



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:55 AM GMT

PDB ID : 2A0F  
Title : Structure of D236A mutant E. coli Aspartate Transcarbamoylase in presence of Phosphonoacetamide at 2.90 Å resolution  
Authors : Stieglitz, K.A.; Dusingberre, K.J.; Cardia, J.P.; Tsuruta, H.; Kantrowitz, E.R.  
Deposited on : 2005-06-16  
Resolution : 2.90 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

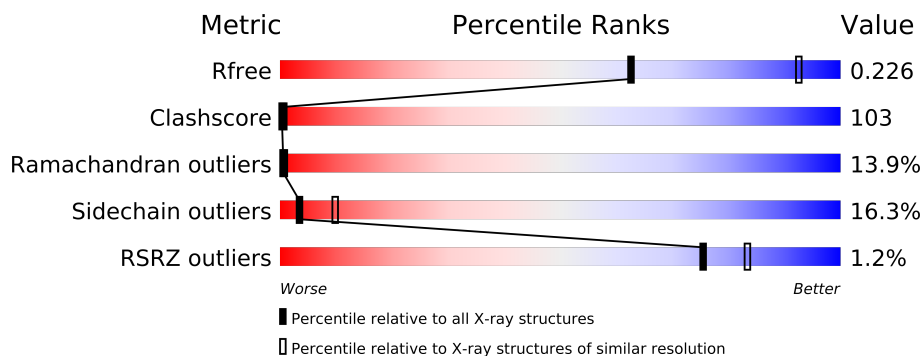
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
$R_{free}$	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	310	
1	C	310	
2	B	153	
2	D	153	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7489 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2412	1526	423	454	9			
1	C	310	Total	C	N	O	S	0	0	0
			2412	1526	423	454	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	ALA	ASP	ENGINEERED	UNP P0A786
C	236	ALA	ASP	ENGINEERED	UNP P0A786

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			
2	D	146	Total	C	N	O	S	0	0	0
			1138	714	201	218	5			

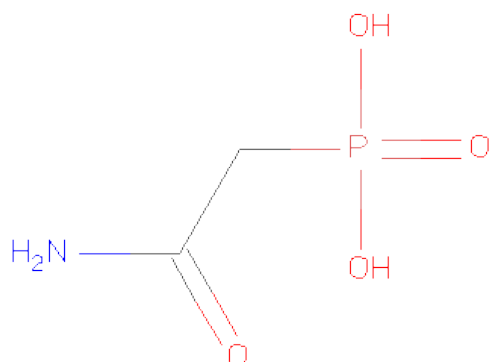
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	INITIATING METHIONINE	UNP P0A7F3
D	1	MET	-	INITIATING METHIONINE	UNP P0A7F3

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PHOSPHONOACETAMIDE (three-letter code: PCT) (formula:  $C_2H_6NO_4P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			8	2	1	4	1		

- Molecule 5 is water.

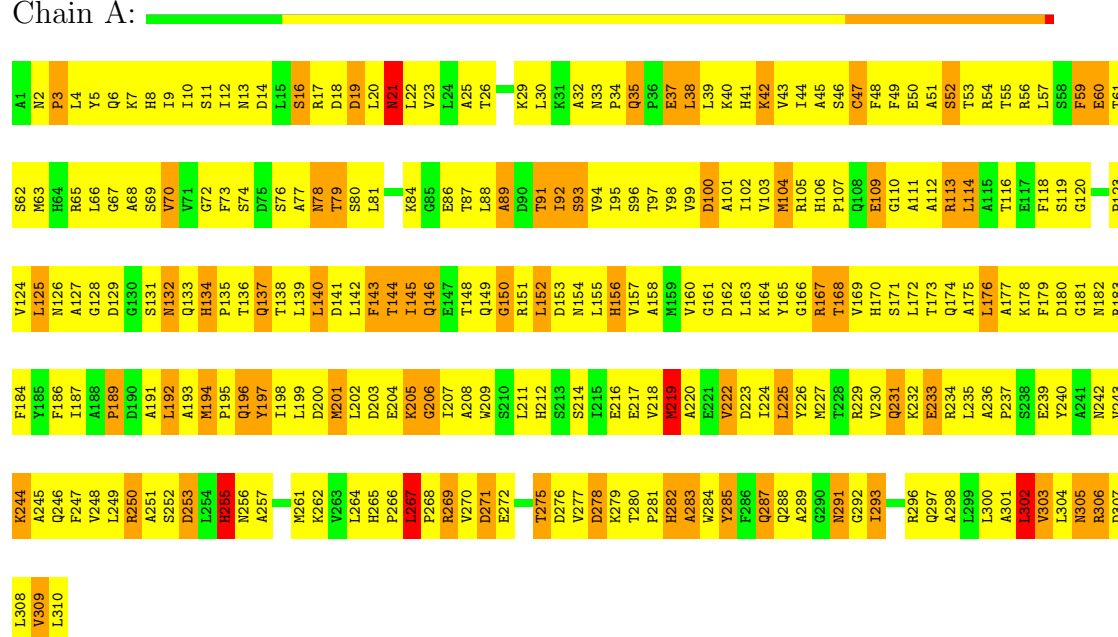
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	130	Total	O	0	0
			130	130		
5	B	82	Total	O	0	0
			82	82		
5	C	110	Total	O	0	0
			110	110		
5	D	57	Total	O	0	0
			57	57		

### 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: Aspartate carbamoyltransferase catalytic chain

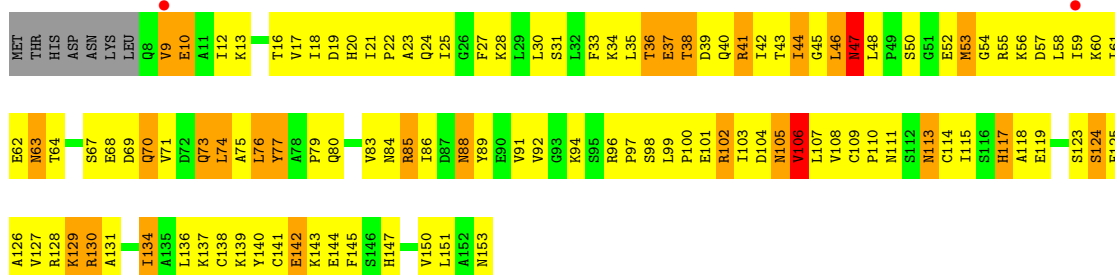
Chain A:





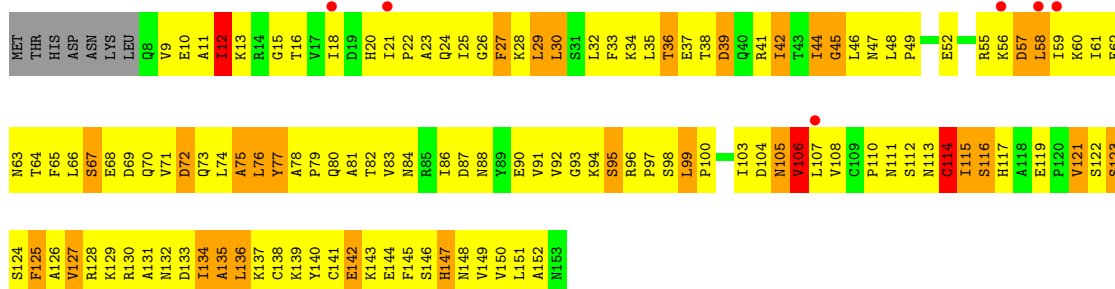
• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain B:



• Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.45Å 120.45Å 155.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.90 36.73 – 2.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.90) 80.9 (36.73-2.79)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.217 , 0.279 0.215 , 0.226	Depositor DCC
$R_{free}$ test set	2697 reflections (11.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 114.4	EDS
Estimated twinning fraction	0.427 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 26586 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7489	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PCT

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	0.62	1/2458 (0.0%)	0.83	1/3335 (0.0%)
1	C	0.53	3/2458 (0.1%)	0.71	0/3335
2	B	0.52	0/1155	0.75	1/1561 (0.1%)
2	D	0.44	0/1155	0.68	0/1561
All	All	0.55	4/7226 (0.1%)	0.75	2/9792 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	60	GLU	CD-OE2	7.41	1.33	1.25
1	A	60	GLU	CD-OE2	6.51	1.32	1.25
1	C	147	GLU	CG-CD	5.70	1.60	1.51
1	C	147	GLU	CD-OE1	5.10	1.31	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	LEU	CA-CB-CG	6.34	129.88	115.30
2	B	74	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	98	TYR	Sidechain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2412	0	2423	452	0
1	C	2412	0	2423	578	0
2	B	1138	0	1152	209	0
2	D	1138	0	1154	295	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	8	0	4	3	0
5	A	130	0	0	22	0
5	B	82	0	0	18	0
5	C	110	0	0	32	0
5	D	57	0	0	3	0
All	All	7489	0	7156	1476	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 103.

