



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 05:11 PM EDT

PDB ID : 3CU7
Title : Human Complement Component 5
Authors : Fredslund, F.; Andersen, G.R.
Deposited on : unknown
Resolution : 3.10 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

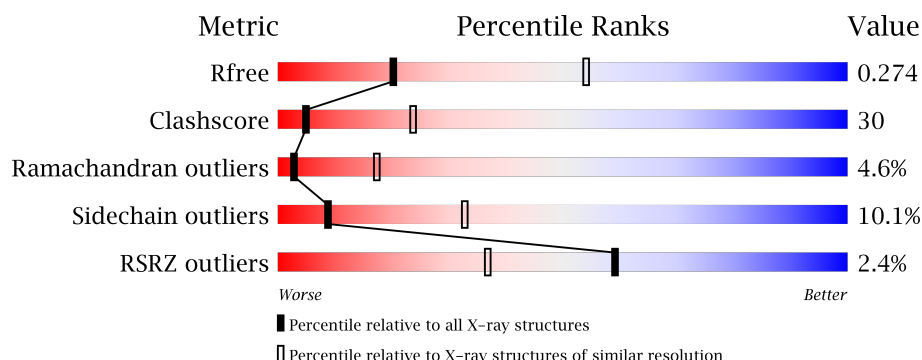
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	1676	<div> <div>3%</div> <div>45%</div> <div>44%</div> <div>8%</div> <div>••</div> </div>
1	B	1676	<div> <div>%</div> <div>42%</div> <div>39%</div> <div>6%</div> <div>12%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24655 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.

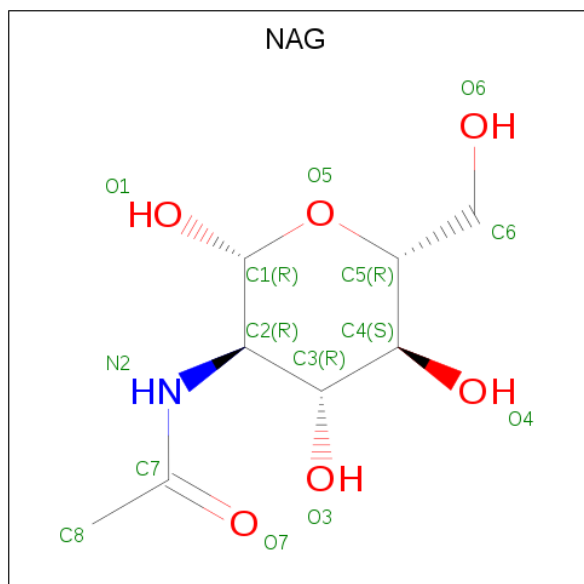
- Molecule 1 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1625	Total	C	N	O	S	0	0	0
			12861	8239	2111	2458	53			
1	B	1481	Total	C	N	O	S	0	0	0
			11701	7493	1930	2232	46			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	802	ILE	VAL	SEE REMARK 999	UNP P01031
B	802	ILE	VAL	SEE REMARK 999	UNP P01031

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

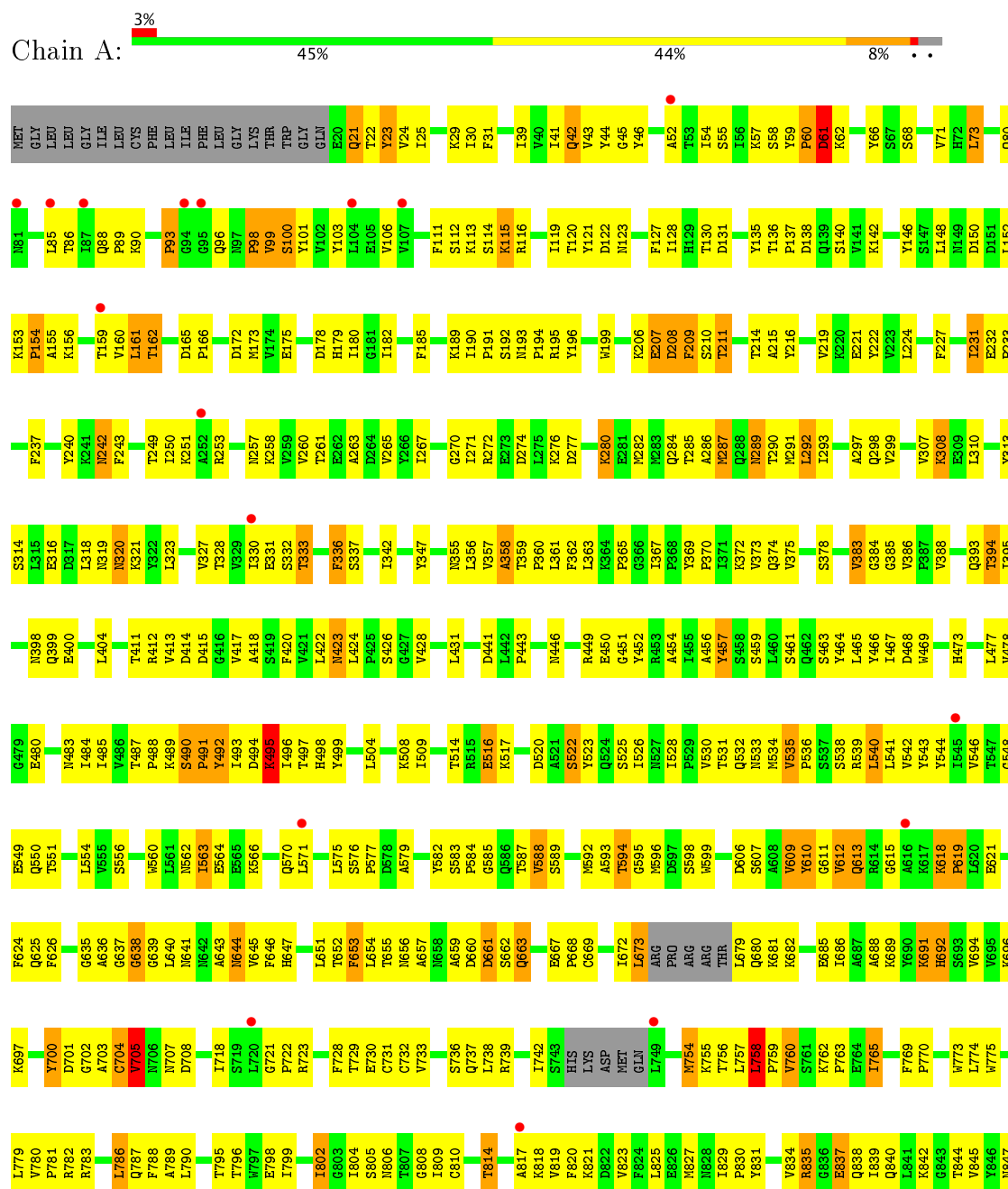
- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

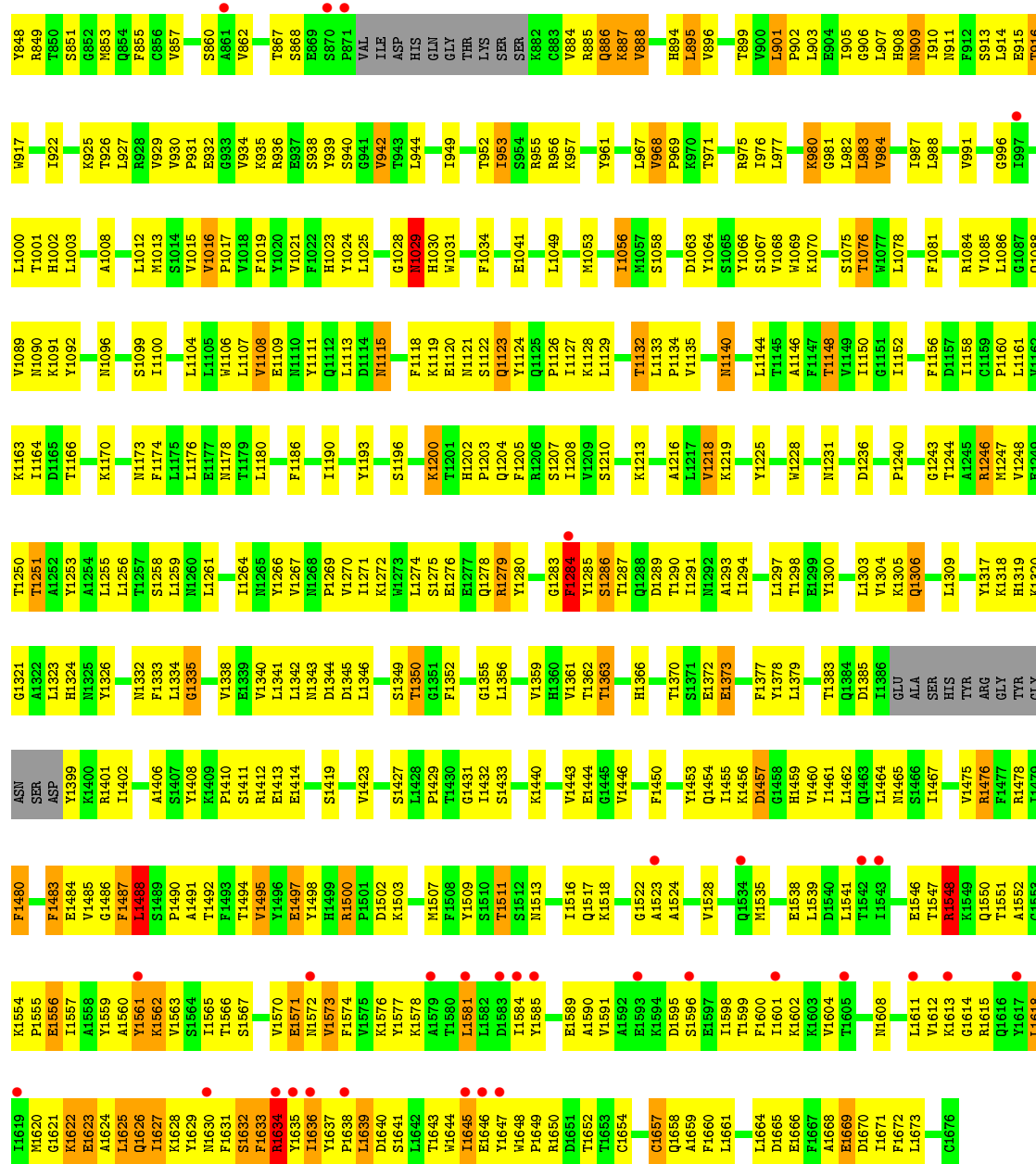
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Cd	0	0
			4	4		
3	A	5	Total	Cd	0	0
			5	5		

3 Residue-property plots

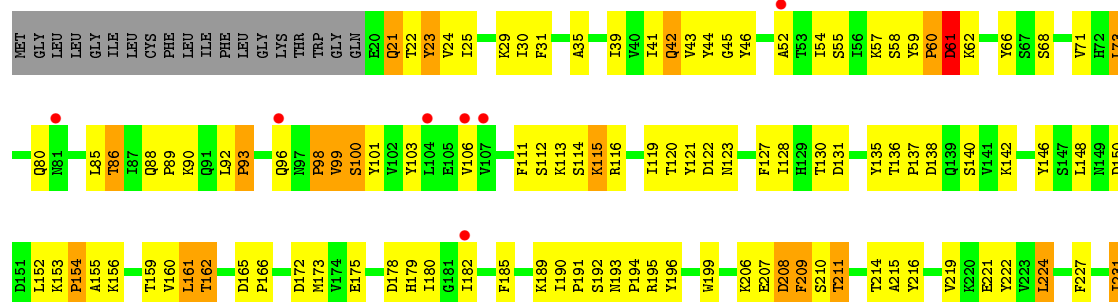
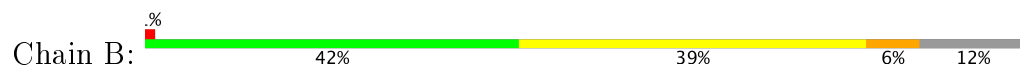
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Complement C5





• Molecule 1: Complement C5





[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	144.26 Å 144.26 Å 241.00 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.29 – 3.10 29.29 – 3.11	Depositor EDS
% Data completeness (in resolution range)	97.5 (29.29-3.10) 97.4 (29.29-3.11)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.11 Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.236 , 0.281 0.229 , 0.274	Depositor DCC
R_{free} test set	4916 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	94.3	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 91.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.468 for h,-h-k,-l 0.009 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24655	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: NAG, CD

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	0.26	0/13137	0.47	1/17820 (0.0%)
1	B	0.26	0/11954	0.47	1/16219 (0.0%)
All	All	0.26	0/25091	0.47	2/34039 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1488	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	1488	LEU	CA-CB-CG	5.05	126.91	115.30

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	12861	0	12817	794	0
1	B	11701	0	11669	700	0
2	A	42	0	38	2	0
2	B	42	0	38	2	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
All	All	24655	0	24562	1484	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 30.

