



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 09:54 pm GMT

PDB ID : 2C9M
Title : Structure of (SR) Calcium-ATPase in the Ca₂E1 state solved in a P1 crystal form.
Authors : Lund Jensen, A.-M.; Sorensen, T.L.-M.; Olesen, C.; Moller, J.V.; Nissen, P.
Deposited on : 2005-12-13
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

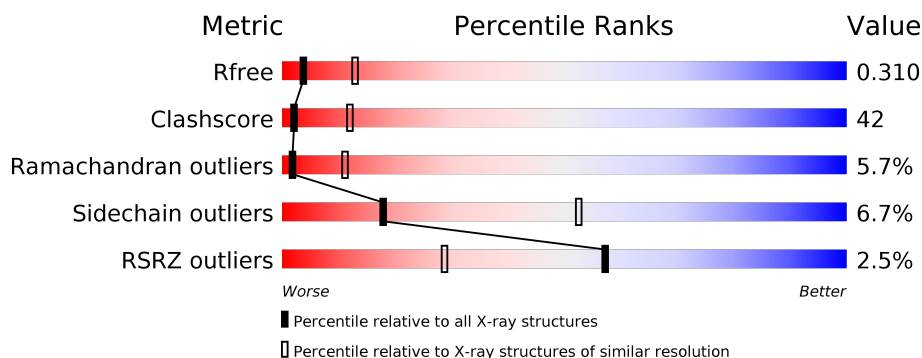
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	994	<div> <div>2%</div> <div> <div></div> <div>41%</div> <div>51%</div> <div>7%</div> </div> </div>
1	B	994	<div> <div>3%</div> <div> <div></div> <div>39%</div> <div>53%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15351 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 SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	0	0	0
			7670	4876	1287	1450	57			
1	B	994	Total	C	N	O	S	0	0	0
			7670	4876	1287	1450	57			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		

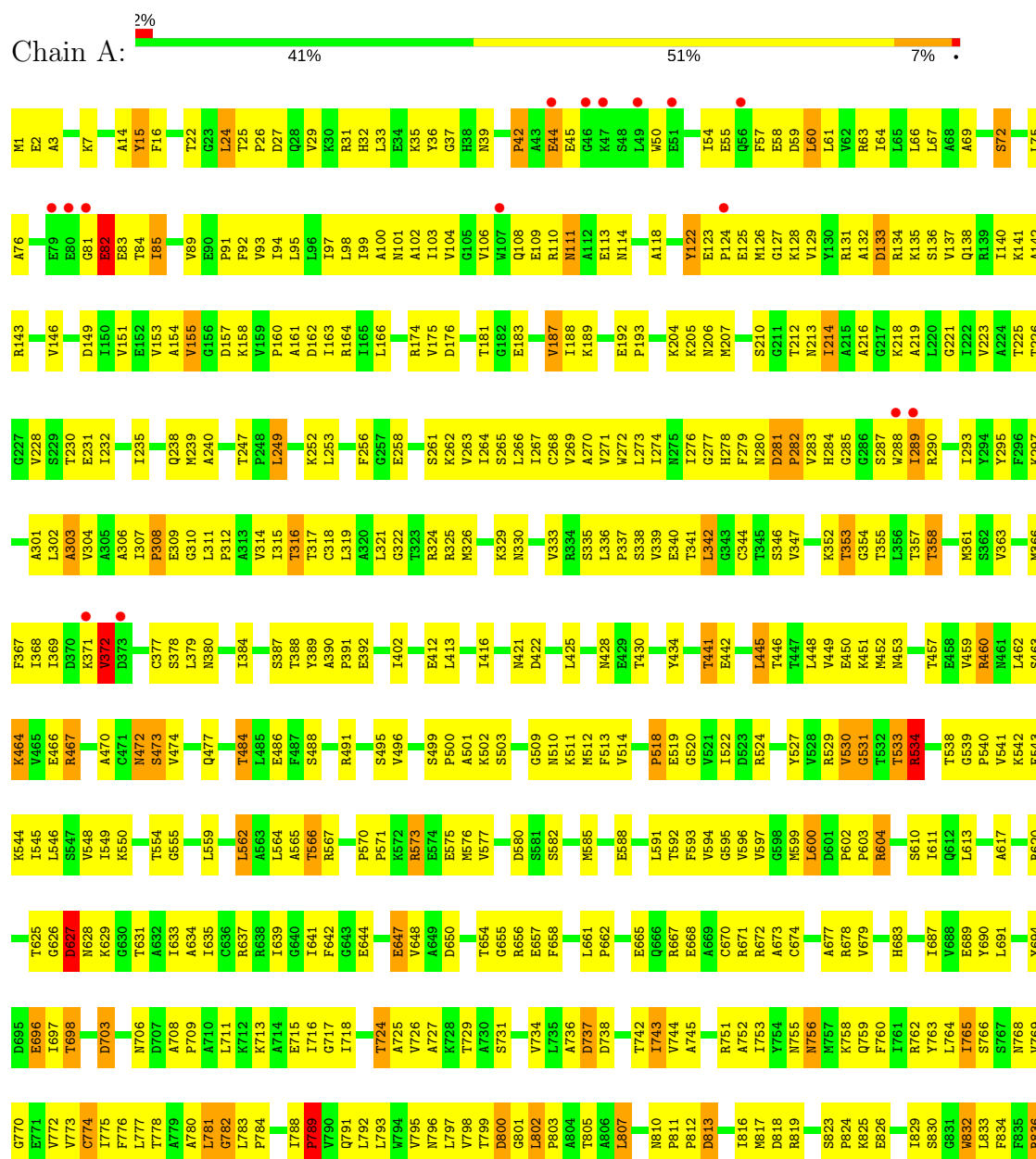
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

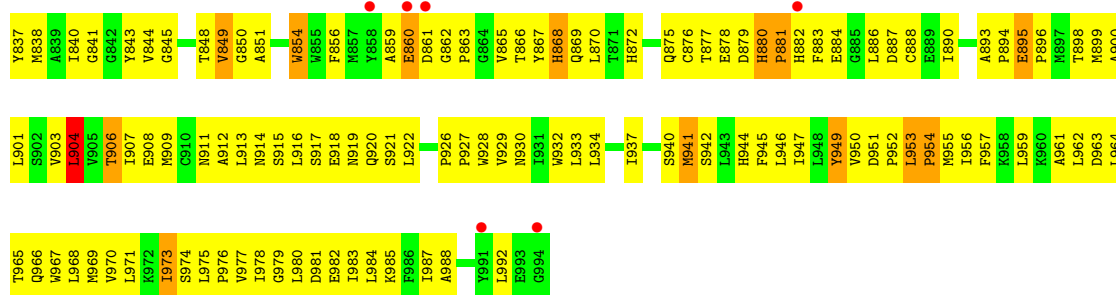
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		

3 Residue-property plots

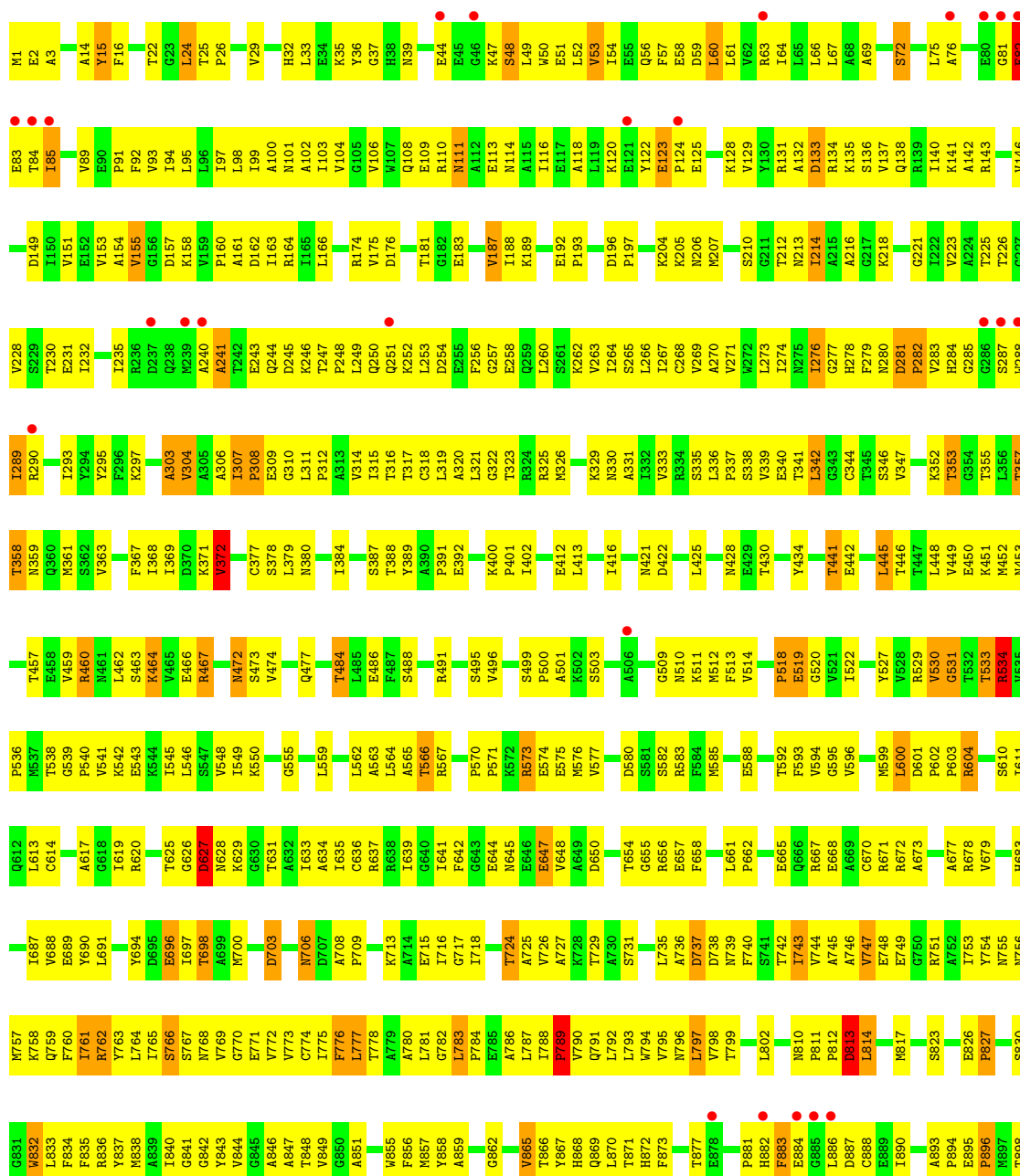
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

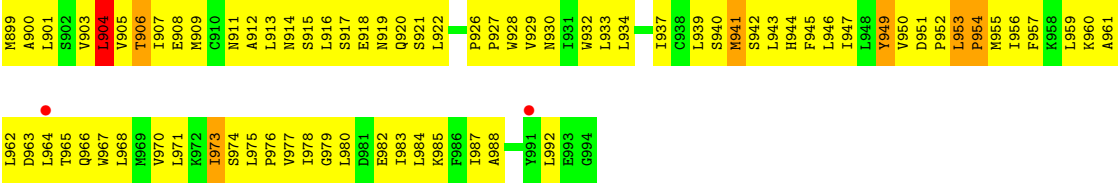
- Molecule 1: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1





• Molecule 1: SARCOPLASMIC/ENDOPLASMIC RETICULUM CALCIUM ATPASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	64.95Å 81.28Å 131.01Å 97.64° 99.94° 95.22°	Depositor
Resolution (Å)	15.00 – 3.00 23.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	80.4 (15.00-3.00) 80.2 (23.79-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.266 , 0.317 0.262 , 0.310	Depositor DCC
R_{free} test set	1158 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	75.2	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	15351	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, CA, CL

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	0.49	1/7811 (0.0%)	0.72	2/10592 (0.0%)
1	B	0.48	0/7811	0.71	1/10592 (0.0%)
All	All	0.48	1/15622 (0.0%)	0.72	3/21184 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	674	CYS	CB-SG	-6.05	1.72	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	GLU	CA-CB-CG	5.91	126.40	113.40
1	A	800	ASP	N-CA-C	-5.73	95.52	111.00
1	B	82	GLU	CA-CB-CG	5.44	125.36	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7670	0	7764	632	0
1	B	7670	0	7766	677	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	0	0	0
2	B	3	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
All	All	15351	0	15530	1309	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 42.