All (1476) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:111:ASN:HD22	2:D:114:CYS:HB2	1.07	1.16
1:A:158:ALA:HB2	1:A:222:VAL:HG11	1.26	1.11
2:D:82:THR:HA	2:D:96:ARG:HH12	1.11	1.08
2:B:44:ILE:HG23	2:D:44:ILE:HB	1.37	1.06
2:D:20:HIS:HB3	2:D:80:GLN:HG2	1.37	1.05
1:C:270:VAL:HG13	1:C:271:ASP:H	1.20	1.04
2:B:75:ALA:HB1	2:B:99:LEU:HD12	1.36	1.03
1:C:249:LEU:HG	1:C:254:LEU:HD11	1.40	1.02
1:C:26:THR:O	1:C:30:LEU:HG	1.58	1.02
1:A:229:ARG:HH21	1:A:270:VAL:HG21	1.22	1.02
1:C:20:LEU:HD12	1:C:20:LEU:H	1.23	1.02
1:A:164:LYS:HA	1:A:195:PRO:HD3	1.42	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:76:LEU:H	2:B:76:LEU:HD23	1.23	1.01
2:D:74:LEU:HG	2:D:97:PRO:HB3	1.40	1.00
1:C:12:ILE:HD11	1:C:135:PRO:HA	1.43	1.00
1:C:219:MET:HB3	1:C:256:ASN:HD21	1.26	0.99
2:D:103:ILE:HB	2:D:125:PHE:H	1.26	0.99
1:A:189:PRO:HG2	1:A:192:LEU:HD12	1.42	0.99
2:D:146:SER:HB2	2:D:148:ASN:HD22	1.28	0.98
1:A:216:GLU:O	1:A:219:MET:HB2	1.61	0.98
1:C:9:ILE:HB	1:C:125:LEU:HA	1.43	0.97
1:C:139:LEU:HA	1:C:142:LEU:HD12	1.42	0.97
1:C:60:GLU:HA	1:C:63:MET:SD	2.05	0.97
1:C:264:LEU:HD12	1:C:288:GLN:HB2	1.46	0.97
2:D:111:ASN:ND2	2:D:114:CYS:HB2	1.79	0.97
2:B:43:THR:HA	2:D:45:GLY:HA2	1.44	0.97
1:A:145:ILE:HG23	1:A:224:ILE:HD12	1.44	0.97
1:A:3:PRO:HD2	1:A:22:LEU:HD21	1.44	0.96
2:D:46:LEU:HD23	2:D:46:LEU:H	1.29	0.96
1:A:8:HIS:CD2	1:A:123:PRO:HA	2.01	0.96
1:A:219:MET:HB3	1:A:256:ASN:HD21	1.30	0.96
1:C:199:LEU:HA	1:C:202:LEU:HD21	1.48	0.95
1:C:121:ASN:HD22	1:C:121:ASN:H	1.15	0.94
1:A:267:LEU:HD23	1:A:268:PRO:HA	1.47	0.93
1:C:237:PRO:HA	1:C:240:TYR:CE2	2.03	0.93
1:A:52:SER:OG	1:A:55:THR:HG22	1.69	0.92
2:D:137:LYS:HA	2:D:144:GLU:HA	1.50	0.92
1:C:55:THR:O	1:C:59:PHE:HB2	1.70	0.91
2:D:82:THR:HA	2:D:96:ARG:NH1	1.85	0.91
1:A:109:GLU:HB3	2:B:141:CYS:HB3	1.52	0.91
1:C:219:MET:HB3	1:C:256:ASN:ND2	1.84	0.91
1:C:92:ILE:HG21	1:C:115:ALA:O	1.71	0.91
1:C:92:ILE:HG13	1:C:115:ALA:HA	1.51	0.90
1:C:237:PRO:HA	1:C:240:TYR:CZ	2.07	0.90
1:C:169:VAL:HA	1:C:172:LEU:HD13	1.53	0.90
2:B:102:ARG:HB3	2:B:126:ALA:HA	1.53	0.90
1:C:19:ASP:O	1:C:22:LEU:HB3	1.72	0.90
2:D:76:LEU:HB3	2:D:134:ILE:HG21	1.51	0.90
1:A:125:LEU:HD12	1:A:125:LEU:N	1.87	0.89
1:A:91:THR:O	1:A:95:ILE:HG12	1.70	0.89
1:C:169:VAL:HB	1:C:172:LEU:HD22	1.53	0.88
1:C:118:PHE:HB2	5:C:329:HOH:O	1.73	0.88
1:A:160:VAL:HG12	1:A:187:ILE:HB	1.52	0.88
1:C:59:PHE:O	1:C:63:MET:HG3	1.74	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:152:LEU:H	1:C:152:LEU:HD12	1.37	0.88
1:C:109:GLU:HB2	2:D:141:CYS:SG	2.13	0.87
2:B:41:ARG:HG3	2:D:48:LEU:HD22	1.56	0.87
2:D:111:ASN:ND2	2:D:114:CYS:H	1.72	0.87
1:C:151:ARG:HH11	1:C:155:LEU:HD11	1.39	0.87
1:A:219:MET:HB3	1:A:256:ASN:ND2	1.89	0.87
2:B:27:PHE:N	2:B:46:LEU:HD21	1.90	0.87
1:A:48:PHE:HE2	1:A:55:THR:HG23	1.38	0.86
1:C:228:THR:HA	1:C:266:PRO:HG2	1.57	0.86
2:D:78:ALA:HB3	2:D:81:ALA:HB2	1.58	0.86
1:C:285:TYR:HA	1:C:288:GLN:OE1	1.76	0.86
1:C:121:ASN:N	1:C:121:ASN:HD22	1.69	0.86
1:A:94:VAL:HG23	1:A:95:ILE:HD13	1.57	0.85
1:C:157:VAL:HG12	1:C:158:ALA:H	1.41	0.85
1:A:200:ASP:O	1:A:203:ASP:HB2	1.75	0.85
2:B:21:ILE:HB	2:B:57:ASP:HB2	1.58	0.85
2:B:41:ARG:HA	2:D:47:ASN:HB2	1.57	0.85
2:D:56:LYS:HD2	2:D:57:ASP:N	1.92	0.84
2:D:42:ILE:HA	2:D:60:LYS:O	1.76	0.84
1:C:207:ILE:HG13	1:C:208:ALA:H	1.38	0.84
1:C:248:VAL:HG12	1:C:249:LEU:H	1.43	0.84
1:C:109:GLU:HB3	5:C:419:HOH:O	1.77	0.84
1:A:183:ARG:HH21	1:A:183:ARG:HG3	1.43	0.83
1:C:104:MET:SD	1:C:112:ALA:HA	2.17	0.83
1:C:13:ASN:N	1:C:174:GLN:HE22	1.75	0.83
1:A:51:ALA:O	1:A:52:SER:HB2	1.76	0.83
1:A:54:ARG:HB2	4:A:1311:PCT:O3P	1.79	0.83
2:D:82:THR:CA	2:D:96:ARG:HH12	1.92	0.83
1:A:92:ILE:HG22	1:A:93:SER:N	1.94	0.83
1:C:264:LEU:HB3	1:C:288:GLN:CD	1.99	0.82
2:D:138:CYS:SG	2:D:141:CYS:HB2	2.19	0.82
2:D:29:LEU:C	2:D:30:LEU:HD13	2.00	0.82
2:B:70:GLN:H	2:B:70:GLN:NE2	1.77	0.82
1:C:183:ARG:HE	1:C:208:ALA:HB1	1.44	0.82
1:C:64:HIS:CD2	1:C:70:VAL:HG23	2.14	0.81
1:A:8:HIS:ND1	1:A:116:THR:HG22	1.95	0.81
1:C:109:GLU:OE1	1:C:132:ASN:HB2	1.81	0.81
1:A:10:ILE:HG13	1:A:11:SER:N	1.95	0.81
1:C:164:LYS:HB2	1:C:192:LEU:HA	1.62	0.81
2:B:137:LYS:HA	2:B:144:GLU:HA	1.63	0.81
1:A:138:THR:HG23	1:A:172:LEU:HA	1.63	0.81
1:C:264:LEU:HD11	1:C:284:TRP:HB3	1.63	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:104:ASP:O	2:D:106:VAL:HG23	1.82	0.80
1:A:116:THR:HA	1:A:119:SER:OG	1.82	0.80
2:B:70:GLN:H	2:B:70:GLN:HE21	1.29	0.80
1:A:243:VAL:HG13	1:A:244:LYS:H	1.47	0.80
1:C:91:THR:O	1:C:95:ILE:HG13	1.82	0.79
2:D:20:HIS:HB3	2:D:80:GLN:CG	2.12	0.79
1:C:142:LEU:HD23	1:C:145:ILE:CD1	2.12	0.79
2:B:141:CYS:O	2:B:143:LYS:HG2	1.82	0.79
2:D:146:SER:HB2	2:D:148:ASN:ND2	1.97	0.79
1:C:96:SER:O	1:C:122:VAL:HG11	1.83	0.79
1:C:218:VAL:O	1:C:222:VAL:HG13	1.82	0.79
1:C:48:PHE:HZ	1:C:52:SER:H	1.30	0.79
2:B:39:ASP:HA	2:D:55:ARG:HH22	1.47	0.79
1:A:3:PRO:CD	1:A:22:LEU:HD21	2.13	0.79
1:C:124:VAL:HG12	1:C:125:LEU:N	1.97	0.78
1:C:225:LEU:HB2	1:C:261:MET:SD	2.24	0.78
1:A:229:ARG:NH2	1:A:270:VAL:HG21	1.98	0.78
2:D:126:ALA:O	2:D:127:VAL:HG13	1.83	0.78
1:A:109:GLU:OE1	2:B:113:ASN:ND2	2.17	0.78
1:A:80:SER:O	1:A:84:LYS:HB2	1.82	0.78
1:C:108:GLN:NE2	2:D:115:ILE:HD12	1.99	0.78
1:A:20:LEU:HD12	1:A:179:PHE:HZ	1.46	0.78
1:C:132:ASN:OD1	2:D:143:LYS:NZ	2.16	0.78
1:C:105:ARG:HH11	1:C:167:ARG:HH12	1.29	0.77
2:B:141:CYS:O	2:B:143:LYS:N	2.17	0.77
2:D:15:GLY:HA2	2:D:64:THR:O	1.85	0.77
2:B:69:ASP:O	2:B:73:GLN:HG3	1.83	0.77
1:C:183:ARG:HA	1:C:208:ALA:HB3	1.66	0.77
2:D:96:ARG:HG3	2:D:97:PRO:HD2	1.65	0.77
2:B:30:LEU:HG	2:D:27:PHE:CZ	2.19	0.77
1:A:302:LEU:HD23	1:A:302:LEU:H	1.50	0.77
1:A:105:ARG:HB2	1:A:127:ALA:HB3	1.64	0.77
1:A:287:GLN:HE21	1:A:287:GLN:N	1.82	0.77
1:C:171:SER:O	1:C:174:GLN:HG3	1.85	0.77
1:A:81:LEU:HG	1:A:86:GLU:O	1.85	0.77
