C:725:VAL:HB	2.02	0.41
1:C:786:PHE:O	1:C:786:PHE:CD1	2.73	0.41
1:C:824:ILE:O	1:C:826:LYS:N	2.49	0.41
1:C:938:PHE:C	1:C:940:GLN:N	2.74	0.41
1:C:992:PHE:CD1	1:C:992:PHE:C	2.94	0.41
1:C:992:PHE:CD1	1:C:993:VAL:N	2.89	0.41
1:A:460:VAL:O	1:A:464:ARG:N	2.51	0.41
1:A:647:GLN:C	1:A:650:PRO:HD2	2.41	0.41
1:A:757:GLU:O	1:A:761:ILE:HG12	2.21	0.41
1:A:803:ILE:HG22	1:A:808:ASP:OD2	2.20	0.41
1:A:871:PHE:C	1:A:873:PRO:HD3	2.40	0.41
1:A:865:ILE:HG21	1:A:910:THR:HG22	2.02	0.41
1:A:959:ALA:O	1:A:963:TYR:HD1	2.04	0.41
1:C:203:GLY:O	1:C:245:GLY:HA3	2.21	0.41
1:C:410:THR:HA	1:C:515:LEU:HD13	2.01	0.41
1:C:566:THR:C	1:C:568:ASP:H	2.24	0.41
1:C:715:SER:CB	1:C:716:PRO:CD	2.93	0.41
1:C:788:ILE:HG13	1:C:788:ILE:H	1.62	0.41
3:H:51:ARG:OXT	3:H:51:ARG:HD2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:CZ	1:A:225:THR:O	2.74	0.41
1:A:282:GLU:O	1:A:284:PHE:N	2.54	0.41
1:A:295:LEU:O	1:A:296:GLY:C	2.59	0.41
1:A:591:ALA:O	1:A:592:VAL:C	2.59	0.41
1:A:651:ARG:NH1	1:A:677:TYR:HE2	2.18	0.41
1:A:674:ILE:N	1:A:674:ILE:CD1	2.84	0.41
1:A:769:ILE:C	1:A:772:THR:HG22	2.40	0.41
1:A:842:LEU:HB2	1:A:1016:TYR:HE1	1.86	0.41
1:A:873:PRO:HG2	2:B:58:LEU:HD21	2.02	0.41
1:A:900:THR:O	1:A:901:TYR:C	2.59	0.41
1:A:923:GLN:NE2	1:A:923:GLN:HA	2.36	0.41
1:A:966:GLY:C	1:A:968:GLY:N	2.73	0.41
1:A:96:LEU:O	1:A:99:ILE:HG22	2.21	0.41
1:C:123:LEU:O	1:C:123:LEU:HD13	2.21	0.41
1:C:304:LEU:O	1:C:304:LEU:HD13	2.20	0.41
1:C:524:ASP:O	1:C:528:LYS:HB2	2.21	0.41
1:C:805:LEU:HD12	1:C:809:MET:HE1	2.02	0.41
1:C:805:LEU:HD12	1:C:809:MET:HE2	2.01	0.41
1:C:858:GLY:HA3	1:C:915:PHE:CE2	2.56	0.41
1:C:910:THR:CG2	1:C:911:CYS:H	2.22	0.41
1:A:108:TYR:HE1	1:A:119:GLN:HA	1.84	0.41
1:A:124:TYR:O	1:A:128:VAL:HG23	2.20	0.41
1:A:270:LEU:HD12	1:A:271:GLU:H	1.86	0.41
1:A:314:VAL:HG23	1:A:315:ILE:N	2.35	0.41
1:A:605:LYS:HZ2	1:A:676:LYS:HE2	1.86	0.41
1:A:651:ARG:NH1	1:A:677:TYR:CD2	2.89	0.41
1:A:662:ASP:O	1:A:666:MET:HG3	2.20	0.41
2:B:37:LEU:HD12	2:B:37:LEU:O	2.21	0.41
2:B:64:PHE:CD1	2:B:65:LYS:O	2.74	0.41
1:C:341:ALA:C	1:C:343:ARG:N	2.73	0.41
1:C:695:VAL:O	1:C:699:GLN:HG3	2.20	0.41
1:C:768:SER:O	1:C:772:THR:HG22	2.21	0.41
1:C:780:ILE:C	1:C:782:PRO:HD2	2.41	0.41
1:C:963:TYR:HD1	1:C:974:TYR:CG	2.39	0.41
1:C:980:TRP:O	1:C:983:CYS:SG	2.78	0.41
1:C:987:TYR:O	1:C:990:LEU:HB3	2.20	0.41
2:D:63:GLU:HG2	2:D:64:PHE:N	2.36	0.41
1:A:183:LEU:CD2	1:A:183:LEU:H	2.34	0.41
1:A:382:ALA:C	1:A:383:HIS:ND1	2.75	0.41
1:A:725:VAL:HG12	1:A:743:LEU:HD23	2.03	0.41
1:A:732:SER:OG	1:A:734:VAL:HG13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:PHE:HD1	1:A:872:LEU:H	1.69	0.41
1:C:288:ILE:C	1:C:290:GLY:N	2.74	0.41
1:C:318:ILE:HD12	1:C:318:ILE:O	2.21	0.41
1:C:337:LEU:O	1:C:340:THR:N	2.54	0.41
1:C:46:ARG:HH11	1:C:46:ARG:HG3	1.85	0.41
1:C:692:LEU:O	1:C:693:ILE:C	2.55	0.41