All (1309) 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:B:830:SER:HB3	1:B:833:LEU:HB2	1.40	1.03
1:A:372:VAL:HG13	1:A:377:CYS:HB3	1.44	0.99
1:A:263:VAL:HG12	1:A:267:ILE:HD11	1.44	0.97
1:B:372:VAL:HG13	1:B:377:CYS:HB3	1.46	0.97
1:B:559:LEU:HD23	1:B:600:LEU:HB3	1.47	0.95
1:A:559:LEU:HD23	1:A:600:LEU:HB3	1.47	0.95
1:B:47:LYS:HB3	1:B:51:GLU:HB3	1.46	0.94
1:A:214:ILE:HD13	1:A:214:ILE:H	1.33	0.94
1:B:263:VAL:HG12	1:B:267:ILE:HD11	1.48	0.93
1:A:658:PHE:HA	1:A:661:LEU:HD12	1.49	0.93
1:A:629:LYS:O	1:A:633:ILE:HG13	1.70	0.92
1:B:907:ILE:HD12	1:B:974:SER:HA	1.50	0.92
1:B:767:SER:HB3	1:B:911:ASN:HD22	1.36	0.91
1:B:658:PHE:HA	1:B:661:LEU:HD12	1.50	0.91
1:B:129:VAL:HG12	1:B:151:VAL:HG22	1.50	0.90
1:A:24:LEU:HD13	1:A:149:ASP:HA	1.51	0.90
1:A:759:GLN:HE21	1:A:917:SER:HA	1.35	0.90
1:B:214:ILE:HD13	1:B:214:ILE:H	1.37	0.90
1:A:755:ASN:O	1:A:759:GLN:HG3	1.72	0.90
1:B:904:LEU:O	1:B:907:ILE:HG22	1.70	0.90
1:B:756:ASN:HA	1:B:759:GLN:HE21	1.37	0.89
1:B:980:LEU:HA	1:B:983:ILE:HD12	1.53	0.89
1:B:629:LYS:O	1:B:633:ILE:HG13	1.73	0.88
1:A:904:LEU:O	1:A:907:ILE:HG22	1.74	0.87
1:A:679:VAL:HG13	1:A:683:HIS:HB2	1.55	0.87
1:B:567:ARG:HD3	1:B:570:PRO:HA	1.57	0.87
1:B:24:LEU:HD13	1:B:149:ASP:HA	1.54	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:VAL:CG2	1:A:845:GLY:HA3	2.05	0.87
1:B:783:LEU:HD13	1:B:870:LEU:HD11	1.55	0.87
1:A:773:VAL:HG23	1:A:845:GLY:HA3	1.55	0.86
1:B:679:VAL:HG13	1:B:683:HIS:HB2	1.56	0.86
1:B:311:LEU:HB3	1:B:312:PRO:HD3	1.58	0.86
1:A:567:ARG:HD3	1:A:570:PRO:HA	1.56	0.86
1:B:530:VAL:HG12	1:B:531:GLY:H	1.39	0.86
1:A:530:VAL:HG12	1:A:531:GLY:H	1.41	0.86
1:B:920:GLN:O	1:B:985:LYS:HD3	1.76	0.86
1:B:319:LEU:HD11	1:B:339:VAL:CG2	2.06	0.85
1:B:319:LEU:HD11	1:B:339:VAL:HG21	1.57	0.85
1:A:783:LEU:HD22	1:A:784:PRO:HD2	1.57	0.85
1:A:813:ASP:OD1	1:A:917:SER:HB2	1.76	0.85
1:A:42:PRO:HG2	1:A:44:GLU:OE1	1.77	0.84
1:A:788:ILE:HG12	1:A:791:GLN:NE2	1.92	0.84
1:A:769:VAL:HG13	1:A:841:GLY:HA3	1.58	0.84
1:B:798:VAL:HG13	1:B:940:SER:HB3	1.59	0.84
1:A:980:LEU:HA	1:A:983:ILE:HD12	1.59	0.83
1:B:886:LEU:HD11	1:B:890:ILE:HD11	1.58	0.83
1:B:767:SER:HB3	1:B:911:ASN:ND2	1.93	0.82
1:A:844:VAL:HG12	1:A:907:ILE:HG12	1.61	0.82
1:B:767:SER:CB	1:B:911:ASN:HD22	1.93	0.81
1:A:311:LEU:HB3	1:A:312:PRO:HD3	1.62	0.81
1:A:679:VAL:CG1	1:A:683:HIS:HB2	2.10	0.81
1:A:125:GLU:HB3	1:A:142:ALA:HB2	1.61	0.81
1:A:907:ILE:HD12	1:A:974:SER:HA	1.63	0.81
1:B:775:ILE:HD11	1:B:787:LEU:HD12	1.62	0.81
1:A:920:GLN:O	1:A:985:LYS:HD3	1.81	0.81
1:A:193:PRO:HD3	4:A:1000:CL:CL	2.18	0.80
1:A:125:GLU:CD	1:A:158:LYS:HB3	2.03	0.79
1:B:679:VAL:CG1	1:B:683:HIS:HB2	2.12	0.79
1:A:759:GLN:NE2	1:A:917:SER:HA	1.97	0.79
1:A:881:PRO:HG2	1:A:882:HIS:H	1.45	0.79
1:B:798:VAL:O	1:B:909:MET:HE1	1.82	0.79
1:A:111:ASN:HD22	1:A:111:ASN:H	1.31	0.79
1:B:111:ASN:H	1:B:111:ASN:HD22	1.32	0.78
1:B:49:LEU:HB3	1:B:254:ASP:HB3	1.64	0.78
1:A:756:ASN:HA	1:A:759:GLN:OE1	1.83	0.78
1:B:276:ILE:HA	1:B:279:PHE:CE2	2.18	0.78
1:A:802:LEU:HB3	1:A:803:PRO:HD3	1.65	0.78
1:A:102:ALA:O	1:A:106:VAL:HG22	1.83	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:ILE:HA	1:B:974:SER:HB3	1.64	0.77
1:B:102:ALA:O	1:B:106:VAL:HG22	1.83	0.77
1:B:573:ARG:HG3	1:B:573:ARG:HH11	1.50	0.77
1:A:276:ILE:HA	1:A:279:PHE:CE2	2.20	0.77
1:B:580:ASP:OD2	1:B:582:SER:HB3	1.85	0.77
1:B:887:ASP:HB2	1:B:890:ILE:HG23	1.64	0.77
1:A:580:ASP:OD2	1:A:582:SER:HB3	1.84	0.76
1:B:814:LEU:HG	1:B:920:GLN:HE21	1.49	0.76
1:B:794:TRP:HD1	1:B:901:LEU:HD11	1.49	0.76
1:B:278:HIS:HA	1:B:281:ASP:OD2	1.86	0.76
1:A:811:PRO:HG2	1:A:929:VAL:HG12	1.67	0.76
1:A:565:ALA:HA	1:A:594:VAL:HG23	1.67	0.76
1:A:125:GLU:OE2	1:A:158:LYS:HB3	1.86	0.75
1:A:769:VAL:O	1:A:773:VAL:HG13	1.85	0.75
1:B:565:ALA:HA	1:B:594:VAL:HG23	1.69	0.75
1:B:795:VAL:HG13	1:B:904:LEU:HG	1.69	0.75
1:A:347:VAL:HG22	1:A:620:ARG:HB2	1.69	0.75
1:A:129:VAL:HG12	1:A:151:VAL:HG22	1.66	0.75
1:A:75:LEU:HD12	1:A:76:ALA:N	2.01	0.75
1:B:811:PRO:HG2	1:B:929:VAL:HG12	1.69	0.75
1:A:573:ARG:HH11	1:A:573:ARG:HG3	1.50	0.74
1:B:318:CYS:SG	1:B:756:ASN:HB3	2.27	0.74
1:A:267:ILE:HG21	1:A:772:VAL:HG11	1.69	0.74
1:B:928:TRP:HA	1:B:934:LEU:HD11	1.69	0.74
1:A:697:ILE:HA	1:A:715:GLU:HG2	1.68	0.74
1:A:278:HIS:HA	1:A:281:ASP:OD2	1.88	0.74
1:A:763:TYR:HB2	1:A:915:SER:OG	1.88	0.74
1:A:907:ILE:HA	1:A:974:SER:HB3	1.69	0.73
1:A:387:SER:HB3	1:A:602:PRO:CG	2.19	0.73
1:B:314:VAL:HG21	1:B:760:PHE:CE2	2.23	0.73
1:B:441:THR:HG22	1:B:599:MET:SD	2.28	0.73
1:B:75:LEU:HD12	1:B:76:ALA:N	2.02	0.73
1:B:678:ARG:HH11	1:B:678:ARG:HG3	1.54	0.73
1:B:161:ALA:HA	1:B:210:SER:HB2	1.70	0.72
1:B:697:ILE:HA	1:B:715:GLU:HG2	1.70	0.72
1:B:962:LEU:HB3	1:B:966:GLN:HB3	1.71	0.72
1:B:941:MET:HA	1:B:941:MET:CE	2.18	0.72
1:B:95:LEU:O	1:B:99:ILE:HG12	1.90	0.72
1:A:175:VAL:HG22	1:A:214:ILE:HG22	1.72	0.72
1:A:678:ARG:HG3	1:A:678:ARG:HH11	1.55	0.72
1:A:941:MET:CE	1:A:941:MET:HA	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:THR:O	1:A:449:VAL:HG22	1.89	0.72
1:A:825:LYS:HG3	1:A:826:GLU:H	1.55	0.72
1:A:95:LEU:O	1:A:99:ILE:HG12	1.90	0.71
1:B:788:ILE:HB	1:B:789:PRO:HD2	1.71	0.71
1:A:823:SER:HB2	1:A:825:LYS:HG2	1.71	0.71
1:A:100:ALA:HA	1:A:103:ILE:HG22	1.72	0.71
1:B:310:GLY:O	1:B:314:VAL:HG23	1.90	0.71
1:A:367:PHE:CD2	1:A:379:LEU:HD13	2.25	0.71
1:B:756:ASN:HA	1:B:759:GLN:NE2	2.06	0.71
1:B:367:PHE:CD2	1:B:379:LEU:HD13	2.25	0.71
1:B:769:VAL:HG12	1:B:841:GLY:HA3	1.71	0.71
1:A:559:LEU:CD2	1:A:600:LEU:HB3	2.20	0.71
1:B:175:VAL:HG22	1:B:214:ILE:HG22	1.73	0.71
1:B:763:TYR:HB2	1:B:915:SER:OG	1.91	0.71
1:B:840:ILE:HD13	1:B:980:LEU:HD23	1.73	0.71
1:B:347:VAL:CG2	1:B:696:GLU:HG2	2.20	0.71
1:B:617:ALA:HB1	1:B:751:ARG:HH12	1.54	0.70
1:A:449:VAL:HG21	1:A:472:ASN:ND2	2.06	0.70
1:A:416:ILE:HD11	1:A:594:VAL:HG21	1.73	0.70
1:B:267:ILE:HG21	1:B:772:VAL:HG11	1.73	0.70
1:A:281:ASP:HB3	1:A:282:PRO:HD2	1.73	0.70
1:A:310:GLY:O	1:A:314:VAL:HG23	1.91	0.70
1:A:319:LEU:HD11	1:A:339:VAL:CG2	2.22	0.70
1:A:988:ALA:HA	1:A:992:LEU:HD12	1.73	0.70
1:A:111:ASN:N	1:A:111:ASN:HD22	1.88	0.70
1:A:2:GLU:CD	1:A:3:ALA:H	1.94	0.70
1:B:346:SER:OG	1:B:696:GLU:HG3	1.91	0.70
1:B:988:ALA:HA	1:B:992:LEU:HD12	1.74	0.70
1:A:926:PRO:O	1:A:929:VAL:HG23	1.91	0.70
1:B:755:ASN:O	1:B:759:GLN:HG3	1.92	0.69
1:B:281:ASP:HB3	1:B:282:PRO:HD2	1.73	0.69
1:B:2:GLU:CD	1:B:3:ALA:H	1.95	0.69
1:A:25:THR:HG22	1:A:132:ALA:HB2	1.73	0.69
1:B:918:GLU:C	1:B:919:ASN:HD22	1.94	0.69
1:B:926:PRO:O	1:B:929:VAL:HG23	1.93	0.69
1:A:962:LEU:HB3	1:A:966:GLN:HB3	1.74	0.69
1:B:111:ASN:N	1:B:111:ASN:HD22	1.89	0.69
1:B:347:VAL:HG22	1:B:620:ARG:HB2	1.74	0.69
1:B:917:SER:OG	1:B:920:GLN:HB2	1.91	0.69
1:B:899:MET:HG2	1:B:962:LEU:HD21	1.73	0.69
1:A:122:TYR:O	1:A:124:PRO:HD3	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:VAL:HA	1:A:462:LEU:HD12	1.74	0.68
1:B:100:ALA:HA	1:B:103:ILE:HG22	1.74	0.68
1:B:783:LEU:CD1	1:B:870:LEU:HD11	2.23	0.68
1:A:361:MET:HE3	1:A:599:MET:HB2	1.75	0.68
1:A:342:LEU:HD12	1:A:716:ILE:HD13	1.73	0.68
1:A:311:LEU:HA	1:A:760:PHE:CE1	2.28	0.68
1:B:319:LEU:CD1	1:B:339:VAL:HG21	2.22	0.68
1:B:416:ILE:HD11	1:B:594:VAL:HG21	1.74	0.68
1:B:628:ASN:HB3	1:B:678:ARG:HH22	1.58	0.68
1:B:832:TRP:O	1:B:835:PHE:HB3	1.94	0.68
1:A:647:GLU:H	1:A:647:GLU:CD	1.97	0.68
1:B:446:THR:O	1:B:449:VAL:HG22	1.92	0.67
1:A:336:LEU:N	1:A:337:PRO:HD2	2.09	0.67
1:B:47:LYS:HD3	1:B:51:GLU:O	1.95	0.67
1:B:559:LEU:CD2	1:B:600:LEU:HB3	2.22	0.67
1:B:25:THR:HG22	1:B:132:ALA:HB2	1.75	0.67
1:A:326:MET:CE	1:A:333:VAL:HG21	2.25	0.67
1:A:742:THR:O	1:A:745:ALA:N	2.27	0.67
1:A:778:THR:HG22	1:A:849:VAL:HG13	1.76	0.67
1:A:811:PRO:HG2	1:A:929:VAL:CG1	2.24	0.67
1:B:459:VAL:HA	1:B:462:LEU:HD12	1.77	0.67
1:B:359:ASN:HA	1:B:601:ASP:OD1	1.94	0.67
1:B:662:PRO:HD2	1:B:665:GLU:HB2	1.76	0.67
1:B:671:ARG:HB3	1:B:694:TYR:CE2	2.30	0.67
1:B:387:SER:HB3	1:B:602:PRO:CG	2.24	0.67
1:A:271:VAL:HA	1:A:274:ILE:HG12	1.76	0.67
1:B:336:LEU:N	1:B:337:PRO:HD2	2.10	0.67
1:B:647:GLU:CD	1:B:647:GLU:H	1.98	0.67
1:A:631:THR:O	1:A:634:ALA:HB3	1.95	0.67
1:A:918:GLU:C	1:A:919:ASN:HD22	1.98	0.67
1:A:308:PRO:HB2	1:A:764:LEU:HD12	1.76	0.66
1:A:928:TRP:HA	1:A:934:LEU:HD11	1.77	0.66
1:B:539:GLY:N	1:B:540:PRO:HD2	2.10	0.66
1:B:306:ALA:O	1:B:768:ASN:ND2	2.28	0.66
1:A:975:LEU:N	1:A:976:PRO:HD2	2.11	0.66
1:A:100:ALA:HB1	1:A:797:LEU:HD11	1.77	0.66
1:A:210:SER:HB3	1:A:230:THR:HG21	1.76	0.66
1:A:54:ILE:HD12	1:A:55:GLU:N	2.10	0.66
1:A:662:PRO:HD2	1:A:665:GLU:HB2	1.78	0.66
1:A:81:GLY:C	1:A:82:GLU:OE1	2.35	0.66
1:A:412:GLU:OE1	1:A:529:ARG:HD2	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:THR:HG22	1:A:599:MET:SD	2.36	0.66
1:B:210:SER:HB3	1:B:230:THR:HG21	1.78	0.66
1:A:230:THR:CG2	1:A:232:ILE:HG22	2.26	0.65
1:A:899:MET:HG2	1:A:962:LEU:HD21	1.77	0.65
1:B:357:THR:HA	1:B:603:PRO:HA	1.77	0.65
1:B:944:HIS:O	1:B:947:ILE:HG22	1.95	0.65
1:A:161:ALA:HA	1:A:210:SER:HB2	1.76	0.65
1:A:162:ASP:OD1	1:A:230:THR:HG23	1.96	0.65
1:A:50:TRP:HB2	1:A:55:GLU:CD	2.16	0.65
1:B:495:SER:HB3	1:B:514:VAL:HA	1.78	0.65
1:B:361:MET:HE3	1:B:599:MET:HB2	1.78	0.65
1:B:347:VAL:HG23	1:B:696:GLU:HG2	1.77	0.65
1:A:317:THR:HG22	1:A:321:LEU:HD12	1.77	0.65
1:A:319:LEU:HD11	1:A:339:VAL:HG21	1.78	0.65
1:A:442:GLU:O	1:A:445:LEU:HB2	1.96	0.65
1:A:495:SER:HB3	1:A:514:VAL:HA	1.78	0.65
1:B:271:VAL:HA	1:B:274:ILE:HG12	1.78	0.65
1:B:317:THR:HG22	1:B:321:LEU:HD12	1.79	0.65
1:B:975:LEU:N	1:B:976:PRO:HD2	2.12	0.65
1:A:539:GLY:N	1:A:540:PRO:HD2	2.12	0.65
1:A:941:MET:HE2	1:A:941:MET:HA	1.78	0.65
1:A:944:HIS:O	1:A:947:ILE:HG22	1.96	0.65
1:A:100:ALA:CB	1:A:797:LEU:HD11	2.27	0.65
1:B:342:LEU:HD12	1:B:716:ILE:HD13	1.79	0.65
1:B:893:ALA:O	1:B:896:PRO:HD2	1.96	0.65
1:B:442:GLU:O	1:B:445:LEU:HB2	1.97	0.65
1:A:82:GLU:N	1:A:82:GLU:OE1	2.30	0.65
1:B:267:ILE:CG2	1:B:772:VAL:HG11	2.28	0.64
1:B:783:LEU:HD13	1:B:870:LEU:CD1	2.26	0.64
1:B:82:GLU:OE1	1:B:82:GLU:N	2.30	0.64
1:A:628:ASN:HB3	1:A:678:ARG:HH22	1.62	0.64
1:B:230:THR:CG2	1:B:232:ILE:HG22	2.26	0.64
1:B:49:LEU:HB3	1:B:254:ASP:CB	2.28	0.64
1:B:610:SER:HB3	1:B:744:VAL:HG21	1.79	0.64
1:B:775:ILE:CD1	1:B:787:LEU:HD12	2.27	0.64
1:B:898:THR:OG1	1:B:959:LEU:HA	1.97	0.64
1:A:770:GLY:HA2	1:A:841:GLY:O	1.96	0.64
1:A:347:VAL:CG2	1:A:696:GLU:HG2	2.27	0.64
1:B:518:PRO:O	1:B:522:ILE:HG12	1.98	0.64
1:B:759:GLN:OE1	1:B:917:SER:HA	1.96	0.64
1:B:883:PHE:O	1:B:884:GLU:HG2	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:C	1:A:413:LEU:HD23	2.17	0.64
1:A:770:GLY:HA3	1:A:844:VAL:CG2	2.28	0.64
1:B:449:VAL:HG21	1:B:472:ASN:ND2	2.12	0.64
1:B:941:MET:HA	1:B:941:MET:HE2	1.79	0.64
1:B:962:LEU:HB3	1:B:966:GLN:CB	2.28	0.64
1:B:1:MET:O	1:B:1:MET:HG3	1.98	0.64
1:B:162:ASP:OD1	1:B:230:THR:HG23	1.97	0.64
1:B:962:LEU:HA	1:B:966:GLN:OE1	1.97	0.64
1:A:263:VAL:O	1:A:267:ILE:HG13	1.97	0.64
1:A:459:VAL:HG23	1:A:460:ARG:H	1.61	0.64
1:A:467:ARG:HH11	1:A:467:ARG:HG2	1.62	0.64
1:A:629:LYS:HD2	1:A:657:GLU:OE1	1.98	0.64
1:A:798:VAL:HG13	1:A:940:SER:HB3	1.78	0.64
1:B:895:GLU:N	1:B:896:PRO:HD2	2.13	0.64
1:A:559:LEU:HD21	1:A:600:LEU:HD13	1.80	0.63
1:A:762:ARG:HG3	1:A:837:TYR:CE1	2.33	0.63
1:B:60:LEU:O	1:B:60:LEU:HD12	1.98	0.63
1:B:886:LEU:HD11	1:B:890:ILE:CD1	2.29	0.63
1:B:907:ILE:CA	1:B:974:SER:HB3	2.29	0.63
1:A:449:VAL:CG2	1:A:472:ASN:ND2	2.61	0.63
1:B:628:ASN:HD21	1:B:631:THR:HG23	1.63	0.63
1:B:766:SER:O	1:B:769:VAL:HG12	1.97	0.63
1:B:894:PRO:HG2	1:B:895:GLU:OE2	1.99	0.63
1:A:679:VAL:HG13	1:A:683:HIS:CB	2.26	0.63
1:A:946:LEU:C	1:A:946:LEU:HD23	2.19	0.63
1:A:843:TYR:OH	1:A:976:PRO:HG2	1.99	0.63
1:B:330:ASN:HB3	1:B:736:ALA:HB3	1.79	0.63
1:B:870:LEU:C	1:B:870:LEU:HD12	2.19	0.63
1:A:118:ALA:HB1	1:A:324:ARG:HE	1.63	0.63
1:B:631:THR:O	1:B:634:ALA:HB3	1.99	0.63
1:B:25:THR:O	1:B:29:VAL:HG23	1.98	0.63
1:B:946:LEU:C	1:B:946:LEU:HD23	2.20	0.63
1:B:467:ARG:HH11	1:B:467:ARG:HG2	1.64	0.62
1:A:610:SER:HB3	1:A:744:VAL:HG21	1.81	0.62
1:A:97:ILE:HG21	1:A:793:LEU:HB3	1.82	0.62
1:B:230:THR:HG21	1:B:232:ILE:HG22	1.81	0.62
1:B:326:MET:CE	1:B:333:VAL:HG21	2.28	0.62
1:B:412:GLU:OE1	1:B:529:ARG:HD2	1.99	0.62
1:B:658:PHE:HA	1:B:661:LEU:CD1	2.26	0.62
1:A:708:ALA:HB3	1:A:709:PRO:HD3	1.80	0.62
1:A:25:THR:O	1:A:29:VAL:HG23	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:THR:HG21	1:A:232:ILE:HG22	1.82	0.62
1:B:559:LEU:HD21	1:B:600:LEU:HD13	1.81	0.62
1:A:369:ILE:N	1:A:369:ILE:HD12	2.13	0.62
1:A:947:ILE:HG12	1:A:957:PHE:CE2	2.34	0.62
1:A:962:LEU:HB3	1:A:966:GLN:CB	2.30	0.62
1:B:957:PHE:O	1:B:959:LEU:HG	1.99	0.62
1:A:230:THR:HG22	1:A:232:ILE:H	1.64	0.62
1:B:683:HIS:O	1:B:687:ILE:HG13	2.00	0.62
1:A:100:ALA:HA	1:A:103:ILE:CG2	2.30	0.62
1:A:264:ILE:HA	1:A:267:ILE:HD12	1.81	0.62
1:B:212:THR:HG22	1:B:213:ASN:N	2.15	0.62
1:B:413:LEU:HD23	1:B:413:LEU:C	2.20	0.62
1:A:330:ASN:HB3	1:A:736:ALA:HB3	1.81	0.61
1:B:742:THR:O	1:B:745:ALA:N	2.33	0.61
1:A:326:MET:HE3	1:A:333:VAL:HG21	1.82	0.61
1:A:658:PHE:HA	1:A:661:LEU:CD1	2.27	0.61
1:B:639:ILE:HD11	1:B:641:ILE:HD12	1.83	0.61
1:B:679:VAL:HG13	1:B:683:HIS:CB	2.28	0.61
1:B:369:ILE:HD12	1:B:369:ILE:N	2.15	0.61
1:A:24:LEU:HD22	1:A:149:ASP:HB3	1.82	0.61
1:A:898:THR:OG1	1:A:959:LEU:HA	2.00	0.61
1:A:769:VAL:CG1	1:A:841:GLY:HA3	2.28	0.61
1:A:448:LEU:O	1:A:452:MET:HG3	2.00	0.61
1:A:263:VAL:HG12	1:A:267:ILE:CD1	2.25	0.61
1:A:367:PHE:CE1	1:A:596:VAL:HB	2.36	0.61
1:B:214:ILE:H	1:B:214:ILE:CD1	2.13	0.61
1:B:836:ARG:HD3	1:B:984:LEU:HD12	1.82	0.61
1:A:57:PHE:O	1:A:61:LEU:HG	2.01	0.61
1:A:953:LEU:H	1:A:954:PRO:HD2	1.65	0.61
1:A:907:ILE:CA	1:A:974:SER:HB3	2.31	0.61
1:A:947:ILE:HG12	1:A:957:PHE:CD2	2.36	0.61
1:B:449:VAL:CG2	1:B:472:ASN:ND2	2.63	0.60
1:B:484:THR:HB	1:B:496:VAL:HG12	1.81	0.60
1:B:843:TYR:O	1:B:846:ALA:HB3	2.00	0.60
1:A:962:LEU:HA	1:A:966:GLN:OE1	2.01	0.60
1:B:459:VAL:HG23	1:B:460:ARG:H	1.65	0.60
1:A:271:VAL:C	1:A:273:LEU:H	2.05	0.60
1:A:518:PRO:O	1:A:522:ILE:HG12	2.02	0.60
1:A:50:TRP:HB2	1:A:55:GLU:OE2	2.01	0.60
1:B:263:VAL:O	1:B:267:ILE:HG13	2.00	0.60
1:A:650:ASP:HB2	1:A:672:ARG:NH2	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:ALA:HB3	1:B:709:PRO:HD3	1.82	0.60
1:B:93:VAL:HB	1:B:790:VAL:HG11	1.83	0.60
1:B:834:PHE:O	1:B:838:MET:HG2	2.01	0.60
1:A:1:MET:HG3	1:A:1:MET:O	2.02	0.60
1:A:347:VAL:HG23	1:A:696:GLU:HG2	1.82	0.60
1:A:917:SER:OG	1:A:920:GLN:HB2	2.01	0.60
1:B:118:ALA:C	1:B:120:LYS:H	2.04	0.60
1:A:214:ILE:H	1:A:214:ILE:CD1	2.11	0.60