1:C:264:LEU:CD1	1:C:284:TRP:HB3	2.14	0.77
2:B:44:ILE:HD11	2:B:46:LEU:HD23	1.65	0.77
1:C:160:VAL:HG12	1:C:161:GLY:H	1.50	0.77
2:D:41:ARG:HB3	2:D:62:GLU:HB2	1.67	0.77
2:B:36:THR:HB	2:D:27:PHE:CD2	2.20	0.77
1:C:264:LEU:HD12	1:C:288:GLN:CB	2.15	0.77
1:A:38:LEU:O	1:A:38:LEU:HD23	1.84	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:43:VAL:HG12	1:C:99:VAL:HG12	1.67	0.76
2:B:30:LEU:HG	2:D:27:PHE:HZ	1.47	0.76
1:A:61:THR:HG22	1:A:65:ARG:HD2	1.67	0.76
1:C:56:ARG:HG2	1:C:56:ARG:NH2	1.99	0.76
1:C:44:ILE:HG13	1:C:101:ALA:HB3	1.68	0.76
1:C:56:ARG:HG2	1:C:56:ARG:HH21	1.50	0.76
1:C:146:GLN:HA	1:C:150:GLY:HA2	1.68	0.76
1:C:45:ALA:HB2	1:C:99:VAL:HG11	1.66	0.76
1:A:156:HIS:ND1	1:A:156:HIS:N	2.31	0.75
1:C:142:LEU:HD23	1:C:145:ILE:HD11	1.68	0.75
2:D:24:GLN:NE2	2:D:47:ASN:HD21	1.85	0.75
1:A:26:THR:HA	1:A:29:LYS:HE3	1.68	0.75
1:A:109:GLU:HG3	1:A:132:ASN:HB2	1.67	0.75
1:C:159:MET:CE	1:C:172:LEU:HD23	2.16	0.75
1:A:43:VAL:HA	1:A:69:SER:O	1.85	0.75
2:B:34:LYS:HB3	2:B:37:GLU:HB2	1.69	0.75
2:D:62:GLU:HG2	2:D:63:ASN:ND2	2.02	0.75
5:B:204:HOH:O	2:D:39:ASP:HA	1.85	0.75
2:D:119:GLU:O	2:D:121:VAL:HG13	1.86	0.75
1:A:166:GLY:HA2	1:A:231:GLN:NE2	2.01	0.75
2:B:76:LEU:H	2:B:76:LEU:CD2	2.00	0.75
1:A:2:ASN:CG	1:A:5:TYR:HB2	2.08	0.74
1:C:132:ASN:HA	1:C:170:HIS:ND1	2.01	0.74
1:C:20:LEU:C	1:C:24:LEU:HG	2.07	0.74
1:A:81:LEU:HD23	1:A:81:LEU:O	1.86	0.74
1:C:214:SER:HB2	1:C:216:GLU:HG3	1.69	0.74
1:C:149:GLN:HB2	5:C:326:HOH:O	1.87	0.74
1:C:270:VAL:HG13	1:C:271:ASP:N	2.01	0.74
2:B:45:GLY:HA3	2:B:48:LEU:HD11	1.68	0.74
2:B:75:ALA:CB	2:B:99:LEU:HD12	2.16	0.74
1:A:267:LEU:CD2	1:A:268:PRO:HA	2.16	0.74
1:C:245:ALA:HB2	1:C:272:GLU:OE1	1.87	0.74
1:A:48:PHE:CE2	1:A:55:THR:HG23	2.22	0.74
2:D:41:ARG:HB3	2:D:62:GLU:CB	2.17	0.74
1:C:152:LEU:N	1:C:152:LEU:HD12	2.03	0.74
1:C:228:THR:HA	1:C:266:PRO:CG	2.18	0.74
2:B:42:ILE:HB	2:D:46:LEU:HD21	1.70	0.74
1:A:231:GLN:HB3	1:A:234:ARG:HB2	1.69	0.73
1:C:174:GLN:O	1:C:178:LYS:HE2	1.87	0.73
1:A:2:ASN:ND2	1:A:5:TYR:HB2	2.03	0.73
1:C:146:GLN:HA	1:C:150:GLY:CA	2.18	0.73
1:C:187:ILE:HD13	1:C:215:ILE:CD1	2.19	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:269:ARG:HH12	1:A:275:THR:HA	1.53	0.73
1:A:59:PHE:HE2	1:A:300:LEU:HD21	1.54	0.73
1:C:296:ARG:C	1:C:300:LEU:HG	2.09	0.73
2:D:148:ASN:O	2:D:152:ALA:HB2	1.87	0.73
2:D:138:CYS:HB3	2:D:143:LYS:H	1.53	0.73
2:B:30:LEU:HD22	2:B:44:ILE:CD1	2.18	0.73
1:C:249:LEU:HG	1:C:254:LEU:CD1	2.17	0.73
1:A:4:LEU:HD12	1:A:302:LEU:HD12	1.70	0.72
2:B:44:ILE:HG23	2:D:44:ILE:CB	2.16	0.72
1:A:141:ASP:O	1:A:145:ILE:HG12	1.88	0.72
1:A:155:LEU:HD22	1:A:223:ASP:CG	2.10	0.72
1:C:308:LEU:O	1:C:308:LEU:HD13	1.89	0.72
1:A:237:PRO:HA	1:A:240:TYR:CD1	2.24	0.72
1:C:287:GLN:H	1:C:287:GLN:NE2	1.86	0.72
1:A:8:HIS:NE2	1:A:123:PRO:HA	2.03	0.72
1:C:151:ARG:HH11	1:C:155:LEU:CD1	2.03	0.72
1:C:158:ALA:HA	1:C:185:TYR:O	1.89	0.72
1:C:245:ALA:HB1	5:C:338:HOH:O	1.90	0.72
1:C:227:MET:O	1:C:266:PRO:HD3	1.89	0.72
1:C:310:LEU:N	1:C:310:LEU:HD12	2.05	0.72
1:C:44:ILE:CG1	1:C:101:ALA:HB3	2.20	0.72
1:C:169:VAL:CA	1:C:172:LEU:HD13	2.20	0.71
1:C:296:ARG:O	1:C:300:LEU:HG	1.90	0.71
2:D:135:ALA:HB1	2:D:145:PHE:O	1.89	0.71
1:C:226:TYR:CZ	1:C:266:PRO:HG3	2.24	0.71
1:C:66:LEU:HD11	1:C:297:GLN:HA	1.73	0.71
2:D:74:LEU:CG	2:D:97:PRO:HB3	2.18	0.71
1:C:163:LEU:HG	1:C:188:ALA:HB2	1.71	0.71
1:A:26:THR:HA	1:A:29:LYS:CE	2.21	0.71
2:D:29:LEU:O	2:D:30:LEU:HD13	1.90	0.71
2:B:85:ARG:HB2	2:B:85:ARG:NH2	2.05	0.71
1:C:285:TYR:HA	1:C:288:GLN:HB3	1.69	0.71
1:A:165:TYR:HE2	1:A:235:LEU:HD23	1.55	0.71
1:C:105:ARG:NH1	1:C:167:ARG:HH12	1.89	0.71
2:D:99:LEU:CD1	2:D:129:LYS:HE3	2.21	0.71
1:A:216:GLU:OE2	1:A:253:ASP:HA	1.89	0.71
1:A:280:THR:HB	1:A:281:PRO:CD	2.21	0.71
1:A:288:GLN:HG2	1:A:288:GLN:O	1.91	0.71
1:C:218:VAL:HG12	1:C:218:VAL:O	1.91	0.70
1:C:164:LYS:HD3	1:C:191:ALA:O	1.91	0.70
1:C:134:HIS:CE1	1:C:137:GLN:HB2	2.27	0.70
1:C:139:LEU:CA	1:C:142:LEU:HD12	2.21	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:20:LEU:O	1:C:24:LEU:HG	1.91	0.70
1:C:160:VAL:HG12	1:C:161:GLY:N	2.05	0.70
2:D:128:ARG:O	2:D:130:ARG:HG3	1.91	0.70
1:A:229:ARG:HH21	1:A:270:VAL:CG2	2.01	0.70
1:A:187:ILE:N	1:A:187:ILE:HD12	2.07	0.70
1:A:164:LYS:HA	1:A:195:PRO:CD	2.20	0.70
1:A:128:GLY:HA2	1:A:133:GLN:O	1.91	0.70
1:C:142:LEU:HA	1:C:145:ILE:CD1	2.22	0.70
1:A:230:VAL:O	1:A:232:LYS:N	2.24	0.70
1:C:111:ALA:O	1:C:114:LEU:HB3	1.91	0.69
1:C:195:PRO:O	1:C:199:LEU:HG	1.91	0.69
1:A:267:LEU:HD23	1:A:269:ARG:H	1.55	0.69
1:A:287:GLN:H	1:A:287:GLN:NE2	1.90	0.69
1:C:222:VAL:HG21	1:C:225:LEU:HD13	1.75	0.69
1:C:30:LEU:HD12	1:C:298:ALA:HA	1.74	0.69
2:D:138:CYS:O	2:D:142:GLU:HA	1.93	0.69
2:B:46:LEU:O	2:D:42:ILE:HG13	1.93	0.69
1:A:160:VAL:HG23	1:A:227:MET:SD	2.32	0.69
2:B:70:GLN:HA	2:B:73:GLN:OE1	1.93	0.69
1:C:133:GLN:O	1:C:167:ARG:HB2	1.92	0.69
2:B:75:ALA:HB2	2:B:97:PRO:O	1.92	0.69
1:C:124:VAL:CG1	1:C:125:LEU:N	2.55	0.69
1:A:2:ASN:HD22	1:A:306:ARG:CA	2.06	0.69
1:C:50:GLU:OE2	1:C:107:PRO:HA	1.93	0.69
1:C:11:SER:HA	1:C:133:GLN:OE1	1.92	0.69
1:A:9:ILE:HD13	1:A:125:LEU:HG	1.74	0.69
2:B:70:GLN:N	2:B:70:GLN:HE21	1.90	0.69
1:A:184:PHE:O	1:A:209:TRP:HA	1.93	0.69
2:D:12:ILE:H	2:D:12:ILE:HD13	1.58	0.69
2:D:105:ASN:HA	2:D:123:SER:O	1.92	0.69
1:C:169:VAL:HA	1:C:172:LEU:CD1	2.23	0.68
1:C:228:THR:HA	1:C:266:PRO:CD	2.23	0.68
1:C:248:VAL:HG12	1:C:249:LEU:N	2.07	0.68
1:C:112:ALA:C	1:C:114:LEU:H	1.97	0.68
1:C:132:ASN:N	5:C:419:HOH:O	2.27	0.68
1:A:153:ASP:OD1	1:A:179:PHE:HB3	1.92	0.68
1:C:124:VAL:CG1	1:C:125:LEU:H	2.06	0.68
1:A:49:PHE:HB2	1:A:107:PRO:HD2	1.76	0.68
1:A:160:VAL:HG12	1:A:187:ILE:HD13	1.76	0.68
1:A:2:ASN:ND2	1:A:306:ARG:HA	2.09	0.68
1:A:8:HIS:CE1	1:A:116:THR:HG22	2.29	0.68
1:C:9:ILE:HG21	1:C:125:LEU:HG	1.76	0.68

