



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:41 PM GMT

PDB ID : 3WX0  
Title : The crystal structure of D-lactate dehydrogenase from Escherichia coli  
Authors : Furukawa, N.; Togawa, M.; Miyanaga, A.; Nakajima, M.; Taguchi, H.  
Deposited on : 2014-07-08  
Resolution : 3.30 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](mailto: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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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-20026982

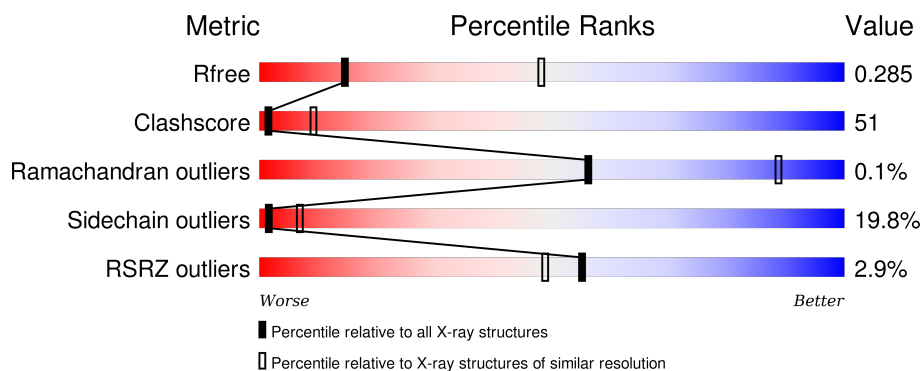
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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  $\geq 3$ , 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	345	<div> <div>3%</div> <div>37% 40% 11% 12%</div> </div>
1	B	345	<div> <div>3%</div> <div>34% 34% 11% 21%</div> </div>
1	C	345	<div> <div>3%</div> <div>32% 36% 9% 23%</div> </div>
1	D	345	<div> <div>2%</div> <div>32% 43% 9% 17%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8746 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 D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2348	1493	399	442	14			
1	B	274	Total	C	N	O	S	0	0	0
			2124	1348	363	398	15			
1	C	264	Total	C	N	O	S	0	0	0
			2057	1307	351	386	13			
1	D	287	Total	C	N	O	S	0	0	0
			2217	1412	373	419	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	EXPRESSION TAG	UNP C6EEW4
A	-14	ASN	-	EXPRESSION TAG	UNP C6EEW4
A	-13	HIS	-	EXPRESSION TAG	UNP C6EEW4
A	-12	LYS	-	EXPRESSION TAG	UNP C6EEW4
A	-11	VAL	-	EXPRESSION TAG	UNP C6EEW4
A	-10	HIS	-	EXPRESSION TAG	UNP C6EEW4
A	-9	HIS	-	EXPRESSION TAG	UNP C6EEW4
A	-8	HIS	-	EXPRESSION TAG	UNP C6EEW4
A	-7	HIS	-	EXPRESSION TAG	UNP C6EEW4
A	-6	HIS	-	EXPRESSION TAG	UNP C6EEW4
A	-5	HIS	-	EXPRESSION TAG	UNP C6EEW4
A	-4	ILE	-	EXPRESSION TAG	UNP C6EEW4
A	-3	GLU	-	EXPRESSION TAG	UNP C6EEW4
A	-2	GLY	-	EXPRESSION TAG	UNP C6EEW4
A	-1	ARG	-	EXPRESSION TAG	UNP C6EEW4
A	0	HIS	-	EXPRESSION TAG	UNP C6EEW4
B	-15	MET	-	EXPRESSION TAG	UNP C6EEW4
B	-14	ASN	-	EXPRESSION TAG	UNP C6EEW4
B	-13	HIS	-	EXPRESSION TAG	UNP C6EEW4
B	-12	LYS	-	EXPRESSION TAG	UNP C6EEW4
B	-11	VAL	-	EXPRESSION TAG	UNP C6EEW4

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	HIS	-	EXPRESSION TAG	UNP C6EEW4
B	-9	HIS	-	EXPRESSION TAG	UNP C6EEW4
B	-8	HIS	-	EXPRESSION TAG	UNP C6EEW4
B	-7	HIS	-	EXPRESSION TAG	UNP C6EEW4
B	-6	HIS	-	EXPRESSION TAG	UNP C6EEW4
B	-5	HIS	-	EXPRESSION TAG	UNP C6EEW4
B	-4	ILE	-	EXPRESSION TAG	UNP C6EEW4
B	-3	GLU	-	EXPRESSION TAG	UNP C6EEW4
B	-2	GLY	-	EXPRESSION TAG	UNP C6EEW4
B	-1	ARG	-	EXPRESSION TAG	UNP C6EEW4
B	0	HIS	-	EXPRESSION TAG	UNP C6EEW4
C	-15	MET	-	EXPRESSION TAG	UNP C6EEW4
C	-14	ASN	-	EXPRESSION TAG	UNP C6EEW4
C	-13	HIS	-	EXPRESSION TAG	UNP C6EEW4
C	-12	LYS	-	EXPRESSION TAG	UNP C6EEW4
C	-11	VAL	-	EXPRESSION TAG	UNP C6EEW4
C	-10	HIS	-	EXPRESSION TAG	UNP C6EEW4
C	-9	HIS	-	EXPRESSION TAG	UNP C6EEW4
C	-8	HIS	-	EXPRESSION TAG	UNP C6EEW4
C	-7	HIS	-	EXPRESSION TAG	UNP C6EEW4
C	-6	HIS	-	EXPRESSION TAG	UNP C6EEW4
C	-5	HIS	-	EXPRESSION TAG	UNP C6EEW4
C	-4	ILE	-	EXPRESSION TAG	UNP C6EEW4
C	-3	GLU	-	EXPRESSION TAG	UNP C6EEW4
C	-2	GLY	-	EXPRESSION TAG	UNP C6EEW4
C	-1	ARG	-	EXPRESSION TAG	UNP C6EEW4
C	0	HIS	-	EXPRESSION TAG	UNP C6EEW4
D	-15	MET	-	EXPRESSION TAG	UNP C6EEW4
D	-14	ASN	-	EXPRESSION TAG	UNP C6EEW4
D	-13	HIS	-	EXPRESSION TAG	UNP C6EEW4
D	-12	LYS	-	EXPRESSION TAG	UNP C6EEW4
D	-11	VAL	-	EXPRESSION TAG	UNP C6EEW4
D	-10	HIS	-	EXPRESSION TAG	UNP C6EEW4
D	-9	HIS	-	EXPRESSION TAG	UNP C6EEW4
D	-8	HIS	-	EXPRESSION TAG	UNP C6EEW4
D	-7	HIS	-	EXPRESSION TAG	UNP C6EEW4
D	-6	HIS	-	EXPRESSION TAG	UNP C6EEW4
D	-5	HIS	-	EXPRESSION TAG	UNP C6EEW4
D	-4	ILE	-	EXPRESSION TAG	UNP C6EEW4
D	-3	GLU	-	EXPRESSION TAG	UNP C6EEW4
D	-2	GLY	-	EXPRESSION TAG	UNP C6EEW4
D	-1	ARG	-	EXPRESSION TAG	UNP C6EEW4

*Continued on next page...*

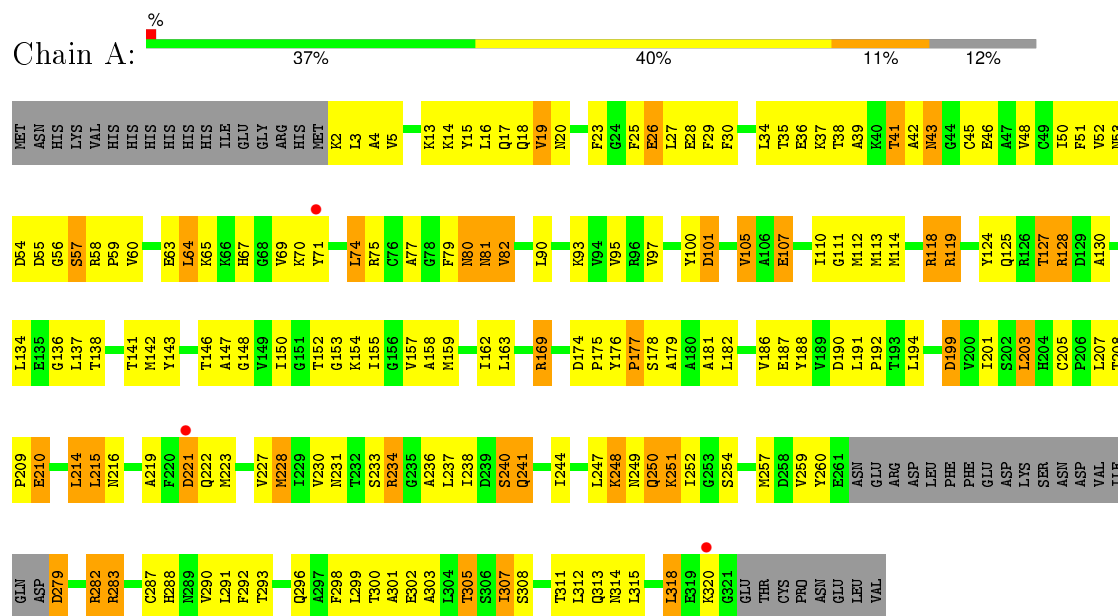
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	EXPRESSION TAG	UNP C6EEW4

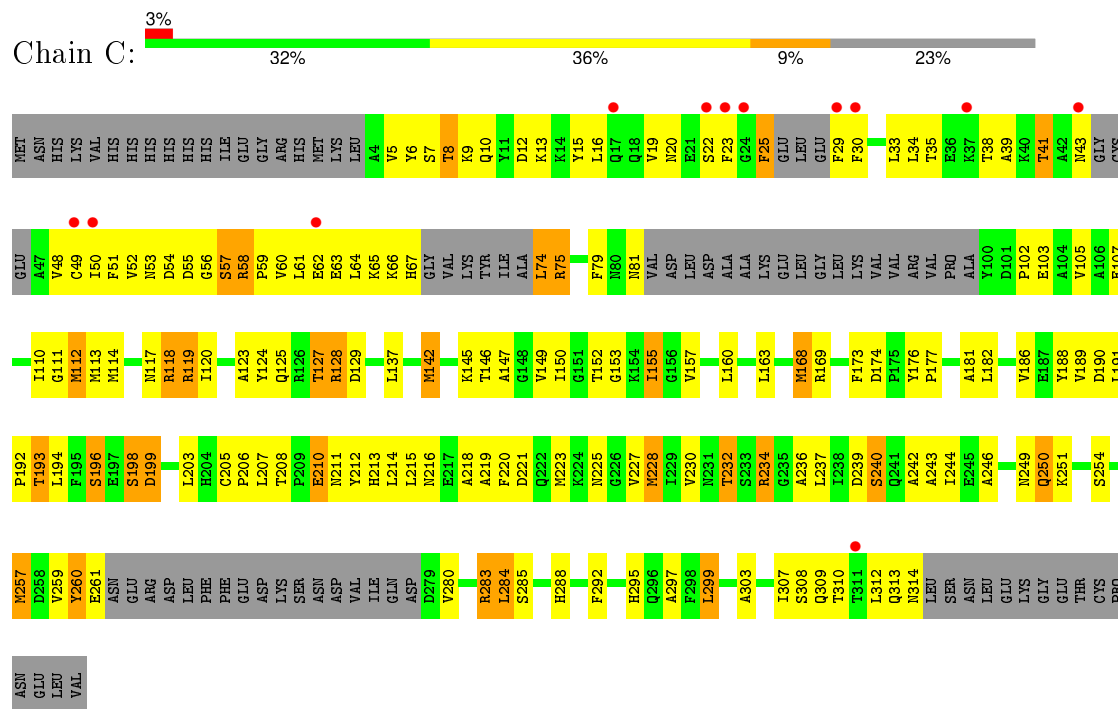
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