1:A:628:ASN:HD21	1:A:631:THR:HG23	1.66	0.60
1:A:642:PHE:CD2	1:A:648:VAL:HG11	2.36	0.60
1:A:957:PHE:O	1:A:959:LEU:HG	2.01	0.60
1:B:100:ALA:HA	1:B:103:ILE:CG2	2.32	0.60
1:A:212:THR:HG22	1:A:213:ASN:N	2.16	0.60
1:A:484:THR:HB	1:A:496:VAL:HG12	1.84	0.60
1:B:788:ILE:HB	1:B:789:PRO:CD	2.31	0.60
1:A:683:HIS:O	1:A:687:ILE:HG13	2.01	0.60
1:B:462:LEU:HD22	1:B:466:GLU:HB3	1.84	0.60
1:B:762:ARG:CZ	1:B:836:ARG:NH1	2.64	0.60
1:A:780:ALA:C	1:A:782:GLY:H	2.05	0.60
1:B:726:VAL:HG13	1:B:727:ALA:N	2.16	0.60
1:A:346:SER:OG	1:A:696:GLU:HG3	2.01	0.59
1:A:387:SER:HB3	1:A:602:PRO:HG3	1.83	0.59
1:A:671:ARG:HB3	1:A:694:TYR:CE2	2.37	0.59
1:A:94:ILE:HD12	1:A:95:LEU:N	2.17	0.59
1:A:689:GLU:HB2	1:A:713:LYS:HZ3	1.68	0.59
1:B:116:ILE:HD13	1:B:320:ALA:HB2	1.84	0.59
1:A:249:LEU:O	1:A:253:LEU:HB2	2.02	0.59
1:A:372:VAL:HG13	1:A:377:CYS:CB	2.25	0.59
1:A:22:THR:HG22	1:A:135:LYS:NZ	2.18	0.59
1:A:311:LEU:HA	1:A:760:PHE:HE1	1.65	0.59
1:B:367:PHE:CE2	1:B:379:LEU:HD13	2.38	0.59
1:B:947:ILE:HG12	1:B:957:PHE:CE2	2.37	0.59
1:A:758:LYS:HE3	1:A:833:LEU:HD21	1.84	0.59
1:B:134:ARG:HH11	1:B:134:ARG:HG3	1.67	0.59
1:A:355:THR:HA	1:A:738:ASP:O	2.02	0.59
1:A:60:LEU:O	1:A:60:LEU:HD12	2.03	0.59
1:A:697:ILE:HG23	1:A:715:GLU:HG2	1.85	0.59
1:B:52:LEU:HD12	1:B:56:GLN:OE1	2.03	0.59
1:B:629:LYS:HD2	1:B:657:GLU:OE1	2.02	0.59
1:A:367:PHE:CE2	1:A:379:LEU:HD13	2.37	0.59
1:B:24:LEU:HD22	1:B:149:ASP:HB3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:THR:HG22	1:B:135:LYS:NZ	2.18	0.59
1:B:725:ALA:O	1:B:729:THR:HG23	2.03	0.59
1:B:953:LEU:H	1:B:954:PRO:HD2	1.68	0.59
1:A:223:VAL:HG11	1:A:226:THR:HG22	1.85	0.58
1:B:131:ARG:HG3	1:B:131:ARG:HH11	1.67	0.58
1:B:530:VAL:O	1:B:531:GLY:C	2.41	0.58
1:B:654:THR:HA	1:B:677:ALA:O	2.03	0.58
1:A:600:LEU:O	1:A:600:LEU:HD23	2.03	0.58
1:A:825:LYS:HG3	1:A:826:GLU:N	2.17	0.58
1:B:230:THR:HG22	1:B:232:ILE:H	1.67	0.58
1:B:603:PRO:HB3	1:B:639:ILE:HG22	1.83	0.58
1:B:264:ILE:HA	1:B:267:ILE:HD12	1.84	0.58
1:B:788:ILE:HG12	1:B:791:GLN:HG3	1.86	0.58
1:B:94:ILE:HD12	1:B:95:LEU:N	2.18	0.58
1:B:212:THR:CG2	1:B:213:ASN:N	2.67	0.58
1:B:271:VAL:C	1:B:273:LEU:H	2.07	0.58
1:B:650:ASP:HB2	1:B:672:ARG:NH2	2.18	0.58
1:B:50:TRP:CZ2	1:B:311:LEU:HD23	2.38	0.58
1:B:154:ALA:O	1:B:214:ILE:HD11	2.03	0.58
1:B:223:VAL:HG11	1:B:226:THR:HG22	1.85	0.58
1:A:879:ASP:C	1:A:881:PRO:HD3	2.24	0.58
1:B:282:PRO:O	1:B:284:HIS:N	2.37	0.58
1:B:794:TRP:HE1	1:B:944:HIS:HD1	1.52	0.58
1:B:573:ARG:HG3	1:B:573:ARG:NH1	2.17	0.58
1:B:57:PHE:O	1:B:61:LEU:HG	2.04	0.58
1:B:770:GLY:CA	1:B:841:GLY:O	2.52	0.58
1:A:726:VAL:HG13	1:A:727:ALA:N	2.18	0.58
1:A:867:TYR:C	1:A:869:GLN:H	2.07	0.58
1:B:933:LEU:O	1:B:937:ILE:HG13	2.04	0.58
1:A:140:ILE:HD12	1:A:141:LYS:H	1.69	0.57
1:B:39:ASN:HB3	1:B:143:ARG:HA	1.86	0.57
1:B:900:ALA:O	1:B:903:VAL:N	2.36	0.57
1:B:762:ARG:NH2	1:B:918:GLU:O	2.37	0.57
1:B:244:GLN:HE21	1:B:247:THR:CG2	2.17	0.57
1:B:847:ALA:HB1	1:B:973:ILE:HD12	1.85	0.57
1:A:134:ARG:HH11	1:A:134:ARG:HG3	1.67	0.57
1:A:39:ASN:HB3	1:A:143:ARG:HA	1.86	0.57
1:A:539:GLY:O	1:A:543:GLU:HG2	2.04	0.57
1:B:146:VAL:O	1:B:149:ASP:OD2	2.22	0.57
1:B:947:ILE:HG12	1:B:957:PHE:CD2	2.40	0.57
1:A:462:LEU:HD22	1:A:466:GLU:HB3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:VAL:HA	1:B:477:GLN:HE21	1.70	0.57
1:A:69:ALA:HA	1:A:297:LYS:HZ1	1.69	0.57
1:A:770:GLY:O	1:A:773:VAL:HG22	2.04	0.57
1:B:530:VAL:HG12	1:B:531:GLY:N	2.16	0.57
1:A:639:ILE:HD11	1:A:641:ILE:HD12	1.87	0.57
1:B:116:ILE:CD1	1:B:320:ALA:HB2	2.35	0.57
1:B:308:PRO:HB3	1:B:764:LEU:HG	1.87	0.57
1:A:125:GLU:OE1	1:A:158:LYS:HB3	2.04	0.57
1:A:783:LEU:CD2	1:A:784:PRO:HD2	2.31	0.57
1:A:950:VAL:O	1:A:954:PRO:HD2	2.05	0.57
1:B:263:VAL:HG12	1:B:267:ILE:CD1	2.28	0.57
1:A:800:ASP:O	1:A:802:LEU:N	2.37	0.57
1:B:353:THR:O	1:B:353:THR:CG2	2.53	0.57
1:B:367:PHE:HA	1:B:380:ASN:O	2.04	0.57
1:B:539:GLY:O	1:B:543:GLU:HG2	2.05	0.57
1:B:567:ARG:HD3	1:B:570:PRO:CA	2.32	0.57
1:A:843:TYR:C	1:A:843:TYR:CD2	2.78	0.57
1:A:867:TYR:O	1:A:869:GLN:N	2.38	0.57
1:A:879:ASP:O	1:A:880:HIS:HB2	2.04	0.57
1:B:448:LEU:O	1:B:452:MET:HG3	2.05	0.57
1:B:812:PRO:O	1:B:813:ASP:O	2.23	0.57
1:B:762:ARG:CZ	1:B:836:ARG:HH12	2.18	0.57
1:A:763:TYR:CE1	1:A:912:ALA:HB2	2.40	0.56
1:A:950:VAL:HG12	1:A:952:PRO:HD2	1.87	0.56
1:B:279:PHE:HE1	1:B:295:TYR:HB2	1.69	0.56
1:B:336:LEU:O	1:B:339:VAL:HG22	2.05	0.56
1:A:573:ARG:NH1	1:A:573:ARG:HG3	2.17	0.56
1:B:881:PRO:HD2	1:B:883:PHE:HE2	1.69	0.56
1:A:33:LEU:O	1:A:37:GLY:N	2.38	0.56
1:A:488:SER:OG	1:A:491:ARG:NH1	2.39	0.56
1:B:950:VAL:O	1:B:954:PRO:HD2	2.05	0.56
1:A:137:VAL:HG12	1:A:138:GLN:N	2.20	0.56
1:A:836:ARG:HH11	1:A:836:ARG:CG	2.17	0.56
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.71	0.56
1:A:154:ALA:O	1:A:214:ILE:HD11	2.06	0.56
1:A:335:SER:OG	1:A:337:PRO:HG2	2.05	0.56
1:A:770:GLY:HA3	1:A:844:VAL:HG23	1.88	0.56
1:A:834:PHE:O	1:A:838:MET:HG2	2.06	0.56
1:A:968:LEU:HD23	1:A:968:LEU:O	2.05	0.56
1:B:240:ALA:O	1:B:241:ALA:C	2.44	0.56
1:B:628:ASN:HD21	1:B:631:THR:CG2	2.17	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:968:LEU:HD23	1:B:968:LEU:O	2.05	0.56
1:A:282:PRO:O	1:A:284:HIS:N	2.39	0.56
1:A:428:ASN:OD1	1:A:430:THR:HB	2.04	0.56
1:A:50:TRP:HB2	1:A:55:GLU:OE1	2.04	0.56
1:A:900:ALA:O	1:A:903:VAL:N	2.38	0.56
1:A:988:ALA:CA	1:A:992:LEU:HD12	2.35	0.56
1:A:25:THR:HB	1:A:26:PRO:HD2	1.87	0.56
1:A:903:VAL:HA	1:A:970:VAL:HG13	1.88	0.56
1:A:66:LEU:HD12	1:A:94:ILE:HD11	1.86	0.56
1:B:137:VAL:HG12	1:B:138:GLN:H	1.70	0.56
1:B:950:VAL:HG12	1:B:952:PRO:HD2	1.87	0.56
1:A:832:TRP:CZ2	1:A:988:ALA:HB2	2.41	0.56
1:A:137:VAL:HG12	1:A:138:GLN:H	1.71	0.56
1:A:146:VAL:O	1:A:149:ASP:OD2	2.24	0.56
1:A:774:CYS:SG	1:A:775:ILE:N	2.79	0.56
1:B:260:LEU:HD11	1:B:765:ILE:HD11	1.88	0.56
1:B:306:ALA:HA	1:B:768:ASN:HD21	1.70	0.55
1:B:777:LEU:HA	1:B:780:ALA:HB3	1.87	0.55
1:B:899:MET:O	1:B:903:VAL:HG23	2.05	0.55
1:A:962:LEU:CD2	1:A:966:GLN:HB3	2.37	0.55
1:B:325:ARG:NH1	1:B:812:PRO:HG3	2.21	0.55
1:A:389:TYR:HB3	1:A:425:LEU:HD21	1.88	0.55
1:A:567:ARG:HD3	1:A:570:PRO:CA	2.31	0.55
1:B:89:VAL:O	1:B:93:VAL:HG23	2.06	0.55
1:A:628:ASN:HD21	1:A:631:THR:CG2	2.20	0.55
1:B:372:VAL:HG13	1:B:377:CYS:CB	2.28	0.55
1:B:66:LEU:HD12	1:B:94:ILE:HD11	1.86	0.55
1:A:329:LYS:O	1:A:330:ASN:HB2	2.06	0.55
1:B:367:PHE:CE1	1:B:596:VAL:HB	2.42	0.55
1:A:192:GLU:HB3	1:A:193:PRO:HD2	1.88	0.55
1:A:325:ARG:NH1	1:A:812:PRO:HG3	2.21	0.55
1:A:872:HIS:O	1:A:875:GLN:HG2	2.06	0.55
1:B:25:THR:HB	1:B:26:PRO:HD2	1.88	0.55
1:B:276:ILE:HA	1:B:279:PHE:CD2	2.41	0.55
1:B:771:GLU:O	1:B:775:ILE:HG12	2.06	0.55
1:B:814:LEU:HG	1:B:920:GLN:NE2	2.20	0.55
1:A:851:ALA:CB	1:A:903:VAL:HG21	2.37	0.55
1:B:137:VAL:HG12	1:B:138:GLN:N	2.21	0.55
1:B:428:ASN:OD1	1:B:430:THR:HB	2.07	0.55
1:B:69:ALA:HA	1:B:297:LYS:HZ1	1.72	0.55
1:A:128:LYS:O	1:A:151:VAL:HG13	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:THR:CG2	1:A:213:ASN:N	2.70	0.55
1:A:913:LEU:HD22	1:A:927:PRO:HB3	1.89	0.55
1:B:855:TRP:CZ2	1:B:895:GLU:HB2	2.42	0.55
1:A:153:VAL:O	1:A:218:LYS:HA	2.06	0.55
1:A:530:VAL:HG12	1:A:531:GLY:N	2.19	0.55
1:A:725:ALA:O	1:A:729:THR:HG23	2.07	0.55
1:B:54:ILE:HG23	1:B:307:ILE:CG2	2.37	0.55
1:B:81:GLY:C	1:B:82:GLU:OE1	2.45	0.55
1:B:903:VAL:HA	1:B:970:VAL:HG13	1.89	0.55
1:A:737:ASP:OD1	1:A:737:ASP:N	2.40	0.54
1:A:823:SER:CB	1:A:825:LYS:HG2	2.37	0.54
1:B:697:ILE:HG23	1:B:715:GLU:HG2	1.89	0.54
1:B:748:GLU:HB2	1:B:817:MET:SD	2.47	0.54
1:A:302:LEU:HA	1:A:792:LEU:HD13	1.89	0.54
1:B:413:LEU:HG	1:B:564:LEU:CD1	2.37	0.54
1:B:988:ALA:CA	1:B:992:LEU:HD12	2.37	0.54
1:A:474:VAL:HA	1:A:477:GLN:HE21	1.71	0.54
1:A:880:HIS:N	1:A:881:PRO:CD	2.71	0.54
1:B:140:ILE:HD12	1:B:141:LYS:H	1.73	0.54
1:B:628:ASN:HA	1:B:678:ARG:NH1	2.22	0.54
1:A:513:PHE:CD1	1:A:566:THR:HG23	2.42	0.54
1:B:389:TYR:HB3	1:B:425:LEU:HD21	1.89	0.54
1:B:571:PRO:HG2	1:B:576:MET:SD	2.48	0.54
1:A:367:PHE:O	1:A:368:ILE:HG23	2.08	0.54
1:B:488:SER:OG	1:B:491:ARG:NH1	2.41	0.54
1:B:724:THR:HB	1:B:726:VAL:HG12	1.88	0.54
1:B:315:ILE:HG12	1:B:757:MET:HG3	1.90	0.54
1:A:836:ARG:HD3	1:A:984:LEU:CD1	2.38	0.54
1:B:155:VAL:HG13	1:B:216:ALA:HA	1.88	0.54
1:B:562:LEU:O	1:B:596:VAL:HG13	2.07	0.54
1:B:355:THR:HA	1:B:738:ASP:O	2.07	0.54
1:B:840:ILE:HG22	1:B:841:GLY:N	2.23	0.54
1:A:155:VAL:HG13	1:A:216:ALA:HA	1.89	0.54
1:A:276:ILE:HA	1:A:279:PHE:CD2	2.42	0.54
1:A:724:THR:HB	1:A:726:VAL:HG12	1.89	0.54
1:B:826:GLU:O	1:B:827:PRO:O	2.26	0.54
1:B:962:LEU:CD2	1:B:966:GLN:HB3	2.38	0.54
1:A:176:ASP:O	1:A:212:THR:HG23	2.07	0.54
1:A:214:ILE:N	1:A:214:ILE:HD13	2.14	0.54
1:A:678:ARG:NH1	1:A:678:ARG:HG3	2.22	0.54
1:B:50:TRP:CE3	1:B:257:GLY:HA3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:PRO:HG2	1:A:576:MET:SD	2.48	0.54
1:B:794:TRP:HZ2	1:B:944:HIS:HA	1.72	0.54
1:A:164:ARG:HA	1:A:207:MET:SD	2.48	0.54
1:A:726:VAL:HG13	1:A:727:ALA:H	1.72	0.54
1:B:153:VAL:O	1:B:218:LYS:HA	2.07	0.54
1:B:192:GLU:HB3	1:B:193:PRO:HD2	1.90	0.54
1:B:726:VAL:HG13	1:B:727:ALA:H	1.72	0.54
1:B:308:PRO:CB	1:B:764:LEU:HG	2.38	0.53
1:A:628:ASN:HA	1:A:678:ARG:NH1	2.23	0.53
1:A:755:ASN:OD1	1:A:819:ARG:NH2	2.40	0.53
1:B:53:VAL:O	1:B:53:VAL:HG12	2.08	0.53
1:B:765:ILE:HG21	1:B:837:TYR:HD2	1.73	0.53
1:B:903:VAL:HG22	1:B:973:ILE:HG21	1.90	0.53
1:B:920:GLN:HA	1:B:920:GLN:OE1	2.08	0.53
1:A:627:ASP:O	1:A:678:ARG:HG2	2.09	0.53
1:A:903:VAL:CG2	1:A:973:ILE:HG21	2.39	0.53
1:B:176:ASP:O	1:B:212:THR:HG23	2.08	0.53
1:A:264:ILE:O	1:A:266:LEU:N	2.42	0.53
1:A:654:THR:HA	1:A:677:ALA:O	2.09	0.53
1:A:89:VAL:O	1:A:93:VAL:HG23	2.07	0.53
1:B:104:VAL:HG21	1:B:797:LEU:HD11	1.91	0.53
1:B:513:PHE:CD1	1:B:566:THR:HG23	2.44	0.53
1:B:322:GLY:HA3	1:B:753:ILE:HD11	1.91	0.53
1:A:279:PHE:HE1	1:A:295:TYR:HB2	1.72	0.53
1:A:788:ILE:HB	1:A:789:PRO:HD2	1.90	0.53
1:A:751:ARG:CB	1:A:816:ILE:HD11	2.38	0.53
1:B:326:MET:HE3	1:B:333:VAL:HG21	1.89	0.53
1:B:82:GLU:HB2	1:B:83:GLU:OE1	2.09	0.53
1:A:110:ARG:HH11	1:A:110:ARG:HG3	1.73	0.53
1:B:2:GLU:CD	1:B:3:ALA:N	2.62	0.53
1:B:794:TRP:CZ2	1:B:944:HIS:HA	2.43	0.53
1:B:98:LEU:HA	1:B:101:ASN:HD22	1.72	0.53
1:A:358:THR:HG23	1:A:602:PRO:O	2.08	0.53
1:A:916:LEU:HD11	1:A:927:PRO:HA	1.91	0.53
1:B:656:ARG:HG2	1:B:656:ARG:HH11	1.73	0.53
1:B:762:ARG:NH2	1:B:836:ARG:HH12	2.07	0.53
1:A:367:PHE:HA	1:A:380:ASN:O	2.09	0.53
1:A:880:HIS:HA	1:A:883:PHE:CD2	2.45	0.52
1:B:123:GLU:O	1:B:123:GLU:HG2	2.09	0.52
1:B:836:ARG:HD3	1:B:984:LEU:CD1	2.40	0.52
1:A:98:LEU:HA	1:A:101:ASN:HD22	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ALA:O	1:B:214:ILE:CG1	2.58	0.52
1:B:246:LYS:HA	1:B:251:GLN:HG3	1.90	0.52
1:B:867:TYR:CG	1:B:868:HIS:N	2.78	0.52
1:B:913:LEU:HD22	1:B:927:PRO:HB3	1.91	0.52
1:B:799:THR:HB	1:B:908:GLU:OE1	2.09	0.52
1:A:459:VAL:HG23	1:A:460:ARG:N	2.23	0.52
1:B:369:ILE:HA	1:B:379:LEU:HD23	1.91	0.52
1:B:459:VAL:HG23	1:B:460:ARG:N	2.25	0.52
1:A:336:LEU:O	1:A:339:VAL:HG22	2.09	0.52
1:A:742:THR:O	1:A:743:ILE:C	2.48	0.52
1:A:765:ILE:HG21	1:A:837:TYR:CD2	2.44	0.52
1:B:228:VAL:HG22	1:B:228:VAL:O	2.09	0.52
1:B:311:LEU:HB3	1:B:312:PRO:CD	2.34	0.52
1:B:49:LEU:HB3	1:B:254:ASP:CG	2.30	0.52
1:A:920:GLN:HA	1:A:920:GLN:OE1	2.10	0.52
1:B:522:ILE:HD12	1:B:545:ILE:HG21	1.92	0.52
1:A:72:SER:HA	1:A:293:ILE:CD1	2.39	0.52
1:A:69:ALA:O	1:A:91:PRO:HG3	2.10	0.52
1:A:2:GLU:CD	1:A:3:ALA:N	2.62	0.52
1:B:627:ASP:O	1:B:678:ARG:HG2	2.10	0.52
1:B:895:GLU:OE2	1:B:960:LYS:HG2	2.10	0.52
1:B:290:ARG:O	1:B:293:ILE:HG12	2.09	0.52
1:B:600:LEU:HD23	1:B:600:LEU:O	2.09	0.52
1:B:916:LEU:HD11	1:B:927:PRO:HA	1.91	0.52
1:A:825:LYS:CG	1:A:826:GLU:H	2.21	0.52
1:A:844:VAL:HG23	1:A:845:GLY:H	1.74	0.52
1:A:975:LEU:N	1:A:976:PRO:CD	2.73	0.52
1:B:620:ARG:NH2	1:B:670:CYS:O	2.42	0.52
1:B:862:GLY:O	1:B:865:VAL:HG13	2.10	0.52
1:A:252:LYS:NZ	1:A:826:GLU:O	2.40	0.51
1:B:100:ALA:O	1:B:104:VAL:HG23	2.10	0.51
1:B:747:VAL:HG12	1:B:748:GLU:N	2.25	0.51
1:B:763:TYR:CE1	1:B:912:ALA:HB2	2.45	0.51
1:A:264:ILE:C	1:A:266:LEU:H	2.14	0.51
1:A:384:ILE:HD12	1:A:384:ILE:N	2.25	0.51
1:B:174:ARG:HA	1:B:187:VAL:O	2.11	0.51
1:B:335:SER:OG	1:B:337:PRO:HG2	2.09	0.51
1:B:402:ILE:HD12	1:B:402:ILE:O	2.10	0.51
1:B:668:GLU:OE2	1:B:671:ARG:NH1	2.40	0.51
1:B:787:LEU:HD13	1:B:792:LEU:HD23	1.91	0.51
1:A:530:VAL:O	1:A:531:GLY:C	2.49	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:CD2	1:A:600:LEU:HD13	2.40	0.51
1:A:762:ARG:HG3	1:A:837:TYR:HE1	1.75	0.51
1:A:763:TYR:CD1	1:A:912:ALA:HA	2.45	0.51
1:A:795:VAL:HG22	1:A:901:LEU:CD1	2.40	0.51
1:B:717:GLY:O	1:B:731:SER:HB2	2.11	0.51
1:B:887:ASP:CB	1:B:890:ILE:HG23	2.36	0.51
1:A:363:VAL:HG11	1:A:448:LEU:HD22	1.93	0.51
1:A:791:GLN:O	1:A:795:VAL:HG23	2.11	0.51
1:B:784:PRO:HA	1:B:873:PHE:CE2	2.46	0.51
1:A:467:ARG:HH11	1:A:467:ARG:CG	2.24	0.51
1:A:836:ARG:NH1	1:A:836:ARG:HG2	2.24	0.51
1:B:72:SER:O	1:B:75:LEU:HG	2.08	0.51
1:A:903:VAL:HG22	1:A:973:ILE:HG21	1.92	0.51
1:B:110:ARG:HG3	1:B:110:ARG:HH11	1.75	0.51
1:B:214:ILE:N	1:B:214:ILE:HD13	2.17	0.51
1:B:367:PHE:O	1:B:368:ILE:HG23	2.10	0.51
1:A:100:ALA:O	1:A:104:VAL:HG23	2.11	0.51
1:A:69:ALA:HA	1:A:297:LYS:NZ	2.25	0.51
1:A:319:LEU:CD1	1:A:339:VAL:HG21	2.40	0.51
1:B:753:ILE:O	1:B:753:ILE:HG22	2.11	0.51
1:A:122:TYR:O	1:A:124:PRO:CD	2.59	0.51
1:A:270:ALA:O	1:A:274:ILE:HG23	2.11	0.51
1:A:44:GLU:OE2	1:A:45:GLU:HG3	2.11	0.51
1:A:840:ILE:HD11	1:A:981:ASP:HB2	1.93	0.51
1:B:249:LEU:O	1:B:252:LYS:N	2.43	0.51
1:B:347:VAL:HG21	1:B:696:GLU:HG2	1.90	0.51
1:A:881:PRO:HG2	1:A:882:HIS:N	2.21	0.51
1:B:49:LEU:HD21	1:B:258:GLU:OE1	2.11	0.51
1:B:883:PHE:HD2	1:B:883:PHE:H	1.58	0.51
1:B:975:LEU:N	1:B:976:PRO:CD	2.74	0.50
1:A:950:VAL:C	1:A:952:PRO:HD2	2.31	0.50
1:B:116:ILE:HG22	1:B:116:ILE:O	2.10	0.50
1:B:154:ALA:O	1:B:214:ILE:HG13	2.11	0.50
1:B:157:ASP:O	1:B:214:ILE:HD13	2.12	0.50
1:B:256:PHE:C	1:B:258:GLU:H	2.15	0.50
1:B:269:VAL:O	1:B:269:VAL:HG12	2.12	0.50
1:A:111:ASN:ND2	1:A:111:ASN:H	2.05	0.50
1:A:522:ILE:HD12	1:A:545:ILE:HG21	1.92	0.50
1:A:881:PRO:CG	1:A:882:HIS:H	2.19	0.50
1:A:843:TYR:HE2	1:A:907:ILE:HD11	1.75	0.50
1:B:315:ILE:O	1:B:317:THR:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:HD3	1:A:585:MET:HA	1.92	0.50
1:A:737:ASP:O	1:A:738:ASP:HB2	2.12	0.50
1:A:833:LEU:O	1:A:836:ARG:HB3	2.11	0.50
1:B:49:LEU:HD23	1:B:254:ASP:HB3	1.93	0.50
1:B:963:ASP:N	1:B:966:GLN:HB2	2.27	0.50
1:A:258:GLU:O	1:A:262:LYS:HG2	2.12	0.50
1:A:54:ILE:CG2	1:A:261:SER:HB3	2.41	0.50
1:A:72:SER:O	1:A:75:LEU:HG	2.09	0.50