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:202:LEU:HB3	1:A:207:ILE:HB	1.75	0.68
1:A:287:GLN:H	1:A:287:GLN:HE21	1.42	0.68
1:A:255:HIS:CD2	1:A:255:HIS:H	2.11	0.68
1:C:159:MET:O	1:C:163:LEU:HD11	1.93	0.67
1:C:295:ALA:O	1:C:297:GLN:N	2.27	0.67
1:C:43:VAL:C	1:C:44:ILE:HD12	2.15	0.67
2:B:41:ARG:HD3	2:D:48:LEU:HD13	1.76	0.67
2:B:36:THR:HB	2:D:27:PHE:CE2	2.28	0.67
1:A:47:CYS:HB3	1:A:73:PHE:CZ	2.29	0.67
1:A:92:ILE:CG2	1:A:93:SER:N	2.58	0.67
1:C:250:ARG:HB2	1:C:252:SER:OG	1.94	0.67
1:C:262:LYS:HG3	1:C:282:HIS:HA	1.77	0.67
1:C:269:ARG:HD3	1:C:273:ILE:H	1.57	0.67
1:A:45:ALA:HB1	1:A:47:CYS:SG	2.35	0.67
1:C:42:LYS:HA	1:C:100:ASP:OD1	1.94	0.67
2:D:66:LEU:HD22	2:D:83:VAL:HG21	1.77	0.67
2:B:129:LYS:HE3	2:B:129:LYS:C	2.15	0.67
1:C:266:PRO:O	1:C:267:LEU:HB2	1.94	0.67
1:C:17:ARG:HG3	1:C:18:ASP:H	1.58	0.67
1:C:102:ILE:HD13	1:C:102:ILE:N	2.09	0.67
2:B:84:ASN:O	2:B:86:ILE:HG13	1.94	0.67
1:C:160:VAL:HG12	5:C:338:HOH:O	1.95	0.67
1:C:202:LEU:HA	1:C:205:LYS:NZ	2.10	0.67
1:C:223:ASP:C	1:C:261:MET:HG2	2.16	0.67
1:A:201:MET:HG2	1:A:205:LYS:HD2	1.77	0.67
2:B:50:SER:HA	2:B:56:LYS:HE2	1.75	0.67
1:A:29:LYS:HB2	1:A:29:LYS:HZ2	1.60	0.67
2:B:138:CYS:SG	5:B:221:HOH:O	2.53	0.67
1:C:114:LEU:HD13	1:C:114:LEU:C	2.15	0.66
1:C:29:LYS:HD3	1:C:310:LEU:HB2	1.77	0.66
1:C:20:LEU:CD1	1:C:20:LEU:H	2.02	0.66
1:A:110:GLY:HA2	1:A:129:ASP:OD1	1.96	0.66
2:B:69:ASP:HB3	2:B:70:GLN:HE21	1.59	0.66
1:C:112:ALA:O	1:C:114:LEU:N	2.28	0.66
2:B:62:GLU:C	2:B:64:THR:H	1.98	0.66
1:C:162:ASP:HB3	1:C:230:VAL:HA	1.76	0.66
1:C:231:GLN:H	1:C:231:GLN:NE2	1.93	0.66
2:B:30:LEU:HD22	2:B:44:ILE:HD13	1.78	0.66
2:D:34:LYS:HB3	2:D:37:GLU:OE1	1.95	0.66
1:C:222:VAL:HG23	1:C:261:MET:HG3	1.77	0.66
2:D:107:LEU:HD21	2:D:136:LEU:HD22	1.77	0.66
1:C:89:ALA:HB1	1:C:118:PHE:CG	2.30	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:ASN:N	1:A:306:ARG:O	2.26	0.66
2:D:132:ASN:ND2	2:D:133:ASP:H	1.93	0.66
1:A:229:ARG:HH22	1:A:232:LYS:HE3	1.59	0.66
1:A:5:TYR:C	1:A:7:LYS:H	1.98	0.66
1:A:138:THR:O	1:A:142:LEU:HG	1.96	0.66
1:C:151:ARG:NH1	1:C:155:LEU:HD21	2.11	0.66
1:A:158:ALA:HB2	1:A:222:VAL:CG1	2.17	0.66
2:B:17:VAL:HG13	2:B:59:ILE:O	1.95	0.66
1:A:99:VAL:HG23	1:A:101:ALA:H	1.61	0.66
1:C:132:ASN:HA	1:C:170:HIS:CE1	2.30	0.65
1:C:59:PHE:CD1	1:C:296:ARG:HD3	2.30	0.65
1:C:88:LEU:O	1:C:92:ILE:HG12	1.95	0.65
2:D:107:LEU:HD11	2:D:151:LEU:HD21	1.78	0.65
1:C:38:LEU:HD12	1:C:39:LEU:CD1	2.26	0.65
1:A:111:ALA:O	1:A:114:LEU:HB2	1.97	0.65
1:A:308:LEU:HD23	1:A:309:VAL:O	1.96	0.65
1:A:138:THR:OG1	1:A:171:SER:HB3	1.96	0.65
2:D:127:VAL:HG21	2:D:129:LYS:HZ2	1.61	0.65
1:A:284:TRP:CD1	1:A:287:GLN:HB2	2.31	0.65
1:C:237:PRO:HG3	1:C:240:TYR:OH	1.96	0.65
2:D:103:ILE:HB	2:D:125:PHE:N	2.07	0.65
2:B:30:LEU:HD12	2:B:35:LEU:HB2	1.78	0.65
1:A:183:ARG:NH2	1:A:208:ALA:O	2.29	0.65
1:C:100:ASP:O	1:C:122:VAL:HG13	1.96	0.65
1:A:293:ILE:O	1:A:297:GLN:HB2	1.97	0.65
2:D:125:PHE:CE2	2:D:138:CYS:HA	2.32	0.65
2:B:13:LYS:HG3	2:B:89:TYR:CE1	2.32	0.64
1:C:179:PHE:HD1	1:C:180:ASP:N	1.95	0.64
1:C:205:LYS:HD2	1:C:205:LYS:H	1.62	0.64
2:B:41:ARG:HA	2:D:47:ASN:CB	2.27	0.64
1:A:26:THR:HA	1:A:29:LYS:NZ	2.12	0.64
1:A:129:ASP:O	1:A:132:ASN:HB3	1.98	0.64
1:C:230:VAL:O	1:C:232:LYS:N	2.30	0.64
1:C:263:VAL:HB	1:C:283:ALA:HA	1.79	0.64
1:C:59:PHE:CE1	1:C:296:ARG:NH2	2.65	0.64
2:D:76:LEU:HB3	2:D:134:ILE:CG2	2.25	0.64
2:D:13:LYS:HA	2:D:88:ASN:HA	1.78	0.64
1:C:162:ASP:OD2	1:C:165:TYR:HB2	1.98	0.64
1:A:169:VAL:O	1:A:170:HIS:C	2.36	0.64
1:C:227:MET:SD	1:C:272:GLU:HB3	2.36	0.64
2:D:114:CYS:O	2:D:116:SER:N	2.30	0.64
1:A:25:ALA:O	1:A:29:LYS:HG3	1.97	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:269:ARG:NH1	1:A:275:THR:HA	2.12	0.64
2:D:103:ILE:CB	2:D:125:PHE:H	2.04	0.64
2:D:86:ILE:HG23	2:D:90:GLU:C	2.17	0.64
1:A:229:ARG:HH12	1:A:232:LYS:HG2	1.63	0.64
1:C:48:PHE:HZ	1:C:52:SER:N	1.96	0.64
1:A:292:GLY:O	1:A:293:ILE:C	2.35	0.64
1:A:40:LYS:O	1:A:42:LYS:N	2.31	0.64
1:C:144:THR:HA	1:C:147:GLU:HB2	1.80	0.63
1:C:157:VAL:O	1:C:185:TYR:HB2	1.98	0.63
1:A:134:HIS:HB2	1:A:167:ARG:HB2	1.80	0.63
2:B:53:MET:SD	2:B:54:GLY:N	2.71	0.63
1:C:11:SER:CB	1:C:133:GLN:HG3	2.27	0.63
2:D:135:ALA:HA	2:D:147:HIS:H	1.63	0.63
1:C:274:ALA:O	1:C:277:VAL:HG23	1.98	0.63
1:C:171:SER:HA	1:C:174:GLN:HG2	1.80	0.63
2:D:48:LEU:HB2	2:D:56:LYS:HZ2	1.61	0.63
2:B:68:GLU:HA	2:B:71:VAL:CG2	2.27	0.63
1:C:183:ARG:NE	1:C:208:ALA:HB1	2.13	0.63
2:B:38:THR:HG23	2:B:42:ILE:HD11	1.81	0.63
2:B:39:ASP:O	2:D:47:ASN:HB3	1.98	0.63
1:A:23:VAL:HA	1:A:302:LEU:HD11	1.81	0.63
1:A:125:LEU:CD1	1:A:125:LEU:N	2.60	0.63
1:A:113:ARG:HH22	2:B:139:LYS:HB2	1.62	0.63
2:B:86:ILE:HG12	2:B:91:VAL:HA	1.80	0.63
1:C:5:TYR:HA	1:C:303:VAL:HA	1.81	0.63
1:A:223:ASP:O	1:A:261:MET:HA	1.99	0.62
2:D:46:LEU:H	2:D:46:LEU:CD2	2.09	0.62
2:B:34:LYS:C	2:B:36:THR:H	2.01	0.62
2:B:39:ASP:CA	2:D:55:ARG:HH22	2.12	0.62
2:D:56:LYS:HE2	2:D:58:LEU:HB3	1.81	0.62
1:A:134:HIS:CE1	1:A:136:THR:OG1	2.52	0.62
1:A:176:LEU:HD12	1:A:184:PHE:CZ	2.34	0.62
2:D:72:ASP:HA	2:D:98:SER:O	2.00	0.62
2:D:48:LEU:HB2	2:D:56:LYS:NZ	2.14	0.62
2:B:71:VAL:HG23	5:B:190:HOH:O	2.00	0.62
1:C:187:ILE:HD13	1:C:215:ILE:HD13	1.79	0.62
2:D:44:ILE:HG22	2:D:45:GLY:H	1.63	0.62
1:A:235:LEU:HB3	1:A:240:TYR:CE2	2.35	0.62
1:A:59:PHE:CE1	1:A:296:ARG:HG2	2.34	0.62
2:D:110:PRO:HD3	2:D:150:VAL:HG13	1.81	0.62
2:D:128:ARG:NH1	2:D:130:ARG:HD2	2.15	0.62
1:C:103:VAL:HA	1:C:125:LEU:O	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:201:MET:CG	1:A:205:LYS:HD2	2.30	0.62
1:A:205:LYS:C	1:A:207:ILE:H	2.03	0.62
1:A:306:ARG:HG3	1:A:307:ASP:N	2.14	0.62
1:A:111:ALA:HA	2:B:115:ILE:HG21	1.81	0.62
2:B:129:LYS:HZ1	2:B:131:ALA:N	1.98	0.62
1:C:306:ARG:NH2	1:C:306:ARG:HB3	2.14	0.62
1:C:306:ARG:HG3	1:C:307:ASP:H	1.65	0.62
2:B:104:ASP:O	2:B:106:VAL:HG22	1.98	0.62
1:C:105:ARG:NH1	1:C:167:ARG:NH1	2.48	0.62
1:A:5:TYR:O	1:A:7:LYS:N	2.32	0.62
1:A:161:GLY:O	1:A:163:LEU:HG	2.00	0.62
1:A:40:LYS:HA	1:A:67:GLY:O	2.00	0.62
1:C:265:HIS:ND1	1:C:266:PRO:HD2	2.15	0.62
1:C:23:VAL:HG11	1:C:299:LEU:HD12	1.81	0.61
1:C:264:LEU:HD22	1:C:264:LEU:N	2.14	0.61
2:B:40:GLN:HB3	2:B:63:ASN:HD22	1.65	0.61
1:A:186:PHE:O	1:A:211:LEU:HD23	1.99	0.61
1:A:77:ALA:O	1:A:79:THR:N	2.28	0.61
1:C:65:ARG:NE	5:C:351:HOH:O	2.33	0.61
2:D:137:LYS:HE3	2:D:142:GLU:OE2	1.99	0.61
2:B:20:HIS:NE2	2:B:52:GLU:CD	2.54	0.61
1:C:144:THR:HG21	1:C:288:GLN:HA	1.83	0.61
2:D:73:GLN:O	2:D:77:TYR:HB2	2.00	0.61
1:C:306:ARG:CB	1:C:306:ARG:HH21	2.14	0.61
1:C:149:GLN:CB	1:C:151:ARG:HH12	2.13	0.61
1:C:284:TRP:HD1	1:C:288:GLN:HB2	1.64	0.61
1:C:303:VAL:HG12	1:C:303:VAL:O	2.01	0.61
2:D:81:ALA:O	2:D:97:PRO:HD3	2.01	0.61
1:A:145:ILE:HG23	1:A:224:ILE:CD1	2.26	0.61
1:C:104:MET:HG3	1:C:126:ASN:HB2	1.81	0.61
2:D:99:LEU:HD22	2:D:99:LEU:O	2.01	0.61
1:A:53:THR:O	1:A:57:LEU:HD12	1.99	0.61
2:B:50:SER:OG	2:B:53:MET:HB3	2.00	0.61
1:C:9:ILE:HB	1:C:125:LEU:CA	2.27	0.61
2:B:44:ILE:O	2:D:44:ILE:HG12	2.01	0.61
2:D:138:CYS:HB3	2:D:143:LYS:N	2.15	0.61
1:C:176:LEU:C	1:C:178:LYS:H	2.05	0.60
2:D:103:ILE:HD11	2:D:127:VAL:HG22	1.81	0.60
1:A:284:TRP:HA	1:A:287:GLN:NE2	2.16	0.60
1:A:183:ARG:NH2	1:A:183:ARG:HG3	2.10	0.60
1:A:138:THR:CG2	1:A:172:LEU:HA	2.31	0.60
1:C:269:ARG:NE	1:C:273:ILE:HB	2.15	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:267:LEU:HD21	1:A:269:ARG:HG2	1.82	0.60
1:C:56:ARG:HH21	1:C:56:ARG:C	2.04	0.60
1:C:36:PRO:O	1:C:38:LEU:N	2.35	0.60
1:C:125:LEU:HD23	1:C:125:LEU:O	2.01	0.60
1:A:245:ALA:HB2	1:A:271:ASP:OD2	2.00	0.60
1:C:162:ASP:OD1	1:C:192:LEU:HD22	2.01	0.60
1:C:215:ILE:CG2	1:C:219:MET:HE2	2.31	0.60
1:C:54:ARG:NH2	1:C:267:LEU:HD12	2.17	0.60