1:C:913:THR:CB	1:C:914:PRO:HD3	2.50	0.41
1:C:915:PHE:HA	1:C:918:THR:OG1	2.21	0.41
1:C:972:ARG:HB3	1:C:973:MET:H	1.73	0.41
2:D:37:LEU:O	2:D:37:LEU:CD1	2.68	0.41
1:A:297:VAL:HG23	1:A:298:SER:N	2.35	0.41
1:A:305:ILE:O	1:A:306:LEU:C	2.58	0.41
1:A:523:LEU:HD21	1:A:528:LYS:CE	2.50	0.41
1:A:625:GLY:C	1:A:627:ILE:N	2.75	0.41
1:A:785:ILE:C	1:A:787:ILE:H	2.24	0.41
1:A:807:THR:HG22	1:A:808:ASP:N	2.36	0.41
1:A:831:ASN:ND2	1:A:834:THR:N	2.52	0.41
1:A:900:THR:CG2	1:A:903:GLN:HE21	2.34	0.41
1:A:910:THR:O	1:A:911:CYS:C	2.58	0.41
1:A:982:PHE:O	1:A:985:PHE:CB	2.68	0.41
1:C:326:PRO:O	1:C:328:GLY:N	2.54	0.41
1:C:674:ILE:CD1	1:C:674:ILE:N	2.84	0.41
1:C:849:GLN:HB2	1:C:849:GLN:HE21	1.57	0.41
2:D:33:PHE:O	2:D:36:LEU:N	2.49	0.41
1:A:111:GLN:NE2	1:A:118:PRO:HB2	2.35	0.40
1:A:157:MET:O	1:A:191:ARG:HD2	2.21	0.40
1:A:224:PHE:CZ	1:A:226:ASN:CG	2.94	0.40
1:A:312:GLU:O	1:A:313:ALA:C	2.59	0.40
1:A:376:GLN:H	1:A:376:GLN:HG2	1.63	0.40
1:A:605:LYS:NZ	1:A:676:LYS:CE	2.84	0.40
1:A:684:ALA:O	1:A:685:ARG:C	2.59	0.40
1:A:763:ASP:C	1:A:765:LEU:N	2.71	0.40
1:A:773:LEU:O	1:A:774:THR:C	2.59	0.40
1:A:915:PHE:O	1:A:916:PHE:C	2.60	0.40
1:C:289:THR:HA	1:C:292:ALA:CB	2.51	0.40
1:C:732:SER:CB	1:C:734:VAL:HG13	2.50	0.40
1:C:150:ILE:HD11	1:C:738:ALA:HB2	2.03	0.40
1:C:815:LEU:HD23	1:C:927:LEU:HD12	2.03	0.40
1:C:785:ILE:HB	1:C:859:PHE:HZ	1.86	0.40
1:C:982:PHE:O	1:C:985:PHE:CB	2.69	0.40
2:D:63:GLU:HG2	2:D:64:PHE:CG	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:GLN:O	1:A:438:ARG:NH2	2.54	0.40
1:A:895:TYR:HD2	1:A:899:TRP:HB3	1.80	0.40
2:B:51:ILE:O	2:B:54:ILE:HB	2.22	0.40
1:C:553:LEU:HA	1:C:554:PRO:HD2	1.88	0.40
1:C:625:GLY:C	1:C:627:ILE:N	2.75	0.40
1:C:680:GLU:CG	1:C:681:ILE:N	2.83	0.40
1:C:210:SER:CB	1:C:712:VAL:HG11	2.51	0.40
1:C:841:GLN:O	1:C:844:SER:HB3	2.22	0.40
1:C:855:ALA:O	1:C:859:PHE:HB2	2.21	0.40
1:C:879:LEU:CD1	1:C:880:ARG:N	2.72	0.40
1:C:913:THR:O	1:C:917:VAL:HG22	2.21	0.40
1:C:960:PHE:O	1:C:960:PHE:CD1	2.74	0.40
1:C:961:LEU:CG	1:C:971:LEU:HD13	2.51	0.40
1:A:483:LEU:HA	1:A:499:VAL:O	2.22	0.40
1:A:524:ASP:O	1:A:528:LYS:HB2	2.22	0.40
1:A:611:GLY:O	1:A:685:ARG:HA	2.21	0.40
1:A:150:ILE:CD1	1:A:738:ALA:HB2	2.51	0.40
1:A:771:TYR:HD2	1:A:772:THR:CA	2.34	0.40
1:A:822:SER:O	1:A:824:ILE:N	2.54	0.40
1:A:863:PHE:HB3	1:A:871:PHE:CE1	2.56	0.40
1:A:902:GLU:HA	1:A:905:LYS:HG3	1.95	0.40
1:C:142:TYR:CG	1:C:142:TYR:O	2.74	0.40
1:C:350:LEU:CG	1:C:351:VAL:N	2.79	0.40
1:C:420:LEU:O	1:C:422:ASN:N	2.55	0.40
1:C:671:LEU:HD23	1:C:671:LEU:O	2.21	0.40
1:C:763:ASP:C	1:C:765:LEU:N	2.74	0.40
1:C:816:ALA:O	1:C:818:GLU:N	2.54	0.40
1:C:919:ILE:O	1:C:920:VAL:C	2.59	0.40
2:D:46:LEU:HD23	2:D:46:LEU:HA	1.75	0.40
1:C:899:TRP:CZ2	2:D:70:ASP:C	2.92	0.40
1:A:634:VAL:C	1:A:636:ASP:N	2.74	0.40
1:A:679:THR:HG22	1:A:681:ILE:CD1	2.39	0.40