1:A:752:ALA:N	1:A:816:ILE:HD11	2.27	0.50
1:A:848:THR:C	1:A:850:GLY:H	2.15	0.50
1:B:347:VAL:HB	1:B:698:THR:HG23	1.93	0.50
1:B:363:VAL:HG11	1:B:448:LEU:HD22	1.94	0.50
1:B:484:THR:CB	1:B:496:VAL:HG12	2.42	0.50
1:B:357:THR:HG23	1:B:601:ASP:OD2	2.12	0.50
1:B:69:ALA:O	1:B:91:PRO:HG3	2.12	0.50
1:B:953:LEU:O	1:B:955:MET:N	2.44	0.50
1:B:921:SER:HA	1:B:982:GLU:OE2	2.12	0.50
1:A:157:ASP:O	1:A:214:ILE:HD13	2.12	0.50
1:A:907:ILE:CG2	1:A:908:GLU:N	2.75	0.50
1:B:104:VAL:HG13	1:B:802:LEU:CD2	2.41	0.50
1:B:353:THR:O	1:B:353:THR:HG22	2.12	0.50
1:B:642:PHE:CD2	1:B:648:VAL:HG11	2.46	0.50
1:B:903:VAL:CG2	1:B:973:ILE:HG21	2.42	0.50
1:A:164:ARG:CZ	1:A:206:ASN:HD22	2.25	0.50
1:A:290:ARG:O	1:A:293:ILE:HG12	2.11	0.50
1:A:798:VAL:O	1:A:909:MET:HE1	2.11	0.50
1:A:907:ILE:HG23	1:A:908:GLU:N	2.27	0.50
1:A:988:ALA:CB	1:A:992:LEU:HD12	2.41	0.50
1:B:111:ASN:H	1:B:111:ASN:ND2	2.06	0.50
1:B:387:SER:HB3	1:B:602:PRO:HG3	1.93	0.50
1:B:368:ILE:HG22	1:B:595:GLY:HA3	1.94	0.50
1:B:870:LEU:O	1:B:873:PHE:HB3	2.12	0.50
1:A:777:LEU:O	1:A:781:LEU:HG	2.11	0.49
1:A:832:TRP:CZ3	1:A:992:LEU:HD11	2.47	0.49
1:A:123:GLU:OE2	1:A:734:VAL:HG21	2.12	0.49
1:A:239:MET:HG3	1:A:240:ALA:H	1.77	0.49
1:A:347:VAL:HB	1:A:698:THR:HG23	1.94	0.49
1:A:963:ASP:N	1:A:966:GLN:HB2	2.27	0.49
1:B:491:ARG:HD3	1:B:585:MET:HA	1.93	0.49
1:B:718:ILE:HD13	1:B:743:ILE:HG12	1.94	0.49
1:B:72:SER:HA	1:B:293:ILE:CD1	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:ILE:HG23	1:B:908:GLU:N	2.27	0.49
1:A:369:ILE:HA	1:A:379:LEU:HD23	1.94	0.49
1:A:620:ARG:NH2	1:A:691:LEU:HD21	2.27	0.49
1:B:122:TYR:O	1:B:124:PRO:N	2.45	0.49
1:B:559:LEU:CD2	1:B:600:LEU:HD13	2.41	0.49
1:A:228:VAL:HG22	1:A:228:VAL:O	2.12	0.49
1:A:463:SER:O	1:A:466:GLU:HB2	2.12	0.49
1:A:836:ARG:HH11	1:A:836:ARG:HG2	1.77	0.49
1:A:953:LEU:N	1:A:954:PRO:HD2	2.27	0.49
1:A:953:LEU:O	1:A:955:MET:N	2.44	0.49
1:B:342:LEU:HD12	1:B:716:ILE:CD1	2.41	0.49
1:B:742:THR:O	1:B:743:ILE:C	2.51	0.49
1:A:342:LEU:HD12	1:A:716:ILE:CD1	2.40	0.49
1:B:264:ILE:O	1:B:266:LEU:N	2.46	0.49
1:A:269:VAL:O	1:A:269:VAL:HG12	2.13	0.49
1:A:780:ALA:O	1:A:782:GLY:N	2.43	0.49
1:B:104:VAL:HG13	1:B:802:LEU:HD21	1.93	0.49
1:B:258:GLU:O	1:B:262:LYS:HG2	2.13	0.49
1:A:333:VAL:HG11	1:A:339:VAL:CG1	2.43	0.49
1:A:603:PRO:HB3	1:A:639:ILE:HG22	1.95	0.49
1:A:668:GLU:OE2	1:A:671:ARG:NH1	2.42	0.49
1:B:188:ILE:HG22	1:B:189:LYS:N	2.27	0.49
1:B:264:ILE:C	1:B:266:LEU:H	2.16	0.49
1:B:495:SER:CB	1:B:514:VAL:HG22	2.43	0.49
1:B:49:LEU:O	1:B:53:VAL:HG23	2.12	0.49
1:B:678:ARG:HG3	1:B:678:ARG:NH1	2.20	0.49
1:A:154:ALA:O	1:A:214:ILE:CG1	2.61	0.49
1:A:799:THR:HG21	1:A:908:GLU:HB2	1.93	0.49
1:B:333:VAL:HG11	1:B:339:VAL:CG1	2.43	0.49
1:B:577:VAL:O	1:B:577:VAL:HG23	2.13	0.49
1:B:783:LEU:HD13	1:B:784:PRO:HD3	1.95	0.49
1:B:893:ALA:C	1:B:896:PRO:HD2	2.33	0.49
1:A:188:ILE:HG22	1:A:189:LYS:N	2.27	0.49
1:A:204:LYS:O	1:A:206:ASN:N	2.43	0.49
1:A:770:GLY:HA3	1:A:844:VAL:HG21	1.92	0.49
1:B:122:TYR:O	1:B:123:GLU:C	2.50	0.49
1:B:463:SER:O	1:B:466:GLU:HB2	2.12	0.49
1:A:287:SER:HB3	1:A:290:ARG:HD3	1.95	0.49
1:A:353:THR:O	1:A:353:THR:CG2	2.61	0.49
1:A:784:PRO:HG3	1:A:856:PHE:CE2	2.47	0.49
1:A:906:THR:HG22	1:A:974:SER:CB	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:O	1:A:293:ILE:HG23	2.13	0.48
1:A:369:ILE:N	1:A:369:ILE:CD1	2.76	0.48
1:A:509:GLY:O	1:A:511:LYS:HG2	2.13	0.48
1:A:530:VAL:HB	1:A:533:THR:OG1	2.12	0.48
1:A:949:TYR:CD1	1:A:949:TYR:N	2.81	0.48
1:B:620:ARG:NH2	1:B:691:LEU:HD21	2.28	0.48
1:B:635:ILE:O	1:B:639:ILE:HG12	2.13	0.48
1:B:69:ALA:HA	1:B:297:LYS:NZ	2.27	0.48
1:A:111:ASN:N	1:A:111:ASN:ND2	2.60	0.48
1:A:163:ILE:CD1	1:A:223:VAL:HG22	2.43	0.48
1:A:230:THR:HG22	1:A:232:ILE:HG22	1.94	0.48
1:A:463:SER:OG	1:A:466:GLU:HG3	2.13	0.48
1:A:823:SER:C	1:A:825:LYS:H	2.16	0.48
1:B:737:ASP:N	1:B:737:ASP:OD1	2.35	0.48
1:B:270:ALA:O	1:B:274:ILE:HG23	2.14	0.48
1:B:287:SER:HB3	1:B:290:ARG:HD3	1.95	0.48
1:B:289:ILE:O	1:B:293:ILE:HG23	2.13	0.48
1:A:204:LYS:C	1:A:206:ASN:H	2.15	0.48
1:B:134:ARG:HG3	1:B:134:ARG:NH1	2.29	0.48
1:B:164:ARG:HA	1:B:207:MET:SD	2.53	0.48
1:B:384:ILE:N	1:B:384:ILE:HD12	2.29	0.48
1:B:823:SER:HB2	1:B:826:GLU:HB2	1.94	0.48
1:B:869:GLN:HA	1:B:871:THR:HG22	1.94	0.48
1:B:794:TRP:CH2	1:B:943:LEU:O	2.66	0.48
1:A:859:ALA:O	1:A:861:ASP:N	2.47	0.48
1:B:293:ILE:O	1:B:297:LYS:HG3	2.13	0.48
1:B:33:LEU:O	1:B:37:GLY:N	2.42	0.48
1:B:756:ASN:CA	1:B:759:GLN:HE21	2.18	0.48
1:B:887:ASP:HB2	1:B:890:ILE:CG2	2.40	0.48
1:A:264:ILE:HD13	1:A:267:ILE:HD12	1.95	0.48
1:A:642:PHE:CG	1:A:648:VAL:HG11	2.48	0.48
1:B:539:GLY:N	1:B:540:PRO:CD	2.75	0.48
1:B:737:ASP:O	1:B:738:ASP:HB2	2.14	0.48
1:A:459:VAL:O	1:A:462:LEU:N	2.43	0.48
1:A:625:THR:OG1	1:A:626:GLY:N	2.46	0.48
1:B:953:LEU:C	1:B:955:MET:H	2.17	0.48
1:A:247:THR:HB	1:A:340:GLU:OE1	2.13	0.48
1:A:368:ILE:HG22	1:A:595:GLY:HA3	1.96	0.48
1:A:921:SER:HA	1:A:982:GLU:OE2	2.13	0.48
1:B:280:ASN:OD1	1:B:281:ASP:N	2.47	0.48
1:A:134:ARG:HG3	1:A:134:ARG:NH1	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:TRP:O	1:A:859:ALA:HB2	2.13	0.48
1:B:22:THR:HG22	1:B:135:LYS:HZ3	1.79	0.48
1:B:134:ARG:HG2	1:B:136:SER:H	1.79	0.48
1:B:163:ILE:CD1	1:B:223:VAL:HG22	2.44	0.48
1:B:288:TRP:HD1	1:B:289:ILE:HG13	1.78	0.48
1:B:540:PRO:O	1:B:543:GLU:HB2	2.14	0.48
1:B:631:THR:O	1:B:635:ILE:HG13	2.13	0.48
1:B:843:TYR:CD2	1:B:843:TYR:C	2.87	0.48
1:A:124:PRO:O	1:A:126:MET:HG2	2.14	0.48
1:A:1:MET:HB2	1:A:16:PHE:CZ	2.48	0.48
1:A:280:ASN:OD1	1:A:281:ASP:N	2.47	0.48
1:A:315:ILE:O	1:A:317:THR:N	2.47	0.48
1:A:369:ILE:CD1	1:A:593:PHE:HE1	2.26	0.48
1:A:865:VAL:HG12	1:A:866:THR:N	2.28	0.48
1:A:868:HIS:C	1:A:870:LEU:H	2.17	0.48
1:B:263:VAL:O	1:B:264:ILE:C	2.53	0.48
1:B:762:ARG:O	1:B:762:ARG:HG2	2.14	0.48
1:B:899:MET:HG2	1:B:962:LEU:CD2	2.42	0.48
1:A:539:GLY:N	1:A:540:PRO:CD	2.77	0.47
1:B:214:ILE:O	1:B:214:ILE:HG12	2.13	0.47
1:B:264:ILE:HD13	1:B:267:ILE:HD12	1.95	0.47
1:B:325:ARG:NH1	1:B:749:GLU:OE1	2.47	0.47
1:B:501:ALA:C	1:B:503:SER:H	2.17	0.47
1:B:689:GLU:HB2	1:B:713:LYS:HZ3	1.79	0.47
1:B:811:PRO:HG2	1:B:929:VAL:CG1	2.43	0.47
1:B:949:TYR:CD1	1:B:949:TYR:N	2.82	0.47
1:B:950:VAL:C	1:B:952:PRO:HD2	2.34	0.47
1:A:256:PHE:C	1:A:258:GLU:H	2.17	0.47
1:A:322:GLY:HA3	1:A:753:ILE:HD11	1.96	0.47
1:A:84:THR:O	1:A:85:ILE:HB	2.14	0.47
1:B:111:ASN:N	1:B:111:ASN:ND2	2.61	0.47
1:B:530:VAL:HB	1:B:533:THR:OG1	2.13	0.47
1:B:745:ALA:O	1:B:746:ALA:C	2.52	0.47
1:B:953:LEU:O	1:B:956:ILE:N	2.48	0.47
1:A:311:LEU:HB3	1:A:312:PRO:CD	2.38	0.47
1:A:797:LEU:O	1:A:797:LEU:HD23	2.13	0.47
1:B:798:VAL:O	1:B:909:MET:CE	2.57	0.47
1:B:794:TRP:HH2	1:B:943:LEU:O	1.97	0.47
1:B:979:GLY:O	1:B:983:ILE:HG13	2.14	0.47
1:A:15:TYR:O	1:A:15:TYR:CD1	2.67	0.47
1:A:371:LYS:O	1:A:377:CYS:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:ARG:HE	1:A:588:GLU:CD	2.18	0.47
1:A:538:THR:HB	1:A:540:PRO:HD2	1.97	0.47
1:B:509:GLY:O	1:B:511:LYS:HG2	2.13	0.47
1:B:717:GLY:C	1:B:731:SER:HB2	2.35	0.47
1:B:794:TRP:HE1	1:B:944:HIS:CE1	2.31	0.47
1:B:826:GLU:HA	1:B:827:PRO:HD2	1.66	0.47
1:A:751:ARG:C	1:A:816:ILE:HD11	2.34	0.47
1:A:895:GLU:N	1:A:896:PRO:HD2	2.29	0.47
1:A:953:LEU:C	1:A:955:MET:H	2.18	0.47
1:B:369:ILE:CD1	1:B:593:PHE:HE1	2.27	0.47
1:B:306:ALA:C	1:B:768:ASN:HD21	2.16	0.47
1:B:271:VAL:HG22	1:B:776:PHE:HE1	1.78	0.47
1:B:887:ASP:O	1:B:890:ILE:HG12	2.14	0.47
1:A:293:ILE:O	1:A:297:LYS:HG3	2.14	0.47
1:A:886:LEU:O	1:A:886:LEU:HD12	2.14	0.47
1:B:245:ASP:OD1	1:B:246:LYS:N	2.47	0.47
1:B:50:TRP:C	1:B:52:LEU:H	2.18	0.47
1:B:549:ILE:HG22	1:B:549:ILE:O	2.15	0.47
1:B:748:GLU:HG3	1:B:817:MET:HG2	1.96	0.47
1:B:756:ASN:HD21	1:B:810:ASN:HB2	1.80	0.47
1:B:857:MET:HE3	1:B:858:TYR:HE1	1.79	0.47
1:A:263:VAL:CG1	1:A:267:ILE:HD11	2.31	0.47
1:A:577:VAL:HG23	1:A:577:VAL:O	2.15	0.47
1:B:467:ARG:CG	1:B:467:ARG:HH11	2.25	0.47
1:A:449:VAL:O	1:A:453:ASN:N	2.37	0.47
1:B:413:LEU:HG	1:B:564:LEU:HD12	1.96	0.47
1:B:786:ALA:O	1:B:787:LEU:HG	2.15	0.47
1:A:288:TRP:HD1	1:A:289:ILE:HG13	1.79	0.47
1:A:467:ARG:O	1:A:467:ARG:HD2	2.15	0.47
1:A:953:LEU:O	1:A:956:ILE:N	2.48	0.47
1:B:369:ILE:CD1	1:B:369:ILE:N	2.77	0.47
1:B:271:VAL:HG22	1:B:776:PHE:CE1	2.50	0.47
1:A:413:LEU:O	1:A:413:LEU:HD23	2.15	0.47
1:A:470:ALA:O	1:A:473:SER:N	2.48	0.47
1:A:484:THR:CB	1:A:496:VAL:HG12	2.45	0.47
1:A:876:CYS:C	1:A:888:CYS:SG	2.92	0.47
1:B:303:ALA:O	1:B:306:ALA:N	2.45	0.47
1:B:474:VAL:HA	1:B:477:GLN:NE2	2.30	0.47
1:A:496:VAL:O	1:A:512:MET:HA	2.15	0.47
1:A:54:ILE:C	1:A:54:ILE:HD12	2.35	0.47
1:A:763:TYR:CD2	1:A:764:LEU:HD23	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:O	1:B:113:GLU:HG2	2.15	0.47
1:B:129:VAL:CG1	1:B:151:VAL:HG22	2.35	0.47
1:B:161:ALA:CA	1:B:210:SER:HB2	2.41	0.47
1:B:253:LEU:HD21	1:B:315:ILE:HD11	1.97	0.47
1:B:895:GLU:N	1:B:896:PRO:CD	2.78	0.47
1:B:953:LEU:N	1:B:954:PRO:HD2	2.29	0.47
1:B:963:ASP:H	1:B:966:GLN:HB2	1.79	0.47
1:A:247:THR:CB	1:A:340:GLU:OE1	2.62	0.46
1:A:895:GLU:H	1:A:895:GLU:CD	2.05	0.46
1:A:933:LEU:O	1:A:937:ILE:HG13	2.14	0.46
1:A:963:ASP:H	1:A:966:GLN:HB2	1.79	0.46
1:B:434:TYR:OH	1:B:464:LYS:HG3	2.15	0.46
1:A:354:GLY:O	1:A:604:ARG:HD2	2.15	0.46
1:A:836:ARG:HD3	1:A:984:LEU:HD13	1.96	0.46
1:B:1:MET:HB2	1:B:16:PHE:CZ	2.49	0.46
1:B:247:THR:H	1:B:251:GLN:CG	2.28	0.46
1:B:400:LYS:HA	1:B:401:PRO:HD3	1.81	0.46
1:B:658:PHE:CA	1:B:661:LEU:HD12	2.35	0.46
1:B:913:LEU:O	1:B:922:LEU:HD21	2.15	0.46
1:A:859:ALA:O	1:A:860:GLU:C	2.53	0.46
1:A:949:TYR:N	1:A:949:TYR:HD1	2.13	0.46
1:B:496:VAL:O	1:B:512:MET:HA	2.15	0.46
1:B:538:THR:HB	1:B:540:PRO:HD2	1.98	0.46
1:B:836:ARG:HH11	1:B:836:ARG:HG2	1.80	0.46
1:B:840:ILE:O	1:B:843:TYR:N	2.49	0.46
1:A:341:THR:O	1:A:344:CYS:N	2.34	0.46
1:A:474:VAL:HA	1:A:477:GLN:NE2	2.31	0.46
1:B:614:CYS:HB3	1:B:619:ILE:HB	1.97	0.46
1:B:352:LYS:HD2	1:B:635:ILE:HG21	1.97	0.46
1:A:867:TYR:CG	1:A:868:HIS:N	2.83	0.46
1:B:140:ILE:HG13	1:B:141:LYS:N	2.31	0.46
1:B:204:LYS:C	1:B:206:ASN:H	2.18	0.46
1:B:837:TYR:HD1	1:B:837:TYR:H	1.64	0.46
1:B:988:ALA:CB	1:B:992:LEU:HD12	2.44	0.46
1:A:140:ILE:HG13	1:A:141:LYS:N	2.31	0.46
1:A:238:GLN:HG3	1:A:238:GLN:O	2.16	0.46
1:A:285:GLY:HA3	1:A:290:ARG:CZ	2.46	0.46
1:A:637:ARG:HA	1:A:642:PHE:O	2.15	0.46
1:A:751:ARG:NH2	1:A:819:ARG:O	2.44	0.46
1:A:895:GLU:OE1	1:A:895:GLU:N	2.25	0.46
1:B:774:CYS:SG	1:B:848:THR:HG21	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:906:THR:HG21	1:B:970:VAL:HG12	1.98	0.46
1:B:974:SER:C	1:B:976:PRO:HD2	2.36	0.46
1:A:134:ARG:HG2	1:A:136:SER:H	1.80	0.46
1:A:154:ALA:O	1:A:214:ILE:HG13	2.15	0.46
1:B:306:ALA:HA	1:B:768:ASN:ND2	2.31	0.46
1:B:907:ILE:CG2	1:B:908:GLU:N	2.78	0.46
1:A:122:TYR:C	1:A:124:PRO:HD3	2.35	0.46
1:B:14:ALA:O	1:B:16:PHE:N	2.49	0.46
1:B:230:THR:HG22	1:B:232:ILE:HG22	1.96	0.46
1:B:795:VAL:CG1	1:B:904:LEU:HG	2.42	0.46
1:B:911:ASN:O	1:B:914:ASN:HB2	2.16	0.46
1:B:341:THR:O	1:B:344:CYS:N	2.35	0.46
1:B:413:LEU:HD23	1:B:413:LEU:O	2.16	0.46
1:B:442:GLU:O	1:B:445:LEU:N	2.48	0.46
1:B:637:ARG:HA	1:B:642:PHE:O	2.16	0.46
1:B:84:THR:O	1:B:85:ILE:HB	2.16	0.46
1:A:25:THR:HG22	1:A:132:ALA:CB	2.43	0.46
1:B:157:ASP:HB2	1:B:214:ILE:HD11	1.98	0.46
1:B:527:TYR:CD1	1:B:534:ARG:HD3	2.51	0.46
1:B:788:ILE:CB	1:B:789:PRO:CD	2.93	0.46
1:B:843:TYR:CD2	1:B:844:VAL:N	2.83	0.46
1:B:869:GLN:OE1	1:B:872:HIS:HD2	1.99	0.46
1:B:953:LEU:C	1:B:955:MET:N	2.69	0.46
1:A:459:VAL:O	1:A:460:ARG:C	2.55	0.45
1:A:540:PRO:O	1:A:543:GLU:HB2	2.16	0.45
1:A:823:SER:O	1:A:826:GLU:HG2	2.15	0.45
1:A:844:VAL:HG23	1:A:845:GLY:N	2.30	0.45
1:B:625:THR:OG1	1:B:626:GLY:N	2.49	0.45
1:B:855:TRP:CE3	1:B:856:PHE:HA	2.51	0.45
1:A:230:THR:HG22	1:A:232:ILE:N	2.29	0.45
1:A:510:ASN:O	1:A:511:LYS:HD3	2.17	0.45
1:A:352:LYS:HE2	1:A:627:ASP:OD1	2.16	0.45
1:A:656:ARG:HH11	1:A:656:ARG:HG2	1.81	0.45
1:A:829:ILE:HD13	1:A:837:TYR:CE2	2.51	0.45
1:B:158:LYS:O	1:B:160:PRO:HD3	2.17	0.45
1:B:15:TYR:CD1	1:B:15:TYR:O	2.69	0.45
1:A:501:ALA:C	1:A:503:SER:H	2.19	0.45
1:A:562:LEU:O	1:A:596:VAL:HG13	2.16	0.45
1:A:82:GLU:HB2	1:A:83:GLU:H	1.43	0.45
1:B:788:ILE:HG12	1:B:791:GLN:CG	2.46	0.45
1:B:798:VAL:CG1	1:B:940:SER:HB3	2.39	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLN:HB3	1:A:805:THR:OG1	2.15	0.45
1:A:263:VAL:O	1:A:264:ILE:C	2.55	0.45
1:A:449:VAL:CG2	1:A:450:GLU:N	2.79	0.45
1:A:718:ILE:HD13	1:A:743:ILE:HG12	1.99	0.45
1:A:75:LEU:HD12	1:A:76:ALA:CB	2.46	0.45
1:A:877:THR:O	1:A:878:GLU:HB3	2.16	0.45
1:B:154:ALA:O	1:B:214:ILE:CD1	2.64	0.45
1:B:230:THR:HG22	1:B:232:ILE:N	2.30	0.45
1:B:637:ARG:HD3	1:B:644:GLU:O	2.17	0.45
1:B:770:GLY:HA3	1:B:841:GLY:O	2.15	0.45
1:B:274:ILE:HD13	1:B:776:PHE:CZ	2.51	0.45
1:B:769:VAL:CG1	1:B:841:GLY:HA3	2.43	0.45
1:A:413:LEU:HG	1:A:564:LEU:CD1	2.47	0.45
1:A:662:PRO:O	1:A:665:GLU:N	2.42	0.45
1:A:783:LEU:HD22	1:A:784:PRO:CD	2.39	0.45
1:B:759:GLN:C	1:B:761:ILE:N	2.68	0.45
1:B:949:TYR:N	1:B:949:TYR:HD1	2.13	0.45
1:B:903:VAL:HG13	1:B:973:ILE:CG2	2.46	0.45
1:A:895:GLU:O	1:A:899:MET:N	2.49	0.45
1:A:974:SER:C	1:A:976:PRO:HD2	2.37	0.45
1:B:110:ARG:O	1:B:114:ASN:N	2.49	0.45
1:B:855:TRP:O	1:B:859:ALA:HB2	2.16	0.45
1:B:869:GLN:C	1:B:871:THR:N	2.67	0.45
1:A:303:ALA:O	1:A:304:VAL:C	2.55	0.45
1:A:766:SER:O	1:A:769:VAL:HG12	2.17	0.45
1:B:326:MET:HE1	1:B:333:VAL:HG21	1.97	0.45
1:B:352:LYS:HE2	1:B:627:ASP:OD1	2.16	0.45
1:B:467:ARG:HA	1:B:467:ARG:HD2	1.64	0.45
1:B:85:ILE:HG22	1:B:85:ILE:O	2.17	0.45
1:A:157:ASP:HB2	1:A:214:ILE:HD11	1.99	0.45
1:A:22:THR:HG22	1:A:135:LYS:HZ1	1.81	0.45
1:B:50:TRP:CE3	1:B:257:GLY:CA	3.00	0.45
1:B:449:VAL:O	1:B:453:ASN:N	2.36	0.45
1:B:633:ILE:O	1:B:636:CYS:HB2	2.17	0.45
1:B:75:LEU:HD12	1:B:76:ALA:CB	2.47	0.45
1:A:100:ALA:CA	1:A:103:ILE:HG22	2.43	0.45
1:A:527:TYR:O	1:A:592:THR:HA	2.17	0.45
1:A:549:ILE:O	1:A:549:ILE:HG22	2.17	0.45
1:A:66:LEU:HD12	1:A:94:ILE:CD1	2.47	0.45
1:B:650:ASP:N	1:B:650:ASP:OD1	2.50	0.45
1:B:66:LEU:HD12	1:B:94:ILE:CD1	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLU:O	1:A:113:GLU:HG2	2.16	0.45
1:A:110:ARG:O	1:A:114:ASN:N	2.49	0.45
1:A:140:ILE:CD1	1:A:141:LYS:H	2.30	0.45
1:B:131:ARG:NH1	1:B:131:ARG:HG3	2.30	0.45
1:B:231:GLU:HA	1:B:231:GLU:OE1	2.16	0.45
1:B:799:THR:HG21	1:B:908:GLU:HB2	1.99	0.45
1:B:980:LEU:HA	1:B:983:ILE:CD1	2.37	0.45
1:A:899:MET:SD	1:A:962:LEU:HD22	2.57	0.44
1:B:204:LYS:O	1:B:206:ASN:N	2.47	0.44
1:B:303:ALA:O	1:B:304:VAL:C	2.56	0.44
1:B:491:ARG:HE	1:B:588:GLU:CD	2.21	0.44
1:B:662:PRO:O	1:B:665:GLU:N	2.42	0.44