1:A:291:ASN:HB2	5:A:1344:HOH:O	2.00	0.60
1:A:138:THR:HG23	1:A:172:LEU:CD1	2.31	0.60
2:B:105:ASN:C	2:B:106:VAL:HG22	2.20	0.60
1:C:219:MET:HB3	1:C:256:ASN:CG	2.20	0.60
2:B:27:PHE:HB2	2:D:36:THR:HG21	1.82	0.60
1:A:49:PHE:CB	1:A:107:PRO:HD2	2.31	0.60
1:A:39:LEU:HD13	1:A:304:LEU:HD12	1.83	0.60
1:C:140:LEU:C	1:C:140:LEU:HD12	2.21	0.60
2:D:28:LYS:HE2	2:D:32:LEU:HB2	1.82	0.60
1:C:17:ARG:HG3	1:C:18:ASP:N	2.16	0.60
1:A:160:VAL:HG12	1:A:187:ILE:CB	2.31	0.60
1:A:4:LEU:O	1:A:7:LYS:HB2	2.00	0.60
1:C:38:LEU:HD12	1:C:39:LEU:HG	1.83	0.60
1:C:162:ASP:CB	1:C:230:VAL:HA	2.31	0.60
2:D:149:VAL:HA	2:D:152:ALA:HB3	1.83	0.60
1:C:199:LEU:O	1:C:202:LEU:HG	2.01	0.60
1:C:189:PRO:HG3	1:C:246:GLN:OE1	2.02	0.60
2:D:83:VAL:O	2:D:94:LYS:HA	2.01	0.60
1:C:183:ARG:NH2	1:C:184:PHE:O	2.34	0.60
1:C:270:VAL:CG1	1:C:271:ASP:H	2.04	0.60
2:D:30:LEU:N	2:D:30:LEU:HD22	2.16	0.60
2:B:42:ILE:HB	2:D:46:LEU:CD2	2.31	0.60
1:A:267:LEU:HD23	1:A:269:ARG:N	2.16	0.60
1:C:214:SER:HB2	1:C:216:GLU:OE2	2.02	0.60
2:B:105:ASN:OD1	2:B:105:ASN:O	2.18	0.60
2:B:105:ASN:O	2:B:106:VAL:HG13	2.01	0.60
2:B:22:PRO:O	2:B:25:ILE:HB	2.02	0.60
1:C:13:ASN:N	1:C:174:GLN:NE2	2.48	0.59
1:A:119:SER:OG	1:A:120:GLY:N	2.35	0.59
2:B:21:ILE:CD1	2:B:59:ILE:HG12	2.32	0.59
1:C:195:PRO:HG2	1:C:198:ILE:HG12	1.82	0.59
2:D:138:CYS:SG	2:D:141:CYS:N	2.75	0.59
1:A:176:LEU:HD12	1:A:184:PHE:HZ	1.68	0.59
1:C:228:THR:CA	1:C:266:PRO:HG2	2.30	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:30:LEU:CD1	1:C:298:ALA:HA	2.33	0.59
1:A:166:GLY:HA2	1:A:231:GLN:HE22	1.66	0.59
2:B:21:ILE:HB	2:B:57:ASP:CB	2.30	0.59
1:A:172:LEU:O	1:A:176:LEU:HG	2.02	0.59
1:A:172:LEU:O	1:A:175:ALA:HB3	2.03	0.59
1:C:214:SER:HB2	1:C:216:GLU:CG	2.31	0.59
1:C:45:ALA:HB1	1:C:72:GLY:H	1.68	0.59
2:D:125:PHE:CD2	2:D:138:CYS:HA	2.38	0.59
1:A:306:ARG:HG3	1:A:307:ASP:H	1.66	0.59
1:A:48:PHE:CE2	1:A:56:ARG:HB2	2.36	0.59
1:A:55:THR:HG21	1:A:105:ARG:HH11	1.68	0.59
1:C:56:ARG:CG	1:C:56:ARG:HH21	2.16	0.59
1:C:220:ALA:N	1:C:256:ASN:ND2	2.50	0.59
1:C:89:ALA:HA	5:C:329:HOH:O	2.02	0.59
1:C:92:ILE:HA	1:C:95:ILE:HB	1.85	0.59
2:D:99:LEU:HD13	2:D:129:LYS:HE3	1.85	0.59
1:A:229:ARG:HG3	1:A:270:VAL:HG23	1.85	0.59
1:A:44:ILE:CG2	1:A:103:VAL:HG23	2.33	0.59
2:B:16:THR:HG22	2:B:17:VAL:N	2.18	0.59
1:C:142:LEU:HA	1:C:145:ILE:HG13	1.85	0.59
1:C:141:ASP:O	1:C:144:THR:N	2.36	0.59
1:C:269:ARG:HD2	1:C:270:VAL:N	2.18	0.59
1:A:23:VAL:HG22	1:A:302:LEU:CD1	2.33	0.59
1:A:140:LEU:HD13	1:A:288:GLN:O	2.03	0.59
2:D:75:ALA:HA	2:D:97:PRO:HB2	1.85	0.58
1:A:235:LEU:CB	1:A:240:TYR:HE2	2.16	0.58
1:C:131:SER:N	5:C:419:HOH:O	2.36	0.58
1:C:136:THR:HB	1:C:296:ARG:NH2	2.18	0.58
2:B:30:LEU:HD22	2:B:44:ILE:HD12	1.84	0.58
1:A:29:LYS:HB2	1:A:29:LYS:NZ	2.18	0.58
1:A:49:PHE:HB2	1:A:106:HIS:HA	1.84	0.58
1:C:215:ILE:HG22	1:C:219:MET:HE2	1.84	0.58
1:A:264:LEU:HD22	1:A:288:GLN:HG3	1.86	0.58
1:A:284:TRP:O	1:A:288:GLN:N	2.33	0.58
2:D:84:ASN:ND2	2:D:91:VAL:HG11	2.17	0.58
1:A:30:LEU:C	1:A:32:ALA:N	2.56	0.58
2:B:62:GLU:HG2	2:B:63:ASN:N	2.18	0.58
2:B:44:ILE:O	2:D:44:ILE:N	2.36	0.58
1:A:146:GLN:HE21	1:A:152:LEU:CB	2.16	0.58
2:D:115:ILE:C	2:D:117:HIS:H	2.07	0.58
1:A:164:LYS:CA	1:A:195:PRO:HD3	2.26	0.58
1:C:282:HIS:O	1:C:284:TRP:N	2.37	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:144:THR:CG2	1:C:288:GLN:HA	2.34	0.58
1:C:113:ARG:HA	1:C:116:THR:OG1	2.04	0.58
2:D:111:ASN:ND2	2:D:114:CYS:N	2.49	0.58
2:B:102:ARG:HA	2:B:127:VAL:HG23	1.85	0.58
2:D:66:LEU:HD13	2:D:83:VAL:HG21	1.84	0.58
1:C:179:PHE:CD1	1:C:180:ASP:N	2.72	0.58
1:C:121:ASN:ND2	1:C:121:ASN:H	1.94	0.58
2:B:69:ASP:HB3	2:B:70:GLN:NE2	2.19	0.58
2:D:12:ILE:HG23	2:D:41:ARG:NH2	2.19	0.58
1:A:124:VAL:C	1:A:125:LEU:HD12	2.24	0.58
2:B:18:ILE:HB	2:B:21:ILE:HD11	1.85	0.57
1:C:134:HIS:HB2	1:C:167:ARG:O	2.04	0.57
1:C:152:LEU:HB2	1:C:179:PHE:CZ	2.39	0.57
2:D:126:ALA:HB3	2:D:137:LYS:O	2.04	0.57
1:A:2:ASN:HD22	1:A:306:ARG:C	2.08	0.57
1:C:184:PHE:HB2	1:C:209:TRP:HA	1.87	0.57
1:A:296:ARG:O	1:A:300:LEU:HG	2.03	0.57
1:A:308:LEU:HD23	1:A:309:VAL:N	2.19	0.57
1:C:151:ARG:HH11	1:C:155:LEU:CG	2.16	0.57
1:C:237:PRO:CA	1:C:240:TYR:CZ	2.85	0.57
2:B:50:SER:HB3	2:B:53:MET:C	2.25	0.57
1:C:112:ALA:C	1:C:114:LEU:N	2.57	0.57
1:C:188:ALA:O	1:C:193:ALA:HB2	2.04	0.57
1:C:4:LEU:HB3	1:C:22:LEU:CD2	2.35	0.57
1:C:23:VAL:HG12	1:C:302:LEU:HD12	1.85	0.57
1:A:177:ALA:HB2	1:A:202:LEU:HD23	1.86	0.57
1:C:207:ILE:HG13	1:C:208:ALA:N	2.16	0.57
1:C:66:LEU:HD11	1:C:297:GLN:CA	2.34	0.57
2:D:143:LYS:HB2	2:D:145:PHE:CE1	2.39	0.57
2:B:62:GLU:HG2	2:B:63:ASN:H	1.69	0.57
2:D:16:THR:HG22	2:D:65:PHE:HA	1.86	0.57
1:A:26:THR:HG21	1:A:302:LEU:HD21	1.85	0.57
1:C:115:ALA:HA	5:C:329:HOH:O	2.05	0.57
1:C:171:SER:HA	1:C:174:GLN:CG	2.35	0.57
1:C:89:ALA:HB1	1:C:118:PHE:CD2	2.40	0.57
2:D:103:ILE:HD11	2:D:127:VAL:HG13	1.85	0.57
2:D:114:CYS:C	2:D:116:SER:H	2.08	0.57
1:A:288:GLN:C	5:A:1344:HOH:O	2.43	0.57
1:C:237:PRO:O	1:C:239:GLU:N	2.38	0.57
1:A:204:GLU:C	1:A:206:GLY:H	2.08	0.57
1:C:44:ILE:CD1	1:C:101:ALA:HB3	2.34	0.57
1:A:189:PRO:HB3	1:A:242:ASN:ND2	2.18	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:114:LEU:HD13	5:C:329:HOH:O	2.05	0.56
1:C:254:LEU:O	1:C:256:ASN:N	2.35	0.56
2:D:128:ARG:HH12	2:D:130:ARG:CZ	2.19	0.56
1:A:163:LEU:HD13	1:A:194:MET:HB2	1.87	0.56
1:A:183:ARG:NE	1:A:208:ALA:HB3	2.20	0.56
1:C:149:GLN:HB3	1:C:151:ARG:HH12	1.69	0.56
1:C:127:ALA:HA	1:C:135:PRO:HD2	1.86	0.56
1:C:180:ASP:O	1:C:182:ASN:OD1	2.24	0.56
1:A:160:VAL:CG1	1:A:187:ILE:HB	2.30	0.56
1:A:3:PRO:CG	1:A:22:LEU:HD21	2.35	0.56
1:A:55:THR:HG21	1:A:105:ARG:HE	1.70	0.56
1:A:138:THR:HG23	1:A:172:LEU:HD13	1.88	0.56
2:B:52:GLU:CD	2:B:52:GLU:H	2.09	0.56
2:B:128:ARG:O	2:B:134:ILE:HG22	2.04	0.56
1:C:29:LYS:CD	1:C:310:LEU:HB2	2.36	0.56
1:C:67:GLY:O	1:C:68:ALA:HB2	2.05	0.56
1:C:3:PRO:O	1:C:7:LYS:HD3	2.05	0.56
2:D:125:PHE:CD1	2:D:136:LEU:HD13	2.40	0.56
1:A:285:TYR:HA	1:A:288:GLN:OE1	2.06	0.56
1:C:237:PRO:C	1:C:239:GLU:H	2.09	0.56
1:C:103:VAL:HG13	1:C:125:LEU:CD2	2.35	0.56
1:C:155:LEU:HD13	1:C:224:ILE:HD11	1.87	0.56
1:A:248:VAL:HG13	1:A:271:ASP:O	2.05	0.56
1:C:75:ASP:C	1:C:77:ALA:H	2.09	0.56
1:C:131:SER:O	1:C:170:HIS:CE1	2.58	0.56
2:B:30:LEU:HD12	2:B:35:LEU:CB	2.35	0.56
1:A:165:TYR:HB3	1:A:231:GLN:HG2	1.86	0.56
1:C:207:ILE:HG23	1:C:208:ALA:N	2.20	0.56
1:C:9:ILE:CG2	1:C:125:LEU:HG	2.35	0.56
1:A:5:TYR:C	1:A:7:LYS:N	2.58	0.56
1:C:104:MET:HG3	1:C:126:ASN:CB	2.35	0.56
1:C:171:SER:C	1:C:174:GLN:HG3	2.25	0.56
1:C:60:GLU:CA	1:C:63:MET:SD	2.90	0.56
2:D:137:LYS:HD2	2:D:142:GLU:O	2.06	0.56
2:D:96:ARG:NH2	2:D:97:PRO:HD2	2.21	0.56
2:B:38:THR:CG2	2:B:42:ILE:HD11	2.34	0.56
2:B:12:ILE:HG12	2:B:13:LYS:N	2.20	0.56
1:C:104:MET:CE	1:C:112:ALA:HA	2.36	0.56
1:C:113:ARG:O	1:C:117:GLU:HG3	2.06	0.56
1:C:44:ILE:HD11	1:C:101:ALA:HB3	1.88	0.56
2:D:24:GLN:NE2	2:D:47:ASN:ND2	2.54	0.56
1:A:94:VAL:HG23	1:A:95:ILE:N	2.19	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:ASN:HD22	1:A:306:ARG:HA	1.67	0.56
1:A:113:ARG:HG2	1:A:113:ARG:HH21	1.70	0.56
1:A:78:ASN:N	1:A:78:ASN:HD22	2.04	0.56
1:C:135:PRO:HG2	1:C:136:THR:H	1.70	0.55
1:C:273:ILE:HG21	1:C:285:TYR:OH	2.06	0.55
2:D:138:CYS:HB3	2:D:142:GLU:N	2.21	0.55
1:A:287:GLN:NE2	1:A:287:GLN:N	2.50	0.55
1:C:253:ASP:OD1	1:C:254:LEU:HD12	2.05	0.55
1:A:196:GLN:C	1:A:198:ILE:H	2.09	0.55
1:A:5:TYR:CE1	1:A:306:ARG:HB3	2.41	0.55
1:A:54:ARG:HH12	1:A:268:PRO:HB3	1.71	0.55
1:A:146:GLN:HE21	1:A:152:LEU:HG	1.70	0.55
1:C:228:THR:HA	1:C:266:PRO:HD2	1.88	0.55
2:D:126:ALA:HB3	2:D:137:LYS:HB3	1.88	0.55
1:A:20:LEU:HD12	1:A:179:PHE:CZ	2.36	0.55
2:B:50:SER:HB3	2:B:53:MET:O	2.06	0.55
1:C:104:MET:CG	1:C:126:ASN:HB2	2.35	0.55