1:A:900:THR:CB	1:A:903:GLN:HE21	2.34	0.40
1:A:914:PRO:O	1:A:918:THR:HG23	2.22	0.40
2:B:37:LEU:CD1	2:B:37:LEU:C	2.86	0.40
2:B:54:ILE:O	2:B:57:MET:HB3	2.21	0.40
1:C:124:TYR:O	1:C:128:VAL:HG23	2.22	0.40
1:C:330:LEU:C	1:C:332:THR:H	2.24	0.40
1:C:354:LEU:O	1:C:355:GLU:C	2.59	0.40
1:C:755:VAL:HG13	1:C:825:MET:HE1	2.02	0.40
1:C:842:LEU:C	1:C:842:LEU:CD1	2.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:960:PHE:HD1	1:C:960:PHE:O	2.05	0.40
1:C:976:LEU:HG	1:C:978:PRO:CD	2.44	0.40
2:D:34:LYS:CA	2:D:37:LEU:HG	2.43	0.40
2:D:64:PHE:HD1	2:D:65:LYS:N	2.20	0.40
1:A:153:SER:OG	1:A:734:VAL:HB	2.22	0.40
1:A:295:LEU:O	1:A:298:SER:N	2.55	0.40
1:A:29:LYS:C	1:A:31:GLU:H	2.23	0.40
1:A:381:VAL:HG11	1:A:384:MET:HE2	2.03	0.40
1:A:651:ARG:O	1:A:653:ALA:N	2.54	0.40
1:A:777:ILE:HD11	1:A:847:TYR:CG	2.56	0.40
1:A:995:ASP:OD2	1:A:998:ARG:CG	2.70	0.40
1:C:224:PHE:CZ	1:C:226:ASN:CG	2.95	0.40
1:C:866:LEU:C	1:C:871:PHE:CB	2.90	0.40
1:C:876:LEU:O	1:C:877:LEU:C	2.59	0.40
1:C:895:TYR:CD2	1:C:899:TRP:HE3	2.37	0.40
1:C:938:PHE:C	1:C:940:GLN:H	2.25	0.40
1:C:944:ASN:HB3	1:C:947:LEU:HD22	2.03	0.40
1:C:951:LEU:HA	1:C:951:LEU:HD23	1.92	0.40
2:D:69:GLN:O	2:D:70:ASP:CB	2.69	0.40
3:H:37:ALA:C	3:H:39:ILE:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	996/998 (100%)	612 (61%)	243 (24%)	141 (14%)	0 3
1	C	996/998 (100%)	599 (60%)	246 (25%)	151 (15%)	0 3
2	B	44/46 (96%)	25 (57%)	9 (20%)	10 (23%)	0 1
2	D	44/46 (96%)	27 (61%)	7 (16%)	10 (23%)	0 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	G	27/29 (93%)	14 (52%)	11 (41%)	2 (7%)	1 11
3	H	27/29 (93%)	20 (74%)	7 (26%)	0	100 100
All	All	2134/2146 (99%)	1297 (61%)	523 (24%)	314 (15%)	0 3

All (314) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	70	PRO
1	A	113	ALA
1	A	115	GLU
1	A	116	GLU
1	A	210	SER
1	A	226	ASN
1	A	227	GLU
1	A	228	ASN
1	A	229	PRO
1	A	302	LEU
1	A	305	ILE
1	A	306	LEU
1	A	402	VAL
1	A	403	SER
1	A	405	ASP
1	A	425	VAL
1	A	491	THR
1	A	494	PRO
1	A	516	ILE
1	A	566	THR
1	A	640	ARG
1	A	641	LEU
1	A	644	PRO
1	A	648	VAL
1	A	715	SER
1	A	764	ASN
1	A	790	ASN
1	A	792	PRO
1	A	802	CYS
1	A	809	MET
1	A	820	ALA
1	A	876	LEU
1	A	877	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	887	TRP
1	A	908	GLU
1	A	911	CYS
1	A	1015	TYR
2	B	62	SER
2	B	65	LYS
2	B	66	PRO
2	B	67	THR
2	B	69	GLN
1	C	33	SER
1	C	70	PRO
1	C	90	PHE
1	C	113	ALA
1	C	115	GLU
1	C	116	GLU
1	C	210	SER
1	C	226	ASN
1	C	227	GLU
1	C	228	ASN
1	C	229	PRO
1	C	240	THR
1	C	402	VAL
1	C	403	SER
1	C	405	ASP
1	C	425	VAL
1	C	491	THR
1	C	494	PRO
1	C	516	ILE
1	C	566	THR
1	C	640	ARG
1	C	641	LEU
1	C	644	PRO
1	C	715	SER
1	C	764	ASN
1	C	845	MET
1	C	877	LEU
1	C	879	LEU
1	C	887	TRP
1	C	897	GLN
1	C	908	GLU
1	C	911	CYS
1	C	945	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	980	TRP
1	C	992	PHE
1	C	1006	PRO
1	C	1009	TRP