1:B:794:TRP:NE1	1:B:944:HIS:ND1	2.63	0.44
1:A:717:GLY:O	1:A:731:SER:HB2	2.18	0.44
1:A:85:ILE:O	1:A:85:ILE:HG22	2.17	0.44
1:A:884:GLU:C	1:A:886:LEU:H	2.20	0.44
1:A:927:PRO:O	1:A:934:LEU:HD21	2.17	0.44
1:B:247:THR:H	1:B:251:GLN:HG2	1.81	0.44
1:B:773:VAL:HG21	1:B:842:GLY:HA2	1.99	0.44
1:A:35:LYS:HE3	1:A:36:TYR:CZ	2.53	0.44
1:A:637:ARG:HD3	1:A:644:GLU:O	2.17	0.44
1:B:611:ILE:HD13	1:B:641:ILE:HG13	2.00	0.44
1:B:977:VAL:HG13	1:B:978:ILE:N	2.32	0.44
1:A:39:ASN:HB3	1:A:142:ALA:O	2.17	0.44
1:A:271:VAL:C	1:A:273:LEU:N	2.70	0.44
1:A:402:ILE:HD12	1:A:402:ILE:O	2.16	0.44
1:A:953:LEU:C	1:A:955:MET:N	2.70	0.44
1:B:249:LEU:O	1:B:250:GLN:C	2.56	0.44
1:B:767:SER:CB	1:B:911:ASN:ND2	2.64	0.44
1:B:832:TRP:CH2	1:B:992:LEU:HD11	2.53	0.44
1:A:390:ALA:HA	1:A:391:PRO:HD3	1.89	0.44
1:A:631:THR:O	1:A:635:ILE:HG13	2.17	0.44
1:A:778:THR:HG22	1:A:849:VAL:CG1	2.47	0.44
1:A:899:MET:O	1:A:903:VAL:HG23	2.17	0.44
1:A:977:VAL:HG13	1:A:978:ILE:N	2.33	0.44
1:B:459:VAL:O	1:B:460:ARG:C	2.56	0.44
1:B:315:ILE:CG1	1:B:757:MET:HG3	2.48	0.44
1:B:771:GLU:O	1:B:774:CYS:HB3	2.17	0.44
1:B:893:ALA:O	1:B:896:PRO:CG	2.66	0.44
1:A:158:LYS:O	1:A:160:PRO:HD3	2.18	0.44
1:A:527:TYR:CD1	1:A:534:ARG:HD3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:ASN:OD1	1:A:916:LEU:HD23	2.18	0.44
1:A:823:SER:C	1:A:825:LYS:N	2.70	0.44
1:B:765:ILE:HG21	1:B:837:TYR:CD2	2.53	0.44
1:A:214:ILE:HG12	1:A:214:ILE:O	2.16	0.44
1:A:445:LEU:O	1:A:448:LEU:HB3	2.18	0.44
1:A:548:VAL:C	1:A:550:LYS:N	2.71	0.44
1:A:737:ASP:O	1:A:738:ASP:CB	2.65	0.44
1:B:39:ASN:HB3	1:B:142:ALA:O	2.17	0.44
1:B:97:ILE:HG21	1:B:793:LEU:HB3	1.99	0.44
1:A:449:VAL:HG23	1:A:450:GLU:N	2.33	0.44
1:A:836:ARG:NH1	1:A:836:ARG:CG	2.78	0.44
1:B:128:LYS:HD2	1:B:137:VAL:HG11	2.00	0.44
1:B:392:GLU:O	1:B:451:LYS:HE2	2.18	0.44
1:B:617:ALA:HB1	1:B:751:ARG:NH1	2.26	0.44
1:B:755:ASN:HA	1:B:758:LYS:HB2	2.00	0.44
1:B:763:TYR:CD1	1:B:912:ALA:HA	2.52	0.44
1:B:765:ILE:HG22	1:B:766:SER:N	2.33	0.44
1:B:778:THR:HG22	1:B:849:VAL:HG13	1.99	0.44
1:A:338:SER:C	1:A:340:GLU:N	2.71	0.44
1:A:764:LEU:O	1:A:765:ILE:C	2.55	0.44
1:A:869:GLN:NE2	1:A:872:HIS:CD2	2.86	0.44
1:A:962:LEU:HD23	1:A:966:GLN:HB3	2.00	0.44
1:B:264:ILE:HA	1:B:267:ILE:CD1	2.47	0.44
1:B:48:SER:HB2	1:B:254:ASP:OD1	2.17	0.44
1:B:881:PRO:O	1:B:882:HIS:HB2	2.18	0.44
1:A:110:ARG:NH1	1:A:110:ARG:HG3	2.33	0.43
1:A:512:MET:HB2	1:A:567:ARG:HB3	1.99	0.43
1:A:906:THR:CG2	1:A:974:SER:HB2	2.48	0.43
1:B:25:THR:HG22	1:B:132:ALA:CB	2.44	0.43
1:B:285:GLY:HA3	1:B:290:ARG:CZ	2.48	0.43
1:B:446:THR:HG23	1:B:472:ASN:ND2	2.33	0.43
1:B:539:GLY:H	1:B:540:PRO:HD2	1.82	0.43
1:B:847:ALA:O	1:B:851:ALA:HB2	2.18	0.43
1:A:166:LEU:HG	1:A:221:GLY:HA2	1.99	0.43
1:A:97:ILE:O	1:A:100:ALA:N	2.51	0.43
1:B:706:ASN:HA	1:B:706:ASN:HD22	1.55	0.43
1:B:836:ARG:NH1	1:B:836:ARG:HG2	2.33	0.43
1:B:893:ALA:O	1:B:896:PRO:CD	2.63	0.43
1:A:388:THR:OG1	1:A:389:TYR:N	2.51	0.43
1:A:499:SER:O	1:A:500:PRO:C	2.57	0.43
1:A:617:ALA:HB2	1:A:817:MET:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ASP:OD1	1:A:650:ASP:N	2.51	0.43
1:A:841:GLY:HA2	1:A:844:VAL:CG2	2.49	0.43
1:A:832:TRP:CH2	1:A:992:LEU:HD11	2.53	0.43
1:B:542:LYS:O	1:B:546:LEU:HD12	2.19	0.43
1:A:131:ARG:NH1	1:A:131:ARG:HG3	2.32	0.43
1:A:239:MET:HG3	1:A:240:ALA:N	2.33	0.43
1:A:542:LYS:O	1:A:546:LEU:HD12	2.18	0.43
1:A:679:VAL:HG13	1:A:683:HIS:ND1	2.33	0.43
1:B:196:ASP:HA	1:B:197:PRO:HD2	1.92	0.43
1:B:565:ALA:HB2	1:B:593:PHE:HA	2.00	0.43
1:B:66:LEU:C	1:B:66:LEU:HD23	2.38	0.43
1:B:355:THR:HG22	1:B:740:PHE:HB2	2.01	0.43
1:A:311:LEU:CA	1:A:760:PHE:HE1	2.31	0.43
1:A:894:PRO:HD2	1:A:895:GLU:OE1	2.19	0.43
1:A:893:ALA:HA	1:A:894:PRO:HD3	1.80	0.43
1:A:930:ASN:C	1:A:930:ASN:OD1	2.57	0.43
1:B:164:ARG:CZ	1:B:206:ASN:HD22	2.32	0.43
1:B:378:SER:O	1:B:379:LEU:HD23	2.19	0.43
1:B:449:VAL:CG2	1:B:450:GLU:N	2.81	0.43
1:A:253:LEU:HD21	1:A:315:ILE:HD11	2.01	0.43
1:A:768:ASN:O	1:A:769:VAL:C	2.54	0.43
1:A:780:ALA:C	1:A:782:GLY:N	2.70	0.43
1:A:899:MET:HG2	1:A:962:LEU:CD2	2.46	0.43
1:B:32:HIS:O	1:B:36:TYR:HD2	2.01	0.43
1:B:358:THR:HG23	1:B:602:PRO:O	2.18	0.43
1:A:932:TRP:HD1	1:A:932:TRP:H	1.67	0.43
1:B:317:THR:O	1:B:318:CYS:C	2.57	0.43
1:B:832:TRP:CZ3	1:B:992:LEU:HD11	2.54	0.43
1:A:830:SER:O	1:A:833:LEU:N	2.51	0.43
1:B:100:ALA:CA	1:B:103:ILE:HG22	2.45	0.43
1:B:573:ARG:O	1:B:573:ARG:HD3	2.19	0.43
1:B:942:SER:C	1:B:944:HIS:N	2.72	0.43
1:B:945:PHE:HE1	1:B:967:TRP:CZ2	2.36	0.43
1:A:181:THR:C	1:A:183:GLU:H	2.22	0.43
1:A:264:ILE:HA	1:A:267:ILE:CD1	2.47	0.43
1:A:467:ARG:NH1	1:A:467:ARG:CG	2.82	0.43
1:B:248:PRO:O	1:B:252:LYS:HB2	2.19	0.43
1:A:378:SER:O	1:A:379:LEU:HD23	2.19	0.42
1:A:911:ASN:O	1:A:914:ASN:HB2	2.19	0.42
1:A:913:LEU:O	1:A:922:LEU:HD21	2.19	0.42
1:B:97:ILE:O	1:B:100:ALA:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ALA:C	1:B:120:LYS:N	2.72	0.42
1:B:125:GLU:HA	1:B:125:GLU:OE1	2.18	0.42
1:B:58:GLU:OE1	1:B:309:GLU:OE2	2.37	0.42
1:B:688:VAL:HG23	1:B:700:MET:HE1	2.01	0.42
1:B:798:VAL:HG12	1:B:798:VAL:O	2.19	0.42
1:B:83:GLU:O	1:B:83:GLU:HG2	2.19	0.42
1:A:346:SER:C	1:A:347:VAL:HG23	2.40	0.42
1:A:654:THR:HG23	1:A:657:GLU:OE1	2.18	0.42
1:B:166:LEU:HG	1:B:221:GLY:HA2	2.01	0.42
1:B:228:VAL:CG2	1:B:228:VAL:O	2.67	0.42
1:B:548:VAL:C	1:B:550:LYS:N	2.71	0.42
1:B:832:TRP:CD1	1:B:833:LEU:N	2.87	0.42
1:A:154:ALA:O	1:A:214:ILE:CD1	2.67	0.42
1:A:14:ALA:O	1:A:16:PHE:N	2.52	0.42
1:A:268:CYS:C	1:A:270:ALA:H	2.22	0.42
1:A:975:LEU:HA	1:A:975:LEU:HD12	1.90	0.42
1:B:271:VAL:CG2	1:B:776:PHE:HE1	2.32	0.42
1:B:679:VAL:HG13	1:B:683:HIS:ND1	2.34	0.42
1:B:691:LEU:HD23	1:B:691:LEU:HA	1.82	0.42
1:B:762:ARG:NE	1:B:836:ARG:NH1	2.67	0.42
1:A:434:TYR:OH	1:A:464:LYS:HG3	2.19	0.42
1:A:829:ILE:HD13	1:A:837:TYR:HE2	1.84	0.42
1:A:887:ASP:O	1:A:890:ILE:HG22	2.20	0.42
1:A:974:SER:O	1:A:977:VAL:HG12	2.18	0.42
1:B:59:ASP:O	1:B:63:ARG:HG3	2.19	0.42
1:A:249:LEU:HB2	1:A:340:GLU:CD	2.40	0.42
1:A:679:VAL:HG13	1:A:683:HIS:CG	2.54	0.42
1:A:825:LYS:CG	1:A:826:GLU:N	2.81	0.42
1:A:865:VAL:O	1:A:866:THR:HG23	2.20	0.42
1:A:945:PHE:HE1	1:A:967:TRP:CZ2	2.37	0.42
1:B:116:ILE:O	1:B:116:ILE:CG2	2.67	0.42
1:B:123:GLU:HA	1:B:124:PRO:HD2	1.76	0.42
1:B:329:LYS:O	1:B:330:ASN:HB2	2.19	0.42
1:B:402:ILE:HD12	1:B:402:ILE:C	2.40	0.42
1:B:656:ARG:HG2	1:B:656:ARG:NH1	2.34	0.42
1:B:755:ASN:O	1:B:756:ASN:C	2.56	0.42
1:A:303:ALA:O	1:A:306:ALA:N	2.50	0.42
1:A:317:THR:O	1:A:318:CYS:C	2.58	0.42
1:A:353:THR:O	1:A:353:THR:HG22	2.20	0.42
1:A:711:LEU:HD23	1:A:711:LEU:HA	1.84	0.42
1:A:753:ILE:HG22	1:A:753:ILE:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:GLU:O	1:A:83:GLU:HG2	2.19	0.42
1:A:867:TYR:C	1:A:869:GLN:N	2.72	0.42
1:B:181:THR:C	1:B:183:GLU:H	2.23	0.42
1:B:271:VAL:C	1:B:273:LEU:N	2.72	0.42
1:B:346:SER:C	1:B:347:VAL:HG23	2.40	0.42
1:B:449:VAL:HG23	1:B:450:GLU:N	2.35	0.42
1:B:499:SER:O	1:B:500:PRO:C	2.57	0.42
1:A:762:ARG:CG	1:A:837:TYR:CE1	3.01	0.42
1:A:851:ALA:HB2	1:A:903:VAL:HG21	2.01	0.42
1:B:35:LYS:HE3	1:B:36:TYR:CZ	2.55	0.42
1:B:306:ALA:CA	1:B:768:ASN:HD21	2.33	0.42
1:B:899:MET:SD	1:B:962:LEU:HD22	2.60	0.42
1:B:974:SER:O	1:B:977:VAL:HG12	2.19	0.42
1:A:335:SER:O	1:A:336:LEU:C	2.58	0.42
1:A:495:SER:CB	1:A:514:VAL:HG22	2.50	0.42
1:A:765:ILE:HG21	1:A:837:TYR:HD2	1.85	0.42
1:A:798:VAL:CG1	1:A:940:SER:HB3	2.48	0.42
1:B:336:LEU:N	1:B:337:PRO:CD	2.81	0.42
1:B:512:MET:HB2	1:B:567:ARG:HB3	2.02	0.42
1:B:964:LEU:O	1:B:968:LEU:HB2	2.19	0.42
1:A:54:ILE:HG22	1:A:261:SER:HB3	2.01	0.42
1:A:946:LEU:O	1:A:946:LEU:HD23	2.19	0.42
1:B:110:ARG:HG3	1:B:110:ARG:NH1	2.35	0.42
1:B:231:GLU:O	1:B:235:ILE:HG12	2.20	0.42
1:B:510:ASN:O	1:B:511:LYS:HD3	2.19	0.42
1:B:574:GLU:C	1:B:576:MET:H	2.22	0.42
1:B:833:LEU:O	1:B:836:ARG:HB3	2.20	0.42
1:A:174:ARG:HA	1:A:187:VAL:O	2.20	0.42
1:A:2:GLU:CG	1:A:3:ALA:N	2.83	0.42
1:A:667:ARG:HA	1:A:690:TYR:CD1	2.55	0.42
1:A:347:VAL:HG21	1:A:696:GLU:HG2	1.98	0.42
1:B:276:ILE:HG12	1:B:279:PHE:HE2	1.85	0.42
1:B:388:THR:OG1	1:B:389:TYR:N	2.53	0.42
1:B:495:SER:HB3	1:B:514:VAL:HG22	2.01	0.42
1:B:932:TRP:H	1:B:932:TRP:HD1	1.68	0.42
1:A:126:MET:HA	1:A:140:ILE:O	2.19	0.41
1:A:24:LEU:HD13	1:A:149:ASP:CA	2.37	0.41
1:A:267:ILE:HG21	1:A:772:VAL:CG1	2.46	0.41
1:A:27:ASP:O	1:A:31:ARG:HB2	2.20	0.41
1:A:66:LEU:HD23	1:A:66:LEU:C	2.40	0.41
1:B:267:ILE:HG13	1:B:267:ILE:H	1.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:PHE:CG	1:B:648:VAL:HG11	2.55	0.41
1:B:688:VAL:HG23	1:B:700:MET:CE	2.50	0.41
1:B:100:ALA:HB1	1:B:797:LEU:HD21	2.02	0.41
1:B:94:ILE:HG22	1:B:790:VAL:HG12	2.01	0.41
1:A:276:ILE:HG12	1:A:279:PHE:HE2	1.85	0.41
1:A:336:LEU:N	1:A:337:PRO:CD	2.81	0.41
1:A:335:SER:C	1:A:337:PRO:HD2	2.40	0.41
1:A:392:GLU:O	1:A:451:LYS:HE2	2.20	0.41
1:A:573:ARG:HD3	1:A:573:ARG:O	2.20	0.41
1:A:59:ASP:O	1:A:63:ARG:HG3	2.20	0.41
1:A:795:VAL:CG2	1:A:901:LEU:CD1	2.98	0.41
1:B:573:ARG:NH1	1:B:573:ARG:CG	2.83	0.41
1:B:811:PRO:HA	1:B:812:PRO:HD3	1.82	0.41
1:B:859:ALA:HB1	1:B:862:GLY:HA3	2.01	0.41
1:B:927:PRO:O	1:B:934:LEU:HD21	2.19	0.41
1:A:231:GLU:O	1:A:235:ILE:HG12	2.20	0.41
1:A:903:VAL:HG13	1:A:973:ILE:CG2	2.50	0.41
1:B:268:CYS:C	1:B:270:ALA:H	2.23	0.41
1:B:352:LYS:CD	1:B:635:ILE:HG21	2.51	0.41
1:B:855:TRP:CE3	1:B:856:PHE:N	2.89	0.41
1:B:89:VAL:HA	1:B:92:PHE:HD2	1.85	0.41
1:A:218:LYS:O	1:A:219:ALA:HB2	2.21	0.41
1:A:58:GLU:OE1	1:A:309:GLU:OE2	2.39	0.41
1:A:352:LYS:CD	1:A:635:ILE:HG21	2.50	0.41
1:B:311:LEU:HA	1:B:760:PHE:CE1	2.55	0.41
1:B:358:THR:HG22	1:B:604:ARG:HA	2.01	0.41
1:B:467:ARG:O	1:B:467:ARG:HD2	2.20	0.41
1:B:754:TYR:CE2	1:B:758:LYS:HG3	2.55	0.41
1:B:760:PHE:O	1:B:760:PHE:CG	2.73	0.41
1:B:926:PRO:HB2	1:B:928:TRP:CE2	2.55	0.41
1:A:262:LYS:O	1:A:263:VAL:C	2.58	0.41
1:A:866:THR:HG22	1:A:886:LEU:HD22	2.02	0.41
1:B:2:GLU:CG	1:B:3:ALA:N	2.83	0.41
1:B:735:LEU:HD13	1:B:739:ASN:O	2.19	0.41
1:B:939:LEU:O	1:B:939:LEU:HG	2.20	0.41
1:A:161:ALA:CA	1:A:210:SER:HB2	2.46	0.41
1:A:253:LEU:O	1:A:256:PHE:HB3	2.21	0.41
1:A:501:ALA:O	1:A:502:LYS:HB2	2.21	0.41
1:A:72:SER:HA	1:A:293:ILE:HD12	2.02	0.41
1:A:755:ASN:HD21	1:A:819:ARG:HH12	1.68	0.41
1:A:964:LEU:O	1:A:968:LEU:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:ALA:HA	1:B:596:VAL:HG22	2.02	0.41
1:B:832:TRP:CZ2	1:B:988:ALA:HB2	2.55	0.41
1:A:125:GLU:OE1	1:A:158:LYS:HG2	2.20	0.41
1:A:840:ILE:O	1:A:843:TYR:N	2.50	0.41
1:A:862:GLY:HA2	1:A:863:PRO:HD3	1.80	0.41
1:B:342:LEU:HG	1:B:747:VAL:HA	2.02	0.41
1:B:759:GLN:C	1:B:761:ILE:H	2.24	0.41
1:B:782:GLY:O	1:B:783:LEU:O	2.38	0.41
1:A:1:MET:HE1	1:A:7:LYS:CD	2.51	0.41
1:A:81:GLY:CA	1:A:82:GLU:OE1	2.69	0.41
1:B:323:THR:HA	1:B:326:MET:HE3	2.03	0.41
1:B:352:LYS:CD	1:B:635:ILE:HD13	2.51	0.41
1:B:772:VAL:O	1:B:773:VAL:C	2.58	0.41
1:B:795:VAL:HG22	1:B:901:LEU:HD13	2.03	0.41
1:A:611:ILE:HD13	1:A:641:ILE:HG13	2.02	0.41
1:B:335:SER:C	1:B:337:PRO:HD2	2.40	0.41
1:B:791:GLN:O	1:B:794:TRP:HB3	2.21	0.41
1:A:140:ILE:CG1	1:A:141:LYS:N	2.84	0.41
1:A:366:MET:CB	1:A:597:VAL:HG12	2.51	0.41
1:A:654:THR:O	1:A:655:GLY:C	2.58	0.41
1:A:717:GLY:C	1:A:731:SER:HB2	2.42	0.41
1:A:89:VAL:HA	1:A:92:PHE:HD2	1.86	0.41
1:A:906:THR:HG22	1:A:974:SER:OG	2.20	0.41
1:B:527:TYR:O	1:B:592:THR:HA	2.21	0.41
1:B:357:THR:C	1:B:604:ARG:HG3	2.41	0.41
1:B:737:ASP:O	1:B:738:ASP:CB	2.68	0.41
1:A:565:ALA:HB2	1:A:593:PHE:HA	2.02	0.41
1:A:620:ARG:NH2	1:A:670:CYS:O	2.53	0.41
1:A:689:GLU:HB2	1:A:713:LYS:NZ	2.34	0.41
1:A:768:ASN:C	1:A:770:GLY:N	2.72	0.41
1:A:979:GLY:O	1:A:983:ILE:HG13	2.21	0.41
1:B:246:LYS:HA	1:B:251:GLN:CG	2.51	0.41
1:B:359:ASN:HA	1:B:601:ASP:CG	2.41	0.41
1:B:527:TYR:HA	1:B:536:PRO:HA	2.03	0.41
1:B:678:ARG:NH1	1:B:678:ARG:CG	2.83	0.41
1:B:930:ASN:C	1:B:930:ASN:OD1	2.60	0.41
1:A:125:GLU:HB3	1:A:142:ALA:CB	2.43	0.40
1:A:316:THR:HG22	1:A:316:THR:O	2.20	0.40
1:A:520:GLY:O	1:A:524:ARG:HG3	2.21	0.40
1:A:658:PHE:CA	1:A:661:LEU:HD12	2.35	0.40
1:A:764:LEU:C	1:A:768:ASN:HD22	2.25	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:988:ALA:HB2	1:A:992:LEU:HD12	2.03	0.40
1:B:108:GLN:OE1	1:B:310:GLY:HA2	2.21	0.40
1:B:326:MET:HB3	1:B:331:ALA:HB3	2.02	0.40
1:B:421:ASN:OD1	1:B:422:ASP:N	2.55	0.40
1:B:671:ARG:HB3	1:B:694:TYR:CD2	2.55	0.40
1:A:108:GLN:OE1	1:A:310:GLY:HA2	2.21	0.40
1:A:32:HIS:O	1:A:36:TYR:HD2	2.03	0.40
1:A:550:LYS:O	1:A:554:THR:HG23	2.21	0.40
1:A:635:ILE:H	1:A:635:ILE:HG13	1.60	0.40
1:B:140:ILE:CG1	1:B:141:LYS:N	2.85	0.40
1:B:14:ALA:C	1:B:16:PHE:N	2.75	0.40
1:B:338:SER:C	1:B:340:GLU:N	2.74	0.40
1:B:604:ARG:HB3	1:B:604:ARG:HE	1.72	0.40
1:B:667:ARG:HA	1:B:690:TYR:CD1	2.57	0.40
1:B:679:VAL:HG13	1:B:683:HIS:CG	2.56	0.40
1:B:770:GLY:HA2	1:B:841:GLY:O	2.21	0.40
1:B:895:GLU:CD	1:B:895:GLU:N	2.74	0.40
1:B:946:LEU:O	1:B:946:LEU:HD23	2.20	0.40
1:A:22:THR:HG22	1:A:135:LYS:HZ2	1.86	0.40
1:A:301:ALA:O	1:A:302:LEU:C	2.59	0.40
1:A:421:ASN:OD1	1:A:422:ASP:N	2.54	0.40
1:A:541:VAL:O	1:A:544:LYS:N	2.55	0.40
1:A:54:ILE:HA	1:A:57:PHE:CB	2.52	0.40
1:A:807:LEU:HD22	1:A:810:ASN:HD21	1.85	0.40
1:A:823:SER:O	1:A:825:LYS:N	2.55	0.40
1:B:519:GLU:O	1:B:520:GLY:C	2.59	0.40
1:B:541:VAL:O	1:B:543:GLU:N	2.55	0.40
1:B:662:PRO:CD	1:B:665:GLU:HB2	2.47	0.40
1:B:855:TRP:CE2	1:B:895:GLU:HB2	2.56	0.40
1:B:906:THR:CG2	1:B:974:SER:HB2	2.50	0.40
1:A:24:LEU:O	1:A:132:ALA:N	2.53	0.40
1:A:319:LEU:HA	1:A:319:LEU:HD12	1.79	0.40
1:A:541:VAL:C	1:A:543:GLU:N	2.75	0.40
1:A:588:GLU:O	1:A:591:LEU:HD11	2.21	0.40
1:A:751:ARG:HB2	1:A:816:ILE:HD11	2.02	0.40
1:A:841:GLY:HA2	1:A:844:VAL:HG22	2.03	0.40
1:A:843:TYR:CD2	1:A:844:VAL:N	2.90	0.40
1:A:942:SER:C	1:A:944:HIS:N	2.74	0.40
1:A:969:MET:O	1:A:970:VAL:C	2.60	0.40
1:B:44:GLU:CD	1:B:44:GLU:O	2.59	0.40
1:B:781:LEU:HA	1:B:781:LEU:HD23	1.82	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:962:LEU:HD23	1:B:966:GLN:HB3	2.03	0.40
1:A:600:LEU:HD23	1:A:600:LEU:C	2.40	0.40
1:A:81:GLY:HA2	1:A:82:GLU:OE1	2.22	0.40
1:A:926:PRO:HB2	1:A:928:TRP:CE2	2.56	0.40
1:B:106:VAL:HA	1:B:109:GLU:HB2	2.03	0.40
1:B:371:LYS:O	1:B:377:CYS:HB2	2.22	0.40
1:B:459:VAL:O	1:B:462:LEU:N	2.48	0.40
1:B:583:ARG:HG3	1:B:583:ARG:HH11	1.86	0.40
1:B:654:THR:O	1:B:655:GLY:C	2.59	0.40
1:B:792:LEU:O	1:B:795:VAL:N	2.55	0.40
1:B:877:THR:HA	1:B:888:CYS:SG	2.61	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	992/994 (100%)	785 (79%)	152 (15%)	55 (6%)	2	12
1	B	992/994 (100%)	774 (78%)	160 (16%)	58 (6%)	2	11
All	All	1984/1988 (100%)	1559 (79%)	312 (16%)	113 (6%)	2	11