1:C:178:LYS:HZ3	1:C:201:MET:CE	2.20	0.55
2:D:137:LYS:HD2	2:D:142:GLU:HG3	1.87	0.55
2:D:15:GLY:HA3	2:D:61:ILE:O	2.05	0.55
2:D:84:ASN:O	2:D:86:ILE:HD12	2.06	0.55
1:C:219:MET:CB	1:C:256:ASN:HD21	2.09	0.55
1:C:46:SER:O	1:C:72:GLY:HA3	2.07	0.55
1:A:166:GLY:O	1:A:167:ARG:C	2.45	0.55
1:C:192:LEU:C	1:C:194:MET:H	2.11	0.55
1:C:226:TYR:OH	1:C:266:PRO:HG3	2.06	0.55
1:C:30:LEU:HD12	1:C:298:ALA:CA	2.36	0.55
2:D:67:SER:O	2:D:71:VAL:HG23	2.07	0.55
1:C:129:ASP:O	5:C:419:HOH:O	2.18	0.55
1:C:11:SER:HB2	1:C:133:GLN:HG3	1.88	0.55
1:C:9:ILE:HG22	1:C:135:PRO:HG3	1.89	0.55
1:C:141:ASP:C	1:C:143:PHE:N	2.59	0.55
2:D:103:ILE:HD11	2:D:127:VAL:CG2	2.37	0.55
2:B:41:ARG:HB2	2:D:47:ASN:O	2.07	0.55
2:D:59:ILE:HD12	2:D:59:ILE:N	2.22	0.55
1:A:59:PHE:O	1:A:63:MET:HE2	2.06	0.55
2:B:137:LYS:HA	2:B:143:LYS:O	2.07	0.55
2:D:105:ASN:O	2:D:106:VAL:HG22	2.07	0.55
1:C:306:ARG:CG	1:C:307:ASP:H	2.19	0.55
1:C:280:THR:C	1:C:282:HIS:H	2.11	0.55
2:D:124:SER:HB2	2:D:139:LYS:HD3	1.89	0.55
2:D:127:VAL:CG2	2:D:129:LYS:HZ2	2.19	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:31:SER:HA	2:D:27:PHE:HE1	1.72	0.55
2:B:9:VAL:HG13	2:B:43:THR:HG21	1.88	0.54
1:A:208:ALA:HA	5:A:1437:HOH:O	2.06	0.54
1:A:146:GLN:NE2	1:A:152:LEU:HG	2.22	0.54
1:C:142:LEU:HD23	1:C:145:ILE:HD12	1.88	0.54
1:C:148:THR:HB	5:C:331:HOH:O	2.08	0.54
1:C:151:ARG:NH2	1:C:151:ARG:HB3	2.22	0.54
1:C:152:LEU:CD1	1:C:152:LEU:H	2.14	0.54
2:D:108:VAL:HG23	2:D:150:VAL:O	2.07	0.54
1:A:235:LEU:HB3	1:A:240:TYR:HE2	1.72	0.54
1:C:237:PRO:HA	1:C:240:TYR:CD2	2.41	0.54
1:C:131:SER:HA	1:C:167:ARG:HB3	1.88	0.54
1:C:160:VAL:CG1	1:C:161:GLY:H	2.20	0.54
1:C:269:ARG:CD	1:C:273:ILE:HB	2.37	0.54
1:C:26:THR:HA	1:C:29:LYS:HG2	1.88	0.54
2:D:30:LEU:O	2:D:34:LYS:HA	2.07	0.54
1:A:10:ILE:HG13	1:A:11:SER:H	1.72	0.54
1:A:168:THR:OG1	1:A:169:VAL:N	2.40	0.54
1:A:92:ILE:HG22	1:A:93:SER:H	1.67	0.54
1:A:155:LEU:HD22	1:A:223:ASP:OD2	2.06	0.54
2:B:85:ARG:HB2	2:B:85:ARG:HH21	1.71	0.54
2:D:122:SER:HB3	5:D:170:HOH:O	2.07	0.54
1:C:103:VAL:HG13	1:C:125:LEU:O	2.05	0.54
1:A:8:HIS:ND1	1:A:116:THR:CG2	2.67	0.54
1:C:167:ARG:NH1	1:C:234:ARG:HH12	2.06	0.54
2:D:74:LEU:HD11	2:D:81:ALA:HB1	1.90	0.54
1:C:20:LEU:N	1:C:20:LEU:HD12	2.08	0.54
2:D:13:LYS:CA	2:D:88:ASN:HA	2.37	0.54
2:D:127:VAL:HG12	2:D:136:LEU:HB3	1.88	0.54
2:D:46:LEU:N	2:D:46:LEU:HD23	2.11	0.54
1:A:59:PHE:HD2	1:A:63:MET:HE2	1.71	0.54
2:B:62:GLU:O	2:B:64:THR:N	2.40	0.54
1:A:47:CYS:HB3	1:A:73:PHE:CE2	2.42	0.54
1:C:103:VAL:HG13	1:C:125:LEU:HD23	1.89	0.54
1:C:153:ASP:CG	1:C:179:PHE:HE1	2.11	0.54
2:D:125:PHE:CE1	2:D:136:LEU:HD13	2.43	0.54
2:D:99:LEU:HD11	2:D:129:LYS:HE3	1.89	0.54
2:D:44:ILE:HD13	2:D:44:ILE:N	2.23	0.54
1:A:177:ALA:HB2	1:A:202:LEU:CD2	2.38	0.54
2:B:13:LYS:O	2:B:88:ASN:N	2.41	0.54
1:C:105:ARG:NH1	1:C:167:ARG:HH22	2.06	0.54
2:D:103:ILE:HG21	2:D:125:PHE:HB2	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:9:VAL:HG13	2:B:43:THR:CG2	2.38	0.54
2:B:27:PHE:HE1	2:D:34:LYS:HZ2	1.55	0.54
1:A:174:GLN:HG2	1:A:198:ILE:HG23	1.90	0.54
1:A:177:ALA:CB	1:A:202:LEU:HD23	2.37	0.54
1:A:129:ASP:CG	1:A:132:ASN:HD22	2.11	0.54
1:A:139:LEU:O	1:A:142:LEU:HB2	2.07	0.54
1:C:81:LEU:HA	1:C:86:GLU:HB2	1.90	0.54
1:C:153:ASP:HA	1:C:179:PHE:CE1	2.43	0.54
2:D:111:ASN:ND2	2:D:114:CYS:CB	2.63	0.54
2:B:47:ASN:HB2	2:D:42:ILE:HD11	1.88	0.54
2:D:87:ASP:O	2:D:88:ASN:HB3	2.07	0.54
1:C:82:GLY:O	1:C:83:LYS:C	2.47	0.54
2:D:99:LEU:HD22	2:D:129:LYS:NZ	2.22	0.53
1:A:280:THR:HB	1:A:281:PRO:HD2	1.89	0.53
1:A:109:GLU:O	2:B:115:ILE:HG22	2.08	0.53
1:C:96:SER:HB2	1:C:122:VAL:HB	1.90	0.53
1:C:265:HIS:N	1:C:288:GLN:OE1	2.39	0.53
2:B:129:LYS:NZ	2:B:130:ARG:N	2.57	0.53
2:B:38:THR:HG21	2:B:61:ILE:HD11	1.91	0.53
1:A:225:LEU:HD12	1:A:226:TYR:N	2.23	0.53
1:A:10:ILE:CG1	1:A:11:SER:N	2.68	0.53
1:A:165:TYR:C	1:A:231:GLN:HE21	2.11	0.53
2:D:90:GLU:OE1	2:D:92:VAL:HG22	2.08	0.53
1:C:306:ARG:HG3	1:C:307:ASP:N	2.24	0.53
1:C:49:PHE:HB2	1:C:105:ARG:O	2.09	0.53
1:C:44:ILE:O	1:C:70:VAL:HA	2.08	0.53
1:A:2:ASN:ND2	1:A:305:ASN:O	2.41	0.53
1:A:54:ARG:NH1	1:A:268:PRO:HB3	2.24	0.53
1:C:92:ILE:HG22	1:C:118:PHE:O	2.09	0.53
1:C:45:ALA:CB	1:C:99:VAL:HG11	2.38	0.53
1:A:251:ALA:O	1:A:253:ASP:N	2.42	0.53
1:A:20:LEU:O	1:A:22:LEU:N	2.41	0.53
2:B:111:ASN:OD1	2:B:114:CYS:N	2.41	0.53
1:C:162:ASP:OD2	1:C:231:GLN:HB2	2.09	0.53
1:A:284:TRP:HA	1:A:287:GLN:CD	2.28	0.53
1:A:95:ILE:N	1:A:95:ILE:HD13	2.23	0.53
1:C:145:ILE:HA	5:C:320:HOH:O	2.09	0.53
1:C:4:LEU:HD21	1:C:299:LEU:CD1	2.39	0.53
1:C:64:HIS:NE2	1:C:70:VAL:HG23	2.24	0.53
1:A:113:ARG:HB3	2:B:140:TYR:HD1	1.74	0.53
2:D:83:VAL:O	2:D:83:VAL:HG13	2.09	0.53
1:C:262:LYS:O	1:C:264:LEU:HD22	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:130:ARG:C	2:D:132:ASN:H	2.12	0.53
2:D:28:LYS:O	2:D:30:LEU:N	2.42	0.53
2:D:41:ARG:HB3	2:D:62:GLU:HB3	1.90	0.53
2:D:9:VAL:C	2:D:11:ALA:H	2.12	0.53
1:C:106:HIS:ND1	1:C:108:GLN:OE1	2.37	0.53
1:A:169:VAL:HG23	1:A:170:HIS:HD2	1.74	0.53
1:A:287:GLN:O	5:A:1344:HOH:O	2.19	0.53
1:C:250:ARG:O	1:C:251:ALA:C	2.47	0.53
2:D:132:ASN:ND2	2:D:133:ASP:OD1	2.42	0.53
2:D:41:ARG:H	2:D:62:GLU:HB3	1.74	0.53
2:B:141:CYS:N	5:B:221:HOH:O	2.15	0.53
2:B:129:LYS:HZ1	2:B:130:ARG:C	2.12	0.53
1:C:178:LYS:NZ	1:C:201:MET:CE	2.73	0.52
2:D:137:LYS:CE	2:D:142:GLU:HG3	2.39	0.52
1:A:49:PHE:HA	1:A:76:SER:HB2	1.90	0.52
1:A:309:VAL:HG22	5:A:1403:HOH:O	2.08	0.52
1:C:184:PHE:HB3	1:C:186:PHE:CE1	2.44	0.52
1:C:231:GLN:H	1:C:231:GLN:HE21	1.57	0.52
1:C:136:THR:CB	1:C:296:ARG:NH2	2.72	0.52
1:A:229:ARG:CG	1:A:270:VAL:HG23	2.39	0.52
1:A:2:ASN:ND2	1:A:5:TYR:CG	2.77	0.52
1:A:278:ASP:HA	1:A:285:TYR:OH	2.09	0.52
2:B:17:VAL:HG13	2:B:60:LYS:HG2	1.91	0.52
1:A:146:GLN:HG2	1:A:152:LEU:HB3	1.90	0.52
1:C:219:MET:HB3	1:C:256:ASN:OD1	2.08	0.52
2:D:107:LEU:HD21	2:D:136:LEU:CD2	2.39	0.52
2:D:124:SER:O	2:D:139:LYS:HB3	2.09	0.52
2:D:24:GLN:HE21	2:D:47:ASN:HD21	1.58	0.52
1:A:287:GLN:HG2	5:A:1326:HOH:O	2.09	0.52
2:B:128:ARG:HD3	5:B:201:HOH:O	2.09	0.52
1:C:155:LEU:HD13	1:C:224:ILE:CD1	2.40	0.52
1:C:201:MET:HA	5:C:337:HOH:O	2.09	0.52
1:A:126:ASN:ND2	1:A:128:GLY:H	2.07	0.52
1:A:76:SER:HA	5:A:1399:HOH:O	2.09	0.52
1:C:193:ALA:HB1	1:C:211:LEU:HD22	1.92	0.52
1:C:54:ARG:NE	1:C:267:LEU:HB3	2.25	0.52
1:C:66:LEU:HG	1:C:297:GLN:HG2	1.92	0.52
1:A:201:MET:O	1:A:202:LEU:C	2.48	0.52
1:A:205:LYS:O	1:A:207:ILE:N	2.43	0.52
1:A:269:ARG:HH22	1:A:278:ASP:CG	2.11	0.52
1:C:45:ALA:HB1	1:C:72:GLY:N	2.25	0.52
2:D:33:PHE:HB3	2:D:35:LEU:HG	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2:ASN:ND2	1:A:5:TYR:CB	2.72	0.52
1:A:169:VAL:HG23	1:A:170:HIS:N	2.25	0.52
1:C:38:LEU:HD12	1:C:39:LEU:CG	2.39	0.52
1:C:157:VAL:HG12	1:C:158:ALA:N	2.17	0.52
1:C:92:ILE:O	1:C:93:SER:C	2.47	0.52
1:A:128:GLY:HA3	1:A:167:ARG:CZ	2.40	0.52
1:A:30:LEU:C	1:A:32:ALA:H	2.13	0.52
1:C:192:LEU:O	1:C:194:MET:N	2.36	0.52
1:C:202:LEU:HA	1:C:205:LYS:HZ2	1.74	0.52
2:B:41:ARG:CD	2:D:48:LEU:HD13	2.40	0.52
1:A:265:HIS:O	1:A:288:GLN:OE1	2.27	0.52
1:C:26:THR:HA	1:C:29:LYS:CG	2.40	0.52
2:D:108:VAL:HG23	2:D:108:VAL:O	2.10	0.52
1:A:157:VAL:HA	1:A:224:ILE:O	2.10	0.52
2:B:18:ILE:N	2:B:18:ILE:HD12	2.24	0.52
2:D:86:ILE:H	2:D:86:ILE:HD12	1.75	0.52
1:C:155:LEU:HA	5:C:363:HOH:O	2.10	0.51
1:C:273:ILE:HG21	1:C:285:TYR:CZ	2.45	0.51
2:D:24:GLN:HE21	2:D:47:ASN:ND2	2.08	0.51
1:A:187:ILE:HG23	1:A:212:HIS:O	2.10	0.51
1:C:48:PHE:CZ	1:C:52:SER:N	2.70	0.51
1:C:164:LYS:CB	1:C:192:LEU:HA	2.38	0.51
1:A:26:THR:HG21	1:A:302:LEU:CD2	2.39	0.51
2:B:103:ILE:HG13	2:B:103:ILE:O	2.10	0.51
1:A:16:SER:O	1:A:178:LYS:HD3	2.11	0.51
1:C:141:ASP:C	1:C:143:PHE:H	2.13	0.51
1:C:142:LEU:HA	1:C:145:ILE:CG1	2.40	0.51