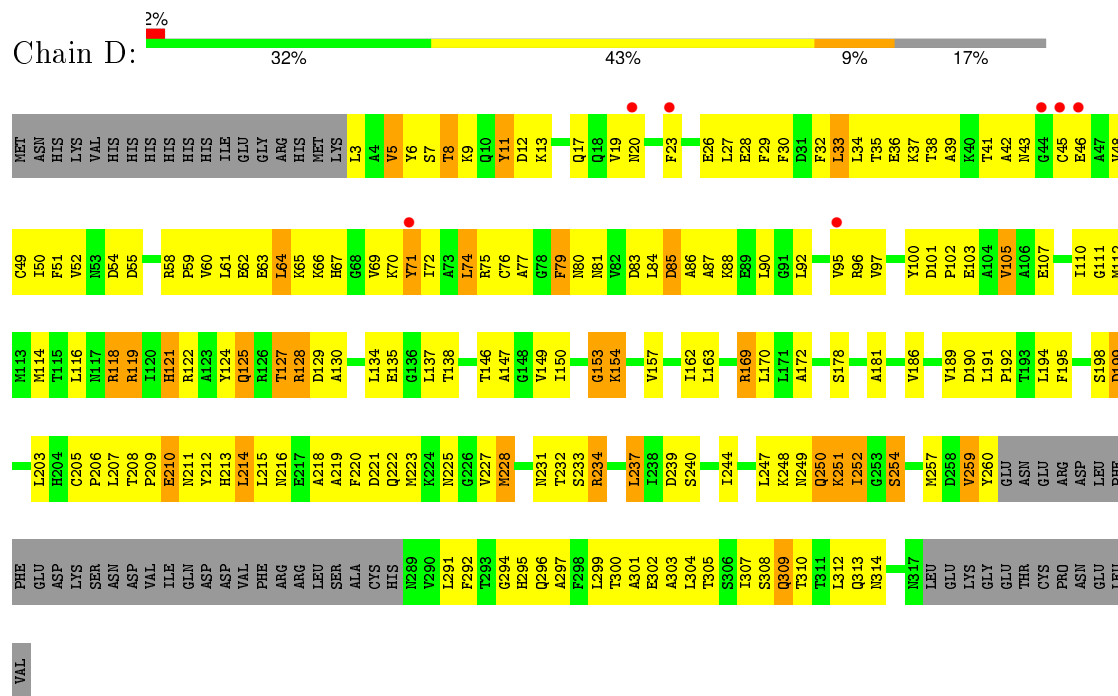
- Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding



• Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding



• Molecule 1: D-isomer specific 2-hydroxyacid dehydrogenase NAD-binding



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.03Å 131.03Å 405.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.03 – 3.30 55.03 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.03-3.30) 100.0 (55.03-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.79 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.231 , 0.271 0.243 , 0.285	Depositor DCC
$R_{free}$ test set	1631 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	72.1	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 67.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 32044 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	8746	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.05	0/2388	0.76	0/3223
1	B	0.97	0/2157	0.78	4/2907 (0.1%)
1	C	1.04	0/2091	0.80	0/2817
1	D	1.05	0/2255	0.78	1/3047 (0.0%)
All	All	1.03	0/8891	0.78	5/11994 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	THR	N-CA-C	-5.84	95.23	111.00
1	B	94	VAL	CB-CA-C	-5.76	100.45	111.40
1	B	325	PRO	CA-N-CD	-5.45	103.86	111.50
1	D	153	GLY	N-CA-C	-5.41	99.59	113.10
1	B	186	VAL	CB-CA-C	-5.01	101.87	111.40

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	2348	0	2353	251	0
1	B	2124	0	2101	234	0
1	C	2057	0	2036	242	0
1	D	2217	0	2220	218	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8746	0	8710	895	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 51.