1	C	1010	VAL
2	D	60	THR
2	D	66	PRO
2	D	69	GLN
2	D	70	ASP
1	A	83	VAL
1	A	90	PHE
1	A	110	ILE
1	A	114	THR
1	A	122	ASN
1	A	167	ASN
1	A	240	THR
1	A	283	HIS
1	A	303	SER
1	A	304	LEU
1	A	338	THR
1	A	342	LYS
1	A	354	LEU
1	A	355	GLU
1	A	428	ALA
1	A	442	GLY
1	A	444	ALA
1	A	480	LYS
1	A	510	ARG
1	A	570	ASN
1	A	638	ALA
1	A	639	ALA
1	A	645	VAL
1	A	726	ALA
1	A	728	GLY
1	A	733	ASP
1	A	772	THR
1	A	825	MET
1	A	835	ASP
1	A	991	ILE
1	A	1008	GLY
2	B	59	LEU
2	B	64	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	83	VAL
1	C	110	ILE
1	C	114	THR
1	C	122	ASN
1	C	167	ASN
1	C	292	ALA
1	C	306	LEU
1	C	309	THR
1	C	334	THR
1	C	354	LEU
1	C	355	GLU
1	C	428	ALA
1	C	442	GLY
1	C	444	ALA
1	C	480	LYS
1	C	510	ARG
1	C	570	ASN
1	C	638	ALA
1	C	639	ALA
1	C	645	VAL
1	C	648	VAL
1	C	726	ALA
1	C	728	GLY
1	C	733	ASP
1	C	806	GLY
1	C	809	MET
1	C	869	ASN
1	C	876	LEU
1	C	886	ARG
1	C	919	ILE
1	C	976	LEU
1	C	991	ILE
1	C	1008	GLY
2	D	59	LEU
2	D	64	PHE
1	A	53	SER
1	A	89	LEU
1	A	146	LYS
1	A	151	MET
1	A	209	SER
1	A	256	ASP
1	A	329	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	348	ASN
1	A	349	CYS
1	A	430	GLN
1	A	454	GLU
1	A	475	PHE
1	A	476	ASN
1	A	507	ILE
1	A	535	TYR
1	A	556	GLU
1	A	626	ILE
1	A	633	THR
1	A	685	ARG
1	A	822	SER
1	A	868	GLU
1	A	897	GLN
1	A	927	LEU
1	A	948	ILE
1	A	965	PRO
2	B	30	GLY
2	B	32	TRP
1	C	53	SER
1	C	146	LYS
1	C	209	SER
1	C	224	PHE
1	C	256	ASP
1	C	276	PRO
1	C	322	VAL
1	C	327	GLU
1	C	338	THR
1	C	348	ASN
1	C	349	CYS
1	C	430	GLN
1	C	454	GLU
1	C	475	PHE
1	C	476	ASN
1	C	507	ILE
1	C	535	TYR
1	C	556	GLU
1	C	626	ILE
1	C	633	THR
1	C	685	ARG
1	C	790	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	817	TYR
1	C	820	ALA
1	C	932	THR
1	C	967	MET
2	D	65	LYS
1	A	142	TYR
1	A	224	PHE
1	A	296	GLY
1	A	324	ASN
1	A	350	LEU
1	A	458	GLY
1	A	474	PRO
1	A	512	SER
1	A	519	LYS
1	A	533	ASN
1	A	643	ILE
1	A	646	SER
1	A	716	PRO
1	A	754	GLY
1	A	905	LYS
1	A	928	VAL
1	A	934	ARG
1	A	980	TRP
3	G	24	GLU
1	C	142	TYR
1	C	151	MET
1	C	298	SER
1	C	305	ILE
1	C	342	LYS
1	C	350	LEU
1	C	458	GLY
1	C	474	PRO
1	C	512	SER
1	C	519	LYS
1	C	567	ASP
1	C	643	ILE
1	C	646	SER
1	C	716	PRO
1	C	754	GLY
1	C	822	SER
1	C	835	ASP
1	C	965	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	994	TYR
2	D	37	LEU
2	D	67	THR
1	A	21	LYS
1	A	79	THR
1	A	276	PRO
1	A	301	ILE
1	A	387	ASP
1	A	394	ASP
1	A	490	ASN
1	A	506	ARG
1	A	524	ASP
1	A	567	ASP
1	A	673	ASP
1	A	781	THR
1	A	869	ASN
1	A	870	GLY
3	G	29	GLY
1	C	21	LYS
1	C	79	THR
1	C	89	LEU
1	C	267	ALA
1	C	394	ASP
1	C	490	ASN
1	C	506	ARG
1	C	524	ASP
1	C	533	ASN
1	C	593	PRO
1	C	673	ASP
1	C	804	ASP
1	C	805	LEU
1	C	825	MET
1	C	847	TYR
1	C	885	ASP
1	C	934	ARG
1	A	61	ALA
1	A	267	ALA
1	A	434	PRO
1	A	593	PRO
1	A	614	PRO
1	A	615	ILE
1	A	793	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	832	PRO
1	A	891	VAL
1	A	977	LYS