1:C:155:LEU:HD22	1:C:224:ILE:CD1	2.40	0.51
2:D:135:ALA:CB	2:D:146:SER:HA	2.40	0.51
1:A:50:GLU:HG2	1:A:105:ARG:HD3	1.92	0.51
1:C:274:ALA:HB3	1:C:277:VAL:HG23	1.92	0.51
1:C:136:THR:OG1	1:C:296:ARG:NH2	2.43	0.51
1:A:23:VAL:O	1:A:26:THR:HB	2.10	0.51
2:B:109:CYS:SG	2:B:110:PRO:HD2	2.50	0.51
1:C:13:ASN:OD1	1:C:178:LYS:CE	2.59	0.51
2:D:103:ILE:HD11	2:D:127:VAL:CG1	2.40	0.51
2:D:28:LYS:C	2:D:30:LEU:H	2.13	0.51
1:A:177:ALA:O	1:A:207:ILE:HD11	2.11	0.51
1:A:26:THR:OG1	1:A:302:LEU:HD21	2.10	0.51
2:B:20:HIS:HA	2:B:56:LYS:HD2	1.91	0.51
1:C:124:VAL:HG12	1:C:125:LEU:H	1.64	0.51
1:C:178:LYS:HZ3	1:C:201:MET:HE1	1.75	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:188:ALA:HB3	1:C:193:ALA:HA	1.92	0.51
1:C:2:ASN:HB2	1:C:3:PRO:HD2	1.93	0.51
2:B:21:ILE:O	2:B:57:ASP:HB2	2.11	0.51
2:B:28:LYS:C	2:B:30:LEU:H	2.12	0.51
1:C:159:MET:HE3	1:C:172:LEU:HD23	1.91	0.51
1:C:261:MET:C	1:C:262:LYS:HD2	2.31	0.51
1:C:4:LEU:HD23	1:C:303:VAL:HG22	1.93	0.51
2:B:27:PHE:H	2:B:46:LEU:HD21	1.74	0.51
2:D:34:LYS:O	2:D:37:GLU:OE1	2.29	0.51
2:B:114:CYS:O	2:B:117:HIS:HE1	1.93	0.51
2:D:16:THR:CG2	2:D:65:PHE:HA	2.41	0.51
2:B:84:ASN:O	2:B:86:ILE:N	2.44	0.51
1:A:279:LYS:HB2	5:A:1418:HOH:O	2.11	0.51
1:C:291:ASN:O	1:C:292:GLY:C	2.49	0.51
2:D:133:ASP:HB2	2:D:147:HIS:HE1	1.74	0.51
2:D:45:GLY:O	2:D:48:LEU:HD23	2.10	0.51
1:A:155:LEU:O	1:A:182:ASN:HA	2.10	0.51
1:A:191:ALA:C	1:A:193:ALA:H	2.14	0.51
1:C:136:THR:CB	1:C:296:ARG:HH22	2.23	0.51
1:C:46:SER:N	1:C:72:GLY:HA3	2.26	0.51
2:B:36:THR:O	2:D:24:GLN:NE2	2.43	0.51
1:A:131:SER:HB2	1:A:165:TYR:HA	1.93	0.51
1:A:129:ASP:OD2	1:A:132:ASN:HB3	2.10	0.50
1:C:186:PHE:C	1:C:187:ILE:HG13	2.31	0.50
1:C:31:LYS:HZ3	1:C:143:PHE:HE2	1.53	0.50
1:C:80:SER:HA	1:C:84:LYS:HB2	1.93	0.50
1:A:225:LEU:C	1:A:225:LEU:HD12	2.32	0.50
1:C:129:ASP:O	1:C:130:GLY:C	2.49	0.50
1:C:220:ALA:HB2	1:C:256:ASN:HD22	1.77	0.50
2:B:42:ILE:O	2:D:46:LEU:N	2.45	0.50
1:A:174:GLN:CG	1:A:198:ILE:HG23	2.41	0.50
1:A:16:SER:HA	5:A:1389:HOH:O	2.11	0.50
1:C:190:ASP:OD1	1:C:191:ALA:N	2.36	0.50
1:C:189:PRO:O	1:C:192:LEU:N	2.45	0.50
2:D:125:PHE:O	2:D:139:LYS:HB2	2.11	0.50
1:A:157:VAL:HG12	1:A:224:ILE:HB	1.92	0.50
2:B:58:LEU:HD22	2:B:60:LYS:HG3	1.92	0.50
1:A:191:ALA:O	1:A:193:ALA:N	2.42	0.50
1:C:155:LEU:HD23	1:C:223:ASP:CG	2.32	0.50
1:C:224:ILE:N	1:C:261:MET:HG2	2.26	0.50
1:C:2:ASN:OD1	1:C:5:TYR:HB2	2.10	0.50
2:D:137:LYS:CD	2:D:142:GLU:HG3	2.42	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:149:VAL:HA	2:D:152:ALA:CB	2.42	0.50
1:C:81:LEU:HD23	1:C:81:LEU:C	2.32	0.50
1:C:263:VAL:HG23	1:C:282:HIS:HB3	1.94	0.50
2:B:9:VAL:O	2:B:10:GLU:HB2	2.11	0.50
2:B:96:ARG:HD2	2:B:97:PRO:HD2	1.93	0.50
1:A:160:VAL:CG1	1:A:187:ILE:HD13	2.42	0.50
1:A:189:PRO:HD2	1:A:192:LEU:HB2	1.92	0.50
1:A:16:SER:OG	1:A:19:ASP:HB2	2.11	0.50
2:B:83:VAL:HG11	2:B:85:ARG:NH1	2.26	0.50
1:C:248:VAL:CG1	1:C:249:LEU:H	2.19	0.49
1:C:295:ALA:O	1:C:296:ARG:C	2.49	0.49
1:C:26:THR:HA	1:C:29:LYS:CD	2.42	0.49
1:C:26:THR:CA	1:C:29:LYS:HG2	2.42	0.49
1:C:43:VAL:O	1:C:44:ILE:HD12	2.12	0.49
2:B:36:THR:HG23	2:B:37:GLU:H	1.77	0.49
1:C:237:PRO:HA	1:C:240:TYR:CE1	2.47	0.49
1:C:26:THR:OG1	1:C:302:LEU:HD11	2.12	0.49
1:C:46:SER:O	1:C:73:PHE:N	2.45	0.49
2:B:61:ILE:O	2:B:61:ILE:HG23	2.11	0.49
1:C:21:ASN:HA	1:C:24:LEU:HD12	1.94	0.49
1:A:128:GLY:HA3	1:A:167:ARG:NH2	2.27	0.49
2:B:55:ARG:O	2:B:56:LYS:HB3	2.13	0.49
1:C:183:ARG:HA	1:C:208:ALA:CB	2.40	0.49
1:C:140:LEU:O	1:C:291:ASN:OD1	2.29	0.49
1:C:5:TYR:O	1:C:6:GLN:HB2	2.12	0.49
1:A:2:ASN:ND2	1:A:306:ARG:CA	2.70	0.49
1:A:48:PHE:CD2	1:A:105:ARG:HD2	2.47	0.49
1:A:109:GLU:OE2	1:A:132:ASN:HB2	2.12	0.49
1:A:134:HIS:ND1	1:A:136:THR:OG1	2.42	0.49
1:A:267:LEU:CD2	1:A:269:ARG:HG2	2.41	0.49
1:C:38:LEU:HB3	1:C:39:LEU:HD12	1.94	0.49
1:C:159:MET:HE2	1:C:172:LEU:HD23	1.91	0.49
1:A:160:VAL:HA	1:A:187:ILE:O	2.12	0.49
1:A:243:VAL:O	1:A:244:LYS:O	2.29	0.49
2:D:16:THR:HG21	2:D:66:LEU:HD12	1.94	0.49
1:C:234:ARG:C	1:C:235:LEU:HD23	2.33	0.49
1:C:61:THR:CG2	5:C:351:HOH:O	2.60	0.49
1:A:39:LEU:HD21	1:A:301:ALA:HA	1.94	0.49
2:D:25:ILE:HG23	5:D:191:HOH:O	2.12	0.49
1:C:260:ASN:O	1:C:262:LYS:HD2	2.12	0.49
1:A:105:ARG:HG2	5:A:1388:HOH:O	2.13	0.49
1:A:78:ASN:HD22	1:A:78:ASN:H	1.61	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:42:ILE:O	2:D:45:GLY:HA2	2.12	0.49
1:A:137:GLN:NE2	1:A:266:PRO:HB3	2.28	0.49
1:A:183:ARG:CG	1:A:183:ARG:NH2	2.74	0.49
2:B:12:ILE:HG12	2:B:13:LYS:H	1.78	0.49
1:C:109:GLU:CB	5:C:419:HOH:O	2.49	0.49
1:C:128:GLY:HA2	1:C:133:GLN:O	2.13	0.49
1:C:249:LEU:HD11	1:C:254:LEU:HD21	1.94	0.49
1:C:60:GLU:O	1:C:63:MET:HB2	2.13	0.49
1:C:110:GLY:HA2	2:D:140:TYR:O	2.12	0.49
1:A:202:LEU:HA	1:A:207:ILE:HB	1.94	0.49
1:A:302:LEU:N	1:A:302:LEU:HD23	2.21	0.49
2:B:70:GLN:HB3	5:B:164:HOH:O	2.13	0.49
1:C:134:HIS:CE1	1:C:137:GLN:CB	2.95	0.49
1:C:155:LEU:HD22	1:C:224:ILE:HD11	1.94	0.49
1:C:292:GLY:HA2	1:C:296:ARG:HG3	1.94	0.49
1:C:5:TYR:CE2	1:C:305:ASN:N	2.81	0.49
2:D:33:PHE:O	2:D:34:LYS:C	2.51	0.49
1:A:160:VAL:CG2	1:A:227:MET:SD	3.00	0.49
1:A:267:LEU:HD23	1:A:268:PRO:CA	2.33	0.49
1:A:255:HIS:N	1:A:255:HIS:CD2	2.75	0.49
1:A:34:PRO:O	1:A:35:GLN:HG3	2.13	0.49
1:C:229:ARG:O	1:C:231:GLN:NE2	2.46	0.49
1:A:92:ILE:HG21	1:A:118:PHE:HB2	1.94	0.49
1:C:160:VAL:CG1	1:C:161:GLY:N	2.75	0.48
1:C:13:ASN:HB2	1:C:174:GLN:NE2	2.27	0.48
1:A:202:LEU:CB	1:A:207:ILE:HB	2.41	0.48
1:A:134:HIS:CE1	1:A:136:THR:HG1	2.31	0.48
1:C:276:ASP:HA	1:C:279:LYS:NZ	2.27	0.48
1:C:141:ASP:OD1	1:C:288:GLN:HG2	2.13	0.48
1:C:167:ARG:HH21	1:C:167:ARG:HG3	1.78	0.48
1:A:9:ILE:N	1:A:9:ILE:HD12	2.28	0.48
1:C:37:GLU:HA	1:C:40:LYS:HE3	1.93	0.48
1:C:9:ILE:CB	1:C:125:LEU:HG	2.43	0.48
1:A:160:VAL:HG12	1:A:187:ILE:CD1	2.43	0.48
1:A:289:ALA:N	5:A:1344:HOH:O	2.46	0.48
2:B:86:ILE:HA	2:B:91:VAL:HA	1.95	0.48
1:C:142:LEU:HA	1:C:145:ILE:HD12	1.94	0.48
1:C:219:MET:HE1	1:C:254:LEU:HG	1.95	0.48
1:C:228:THR:HG23	1:C:266:PRO:HG2	1.96	0.48
1:C:4:LEU:HD13	1:C:23:VAL:HG13	1.96	0.48
1:C:260:ASN:O	1:C:262:LYS:CD	2.61	0.48
1:C:107:PRO:HB2	5:C:316:HOH:O	2.13	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:146:GLN:OE1	1:C:146:GLN:N	2.47	0.48
1:A:164:LYS:HD3	5:A:1376:HOH:O	2.12	0.48
1:A:162:ASP:OD1	1:A:192:LEU:HD22	2.13	0.48
1:A:48:PHE:CZ	1:A:56:ARG:HA	2.49	0.48
1:A:55:THR:HB	4:A:1311:PCT:C1	2.43	0.48
1:C:137:GLN:O	1:C:137:GLN:HG3	2.14	0.48
1:C:105:ARG:NH1	1:C:167:ARG:NH2	2.60	0.48
1:C:49:PHE:CD1	1:C:49:PHE:N	2.82	0.48
1:A:13:ASN:OD1	1:A:174:GLN:CD	2.51	0.48
2:B:50:SER:OG	2:B:56:LYS:HD3	2.13	0.48
1:A:146:GLN:HE21	1:A:152:LEU:CG	2.26	0.48
1:C:231:GLN:N	1:C:231:GLN:NE2	2.60	0.48
1:C:310:LEU:N	1:C:310:LEU:CD1	2.74	0.48
1:C:65:ARG:C	1:C:67:GLY:H	2.16	0.48
2:D:147:HIS:HB2	2:D:151:LEU:CD1	2.44	0.48
1:A:167:ARG:HD2	5:A:1319:HOH:O	2.13	0.48
1:C:125:LEU:HD23	1:C:125:LEU:C	2.33	0.48
1:C:151:ARG:NH1	1:C:155:LEU:HD11	2.19	0.48
1:C:92:ILE:HG13	1:C:115:ALA:CA	2.32	0.48
2:B:74:LEU:HB2	2:B:97:PRO:HB3	1.96	0.48
2:B:75:ALA:CB	2:B:97:PRO:O	2.60	0.48
1:A:87:THR:O	1:A:91:THR:OG1	2.31	0.48
1:C:306:ARG:NH2	1:C:306:ARG:CB	2.73	0.48
1:C:163:LEU:CG	1:C:188:ALA:HB2	2.41	0.48
1:C:202:LEU:HA	1:C:205:LYS:HZ3	1.77	0.48
1:C:245:ALA:O	1:C:247:PHE:N	2.46	0.48
1:C:219:MET:O	1:C:257:ALA:HA	2.14	0.48
2:D:72:ASP:N	2:D:72:ASP:OD2	2.46	0.48
2:B:30:LEU:O	2:B:33:PHE:O	2.31	0.48
2:B:47:ASN:O	2:B:48:LEU:HD23	2.14	0.48
1:A:106:HIS:HB3	1:A:111:ALA:HB3	1.95	0.48
1:C:228:THR:CB	1:C:266:PRO:HG2	2.43	0.47
2:D:28:LYS:HE2	2:D:32:LEU:HD22	1.96	0.47
2:D:62:GLU:O	2:D:63:ASN:HB2	2.13	0.47
1:A:165:TYR:CE2	1:A:235:LEU:HD23	2.43	0.47
1:A:57:LEU:O	1:A:60:GLU:N	2.47	0.47
2:D:86:ILE:N	2:D:86:ILE:HD12	2.29	0.47