All (895) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ARG:HG3	1:C:59:PRO:CD	1.34	1.52
1:B:51:PHE:CD2	1:B:52:VAL:HG23	1.54	1.42
1:C:58:ARG:CG	1:C:59:PRO:HD3	1.55	1.35
1:D:212:TYR:CE1	1:D:213:HIS:CD2	2.26	1.22
1:B:51:PHE:CE2	1:B:52:VAL:HG23	1.73	1.21
1:C:15:TYR:O	1:C:19:VAL:HG23	1.34	1.20
1:B:51:PHE:CE2	1:B:52:VAL:CG2	2.24	1.19
1:C:181:ALA:O	1:C:186:VAL:HG12	1.43	1.18
1:A:105:VAL:HG21	1:A:155:ILE:HD13	1.23	1.17
1:A:19:VAL:HG11	1:A:312:LEU:HD12	1.24	1.15
1:A:207:LEU:HD13	1:A:237:LEU:HD23	1.24	1.15
1:A:19:VAL:CG1	1:A:312:LEU:HD12	1.77	1.13
1:D:259:VAL:O	1:D:294:GLY:HA2	1.50	1.11
1:B:15:TYR:O	1:B:19:VAL:HG23	1.51	1.11
1:A:70:LYS:HB3	1:A:71:TYR:CE1	1.85	1.11
1:A:19:VAL:CG1	1:A:312:LEU:CD1	2.30	1.09
1:D:50:ILE:HG13	1:D:74:LEU:CD1	1.82	1.08
1:B:51:PHE:CD2	1:B:52:VAL:CG2	2.37	1.08
1:C:239:ASP:OD2	1:C:242:ALA:HB2	1.53	1.06
1:C:60:VAL:O	1:C:64:LEU:HD13	1.56	1.05
1:D:50:ILE:CG1	1:D:74:LEU:CD1	2.35	1.05
1:B:212:TYR:CZ	1:B:213:HIS:CE1	2.43	1.05
1:C:125:GLN:HE22	1:D:125:GLN:HG2	0.93	1.05
1:A:302:GLU:N	1:A:302:GLU:OE1	1.87	1.05
1:C:181:ALA:HB1	1:C:186:VAL:HG11	1.36	1.05
1:C:105:VAL:HG21	1:C:155:ILE:CD1	1.85	1.05
1:A:207:LEU:HD13	1:A:237:LEU:CD2	1.86	1.04
1:D:247:LEU:HD23	1:D:252:ILE:HG22	1.40	1.04
1:C:125:GLN:NE2	1:D:125:GLN:HG2	1.72	1.03
1:C:189:VAL:HB	1:C:193:THR:HG21	1.40	1.02
1:D:210:GLU:OE2	1:D:210:GLU:N	1.92	1.02
1:C:61:LEU:O	1:C:64:LEU:HB2	1.59	1.02
1:D:146:THR:HG23	1:D:169:ARG:NH1	1.72	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ALA:O	1:A:186:VAL:HG12	1.60	1.01
1:C:105:VAL:CG2	1:C:155:ILE:HD13	1.90	1.01
1:D:97:VAL:HG23	1:D:310:THR:HG21	1.43	1.00
1:C:125:GLN:HE22	1:D:125:GLN:CG	1.74	1.00
1:B:51:PHE:HD2	1:B:52:VAL:HG23	1.22	0.99
1:D:50:ILE:HG13	1:D:74:LEU:HD12	1.42	0.99
1:C:105:VAL:HG21	1:C:155:ILE:HD13	1.43	0.99
1:B:239:ASP:HB3	1:B:242:ALA:HB3	1.39	0.99
1:A:208:THR:HG22	1:A:210:GLU:HG2	1.40	0.99
1:D:260:TYR:CE1	1:D:295:HIS:ND1	2.30	0.98
1:A:13:LYS:O	1:A:17:GLN:HG3	1.61	0.98
1:C:23:PHE:HB3	1:C:25:PHE:CE1	1.98	0.98
1:C:207:LEU:HD13	1:C:237:LEU:CD2	1.94	0.98
1:A:3:LEU:HD12	1:A:4:ALA:N	1.78	0.97
1:C:58:ARG:CG	1:C:59:PRO:CD	2.23	0.97
1:D:212:TYR:CE1	1:D:213:HIS:HD2	1.73	0.96
1:A:208:THR:HG22	1:A:209:PRO:HD2	1.44	0.96
1:B:152:THR:HG23	1:B:174:ASP:CB	1.96	0.95
1:D:302:GLU:N	1:D:302:GLU:OE1	2.00	0.95
1:D:146:THR:CG2	1:D:169:ARG:NH1	2.29	0.95
1:B:105:VAL:HG21	1:B:155:ILE:HD13	1.46	0.95
1:C:23:PHE:HB3	1:C:25:PHE:HE1	1.27	0.94
1:C:190:ASP:HB3	1:C:193:THR:HB	1.50	0.94
1:B:83:ASP:OD1	1:B:84:LEU:N	1.99	0.94
1:B:212:TYR:OH	1:B:213:HIS:HE1	1.51	0.93
1:B:302:GLU:N	1:B:302:GLU:OE1	2.00	0.93
1:A:208:THR:CG2	1:A:210:GLU:HG2	1.97	0.93
1:D:181:ALA:O	1:D:186:VAL:HG12	1.67	0.93
1:C:189:VAL:HB	1:C:193:THR:CG2	1.97	0.93
1:B:152:THR:HG23	1:B:174:ASP:HB2	1.48	0.92
1:A:23:PHE:HD2	1:A:25:PHE:HE1	1.10	0.92
1:D:38:THR:O	1:D:41:THR:HG23	1.70	0.91
1:B:213:HIS:HD2	1:B:239:ASP:HA	1.35	0.91
1:B:322:GLU:N	1:B:322:GLU:OE1	2.02	0.91
1:A:107:GLU:O	1:A:110:ILE:HG22	1.70	0.91
1:A:105:VAL:CG2	1:A:155:ILE:HD13	2.01	0.91
1:D:64:LEU:HD23	1:D:69:VAL:HG21	1.53	0.91
1:A:169:ARG:HG2	1:A:169:ARG:HH11	1.32	0.90
1:A:23:PHE:HB3	1:A:25:PHE:CD1	2.07	0.90
1:A:42:ALA:O	1:A:45:CYS:HB2	1.70	0.90
1:B:58:ARG:HB3	1:B:59:PRO:HD3	1.51	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:CYS:SG	1:B:75:ARG:HD3	2.12	0.89
1:C:6:TYR:HE1	1:C:30:PHE:CD2	1.91	0.88
1:D:225:ASN:OD1	1:D:251:LYS:HE2	1.72	0.88
1:A:70:LYS:HB3	1:A:71:TYR:CD1	2.08	0.88
1:D:35:THR:HG22	1:D:36:GLU:H	1.39	0.88
1:C:261:GLU:OE1	1:C:261:GLU:N	2.07	0.87
1:A:23:PHE:CD2	1:A:25:PHE:HE1	1.93	0.87
1:A:207:LEU:CD1	1:A:237:LEU:CD2	2.53	0.86
1:A:207:LEU:CD1	1:A:237:LEU:HD23	2.06	0.85
1:D:121:HIS:HD2	1:D:122:ARG:H	1.23	0.85
1:A:65:LYS:HE3	1:A:90:LEU:O	1.77	0.85
1:A:234:ARG:HH11	1:A:234:ARG:HG3	1.42	0.85
1:B:94:VAL:O	1:B:325:PRO:CB	2.25	0.84
1:D:247:LEU:HD23	1:D:252:ILE:CG2	2.06	0.84
1:B:214:LEU:O	1:B:214:LEU:HD12	1.76	0.84
1:D:50:ILE:CG1	1:D:74:LEU:HD12	2.03	0.84
1:C:239:ASP:HB3	1:C:242:ALA:HB3	1.60	0.84
1:B:124:TYR:O	1:B:128:ARG:HG2	1.78	0.83
1:A:2:LYS:N	1:A:26:GLU:HG2	1.94	0.83
1:C:118:ARG:HH11	1:C:118:ARG:HG3	1.41	0.83
1:A:208:THR:HG22	1:A:209:PRO:CD	2.08	0.83
1:C:176:TYR:CD1	1:C:177:PRO:HD2	2.14	0.83
1:A:2:LYS:N	1:A:26:GLU:CG	2.42	0.83
1:B:51:PHE:HE2	1:B:52:VAL:CG2	1.90	0.82
1:B:212:TYR:CZ	1:B:213:HIS:ND1	2.47	0.82
1:C:6:TYR:HD1	1:C:30:PHE:HB2	1.44	0.82
1:B:152:THR:HG21	1:B:188:TYR:OH	1.81	0.81
1:D:212:TYR:HE1	1:D:213:HIS:CD2	1.94	0.81
1:B:212:TYR:CE2	1:B:213:HIS:ND1	2.48	0.81
1:C:216:ASN:OD1	1:C:218:ALA:HB3	1.79	0.81
1:A:114:MET:HA	1:A:114:MET:HE3	1.62	0.81
1:C:292:PHE:HB2	1:D:127:THR:CG2	2.11	0.81
1:D:259:VAL:O	1:D:294:GLY:CA	2.29	0.81
1:D:247:LEU:CD2	1:D:252:ILE:CG2	2.58	0.81
1:B:118:ARG:HH11	1:B:118:ARG:HG3	1.45	0.80
1:A:2:LYS:N	1:A:26:GLU:HB3	1.97	0.80
1:C:5:VAL:HG11	1:C:29:PHE:HE1	1.46	0.80
1:D:35:THR:HG22	1:D:36:GLU:N	1.96	0.80
1:C:5:VAL:HG22	1:C:29:PHE:HD1	1.45	0.80
1:A:3:LEU:HD12	1:A:4:ALA:H	1.45	0.80
1:C:223:MET:O	1:C:251:LYS:HE2	1.81	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:VAL:HG23	1:D:310:THR:CG2	2.12	0.80
1:D:12:ASP:CG	1:D:75:ARG:NH1	2.35	0.80
1:B:213:HIS:CD2	1:B:239:ASP:HA	2.15	0.80
1:D:50:ILE:HG13	1:D:74:LEU:HD11	1.62	0.79
1:C:207:LEU:CD1	1:C:237:LEU:CD2	2.60	0.79
1:C:124:TYR:O	1:C:128:ARG:HG2	1.82	0.79
1:B:152:THR:CG2	1:B:188:TYR:OH	2.30	0.79
1:D:146:THR:CG2	1:D:169:ARG:HH12	1.93	0.79
1:B:58:ARG:HB3	1:B:59:PRO:CD	2.10	0.79
1:A:181:ALA:HB1	1:A:186:VAL:HG11	1.65	0.79
1:A:292:PHE:HB2	1:B:127:THR:CG2	2.13	0.79
1:A:93:LYS:HD2	1:A:318:LEU:HD23	1.64	0.79
1:B:212:TYR:OH	1:B:213:HIS:CE1	2.34	0.79
1:C:19:VAL:HG21	1:C:308:SER:HB2	1.65	0.78
1:C:207:LEU:HD13	1:C:237:LEU:HD21	1.64	0.78
1:D:121:HIS:CD2	1:D:122:ARG:H	2.01	0.78
1:A:214:LEU:O	1:A:214:LEU:HD12	1.83	0.78
1:B:152:THR:CG2	1:B:174:ASP:HB3	2.13	0.78
1:C:181:ALA:CB	1:C:186:VAL:HG11	2.14	0.78
1:B:49:CYS:SG	1:B:75:ARG:CD	2.71	0.78
1:C:15:TYR:O	1:C:19:VAL:CG2	2.25	0.78
1:C:35:THR:OG1	1:C:38:THR:HG23	1.84	0.78
1:B:5:VAL:HG23	1:B:8:THR:CG2	2.13	0.77
1:A:19:VAL:HG12	1:A:312:LEU:CD1	2.11	0.77
1:B:212:TYR:HD1	1:B:236:ALA:HB1	1.49	0.77
1:C:58:ARG:N	1:C:59:PRO:HD2	2.00	0.77
1:C:105:VAL:HG21	1:C:155:ILE:HD12	1.64	0.77
1:B:94:VAL:O	1:B:325:PRO:HB2	1.85	0.77
1:C:58:ARG:HG3	1:C:59:PRO:HD2	1.63	0.77
1:A:240:SER:O	1:A:244:ILE:HG13	1.84	0.77
1:C:6:TYR:CD1	1:C:30:PHE:HB2	2.19	0.77
1:D:124:TYR:O	1:D:128:ARG:HG2	1.85	0.77
1:D:125:GLN:HE21	1:D:125:GLN:C	1.88	0.76
1:A:283:ARG:HG3	1:C:283:ARG:HG2	1.65	0.76
1:A:35:THR:HG22	1:A:36:GLU:N	2.00	0.76
1:B:5:VAL:HG23	1:B:8:THR:HG22	1.68	0.76
1:C:189:VAL:CB	1:C:193:THR:HG21	2.14	0.76
1:B:84:LEU:N	1:B:84:LEU:HD12	2.01	0.76
1:C:61:LEU:O	1:C:64:LEU:CB	2.32	0.76
1:A:105:VAL:CG2	1:A:155:ILE:HG21	2.16	0.76
1:B:212:TYR:CD1	1:B:236:ALA:HB1	2.21	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:VAL:HG11	1:C:29:PHE:CE1	2.21	0.75
1:B:208:THR:OG1	1:B:211:ASN:HB2	1.87	0.75
1:A:2:LYS:N	1:A:26:GLU:CB	2.49	0.75
1:D:12:ASP:CG	1:D:75:ARG:HH12	1.89	0.75
1:A:287:CYS:O	1:A:288:HIS:ND1	2.19	0.75
1:B:191:LEU:HB2	1:B:192:PRO:HD3	1.68	0.75
1:C:64:LEU:O	1:C:65:LYS:C	2.20	0.75
1:A:118:ARG:HG3	1:A:118:ARG:HH11	1.52	0.75
1:B:5:VAL:CG2	1:B:8:THR:CG2	2.65	0.75
1:C:19:VAL:HG21	1:C:308:SER:CB	2.16	0.74
1:C:181:ALA:O	1:C:186:VAL:CG1	2.31	0.74
1:A:35:THR:HG22	1:A:36:GLU:H	1.51	0.74
1:D:77:ALA:O	1:D:96:ARG:NH1	2.20	0.74
1:C:193:THR:CG2	1:C:194:LEU:N	2.51	0.74
1:D:95:VAL:HG21	1:D:314:ASN:HB3	1.69	0.74
1:A:60:VAL:O	1:A:64:LEU:HD12	1.88	0.74
1:D:299:LEU:HD12	1:D:304:LEU:HD11	1.69	0.74
1:C:190:ASP:CB	1:C:193:THR:HB	2.17	0.74
1:D:13:LYS:O	1:D:17:GLN:HG3	1.88	0.74
1:A:105:VAL:CG2	1:A:155:ILE:CG2	2.66	0.73
1:C:292:PHE:HB2	1:D:127:THR:HG23	1.70	0.73
1:D:125:GLN:HE21	1:D:125:GLN:CA	2.01	0.73