1	C	61	ALA
1	C	387	ASP
1	C	614	PRO
1	C	615	ILE
1	C	632	GLU
1	C	778	PRO
1	C	920	VAL
1	C	983	CYS
1	A	417	ILE
1	A	806	GLY
2	B	51	ILE
1	C	417	ILE
1	C	434	PRO
1	C	881	VAL
1	C	966	GLY
1	C	993	VAL
1	A	251	VAL
1	A	681	ILE
1	C	251	VAL
1	C	681	ILE
1	C	777	ILE
2	D	56	VAL
1	A	326	PRO
1	C	592	VAL
1	C	941	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	848/848 (100%)	728 (86%)	120 (14%)	3 19
1	C	848/848 (100%)	729 (86%)	119 (14%)	3 19
2	B	39/39 (100%)	32 (82%)	7 (18%)	2 9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	39/39 (100%)	31 (80%)	8 (20%)	1 6
3	G	23/23 (100%)	19 (83%)	4 (17%)	2 11
3	H	23/23 (100%)	21 (91%)	2 (9%)	10 38
All	All	1820/1820 (100%)	1560 (86%)	260 (14%)	3 19

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	MET
1	A	32	VAL
1	A	35	ASP
1	A	39	LEU
1	A	54	ARG
1	A	57	THR
1	A	70	PRO
1	A	74	THR
1	A	88	GLN
1	A	89	LEU
1	A	95	MET
1	A	97	LEU
1	A	104	CYS
1	A	105	PHE
1	A	134	ILE
1	A	154	PHE
1	A	163	LEU
1	A	169	GLU
1	A	183	LEU
1	A	184	VAL
1	A	198	ILE
1	A	211	LEU
1	A	215	SER
1	A	221	SER
1	A	226	ASN
1	A	228	ASN
1	A	229	PRO
1	A	241	ASN
1	A	246	THR
1	A	275	THR
1	A	277	ILE
1	A	282	GLU
1	A	284	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	287	ILE
1	A	288	ILE
1	A	293	VAL
1	A	304	LEU
1	A	310	TRP
1	A	311	LEU
1	A	318	ILE
1	A	329	LEU
1	A	334	THR
1	A	337	LEU
1	A	378	ARG
1	A	404	PHE
1	A	425	VAL
1	A	429	ASN
1	A	451	LYS
1	A	455	LEU
1	A	456	CYS
1	A	457	CYS
1	A	478	THR
1	A	481	TYR
1	A	493	GLU
1	A	494	PRO
1	A	498	LEU
1	A	509	ASP
1	A	545	VAL
1	A	546	LEU
1	A	550	HIS
1	A	560	GLU
1	A	574	ASP
1	A	606	VAL
1	A	615	ILE
1	A	620	ILE
1	A	631	ASN
1	A	632	GLU
1	A	663	LEU
1	A	678	HIS
1	A	679	THR
1	A	680	GLU
1	A	693	ILE
1	A	694	ILE
1	A	712	VAL
1	A	725	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	734	VAL
1	A	743	LEU
1	A	744	LEU
1	A	751	ILE
1	A	765	LEU
1	A	771	TYR
1	A	773	LEU
1	A	776	ASN
1	A	780	ILE
1	A	791	ILE
1	A	792	PRO
1	A	795	LEU
1	A	804	ASP
1	A	810	VAL
1	A	814	SER
1	A	824	ILE
1	A	839	ASN
1	A	844	SER
1	A	845	MET
1	A	847	TYR
1	A	849	GLN
1	A	852	MET
1	A	859	PHE
1	A	860	PHE
1	A	871	PHE
1	A	876	LEU
1	A	877	LEU
1	A	879	LEU
1	A	915	PHE
1	A	916	PHE
1	A	919	ILE
1	A	931	LYS
1	A	932	THR
1	A	934	ARG
1	A	942	MET
1	A	947	LEU
1	A	955	THR
1	A	972	ARG
1	A	979	THR
1	A	980	TRP
1	A	982	PHE
1	A	989	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	992	PHE
1	A	1011	GLU
1	A	1015	TYR
2	B	33	PHE
2	B	37	LEU
2	B	39	TYR
2	B	63	GLU
2	B	64	PHE
2	B	65	LYS
2	B	67	THR
3	G	23	TYR
3	G	26	VAL
3	G	45	ILE
3	G	48	LYS
1	C	25	MET
1	C	32	VAL
1	C	35	ASP
1	C	39	LEU
1	C	54	ARG
1	C	57	THR
1	C	70	PRO
1	C	74	THR
1	C	88	GLN
1	C	89	LEU
1	C	95	MET
1	C	97	LEU
1	C	104	CYS
1	C	105	PHE
1	C	134	ILE
1	C	154	PHE
1	C	163	LEU
1	C	169	GLU
1	C	183	LEU
1	C	184	VAL
1	C	198	ILE
1	C	211	LEU
1	C	215	SER
1	C	221	SER
1	C	226	ASN