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	ILE
1	A	205	LYS
1	A	283	VAL
1	A	518	PRO
1	A	519	GLU
1	A	801	GLY
1	A	860	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	868	HIS
1	A	880	HIS
1	A	881	PRO
1	B	85	ILE
1	B	205	LYS
1	B	241	ALA
1	B	283	VAL
1	B	518	PRO
1	B	519	GLU
1	B	789	PRO
1	B	813	ASP
1	B	827	PRO
1	B	865	VAL
1	A	82	GLU
1	A	127	GLY
1	A	265	SER
1	A	316	THR
1	A	342	LEU
1	A	531	GLY
1	A	555	GLY
1	A	627	ASP
1	A	781	LEU
1	A	782	GLY
1	A	807	LEU
1	A	987	ILE
1	B	15	TYR
1	B	82	GLU
1	B	243	GLU
1	B	265	SER
1	B	316	THR
1	B	531	GLY
1	B	555	GLY
1	B	604	ARG
1	B	627	ASP
1	B	673	ALA
1	B	766	SER
1	B	797	LEU
1	B	866	THR
1	B	904	LEU
1	B	987	ILE
1	A	15	TYR
1	A	24	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	72	SER
1	A	133	ASP
1	A	307	ILE
1	A	534	ARG
1	A	575	GLU
1	A	604	ARG
1	A	673	ALA
1	A	703	ASP
1	A	904	LEU
1	B	24	LEU
1	B	72	SER
1	B	133	ASP
1	B	342	LEU
1	B	534	ARG
1	B	575	GLU
1	B	703	ASP
1	B	796	ASN
1	A	303	ALA
1	A	372	VAL
1	A	460	ARG
1	A	533	THR
1	A	743	ILE
1	A	796	ASN
1	B	303	ALA
1	B	372	VAL
1	B	533	THR
1	B	743	ILE
1	B	783	LEU
1	A	42	PRO
1	A	282	PRO
1	A	789	PRO
1	A	802	LEU
1	A	961	ALA
1	B	48	SER
1	B	123	GLU
1	B	282	PRO
1	B	953	LEU
1	A	272	TRP
1	A	281	ASP
1	A	289	ILE
1	A	951	ASP
1	A	953	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	954	PRO
1	B	53	VAL
1	B	281	ASP
1	B	289	ILE
1	B	307	ILE
1	B	460	ARG
1	B	747	VAL
1	B	951	ASP
1	B	954	PRO
1	B	961	ALA
1	A	849	VAL
1	B	304	VAL
1	A	765	ILE
1	B	391	PRO
1	B	896	PRO
1	A	277	GLY
1	A	308	PRO
1	A	530	VAL
1	B	277	GLY
1	B	530	VAL
1	B	905	VAL
1	B	308	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	840/840 (100%)	782 (93%)	58 (7%)	17	51
1	B	840/840 (100%)	786 (94%)	54 (6%)	19	55
All	All	1680/1680 (100%)	1568 (93%)	112 (7%)	18	52