All (1484) 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:1538:GLU:HG2	1:A:1539:LEU:HG	1.31	1.12
1:A:253:ARG:HH22	1:A:257:ASN:HA	1.13	1.11
1:B:253:ARG:HH22	1:B:257:ASN:HA	1.12	1.10
1:A:1279:ARG:HG3	1:A:1284:PHE:HB2	1.30	1.08
1:B:1279:ARG:HG3	1:B:1284:PHE:HB2	1.31	1.06
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.38	1.05
1:B:535:VAL:HG23	1:B:536:PRO:HD3	1.38	1.04
1:B:270:GLY:HA3	1:B:282:MET:HE1	1.41	1.02
1:A:543:TYR:HB3	1:A:556:SER:HB3	1.41	1.02
1:A:835:ARG:HG2	1:A:835:ARG:HH11	1.22	1.01
1:B:543:TYR:HB3	1:B:556:SER:HB3	1.42	1.01
1:A:270:GLY:HA3	1:A:282:MET:HE1	1.42	1.01
1:B:835:ARG:HG2	1:B:835:ARG:HH11	1.23	0.99
1:A:1429:PRO:HG2	1:A:1511:THR:HB	1.44	0.99
1:B:1429:PRO:HG2	1:B:1511:THR:HB	1.45	0.99
1:B:59:TYR:CG	1:B:60:PRO:HD2	1.98	0.98
1:A:1539:LEU:HD13	1:A:1657:CYS:HB3	1.45	0.97
1:A:59:TYR:CG	1:A:60:PRO:HD2	1.98	0.97
1:A:1612:VAL:HB	1:A:1615:ARG:HD2	1.51	0.91
1:A:160:VAL:HG22	1:A:175:GLU:HB3	1.53	0.90
1:A:1632:SER:O	1:A:1633:PHE:HB2	1.72	0.90
1:B:829:ILE:HG13	1:B:925:LYS:HG2	1.53	0.89
1:A:829:ILE:HG13	1:A:925:LYS:HG2	1.53	0.89
1:B:160:VAL:HG22	1:B:175:GLU:HB3	1.52	0.89
1:B:473:HIS:HE1	1:B:477:LEU:HG	1.38	0.88
1:B:653:PHE:CZ	1:B:660:ASP:HA	2.08	0.88
1:A:473:HIS:HE1	1:A:477:LEU:HG	1.40	0.87
1:A:773:TRP:HZ3	1:A:788:PHE:HE1	1.18	0.87
1:A:1096:ASN:HD22	1:A:1099:SER:H	1.18	0.87
1:A:653:PHE:CZ	1:A:660:ASP:HA	2.08	0.87
1:B:773:TRP:HZ3	1:B:788:PHE:HE1	1.18	0.86
1:B:1096:ASN:HD22	1:B:1099:SER:H	1.18	0.86
1:A:253:ARG:NH2	1:A:257:ASN:HA	1.92	0.85
1:B:977:LEU:HD12	1:B:1361:VAL:HG22	1.58	0.84
1:B:639:GLY:H	1:B:645:VAL:HG22	1.42	0.84
1:A:977:LEU:HD12	1:A:1361:VAL:HG22	1.58	0.84
1:B:253:ARG:NH2	1:B:257:ASN:HA	1.92	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:GLY:H	1:A:645:VAL:HG22	1.43	0.83
1:B:1500:ARG:HD3	1:B:1503:LYS:HD3	1.61	0.82
1:A:1202:HIS:HD2	1:A:1204:GLN:H	1.28	0.82
1:A:1673:LEU:HB3	1:B:258:LYS:NZ	1.95	0.82
1:B:25:ILE:HB	1:B:654:LEU:HB3	1.62	0.81
1:B:1023:HIS:HD2	1:B:1092:TYR:OH	1.64	0.81
1:B:981:GLY:HA3	1:B:1333:PHE:HB2	1.60	0.81
1:A:1500:ARG:HD3	1:A:1503:LYS:HD3	1.61	0.81
1:A:981:GLY:HA3	1:A:1333:PHE:HB2	1.61	0.81
1:B:640:LEU:H	1:B:644:ASN:HB3	1.46	0.81
1:B:504:LEU:HD21	1:B:651:LEU:HG	1.62	0.81
1:A:362:PHE:HD1	1:A:638:GLY:O	1.64	0.81
1:A:1023:HIS:HD2	1:A:1092:TYR:OH	1.64	0.80
1:A:25:ILE:HB	1:A:654:LEU:HB3	1.64	0.80
1:B:886:GLN:HG3	1:B:887:LYS:H	1.47	0.80
1:A:1541:LEU:HD21	1:A:1659:ALA:HB1	1.64	0.80
1:A:640:LEU:H	1:A:644:ASN:HB3	1.46	0.80
1:A:1244:THR:HG22	1:A:1247:MET:H	1.47	0.79
1:A:468:ASP:O	1:A:484:ILE:HG13	1.83	0.79
1:B:1096:ASN:ND2	1:B:1099:SER:H	1.79	0.79
1:B:468:ASP:O	1:B:484:ILE:HG13	1.83	0.79
1:B:770:PRO:HG2	1:B:795:THR:HG21	1.65	0.79
1:A:1096:ASN:ND2	1:A:1099:SER:H	1.79	0.79
1:B:934:VAL:HG22	1:B:1366:HIS:CD2	2.18	0.79
1:B:1202:HIS:HD2	1:B:1204:GLN:H	1.28	0.79
1:B:362:PHE:HD1	1:B:638:GLY:O	1.66	0.79
1:A:922:ILE:HD12	2:A:2001:NAG:H82	1.65	0.78
1:B:115:LYS:HG2	1:B:654:LEU:HD13	1.66	0.78
1:A:934:VAL:HG22	1:A:1366:HIS:CD2	2.18	0.78
1:A:504:LEU:HD21	1:A:651:LEU:HG	1.64	0.78
1:B:1244:THR:HG22	1:B:1247:MET:H	1.48	0.78
1:A:1497:GLU:HB3	1:A:1500:ARG:HG3	1.66	0.78
1:A:886:GLN:HG3	1:A:887:LYS:H	1.47	0.78
1:B:838:GLN:HB3	1:B:1486:GLY:HA3	1.64	0.78
1:A:770:PRO:HG2	1:A:795:THR:HG21	1.65	0.77
1:B:1497:GLU:HB3	1:B:1500:ARG:HG3	1.67	0.77
1:B:1279:ARG:HG3	1:B:1284:PHE:CB	2.13	0.77
1:A:1565:ILE:HD11	1:A:1614:GLY:H	1.50	0.77
1:A:128:ILE:HB	1:A:215:ALA:HB2	1.65	0.77
1:A:961:TYR:OH	1:A:1343:ASN:HA	1.84	0.76
1:B:961:TYR:OH	1:B:1343:ASN:HA	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:ASN:HB3	1:A:739:ARG:HH12	1.50	0.76
1:B:128:ILE:HB	1:B:215:ALA:HB2	1.65	0.76
1:B:473:HIS:CE1	1:B:477:LEU:HG	2.21	0.76
1:B:707:ASN:HB3	1:B:739:ARG:HH12	1.49	0.76
1:A:115:LYS:HG2	1:A:654:LEU:HD13	1.65	0.76
1:A:576:SER:HB2	1:A:577:PRO:HD3	1.68	0.76
1:A:1290:THR:O	1:A:1294:ILE:HG12	1.84	0.76
1:B:576:SER:HB2	1:B:577:PRO:HD3	1.68	0.76
1:A:635:GLY:HA2	1:A:672:ILE:HG23	1.67	0.76
1:B:359:THR:HG21	1:B:372:LYS:H	1.50	0.76
1:B:1290:THR:O	1:B:1294:ILE:HG12	1.84	0.76
1:B:635:GLY:HA2	1:B:672:ILE:HG23	1.68	0.75
1:A:359:THR:HG21	1:A:372:LYS:H	1.51	0.75
1:A:838:GLN:HB3	1:A:1486:GLY:HA3	1.65	0.75
1:B:987:ILE:HD13	1:B:1294:ILE:HG23	1.69	0.75
1:B:566:LYS:HE2	1:B:570:GLN:HE22	1.52	0.75
1:B:23:TYR:HE1	1:B:656:ASN:H	1.35	0.74
1:A:1108:VAL:HG11	1:A:1164:ILE:HG22	1.70	0.74
1:A:55:SER:HB3	1:A:68:SER:HB3	1.69	0.74
1:A:987:ILE:HD13	1:A:1294:ILE:HG23	1.69	0.74
1:B:1056:ILE:HD11	1:B:1066:TYR:CE2	2.23	0.74
1:B:1383:THR:HG21	1:B:1511:THR:HA	1.70	0.74
1:B:1219:LYS:HB2	1:B:1225:TYR:HB2	1.70	0.73
1:A:1279:ARG:HG3	1:A:1284:PHE:CB	2.12	0.73
1:A:1056:ILE:HD11	1:A:1066:TYR:CE2	2.23	0.73
1:A:1219:LYS:HB2	1:A:1225:TYR:HB2	1.70	0.73
1:A:1383:THR:HG21	1:A:1511:THR:HA	1.71	0.73
1:A:23:TYR:HE1	1:A:656:ASN:H	1.37	0.73
1:B:231:ILE:HD12	1:B:327:VAL:HG23	1.71	0.73
1:B:263:ALA:HB3	1:B:292:LEU:HB3	1.71	0.73
1:B:1108:VAL:HG11	1:B:1164:ILE:HG22	1.69	0.73
1:B:57:LYS:HD3	1:B:62:LYS:HB3	1.71	0.73
1:A:467:ILE:HD12	1:A:484:ILE:HD11	1.71	0.72
1:A:566:LYS:HE2	1:A:570:GLN:HE22	1.53	0.72
1:B:1264:ILE:HG12	1:B:1303:LEU:HD11	1.72	0.72
1:B:55:SER:HB3	1:B:68:SER:HB3	1.69	0.72
1:A:473:HIS:CE1	1:A:477:LEU:HG	2.22	0.72
1:B:1132:THR:HB	1:B:1134:PRO:HD2	1.72	0.72
1:B:516:GLU:H	1:B:516:GLU:CD	1.91	0.72
1:A:640:LEU:HB3	1:A:644:ASN:OD1	1.90	0.72
1:B:640:LEU:HB3	1:B:644:ASN:OD1	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:THR:HB	1:A:1134:PRO:HD2	1.72	0.71
1:B:1000:LEU:HD11	1:B:1017:PRO:HG3	1.72	0.71
1:A:57:LYS:HD3	1:A:62:LYS:HB3	1.72	0.71
1:B:415:ASP:HB3	1:B:417:VAL:H	1.54	0.71
1:A:1516:ILE:HG22	1:A:1517:GLN:H	1.55	0.71
1:A:516:GLU:H	1:A:516:GLU:CD	1.91	0.71
1:A:535:VAL:HA	1:A:563:ILE:HD11	1.73	0.71
1:B:467:ILE:HD12	1:B:484:ILE:HD11	1.72	0.71
1:A:1193:TYR:CE1	1:A:1256:LEU:HB3	2.26	0.71
1:A:1567:SER:HB2	1:A:1578:LYS:HD3	1.73	0.71
1:A:231:ILE:HD12	1:A:327:VAL:HG23	1.70	0.71
1:A:415:ASP:HB3	1:A:417:VAL:H	1.54	0.71
1:A:1000:LEU:HD11	1:A:1017:PRO:HG3	1.73	0.70
1:A:1668:ALA:O	1:A:1671:ILE:HG22	1.90	0.70
1:B:956:ARG:HG2	1:B:1349:SER:HB3	1.71	0.70
1:A:263:ALA:HB3	1:A:292:LEU:HB3	1.72	0.70
1:A:862:VAL:HG21	1:A:909:ASN:O	1.91	0.70
1:A:956:ARG:HG2	1:A:1349:SER:HB3	1.72	0.70
1:B:1259:LEU:HD11	1:B:1300:TYR:HB2	1.73	0.70
1:B:1304:VAL:HG12	1:B:1305:LYS:N	2.07	0.70
1:A:1264:ILE:HG12	1:A:1303:LEU:HD11	1.71	0.70
1:B:285:THR:HG23	1:B:681:LYS:HD3	1.73	0.70
1:A:612:VAL:HG23	1:A:613:GLN:H	1.55	0.70
1:B:1193:TYR:CE1	1:B:1256:LEU:HB3	2.26	0.70
1:A:1304:VAL:HG12	1:A:1305:LYS:N	2.06	0.69
1:A:667:GLU:N	1:A:668:PRO:HD3	2.06	0.69
1:A:835:ARG:CG	1:A:835:ARG:HH11	2.00	0.69
1:B:1246:ARG:O	1:B:1250:THR:HG23	1.92	0.69
1:B:612:VAL:HG23	1:B:613:GLN:H	1.55	0.69
1:A:1629:TYR:CZ	1:A:1632:SER:HB2	2.27	0.69
1:A:123:ASN:H	1:A:211:THR:HG23	1.57	0.69
1:A:1259:LEU:HD11	1:A:1300:TYR:HB2	1.73	0.69
1:B:535:VAL:HA	1:B:563:ILE:HD11	1.73	0.69
1:B:123:ASN:H	1:B:211:THR:HG23	1.58	0.69
1:A:1246:ARG:O	1:A:1250:THR:HG23	1.92	0.69
1:B:862:VAL:HG21	1:B:909:ASN:O	1.92	0.69
1:B:835:ARG:CG	1:B:835:ARG:HH11	2.00	0.68
1:A:285:THR:HG23	1:A:681:LYS:HD3	1.74	0.68
1:B:232:GLU:OE2	1:B:251:LYS:HE2	1.93	0.68
1:B:667:GLU:N	1:B:668:PRO:HD3	2.06	0.68
1:A:361:LEU:O	1:A:454:ALA:HA	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1247:MET:O	1:B:1251:THR:HG23	1.94	0.67
1:B:1488:LEU:O	1:B:1488:LEU:HD12	1.95	0.67
1:A:1488:LEU:HD12	1:A:1488:LEU:O	1.95	0.67
1:A:232:GLU:OE2	1:A:251:LYS:HE2	1.94	0.67
1:B:1000:LEU:CD1	1:B:1017:PRO:HG3	2.24	0.67
1:A:280:LYS:HG3	1:A:282:MET:HE3	1.77	0.67
1:A:704:CYS:O	1:A:705:VAL:HG13	1.95	0.67
1:B:988:LEU:HD23	1:B:1021:VAL:HG22	1.77	0.67
1:A:1068:VAL:HA	1:A:1078:LEU:HD13	1.77	0.67
1:A:1090:ASN:HD22	1:A:1158:ILE:HD13	1.59	0.67
1:B:280:LYS:HG3	1:B:282:MET:HE3	1.77	0.67
1:B:96:GLN:O	1:B:98:PRO:HD3	1.95	0.67
1:A:242:ASN:ND2	1:A:242:ASN:H	1.93	0.66
1:B:123:ASN:N	1:B:211:THR:HG23	2.11	0.66
1:A:1462:LEU:HD11	1:A:1475:VAL:HG21	1.78	0.66
1:B:1090:ASN:HD22	1:B:1158:ILE:HD13	1.59	0.66
1:A:1000:LEU:CD1	1:A:1017:PRO:HG3	2.25	0.66
1:A:641:ASN:H	1:A:644:ASN:HB2	1.61	0.66
1:A:54:ILE:HG12	1:A:106:VAL:HG22	1.78	0.66
1:A:886:GLN:HE22	1:A:1623:GLU:HG2	1.59	0.66
1:A:96:GLN:O	1:A:98:PRO:HD3	1.95	0.66
1:B:361:LEU:O	1:B:454:ALA:HA	1.96	0.66
1:B:242:ASN:ND2	1:B:242:ASN:H	1.93	0.66
1:B:488:PRO:O	1:B:491:PRO:HD2	1.95	0.66
1:A:1570:VAL:O	1:A:1571:GLU:HB2	1.94	0.66
1:B:386:VAL:H	1:B:411:THR:CG2	2.09	0.66
1:A:1673:LEU:HB3	1:B:258:LYS:HZ2	1.60	0.66
1:A:123:ASN:N	1:A:211:THR:HG23	2.10	0.65
1:B:704:CYS:O	1:B:705:VAL:HG13	1.95	0.65
1:A:496:ILE:HD12	1:A:496:ILE:H	1.61	0.65
1:B:1068:VAL:HA	1:B:1078:LEU:HD13	1.77	0.65
1:B:1462:LEU:HD11	1:B:1475:VAL:HG21	1.78	0.65
1:A:386:VAL:H	1:A:411:THR:CG2	2.09	0.65
1:A:988:LEU:HD23	1:A:1021:VAL:HG22	1.77	0.65
1:A:1247:MET:O	1:A:1251:THR:HG23	1.95	0.65
1:A:1304:VAL:HG12	1:A:1305:LYS:H	1.61	0.65
1:A:488:PRO:O	1:A:491:PRO:HD2	1.95	0.65
1:A:1019:PHE:CZ	1:A:1088:GLN:HB3	2.32	0.65
1:B:54:ILE:HG12	1:B:106:VAL:HG22	1.79	0.65
1:B:412:ARG:HD2	1:B:415:ASP:HB2	1.78	0.65
1:A:120:THR:HG22	1:A:122:ASP:H	1.62	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ALA:HB3	1:A:73:LEU:HD21	1.79	0.65
1:A:1669:GLU:O	1:A:1673:LEU:HG	1.96	0.65
1:A:820:PHE:HE2	1:A:848:TYR:HD2	1.45	0.65
1:B:1019:PHE:CZ	1:B:1088:GLN:HB3	2.32	0.65
1:B:1200:LYS:HE3	1:B:1261:LEU:HD23	1.79	0.65
1:B:464:TYR:H	1:B:491:PRO:HD3	1.62	0.65
1:A:1633:PHE:CD2	1:A:1634:ARG:HB2	2.33	0.64
1:A:412:ARG:HD2	1:A:415:ASP:HB2	1.78	0.64
1:A:59:TYR:CD2	1:A:60:PRO:HD2	2.32	0.64
1:A:1598:ILE:HG13	1:A:1599:THR:H	1.61	0.64
1:B:496:ILE:H	1:B:496:ILE:HD12	1.61	0.64
1:B:59:TYR:CD2	1:B:60:PRO:HD2	2.32	0.64
1:B:829:ILE:CG1	1:B:925:LYS:HG2	2.24	0.64
1:B:120:THR:HG22	1:B:122:ASP:H	1.63	0.64
1:B:499:TYR:CE2	1:B:517:LYS:HG2	2.32	0.64
1:B:754:MET:O	1:B:755:LYS:HG2	1.98	0.64
1:A:618:LYS:HB2	1:A:621:GLU:HB2	1.79	0.64
1:B:1304:VAL:HG12	1:B:1305:LYS:H	1.62	0.64
1:B:641:ASN:H	1:B:644:ASN:HB2	1.61	0.64
1:A:1503:LYS:N	1:A:1503:LYS:HD2	2.13	0.64
1:A:375:VAL:HG12	1:A:383:VAL:HG13	1.80	0.64
1:A:820:PHE:CE2	1:A:848:TYR:HD2	2.15	0.64
1:B:52:ALA:HB3	1:B:73:LEU:HD21	1.79	0.64
1:A:560:TRP:CH2	1:A:562:ASN:HB2	2.33	0.64
1:A:829:ILE:CG1	1:A:925:LYS:HG2	2.24	0.64
1:A:464:TYR:H	1:A:491:PRO:HD3	1.62	0.64
1:B:1323:LEU:HD12	1:B:1324:HIS:H	1.63	0.64
1:B:367:ILE:HD11	1:B:489:LYS:HB3	1.80	0.64
1:A:1200:LYS:HE3	1:A:1261:LEU:HD23	1.79	0.64
1:A:855:PHE:CE2	1:A:888:VAL:HG13	2.33	0.64
1:A:560:TRP:CZ3	1:A:562:ASN:HB2	2.33	0.63
1:A:1630:ASN:O	1:A:1631:PHE:HB2	1.98	0.63
1:A:647:HIS:CD2	1:A:662:SER:HB2	2.33	0.63
1:A:1673:LEU:HB3	1:B:258:LYS:HZ3	1.63	0.63
1:A:499:TYR:CE2	1:A:517:LYS:HG2	2.33	0.63
1:A:1638:PRO:O	1:A:1639:LEU:HB3	1.99	0.63
1:B:823:VAL:HG22	1:B:847:ASN:HA	1.80	0.63
1:B:1399:TYR:OH	1:B:1478:ARG:HD3	1.98	0.62
1:B:1503:LYS:N	1:B:1503:LYS:HD2	2.13	0.62
1:A:367:ILE:HD11	1:A:489:LYS:HB3	1.81	0.62
1:B:271:ILE:HG22	1:B:272:ARG:H	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:TRP:CZ3	1:B:562:ASN:HB2	2.34	0.62
1:B:618:LYS:HB2	1:B:621:GLU:HB2	1.79	0.62
1:B:855:PHE:CE2	1:B:888:VAL:HG13	2.33	0.62
1:A:1669:GLU:HG3	1:A:1672:PHE:CZ	2.34	0.62
1:A:1399:TYR:OH	1:A:1478:ARG:HD3	1.99	0.62
1:A:271:ILE:HG22	1:A:272:ARG:H	1.64	0.62
1:A:1614:GLY:O	1:B:1519:VAL:HG21	2.00	0.62
1:B:647:HIS:CD2	1:B:662:SER:HB2	2.34	0.62
1:B:702:GLY:HA2	1:B:728:PHE:CE1	2.35	0.62
1:A:1488:LEU:HD21	1:A:1511:THR:HG22	1.82	0.62
1:A:1631:PHE:O	1:A:1632:SER:HB3	1.98	0.62
1:A:696:LYS:HE3	1:A:700:TYR:HD2	1.65	0.62
1:B:1488:LEU:HD21	1:B:1511:THR:HG22	1.81	0.62
1:B:647:HIS:HE1	1:B:667:GLU:HG3	1.65	0.62
1:B:707:ASN:HB3	1:B:739:ARG:NH1	2.15	0.62
1:A:1323:LEU:HD12	1:A:1324:HIS:H	1.64	0.62
1:A:647:HIS:HE1	1:A:667:GLU:HG3	1.65	0.61
1:B:153:LYS:HG2	1:B:806:ASN:O	2.00	0.61
1:A:39:ILE:HG13	1:A:85:LEU:HD23	1.83	0.61
1:B:487:THR:HG22	1:B:523:TYR:HB3	1.82	0.61
1:B:39:ILE:HG13	1:B:85:LEU:HD23	1.82	0.61
1:A:153:LYS:HG2	1:A:806:ASN:O	2.00	0.61
1:A:823:VAL:HG22	1:A:847:ASN:HA	1.80	0.61
1:B:560:TRP:CH2	1:B:562:ASN:HB2	2.35	0.61
1:A:1056:ILE:HD11	1:A:1066:TYR:HE2	1.64	0.61
1:A:702:GLY:HA2	1:A:728:PHE:CE1	2.35	0.61
1:B:172:ASP:OD2	1:B:173:MET:N	2.32	0.61
1:A:1431:GLY:HA3	1:A:1483:PHE:CE1	2.36	0.61
1:A:172:ASP:OD2	1:A:173:MET:N	2.32	0.61
1:A:487:THR:HG22	1:A:523:TYR:HB3	1.81	0.61
1:B:1186:PHE:HD1	1:B:1250:THR:HG22	1.65	0.61
1:B:820:PHE:CE2	1:B:848:TYR:HD2	2.19	0.61
1:A:1204:GLN:O	1:A:1208:ILE:HG13	2.00	0.61
1:A:21:GLN:NE2	1:A:45:GLY:HA2	2.16	0.61
1:B:1056:ILE:HD11	1:B:1066:TYR:HE2	1.64	0.61
1:B:820:PHE:HE2	1:B:848:TYR:HD2	1.49	0.60
1:A:24:VAL:HA	1:A:655:THR:HG1	1.67	0.60
1:B:375:VAL:HG12	1:B:383:VAL:HG13	1.81	0.60
1:A:534:MET:HB3	1:A:538:SER:OG	2.01	0.60
1:A:857:VAL:HA	1:A:913:SER:O	2.01	0.60
1:B:1204:GLN:O	1:B:1208:ILE:HG13	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLN:NE2	1:B:45:GLY:HA2	2.16	0.60
1:B:733:VAL:HG13	1:B:737:GLN:HE21	1.67	0.60
1:B:773:TRP:HZ3	1:B:788:PHE:CE1	2.10	0.60
1:B:857:VAL:HA	1:B:913:SER:O	2.02	0.60
1:A:944:LEU:HD22	1:A:1350:THR:HG22	1.84	0.60
1:B:1431:GLY:HA3	1:B:1483:PHE:CE1	2.37	0.60
1:B:696:LYS:HE3	1:B:700:TYR:HD2	1.65	0.60
1:A:576:SER:OG	1:A:589:SER:HB2	2.02	0.60
1:B:942:VAL:HG23	1:B:1359:VAL:HB	1.83	0.60
1:B:534:MET:HB3	1:B:538:SER:OG	2.01	0.60
1:A:1186:PHE:HD1	1:A:1250:THR:HG22	1.66	0.60
1:B:412:ARG:HB3	1:B:415:ASP:HB2	1.83	0.60
1:B:576:SER:OG	1:B:589:SER:HB2	2.01	0.60
1:A:956:ARG:CG	1:A:1349:SER:HB3	2.32	0.60
1:A:961:TYR:CZ	1:A:1343:ASN:HA	2.37	0.60
1:B:956:ARG:CG	1:B:1349:SER:HB3	2.32	0.60
1:A:885:ARG:NH2	1:A:1628:LYS:HD2	2.17	0.60
1:B:647:HIS:CE1	1:B:667:GLU:HG3	2.37	0.60
1:B:961:TYR:CZ	1:B:1343:ASN:HA	2.37	0.60
1:A:733:VAL:HG13	1:A:737:GLN:HE21	1.66	0.60
1:A:154:PRO:HB3	1:A:180:ILE:O	2.01	0.59
1:B:1003:LEU:HB3	1:B:1498:TYR:CE1	2.37	0.59
1:B:532:GLN:O	1:B:535:VAL:HG22	2.02	0.59
1:B:944:LEU:HD22	1:B:1350:THR:HG22	1.84	0.59
1:A:707:ASN:HB3	1:A:739:ARG:NH1	2.15	0.59
1:A:773:TRP:HZ3	1:A:788:PHE:CE1	2.10	0.59
1:B:154:PRO:HB3	1:B:180:ILE:O	2.01	0.59
1:B:982:LEU:HD23	1:B:1309:LEU:HD11	1.83	0.59
1:A:982:LEU:HD23	1:A:1309:LEU:HD11	1.83	0.59
1:A:313:TYR:HE2	1:A:321:LYS:HZ1	1.51	0.59
1:A:1565:ILE:HD11	1:A:1614:GLY:N	2.17	0.59
1:A:320:ASN:HD22	1:A:320:ASN:N	1.99	0.59
1:A:942:VAL:HG23	1:A:1359:VAL:HB	1.84	0.59
1:A:1485:VAL:CG2	1:A:1488:LEU:HB3	2.32	0.59
1:B:320:ASN:HD22	1:B:320:ASN:N	2.00	0.59
1:A:1562:LYS:HG3	1:A:1648:TRP:CE3	2.38	0.59
1:A:609:VAL:HG23	1:A:610:TYR:H	1.67	0.59
1:A:412:ARG:HB3	1:A:415:ASP:HB2	1.85	0.58
1:A:647:HIS:CE1	1:A:667:GLU:HG3	2.37	0.58
1:A:41:ILE:O	1:A:80:GLN:HA	2.04	0.58
1:B:576:SER:CB	1:B:577:PRO:HD3	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:ASN:HB2	1:B:644:ASN:H	1.68	0.58
1:B:1485:VAL:CG2	1:B:1488:LEU:HB3	2.33	0.58
1:A:1649:PRO:HG2	1:A:1661:LEU:HG	1.84	0.58
1:A:543:TYR:CB	1:A:556:SER:HB3	2.27	0.58
1:A:1003:LEU:HB3	1:A:1498:TYR:CE1	2.38	0.58
1:B:272:ARG:O	1:B:321:LYS:HB2	2.04	0.58
1:B:284:GLN:NE2	1:B:310:LEU:HD22	2.19	0.58
1:B:356:LEU:HG	1:B:452:TYR:CZ	2.38	0.58
1:A:641:ASN:HB2	1:A:644:ASN:H	1.68	0.58
1:B:231:ILE:HD12	1:B:327:VAL:CG2	2.34	0.58
1:A:1084:ARG:O	1:A:1088:GLN:HG3	2.03	0.58
1:A:532:GLN:O	1:A:535:VAL:HG22	2.02	0.58
1:A:1001:THR:HG22	1:A:1002:HIS:H	1.69	0.58
1:A:1255:LEU:HD22	1:A:1270:VAL:HG12	1.86	0.58
1:A:1274:LEU:C	1:A:1276:GLU:H	2.07	0.58
1:A:1669:GLU:HG3	1:A:1672:PHE:HZ	1.67	0.58
1:B:1271:ILE:C	1:B:1271:ILE:HD12	2.24	0.58
1:B:609:VAL:HG23	1:B:610:TYR:H	1.68	0.58
1:A:1271:ILE:C	1:A:1271:ILE:HD12	2.24	0.57
1:A:884:VAL:HG12	1:A:1625:LEU:HB3	1.86	0.57
1:B:41:ILE:O	1:B:80:GLN:HA	2.03	0.57
1:A:138:ASP:OD1	1:A:192:SER:HA	2.04	0.57
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.40	0.57
1:A:1554:LYS:HD2	1:A:1555:PRO:HD2	1.85	0.57
1:A:272:ARG:O	1:A:321:LYS:HB2	2.04	0.57
1:A:323:LEU:HB2	1:A:347:TYR:CE2	2.39	0.57
1:A:386:VAL:O	1:A:411:THR:HG22	2.04	0.57
1:B:323:LEU:HB2	1:B:347:TYR:CE2	2.39	0.57
1:B:786:LEU:HD23	1:B:786:LEU:N	2.19	0.57
1:A:365:PRO:HG2	1:A:464:TYR:CZ	2.38	0.57
1:A:786:LEU:N	1:A:786:LEU:HD23	2.19	0.57
1:B:138:ASP:OD1	1:B:192:SER:HA	2.04	0.57
1:A:356:LEU:HG	1:A:452:TYR:CZ	2.40	0.57
1:B:981:GLY:CA	1:B:1333:PHE:HB2	2.34	0.57
1:B:386:VAL:O	1:B:411:THR:HG22	2.04	0.57
1:B:365:PRO:HG2	1:B:464:TYR:CZ	2.39	0.57
1:B:908:HIS:HB3	1:B:926:THR:HB	1.86	0.57
1:A:1550:GLN:C	1:A:1552:ALA:H	2.06	0.57
1:A:641:ASN:H	1:A:644:ASN:CB	2.17	0.57
1:B:541:LEU:HD21	1:B:646:PHE:CZ	2.40	0.57
1:B:782:ARG:O	1:B:783:ARG:HG3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1001:THR:HG22	1:B:1002:HIS:H	1.70	0.57
1:B:1213:LYS:HG3	1:B:1266:TYR:OH	2.05	0.57
1:A:284:GLN:NE2	1:A:310:LEU:HD22	2.19	0.57
1:A:782:ARG:O	1:A:783:ARG:HG3	2.04	0.57