1:B:170:LEU:N	1:B:170:LEU:HD23	2.02	0.73
1:A:14:LYS:O	1:A:18:GLN:HG3	1.87	0.73
1:C:193:THR:HG22	1:C:194:LEU:N	2.02	0.73
1:B:125:GLN:NE2	1:C:129:ASP:OD2	2.22	0.73
1:A:23:PHE:HB3	1:A:25:PHE:HD1	1.53	0.73
1:A:124:TYR:O	1:A:128:ARG:HG2	1.88	0.73
1:A:208:THR:CG2	1:A:209:PRO:HD2	2.18	0.73
1:C:113:MET:HE2	1:C:230:VAL:HG21	1.72	0.72
1:A:194:LEU:HD23	1:A:194:LEU:O	1.89	0.72
1:D:33:LEU:O	1:D:38:THR:HG21	1.89	0.72
1:A:23:PHE:HD2	1:A:25:PHE:CE1	2.01	0.72
1:B:19:VAL:HG21	1:B:308:SER:HB2	1.69	0.72
1:B:239:ASP:HB3	1:B:242:ALA:CB	2.18	0.72
1:D:30:PHE:HB3	1:D:32:PHE:CE2	2.25	0.72
1:B:45:CYS:O	1:B:69:VAL:HG22	1.89	0.72
1:B:34:LEU:HD23	1:B:55:ASP:O	1.90	0.72
1:D:234:ARG:HH11	1:D:234:ARG:HG3	1.55	0.72
1:C:292:PHE:O	1:D:127:THR:HG21	1.89	0.71
1:A:5:VAL:HG22	1:A:29:PHE:HD1	1.55	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:LEU:HD12	1:D:214:LEU:O	1.90	0.71
1:B:23:PHE:HE2	1:B:313:GLN:HA	1.55	0.71
1:B:283:ARG:O	1:B:287:CYS:SG	2.49	0.71
1:C:58:ARG:O	1:C:62:GLU:HG3	1.91	0.71
1:A:23:PHE:HB3	1:A:25:PHE:CE1	2.26	0.71
1:D:64:LEU:CD2	1:D:69:VAL:HG21	2.19	0.71
1:D:234:ARG:HG3	1:D:234:ARG:NH1	2.05	0.70
1:B:58:ARG:CB	1:B:59:PRO:CD	2.68	0.70
1:B:6:TYR:O	1:B:7:SER:OG	2.09	0.70
1:B:51:PHE:CE2	1:B:52:VAL:HG22	2.24	0.70
1:C:181:ALA:C	1:C:186:VAL:HG12	2.11	0.70
1:D:212:TYR:CD1	1:D:213:HIS:CD2	2.79	0.70
1:A:190:ASP:OD2	1:A:192:PRO:HD2	1.91	0.70
1:D:249:ASN:O	1:D:249:ASN:OD1	2.09	0.70
1:A:43:ASN:OD1	1:A:67:HIS:ND1	2.22	0.70
1:B:240:SER:O	1:B:244:ILE:HG13	1.92	0.69
1:D:303:ALA:O	1:D:307:ILE:HG13	1.92	0.69
1:B:51:PHE:HD2	1:B:52:VAL:H	1.40	0.69
1:B:211:ASN:O	1:B:214:LEU:HB2	1.91	0.69
1:B:83:ASP:O	1:B:84:LEU:HG	1.92	0.69
1:A:169:ARG:HG2	1:A:169:ARG:NH1	2.05	0.69
1:C:190:ASP:HB3	1:C:193:THR:H	1.57	0.69
1:C:5:VAL:HG22	1:C:29:PHE:CD1	2.27	0.69
1:B:124:TYR:O	1:B:128:ARG:CG	2.40	0.69
1:C:5:VAL:O	1:C:30:PHE:N	2.25	0.69
1:D:107:GLU:O	1:D:110:ILE:HG22	1.93	0.69
1:A:119:ARG:HG3	1:A:137:LEU:HA	1.73	0.69
1:B:323:THR:O	1:B:325:PRO:HD3	1.93	0.68
1:B:282:ARG:HH11	1:B:282:ARG:HG3	1.55	0.68
1:B:249:ASN:O	1:B:250:GLN:HB2	1.92	0.68
1:A:19:VAL:HG11	1:A:312:LEU:CD1	2.03	0.68
1:D:260:TYR:CZ	1:D:295:HIS:ND1	2.56	0.68
1:A:283:ARG:HG3	1:C:283:ARG:CG	2.23	0.68
1:A:60:VAL:HG12	1:A:64:LEU:CD1	2.24	0.68
1:C:191:LEU:N	1:C:192:PRO:CD	2.54	0.68
1:A:279:ASP:OD1	1:A:282:ARG:HD2	1.93	0.68
1:B:186:VAL:HG22	1:B:187:GLU:H	1.59	0.68
1:D:86:ALA:O	1:D:90:LEU:HD12	1.93	0.68
1:D:194:LEU:HD23	1:D:194:LEU:C	2.14	0.68
1:C:207:LEU:HD13	1:C:237:LEU:HD23	1.72	0.68
1:A:241:GLN:NE2	1:A:241:GLN:O	2.26	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:LEU:HD23	1:C:194:LEU:C	2.14	0.68
1:C:25:PHE:H	1:C:25:PHE:HD1	1.38	0.68
1:D:19:VAL:HG12	1:D:312:LEU:HD12	1.76	0.68
1:D:146:THR:OG1	1:D:169:ARG:NH1	2.26	0.68
1:C:6:TYR:CE1	1:C:30:PHE:CD2	2.78	0.68
1:D:225:ASN:HA	1:D:251:LYS:HD3	1.75	0.67
1:D:62:GLU:O	1:D:66:LYS:HG3	1.93	0.67
1:D:43:ASN:OD1	1:D:67:HIS:ND1	2.20	0.67
1:A:208:THR:CG2	1:A:209:PRO:CD	2.72	0.67
1:B:194:LEU:HD23	1:B:194:LEU:C	2.15	0.67
1:B:258:ASP:OD1	1:B:293:THR:HG23	1.95	0.67
1:C:5:VAL:CG2	1:C:29:PHE:HD1	2.06	0.67
1:B:194:LEU:HD23	1:B:195:PHE:N	2.10	0.67
1:C:107:GLU:O	1:C:110:ILE:HG22	1.94	0.67
1:B:46:GLU:O	1:B:70:LYS:N	2.28	0.66
1:B:203:LEU:HD21	1:B:215:LEU:HD22	1.77	0.66
1:D:153:GLY:O	1:D:157:VAL:HG23	1.95	0.66
1:C:105:VAL:HG22	1:C:155:ILE:HD13	1.77	0.66
1:B:77:ALA:HA	1:B:97:VAL:O	1.94	0.66
1:D:50:ILE:CG1	1:D:74:LEU:HD11	2.18	0.66
1:A:234:ARG:HG3	1:A:234:ARG:NH1	2.11	0.66
1:D:189:VAL:HG23	1:D:190:ASP:O	1.95	0.66
1:C:58:ARG:CG	1:C:59:PRO:HD2	2.23	0.66
1:C:190:ASP:O	1:C:193:THR:HG22	1.95	0.65
1:C:64:LEU:O	1:C:66:LYS:N	2.29	0.65
1:D:191:LEU:N	1:D:192:PRO:CD	2.59	0.65
1:B:95:VAL:HG12	1:B:325:PRO:HB3	1.77	0.65
1:A:51:PHE:CD2	1:A:52:VAL:HG22	2.32	0.65
1:A:227:VAL:HG22	1:A:228:MET:N	2.12	0.65
1:B:105:VAL:CG2	1:B:155:ILE:HD13	2.25	0.65
1:A:207:LEU:CD2	1:A:236:ALA:HB3	2.26	0.65
1:D:212:TYR:CD1	1:D:213:HIS:HD2	2.14	0.65
1:D:247:LEU:CD2	1:D:252:ILE:HG22	2.18	0.65
1:B:152:THR:CG2	1:B:174:ASP:CB	2.68	0.65
1:C:292:PHE:HB2	1:D:127:THR:HG21	1.79	0.65
1:D:125:GLN:NE2	1:D:125:GLN:O	2.29	0.64
1:A:60:VAL:HG12	1:A:64:LEU:HD11	1.77	0.64
1:C:12:ASP:OD2	1:C:75:ARG:NH2	2.30	0.64
1:C:5:VAL:CG2	1:C:29:PHE:CD1	2.81	0.64
1:A:283:ARG:CG	1:C:283:ARG:CG	2.76	0.64
1:D:51:PHE:N	1:D:54:ASP:OD2	2.23	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PHE:HB2	1:B:127:THR:HG21	1.78	0.64
1:D:5:VAL:HG22	1:D:29:PHE:HD1	1.63	0.64
1:B:33:LEU:HD23	1:B:54:ASP:HA	1.79	0.64
1:B:223:MET:O	1:B:251:LYS:CE	2.46	0.64
1:C:60:VAL:O	1:C:64:LEU:CD1	2.41	0.64
1:A:208:THR:CG2	1:A:210:GLU:CG	2.72	0.64
1:D:38:THR:O	1:D:41:THR:CG2	2.46	0.64
1:A:134:LEU:HD11	1:B:294:GLY:O	1.98	0.64
1:D:121:HIS:CD2	1:D:122:ARG:N	2.65	0.64
1:A:30:PHE:CE2	1:A:41:THR:HB	2.33	0.64
1:A:58:ARG:N	1:A:59:PRO:HD2	2.13	0.64
1:B:110:ILE:HD13	1:B:162:ILE:CG2	2.28	0.64
1:C:212:TYR:CE1	1:C:213:HIS:CD2	2.86	0.64
1:C:5:VAL:CG1	1:C:29:PHE:CE1	2.81	0.64
1:C:214:LEU:HD12	1:C:214:LEU:O	1.98	0.64
1:B:208:THR:H	1:B:211:ASN:HB2	1.63	0.63
1:B:5:VAL:CG2	1:B:8:THR:HG22	2.26	0.63
1:C:181:ALA:C	1:C:186:VAL:CG1	2.67	0.63
1:A:23:PHE:CE2	1:A:313:GLN:HA	2.33	0.63
1:C:190:ASP:OD1	1:C:192:PRO:HD2	1.97	0.63
1:C:310:THR:O	1:C:314:ASN:ND2	2.26	0.63
1:A:194:LEU:C	1:A:194:LEU:HD23	2.17	0.63
1:B:10:GLN:OE1	1:B:10:GLN:HA	1.96	0.63
1:D:225:ASN:OD1	1:D:251:LYS:CE	2.44	0.63
1:A:39:ALA:HB3	1:A:63:GLU:HG2	1.79	0.63
1:A:105:VAL:HG22	1:A:155:ILE:HG23	1.81	0.63
1:C:142:MET:O	1:C:168:MET:HE3	1.98	0.63
1:A:23:PHE:HZ	1:A:313:GLN:HG2	1.62	0.63
1:B:231:ASN:OD1	1:B:233:SER:N	2.32	0.63
1:B:152:THR:HG21	1:B:188:TYR:CE1	2.33	0.63
1:B:83:ASP:C	1:B:84:LEU:HD12	2.19	0.63
1:C:58:ARG:N	1:C:59:PRO:CD	2.62	0.63
1:C:118:ARG:HH11	1:C:118:ARG:CG	2.09	0.63
1:C:119:ARG:HB2	1:C:137:LEU:HD22	1.81	0.62
1:A:37:LYS:NZ	1:D:28:GLU:OE2	2.23	0.62
1:B:214:LEU:HD12	1:B:214:LEU:C	2.19	0.62
1:A:16:LEU:HD23	1:A:308:SER:OG	1.99	0.62
1:D:35:THR:HB	1:D:38:THR:HG23	1.81	0.62
1:C:146:THR:HG23	1:C:169:ARG:HD3	1.79	0.62
1:A:314:ASN:O	1:A:318:LEU:HD12	2.00	0.62
1:D:50:ILE:CD1	1:D:74:LEU:HD11	2.29	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ARG:HB3	1:A:59:PRO:HD3	1.81	0.62
1:B:152:THR:HG21	1:B:174:ASP:HB3	1.80	0.61
1:D:42:ALA:O	1:D:45:CYS:HB2	2.00	0.61
1:A:70:LYS:CB	1:A:71:TYR:CE1	2.74	0.61
1:B:94:VAL:O	1:B:325:PRO:HB3	1.99	0.61
1:D:205:CYS:HB2	1:D:206:PRO:HD2	1.82	0.61
1:A:70:LYS:C	1:A:71:TYR:CD1	2.74	0.61
1:A:127:THR:HG21	1:B:292:PHE:O	1.99	0.61
1:C:12:ASP:CG	1:C:75:ARG:NH2	2.54	0.61
1:B:199:ASP:N	1:B:199:ASP:OD1	2.32	0.61
1:C:113:MET:HE2	1:C:230:VAL:CG2	2.31	0.61
1:A:150:ILE:HD12	1:A:203:LEU:HD23	1.82	0.61
1:A:23:PHE:CD2	1:A:25:PHE:CE1	2.82	0.61
1:C:114:MET:HE3	1:C:114:MET:HA	1.82	0.61
1:C:303:ALA:O	1:C:307:ILE:HG13	2.00	0.61
1:C:12:ASP:CG	1:C:75:ARG:HH21	2.04	0.61
1:A:283:ARG:CG	1:C:283:ARG:HG2	2.31	0.60
1:D:234:ARG:HH11	1:D:234:ARG:CG	2.12	0.60
1:A:80:ASN:C	1:A:80:ASN:HD22	2.02	0.60
1:D:119:ARG:HG3	1:D:137:LEU:HA	1.82	0.60
1:A:216:ASN:O	1:A:219:ALA:N	2.34	0.60
1:D:3:LEU:HD11	1:D:49:CYS:HB2	1.84	0.60
1:A:81:ASN:OD1	1:A:81:ASN:N	2.29	0.60
1:C:5:VAL:HG13	1:C:29:PHE:CD1	2.37	0.60
1:C:239:ASP:HB3	1:C:242:ALA:CB	2.29	0.60
1:C:237:LEU:N	1:C:237:LEU:HD23	2.15	0.60
1:B:282:ARG:NH1	1:B:282:ARG:HG3	2.15	0.60
1:A:259:VAL:HG12	1:A:260:TYR:O	2.02	0.60
1:D:50:ILE:HG12	1:D:74:LEU:CD1	2.27	0.60
1:A:64:LEU:O	1:A:69:VAL:HG23	2.01	0.60
1:B:23:PHE:HB3	1:B:25:PHE:CD1	2.36	0.60
1:D:55:ASP:HB3	1:D:60:VAL:HG21	1.82	0.60
1:B:122:ARG:HH21	1:C:129:ASP:CG	2.04	0.60
1:C:119:ARG:HG3	1:C:137:LEU:HA	1.84	0.60
1:C:127:THR:HG21	1:D:292:PHE:O	2.01	0.60
1:A:70:LYS:CB	1:A:71:TYR:CD1	2.83	0.59
1:D:211:ASN:O	1:D:214:LEU:HB2	2.02	0.59
1:A:153:GLY:O	1:A:157:VAL:HG23	2.03	0.59
1:A:114:MET:HA	1:A:114:MET:CE	2.29	0.59
1:C:6:TYR:CE1	1:C:30:PHE:HD2	2.19	0.59