1	C	228	ASN
1	C	229	PRO
1	C	241	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	246	THR
1	C	275	THR
1	C	276	PRO
1	C	277	ILE
1	C	310	TRP
1	C	318	ILE
1	C	330	LEU
1	C	333	VAL
1	C	336	CYS
1	C	337	LEU
1	C	339	LEU
1	C	340	THR
1	C	378	ARG
1	C	404	PHE
1	C	425	VAL
1	C	429	ASN
1	C	451	LYS
1	C	455	LEU
1	C	456	CYS
1	C	457	CYS
1	C	478	THR
1	C	481	TYR
1	C	493	GLU
1	C	494	PRO
1	C	498	LEU
1	C	509	ASP
1	C	545	VAL
1	C	546	LEU
1	C	550	HIS
1	C	560	GLU
1	C	574	ASP
1	C	606	VAL
1	C	615	ILE
1	C	620	ILE
1	C	631	ASN
1	C	632	GLU
1	C	663	LEU
1	C	678	HIS
1	C	679	THR
1	C	680	GLU
1	C	693	ILE
1	C	694	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	712	VAL
1	C	725	VAL
1	C	734	VAL
1	C	743	LEU
1	C	744	LEU
1	C	751	ILE
1	C	765	LEU
1	C	772	THR
1	C	773	LEU
1	C	795	LEU
1	C	815	LEU
1	C	826	LYS
1	C	828	GLN
1	C	830	ARG
1	C	835	ASP
1	C	840	GLU
1	C	842	LEU
1	C	847	TYR
1	C	849	GLN
1	C	852	MET
1	C	859	PHE
1	C	872	LEU
1	C	900	THR
1	C	904	ARG
1	C	908	GLU
1	C	909	PHE
1	C	913	THR
1	C	915	PHE
1	C	916	PHE
1	C	917	VAL
1	C	922	VAL
1	C	930	CYS
1	C	932	THR
1	C	942	MET
1	C	947	LEU
1	C	952	PHE
1	C	955	THR
1	C	957	LEU
1	C	972	ARG
1	C	973	MET
1	C	974	TYR
1	C	980	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	983	CYS
1	C	985	PHE
1	C	989	LEU
1	C	992	PHE
1	C	1011	GLU
1	C	1015	TYR
1	C	1016	TYR
2	D	32	TRP
2	D	33	PHE
2	D	39	TYR
2	D	46	LEU
2	D	53	THR
2	D	57	MET
2	D	64	PHE
2	D	67	THR
3	H	24	GLU
3	H	48	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	111	GLN
1	A	156	ASN
1	A	228	ASN
1	A	353	ASN
1	A	377	ASN
1	A	427	GLN
1	A	476	ASN
1	A	490	ASN
1	A	521	GLN
1	A	532	GLN
1	A	570	ASN
1	A	647	GLN
1	A	670	GLN
1	A	678	HIS
1	A	690	GLN
1	A	737	GLN
1	A	764	ASN
1	A	831	ASN
1	A	839	ASN
1	A	849	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	903	GLN
1	A	912	HIS
1	C	71	ASN
1	C	88	GLN
1	C	156	ASN
1	C	228	ASN
1	C	353	ASN
1	C	377	ASN
1	C	427	GLN
1	C	476	ASN
1	C	482	GLN
1	C	490	ASN
1	C	521	GLN
1	C	532	GLN
1	C	570	ASN
1	C	647	GLN
1	C	670	GLN
1	C	678	HIS
1	C	690	GLN
1	C	737	GLN
1	C	764	ASN
1	C	828	GLN
1	C	831	ASN
1	C	839	ASN
1	C	849	GLN
1	C	854	GLN
1	C	889	ASN
1	C	898	GLN
1	C	912	HIS
1	C	923	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	PC1	B	1	-	11,11,53	0.85	0	15,16,61	0.64	0
6	MF4	A	2001	-	0,4,4	0.00	-	-		
6	MF4	C	2001	-	0,4,4	0.00	-	-		
7	PC1	C	1	-	11,11,53	0.84	0	15,16,61	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PC1	B	1	-	-	5/11/11/57	-
7	PC1	C	1	-	-	1/11/11/57	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	1	PC1	C11-O13-P-O12
7	B	1	PC1	C11-O13-P-O14
7	B	1	PC1	C11-O13-P-O11
7	B	1	PC1	C1-O11-P-O14
7	C	1	PC1	O13-C11-C12-N

Continued on next page...

Continued from previous page...

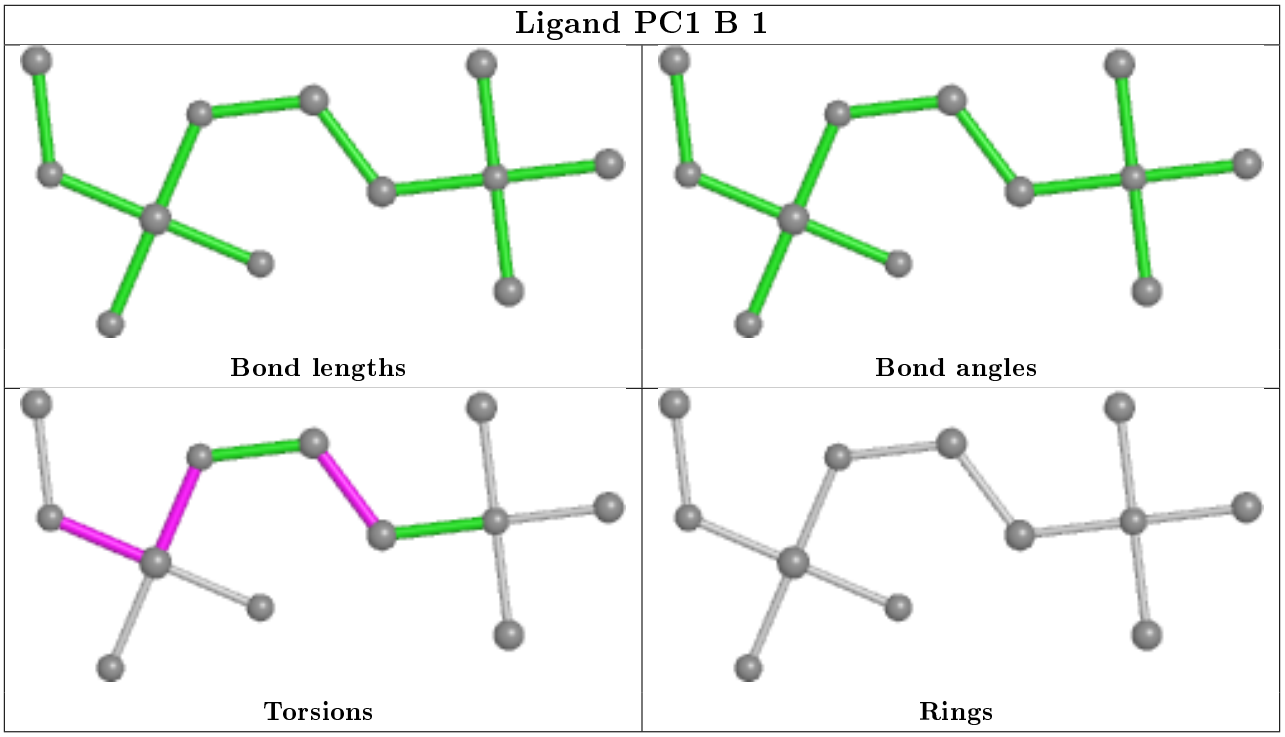
Mol	Chain	Res	Type	Atoms
7	B	1	PC1	O13-C11-C12-N

There are no ring outliers.