1:A:885:ARG:HH22	1:A:1628:LYS:HD2	1.69	0.57
1:B:1084:ARG:O	1:B:1088:GLN:HG3	2.04	0.57
1:B:641:ASN:H	1:B:644:ASN:CB	2.18	0.57
1:B:718:ILE:HG12	1:B:1446:VAL:HG12	1.85	0.57
1:B:961:TYR:HH	1:B:1343:ASN:HA	1.69	0.57
1:B:968:VAL:HG22	1:B:1366:HIS:O	2.04	0.57
1:A:1411:SER:H	1:A:1414:GLU:HG3	1.70	0.57
1:A:1557:ILE:HG22	1:A:1559:TYR:O	2.04	0.57
1:A:576:SER:CB	1:A:577:PRO:HD3	2.33	0.57
1:A:908:HIS:HB3	1:A:926:THR:HB	1.86	0.57
1:B:99:VAL:HB	1:B:121:TYR:OH	2.05	0.57
1:B:1320:LYS:HG3	1:B:1321:GLY:N	2.20	0.57
1:B:59:TYR:CG	1:B:60:PRO:CD	2.82	0.57
1:A:1433:SER:HB2	1:A:1480:PHE:CD1	2.40	0.57
1:A:231:ILE:HD12	1:A:327:VAL:CG2	2.34	0.57
1:B:42:GLN:HG3	1:B:80:GLN:HE21	1.70	0.57
1:A:1025:LEU:HD13	1:A:1031:TRP:CZ3	2.40	0.56
1:A:42:GLN:HG3	1:A:80:GLN:HE21	1.70	0.56
1:A:478:VAL:HG11	1:A:566:LYS:HD3	1.87	0.56
1:A:739:ARG:HD3	1:A:754:MET:SD	2.45	0.56
1:A:894:HIS:CE1	1:A:1589:GLU:OE2	2.59	0.56
1:B:1255:LEU:HB2	1:B:1270:VAL:HG11	1.88	0.56
1:A:1127:ILE:HD13	1:A:1129:LEU:HG	1.87	0.56
1:B:700:TYR:CZ	1:B:758:LEU:HD12	2.40	0.56
1:B:834:VAL:O	1:B:837:GLU:HB2	2.06	0.56
1:A:1557:ILE:HD12	1:A:1621:GLY:HA2	1.86	0.56
1:A:1624:ALA:HA	1:A:1637:TYR:HA	1.87	0.56
1:A:834:VAL:O	1:A:837:GLU:HB2	2.05	0.56
1:A:839:ILE:HD11	1:A:1483:PHE:CZ	2.40	0.56
1:B:1025:LEU:HD13	1:B:1031:TRP:CZ3	2.40	0.56
1:B:1127:ILE:HD13	1:B:1129:LEU:HG	1.87	0.56
1:B:1411:SER:H	1:B:1414:GLU:HG3	1.70	0.56
1:A:830:PRO:HG3	1:A:1483:PHE:CE2	2.40	0.56
1:A:1554:LYS:HE3	1:A:1556:GLU:HG2	1.87	0.56
1:B:1433:SER:HB2	1:B:1480:PHE:CD1	2.41	0.56
1:B:237:PHE:CE1	1:B:378:SER:HB2	2.41	0.56
1:B:59:TYR:CD1	1:B:60:PRO:HD2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1320:LYS:HG3	1:A:1321:GLY:N	2.20	0.56
1:A:1669:GLU:HA	1:A:1672:PHE:CE1	2.41	0.56
1:A:835:ARG:HD3	1:A:903:LEU:O	2.05	0.56
1:B:1274:LEU:C	1:B:1276:GLU:H	2.08	0.56
1:A:1213:LYS:HG3	1:A:1266:TYR:OH	2.05	0.56
1:A:981:GLY:CA	1:A:1333:PHE:HB2	2.35	0.56
1:A:1554:LYS:HE3	1:A:1556:GLU:CG	2.36	0.56
1:A:804:ILE:HG22	1:A:809:ILE:HA	1.88	0.56
1:A:855:PHE:CZ	1:A:886:GLN:HB3	2.41	0.56
1:B:1255:LEU:HD22	1:B:1270:VAL:HG12	1.87	0.56
1:B:835:ARG:HG2	1:B:835:ARG:NH1	2.04	0.56
1:B:496:ILE:HG23	1:B:544:TYR:HB2	1.88	0.56
1:A:1255:LEU:HB2	1:A:1270:VAL:HG11	1.86	0.56
1:A:541:LEU:HD21	1:A:646:PHE:CZ	2.41	0.56
1:B:24:VAL:HA	1:B:655:THR:HG1	1.71	0.56
1:A:1107:LEU:H	1:A:1107:LEU:HD12	1.71	0.56
1:A:59:TYR:CG	1:A:60:PRO:CD	2.82	0.56
1:A:88:GLN:HB3	1:A:89:PRO:HD2	1.88	0.56
1:B:1450:PHE:CZ	1:B:1475:VAL:HB	2.40	0.56
1:B:88:GLN:HB3	1:B:89:PRO:HD2	1.88	0.56
1:B:835:ARG:HD3	1:B:903:LEU:O	2.05	0.56
1:A:625:GLN:HG3	1:A:626:PHE:N	2.21	0.56
1:A:885:ARG:HH12	1:A:1628:LYS:HZ3	1.53	0.56
1:B:385:GLY:N	1:B:411:THR:HG23	2.21	0.56
1:B:697:LYS:HE3	1:B:701:ASP:OD2	2.06	0.56
1:A:1590:ALA:O	1:A:1591:VAL:HG12	2.06	0.55
1:A:99:VAL:HB	1:A:121:TYR:OH	2.06	0.55
1:B:478:VAL:HG11	1:B:566:LYS:HD3	1.87	0.55
1:B:955:ARG:O	1:B:956:ARG:HG3	2.05	0.55
1:A:587:THR:HG22	1:A:789:ALA:HB2	1.88	0.55
1:B:855:PHE:CZ	1:B:886:GLN:HB3	2.41	0.55
1:B:1320:LYS:HG2	1:B:1342:LEU:HD12	1.89	0.55
1:B:357:VAL:O	1:B:359:THR:HG23	2.07	0.55
1:B:250:ILE:HD11	1:B:265:VAL:HG21	1.89	0.55
1:B:587:THR:HG22	1:B:789:ALA:HB2	1.89	0.55
1:B:696:LYS:HE3	1:B:700:TYR:CD2	2.41	0.55
1:A:385:GLY:N	1:A:411:THR:HG23	2.21	0.55
1:A:496:ILE:HG23	1:A:544:TYR:HB2	1.88	0.55
1:A:1069:TRP:HH2	1:A:1465:ASN:OD1	1.88	0.55
1:A:955:ARG:O	1:A:956:ARG:HG3	2.07	0.55
1:B:489:LYS:O	1:B:490:SER:HB2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:625:GLN:HG3	1:B:626:PHE:N	2.21	0.55
1:B:804:ILE:HG22	1:B:809:ILE:HA	1.88	0.55
1:A:967:LEU:HD12	1:A:1366:HIS:O	2.06	0.55
1:B:640:LEU:HD12	1:B:640:LEU:O	2.07	0.55
1:A:237:PHE:CE1	1:A:378:SER:HB2	2.41	0.55
1:A:968:VAL:HG22	1:A:1366:HIS:O	2.06	0.55
1:B:1056:ILE:HG12	1:B:1056:ILE:O	2.07	0.55
1:B:1069:TRP:HH2	1:B:1465:ASN:OD1	1.89	0.55
1:A:1652:THR:HG21	1:B:868:SER:OG	2.07	0.55
1:A:1570:VAL:O	1:A:1571:GLU:CB	2.55	0.55
1:B:938:SER:OG	1:B:1279:ARG:CZ	2.55	0.55
1:B:967:LEU:HD12	1:B:1366:HIS:O	2.07	0.55
1:A:1202:HIS:CD2	1:A:1203:PRO:HD2	2.41	0.54
1:A:308:LYS:HG3	1:A:314:SER:HB3	1.89	0.54
1:A:243:PHE:CD1	1:A:316:GLU:HG3	2.43	0.54
1:B:271:ILE:HG22	1:B:272:ARG:N	2.22	0.54
1:A:271:ILE:HG22	1:A:272:ARG:N	2.23	0.54
1:A:357:VAL:O	1:A:359:THR:HG23	2.06	0.54
1:A:696:LYS:HE3	1:A:700:TYR:CD2	2.41	0.54
1:B:1202:HIS:CD2	1:B:1203:PRO:HD2	2.42	0.54
1:B:639:GLY:N	1:B:645:VAL:HG22	2.18	0.54
1:B:692:HIS:HD2	1:B:694:VAL:HG23	1.72	0.54
1:A:1516:ILE:HG22	1:A:1517:GLN:N	2.20	0.54
1:A:1599:THR:HG22	1:A:1600:PHE:H	1.72	0.54
1:A:692:HIS:HD2	1:A:694:VAL:HG23	1.72	0.54
1:A:1076:THR:CG2	1:A:1120:GLU:HA	2.37	0.54
1:B:1107:LEU:HD12	1:B:1107:LEU:H	1.71	0.54
1:B:161:LEU:HD11	1:B:185:PHE:CD1	2.43	0.54
1:B:465:LEU:HD12	1:B:466:TYR:H	1.72	0.54
1:A:1056:ILE:HG12	1:A:1056:ILE:O	2.07	0.54
1:A:1320:LYS:HG2	1:A:1342:LEU:HD12	1.89	0.54
1:A:697:LYS:HE3	1:A:701:ASP:OD2	2.07	0.54
1:B:331:GLU:OE2	1:B:333:THR:HG23	2.08	0.54
1:A:307:VAL:CG1	1:A:313:TYR:HB2	2.38	0.54
1:A:489:LYS:O	1:A:490:SER:HB2	2.07	0.54
1:B:1115:ASN:H	1:B:1115:ASN:HD22	1.54	0.54
1:B:308:LYS:HG3	1:B:314:SER:HB3	1.89	0.54
1:B:765:ILE:O	1:B:765:ILE:HG23	2.08	0.54
1:A:103:TYR:HA	1:A:115:LYS:O	2.08	0.54
1:B:191:PRO:HD2	1:B:194:PRO:HB3	1.89	0.54
1:B:823:VAL:HG21	1:B:853:MET:SD	2.48	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:839:ILE:HD11	1:B:1483:PHE:CZ	2.42	0.54
1:A:1146:ALA:O	1:A:1150:ILE:HG13	2.08	0.54
1:A:1554:LYS:HG3	1:A:1556:GLU:HG2	1.88	0.54
1:A:29:LYS:HG3	1:A:30:ILE:HG12	1.89	0.54
1:B:1255:LEU:O	1:B:1255:LEU:HD12	2.07	0.54
1:B:1001:THR:HG23	1:B:1284:PHE:CD2	2.43	0.54
1:B:191:PRO:O	1:B:194:PRO:HG3	2.08	0.54
1:A:1019:PHE:CE2	1:A:1088:GLN:HB3	2.43	0.54
1:A:161:LEU:HD11	1:A:185:PHE:CD1	2.43	0.54
1:A:1638:PRO:O	1:A:1639:LEU:CB	2.55	0.54
1:A:263:ALA:HB3	1:A:292:LEU:CB	2.38	0.54
1:A:465:LEU:HD12	1:A:466:TYR:H	1.72	0.54
1:B:1525:CYS:O	1:B:1526:LYS:HG2	2.08	0.54
1:B:42:GLN:HG2	1:B:43:VAL:N	2.23	0.54
1:B:830:PRO:HG3	1:B:1483:PHE:CE2	2.43	0.54
1:A:1565:ILE:HD11	1:A:1613:LYS:HA	1.89	0.54
1:A:191:PRO:HD2	1:A:194:PRO:HB3	1.90	0.54
1:A:509:ILE:HD11	1:A:651:LEU:HD21	1.89	0.54
1:B:103:TYR:HA	1:B:115:LYS:O	2.07	0.54
1:B:307:VAL:CG1	1:B:313:TYR:HB2	2.38	0.54
1:B:544:TYR:CE2	1:B:546:VAL:HG23	2.43	0.54
1:A:42:GLN:HG2	1:A:43:VAL:N	2.23	0.53
1:A:718:ILE:HG12	1:A:1446:VAL:HG12	1.89	0.53
1:A:191:PRO:O	1:A:194:PRO:HG3	2.08	0.53
1:A:544:TYR:CE2	1:A:546:VAL:HG23	2.43	0.53
1:A:606:ASP:O	1:A:609:VAL:HG22	2.09	0.53
1:B:1411:SER:HB2	1:B:1414:GLU:HG2	1.90	0.53
1:B:29:LYS:HG3	1:B:30:ILE:HG12	1.89	0.53
1:B:540:LEU:C	1:B:540:LEU:HD12	2.29	0.53
1:A:274:ASP:OD2	1:A:277:ASP:HB2	2.07	0.53
1:A:59:TYR:CD1	1:A:60:PRO:HD2	2.41	0.53
1:A:653:PHE:N	1:A:653:PHE:CD2	2.76	0.53
1:A:823:VAL:HG21	1:A:853:MET:SD	2.48	0.53
1:A:938:SER:OG	1:A:1279:ARG:CZ	2.57	0.53
1:B:1111:TYR:HD1	1:B:1119:LYS:HG3	1.73	0.53
1:B:1146:ALA:O	1:B:1150:ILE:HG13	2.08	0.53
1:B:1213:LYS:HG3	1:B:1266:TYR:CZ	2.43	0.53
1:B:263:ALA:HB3	1:B:292:LEU:CB	2.37	0.53
1:B:243:PHE:CD1	1:B:316:GLU:HG3	2.43	0.53
1:A:1001:THR:HG23	1:A:1284:PHE:CD2	2.43	0.53
1:A:162:THR:HB	1:A:173:MET:HG3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:THR:HG23	1:A:428:VAL:HG23	1.89	0.53
1:A:540:LEU:HD12	1:A:540:LEU:C	2.29	0.53
1:A:24:VAL:HA	1:A:655:THR:OG1	2.09	0.53
1:A:827:MET:HE3	1:A:842:LYS:O	2.09	0.53
1:B:274:ASP:OD2	1:B:277:ASP:HB2	2.08	0.53
1:A:250:ILE:HD11	1:A:265:VAL:HG21	1.89	0.53
1:A:640:LEU:O	1:A:640:LEU:HD12	2.08	0.53
1:B:394:THR:HG23	1:B:428:VAL:HG23	1.89	0.53
1:B:509:ILE:HD11	1:B:651:LEU:HD21	1.89	0.53
1:A:1111:TYR:HD1	1:A:1119:LYS:HG3	1.73	0.53
1:A:1629:TYR:OH	1:A:1632:SER:HB2	2.07	0.53
1:A:845:VAL:HG12	1:A:894:HIS:O	2.09	0.53
1:B:356:LEU:HG	1:B:452:TYR:CE1	2.42	0.53
1:A:1560:ALA:HA	1:A:1620:MET:HG2	1.90	0.53
1:A:1627:ILE:HD13	1:A:1627:ILE:H	1.73	0.53
1:A:765:ILE:HG23	1:A:765:ILE:O	2.08	0.53
1:B:1019:PHE:CE2	1:B:1088:GLN:HB3	2.44	0.53
1:B:1076:THR:CG2	1:B:1120:GLU:HA	2.39	0.53
1:A:443:PRO:HA	1:B:443:PRO:HA	1.90	0.53
1:A:1255:LEU:O	1:A:1255:LEU:HD12	2.09	0.53
1:A:1411:SER:HB2	1:A:1414:GLU:HG2	1.90	0.53
1:A:739:ARG:HB3	1:A:754:MET:SD	2.49	0.53
1:B:1063:ASP:O	1:B:1064:TYR:HB2	2.09	0.53
1:B:307:VAL:HG12	1:B:313:TYR:O	2.09	0.53
1:B:543:TYR:CB	1:B:556:SER:HB3	2.27	0.53
1:A:1063:ASP:O	1:A:1064:TYR:HB2	2.09	0.53
1:A:1581:LEU:O	1:A:1595:ASP:HA	2.09	0.53
1:A:331:GLU:OE2	1:A:333:THR:HG23	2.09	0.53
1:A:494:ASP:C	1:A:496:ILE:HD12	2.30	0.53
1:A:796:THR:HA	1:A:818:LYS:HA	1.91	0.53
1:B:131:ASP:HB3	1:B:142:LYS:HB2	1.91	0.53
1:B:796:THR:HA	1:B:818:LYS:HA	1.91	0.53
1:B:1213:LYS:HD2	1:B:1266:TYR:CE2	2.44	0.52
1:B:162:THR:HB	1:B:173:MET:HG3	1.90	0.52
1:B:922:ILE:HD12	2:B:2001:NAG:H82	1.91	0.52
1:A:1213:LYS:HG3	1:A:1266:TYR:CZ	2.44	0.52
1:B:313:TYR:HE2	1:B:321:LYS:HZ1	1.56	0.52
1:B:24:VAL:HA	1:B:655:THR:OG1	2.08	0.52
1:A:1115:ASN:HD22	1:A:1115:ASN:H	1.54	0.52
1:A:1372:GLU:HG3	1:A:1373:GLU:H	1.75	0.52
1:A:1535:MET:HB2	1:A:1645:ILE:HD11	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:GLY:N	1:A:645:VAL:HG22	2.18	0.52
1:B:1283:GLY:O	1:B:1285:TYR:N	2.42	0.52
1:B:606:ASP:O	1:B:609:VAL:HG22	2.09	0.52
1:B:661:ASP:OD2	1:B:663:GLN:HG2	2.09	0.52
1:A:661:ASP:OD2	1:A:663:GLN:HG2	2.09	0.52
1:B:739:ARG:HD3	1:B:754:MET:SD	2.50	0.52
1:A:1670:ASP:HA	1:A:1673:LEU:HD12	1.92	0.52
1:B:1084:ARG:NE	1:B:1088:GLN:OE1	2.39	0.52
1:B:494:ASP:C	1:B:496:ILE:HD12	2.29	0.52
1:B:1377:PHE:CE1	1:B:1467:ILE:HD12	2.45	0.52
1:B:835:ARG:HH21	1:B:971:THR:HG22	1.75	0.52
1:A:1652:THR:OG1	1:B:868:SER:HB3	2.10	0.52
1:A:1204:GLN:OE1	1:A:1204:GLN:HA	2.10	0.52
1:A:489:LYS:C	1:A:491:PRO:HD2	2.30	0.52
1:B:1068:VAL:HG13	1:B:1069:TRP:CE3	2.45	0.52
1:A:1304:VAL:CG1	1:A:1305:LYS:N	2.73	0.52
1:A:1522:GLY:O	1:A:1523:ALA:HB3	2.10	0.52
1:A:356:LEU:HG	1:A:452:TYR:CE1	2.44	0.52
1:A:942:VAL:HG22	1:A:957:LYS:HD3	1.92	0.52
1:B:700:TYR:CE1	1:B:758:LEU:HD12	2.45	0.52
1:B:835:ARG:CG	1:B:835:ARG:NH1	2.67	0.52
1:A:1599:THR:HB	1:A:1636:ILE:HD12	1.91	0.52
1:B:1166:THR:O	1:B:1170:LYS:HG2	2.10	0.52
1:B:492:TYR:CD2	1:B:493:ILE:N	2.78	0.52
1:B:739:ARG:HB3	1:B:754:MET:SD	2.50	0.52
1:A:131:ASP:HB3	1:A:142:LYS:HB2	1.91	0.51
1:A:1068:VAL:HG13	1:A:1069:TRP:CE3	2.45	0.51
1:A:1111:TYR:CE1	1:A:1121:ASN:HB2	2.45	0.51
1:A:307:VAL:HG12	1:A:313:TYR:O	2.10	0.51
1:B:1034:PHE:CZ	1:B:1041:GLU:HG2	2.45	0.51
1:B:1243:GLY:HA3	1:B:1285:TYR:OH	2.10	0.51
1:B:531:THR:HG23	1:B:533:ASN:H	1.75	0.51
1:A:208:ASP:O	1:A:209:PHE:HB2	2.10	0.51
1:B:1372:GLU:HG3	1:B:1373:GLU:H	1.75	0.51
1:B:166:PRO:HG3	1:B:199:TRP:CD1	2.46	0.51
1:B:489:LYS:C	1:B:491:PRO:HD2	2.30	0.51
1:B:587:THR:HA	1:B:789:ALA:HA	1.92	0.51
1:A:1034:PHE:CZ	1:A:1041:GLU:HG2	2.45	0.51
1:A:1166:THR:O	1:A:1170:LYS:HG2	2.10	0.51
1:A:1213:LYS:HD2	1:A:1266:TYR:CE2	2.45	0.51
1:B:60:PRO:HD3	1:B:103:TYR:HE1	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1111:TYR:CE1	1:B:1121:ASN:HB2	2.45	0.51
1:B:640:LEU:H	1:B:644:ASN:CB	2.21	0.51
1:B:968:VAL:HG23	1:B:971:THR:OG1	2.10	0.51
1:A:1003:LEU:HD11	1:A:1286:SER:HA	1.92	0.51
1:A:1243:GLY:HA3	1:A:1285:TYR:OH	2.11	0.51
1:A:1274:LEU:O	1:A:1276:GLU:N	2.44	0.51
1:A:1283:GLY:O	1:A:1285:TYR:N	2.43	0.51
1:A:39:ILE:CG1	1:A:85:LEU:HD23	2.40	0.51
1:A:909:ASN:H	1:A:926:THR:HG22	1.75	0.51
1:A:968:VAL:HG23	1:A:971:THR:OG1	2.09	0.51
1:B:566:LYS:HE2	1:B:570:GLN:NE2	2.23	0.51
1:B:749:LEU:HG	1:B:750:GLY:H	1.76	0.51
1:B:827:MET:HE3	1:B:842:LYS:O	2.10	0.51
1:A:357:VAL:HG23	1:A:374:GLN:HB2	1.93	0.51
1:A:981:GLY:O	1:A:982:LEU:HD23	2.10	0.51
1:B:1024:TYR:OH	1:B:1306:GLN:NE2	2.44	0.51
1:B:59:TYR:CD1	1:B:60:PRO:CD	2.94	0.51
1:A:1115:ASN:HD22	1:A:1115:ASN:N	2.09	0.51
1:A:153:LYS:HB3	1:A:154:PRO:HD2	1.93	0.51
1:A:182:ILE:HG12	1:A:804:ILE:HD11	1.93	0.51
1:A:492:TYR:CD2	1:A:493:ILE:N	2.78	0.51
1:A:855:PHE:HD2	1:A:888:VAL:HG22	1.76	0.51
1:B:39:ILE:CG1	1:B:85:LEU:HD23	2.40	0.51
1:B:44:TYR:CE1	1:B:497:THR:HG21	2.46	0.51
1:A:1377:PHE:CE1	1:A:1467:ILE:HD12	2.46	0.51
1:A:1673:LEU:HD22	1:B:258:LYS:HG2	1.93	0.51
1:A:916:THR:HG22	1:A:917:TRP:H	1.75	0.51
1:B:1123:GLN:NE2	1:B:1123:GLN:H	2.09	0.51
1:B:1204:GLN:HA	1:B:1204:GLN:OE1	2.10	0.51
1:B:916:THR:HG22	1:B:917:TRP:H	1.75	0.51
1:A:1001:THR:HG23	1:A:1284:PHE:HD2	1.75	0.51
1:A:227:PHE:HB2	1:A:253:ARG:O	2.10	0.51
1:A:635:GLY:CA	1:A:672:ILE:HG23	2.39	0.51
1:B:886:GLN:HG2	1:B:894:HIS:CD2	2.46	0.51
1:A:1028:GLY:C	1:A:1029:ASN:HD22	2.15	0.51
1:A:839:ILE:HD12	1:A:1485:VAL:HG12	1.93	0.51
1:B:1003:LEU:HD11	1:B:1286:SER:HA	1.92	0.51
1:B:855:PHE:HD2	1:B:888:VAL:HG22	1.76	0.51
1:A:1076:THR:HG22	1:A:1120:GLU:HA	1.93	0.50
1:A:1084:ARG:NE	1:A:1088:GLN:OE1	2.39	0.50
1:A:498:HIS:HB3	1:A:514:THR:HG23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PRO:HD3	1:A:103:TYR:HE1	1.76	0.50
1:B:1186:PHE:CD1	1:B:1250:THR:HG22	2.46	0.50
1:B:1429:PRO:HB3	1:B:1488:LEU:HD22	1.93	0.50
1:B:909:ASN:H	1:B:926:THR:HG22	1.75	0.50
1:B:942:VAL:HG22	1:B:957:LYS:HD3	1.92	0.50
1:A:1577:TYR:HB2	1:A:1600:PHE:O	2.12	0.50
1:A:362:PHE:CD1	1:A:638:GLY:O	2.54	0.50
1:A:733:VAL:O	1:A:737:GLN:HG2	2.11	0.50
1:B:227:PHE:HB2	1:B:253:ARG:O	2.11	0.50
1:B:292:LEU:HD13	1:B:293:ILE:N	2.27	0.50
1:B:363:LEU:HD12	1:B:456:ALA:HA	1.93	0.50
1:B:544:TYR:HE2	1:B:546:VAL:HG23	1.76	0.50
1:B:653:PHE:N	1:B:653:PHE:CD2	2.76	0.50
1:A:1024:TYR:OH	1:A:1306:GLN:NE2	2.44	0.50
1:A:131:ASP:OD1	1:A:135:TYR:OH	2.21	0.50
1:A:587:THR:HA	1:A:789:ALA:HA	1.93	0.50
1:B:1028:GLY:C	1:B:1029:ASN:HD22	2.15	0.50
1:B:733:VAL:O	1:B:737:GLN:HG2	2.10	0.50
1:B:855:PHE:HA	1:B:915:GLU:O	2.11	0.50
1:A:1016:VAL:HG12	1:A:1017:PRO:N	2.26	0.50
1:A:1207:SER:O	1:A:1210:SER:HB3	2.12	0.50
1:A:1378:TYR:O	1:A:1406:ALA:HA	2.11	0.50
1:A:1637:TYR:CE1	1:A:1639:LEU:HA	2.46	0.50
1:B:1378:TYR:O	1:B:1406:ALA:HA	2.12	0.50
1:A:1123:GLN:H	1:A:1123:GLN:NE2	2.09	0.50
1:A:798:GLU:HG3	1:A:814:THR:OG1	2.11	0.50
1:A:938:SER:O	1:A:940:SER:N	2.45	0.50
1:B:1016:VAL:HG12	1:B:1017:PRO:N	2.27	0.50
1:B:1207:SER:O	1:B:1210:SER:HB3	2.12	0.50
1:B:1304:VAL:CG1	1:B:1305:LYS:H	2.25	0.50
1:B:743:SER:OG	1:B:752:LEU:HD22	2.12	0.50
1:A:830:PRO:HG3	1:A:1483:PHE:HE2	1.77	0.50
1:A:166:PRO:HG3	1:A:199:TRP:CD1	2.46	0.50
1:A:363:LEU:HD12	1:A:456:ALA:HA	1.93	0.50
1:A:680:GLN:HG3	1:A:756:THR:HG23	1.93	0.50
1:B:357:VAL:HG23	1:B:374:GLN:HB2	1.93	0.50
1:A:1279:ARG:CZ	1:A:1284:PHE:CD1	2.94	0.50
1:A:44:TYR:CE1	1:A:497:THR:HG21	2.47	0.50
1:A:531:THR:HG23	1:A:533:ASN:H	1.75	0.50
1:A:700:TYR:CE1	1:A:758:LEU:HD12	2.47	0.50
1:B:1001:THR:HG23	1:B:1284:PHE:HD2	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:PRO:HG2	1:A:821:LYS:HB2	1.94	0.50
1:B:1115:ASN:N	1:B:1115:ASN:HD22	2.09	0.50
1:B:1279:ARG:CZ	1:B:1284:PHE:CD1	2.95	0.50
1:B:208:ASP:O	1:B:209:PHE:HB2	2.11	0.50
1:B:196:TYR:HD1	1:B:219:VAL:HG12	1.77	0.50
1:A:1585:TYR:CD1	1:A:1671:ILE:HG21	2.47	0.50
1:A:292:LEU:HD13	1:A:293:ILE:N	2.26	0.50
1:A:1385:ASP:O	1:A:1399:TYR:HD2	1.94	0.49
1:A:981:GLY:O	1:A:1309:LEU:HD21	2.12	0.49
1:B:1274:LEU:O	1:B:1276:GLU:N	2.45	0.49
1:B:1300:TYR:CZ	1:B:1304:VAL:HG21	2.47	0.49
1:B:1385:ASP:O	1:B:1399:TYR:HD2	1.94	0.49
1:A:43:VAL:HG22	1:A:44:TYR:N	2.27	0.49
1:A:835:ARG:HH21	1:A:971:THR:HG22	1.77	0.49
1:A:982:LEU:CD2	1:A:1309:LEU:HD11	2.41	0.49
1:B:373:VAL:HG21	1:B:388:VAL:HG11	1.93	0.49
1:B:498:HIS:HB3	1:B:514:THR:HG23	1.93	0.49
1:A:1300:TYR:CZ	1:A:1304:VAL:HG21	2.48	0.49
1:B:1076:THR:HG22	1:B:1120:GLU:HA	1.94	0.49
1:B:153:LYS:HB3	1:B:154:PRO:HD2	1.93	0.49
1:B:798:GLU:HG3	1:B:814:THR:OG1	2.11	0.49
1:A:114:SER:O	1:A:115:LYS:HE2	2.12	0.49
1:A:1286:SER:OG	1:A:1287:THR:N	2.45	0.49
1:A:1304:VAL:CG1	1:A:1305:LYS:H	2.24	0.49
1:A:136:THR:HG21	1:A:222:TYR:HB2	1.95	0.49
1:B:233:PRO:HG3	1:B:342:ILE:HD13	1.94	0.49
1:A:360:PRO:HA	1:A:636:ALA:HB3	1.95	0.49
1:A:240:TYR:HB3	1:A:446:ASN:ND2	2.28	0.49
1:B:1003:LEU:HB3	1:B:1498:TYR:HE1	1.77	0.49
1:B:953:ILE:O	1:B:953:ILE:HG13	2.11	0.49
1:A:1066:TYR:N	1:A:1066:TYR:CD1	2.81	0.49
1:A:1429:PRO:HB3	1:A:1488:LEU:HD22	1.93	0.49
1:A:820:PHE:HZ	1:A:848:TYR:HB2	1.76	0.49
1:A:930:VAL:HG12	1:A:931:PRO:O	2.12	0.49
1:B:115:LYS:HA	1:B:115:LYS:HE2	1.95	0.49
1:B:886:GLN:HG3	1:B:887:LYS:N	2.23	0.49
1:A:1293:ALA:O	1:A:1297:LEU:HD12	2.12	0.49
1:A:1578:LYS:HA	1:A:1599:THR:HG23	1.94	0.49
1:A:373:VAL:HG21	1:A:388:VAL:HG11	1.94	0.49
1:A:703:ALA:HB2	1:A:732:CYS:HA	1.95	0.49
1:B:114:SER:O	1:B:115:LYS:HE2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:GLY:HA2	1:B:411:THR:HG23	1.94	0.49
1:B:931:PRO:HA	1:B:932:GLU:OE1	2.13	0.49
1:A:196:TYR:HD1	1:A:219:VAL:HG12	1.78	0.49
1:A:233:PRO:HG3	1:A:342:ILE:HD13	1.94	0.49
1:A:59:TYR:CD1	1:A:60:PRO:CD	2.94	0.49
1:A:931:PRO:HA	1:A:932:GLU:OE1	2.12	0.49
1:B:635:GLY:CA	1:B:672:ILE:HG23	2.40	0.49