1:A:2:LYS:N	1:A:26:GLU:O	2.36	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ALA:O	1:A:186:VAL:CG1	2.44	0.58
1:D:313:GLN:OE1	1:D:313:GLN:HA	2.03	0.58
1:A:208:THR:HG21	1:A:210:GLU:CG	2.34	0.58
1:D:35:THR:CG2	1:D:36:GLU:H	2.14	0.58
1:C:34:LEU:C	1:C:34:LEU:HD23	2.23	0.58
1:C:153:GLY:O	1:C:157:VAL:HG23	2.02	0.58
1:D:260:TYR:HE1	1:D:295:HIS:ND1	1.94	0.58
1:D:208:THR:H	1:D:211:ASN:HD22	1.52	0.58
1:A:298:PHE:O	1:A:303:ALA:HB3	2.03	0.58
1:C:5:VAL:CG1	1:C:29:PHE:CD1	2.87	0.58
1:A:296:GLN:HG3	1:B:134:LEU:HD22	1.84	0.58
1:B:152:THR:HG21	1:B:188:TYR:CZ	2.39	0.58
1:B:50:ILE:HG13	1:B:74:LEU:CD1	2.33	0.58
1:C:51:PHE:CD2	1:C:52:VAL:HG13	2.38	0.58
1:B:239:ASP:CB	1:B:242:ALA:HB3	2.25	0.58
1:D:6:TYR:O	1:D:75:ARG:NH2	2.36	0.58
1:A:203:LEU:HD12	1:A:231:ASN:CG	2.24	0.58
1:D:146:THR:CB	1:D:169:ARG:HH12	2.15	0.58
1:D:69:VAL:O	1:D:92:LEU:CD2	2.52	0.58
1:D:223:MET:O	1:D:251:LYS:HD2	2.03	0.58
1:D:58:ARG:N	1:D:59:PRO:HD2	2.17	0.58
1:C:189:VAL:HB	1:C:193:THR:HG22	1.85	0.58
1:D:84:LEU:O	1:D:87:ALA:HB3	2.03	0.58
1:D:85:ASP:O	1:D:88:LYS:N	2.37	0.57
1:C:297:ALA:O	1:D:118:ARG:NH2	2.37	0.57
1:D:5:VAL:CG2	1:D:8:THR:HG23	2.35	0.57
1:C:207:LEU:HD21	1:C:236:ALA:HB3	1.85	0.57
1:D:7:SER:OG	1:D:54:ASP:OD1	2.22	0.57
1:B:118:ARG:HH11	1:B:118:ARG:CG	2.14	0.57
1:B:169:ARG:C	1:B:170:LEU:HD23	2.24	0.57
1:D:19:VAL:HG21	1:D:308:SER:HB2	1.85	0.57
1:D:63:GLU:OE2	1:D:67:HIS:CD2	2.58	0.57
1:C:34:LEU:HD23	1:C:35:THR:N	2.20	0.57
1:A:107:GLU:O	1:A:110:ILE:CG2	2.48	0.57
1:C:221:ASP:O	1:C:251:LYS:NZ	2.34	0.57
1:D:50:ILE:CD1	1:D:74:LEU:CD1	2.82	0.57
1:A:191:LEU:N	1:A:192:PRO:CD	2.67	0.57
1:D:244:ILE:O	1:D:248:LYS:HG3	2.05	0.57
1:B:79:PHE:N	1:B:79:PHE:CD2	2.73	0.57
1:A:221:ASP:OD1	1:A:251:LYS:NZ	2.30	0.57
1:A:205:CYS:SG	1:A:237:LEU:CD1	2.93	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HD21	1:B:53:ASN:O	2.05	0.57
1:C:58:ARG:O	1:C:61:LEU:HB2	2.05	0.57
1:B:110:ILE:HD13	1:B:162:ILE:HG22	1.86	0.57
1:A:105:VAL:CG2	1:A:155:ILE:HG23	2.33	0.56
1:B:317:ASN:HD22	1:B:323:THR:HB	1.70	0.56
1:D:146:THR:O	1:D:199:ASP:OD1	2.21	0.56
1:C:58:ARG:HG3	1:C:59:PRO:HD3	0.59	0.56
1:A:19:VAL:HG12	1:A:20:ASN:N	2.20	0.56
1:D:209:PRO:HB2	1:D:210:GLU:OE2	2.05	0.56
1:B:105:VAL:CG2	1:B:155:ILE:CG2	2.83	0.56
1:B:302:GLU:O	1:B:305:THR:OG1	2.21	0.56
1:B:110:ILE:O	1:B:113:MET:N	2.39	0.56
1:C:249:ASN:O	1:C:249:ASN:OD1	2.22	0.56
1:A:301:ALA:O	1:A:305:THR:OG1	2.24	0.56
1:A:56:GLY:HA3	1:A:82:VAL:HA	1.86	0.56
1:B:119:ARG:HG3	1:B:137:LEU:HA	1.87	0.56
1:B:5:VAL:HG22	1:B:8:THR:HG21	1.86	0.56
1:A:23:PHE:CE2	1:A:312:LEU:C	2.79	0.56
1:D:12:ASP:OD2	1:D:75:ARG:NH1	2.33	0.56
1:A:283:ARG:CG	1:C:283:ARG:HG3	2.36	0.56
1:A:137:LEU:HD23	1:A:137:LEU:N	2.21	0.56
1:A:56:GLY:O	1:A:57:SER:O	2.23	0.56
1:A:19:VAL:HG12	1:A:312:LEU:HD11	1.88	0.56
1:A:35:THR:CG2	1:A:36:GLU:N	2.69	0.56
1:A:112:MET:HE1	1:A:293:THR:HG23	1.87	0.56
1:C:150:ILE:HD12	1:C:203:LEU:CD2	2.36	0.56
1:D:203:LEU:HD12	1:D:231:ASN:CG	2.26	0.56
1:A:5:VAL:CG2	1:A:29:PHE:HD1	2.18	0.56
1:D:249:ASN:O	1:D:250:GLN:HB2	2.06	0.56
1:C:51:PHE:CE2	1:C:52:VAL:HG13	2.41	0.56
1:C:10:GLN:NE2	1:C:10:GLN:HA	2.20	0.56
1:B:110:ILE:HG23	1:B:111:GLY:N	2.21	0.56
1:D:227:VAL:HG22	1:D:228:MET:N	2.21	0.56
1:D:39:ALA:HB3	1:D:63:GLU:HG2	1.89	0.55
1:B:227:VAL:HG22	1:B:228:MET:N	2.22	0.55
1:C:7:SER:OG	1:C:54:ASP:OD2	2.24	0.55
1:C:61:LEU:C	1:C:64:LEU:HB2	2.24	0.55
1:B:213:HIS:HD2	1:B:239:ASP:CA	2.14	0.55
1:C:189:VAL:CB	1:C:193:THR:CG2	2.79	0.55
1:C:39:ALA:HB1	1:C:64:LEU:HD12	1.89	0.55
1:A:128:ARG:O	1:B:282:ARG:HG2	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:O	1:B:110:ILE:HG22	2.06	0.55
1:C:6:TYR:O	1:C:7:SER:OG	2.20	0.55
1:B:49:CYS:SG	1:B:75:ARG:HG3	2.46	0.55
1:D:259:VAL:O	1:D:295:HIS:N	2.39	0.55
1:D:205:CYS:HB2	1:D:206:PRO:CD	2.35	0.55
1:A:114:MET:CA	1:A:114:MET:HE3	2.36	0.55
1:D:178:SER:OG	1:D:181:ALA:CB	2.55	0.55
1:B:128:ARG:NH2	1:D:128:ARG:NH2	2.55	0.55
1:B:58:ARG:CG	1:B:58:ARG:HH11	2.19	0.55
1:A:118:ARG:HH11	1:A:118:ARG:CG	2.18	0.55
1:A:127:THR:O	1:A:130:ALA:N	2.30	0.55
1:A:71:TYR:CD1	1:A:71:TYR:N	2.72	0.55
1:A:112:MET:CE	1:A:293:THR:HG23	2.37	0.55
1:A:23:PHE:HE2	1:A:313:GLN:HA	1.71	0.54
1:A:279:ASP:HA	1:A:282:ARG:HG3	1.90	0.54
1:A:178:SER:O	1:A:182:LEU:HG	2.07	0.54
1:C:33:LEU:O	1:C:38:THR:HG21	2.07	0.54
1:D:50:ILE:HD11	1:D:74:LEU:HD11	1.87	0.54
1:B:211:ASN:O	1:B:214:LEU:CB	2.55	0.54
1:B:23:PHE:N	1:B:23:PHE:CD1	2.74	0.54
1:C:117:ASN:HB2	1:C:228:MET:HE1	1.89	0.54
1:D:19:VAL:CG1	1:D:312:LEU:HD12	2.36	0.54
1:C:25:PHE:CD1	1:C:25:PHE:N	2.73	0.54
1:D:207:LEU:HD13	1:D:237:LEU:CD2	2.37	0.54
1:A:58:ARG:HH11	1:A:58:ARG:HG3	1.72	0.54
1:C:55:ASP:CG	1:C:57:SER:HG	2.09	0.54
1:D:208:THR:OG1	1:D:211:ASN:ND2	2.41	0.54
1:D:5:VAL:CG2	1:D:29:PHE:HD1	2.20	0.54
1:C:227:VAL:HG22	1:C:228:MET:N	2.22	0.54
1:C:112:MET:HE1	1:C:257:MET:N	2.22	0.54
1:A:241:GLN:HE21	1:A:241:GLN:C	2.10	0.54
1:C:191:LEU:HB2	1:C:192:PRO:HD3	1.90	0.54
1:D:181:ALA:O	1:D:186:VAL:CG1	2.50	0.54
1:B:323:THR:OG1	1:B:324:CYS:N	2.41	0.54
1:B:118:ARG:HG3	1:B:118:ARG:NH1	2.21	0.54
1:B:105:VAL:CG2	1:B:155:ILE:HG23	2.37	0.53
1:A:147:ALA:HB1	1:A:163:LEU:HD13	1.89	0.53
1:B:23:PHE:HE2	1:B:313:GLN:CA	2.21	0.53
1:C:23:PHE:HB3	1:C:25:PHE:CD1	2.43	0.53
1:A:3:LEU:HD22	1:A:315:LEU:CD1	2.39	0.53
1:B:203:LEU:HD21	1:B:215:LEU:CD2	2.39	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:PHE:N	1:D:32:PHE:CD2	2.73	0.53
1:C:38:THR:O	1:C:41:THR:OG1	2.26	0.53
1:A:58:ARG:HB3	1:A:59:PRO:CD	2.39	0.53
1:D:149:VAL:O	1:D:172:ALA:HA	2.09	0.53
1:B:186:VAL:HG22	1:B:187:GLU:N	2.22	0.53
1:A:207:LEU:HD22	1:A:236:ALA:HB3	1.90	0.53
1:A:63:GLU:O	1:A:67:HIS:HD2	1.92	0.53
1:C:8:THR:O	1:C:9:LYS:HD3	2.09	0.52
1:C:189:VAL:CG1	1:C:193:THR:HG21	2.38	0.52
1:B:51:PHE:HB2	1:B:75:ARG:NH2	2.24	0.52
1:C:223:MET:O	1:C:251:LYS:CE	2.56	0.52
1:A:158:ALA:O	1:A:162:ILE:HG13	2.09	0.52
1:B:15:TYR:O	1:B:19:VAL:CG2	2.42	0.52
1:A:42:ALA:O	1:A:45:CYS:CB	2.51	0.52
1:B:146:THR:O	1:B:199:ASP:OD1	2.26	0.52
1:C:51:PHE:CD2	1:C:52:VAL:N	2.72	0.52
1:D:52:VAL:HG12	1:D:76:CYS:SG	2.50	0.52
1:C:234:ARG:O	1:C:237:LEU:HG	2.10	0.52
1:B:23:PHE:N	1:B:23:PHE:HD1	2.08	0.52
1:C:142:MET:O	1:C:168:MET:CE	2.57	0.52
1:A:118:ARG:HG3	1:A:118:ARG:NH1	2.24	0.52
1:A:207:LEU:HD21	1:A:236:ALA:HB3	1.91	0.52
1:D:247:LEU:CD2	1:D:252:ILE:HG21	2.40	0.52
1:D:30:PHE:CD1	1:D:32:PHE:CE2	2.98	0.52
1:C:25:PHE:HD1	1:C:25:PHE:N	2.06	0.52
1:B:191:LEU:N	1:B:192:PRO:CD	2.72	0.52
1:C:19:VAL:HG21	1:C:308:SER:HB3	1.91	0.52
1:B:213:HIS:N	1:B:236:ALA:O	2.35	0.52
1:C:105:VAL:HG23	1:C:155:ILE:HG23	1.92	0.52
1:A:128:ARG:NH2	1:B:125:GLN:OE1	2.42	0.51
1:A:291:LEU:HD21	1:B:120:ILE:HG21	1.92	0.51
1:D:50:ILE:HD11	1:D:74:LEU:CD1	2.39	0.51
1:C:239:ASP:OD2	1:C:242:ALA:CB	2.42	0.51
1:B:4:ALA:HB2	1:B:45:CYS:SG	2.50	0.51
1:D:65:LYS:HE3	1:D:90:LEU:O	2.10	0.51
1:C:211:ASN:O	1:C:214:LEU:HB2	2.10	0.51
1:C:152:THR:HG23	1:C:174:ASP:HB2	1.92	0.51
1:D:114:MET:HA	1:D:114:MET:HE3	1.92	0.51
1:A:207:LEU:HD13	1:A:237:LEU:HD21	1.87	0.51
1:B:34:LEU:HB3	1:B:54:ASP:HB3	1.92	0.51
1:A:58:ARG:N	1:A:59:PRO:CD	2.73	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:PHE:CD1	1:C:79:PHE:C	2.83	0.51
1:D:247:LEU:HG	1:D:252:ILE:HG21	1.92	0.51
1:A:214:LEU:C	1:A:214:LEU:HD12	2.27	0.51
1:D:191:LEU:HB2	1:D:192:PRO:HD3	1.93	0.51
1:B:5:VAL:CG2	1:B:8:THR:HG21	2.40	0.51
1:D:125:GLN:NE2	1:D:125:GLN:CA	2.73	0.51
1:D:208:THR:CG2	1:D:210:GLU:HG2	2.40	0.51
1:D:50:ILE:HG12	1:D:74:LEU:HD12	1.90	0.51
1:B:58:ARG:CB	1:B:59:PRO:HD3	2.29	0.51
1:A:241:GLN:NE2	1:A:241:GLN:CA	2.73	0.51
1:C:249:ASN:O	1:C:250:GLN:HB2	2.11	0.51
1:A:58:ARG:HG3	1:A:58:ARG:NH1	2.26	0.51
1:C:6:TYR:HD2	1:C:34:LEU:HD12	1.74	0.51
1:B:223:MET:O	1:B:251:LYS:HE2	2.11	0.51
1:B:110:ILE:HD11	1:B:166:PHE:CE1	2.45	0.51
1:A:105:VAL:HG23	1:A:155:ILE:HG21	1.92	0.51