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	60	LEU
1	A	64	ILE
1	A	67	LEU
1	A	82	GLU
1	A	111	ASN
1	A	122	TYR
1	A	133	ASP
1	A	155	VAL
1	A	187	VAL
1	A	214	ILE
1	A	225	THR
1	A	249	LEU
1	A	353	THR
1	A	357	THR
1	A	358	THR
1	A	372	VAL
1	A	441	THR
1	A	445	LEU
1	A	457	THR
1	A	464	LYS
1	A	467	ARG
1	A	472	ASN
1	A	473	SER
1	A	484	THR
1	A	486	GLU
1	A	534	ARG
1	A	562	LEU
1	A	566	THR
1	A	573	ARG
1	A	600	LEU
1	A	613	LEU
1	A	627	ASP
1	A	647	GLU
1	A	696	GLU
1	A	698	THR
1	A	703	ASP
1	A	706	ASN
1	A	724	THR
1	A	737	ASP
1	A	756	ASN
1	A	774	CYS
1	A	776	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	789	PRO
1	A	813	ASP
1	A	818	ASP
1	A	824	PRO
1	A	832	TRP
1	A	836	ARG
1	A	854	TRP
1	A	895	GLU
1	A	904	LEU
1	A	906	THR
1	A	941	MET
1	A	949	TYR
1	A	965	THR
1	A	971	LEU
1	A	973	ILE
1	B	60	LEU
1	B	64	ILE
1	B	67	LEU
1	B	82	GLU
1	B	111	ASN
1	B	133	ASP
1	B	155	VAL
1	B	187	VAL
1	B	214	ILE
1	B	225	THR
1	B	276	ILE
1	B	353	THR
1	B	357	THR
1	B	358	THR
1	B	372	VAL
1	B	441	THR
1	B	445	LEU
1	B	457	THR
1	B	464	LYS
1	B	467	ARG
1	B	472	ASN
1	B	473	SER
1	B	484	THR
1	B	486	GLU
1	B	534	ARG
1	B	566	THR
1	B	573	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	600	LEU
1	B	613	LEU
1	B	627	ASP
1	B	645	ASN
1	B	647	GLU
1	B	696	GLU
1	B	698	THR
1	B	703	ASP
1	B	706	ASN
1	B	724	THR
1	B	737	ASP
1	B	761	ILE
1	B	762	ARG
1	B	776	PHE
1	B	777	LEU
1	B	789	PRO
1	B	813	ASP
1	B	814	LEU
1	B	832	TRP
1	B	883	PHE
1	B	904	LEU
1	B	906	THR
1	B	941	MET
1	B	949	TYR
1	B	965	THR
1	B	971	LEU
1	B	973	ILE