1:B:982:LEU:CD2	1:B:1309:LEU:HD11	2.42	0.49
1:A:1053:MET:CE	1:A:1086:LEU:HD13	2.43	0.49
1:A:1289:ASP:OD2	1:A:1290:THR:N	2.46	0.49
1:A:1584:ILE:HG22	1:A:1585:TYR:N	2.27	0.49
1:A:544:TYR:HE2	1:A:546:VAL:HG23	1.77	0.49
1:A:595:GLY:O	1:A:596:MET:HB2	2.13	0.49
1:A:708:ASP:OD2	1:A:1401:ARG:NH2	2.46	0.49
1:A:592:MET:HB3	1:A:780:VAL:HG11	1.94	0.49
1:A:855:PHE:HA	1:A:915:GLU:O	2.12	0.49
1:B:1053:MET:CE	1:B:1086:LEU:HD13	2.43	0.49
1:B:1309:LEU:HD23	1:B:1355:GLY:HA3	1.94	0.49
1:B:271:ILE:O	1:B:280:LYS:HB2	2.13	0.49
1:B:592:MET:HB3	1:B:780:VAL:HG11	1.94	0.49
1:A:267:ILE:HG12	1:A:327:VAL:HG13	1.94	0.49
1:A:835:ARG:HG2	1:A:835:ARG:NH1	2.04	0.49
1:B:43:VAL:HG22	1:B:44:TYR:N	2.28	0.49
1:A:1637:TYR:CD2	1:A:1638:PRO:HD2	2.47	0.48
1:A:384:GLY:HA2	1:A:411:THR:HG23	1.95	0.48
1:B:267:ILE:HG12	1:B:327:VAL:HG13	1.94	0.48
1:B:412:ARG:HG2	1:B:413:VAL:N	2.28	0.48
1:B:52:ALA:CB	1:B:73:LEU:HD21	2.43	0.48
1:B:757:LEU:O	1:B:758:LEU:HB2	2.12	0.48
1:B:584:PRO:HG2	1:B:821:LYS:HB2	1.94	0.48
1:B:938:SER:O	1:B:940:SER:N	2.45	0.48
1:A:1572:ASN:O	1:A:1573:VAL:HG22	2.12	0.48
1:A:1598:ILE:HG13	1:A:1599:THR:N	2.29	0.48
1:A:1622:LYS:HG3	1:A:1623:GLU:H	1.78	0.48
1:A:386:VAL:N	1:A:411:THR:HG22	2.28	0.48
1:B:1193:TYR:O	1:B:1196:SER:HB3	2.13	0.48
1:B:489:LYS:O	1:B:490:SER:CB	2.61	0.48
1:B:703:ALA:HB2	1:B:732:CYS:HA	1.95	0.48
1:A:831:TYR:CE1	1:A:1457:ASP:HB3	2.47	0.48
1:A:640:LEU:H	1:A:644:ASN:CB	2.21	0.48
1:A:835:ARG:NH1	1:A:835:ARG:CG	2.68	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:GLY:O	1:A:908:HIS:CE1	2.66	0.48
1:A:942:VAL:HG13	1:A:957:LYS:HD2	1.95	0.48
1:A:953:ILE:HG13	1:A:953:ILE:O	2.12	0.48
1:B:1289:ASP:OD2	1:B:1290:THR:N	2.46	0.48
1:B:981:GLY:O	1:B:1309:LEU:HD21	2.13	0.48
1:A:1589:GLU:HB2	1:A:1623:GLU:OE1	2.13	0.48
1:A:271:ILE:O	1:A:280:LYS:HB2	2.13	0.48
1:B:1176:LEU:HB3	1:B:1204:GLN:HG2	1.95	0.48
1:B:1293:ALA:O	1:B:1297:LEU:HD12	2.13	0.48
1:B:708:ASP:OD2	1:B:1401:ARG:NH2	2.46	0.48
1:B:736:SER:O	1:B:739:ARG:HG2	2.14	0.48
1:B:845:VAL:HG12	1:B:894:HIS:O	2.14	0.48
1:B:981:GLY:O	1:B:982:LEU:HD23	2.12	0.48
1:A:1652:THR:O	1:A:1658:GLN:HB2	2.13	0.48
1:B:127:PHE:HB2	1:B:146:TYR:HB2	1.96	0.48
1:A:1673:LEU:CA	1:B:258:LYS:HG3	2.43	0.48
1:B:484:ILE:HG22	1:B:526:ILE:O	2.14	0.48
1:B:595:GLY:O	1:B:596:MET:HB2	2.13	0.48
1:B:692:HIS:CD2	1:B:694:VAL:HG23	2.48	0.48
1:B:831:TYR:CE1	1:B:1457:ASP:HB3	2.49	0.48
1:A:1309:LEU:HD23	1:A:1355:GLY:HA3	1.94	0.48
1:A:1340:VAL:HG21	1:A:1346:LEU:HD22	1.96	0.48
1:B:386:VAL:N	1:B:411:THR:HG22	2.27	0.48
1:B:686:ILE:C	1:B:688:ALA:H	2.17	0.48
1:B:930:VAL:HG12	1:B:931:PRO:O	2.14	0.48
1:A:1132:THR:H	1:A:1135:VAL:HB	1.79	0.48
1:A:1279:ARG:CZ	1:A:1284:PHE:HD1	2.27	0.48
1:A:412:ARG:HG2	1:A:413:VAL:N	2.28	0.48
1:A:566:LYS:HE2	1:A:570:GLN:NE2	2.24	0.48
1:A:182:ILE:CG1	1:A:804:ILE:HD11	2.43	0.48
1:A:922:ILE:HG21	2:A:2001:NAG:C7	2.44	0.48
1:B:1244:THR:HG22	1:B:1246:ARG:N	2.28	0.48
1:B:849:ARG:HG3	1:B:851:SER:H	1.78	0.48
1:A:115:LYS:HA	1:A:115:LYS:HE2	1.94	0.48
1:A:156:LYS:HB3	1:A:178:ASP:O	2.13	0.48
1:A:480:GLU:O	1:A:530:VAL:HG12	2.13	0.48
1:B:1320:LYS:HD2	1:B:1321:GLY:H	1.78	0.48
1:B:182:ILE:HG12	1:B:804:ILE:HD11	1.95	0.48
1:B:136:THR:HG21	1:B:222:TYR:HB2	1.95	0.48
1:B:589:SER:HA	1:B:787:GLN:HA	1.96	0.48
1:A:1176:LEU:HB3	1:A:1204:GLN:HG2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:LEU:HA	1:A:1180:LEU:HD23	1.52	0.48
1:A:1320:LYS:HD2	1:A:1321:GLY:H	1.79	0.48
1:A:1378:TYR:O	1:A:1379:LEU:HD23	2.13	0.48
1:A:563:ILE:HG13	1:A:564:GLU:N	2.28	0.48
1:A:736:SER:O	1:A:739:ARG:HG2	2.13	0.48
1:A:849:ARG:HG3	1:A:851:SER:H	1.78	0.48
1:B:1304:VAL:CG1	1:B:1305:LYS:N	2.73	0.48
1:B:1378:TYR:O	1:B:1379:LEU:HD23	2.14	0.48
1:B:480:GLU:O	1:B:530:VAL:HG12	2.14	0.48
1:B:490:SER:O	1:B:491:PRO:C	2.51	0.48
1:B:362:PHE:CD1	1:B:638:GLY:O	2.56	0.48
1:B:182:ILE:CG1	1:B:804:ILE:HD11	2.44	0.48
1:A:1193:TYR:O	1:A:1196:SER:HB3	2.14	0.48
1:A:1244:THR:HG22	1:A:1246:ARG:N	2.28	0.48
1:A:127:PHE:HB2	1:A:146:TYR:HB2	1.96	0.48
1:B:1076:THR:HA	1:B:1106:TRP:HZ3	1.79	0.48
1:B:493:ILE:CG2	1:B:495:LYS:HE2	2.44	0.48
1:B:942:VAL:HG13	1:B:957:LYS:HD2	1.95	0.48
1:A:931:PRO:HB2	1:A:1366:HIS:CD2	2.49	0.47
1:A:1565:ILE:O	1:A:1565:ILE:HD12	2.14	0.47
1:A:702:GLY:HA2	1:A:728:PHE:CD1	2.49	0.47
1:B:1066:TYR:N	1:B:1066:TYR:CD1	2.82	0.47
1:B:1320:LYS:CG	1:B:1321:GLY:N	2.77	0.47
1:B:760:VAL:HG21	1:B:1444:GLU:OE2	2.14	0.47
1:B:156:LYS:HB3	1:B:178:ASP:O	2.14	0.47
1:A:987:ILE:HG22	1:A:1021:VAL:HG23	1.96	0.47
1:A:490:SER:O	1:A:491:PRO:C	2.50	0.47
1:A:54:ILE:O	1:A:68:SER:HA	2.14	0.47
1:B:679:LEU:HD13	1:B:742:ILE:HD13	1.96	0.47
1:A:1258:SER:HB3	1:A:1267:VAL:HG23	1.96	0.47
1:A:1585:TYR:HB3	1:A:1671:ILE:HG12	1.95	0.47
1:A:1633:PHE:CE2	1:A:1634:ARG:HD2	2.49	0.47
1:A:1576:LYS:HE3	1:A:1601:ILE:HG21	1.97	0.47
1:A:330:ILE:O	1:A:330:ILE:HG13	2.14	0.47
1:B:1286:SER:OG	1:B:1287:THR:N	2.44	0.47
1:B:931:PRO:HB2	1:B:1366:HIS:CD2	2.49	0.47
1:B:1525:CYS:SG	1:B:1526:LYS:N	2.87	0.47
1:B:123:ASN:HB3	1:B:209:PHE:CD2	2.49	0.47
1:A:1146:ALA:HB1	1:A:1190:ILE:HG22	1.97	0.47
1:A:1320:LYS:HG2	1:A:1342:LEU:CD1	2.44	0.47
1:A:1326:TYR:N	1:A:1326:TYR:CD2	2.83	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:LEU:HB3	1:A:1498:TYR:HE1	1.78	0.47
1:B:1132:THR:H	1:B:1135:VAL:HB	1.78	0.47
1:B:1379:LEU:HB2	1:B:1507:MET:CE	2.44	0.47
1:B:1379:LEU:HD21	1:B:1495:VAL:CG1	2.44	0.47
1:B:266:TYR:CE2	1:B:755:LYS:HB2	2.49	0.47
1:B:330:ILE:HG13	1:B:330:ILE:O	2.15	0.47
1:B:386:VAL:N	1:B:411:THR:CG2	2.77	0.47
1:B:54:ILE:O	1:B:68:SER:HA	2.15	0.47
1:A:1576:LYS:HG3	1:A:1601:ILE:HG22	1.97	0.47
1:A:489:LYS:O	1:A:490:SER:CB	2.62	0.47
1:B:829:ILE:HG13	1:B:925:LYS:CG	2.35	0.47
1:A:1561:TYR:O	1:A:1561:TYR:HD2	1.98	0.47
1:A:457:TYR:HE2	1:A:459:SER:HB2	1.80	0.47
1:A:484:ILE:HG22	1:A:526:ILE:O	2.14	0.47
1:B:598:SER:HA	1:B:805:SER:OG	2.15	0.47
1:B:820:PHE:HZ	1:B:848:TYR:HB2	1.79	0.47
1:A:123:ASN:HB3	1:A:209:PHE:CD2	2.50	0.47
1:A:258:LYS:HD3	1:A:258:LYS:HA	1.59	0.47
1:A:757:LEU:HG	1:A:759:PRO:HD3	1.97	0.47
1:A:760:VAL:HG12	1:A:760:VAL:O	2.15	0.47
1:B:1326:TYR:N	1:B:1326:TYR:CD2	2.83	0.47
1:B:760:VAL:O	1:B:760:VAL:HG12	2.15	0.47
1:A:1290:THR:O	1:A:1294:ILE:CG1	2.58	0.47
1:A:1379:LEU:HB2	1:A:1507:MET:CE	2.44	0.47
1:A:465:LEU:HD21	1:A:542:VAL:HG12	1.97	0.47
1:A:493:ILE:CG2	1:A:495:LYS:HG2	2.45	0.47
1:A:52:ALA:CB	1:A:73:LEU:HD21	2.43	0.47
1:B:987:ILE:HG22	1:B:1021:VAL:HG23	1.96	0.47
1:B:423:ASN:ND2	1:B:423:ASN:N	2.63	0.47
1:B:702:GLY:HA2	1:B:728:PHE:CD1	2.49	0.47
1:B:839:ILE:HD12	1:B:1485:VAL:HG12	1.97	0.47
1:B:838:GLN:HA	1:B:901:LEU:HB2	1.97	0.47
1:A:1034:PHE:CE1	1:A:1041:GLU:HG2	2.50	0.47
1:A:1144:LEU:O	1:A:1148:THR:HG22	2.15	0.47
1:A:1186:PHE:CD1	1:A:1250:THR:HG22	2.47	0.47
1:A:1370:THR:O	1:A:1370:THR:HG22	2.15	0.47
1:A:493:ILE:CG2	1:A:495:LYS:HE2	2.45	0.47
1:A:599:TRP:HB2	1:A:804:ILE:O	2.15	0.47
1:B:1340:VAL:HG21	1:B:1346:LEU:HD22	1.97	0.47
1:B:493:ILE:CG2	1:B:495:LYS:HG2	2.45	0.47
1:B:906:GLY:O	1:B:908:HIS:CE1	2.67	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LEU:N	1:A:404:LEU:HD23	2.30	0.47
1:A:423:ASN:ND2	1:A:423:ASN:N	2.63	0.47
1:A:598:SER:HA	1:A:805:SER:OG	2.15	0.47
1:A:829:ILE:HG13	1:A:925:LYS:CG	2.35	0.47
1:B:1146:ALA:HB1	1:B:1190:ILE:HG22	1.96	0.47
1:A:692:HIS:CD2	1:A:694:VAL:HG23	2.48	0.46
1:B:563:ILE:HG13	1:B:564:GLU:N	2.28	0.46
1:A:1180:LEU:CD2	1:A:1208:ILE:HG12	2.44	0.46
1:A:1193:TYR:HE1	1:A:1256:LEU:HB3	1.77	0.46
1:A:467:ILE:HG13	1:A:467:ILE:O	2.15	0.46
1:B:465:LEU:HD21	1:B:542:VAL:HG12	1.96	0.46
1:A:1379:LEU:HD21	1:A:1495:VAL:CG1	2.45	0.46
1:A:1546:GLU:HG2	1:A:1547:THR:N	2.30	0.46
1:A:679:LEU:HD13	1:A:742:ILE:HD13	1.96	0.46
1:A:686:ILE:C	1:A:688:ALA:H	2.17	0.46
1:B:1144:LEU:O	1:B:1148:THR:HG22	2.16	0.46
1:B:214:THR:HG22	1:B:216:TYR:CE2	2.50	0.46
1:B:363:LEU:O	1:B:363:LEU:HD12	2.14	0.46
1:A:1320:LYS:CG	1:A:1321:GLY:N	2.77	0.46
1:A:363:LEU:O	1:A:363:LEU:HD12	2.14	0.46
1:A:546:VAL:HG12	1:A:546:VAL:O	2.14	0.46
1:B:1034:PHE:CE1	1:B:1041:GLU:HG2	2.50	0.46
1:B:1180:LEU:CD2	1:B:1208:ILE:HG12	2.45	0.46
1:B:1290:THR:O	1:B:1294:ILE:CG1	2.58	0.46
1:B:1320:LYS:HG2	1:B:1342:LEU:CD1	2.44	0.46
1:B:457:TYR:HE2	1:B:459:SER:HB2	1.80	0.46
1:B:546:VAL:HG12	1:B:546:VAL:O	2.14	0.46
1:B:152:LEU:O	1:B:808:GLY:HA2	2.16	0.46
1:A:1076:THR:HA	1:A:1106:TRP:HZ3	1.80	0.46
1:A:618:LYS:HA	1:A:619:PRO:HD3	1.73	0.46
1:A:838:GLN:HA	1:A:901:LEU:HB2	1.97	0.46
1:B:1015:VAL:HG22	1:B:1015:VAL:O	2.15	0.46
1:A:1264:ILE:HG12	1:A:1303:LEU:CD1	2.43	0.46
1:A:360:PRO:HB3	1:A:637:GLY:O	2.15	0.46
1:B:1303:LEU:HD13	1:B:1303:LEU:C	2.35	0.46
1:B:1319:HIS:HD2	1:B:1344:ASP:OD1	1.99	0.46
1:B:360:PRO:HA	1:B:636:ALA:HB3	1.97	0.46
1:B:582:TYR:CB	1:B:819:VAL:HG12	2.46	0.46
1:A:286:ALA:O	1:A:287:MET:C	2.53	0.46
1:A:589:SER:HA	1:A:787:GLN:HA	1.96	0.46
1:B:1457:ASP:O	1:B:1459:HIS:HD2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ALA:O	1:B:287:MET:C	2.53	0.46
1:A:152:LEU:O	1:A:808:GLY:HA2	2.16	0.46
1:A:1559:TYR:CD2	1:A:1559:TYR:C	2.89	0.46
1:A:1641:SER:C	1:A:1643:THR:H	2.18	0.46
1:A:587:THR:CG2	1:A:789:ALA:HB2	2.45	0.46
1:B:1015:VAL:HG23	1:B:1049:LEU:HD12	1.98	0.46
1:B:473:HIS:HE1	1:B:477:LEU:CG	2.20	0.46
1:A:1015:VAL:O	1:A:1015:VAL:HG22	2.16	0.46
1:A:1303:LEU:C	1:A:1303:LEU:HD13	2.35	0.46
1:A:412:ARG:HD3	1:A:414:ASP:OD2	2.16	0.46
1:B:1258:SER:HB3	1:B:1267:VAL:HG23	1.97	0.46
1:B:1520:CYS:HA	1:B:1525:CYS:CB	2.46	0.46
1:A:441:ASP:OD2	1:A:441:ASP:N	2.46	0.46
1:A:781:PRO:C	1:A:783:ARG:H	2.19	0.46
1:A:838:GLN:HB3	1:A:1486:GLY:CA	2.40	0.46
1:B:830:PRO:HG3	1:B:1483:PHE:HE2	1.80	0.46
1:B:360:PRO:HB3	1:B:637:GLY:O	2.15	0.46
1:B:369:TYR:HA	1:B:370:PRO:HD3	1.70	0.46
1:B:485:ILE:N	1:B:485:ILE:HD12	2.32	0.46
1:B:594:THR:HG21	1:B:598:SER:HB3	1.98	0.46
1:B:599:TRP:CZ3	1:B:779:LEU:HB2	2.51	0.46
1:A:1202:HIS:CD2	1:A:1204:GLN:HB3	2.52	0.45
1:A:1548:ARG:NH2	1:A:1646:GLU:OE1	2.48	0.45
1:B:1370:THR:O	1:B:1370:THR:HG22	2.15	0.45
1:B:232:GLU:HA	1:B:233:PRO:HD3	1.73	0.45
1:A:1076:THR:N	1:A:1120:GLU:OE2	2.49	0.45
1:A:895:LEU:HD13	1:A:1555:PRO:HB2	1.97	0.45
1:A:214:THR:HG22	1:A:216:TYR:CE2	2.51	0.45
1:A:643:ALA:O	1:A:647:HIS:N	2.49	0.45
1:A:758:LEU:HD22	1:A:760:VAL:H	1.80	0.45
1:A:93:PRO:HD2	1:A:96:GLN:O	2.16	0.45
1:B:1012:LEU:O	1:B:1015:VAL:HG12	2.16	0.45
1:B:31:PHE:HB2	1:B:119:ILE:HG22	1.98	0.45
1:B:1408:TYR:O	1:B:1410:PRO:HD3	2.17	0.45
1:B:240:TYR:HB3	1:B:446:ASN:ND2	2.31	0.45
1:B:922:ILE:HG21	2:B:2001:NAG:N2	2.32	0.45
1:B:949:ILE:HG12	1:B:949:ILE:H	1.57	0.45
1:A:1180:LEU:HD21	1:A:1208:ILE:HG12	1.97	0.45
1:B:599:TRP:HB2	1:B:804:ILE:O	2.16	0.45
1:A:1015:VAL:HG23	1:A:1049:LEU:HD12	1.98	0.45
1:A:1104:LEU:HD13	1:A:1164:ILE:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1456:LYS:O	1:A:1457:ASP:C	2.55	0.45
1:A:1457:ASP:O	1:A:1459:HIS:HD2	1.99	0.45
1:B:1318:LYS:HG2	1:B:1319:HIS:NE2	2.31	0.45
1:B:265:VAL:O	1:B:289:ASN:HA	2.17	0.45
1:B:577:PRO:HD3	1:B:588:VAL:HG23	1.98	0.45
1:B:587:THR:CG2	1:B:789:ALA:HB2	2.46	0.45
1:B:66:TYR:OH	1:B:90:LYS:HD2	2.17	0.45
1:B:779:LEU:O	1:B:781:PRO:HD3	2.17	0.45
1:B:905:ILE:HG22	1:B:906:GLY:N	2.32	0.45
1:A:1524:ALA:O	1:A:1528:VAL:HG23	2.16	0.45
1:A:265:VAL:O	1:A:289:ASN:HA	2.17	0.45
1:A:839:ILE:HD11	1:A:1483:PHE:CE1	2.52	0.45
1:B:131:ASP:OD1	1:B:135:TYR:OH	2.22	0.45
1:B:909:ASN:HD22	1:B:910:ILE:N	2.14	0.45
1:A:1076:THR:HG22	1:A:1120:GLU:OE2	2.16	0.45
1:A:388:VAL:O	1:A:420:PHE:HZ	2.00	0.45
1:A:980:LYS:HB3	1:A:980:LYS:HE3	1.64	0.45
1:B:541:LEU:HD13	1:B:645:VAL:HG12	1.98	0.45
1:A:1319:HIS:HD2	1:A:1344:ASP:OD1	1.99	0.45
1:A:1433:SER:HB2	1:A:1480:PHE:HD1	1.81	0.45
1:A:150:ASP:HB2	1:A:508:LYS:NZ	2.31	0.45
1:A:451:GLY:C	1:A:452:TYR:CD2	2.90	0.45
1:A:949:ILE:HG12	1:A:949:ILE:H	1.56	0.45
1:B:113:LYS:HG3	1:B:114:SER:N	2.31	0.45
1:B:1323:LEU:CD1	1:B:1324:HIS:H	2.30	0.45
1:A:1631:PHE:O	1:A:1632:SER:CB	2.64	0.45
1:A:599:TRP:CZ3	1:A:779:LEU:HB2	2.51	0.45
1:A:909:ASN:HD22	1:A:909:ASN:C	2.20	0.45
1:B:1076:THR:HG22	1:B:1120:GLU:OE2	2.17	0.45
1:B:1076:THR:N	1:B:1120:GLU:OE2	2.50	0.45
1:B:1180:LEU:HD21	1:B:1208:ILE:HG12	1.99	0.45
1:B:1427:SER:HB3	1:B:1492:THR:H	1.82	0.45
1:B:404:LEU:HD23	1:B:404:LEU:N	2.32	0.45
1:B:467:ILE:HG13	1:B:467:ILE:O	2.16	0.45
1:B:592:MET:HG2	1:B:780:VAL:HG21	1.98	0.45
1:B:560:TRP:CD2	1:B:673:LEU:HD12	2.52	0.45
1:A:1539:LEU:CD1	1:A:1657:CYS:HB3	2.31	0.45
1:A:577:PRO:HD3	1:A:588:VAL:HG23	1.98	0.45
1:A:779:LEU:O	1:A:781:PRO:HD3	2.17	0.45
1:A:575:LEU:HD11	1:A:817:ALA:HB2	1.99	0.45
1:B:667:GLU:N	1:B:668:PRO:CD	2.79	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1408:TYR:O	1:A:1410:PRO:HD3	2.17	0.45
1:A:1497:GLU:OE1	1:A:1500:ARG:HD2	2.17	0.45
1:A:1665:ASP:O	1:A:1668:ALA:HB3	2.17	0.45
1:A:190:ILE:HG22	1:A:194:PRO:CG	2.47	0.45
1:B:1202:HIS:CD2	1:B:1204:GLN:HB3	2.51	0.45
1:B:583:SER:HA	1:B:584:PRO:HD3	1.80	0.45
1:B:738:LEU:HG	1:B:742:ILE:HD11	1.98	0.45
1:B:575:LEU:HD11	1:B:817:ALA:HB2	1.99	0.45
1:A:1490:PRO:HB3	1:A:1509:TYR:O	2.17	0.44
1:A:576:SER:HB2	1:A:588:VAL:HG23	1.98	0.44
1:A:818:LYS:HG3	1:A:818:LYS:O	2.16	0.44
1:A:909:ASN:HD22	1:A:910:ILE:N	2.15	0.44
1:B:292:LEU:HA	1:B:297:ALA:HB2	1.99	0.44
1:B:818:LYS:O	1:B:818:LYS:HG3	2.16	0.44
1:A:1323:LEU:CD1	1:A:1324:HIS:H	2.30	0.44
1:A:1599:THR:HG22	1:A:1600:PHE:N	2.32	0.44
1:A:319:ASN:C	1:A:320:ASN:HD22	2.20	0.44
1:A:594:THR:HG21	1:A:598:SER:HB3	1.98	0.44
1:A:738:LEU:HG	1:A:742:ILE:HD11	1.99	0.44
1:B:373:VAL:HG22	1:B:418:ALA:HB3	1.99	0.44
1:B:774:LEU:HD23	1:B:774:LEU:HA	1.80	0.44
1:B:909:ASN:C	1:B:909:ASN:HD22	2.20	0.44
1:A:1090:ASN:HD22	1:A:1158:ILE:CD1	2.27	0.44
1:A:1618:LEU:HG	1:A:1618:LEU:O	2.17	0.44
1:A:260:VAL:HG11	1:A:263:ALA:HB2	1.99	0.44
1:A:292:LEU:HA	1:A:297:ALA:HB2	1.99	0.44
1:A:535:VAL:CG2	1:A:536:PRO:HD3	2.28	0.44
1:A:539:ARG:NH2	1:A:635:GLY:O	2.50	0.44
1:A:582:TYR:CB	1:A:819:VAL:HG12	2.46	0.44
1:A:66:TYR:OH	1:A:90:LYS:HD2	2.17	0.44
1:B:1104:LEU:HD13	1:B:1164:ILE:HD12	1.99	0.44
1:B:121:TYR:HB2	1:B:210:SER:HB2	2.00	0.44
1:B:388:VAL:O	1:B:420:PHE:HZ	2.01	0.44
1:B:61:ASP:CG	1:B:61:ASP:O	2.56	0.44
1:A:1318:LYS:HG2	1:A:1319:HIS:NE2	2.32	0.44
1:A:1440:LYS:HD2	1:A:1444:GLU:OE1	2.17	0.44
1:A:838:GLN:O	1:A:1485:VAL:HA	2.17	0.44
1:A:1518:LYS:HE2	1:A:1518:LYS:HB2	1.82	0.44
1:A:290:THR:HG22	1:A:290:THR:O	2.17	0.44
1:A:689:LYS:HB3	1:A:689:LYS:HE2	1.76	0.44
1:A:905:ILE:HG22	1:A:906:GLY:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1053:MET:HE2	1:B:1086:LEU:HD13	1.99	0.44
1:B:189:LYS:HE2	1:B:190:ILE:O	2.18	0.44
1:B:190:ILE:HG22	1:B:194:PRO:CG	2.47	0.44
1:B:497:THR:HG23	1:B:498:HIS:H	1.82	0.44
1:A:193:ASN:OD1	1:A:1070:LYS:HE2	2.17	0.44
1:A:1626:GLN:HG2	1:A:1635:TYR:CD2	2.52	0.44
1:A:541:LEU:HD13	1:A:645:VAL:HG12	1.99	0.44
1:A:592:MET:HG2	1:A:780:VAL:HG21	1.98	0.44
1:B:1309:LEU:CD2	1:B:1356:LEU:H	2.31	0.44
1:B:1485:VAL:HG23	1:B:1488:LEU:HB3	1.99	0.44
1:B:576:SER:HB2	1:B:588:VAL:HG23	1.98	0.44
1:B:775:TRP:O	1:B:775:TRP:CD1	2.71	0.44
1:A:113:LYS:HG3	1:A:114:SER:N	2.32	0.44
1:A:1484:GLU:OE1	1:A:1484:GLU:N	2.45	0.44
1:B:1379:LEU:HD21	1:B:1495:VAL:HG11	1.99	0.44
1:B:539:ARG:NH2	1:B:635:GLY:O	2.51	0.44
1:B:93:PRO:HD2	1:B:96:GLN:O	2.16	0.44
1:A:1012:LEU:O	1:A:1015:VAL:HG12	2.17	0.44
1:A:1109:GLU:HG2	1:A:1163:LYS:HE2	2.00	0.44
1:A:1216:ALA:HB2	1:A:1228:TRP:CZ2	2.53	0.44
1:A:189:LYS:HE2	1:A:190:ILE:O	2.18	0.44
1:A:497:THR:HG23	1:A:498:HIS:N	2.33	0.44
1:A:681:LYS:H	1:A:681:LYS:HG3	1.67	0.44
1:A:775:TRP:O	1:A:775:TRP:CD1	2.71	0.44
1:B:1090:ASN:HD22	1:B:1158:ILE:CD1	2.27	0.44
1:B:1180:LEU:HD23	1:B:1180:LEU:HA	1.52	0.44
1:B:1030:HIS:CE1	1:B:1306:GLN:HE21	2.36	0.44
1:B:733:VAL:HG13	1:B:737:GLN:NE2	2.33	0.44
1:B:781:PRO:C	1:B:783:ARG:H	2.19	0.44
1:A:1644:TRP:O	1:A:1644:TRP:CD1	2.71	0.44
1:A:485:ILE:N	1:A:485:ILE:HD12	2.32	0.44
1:A:610:TYR:O	1:A:612:VAL:HG22	2.18	0.44
1:A:969:PRO:O	1:A:971:THR:HG23	2.18	0.44
1:B:58:SER:O	1:B:103:TYR:HD1	2.01	0.44
1:B:1109:GLU:HG2	1:B:1163:LYS:HE2	2.00	0.44
1:B:1264:ILE:HG12	1:B:1303:LEU:CD1	2.44	0.44
1:B:1266:TYR:O	1:B:1269:PRO:HD2	2.18	0.44
1:B:1300:TYR:CD2	1:B:1300:TYR:C	2.90	0.44
1:A:1091:LYS:HB3	1:A:1091:LYS:HE2	1.70	0.44
1:A:1300:TYR:CD2	1:A:1300:TYR:C	2.91	0.44
1:A:544:TYR:HE2	1:A:546:VAL:CG2	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ASP:O	1:A:61:ASP:CG	2.56	0.44
1:A:885:ARG:HH12	1:A:1628:LYS:NZ	2.16	0.44
1:B:1216:ALA:HB2	1:B:1228:TRP:CZ2	2.53	0.44
1:B:1279:ARG:CZ	1:B:1284:PHE:HD1	2.29	0.44
1:B:1429:PRO:HB2	1:B:1432:ILE:HG13	2.00	0.44
1:B:1484:GLU:N	1:B:1484:GLU:OE1	2.45	0.44
1:B:260:VAL:HG11	1:B:263:ALA:HB2	1.98	0.44
1:B:412:ARG:HD3	1:B:414:ASP:OD2	2.17	0.44
1:B:610:TYR:O	1:B:612:VAL:HG22	2.18	0.44
1:B:802:ILE:HD11	1:B:809:ILE:HG13	2.00	0.44