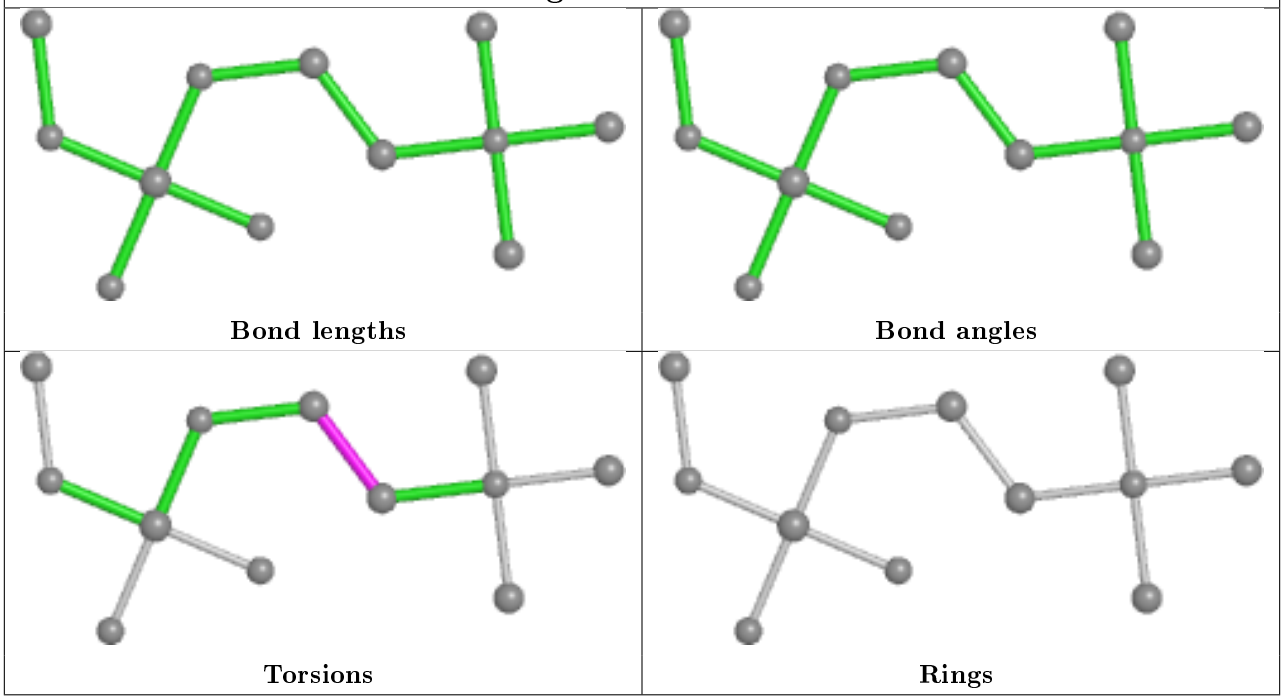
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1	PC1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand PC1 C 1



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, 95^{th} 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	998/998 (100%)	-0.50	8 (0%) 86 81	38, 95, 173, 251	0
1	C	998/998 (100%)	-0.47	10 (1%) 82 77	40, 92, 171, 245	0
2	B	46/46 (100%)	-0.49	0 100 100	67, 107, 177, 199	0
2	D	46/46 (100%)	-0.52	0 100 100	66, 116, 183, 213	0
3	G	29/29 (100%)	1.75	10 (34%) 0 0	145, 185, 217, 251	0
3	H	29/29 (100%)	1.37	7 (24%) 0 0	133, 185, 213, 232	0
All	All	2146/2146 (100%)	-0.43	35 (1%) 72 66	38, 96, 185, 251	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	113	ALA	4.4
1	A	898	GLN	4.2
3	H	28	ASN	4.1
1	C	118	PRO	3.9
3	G	39	ILE	3.8
3	H	43	ILE	3.7
3	G	38	PHE	3.5
3	G	32	ILE	3.4
1	A	30	LYS	3.2
1	A	113	ALA	3.1
1	A	114	THR	3.1
3	H	38	PHE	3.1
3	G	41	GLY	3.0
3	G	34	ALA	3.0
1	C	978	PRO	3.0
1	A	19	ALA	2.9
3	G	43	ILE	2.7
1	C	19	ALA	2.5
3	H	26	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	977	LYS	2.5
3	H	42	LEU	2.4
1	C	117	GLU	2.3
1	A	649	ASN	2.3
3	H	27	ARG	2.3
1	C	906	ILE	2.3
1	A	978	PRO	2.3
1	A	887	TRP	2.2
3	G	33	PHE	2.2
3	H	45	ILE	2.2
3	G	50	LEU	2.2
1	C	646	SER	2.2
3	G	49	ARG	2.2
1	C	79	THR	2.2
3	G	45	ILE	2.0
1	C	885	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PC1	B	1	12/54	0.85	0.27	105,120,120,120	0
5	RB	A	2005	1/1	0.86	0.20	178,178,178,178	0
7	PC1	C	1	12/54	0.90	0.21	105,120,120,120	0
5	RB	A	2003	1/1	0.94	0.19	122,122,122,122	0
5	RB	C	2005	1/1	0.95	0.10	179,179,179,179	0
6	MF4	C	2001	5/5	0.96	0.26	98,98,98,98	0
5	RB	C	2004	1/1	0.97	0.22	115,115,115,115	0

Continued on next page...