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

Mol	Chain	Res	Type
1	A	101	ASN
1	A	111	ASN
1	A	114	ASN
1	A	138	GLN
1	A	284	HIS
1	A	359	ASN
1	A	360	GLN
1	A	472	ASN
1	A	477	GLN
1	A	510	ASN
1	A	706	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	759	GLN
1	A	768	ASN
1	A	869	GLN
1	A	872	HIS
1	A	919	ASN
1	B	101	ASN
1	B	111	ASN
1	B	114	ASN
1	B	138	GLN
1	B	244	GLN
1	B	284	HIS
1	B	360	GLN
1	B	472	ASN
1	B	477	GLN
1	B	510	ASN
1	B	706	ASN
1	B	756	ASN
1	B	768	ASN
1	B	791	GLN
1	B	872	HIS
1	B	911	ASN
1	B	914	ASN
1	B	919	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	994/994 (100%)	-0.32	21 (2%) 63 34	24, 73, 138, 174	0
1	B	994/994 (100%)	-0.21	28 (2%) 53 24	24, 77, 138, 175	0
All	All	1988/1988 (100%)	-0.27	49 (2%) 57 29	24, 75, 138, 175	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	GLU	8.0
1	B	287	SER	6.8
1	B	85	ILE	5.1
1	B	83	GLU	4.7
1	A	49	LEU	4.7
1	B	80	GLU	4.5
1	A	858	TYR	4.4
1	A	46	GLY	4.0
1	B	81	GLY	3.9
1	B	885	GLY	3.8
1	B	237	ASP	3.5
1	A	288	TRP	3.4
1	B	239	MET	3.3
1	B	991	TYR	3.2
1	B	46	GLY	3.0
1	A	44	GLU	2.9
1	A	861	ASP	2.9
1	A	289	ILE	2.8
1	B	76	ALA	2.8
1	A	124	PRO	2.8
1	B	882	HIS	2.7
1	B	878	GLU	2.7
1	B	44	GLU	2.6
1	B	82	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	290	ARG	2.5
1	B	964	LEU	2.4
1	B	506	ALA	2.4
1	A	79	GLU	2.4
1	A	373	ASP	2.4
1	B	63	ARG	2.4
1	A	81	GLY	2.3
1	B	240	ALA	2.3
1	A	882	HIS	2.3
1	A	991	TYR	2.3
1	B	124	PRO	2.3
1	B	121	GLU	2.2
1	A	47	LYS	2.2
1	B	84	THR	2.2
1	A	107	TRP	2.2
1	B	286	GLY	2.2
1	A	860	GLU	2.1
1	B	251	GLN	2.1
1	B	288	TRP	2.1
1	A	994	GLY	2.1
1	A	56	GLN	2.1
1	B	886	LEU	2.1
1	B	884	GLU	2.1
1	A	51	GLU	2.1
1	A	371	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th 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(\AA^2)	Q<0.9
3	K	A	997	1/1	0.88	0.20	91,91,91,91	0
2	CA	A	999	1/1	0.88	0.11	83,83,83,83	0
2	CA	A	998	1/1	0.89	0.14	64,64,64,64	0
2	CA	B	995	1/1	0.93	0.27	70,70,70,70	0
3	K	B	997	1/1	0.94	0.28	69,69,69,69	0
2	CA	B	998	1/1	0.95	0.23	84,84,84,84	0
4	CL	B	999	1/1	0.95	0.11	40,40,40,40	0
2	CA	B	996	1/1	0.96	0.31	52,52,52,52	0
2	CA	A	995	1/1	0.97	0.28	49,49,49,49	0
4	CL	A	1000	1/1	0.97	0.13	56,56,56,56	0
2	CA	A	996	1/1	0.98	0.25	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.