1:A:58:SER:O	1:A:103:TYR:HD1	2.01	0.43
1:A:1309:LEU:CD2	1:A:1356:LEU:H	2.31	0.43
1:A:757:LEU:O	1:A:758:LEU:HB2	2.18	0.43
1:B:1497:GLU:OE1	1:B:1500:ARG:HD2	2.18	0.43
1:B:840:GLN:HG3	1:B:899:THR:CG2	2.48	0.43
1:B:984:VAL:HG13	1:B:988:LEU:HG	2.00	0.43
1:A:1379:LEU:HD21	1:A:1495:VAL:HG11	2.00	0.43
1:A:1584:ILE:CG2	1:A:1585:TYR:N	2.80	0.43
1:A:886:GLN:HG3	1:A:887:LYS:N	2.23	0.43
1:B:1202:HIS:CD2	1:B:1204:GLN:H	2.20	0.43
1:A:1673:LEU:HA	1:B:258:LYS:HG3	2.00	0.43
1:B:969:PRO:O	1:B:971:THR:HG23	2.18	0.43
1:B:977:LEU:HD12	1:B:1361:VAL:CG2	2.39	0.43
1:A:31:PHE:HB2	1:A:119:ILE:HG22	1.98	0.43
1:A:1427:SER:OG	1:A:1491:ALA:HB1	2.18	0.43
1:A:1454:GLN:HG3	1:A:1461:ILE:HB	1.99	0.43
1:A:276:LYS:HD3	1:A:276:LYS:HA	1.89	0.43
1:A:554:LEU:HD23	1:A:554:LEU:HA	1.88	0.43
1:A:659:ALA:C	1:A:661:ASP:H	2.22	0.43
1:A:901:LEU:HA	1:A:902:PRO:HD3	1.78	0.43
1:B:150:ASP:HB2	1:B:508:LYS:NZ	2.33	0.43
1:B:758:LEU:C	1:B:760:VAL:H	2.21	0.43
1:B:142:LYS:HD3	1:B:775:TRP:CG	2.53	0.43
1:A:1671:ILE:HG23	1:A:1672:PHE:N	2.34	0.43
1:B:1244:THR:HB	1:B:1247:MET:HB2	2.01	0.43
1:B:1454:GLN:HG3	1:B:1461:ILE:HB	2.00	0.43
1:B:504:LEU:N	1:B:504:LEU:HD12	2.33	0.43
1:B:571:LEU:HA	1:B:593:ALA:O	2.18	0.43
1:B:691:LYS:O	1:B:692:HIS:HB2	2.18	0.43
1:A:1075:SER:HB2	1:A:1120:GLU:OE1	2.19	0.43
1:A:1202:HIS:CD2	1:A:1204:GLN:H	2.20	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1318:LYS:O	1:A:1318:LYS:HG3	2.18	0.43
1:A:691:LYS:O	1:A:692:HIS:HB2	2.18	0.43
1:B:1440:LYS:HD2	1:B:1444:GLU:OE1	2.18	0.43
1:B:1516:ILE:HG21	1:B:1518:LYS:HE3	2.00	0.43
1:B:290:THR:HG22	1:B:290:THR:O	2.18	0.43
1:B:367:ILE:HD12	1:B:489:LYS:HD3	2.00	0.43
1:B:544:TYR:HE2	1:B:546:VAL:CG2	2.30	0.43
1:B:980:LYS:HE3	1:B:980:LYS:HB3	1.63	0.43
1:A:1174:PHE:O	1:A:1178:ASN:HB2	2.18	0.43
1:A:1318:LYS:HG2	1:A:1319:HIS:CD2	2.54	0.43
1:A:1402:ILE:O	1:A:1476:ARG:HA	2.19	0.43
1:A:1429:PRO:HB2	1:A:1432:ILE:HG13	2.01	0.43
1:A:214:THR:HG22	1:A:215:ALA:N	2.34	0.43
1:A:367:ILE:HD12	1:A:489:LYS:HD3	2.01	0.43
1:A:497:THR:HG23	1:A:498:HIS:H	1.82	0.43
1:A:774:LEU:HA	1:A:774:LEU:HD23	1.80	0.43
1:B:1186:PHE:CD1	1:B:1246:ARG:HD2	2.53	0.43
1:B:1433:SER:HB2	1:B:1480:PHE:HD1	1.82	0.43
1:B:451:GLY:C	1:B:452:TYR:CD2	2.92	0.43
1:B:592:MET:HE3	1:B:780:VAL:CG2	2.48	0.43
1:B:758:LEU:HD22	1:B:760:VAL:H	1.83	0.43
1:A:1200:LYS:HA	1:A:1205:PHE:CD2	2.54	0.43
1:A:1030:HIS:CE1	1:A:1306:GLN:HE21	2.36	0.43
1:A:154:PRO:O	1:A:155:ALA:HB3	2.19	0.43
1:A:1554:LYS:CG	1:A:1556:GLU:HG2	2.49	0.43
1:A:1604:VAL:HG22	1:A:1604:VAL:O	2.19	0.43
1:A:1630:ASN:O	1:A:1631:PHE:CB	2.65	0.43
1:A:1535:MET:CG	1:A:1645:ILE:HD11	2.49	0.43
1:A:1649:PRO:CG	1:A:1660:PHE:HD2	2.32	0.43
1:A:23:TYR:HA	1:A:43:VAL:HG23	2.01	0.43
1:A:906:GLY:H	1:A:929:VAL:HB	1.83	0.43
1:B:1075:SER:HB2	1:B:1120:GLU:OE1	2.19	0.43
1:B:1152:ILE:O	1:B:1156:PHE:HB2	2.19	0.43
1:B:1243:GLY:HA3	1:B:1285:TYR:CZ	2.54	0.43
1:B:1002:HIS:HD1	1:B:1284:PHE:HZ	1.66	0.43
1:B:1379:LEU:HB2	1:B:1507:MET:HE1	2.00	0.43
1:B:161:LEU:HD21	1:B:185:PHE:CD2	2.54	0.43
1:B:757:LEU:HG	1:B:758:LEU:N	2.34	0.43
1:A:1202:HIS:HD2	1:A:1204:GLN:N	2.07	0.43
1:A:1485:VAL:HG23	1:A:1488:LEU:HB3	1.99	0.43
1:A:571:LEU:HA	1:A:593:ALA: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:682:LYS:O	1:A:685:GLU:HG2	2.18	0.43
1:A:769:PHE:HA	1:A:770:PRO:HD3	1.82	0.43
1:A:809:ILE:HG12	1:A:810:CYS:N	2.34	0.43
1:B:1334:LEU:H	1:B:1334:LEU:HD22	1.83	0.43
1:B:1456:LYS:O	1:B:1457:ASP:C	2.56	0.43
1:B:258:LYS:HA	1:B:258:LYS:HD3	1.59	0.43
1:B:689:LYS:HE2	1:B:689:LYS:HB3	1.76	0.43
1:B:838:GLN:HB3	1:B:1486:GLY:CA	2.41	0.43
1:A:1107:LEU:HB3	1:A:1118:PHE:HE2	1.84	0.43
1:A:121:TYR:HB2	1:A:210:SER:HB2	2.00	0.43
1:A:1487:PHE:O	1:A:1488:LEU:C	2.57	0.43
1:A:1649:PRO:HB2	1:A:1661:LEU:HD11	2.01	0.43
1:A:290:THR:HG21	1:A:298:GLN:O	2.19	0.43
1:A:733:VAL:HG13	1:A:737:GLN:NE2	2.32	0.43
1:B:1427:SER:OG	1:B:1491:ALA:HB1	2.18	0.43
1:B:398:ASN:O	1:B:399:GLN:HB2	2.19	0.43
1:B:23:TYR:OH	1:B:656:ASN:HB2	2.18	0.43
1:A:1186:PHE:CD1	1:A:1246:ARG:HD2	2.53	0.43
1:A:760:VAL:HG21	1:A:1444:GLU:OE2	2.18	0.43
1:A:23:TYR:HD1	1:A:23:TYR:O	2.02	0.43
1:B:1174:PHE:O	1:B:1178:ASN:HB2	2.17	0.43
1:B:468:ASP:CG	1:B:469:TRP:H	2.23	0.43
1:B:548:GLY:C	1:B:549:GLU:HG3	2.38	0.43
1:A:1152:ILE:O	1:A:1156:PHE:HB2	2.19	0.42
1:A:1535:MET:CB	1:A:1645:ILE:HD11	2.49	0.42
1:A:287:MET:CE	1:A:299:VAL:HB	2.49	0.42
1:B:1132:THR:HG22	1:B:1133:LEU:H	1.83	0.42
1:B:1318:LYS:HG3	1:B:1318:LYS:O	2.18	0.42
1:B:287:MET:CE	1:B:299:VAL:HB	2.49	0.42
1:B:25:ILE:HD13	1:B:41:ILE:HG13	2.01	0.42
1:B:497:THR:HG23	1:B:498:HIS:N	2.33	0.42
1:B:542:VAL:O	1:B:556:SER:HA	2.19	0.42
1:B:809:ILE:HG12	1:B:810:CYS:N	2.33	0.42
1:B:959:PHE:HA	1:B:960:PRO:HD3	1.80	0.42
1:B:1096:ASN:O	1:B:1100:ILE:HG12	2.20	0.42
1:B:1200:LYS:HA	1:B:1205:PHE:CD2	2.54	0.42
1:B:266:TYR:CZ	1:B:755:LYS:HB2	2.55	0.42
1:B:290:THR:HG21	1:B:298:GLN:O	2.18	0.42
1:B:60:PRO:O	1:B:61:ASP:HB3	2.18	0.42
1:B:682:LYS:O	1:B:685:GLU:HG2	2.18	0.42
1:B:71:VAL:O	1:B:71:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1244:THR:HB	1:A:1247:MET:HB2	2.01	0.42
1:A:161:LEU:HD21	1:A:185:PHE:CD2	2.54	0.42
1:A:548:GLY:C	1:A:549:GLU:HG3	2.38	0.42
1:A:802:ILE:HD11	1:A:809:ILE:HG13	2.00	0.42
1:A:840:GLN:HG3	1:A:899:THR:CG2	2.48	0.42
1:B:1487:PHE:N	1:B:1487:PHE:CD2	2.87	0.42
1:B:154:PRO:O	1:B:155:ALA:HB3	2.19	0.42
1:B:319:ASN:C	1:B:320:ASN:HD22	2.22	0.42
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.93	0.42
1:A:1332:ASN:CG	1:A:1332:ASN:O	2.58	0.42
1:A:721:GLY:HA2	1:A:722:PRO:HD3	1.87	0.42
1:A:142:LYS:HD3	1:A:775:TRP:CG	2.54	0.42
1:A:938:SER:HB2	1:A:1362:THR:HA	2.01	0.42
1:B:611:GLY:O	1:B:612:VAL:C	2.58	0.42
1:B:886:GLN:CG	1:B:887:LYS:H	2.23	0.42
1:A:1180:LEU:HD21	1:A:1208:ILE:HA	2.01	0.42
1:A:1266:TYR:O	1:A:1269:PRO:HD2	2.18	0.42
1:A:1372:GLU:HG3	1:A:1373:GLU:N	2.34	0.42
1:A:373:VAL:HG22	1:A:418:ALA:HB3	2.00	0.42
1:A:504:LEU:HD11	1:A:651:LEU:HD11	2.02	0.42
1:A:829:ILE:HA	1:A:830:PRO:HD3	1.94	0.42
1:A:938:SER:C	1:A:940:SER:H	2.23	0.42
1:A:940:SER:OG	1:A:1361:VAL:HB	2.19	0.42
1:B:1180:LEU:HD21	1:B:1208:ILE:HA	2.02	0.42
1:B:975:ARG:HB3	1:B:1363:THR:HB	2.01	0.42
1:B:137:PRO:O	1:B:138:ASP:HB2	2.19	0.42
1:B:535:VAL:CG2	1:B:536:PRO:HD3	2.28	0.42
1:B:773:TRP:CZ3	1:B:788:PHE:HE1	2.11	0.42
1:A:1008:ALA:HB3	1:A:1078:LEU:HD11	2.00	0.42
1:A:30:ILE:HG21	1:A:120:THR:OG1	2.20	0.42
1:A:25:ILE:HD13	1:A:41:ILE:HG13	2.02	0.42
1:A:71:VAL:HG23	1:A:71:VAL:O	2.19	0.42
1:A:887:LYS:N	1:A:887:LYS:HD2	2.35	0.42
1:B:1274:LEU:C	1:B:1276:GLU:N	2.73	0.42
1:B:1318:LYS:HG2	1:B:1319:HIS:CD2	2.54	0.42
1:B:1317:TYR:CB	1:B:1320:LYS:HB3	2.49	0.42
1:B:23:TYR:O	1:B:23:TYR:HD1	2.02	0.42
1:B:449:ARG:O	1:B:450:GLU:HG2	2.19	0.42
1:B:751:ARG:HA	1:B:751:ARG:HD3	1.88	0.42
1:B:839:ILE:HD11	1:B:1483:PHE:CE1	2.55	0.42
1:B:938:SER:C	1:B:940:SER:H	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1487:PHE:N	1:A:1487:PHE:CD2	2.88	0.42
1:A:1572:ASN:C	1:A:1574:PHE:H	2.23	0.42
1:A:468:ASP:CG	1:A:469:TRP:H	2.22	0.42
1:A:60:PRO:O	1:A:61:ASP:HB3	2.18	0.42
1:A:611:GLY:O	1:A:612:VAL:C	2.58	0.42
1:A:755:LYS:HD2	1:A:755:LYS:HA	1.82	0.42
1:B:193:ASN:OD1	1:B:1070:LYS:HE2	2.19	0.42
1:B:1402:ILE:O	1:B:1476:ARG:HA	2.19	0.42
1:B:23:TYR:HA	1:B:43:VAL:HG23	2.01	0.42
1:B:643:ALA:O	1:B:647:HIS:N	2.49	0.42
1:B:983:LEU:HD13	1:B:1356:LEU:HD13	2.02	0.42
1:A:1317:TYR:CB	1:A:1320:LYS:HB3	2.50	0.42
1:A:1379:LEU:CB	1:A:1507:MET:HE1	2.50	0.42
1:A:1637:TYR:HA	1:A:1638:PRO:HD2	1.76	0.42
1:A:520:ASP:N	1:A:520:ASP:OD1	2.52	0.42
1:B:1200:LYS:H	1:B:1200:LYS:HG2	1.54	0.42
1:B:1515:LYS:HG3	1:B:1515:LYS:O	2.20	0.42
1:B:159:THR:HG22	1:B:160:VAL:N	2.34	0.42
1:B:214:THR:HG22	1:B:215:ALA:N	2.35	0.42
1:B:487:THR:HG22	1:B:523:TYR:CB	2.49	0.42
1:B:582:TYR:HB2	1:B:819:VAL:HG12	2.02	0.42
1:B:906:GLY:H	1:B:929:VAL:HB	1.83	0.42
1:A:1248:VAL:HG21	1:A:1285:TYR:HD2	1.85	0.42
1:A:1320:LYS:CD	1:A:1321:GLY:H	2.33	0.42
1:A:1427:SER:HB3	1:A:1492:THR:H	1.83	0.42
1:A:1557:ILE:HG23	1:A:1621:GLY:N	2.34	0.42
1:A:336:PHE:HB3	1:A:337:SER:H	1.64	0.42
1:A:504:LEU:HD12	1:A:504:LEU:N	2.34	0.42
1:A:825:LEU:HD12	1:A:844:THR:O	2.20	0.42
1:A:984:VAL:HG13	1:A:988:LEU:HG	2.00	0.42
1:B:1320:LYS:CD	1:B:1321:GLY:H	2.33	0.42
1:B:73:LEU:HD23	1:B:73:LEU:N	2.35	0.42
1:B:607:SER:HB3	1:B:798:GLU:HB2	2.01	0.42
1:B:907:LEU:HD12	1:B:908:HIS:H	1.84	0.42
1:A:1132:THR:HG22	1:A:1133:LEU:H	1.84	0.42
1:A:1243:GLY:HA3	1:A:1285:TYR:CZ	2.55	0.42
1:A:1379:LEU:HB2	1:A:1507:MET:HE1	2.00	0.42
1:A:1627:ILE:N	1:A:1627:ILE:HD13	2.35	0.42
1:A:323:LEU:HB2	1:A:347:TYR:HE2	1.85	0.42
1:A:398:ASN:O	1:A:399:GLN:HB2	2.20	0.42
1:A:424:LEU:HB3	1:A:428:VAL:HG11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:LYS:HE3	1:A:756:THR:H	1.84	0.42
1:B:1090:ASN:ND2	1:B:1158:ILE:HD13	2.33	0.42
1:B:1248:VAL:HG21	1:B:1285:TYR:HD2	1.85	0.42
1:B:1412:ARG:HG3	1:B:1413:GLU:CD	2.40	0.42
1:B:1487:PHE:O	1:B:1488:LEU:C	2.57	0.42
1:B:196:TYR:CZ	1:B:221:GLU:HB2	2.55	0.42
1:B:659:ALA:C	1:B:661:ASP:H	2.22	0.42
1:A:1334:LEU:HD22	1:A:1334:LEU:H	1.84	0.41
1:A:1648:TRP:CZ3	1:A:1664:LEU:HD22	2.55	0.41
1:A:412:ARG:CG	1:A:413:VAL:N	2.83	0.41
1:A:583:SER:HA	1:A:584:PRO:HD3	1.80	0.41
1:A:721:GLY:C	1:A:723:ARG:H	2.24	0.41
1:A:981:GLY:C	1:A:982:LEU:HD23	2.40	0.41
1:B:991:VAL:HG21	1:B:1017:PRO:O	2.20	0.41
1:B:1008:ALA:HB3	1:B:1078:LEU:HD11	2.01	0.41
1:B:1107:LEU:HB3	1:B:1118:PHE:HE2	1.84	0.41
1:B:1490:PRO:HB3	1:B:1509:TYR:O	2.18	0.41
1:B:1520:CYS:HA	1:B:1525:CYS:HB2	2.01	0.41
1:B:888:VAL:HG12	1:B:894:HIS:HB2	2.02	0.41
1:B:976:ILE:O	1:B:1361:VAL:HA	2.20	0.41
1:A:1096:ASN:O	1:A:1100:ILE:HG12	2.20	0.41
1:A:975:ARG:HB3	1:A:1363:THR:HB	2.02	0.41
1:A:73:LEU:N	1:A:73:LEU:HD23	2.35	0.41
1:A:907:LEU:HD12	1:A:908:HIS:H	1.85	0.41
1:B:1190:ILE:HG12	1:B:1253:TYR:CE2	2.56	0.41
1:B:504:LEU:HD11	1:B:651:LEU:HD11	2.02	0.41
1:B:860:SER:HB3	1:B:911:ASN:HB2	2.02	0.41
1:B:866:CYS:SG	1:B:903:LEU:HD21	2.60	0.41
1:A:1309:LEU:HD23	1:A:1356:LEU:H	1.86	0.41
1:A:1124:TYR:HA	1:A:1465:ASN:OD1	2.19	0.41
1:A:483:ASN:ND2	1:A:525:SER:HB3	2.36	0.41
1:A:762:LYS:HA	1:A:763:PRO:HD3	1.91	0.41
1:B:1372:GLU:HG3	1:B:1373:GLU:N	2.34	0.41
1:B:412:ARG:CG	1:B:413:VAL:N	2.83	0.41
1:B:825:LEU:HD12	1:B:844:THR:O	2.19	0.41
1:B:906:GLY:N	1:B:929:VAL:HB	2.35	0.41
1:B:940:SER:OG	1:B:1361:VAL:HB	2.20	0.41
1:A:1193:TYR:CD1	1:A:1256:LEU:HB3	2.55	0.41
1:A:357:VAL:O	1:A:358:ALA:C	2.59	0.41
1:A:493:ILE:CG2	1:A:494:ASP:N	2.84	0.41
1:A:906:GLY:N	1:A:929:VAL:HB	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:SER:HB3	1:A:911:ASN:HB2	2.02	0.41
1:A:977:LEU:HD12	1:A:1361:VAL:CG2	2.40	0.41
1:B:308:LYS:HA	1:B:313:TYR:O	2.20	0.41
1:B:350:SER:HA	1:B:351:PRO:HD3	1.89	0.41
1:B:703:ALA:HB2	1:B:731:CYS:C	2.41	0.41
1:B:901:LEU:HA	1:B:902:PRO:HD3	1.77	0.41
1:A:991:VAL:HG21	1:A:1017:PRO:O	2.20	0.41
1:A:1013:MET:HE1	1:A:1081:PHE:HZ	1.86	0.41
1:A:1272:LYS:O	1:A:1272:LYS:HG3	2.20	0.41
1:A:137:PRO:O	1:A:138:ASP:HB2	2.20	0.41
1:A:196:TYR:CZ	1:A:221:GLU:HB2	2.55	0.41
1:A:280:LYS:HG3	1:A:282:MET:CE	2.47	0.41
1:B:1024:TYR:HB2	1:B:1298:THR:HG23	2.03	0.41
1:B:1213:LYS:HD2	1:B:1266:TYR:CZ	2.55	0.41
1:B:1278:GLN:HA	1:B:1278:GLN:NE2	2.35	0.41
1:B:395:ILE:HA	1:B:400:GLU:O	2.21	0.41
1:B:577:PRO:C	1:B:579:ALA:H	2.23	0.41
1:B:59:TYR:CD1	1:B:103:TYR:CE1	3.08	0.41
1:B:618:LYS:HA	1:B:619:PRO:HD3	1.73	0.41
1:B:834:VAL:HG12	1:B:835:ARG:O	2.20	0.41
1:B:887:LYS:N	1:B:887:LYS:HD2	2.35	0.41
1:B:88:GLN:HE21	1:B:88:GLN:HB3	1.73	0.41
1:B:938:SER:OG	1:B:1279:ARG:NH1	2.52	0.41
1:A:1113:LEU:C	1:A:1115:ASN:H	2.24	0.41
1:A:1190:ILE:HG12	1:A:1253:TYR:CE2	2.56	0.41
1:A:1274:LEU:C	1:A:1276:GLU:N	2.73	0.41
1:A:308:LYS:HA	1:A:313:TYR:O	2.20	0.41
1:A:356:LEU:HD12	1:A:361:LEU:HD11	2.02	0.41
1:A:59:TYR:CD1	1:A:103:TYR:CE1	3.08	0.41
1:A:857:VAL:HG21	1:A:896:VAL:CG1	2.50	0.41
1:B:1370:THR:HG23	1:B:1373:GLU:OE1	2.21	0.41
1:B:357:VAL:O	1:B:358:ALA:C	2.58	0.41
1:B:412:ARG:CD	1:B:415:ASP:HB2	2.48	0.41
1:A:1511:THR:HG23	1:A:1511:THR:O	2.19	0.41
1:A:1559:TYR:OH	1:A:1637:TYR:CD1	2.73	0.41
1:A:175:GLU:OE1	1:A:206:LYS:HD2	2.20	0.41
1:A:530:VAL:HG13	1:A:530:VAL:O	2.21	0.41
1:A:542:VAL:O	1:A:556:SER:HA	2.20	0.41
1:A:612:VAL:HG23	1:A:613:GLN:N	2.30	0.41
1:A:23:TYR:OH	1:A:656:ASN:HB2	2.20	0.41
1:A:884:VAL:HG12	1:A:1625:LEU:CB	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1124:TYR:HA	1:B:1465:ASN:OD1	2.20	0.41
1:B:1511:THR:HG23	1:B:1511:THR:O	2.20	0.41
1:A:1133:LEU:N	1:A:1134:PRO:CD	2.84	0.41
1:A:1333:PHE:C	1:A:1335:GLY:H	2.24	0.41
1:A:592:MET:HE3	1:A:780:VAL:CG2	2.51	0.41
1:A:607:SER:HB3	1:A:798:GLU:HB2	2.03	0.41
1:A:667:GLU:N	1:A:668:PRO:CD	2.79	0.41
1:A:838:GLN:O	1:A:1486:GLY:N	2.54	0.41
1:A:449:ARG:O	1:A:450:GLU:HG2	2.21	0.41
1:A:487:THR:HG22	1:A:523:TYR:CB	2.48	0.41
1:B:1225:TYR:CE1	1:B:1272:LYS:HG3	2.56	0.41
1:B:1332:ASN:O	1:B:1332:ASN:CG	2.59	0.41
1:B:35:ALA:HA	1:B:150:ASP:OD1	2.21	0.41
1:B:356:LEU:HD12	1:B:361:LEU:HD11	2.02	0.41
1:B:483:ASN:HD21	1:B:525:SER:HB3	1.86	0.41
1:B:758:LEU:O	1:B:760:VAL:N	2.54	0.41
1:A:1002:HIS:HD1	1:A:1284:PHE:HZ	1.67	0.41
1:A:1218:VAL:HA	1:A:1225:TYR:O	2.21	0.41
1:A:1412:ARG:HG3	1:A:1413:GLU:CD	2.41	0.41
1:A:1455:ILE:HG13	1:A:1460:VAL:HG22	2.03	0.41
1:A:1548:ARG:HG2	1:A:1548:ARG:NH1	2.36	0.41
1:A:1666:GLU:HA	1:A:1666:GLU:OE2	2.21	0.41
1:A:243:PHE:CZ	1:A:316:GLU:HB2	2.56	0.41
1:A:461:SER:C	1:A:463:SER:N	2.74	0.41
1:A:532:GLN:NE2	1:A:535:VAL:HG11	2.35	0.41
1:B:1420:SER:O	1:B:1421:HIS:C	2.60	0.41
1:B:327:VAL:HG12	1:B:328:THR:N	2.36	0.41
1:B:532:GLN:NE2	1:B:535:VAL:HG11	2.35	0.41
1:B:721:GLY:C	1:B:723:ARG:H	2.23	0.41
1:A:1024:TYR:HB2	1:A:1298:THR:HG23	2.03	0.41
1:A:560:TRP:CD2	1:A:673:LEU:HD12	2.55	0.41
1:A:834:VAL:HG12	1:A:835:ARG:O	2.21	0.41
1:B:1008:ALA:HB2	1:B:1059:TYR:CD2	2.55	0.41
1:B:1039:LEU:HD12	1:B:1039:LEU:HA	1.85	0.41
1:B:1113:LEU:C	1:B:1115:ASN:H	2.24	0.41
1:B:1119:LYS:HG3	1:B:1119:LYS:O	2.20	0.41
1:B:1333:PHE:C	1:B:1335:GLY:H	2.24	0.41
1:B:838:GLN:O	1:B:1486:GLY:N	2.54	0.41
1:B:29:LYS:O	1:B:30:ILE:HD13	2.21	0.41
1:B:721:GLY:HA2	1:B:722:PRO:HD3	1.88	0.41
1:A:1001:THR:HG22	1:A:1002:HIS:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:CD2	1:A:112:SER:N	2.89	0.40
1:A:1213:LYS:HD2	1:A:1266:TYR:CZ	2.56	0.40
1:A:159:THR:HG22	1:A:160:VAL:N	2.35	0.40
1:A:1577:TYR:CE2	1:A:1611:LEU:HB3	2.56	0.40
1:A:290:THR:O	1:A:291:MET:C	2.60	0.40
1:A:976:ILE:O	1:A:1361:VAL:HA	2.20	0.40
1:B:1193:TYR:HE1	1:B:1256:LEU:HB3	1.78	0.40
1:B:530:VAL:HG13	1:B:530:VAL:O	2.22	0.40
1:A:983:LEU:HD13	1:A:1356:LEU:HD13	2.03	0.40
1:A:1563:VAL:HG12	1:A:1581:LEU:HG	2.03	0.40
1:B:1053:MET:CE	1:B:1086:LEU:HD22	2.52	0.40
1:B:290:THR:O	1:B:291:MET:C	2.59	0.40
1:B:323:LEU:HB2	1:B:347:TYR:HE2	1.85	0.40
1:B:495:LYS:HA	1:B:495:LYS:CE	2.51	0.40
1:B:592:MET:HE3	1:B:780:VAL:HG21	2.03	0.40
1:B:838:GLN:O	1:B:1485:VAL:HA	2.20	0.40
1:B:85:LEU:O	1:B:86:THR:HB	2.21	0.40
1:A:1591:VAL:HG13	1:A:1591:VAL:O	2.20	0.40
1:A:1615:ARG:NE	1:A:1647:TYR:HE1	2.19	0.40
1:A:308:LYS:HG3	1:A:314:SER:CB	2.51	0.40
1:A:369:TYR:HA	1:A:370:PRO:HD3	1.70	0.40
1:A:483:ASN:HD21	1:A:525:SER:HB3	1.86	0.40
1:A:703:ALA:HB2	1:A:731:CYS:C	2.41	0.40
1:A:987:ILE:HG12	1:A:1294:ILE:HD12	2.03	0.40
1:B:1279:ARG:CG	1:B:1284:PHE:HB2	2.23	0.40
1:B:520:ASP:N	1:B:520:ASP:OD1	2.52	0.40
1:B:540:LEU:CD1	1:B:542:VAL:HG23	2.51	0.40
1:A:1053:MET:CE	1:A:1086:LEU:HD22	2.51	0.40
1:A:1085:VAL:O	1:A:1089:VAL:HG23	2.22	0.40
1:A:1278:GLN:NE2	1:A:1278:GLN:HA	2.36	0.40
1:A:1557:ILE:HG23	1:A:1621:GLY:CA	2.51	0.40
1:A:327:VAL:HG12	1:A:328:THR:N	2.37	0.40
1:A:582:TYR:HB2	1:A:819:VAL:HG12	2.03	0.40
1:B:1133:LEU:N	1:B:1134:PRO:CD	2.83	0.40
1:B:1193:TYR:CD1	1:B:1256:LEU:HB3	2.55	0.40
1:B:1378:TYR:CE2	1:B:1409:LYS:HG2	2.57	0.40
1:B:175:GLU:OE1	1:B:206:LYS:HD2	2.21	0.40
1:B:224:LEU:HA	1:B:224:LEU:HD22	1.90	0.40
1:B:423:ASN:HD22	1:B:423:ASN:H	1.69	0.40
1:B:493:ILE:CG2	1:B:494:ASP:N	2.83	0.40
1:B:769:PHE:HA	1:B:770:PRO:HD3	1.83	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1140:ASN:HA	1:A:1140:ASN:HD22	1.72	0.40
1:A:1370:THR:HG23	1:A:1373:GLU:OE1	2.21	0.40
1:A:1444:GLU:O	1:A:1444:GLU:HG2	2.22	0.40
1:A:207:GLU:HB3	1:A:208:ASP:H	1.66	0.40
1:A:395:ILE:HA	1:A:400:GLU:O	2.20	0.40
1:A:21:GLN:HE22	1:A:45:GLY:HA2	1.87	0.40
1:A:540:LEU:CD1	1:A:542:VAL:HG23	2.51	0.40
1:A:577:PRO:C	1:A:579:ALA:H	2.24	0.40
1:A:773:TRP:CZ3	1:A:788:PHE:HE1	2.11	0.40
1:B:1091:LYS:HB3	1:B:1091:LYS:HE2	1.69	0.40
1:B:111:PHE:CD2	1:B:112:SER:N	2.89	0.40
1:B:493:ILE:HG21	1:B:495:LYS:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1615/1676 (96%)	1282 (79%)	257 (16%)	76 (5%)	3	17
1	B	1471/1676 (88%)	1191 (81%)	214 (14%)	66 (4%)	3	17
All	All	3086/3352 (92%)	2473 (80%)	471 (15%)	142 (5%)	3	17