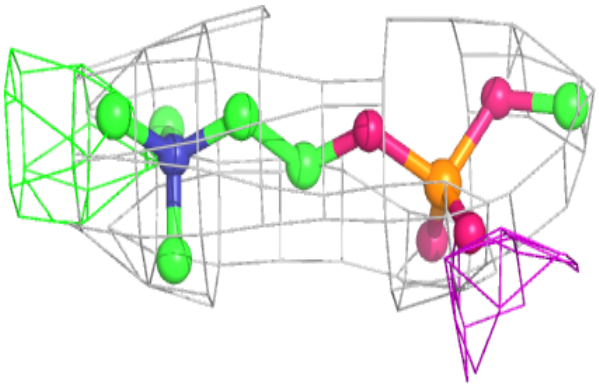
Continued from previous page...

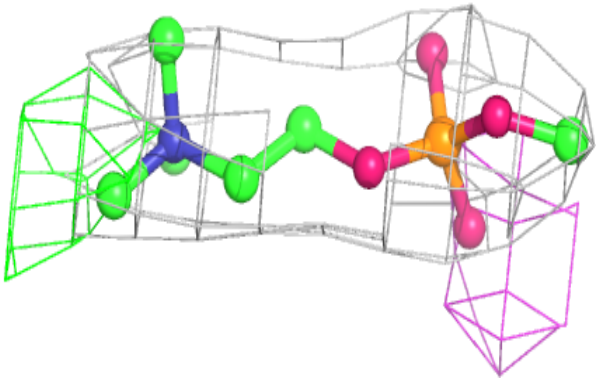
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	RB	A	2004	1/1	0.97	0.20	104,104,104,104	0
4	MG	C	2002	1/1	0.98	0.37	98,98,98,98	0
6	MF4	A	2001	5/5	0.98	0.26	98,98,98,98	0
4	MG	A	2002	1/1	0.99	0.34	98,98,98,98	0
5	RB	C	2003	1/1	0.99	0.28	126,126,126,126	0

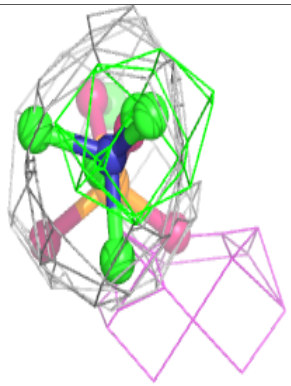
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PC1 B 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

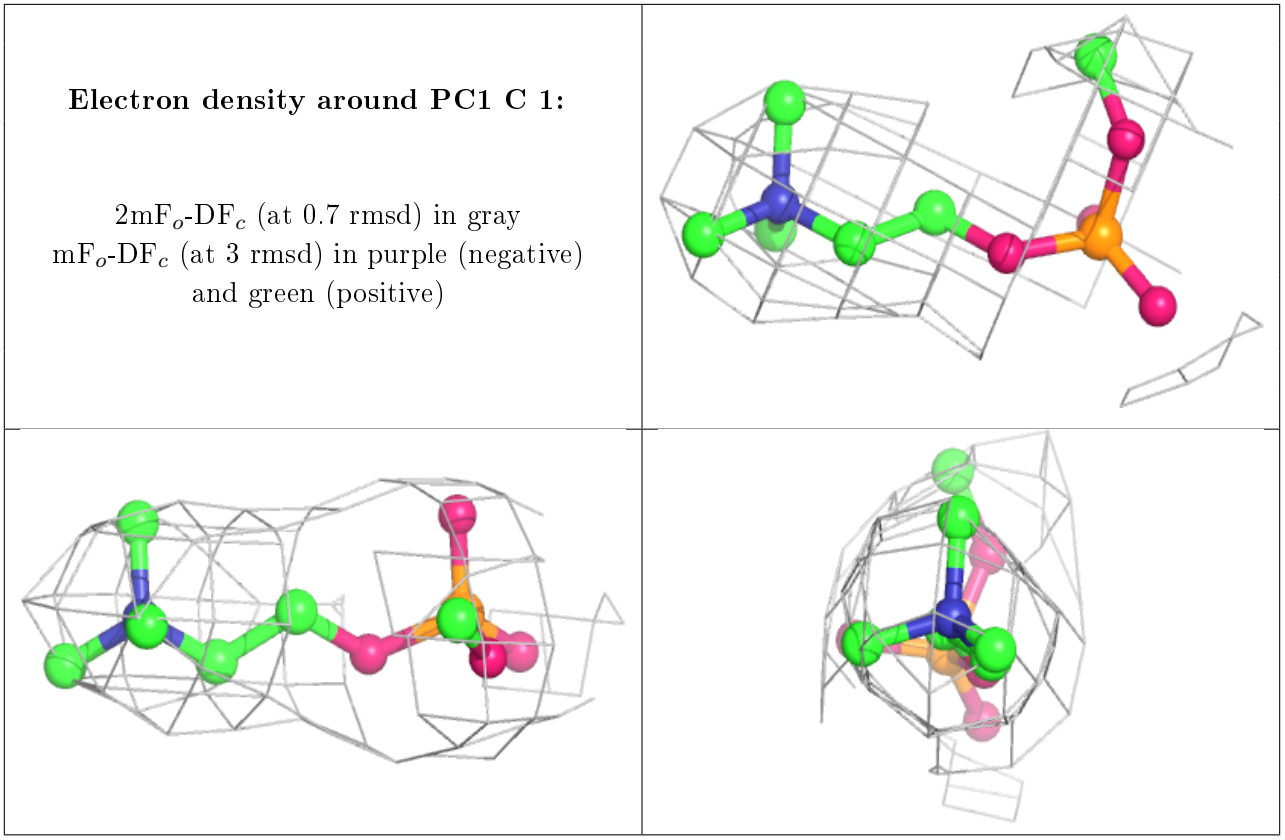






Electron density around PC1 C 1:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.