1:C:51:PHE:HD2	1:C:52:VAL:H	1.53	0.51
1:C:58:ARG:O	1:C:62:GLU:CG	2.59	0.50
1:A:64:LEU:HD23	1:A:69:VAL:HG21	1.93	0.50
1:D:213:HIS:CE1	1:D:239:ASP:OD1	2.63	0.50
1:C:207:LEU:CD1	1:C:237:LEU:HD23	2.35	0.50
1:A:4:ALA:HA	1:A:28:GLU:O	2.11	0.50
1:B:82:VAL:CG2	1:B:83:ASP:N	2.74	0.50
1:C:64:LEU:C	1:C:66:LYS:N	2.60	0.50
1:C:118:ARG:NH1	1:C:118:ARG:CG	2.72	0.50
1:D:110:ILE:HG23	1:D:111:GLY:N	2.27	0.50
1:A:146:THR:OG1	1:A:169:ARG:NH1	2.44	0.50
1:A:93:LYS:HD2	1:A:318:LEU:CD2	2.38	0.50
1:D:30:PHE:CD1	1:D:32:PHE:CZ	2.99	0.50
1:B:79:PHE:HD2	1:B:79:PHE:H	1.56	0.50
1:A:23:PHE:CD2	1:A:312:LEU:HB3	2.47	0.50
1:B:118:ARG:CG	1:B:118:ARG:NH1	2.72	0.50
1:A:244:ILE:O	1:A:248:LYS:HG3	2.12	0.50
1:A:292:PHE:HB2	1:B:127:THR:HG23	1.90	0.50
1:A:118:ARG:NH1	1:A:118:ARG:CG	2.72	0.50
1:D:190:ASP:HB2	1:D:192:PRO:HD2	1.92	0.50
1:D:70:LYS:HB3	1:D:71:TYR:CE1	2.47	0.50
1:C:173:PHE:CE1	1:C:191:LEU:HG	2.47	0.50
1:A:118:ARG:NH1	1:B:300:THR:HG22	2.27	0.50
1:B:23:PHE:HB3	1:B:25:PHE:HD1	1.77	0.50
1:A:15:TYR:O	1:A:19:VAL:HB	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:ARG:O	1:D:314:ASN:ND2	2.41	0.50
1:B:82:VAL:HG22	1:B:83:ASP:N	2.27	0.50
1:D:63:GLU:OE2	1:D:67:HIS:NE2	2.44	0.50
1:A:38:THR:O	1:A:41:THR:OG1	2.29	0.50
1:D:81:ASN:N	1:D:81:ASN:OD1	2.39	0.49
1:C:205:CYS:HB2	1:C:206:PRO:CD	2.41	0.49
1:B:5:VAL:HG22	1:B:29:PHE:HD1	1.77	0.49
1:D:34:LEU:HB3	1:D:54:ASP:HB3	1.94	0.49
1:C:225:ASN:OD1	1:C:251:LYS:CE	2.60	0.49
1:A:176:TYR:CD1	1:A:177:PRO:HD2	2.47	0.49
1:D:79:PHE:CD1	1:D:79:PHE:C	2.85	0.49
1:D:17:GLN:HE21	1:D:29:PHE:HE2	1.60	0.49
1:B:113:MET:SD	1:B:200:VAL:HG11	2.51	0.49
1:B:90:LEU:H	1:B:90:LEU:HD12	1.77	0.49
1:A:35:THR:CG2	1:A:36:GLU:H	2.20	0.49
1:C:48:VAL:HG22	1:C:49:CYS:N	2.27	0.49
1:A:105:VAL:HG23	1:A:155:ILE:CG2	2.42	0.49
1:B:77:ALA:O	1:B:96:ARG:NH1	2.38	0.49
1:C:125:GLN:NE2	1:D:125:GLN:CG	2.52	0.49
1:B:212:TYR:CE1	1:B:213:HIS:CE1	2.98	0.49
1:B:110:ILE:O	1:B:113:MET:HB3	2.12	0.49
1:C:194:LEU:HD23	1:C:194:LEU:O	2.12	0.49
1:A:95:VAL:HG11	1:A:318:LEU:HD11	1.95	0.49
1:C:34:LEU:C	1:C:34:LEU:CD2	2.81	0.49
1:D:97:VAL:HG13	1:D:97:VAL:O	2.11	0.49
1:B:313:GLN:O	1:B:316:SER:N	2.46	0.49
1:B:173:PHE:CD2	1:B:173:PHE:C	2.85	0.49
1:B:243:ALA:O	1:B:246:ALA:HB3	2.12	0.49
1:C:34:LEU:CD2	1:C:60:VAL:HG11	2.43	0.48
1:D:181:ALA:HB1	1:D:186:VAL:HG11	1.95	0.48
1:B:287:CYS:O	1:B:288:HIS:ND1	2.46	0.48
1:B:6:TYR:C	1:B:7:SER:OG	2.51	0.48
1:C:117:ASN:HB2	1:C:228:MET:CE	2.43	0.48
1:C:173:PHE:CD2	1:C:173:PHE:C	2.86	0.48
1:C:191:LEU:N	1:C:192:PRO:HD2	2.26	0.48
1:B:54:ASP:N	1:B:54:ASP:OD2	2.47	0.48
1:C:118:ARG:C	1:C:119:ARG:HG2	2.33	0.48
1:C:6:TYR:CE2	1:C:34:LEU:HG	2.48	0.48
1:D:260:TYR:CE1	1:D:295:HIS:CG	3.00	0.48
1:D:208:THR:N	1:D:211:ASN:HD22	2.09	0.48
1:A:292:PHE:O	1:B:127:THR:HG21	2.13	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ILE:CG2	1:B:111:GLY:N	2.77	0.48
1:C:120:ILE:CG2	1:D:291:LEU:HD21	2.43	0.48
1:D:208:THR:HG21	1:D:210:GLU:HG2	1.95	0.48
1:A:288:HIS:CB	1:A:290:VAL:HG23	2.44	0.48
1:C:120:ILE:HG21	1:D:291:LEU:HD21	1.94	0.48
1:A:60:VAL:HG12	1:A:64:LEU:HD12	1.95	0.48
1:A:110:ILE:O	1:A:113:MET:HB3	2.14	0.48
1:B:58:ARG:CG	1:B:58:ARG:NH1	2.76	0.48
1:A:227:VAL:CG2	1:A:228:MET:N	2.76	0.48
1:A:177:PRO:HG2	1:A:177:PRO:O	2.14	0.47
1:C:6:TYR:CD2	1:C:34:LEU:HB2	2.49	0.47
1:A:70:LYS:C	1:A:71:TYR:HD1	2.16	0.47
1:B:23:PHE:HD2	1:B:25:PHE:HE1	1.63	0.47
1:D:150:ILE:HD12	1:D:203:LEU:HD23	1.95	0.47
1:C:313:GLN:NE2	1:C:313:GLN:HA	2.28	0.47
1:A:208:THR:HG21	1:A:210:GLU:HG3	1.96	0.47
1:B:105:VAL:CG2	1:B:155:ILE:HG21	2.44	0.47
1:A:205:CYS:SG	1:A:237:LEU:HD11	2.54	0.47
1:A:298:PHE:N	1:A:298:PHE:CD2	2.79	0.47
1:C:50:ILE:HG13	1:C:74:LEU:HD12	1.95	0.47
1:C:61:LEU:O	1:C:65:LYS:N	2.45	0.47
1:B:23:PHE:HB3	1:B:25:PHE:CE1	2.49	0.47
1:C:13:LYS:HG3	1:C:29:PHE:CE2	2.50	0.47
1:C:239:ASP:O	1:C:242:ALA:HB3	2.14	0.47
1:C:127:THR:CG2	1:D:292:PHE:HB2	2.44	0.47
1:C:60:VAL:HG12	1:C:64:LEU:HD13	1.95	0.47
1:D:213:HIS:CE1	1:D:239:ASP:HA	2.49	0.47
1:C:193:THR:HG22	1:C:194:LEU:H	1.76	0.47
1:B:279:ASP:CG	1:B:282:ARG:NH1	2.68	0.47
1:B:279:ASP:OD2	1:B:282:ARG:NH1	2.48	0.47
1:A:288:HIS:HB2	1:A:290:VAL:HG23	1.96	0.47
1:B:4:ALA:HA	1:B:28:GLU:O	2.15	0.47
1:B:50:ILE:HB	1:B:54:ASP:HB2	1.97	0.47
1:C:280:VAL:HG13	1:C:284:LEU:HD22	1.97	0.47
1:D:260:TYR:OH	1:D:295:HIS:ND1	2.46	0.47
1:A:251:LYS:HB2	1:A:251:LYS:HE3	1.54	0.47
1:C:54:ASP:O	1:C:81:ASN:ND2	2.47	0.47
1:A:136:GLY:C	1:A:137:LEU:HD23	2.35	0.47
1:A:56:GLY:C	1:A:57:SER:O	2.48	0.47
1:D:20:ASN:O	1:D:23:PHE:N	2.47	0.47
1:D:208:THR:CB	1:D:211:ASN:ND2	2.78	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ASN:O	1:D:250:GLN:CB	2.63	0.47
1:C:149:VAL:HG21	1:C:160:LEU:CD2	2.45	0.47
1:D:5:VAL:HG22	1:D:29:PHE:CD1	2.47	0.46
1:D:116:LEU:HD22	1:D:254:SER:HB3	1.97	0.46
1:B:49:CYS:SG	1:B:75:ARG:CG	3.03	0.46
1:D:259:VAL:O	1:D:294:GLY:C	2.53	0.46
1:B:284:LEU:O	1:B:288:HIS:HB2	2.16	0.46
1:A:107:GLU:OE1	1:B:142:MET:N	2.39	0.46
1:A:58:ARG:CB	1:A:59:PRO:CD	2.94	0.46
1:C:57:SER:OG	1:C:60:VAL:HG23	2.16	0.46
1:A:207:LEU:HD21	1:A:236:ALA:CB	2.45	0.46
1:D:60:VAL:HG12	1:D:64:LEU:HD12	1.97	0.46
1:B:191:LEU:CB	1:B:192:PRO:HD3	2.41	0.46
1:B:50:ILE:O	1:B:50:ILE:HG13	2.15	0.46
1:B:204:HIS:HA	1:B:233:SER:OG	2.15	0.46
1:B:51:PHE:HE2	1:B:52:VAL:HG21	1.75	0.46
1:A:110:ILE:HG23	1:A:111:GLY:N	2.30	0.46
1:A:152:THR:OG1	1:A:174:ASP:CG	2.54	0.46
1:A:77:ALA:HA	1:A:97:VAL:O	2.16	0.46
1:D:146:THR:CB	1:D:169:ARG:NH1	2.75	0.46
1:A:51:PHE:HD2	1:A:52:VAL:HG22	1.77	0.46
1:C:10:GLN:NE2	1:C:10:GLN:CA	2.77	0.46
1:D:11:TYR:HB2	1:D:304:LEU:HD13	1.97	0.46
1:A:182:LEU:CD2	1:A:188:TYR:HE2	2.29	0.46
1:B:188:TYR:C	1:B:189:VAL:CG1	2.84	0.46
1:C:299:LEU:HD23	1:D:138:THR:HA	1.97	0.46
1:D:301:ALA:O	1:D:305:THR:OG1	2.28	0.46
1:B:188:TYR:C	1:B:189:VAL:HG13	2.35	0.46
1:A:234:ARG:CG	1:A:234:ARG:NH1	2.73	0.46
1:B:194:LEU:HD23	1:B:195:PHE:CA	2.46	0.46
1:A:191:LEU:HB2	1:A:192:PRO:HD3	1.96	0.46
1:D:216:ASN:O	1:D:219:ALA:N	2.49	0.45
1:A:141:THR:HG22	1:A:143:TYR:H	1.80	0.45
1:D:220:PHE:HE1	1:D:252:ILE:HD11	1.81	0.45
1:A:146:THR:O	1:A:199:ASP:OD1	2.35	0.45
1:D:191:LEU:HB3	1:D:195:PHE:CE2	2.52	0.45
1:A:52:VAL:HG23	1:A:53:ASN:N	2.30	0.45
1:B:79:PHE:N	1:B:79:PHE:HD2	2.14	0.45
1:B:152:THR:HG21	1:B:188:TYR:HE1	1.79	0.45
1:B:33:LEU:CD2	1:B:53:ASN:O	2.63	0.45
1:D:216:ASN:OD1	1:D:218:ALA:HB3	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLY:O	1:A:201:ILE:HA	2.16	0.45
1:A:138:THR:HA	1:B:299:LEU:HD23	1.98	0.45
1:C:10:GLN:HB2	1:D:135:GLU:OE1	2.17	0.45
1:C:207:LEU:HD12	1:C:207:LEU:HA	1.81	0.45
1:D:34:LEU:HD12	1:D:38:THR:HG1	1.81	0.45
1:D:225:ASN:CG	1:D:251:LYS:CE	2.84	0.45
1:B:208:THR:OG1	1:B:211:ASN:CB	2.63	0.45
1:A:303:ALA:O	1:A:307:ILE:HG12	2.16	0.45
1:C:173:PHE:CD1	1:C:191:LEU:HG	2.52	0.45
1:D:77:ALA:HA	1:D:97:VAL:O	2.17	0.45
1:B:81:ASN:OD1	1:B:82:VAL:N	2.49	0.45
1:B:83:ASP:C	1:B:84:LEU:CG	2.85	0.45
1:D:178:SER:OG	1:D:181:ALA:HB2	2.17	0.45
1:A:113:MET:HE3	1:A:230:VAL:HG21	1.98	0.45
1:A:169:ARG:CG	1:A:169:ARG:NH1	2.73	0.45
1:A:80:ASN:ND2	1:A:80:ASN:O	2.29	0.45
1:A:152:THR:HG21	1:A:188:TYR:CE1	2.51	0.45
1:A:79:PHE:O	1:A:79:PHE:HD1	2.00	0.45
1:B:188:TYR:O	1:B:189:VAL:HG12	2.17	0.45
1:A:55:ASP:CG	1:A:57:SER:HG	2.20	0.45
1:C:199:ASP:OD1	1:C:199:ASP:N	2.49	0.45
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.79	0.45
1:A:23:PHE:CE2	1:A:313:GLN:CA	3.00	0.45
1:C:110:ILE:HG23	1:C:111:GLY:N	2.32	0.45
1:B:145:LYS:HD3	1:B:199:ASP:OD2	2.17	0.44
1:A:216:ASN:O	1:A:219:ALA:HB3	2.17	0.44
1:A:207:LEU:HD12	1:A:237:LEU:CD2	2.43	0.44
1:A:249:ASN:O	1:A:250:GLN:HB2	2.17	0.44
1:A:287:CYS:O	1:A:288:HIS:CG	2.69	0.44
1:B:249:ASN:O	1:B:249:ASN:OD1	2.35	0.44
1:C:216:ASN:OD1	1:C:218:ALA:CB	2.60	0.44
1:C:35:THR:H	1:C:38:THR:CG2	2.31	0.44
1:A:105:VAL:HG22	1:A:155:ILE:CG2	2.40	0.44
1:A:3:LEU:C	1:A:3:LEU:HD12	2.33	0.44