All (142) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	PRO
1	A	261	THR
1	A	308	LYS
1	A	336	PHE
1	A	490	SER
1	A	612	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	705	VAL
1	A	1275	SER
1	A	1284	PHE
1	A	1352	PHE
1	A	1548	ARG
1	A	1571	GLU
1	A	1633	PHE
1	A	1639	LEU
1	B	60	PRO
1	B	261	THR
1	B	308	LYS
1	B	336	PHE
1	B	490	SER
1	B	612	VAL
1	B	705	VAL
1	B	1275	SER
1	B	1284	PHE
1	B	1352	PHE
1	A	99	VAL
1	A	100	SER
1	A	207	GLU
1	A	638	GLY
1	A	657	ALA
1	A	663	GLN
1	A	996	GLY
1	A	1029	ASN
1	A	1240	PRO
1	A	1286	SER
1	A	1335	GLY
1	A	1419	SER
1	A	1457	ASP
1	A	1632	SER
1	A	1634	ARG
1	A	1657	CYS
1	B	99	VAL
1	B	100	SER
1	B	207	GLU
1	B	638	GLY
1	B	657	ALA
1	B	663	GLN
1	B	996	GLY
1	B	1029	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1240	PRO
1	B	1286	SER
1	B	1335	GLY
1	B	1419	SER
1	B	1457	ASP
1	A	46	TYR
1	A	93	PRO
1	A	101	TYR
1	A	289	ASN
1	A	704	CYS
1	A	939	TYR
1	A	1126	PRO
1	A	1236	ASP
1	A	1596	SER
1	A	1608	ASN
1	A	1636	ILE
1	A	1640	ASP
1	B	46	TYR
1	B	93	PRO
1	B	101	TYR
1	B	289	ASN
1	B	615	GLY
1	B	704	CYS
1	B	939	TYR
1	B	1126	PRO
1	B	1236	ASP
1	A	61	ASP
1	A	98	PRO
1	A	318	LEU
1	A	522	SER
1	A	613	GLN
1	A	615	GLY
1	A	669	CYS
1	A	691	LYS
1	A	700	TYR
1	A	765	ILE
1	A	868	SER
1	A	1373	GLU
1	A	1650	ARG
1	B	61	ASP
1	B	98	PRO
1	B	318	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	522	SER
1	B	613	GLN
1	B	669	CYS
1	B	691	LYS
1	B	700	TYR
1	B	765	ILE
1	B	868	SER
1	B	1373	GLU
1	B	1519	VAL
1	B	1524	ALA
1	A	86	THR
1	A	231	ILE
1	A	355	ASN
1	A	358	ALA
1	A	491	PRO
1	A	495	LYS
1	A	692	HIS
1	A	730	GLU
1	A	1122	SER
1	A	1573	VAL
1	B	86	THR
1	B	355	ASN
1	B	358	ALA
1	B	491	PRO
1	B	495	LYS
1	B	692	HIS
1	B	730	GLU
1	B	1122	SER
1	B	1525	CYS
1	A	154	PRO
1	A	209	PHE
1	A	287	MET
1	A	551	THR
1	A	619	PRO
1	A	754	MET
1	B	154	PRO
1	B	209	PHE
1	B	231	ILE
1	B	551	THR
1	B	619	PRO
1	B	758	LEU
1	A	760	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	585	GLY
1	B	585	GLY
1	B	760	VAL
1	A	758	LEU
1	A	1160	PRO
1	B	759	PRO
1	B	1160	PRO
1	B	1296	GLY
1	A	618	LYS
1	B	618	LYS

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	1441/1484 (97%)	1294 (90%)	147 (10%)	8	32
1	B	1314/1484 (88%)	1183 (90%)	131 (10%)	9	33
All	All	2755/2968 (93%)	2477 (90%)	278 (10%)	9	33

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	22	THR
1	A	23	TYR
1	A	42	GLN
1	A	61	ASP
1	A	73	LEU
1	A	100	SER
1	A	115	LYS
1	A	116	ARG
1	A	130	THR
1	A	140	SER
1	A	148	LEU
1	A	161	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	162	THR
1	A	165	ASP
1	A	179	HIS
1	A	195	ARG
1	A	208	ASP
1	A	211	THR
1	A	224	LEU
1	A	242	ASN
1	A	249	THR
1	A	280	LYS
1	A	292	LEU
1	A	320	ASN
1	A	332	SER
1	A	333	THR
1	A	383	VAL
1	A	393	GLN
1	A	394	THR
1	A	422	LEU
1	A	423	ASN
1	A	426	SER
1	A	431	LEU
1	A	457	TYR
1	A	492	TYR
1	A	495	LYS
1	A	516	GLU
1	A	522	SER
1	A	528	ILE
1	A	535	VAL
1	A	540	LEU
1	A	550	GLN
1	A	563	ILE
1	A	588	VAL
1	A	594	THR
1	A	609	VAL
1	A	610	TYR
1	A	624	PHE
1	A	644	ASN
1	A	652	THR
1	A	653	PHE
1	A	661	ASP
1	A	673	LEU
1	A	705	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	729	THR
1	A	758	LEU
1	A	786	LEU
1	A	790	LEU
1	A	799	ILE
1	A	802	ILE
1	A	814	THR
1	A	835	ARG
1	A	837	GLU
1	A	867	THR
1	A	886	GLN
1	A	887	LYS
1	A	888	VAL
1	A	895	LEU
1	A	901	LEU
1	A	909	ASN
1	A	914	LEU
1	A	916	THR
1	A	927	LEU
1	A	935	LYS
1	A	936	ARG
1	A	942	VAL
1	A	952	THR
1	A	953	ILE
1	A	968	VAL
1	A	980	LYS
1	A	983	LEU
1	A	984	VAL
1	A	1016	VAL
1	A	1029	ASN
1	A	1056	ILE
1	A	1058	SER
1	A	1067	SER
1	A	1076	THR
1	A	1108	VAL
1	A	1115	ASN
1	A	1123	GLN
1	A	1128	LYS
1	A	1132	THR
1	A	1140	ASN
1	A	1148	THR
1	A	1161	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1173	ASN
1	A	1200	LYS
1	A	1218	VAL
1	A	1231	ASN
1	A	1246	ARG
1	A	1251	THR
1	A	1279	ARG
1	A	1280	TYR
1	A	1284	PHE
1	A	1291	ILE
1	A	1306	GLN
1	A	1338	VAL
1	A	1341	LEU
1	A	1345	ASP
1	A	1350	THR
1	A	1363	THR
1	A	1423	VAL
1	A	1443	VAL
1	A	1453	TYR
1	A	1464	LEU
1	A	1476	ARG
1	A	1480	PHE
1	A	1483	PHE
1	A	1487	PHE
1	A	1488	LEU
1	A	1494	THR
1	A	1495	VAL
1	A	1497	GLU
1	A	1500	ARG
1	A	1502	ASP
1	A	1511	THR
1	A	1513	ASN
1	A	1548	ARG
1	A	1551	THR
1	A	1556	GLU
1	A	1561	TYR
1	A	1562	LYS
1	A	1566	THR
1	A	1581	LEU
1	A	1602	LYS
1	A	1618	LEU
1	A	1622	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1623	GLU
1	A	1625	LEU
1	A	1626	GLN
1	A	1627	ILE
1	A	1634	ARG
1	A	1645	ILE
1	A	1654	CYS
1	A	1669	GLU
1	B	21	GLN
1	B	22	THR
1	B	23	TYR
1	B	42	GLN
1	B	61	ASP
1	B	73	LEU
1	B	100	SER
1	B	115	LYS
1	B	116	ARG
1	B	130	THR
1	B	140	SER
1	B	148	LEU
1	B	161	LEU
1	B	162	THR
1	B	165	ASP
1	B	179	HIS
1	B	195	ARG
1	B	208	ASP
1	B	211	THR
1	B	224	LEU
1	B	242	ASN
1	B	249	THR
1	B	280	LYS
1	B	292	LEU
1	B	320	ASN
1	B	332	SER
1	B	333	THR
1	B	383	VAL
1	B	393	GLN
1	B	394	THR
1	B	422	LEU
1	B	423	ASN
1	B	426	SER
1	B	431	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	436	LYS
1	B	457	TYR
1	B	492	TYR
1	B	495	LYS
1	B	522	SER
1	B	528	ILE
1	B	535	VAL
1	B	540	LEU
1	B	550	GLN
1	B	563	ILE
1	B	588	VAL
1	B	594	THR
1	B	609	VAL
1	B	610	TYR
1	B	624	PHE
1	B	644	ASN
1	B	652	THR
1	B	653	PHE
1	B	661	ASP
1	B	673	LEU
1	B	705	VAL
1	B	729	THR
1	B	758	LEU
1	B	786	LEU
1	B	790	LEU
1	B	799	ILE
1	B	802	ILE
1	B	814	THR
1	B	835	ARG
1	B	837	GLU
1	B	867	THR
1	B	886	GLN
1	B	887	LYS
1	B	888	VAL
1	B	894	HIS
1	B	901	LEU
1	B	909	ASN
1	B	914	LEU
1	B	916	THR
1	B	927	LEU
1	B	935	LYS
1	B	936	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	942	VAL
1	B	952	THR
1	B	953	ILE
1	B	968	VAL
1	B	980	LYS
1	B	983	LEU
1	B	984	VAL
1	B	1016	VAL
1	B	1029	ASN
1	B	1056	ILE
1	B	1058	SER
1	B	1067	SER
1	B	1076	THR
1	B	1108	VAL
1	B	1115	ASN
1	B	1123	GLN
1	B	1128	LYS
1	B	1132	THR
1	B	1140	ASN
1	B	1148	THR
1	B	1161	LEU
1	B	1162	VAL
1	B	1173	ASN
1	B	1200	LYS
1	B	1218	VAL
1	B	1231	ASN
1	B	1246	ARG
1	B	1251	THR
1	B	1279	ARG
1	B	1280	TYR
1	B	1284	PHE
1	B	1291	ILE
1	B	1306	GLN
1	B	1338	VAL
1	B	1341	LEU
1	B	1345	ASP
1	B	1350	THR
1	B	1363	THR
1	B	1423	VAL
1	B	1443	VAL
1	B	1464	LEU
1	B	1476	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1480	PHE
1	B	1483	PHE
1	B	1487	PHE
1	B	1488	LEU
1	B	1494	THR
1	B	1495	VAL
1	B	1497	GLU
1	B	1500	ARG
1	B	1502	ASP
1	B	1511	THR
1	B	1513	ASN
1	B	1520	CYS
1	B	1527	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	42	GLN
1	A	72	HIS
1	A	80	GLN
1	A	81	ASN
1	A	88	GLN
1	A	242	ASN
1	A	289	ASN
1	A	298	GLN
1	A	320	ASN
1	A	381	GLN
1	A	393	GLN
1	A	423	ASN
1	A	446	ASN
1	A	483	ASN
1	A	647	HIS
1	A	656	ASN
1	A	692	HIS
1	A	737	GLN
1	A	787	GLN
1	A	909	ASN
1	A	1023	HIS
1	A	1029	ASN
1	A	1090	ASN
1	A	1096	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1115	ASN
1	A	1123	GLN
1	A	1140	ASN
1	A	1173	ASN
1	A	1202	HIS
1	A	1221	ASN
1	A	1231	ASN
1	A	1234	HIS
1	A	1278	GLN
1	A	1306	GLN
1	A	1319	HIS
1	A	1366	HIS
1	A	1459	HIS
1	A	1463	GLN
1	A	1536	GLN
1	A	1572	ASN
1	A	1626	GLN
1	B	21	GLN
1	B	42	GLN
1	B	72	HIS
1	B	80	GLN
1	B	81	ASN
1	B	88	GLN
1	B	242	ASN
1	B	289	ASN
1	B	298	GLN
1	B	320	ASN
1	B	381	GLN
1	B	393	GLN
1	B	423	ASN
1	B	446	ASN
1	B	483	ASN
1	B	647	HIS
1	B	656	ASN
1	B	692	HIS
1	B	737	GLN
1	B	787	GLN
1	B	894	HIS
1	B	909	ASN
1	B	1023	HIS
1	B	1029	ASN
1	B	1090	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1096	ASN
1	B	1115	ASN
1	B	1123	GLN
1	B	1140	ASN
1	B	1173	ASN
1	B	1202	HIS
1	B	1221	ASN
1	B	1231	ASN
1	B	1234	HIS
1	B	1278	GLN
1	B	1306	GLN
1	B	1319	HIS
1	B	1366	HIS
1	B	1459	HIS
1	B	1463	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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
2	NAG	A	2001	1,2	14,14,15	0.50	0	15,19,21	0.73	0
2	NAG	A	2002	2	14,14,15	0.47	0	15,19,21	0.79	1 (6%)
2	NAG	A	2003	1	14,14,15	0.57	0	15,19,21	0.91	1 (6%)
2	NAG	B	2001	1,2	14,14,15	0.50	0	15,19,21	0.72	0
2	NAG	B	2002	2	14,14,15	0.47	0	15,19,21	0.81	1 (6%)
2	NAG	B	2003	1	14,14,15	0.60	0	15,19,21	1.09	1 (6%)