1:A:182:LEU:HD21	1:A:188:TYR:CE2	2.52	0.44
1:D:100:TYR:O	1:D:102:PRO:HD3	2.17	0.44
1:C:8:THR:OG1	1:C:30:PHE:O	2.23	0.44
1:B:212:TYR:O	1:B:213:HIS:C	2.55	0.44
1:A:79:PHE:O	1:A:79:PHE:CD1	2.70	0.44
1:D:296:GLN:HG2	1:D:296:GLN:O	2.18	0.44
1:A:182:LEU:HD21	1:A:188:TYR:HE2	1.81	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ARG:H	1:C:59:PRO:HD2	1.77	0.44
1:A:19:VAL:HG13	1:A:312:LEU:CD1	2.40	0.44
1:B:105:VAL:HG22	1:B:155:ILE:HG23	2.00	0.44
1:A:283:ARG:HE	1:C:283:ARG:HG3	1.83	0.44
1:A:291:LEU:HD21	1:B:120:ILE:CG2	2.48	0.44
1:A:34:LEU:HB3	1:A:54:ASP:HB3	2.00	0.44
1:B:257:MET:HB3	1:B:257:MET:HE2	1.95	0.44
1:C:63:GLU:O	1:C:66:LYS:HB2	2.17	0.43
1:B:34:LEU:O	1:B:55:ASP:HB3	2.18	0.43
1:B:23:PHE:HZ	1:B:313:GLN:HG2	1.83	0.43
1:B:313:GLN:O	1:B:314:ASN:C	2.52	0.43
1:D:169:ARG:C	1:D:170:LEU:HD23	2.38	0.43
1:C:102:PRO:HG2	1:C:103:GLU:N	2.33	0.43
1:C:61:LEU:O	1:C:64:LEU:N	2.51	0.43
1:D:8:THR:OG1	1:D:30:PHE:O	2.34	0.43
1:C:16:LEU:O	1:C:20:ASN:HB2	2.19	0.43
1:B:191:LEU:N	1:B:192:PRO:HD2	2.33	0.43
1:A:114:MET:CA	1:A:114:MET:CE	2.95	0.43
1:B:51:PHE:CD2	1:B:52:VAL:N	2.62	0.43
1:A:55:ASP:OD1	1:A:57:SER:OG	2.37	0.43
1:D:214:LEU:HD12	1:D:214:LEU:C	2.38	0.43
1:A:194:LEU:C	1:A:194:LEU:CD2	2.86	0.43
1:B:194:LEU:HD23	1:B:195:PHE:HA	2.00	0.43
1:D:20:ASN:ND2	1:D:27:LEU:CD1	2.82	0.43
1:B:259:VAL:HG21	1:B:292:PHE:HD1	1.84	0.43
1:A:127:THR:CG2	1:B:292:PHE:HB2	2.49	0.43
1:C:259:VAL:O	1:C:295:HIS:HB2	2.19	0.43
1:C:261:GLU:CD	1:C:261:GLU:H	2.04	0.43
1:C:145:LYS:HB2	1:C:168:MET:CE	2.49	0.43
1:A:298:PHE:O	1:A:303:ALA:CB	2.67	0.43
1:C:52:VAL:CG2	1:C:53:ASN:N	2.82	0.43
1:C:225:ASN:OD1	1:C:251:LYS:HE3	2.18	0.43
1:D:191:LEU:O	1:D:195:PHE:N	2.41	0.43
1:A:203:LEU:O	1:A:233:SER:OG	2.27	0.43
1:B:227:VAL:CG2	1:B:228:MET:N	2.82	0.43
1:C:227:VAL:CG2	1:C:228:MET:N	2.82	0.43
1:B:81:ASN:OD1	1:B:82:VAL:HG12	2.19	0.42
1:B:82:VAL:HG22	1:B:83:ASP:O	2.19	0.42
1:A:231:ASN:HB2	1:A:238:ILE:HD11	2.00	0.42
1:C:284:LEU:O	1:C:288:HIS:HB2	2.19	0.42
1:A:299:LEU:HG	1:B:138:THR:HG23	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ASP:N	1:D:190:ASP:OD1	2.51	0.42
1:C:249:ASN:O	1:C:250:GLN:CB	2.67	0.42
1:B:208:THR:OG1	1:B:211:ASN:ND2	2.46	0.42
1:A:283:ARG:HG2	1:C:283:ARG:HG3	2.00	0.42
1:B:194:LEU:CD2	1:B:195:PHE:CD1	3.03	0.42
1:A:23:PHE:CE2	1:A:312:LEU:HB3	2.54	0.42
1:B:83:ASP:C	1:B:84:LEU:CD1	2.86	0.42
1:B:58:ARG:NH1	1:B:58:ARG:HG3	2.34	0.42
1:C:173:PHE:CD2	1:C:173:PHE:O	2.73	0.42
1:C:220:PHE:O	1:C:251:LYS:NZ	2.50	0.42
1:B:113:MET:SD	1:B:200:VAL:CG1	3.07	0.42
1:C:6:TYR:CD2	1:C:34:LEU:HD12	2.53	0.42
1:C:61:LEU:O	1:C:64:LEU:CA	2.67	0.42
1:C:6:TYR:HD2	1:C:34:LEU:HB2	1.83	0.42
1:D:194:LEU:HD23	1:D:195:PHE:N	2.34	0.42
1:B:100:TYR:O	1:B:101:ASP:C	2.57	0.42
1:B:191:LEU:CD1	1:B:214:LEU:HD11	2.50	0.42
1:B:145:LYS:CD	1:B:199:ASP:OD2	2.67	0.42
1:D:79:PHE:C	1:D:79:PHE:HD1	2.23	0.42
1:C:79:PHE:C	1:C:81:ASN:H	2.23	0.42
1:A:23:PHE:CZ	1:A:313:GLN:HA	2.54	0.42
1:A:128:ARG:HH22	1:C:128:ARG:HD3	1.85	0.42
1:A:5:VAL:CG2	1:A:29:PHE:CD1	3.02	0.42
1:B:23:PHE:CZ	1:B:313:GLN:HG2	2.54	0.42
1:A:37:LYS:HD3	1:D:28:GLU:OE2	2.19	0.42
1:C:150:ILE:HD12	1:C:203:LEU:HD23	2.01	0.42
1:C:232:THR:O	1:C:260:TYR:OH	2.21	0.42
1:B:5:VAL:HB	1:B:49:CYS:HB3	2.01	0.42
1:D:9:LYS:O	1:D:12:ASP:HB2	2.20	0.42
1:C:127:THR:HG21	1:D:292:PHE:HB2	2.02	0.42
1:C:299:LEU:HD13	1:D:134:LEU:HD13	2.01	0.42
1:B:92:LEU:HD23	1:B:92:LEU:HA	1.90	0.42
1:C:59:PRO:HA	1:C:62:GLU:HG3	2.02	0.42
1:A:303:ALA:O	1:A:307:ILE:CG1	2.68	0.42
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.85	0.42
1:C:20:ASN:HA	1:C:312:LEU:CD1	2.50	0.42
1:D:129:ASP:O	1:D:130:ALA:HB3	2.19	0.42
1:A:247:LEU:HD23	1:A:252:ILE:HB	2.00	0.42
1:D:213:HIS:HE1	1:D:239:ASP:OD1	2.03	0.41
1:D:247:LEU:HD21	1:D:252:ILE:CG2	2.48	0.41
1:C:190:ASP:CG	1:C:192:PRO:HD2	2.39	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:TYR:O	1:B:189:VAL:CG1	2.68	0.41
1:B:220:PHE:O	1:B:251:LYS:HG2	2.20	0.41
1:C:52:VAL:HG23	1:C:53:ASN:N	2.35	0.41
1:A:50:ILE:HG13	1:A:74:LEU:HD13	2.01	0.41
1:A:300:THR:OG1	1:A:303:ALA:CB	2.68	0.41
1:D:228:MET:HE2	1:D:228:MET:HB2	1.64	0.41
1:B:163:LEU:HD23	1:B:163:LEU:HA	1.79	0.41
1:B:16:LEU:HD23	1:B:16:LEU:HA	1.95	0.41
1:C:216:ASN:O	1:C:219:ALA:N	2.53	0.41
1:A:118:ARG:HG2	1:B:108:HIS:HD1	1.85	0.41
1:A:79:PHE:CD1	1:A:79:PHE:C	2.94	0.41
1:C:194:LEU:CD2	1:C:194:LEU:C	2.85	0.41
1:C:194:LEU:O	1:C:198:SER:OG	2.35	0.41
1:D:95:VAL:CG2	1:D:314:ASN:HB3	2.46	0.41
1:D:105:VAL:HB	1:D:297:ALA:HB1	2.02	0.41
1:D:191:LEU:HD22	1:D:195:PHE:CZ	2.55	0.41
1:A:58:ARG:CB	1:A:59:PRO:HD3	2.49	0.41
1:B:281:PHE:CD1	1:B:292:PHE:CE1	3.08	0.41
1:A:179:ALA:O	1:A:182:LEU:N	2.54	0.41
1:C:147:ALA:HB1	1:C:163:LEU:HD13	2.02	0.41
1:A:113:MET:CE	1:A:230:VAL:HG21	2.50	0.41
1:A:203:LEU:HD12	1:A:231:ASN:OD1	2.20	0.41
1:D:220:PHE:CE1	1:D:252:ILE:HD11	2.55	0.41
1:B:124:TYR:O	1:B:128:ARG:HG3	2.20	0.41
1:A:241:GLN:NE2	1:A:241:GLN:C	2.73	0.41
1:A:100:TYR:O	1:A:101:ASP:C	2.58	0.41
1:A:222:GLN:HB3	1:A:222:GLN:HE21	1.76	0.41
1:B:239:ASP:O	1:B:242:ALA:HB3	2.20	0.41
1:B:83:ASP:C	1:B:84:LEU:HG	2.40	0.41
1:C:118:ARG:NH2	1:D:300:THR:CG2	2.82	0.41
1:B:299:LEU:C	1:B:300:THR:HG23	2.41	0.41
1:B:203:LEU:HD12	1:B:231:ASN:CG	2.41	0.41
1:B:110:ILE:O	1:B:113:MET:CB	2.69	0.41
1:C:211:ASN:O	1:C:214:LEU:CB	2.69	0.41
1:C:43:ASN:HB2	1:C:67:HIS:HD1	1.85	0.41
1:C:56:GLY:HA3	1:C:81:ASN:O	2.21	0.41
1:D:225:ASN:CG	1:D:251:LYS:HE2	2.38	0.41
1:B:299:LEU:O	1:B:300:THR:CG2	2.69	0.41
1:B:186:VAL:HG13	1:B:187:GLU:N	2.35	0.41
1:D:19:VAL:HG12	1:D:312:LEU:CD1	2.50	0.41
1:B:223:MET:O	1:B:251:LYS:HE3	2.19	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LEU:HG	1:C:215:LEU:HD12	2.03	0.41
1:A:231:ASN:HD22	1:A:238:ILE:HD12	1.85	0.41
1:C:123:ALA:O	1:C:127:THR:N	2.33	0.41
1:D:218:ALA:O	1:D:222:GLN:HG3	2.21	0.41
1:B:216:ASN:OD1	1:B:218:ALA:HB3	2.21	0.41
1:D:169:ARG:HH11	1:D:169:ARG:HB3	1.86	0.41
1:B:284:LEU:HA	1:B:284:LEU:HD23	1.85	0.41
1:D:110:ILE:CG2	1:D:111:GLY:N	2.84	0.41
1:D:83:ASP:OD1	1:D:85:ASP:OD2	2.38	0.41
1:C:16:LEU:HA	1:C:16:LEU:HD23	1.88	0.41
1:C:210:GLU:HG2	1:C:210:GLU:H	1.60	0.41
1:D:213:HIS:ND1	1:D:239:ASP:HB2	2.36	0.40
1:C:19:VAL:HG11	1:C:309:GLN:CA	2.51	0.40
1:C:207:LEU:CD2	1:C:236:ALA:HB3	2.50	0.40
1:C:225:ASN:OD1	1:C:251:LYS:CD	2.69	0.40
1:B:47:ALA:HA	1:B:69:VAL:HG13	2.03	0.40
1:B:312:LEU:HA	1:B:312:LEU:HD23	1.75	0.40
1:C:243:ALA:O	1:C:246:ALA:HB3	2.21	0.40
1:D:147:ALA:HB1	1:D:163:LEU:HD13	2.02	0.40
1:D:309:GLN:HE21	1:D:309:GLN:HB2	1.59	0.40
1:D:61:LEU:HD22	1:D:72:ILE:HD11	2.04	0.40
1:A:105:VAL:HG21	1:A:155:ILE:HG21	2.00	0.40
1:A:23:PHE:CE2	1:A:313:GLN:N	2.90	0.40
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.87	0.40
1:D:124:TYR:O	1:D:128:ARG:CG	2.62	0.40
1:A:118:ARG:NH1	1:B:299:LEU:O	2.53	0.40
1:B:23:PHE:CD2	1:B:312:LEU:HB3	2.56	0.40
1:A:20:ASN:CB	1:A:27:LEU:HD11	2.52	0.40
1:C:192:PRO:O	1:C:196:SER:OG	2.38	0.40
1:C:188:TYR:O	1:C:189:VAL:HG13	2.21	0.40
1:D:249:ASN:C	1:D:249:ASN:OD1	2.59	0.40
1:D:237:LEU:HD23	1:D:237:LEU:N	2.36	0.40
1:D:154:LYS:H	1:D:154:LYS:HG2	1.62	0.40
1:A:125:GLN:NE2	1:D:125:GLN:OE1	2.54	0.40
1:B:23:PHE:CE2	1:B:313:GLN:HA	2.45	0.40
1:A:63:GLU:OE2	1:A:67:HIS:NE2	2.55	0.40
1:C:110:ILE:CG2	1:C:111:GLY:N	2.84	0.40
1:D:227:VAL:CG2	1:D:228:MET:N	2.84	0.40
1:D:79:PHE:O	1:D:79:PHE:HD1	2.04	0.40
1:B:216:ASN:O	1:B:219:ALA:N	2.55	0.40
1:C:240:SER:O	1:C:244:ILE:HG13	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HD12	1:A:215:LEU:HA	1.83	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	299/345 (87%)	293 (98%)	5 (2%)	1 (0%)	46	81
1	B	260/345 (75%)	255 (98%)	5 (2%)	0	100	100
1	C	252/345 (73%)	245 (97%)	7 (3%)	0	100	100
1	D	283/345 (82%)	280 (99%)	3 (1%)	0	100	100
All	All	1094/1380 (79%)	1073 (98%)	20 (2%)	1 (0%)	56	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	PRO