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
2	NAG	A	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2002	2	-	0/6/23/26	0/1/1/1
2	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
2	NAG	B	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2002	2	-	2/6/23/26	0/1/1/1
2	NAG	B	2003	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2002	NAG	C1-O5-C5	2.14	115.12	112.17
2	A	2003	NAG	O5-C1-C2	2.20	114.54	111.47
2	A	2002	NAG	C1-O5-C5	2.21	115.22	112.17
2	B	2003	NAG	O5-C1-C2	2.91	115.52	111.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2002	NAG	O7-C7-N2-C2
2	B	2002	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	NAG	2	0
2	B	2001	NAG	2	0

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	1625/1676 (96%)	0.17	49 (3%)	51	27	73, 136, 224, 290	0
1	B	1481/1676 (88%)	0.10	25 (1%)	70	49	75, 131, 205, 267	0
All	All	3106/3352 (92%)	0.14	74 (2%)	59	37	73, 133, 215, 290	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	871	PRO	10.0
1	B	871	PRO	6.1
1	A	1534	GLN	4.9
1	A	1635	TYR	4.1
1	B	1518	LYS	4.1
1	A	1617	TYR	4.1
1	A	1645	ILE	4.0
1	A	1630	ASN	4.0
1	B	81	ASN	3.7
1	B	870	SER	3.6
1	A	1619	ILE	3.6
1	B	52	ALA	3.5
1	B	104	LEU	3.5
1	B	107	VAL	3.4
1	A	1605	THR	3.3
1	B	96	GLN	3.3
1	B	309	GLU	3.3
1	B	1519	VAL	3.2
1	A	1596	SER	3.2
1	A	1543	ILE	3.2
1	A	1583	ASP	3.2
1	A	720	LEU	3.1
1	A	616	ALA	3.1
1	A	1636	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	252	ALA	3.1
1	A	1581	LEU	3.0
1	A	330	ILE	3.0
1	A	1613	LYS	3.0
1	B	720	LEU	3.0
1	B	552	ALA	3.0
1	B	857	VAL	3.0
1	A	1634	ARG	2.9
1	A	749	LEU	2.8
1	A	159	THR	2.7
1	A	1593	GLU	2.7
1	A	1646	GLU	2.7
1	A	85	LEU	2.7
1	A	545	ILE	2.7
1	A	861	ALA	2.7
1	A	104	LEU	2.7
1	A	81	ASN	2.7
1	A	1601	ILE	2.6
1	B	809	ILE	2.6
1	A	1584	ILE	2.6
1	A	817	ALA	2.5
1	A	1523	ALA	2.5
1	B	1236	ASP	2.5
1	B	482	LEU	2.5
1	B	839	ILE	2.5
1	A	1611	LEU	2.5
1	A	1585	TYR	2.4
1	A	1284	PHE	2.3
1	A	870	SER	2.3
1	A	1542	THR	2.3
1	A	94	GLY	2.2
1	B	106	VAL	2.2
1	A	87	ILE	2.2
1	B	182	ILE	2.2
1	B	1480	PHE	2.2
1	B	252	ALA	2.1
1	B	616	ALA	2.1
1	A	1638	PRO	2.1
1	B	329	VAL	2.1
1	A	1579	ALA	2.1
1	A	1647	TYR	2.1
1	A	997	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	571	LEU	2.1
1	A	52	ALA	2.1
1	B	330	ILE	2.1
1	A	107	VAL	2.0
1	A	1561	TYR	2.0
1	B	683	ILE	2.0
1	A	95	GLY	2.0
1	A	1572	ASN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	CD	B	2006	1/1	0.76	0.19	-	183,183,183,183	0
2	NAG	A	2001	14/15	0.81	0.33	-	257,259,270,271	0
2	NAG	B	2003	14/15	0.81	0.57	-	246,252,259,262	0
3	CD	A	2007	1/1	0.94	0.21	-	184,184,184,184	0
3	CD	B	2007	1/1	0.78	0.13	-	264,264,264,264	0
3	CD	A	2006	1/1	0.68	0.18	-	189,189,189,189	0
3	CD	B	2004	1/1	0.99	0.18	-	239,239,239,239	0
2	NAG	B	2001	14/15	0.89	0.38	-	263,269,274,275	0
2	NAG	A	2003	14/15	0.85	0.25	-	215,223,233,237	0
3	CD	B	2005	1/1	0.75	0.20	-	181,181,181,181	0
2	NAG	A	2002	14/15	0.79	0.24	-	249,258,261,262	0
3	CD	A	2005	1/1	0.97	0.16	-	243,243,243,243	0
2	NAG	B	2002	14/15	0.58	0.51	-	251,259,262,262	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CD	A	2008	1/1	0.73	0.11	-	282,282,282,282	0
3	CD	A	2004	1/1	0.95	0.35	-	123,123,123,123	1

6.5 Other polymers [i](#)

There are no such residues in this entry.