### 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	250/291 (86%)	200 (80%)	50 (20%)	1	6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	228/291 (78%)	173 (76%)	55 (24%)	1	3
1	C	219/291 (75%)	185 (84%)	34 (16%)	3	16
1	D	236/291 (81%)	190 (80%)	46 (20%)	2	7
All	All	933/1164 (80%)	748 (80%)	185 (20%)	1	7

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	26	GLU
1	A	41	THR
1	A	43	ASN
1	A	46	GLU
1	A	48	VAL
1	A	57	SER
1	A	64	LEU
1	A	74	LEU
1	A	75	ARG
1	A	80	ASN
1	A	81	ASN
1	A	82	VAL
1	A	101	ASP
1	A	105	VAL
1	A	107	GLU
1	A	118	ARG
1	A	119	ARG
1	A	127	THR
1	A	128	ARG
1	A	142	MET
1	A	154	LYS
1	A	159	MET
1	A	169	ARG
1	A	175	PRO
1	A	187	GLU
1	A	199	ASP
1	A	203	LEU
1	A	210	GLU
1	A	214	LEU
1	A	215	LEU
1	A	221	ASP
1	A	223	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	228	MET
1	A	234	ARG
1	A	240	SER
1	A	241	GLN
1	A	248	LYS
1	A	250	GLN
1	A	251	LYS
1	A	254	SER
1	A	257	MET
1	A	279	ASP
1	A	282	ARG
1	A	283	ARG
1	A	305	THR
1	A	307	ILE
1	A	311	THR
1	A	318	LEU
1	A	320	LYS
1	B	10	GLN
1	B	21	GLU
1	B	22	SER
1	B	23	PHE
1	B	26	GLU
1	B	28	GLU
1	B	33	LEU
1	B	41	THR
1	B	46	GLU
1	B	52	VAL
1	B	54	ASP
1	B	58	ARG
1	B	71	TYR
1	B	74	LEU
1	B	79	PHE
1	B	80	ASN
1	B	84	LEU
1	B	93	LYS
1	B	97	VAL
1	B	101	ASP
1	B	103	GLU
1	B	105	VAL
1	B	118	ARG
1	B	119	ARG
1	B	121	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	125	GLN
1	B	128	ARG
1	B	138	THR
1	B	142	MET
1	B	159	MET
1	B	169	ARG
1	B	170	LEU
1	B	187	GLU
1	B	194	LEU
1	B	198	SER
1	B	199	ASP
1	B	203	LEU
1	B	211	ASN
1	B	214	LEU
1	B	215	LEU
1	B	221	ASP
1	B	228	MET
1	B	232	THR
1	B	234	ARG
1	B	248	LYS
1	B	254	SER
1	B	257	MET
1	B	279	ASP
1	B	289	ASN
1	B	296	GLN
1	B	299	LEU
1	B	309	GLN
1	B	313	GLN
1	B	322	GLU
1	B	323	THR
1	C	8	THR
1	C	22	SER
1	C	25	PHE
1	C	41	THR
1	C	57	SER
1	C	58	ARG
1	C	74	LEU
1	C	75	ARG
1	C	112	MET
1	C	118	ARG
1	C	119	ARG
1	C	127	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	128	ARG
1	C	142	MET
1	C	155	ILE
1	C	168	MET
1	C	193	THR
1	C	196	SER
1	C	198	SER
1	C	199	ASP
1	C	208	THR
1	C	210	GLU
1	C	228	MET
1	C	232	THR
1	C	234	ARG
1	C	240	SER
1	C	250	GLN
1	C	254	SER
1	C	257	MET
1	C	260	TYR
1	C	283	ARG
1	C	284	LEU
1	C	285	SER
1	C	299	LEU
1	D	5	VAL
1	D	8	THR
1	D	11	TYR
1	D	26	GLU
1	D	33	LEU
1	D	37	LYS
1	D	46	GLU
1	D	48	VAL
1	D	64	LEU
1	D	71	TYR
1	D	74	LEU
1	D	79	PHE
1	D	80	ASN
1	D	85	ASP
1	D	101	ASP
1	D	103	GLU
1	D	105	VAL
1	D	112	MET
1	D	118	ARG
1	D	119	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	121	HIS
1	D	125	GLN
1	D	127	THR
1	D	128	ARG
1	D	154	LYS
1	D	162	ILE
1	D	169	ARG
1	D	198	SER
1	D	199	ASP
1	D	210	GLU
1	D	214	LEU
1	D	215	LEU
1	D	221	ASP
1	D	228	MET
1	D	232	THR
1	D	233	SER
1	D	234	ARG
1	D	237	LEU
1	D	240	SER
1	D	250	GLN
1	D	251	LYS
1	D	252	ILE
1	D	254	SER
1	D	257	MET
1	D	259	VAL
1	D	309	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	A	222	GLN
1	A	241	GLN
1	A	309	GLN
1	B	211	ASN
1	B	213	HIS
1	B	289	ASN
1	C	10	GLN
1	C	43	ASN
1	C	125	GLN
1	C	213	HIS
1	C	313	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	17	GLN
1	D	80	ASN
1	D	121	HIS
1	D	125	GLN
1	D	211	ASN
1	D	213	HIS
1	D	222	GLN
1	D	309	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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	303/345 (87%)	0.02	3 (0%) 84 80	48, 69, 89, 111	0
1	B	274/345 (79%)	0.37	11 (4%) 42 34	47, 77, 105, 126	0
1	C	264/345 (76%)	0.12	12 (4%) 37 30	42, 70, 113, 144	0
1	D	287/345 (83%)	0.05	7 (2%) 62 55	41, 68, 94, 111	0
All	All	1128/1380 (81%)	0.14	33 (2%) 55 49	41, 70, 104, 144	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	23	PHE	3.7
1	B	71	TYR	3.6
1	C	24	GLY	3.6
1	C	30	PHE	3.6
1	C	29	PHE	3.5
1	B	70	LYS	3.0
1	C	37	LYS	3.0
1	B	28	GLU	2.7
1	D	71	TYR	2.7
1	A	71	TYR	2.7
1	D	23	PHE	2.6
1	B	20	ASN	2.6
1	C	22	SER	2.5
1	B	25	PHE	2.5
1	D	46	GLU	2.5
1	B	43	ASN	2.4
1	A	221	ASP	2.4
1	C	17	GLN	2.4
1	A	320	LYS	2.4
1	B	249	ASN	2.4
1	B	58	ARG	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	92	LEU	2.3
1	C	43	ASN	2.3
1	B	72	ILE	2.3
1	D	95	VAL	2.2
1	D	44	GLY	2.2
1	D	45	CYS	2.2
1	C	62	GLU	2.2
1	C	311	THR	2.1
1	D	20	ASN	2.1
1	C	50	ILE	2.1
1	C	49	CYS	2.0
1	B	89	GLU	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.