1:C:5:TYR:HE2	1:C:305:ASN:N	2.12	0.47
1:C:26:THR:HG23	1:C:310:LEU:HD22	1.95	0.47
1:C:54:ARG:HH11	1:C:268:PRO:HD3	1.78	0.47
2:D:137:LYS:HB2	2:D:144:GLU:CG	2.44	0.47
2:D:28:LYS:HB3	2:D:32:LEU:HB3	1.97	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:44:ILE:HG21	1:A:103:VAL:CG2	2.44	0.47
1:A:237:PRO:HD3	5:A:1392:HOH:O	2.14	0.47
1:C:287:GLN:CD	1:C:287:GLN:N	2.67	0.47
1:C:146:GLN:HA	1:C:150:GLY:N	2.30	0.47
2:D:96:ARG:CZ	2:D:96:ARG:HA	2.44	0.47
2:D:23:ALA:HB2	2:D:55:ARG:HG3	1.95	0.47
2:D:56:LYS:HD2	2:D:57:ASP:CA	2.44	0.47
1:A:197:TYR:CZ	1:A:198:ILE:HD11	2.50	0.47
1:A:109:GLU:HB3	2:B:141:CYS:CB	2.34	0.47
1:A:50:GLU:HB3	1:A:107:PRO:HD3	1.96	0.47
2:B:129:LYS:HE3	2:B:129:LYS:O	2.14	0.47
1:C:291:ASN:O	1:C:293:ILE:N	2.47	0.47
2:D:149:VAL:O	2:D:150:VAL:C	2.53	0.47
1:A:160:VAL:HG22	1:A:225:LEU:HD11	1.95	0.47
1:A:170:HIS:CD2	1:A:170:HIS:H	2.30	0.47
1:C:100:ASP:O	1:C:122:VAL:CG1	2.62	0.47
1:A:48:PHE:HE2	1:A:55:THR:CG2	2.19	0.47
1:A:41:HIS:O	1:A:42:LYS:C	2.53	0.47
1:A:233:GLU:H	1:A:233:GLU:CD	2.17	0.47
1:C:208:ALA:O	1:C:209:TRP:HB3	2.14	0.47
1:C:253:ASP:OD1	1:C:254:LEU:CD1	2.63	0.47
2:D:115:ILE:O	2:D:115:ILE:HG12	2.15	0.47
1:C:287:GLN:NE2	1:C:287:GLN:N	2.60	0.47
1:C:80:SER:OG	1:C:84:LYS:HD2	2.14	0.47
1:C:108:GLN:HE22	2:D:115:ILE:HD12	1.74	0.47
1:C:89:ALA:HB1	1:C:118:PHE:CD1	2.49	0.47
1:C:204:GLU:N	1:C:204:GLU:OE2	2.48	0.47
1:C:126:ASN:ND2	1:C:128:GLY:H	2.12	0.47
1:C:249:LEU:HD23	1:C:249:LEU:O	2.15	0.47
1:C:303:VAL:O	1:C:304:LEU:HD23	2.15	0.47
2:D:146:SER:CB	2:D:148:ASN:HD22	2.13	0.47
2:B:42:ILE:O	2:D:46:LEU:HD23	2.15	0.47
2:B:77:TYR:O	2:B:79:PRO:HD3	2.14	0.47
1:A:3:PRO:C	1:A:5:TYR:H	2.16	0.47
1:A:119:SER:HG	1:A:120:GLY:H	1.60	0.47
2:B:141:CYS:C	2:B:143:LYS:H	2.18	0.47
1:C:237:PRO:C	1:C:239:GLU:N	2.68	0.47
2:B:21:ILE:HD13	2:B:59:ILE:HG12	1.96	0.47
2:D:104:ASP:O	2:D:106:VAL:N	2.48	0.47
2:B:84:ASN:HB3	2:B:91:VAL:HG13	1.96	0.47
1:C:148:THR:HB	1:C:149:GLN:OE1	2.15	0.47
1:C:43:VAL:O	1:C:99:VAL:HA	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:SER:O	1:A:96:SER:OG	2.33	0.47
2:B:18:ILE:HD13	2:B:59:ILE:HB	1.97	0.47
2:B:86:ILE:HG12	2:B:91:VAL:HG22	1.95	0.47
1:C:66:LEU:CD1	1:C:300:LEU:HB2	2.45	0.47
2:D:12:ILE:N	2:D:12:ILE:HD13	2.29	0.47
1:A:4:LEU:O	1:A:303:VAL:HG13	2.15	0.47
1:A:9:ILE:HB	1:A:125:LEU:HA	1.96	0.47
2:B:108:VAL:HA	5:B:178:HOH:O	2.15	0.47
1:C:253:ASP:CG	1:C:254:LEU:HD12	2.34	0.47
2:D:114:CYS:C	2:D:116:SER:N	2.69	0.47
1:A:8:HIS:CD2	1:A:124:VAL:H	2.33	0.47
1:C:44:ILE:HG13	1:C:101:ALA:O	2.16	0.46
1:C:23:VAL:HG12	1:C:302:LEU:CD1	2.45	0.46
1:C:264:LEU:HB3	1:C:288:GLN:OE1	2.15	0.46
1:C:88:LEU:HD13	1:C:106:HIS:NE2	2.30	0.46
2:D:74:LEU:O	2:D:75:ALA:O	2.33	0.46
2:B:62:GLU:C	2:B:64:THR:N	2.67	0.46
1:A:284:TRP:CG	1:A:287:GLN:HB2	2.50	0.46
2:B:137:LYS:HB2	2:B:144:GLU:CD	2.36	0.46
2:B:137:LYS:HB2	2:B:144:GLU:OE2	2.15	0.46
2:D:16:THR:HG23	2:D:61:ILE:HD12	1.97	0.46
2:B:86:ILE:HG12	2:B:91:VAL:CA	2.42	0.46
1:C:196:GLN:OE1	1:C:196:GLN:O	2.33	0.46
2:D:113:ASN:O	2:D:115:ILE:N	2.48	0.46
2:B:39:ASP:CG	2:D:55:ARG:HH12	2.18	0.46
1:A:264:LEU:HD22	1:A:288:GLN:CG	2.45	0.46
2:B:21:ILE:O	2:B:57:ASP:N	2.49	0.46
2:B:55:ARG:NH1	5:B:204:HOH:O	2.47	0.46
1:C:105:ARG:HH11	1:C:167:ARG:NH1	2.05	0.46
1:C:26:THR:C	1:C:29:LYS:HG2	2.36	0.46
1:A:23:VAL:HG22	1:A:302:LEU:HD12	1.98	0.46
1:A:176:LEU:HB2	1:A:184:PHE:HZ	1.79	0.46
1:C:10:ILE:O	1:C:135:PRO:HD3	2.15	0.46
1:C:105:ARG:NH2	1:C:134:HIS:NE2	2.63	0.46
1:C:145:ILE:HB	1:C:146:GLN:OE1	2.15	0.46
2:D:135:ALA:HB1	2:D:146:SER:HA	1.98	0.46
2:D:81:ALA:O	2:D:96:ARG:NH2	2.48	0.46
1:A:169:VAL:O	1:A:173:THR:N	2.42	0.46
1:C:38:LEU:HD12	1:C:39:LEU:HD12	1.95	0.46
1:C:199:LEU:HD13	1:C:209:TRP:CE3	2.51	0.46
1:C:220:ALA:HA	1:C:256:ASN:O	2.15	0.46
1:C:59:PHE:CE1	1:C:296:ARG:HD3	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:222:VAL:HG23	1:A:222:VAL:O	2.15	0.46
1:A:131:SER:HB2	1:A:165:TYR:CA	2.46	0.46
2:B:113:ASN:O	2:B:114:CYS:C	2.53	0.46
2:B:59:ILE:HG22	2:B:60:LYS:N	2.30	0.46
1:A:38:LEU:C	1:A:38:LEU:HD23	2.36	0.46
2:D:127:VAL:CG1	2:D:136:LEU:HB3	2.46	0.46
2:B:79:PRO:HG2	2:B:80:GLN:H	1.80	0.46
1:A:243:VAL:HG22	1:A:244:LYS:N	2.29	0.46
1:C:288:GLN:O	1:C:291:ASN:OD1	2.33	0.46
2:D:99:LEU:HD22	2:D:99:LEU:C	2.36	0.46
2:B:31:SER:HA	2:D:27:PHE:CE1	2.51	0.46
1:C:21:ASN:HA	1:C:24:LEU:HB2	1.97	0.46
1:A:152:LEU:H	1:A:152:LEU:HD12	1.79	0.46
1:C:139:LEU:HA	1:C:142:LEU:CD1	2.29	0.46
2:B:56:LYS:HE3	5:B:228:HOH:O	2.15	0.46
1:C:195:PRO:HB2	1:C:197:TYR:CD2	2.50	0.46
1:A:202:LEU:CA	1:A:207:ILE:HB	2.45	0.46
1:A:246:GLN:HB3	1:A:247:PHE:CD1	2.50	0.46
1:A:236:ALA:HA	5:A:1392:HOH:O	2.16	0.46
1:A:277:VAL:HA	1:A:280:THR:HG23	1.97	0.46
2:B:117:HIS:O	2:B:119:GLU:N	2.49	0.46
1:A:176:LEU:HG	1:A:176:LEU:H	1.57	0.46
2:D:66:LEU:CD2	2:D:83:VAL:HG21	2.44	0.46
1:A:154:ASN:N	1:A:181:GLY:O	2.49	0.46
2:D:84:ASN:O	2:D:86:ILE:CD1	2.63	0.46
1:C:280:THR:CG2	1:C:281:PRO:HD2	2.46	0.46
2:D:111:ASN:O	2:D:117:HIS:CE1	2.69	0.46
1:A:3:PRO:CG	1:A:22:LEU:CD2	2.94	0.46
1:C:121:ASN:N	1:C:121:ASN:ND2	2.43	0.46
1:A:92:ILE:O	1:A:94:VAL:N	2.49	0.46
2:B:83:VAL:HG11	2:B:85:ARG:HH12	1.80	0.46
1:C:227:MET:HG3	1:C:265:HIS:ND1	2.30	0.45
1:C:280:THR:C	1:C:282:HIS:N	2.70	0.45
1:A:44:ILE:HG21	1:A:103:VAL:HG23	1.97	0.45
1:A:12:ILE:HD13	5:A:1429:HOH:O	2.16	0.45
2:D:143:LYS:CB	2:D:145:PHE:CE1	2.99	0.45
1:C:293:ILE:HB	1:C:294:PHE:H	1.62	0.45
1:C:92:ILE:O	1:C:95:ILE:N	2.48	0.45
2:D:146:SER:O	2:D:148:ASN:N	2.49	0.45
2:D:110:PRO:HG3	2:D:150:VAL:HG22	1.97	0.45
2:D:34:LYS:HD3	2:D:37:GLU:OE2	2.16	0.45
1:A:92:ILE:CG2	1:A:118:PHE:HB2	2.46	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:132:ASN:ND2	2:B:142:GLU:OE1	2.37	0.45
1:A:30:LEU:O	1:A:32:ALA:N	2.50	0.45
1:A:249:LEU:HG	1:A:250:ARG:N	2.31	0.45
1:C:145:ILE:HG23	5:C:320:HOH:O	2.16	0.45
1:C:151:ARG:CG	1:C:153:ASP:HB2	2.46	0.45
2:D:72:ASP:HB3	2:D:100:PRO:HD2	1.97	0.45
2:D:99:LEU:HD22	2:D:100:PRO:O	2.16	0.45
1:A:106:HIS:HA	5:A:1388:HOH:O	2.15	0.45
1:A:278:ASP:N	1:A:278:ASP:OD2	2.49	0.45
2:D:16:THR:CG2	2:D:61:ILE:HD12	2.46	0.45
1:C:205:LYS:HD2	1:C:205:LYS:N	2.28	0.45
1:A:283:ALA:O	1:A:287:GLN:OE1	2.34	0.45
2:B:103:ILE:HG22	5:B:187:HOH:O	2.16	0.45
1:C:265:HIS:CE1	1:C:266:PRO:HD2	2.52	0.45
2:D:149:VAL:O	2:D:152:ALA:N	2.50	0.45
2:B:44:ILE:HG13	5:B:188:HOH:O	2.15	0.45
1:A:3:PRO:HB2	1:A:22:LEU:CD2	2.46	0.45
1:A:103:VAL:HG22	1:A:125:LEU:HD13	1.97	0.45
1:A:86:GLU:OE1	1:A:91:THR:HG23	2.17	0.45
1:C:48:PHE:O	1:C:74:SER:O	2.34	0.45
1:C:157:VAL:O	1:C:158:ALA:HB2	2.16	0.45
1:C:163:LEU:HB2	1:C:192:LEU:O	2.17	0.45
1:C:176:LEU:C	1:C:178:LYS:N	2.70	0.45
2:D:128:ARG:HH21	2:D:128:ARG:HG2	1.82	0.45
2:D:76:LEU:HD12	2:D:77:TYR:N	2.32	0.45
2:D:64:THR:HG22	2:D:65:PHE:N	2.32	0.45
2:D:13:LYS:C	2:D:88:ASN:HA	2.36	0.45
1:C:154:ASN:O	1:C:155:LEU:HG	2.16	0.45
1:C:59:PHE:CG	1:C:296:ARG:HD3	2.51	0.45
2:D:126:ALA:N	2:D:137:LYS:O	2.50	0.45
1:A:189:PRO:HA	1:A:246:GLN:OE1	2.17	0.45
1:A:2:ASN:OD1	1:A:5:TYR:HB2	2.15	0.45
1:A:10:ILE:HD12	1:A:113:ARG:CD	2.47	0.45
1:A:81:LEU:HA	1:A:86:GLU:HB3	1.99	0.45
1:A:39:LEU:HD12	1:A:66:LEU:HD12	1.99	0.45
1:C:249:LEU:C	1:C:249:LEU:HD23	2.38	0.45
2:D:128:ARG:CZ	2:D:130:ARG:HD2	2.47	0.45
2:D:76:LEU:CB	2:D:134:ILE:HG21	2.37	0.45
2:D:141:CYS:O	2:D:143:LYS:N	2.49	0.45
1:A:227:MET:CE	1:A:272:GLU:HB2	2.47	0.45
1:A:44:ILE:O	1:A:70:VAL:HG23	2.17	0.45
1:A:109:GLU:HB2	2:B:114:CYS:HA	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:284:TRP:O	1:A:285:TYR:C	2.55	0.45
1:A:49:PHE:CZ	1:A:73:PHE:HZ	2.35	0.45
1:A:146:GLN:NE2	1:A:151:ARG:C	2.71	0.45
1:C:264:LEU:HD12	1:C:288:GLN:CG	2.47	0.45
2:D:138:CYS:SG	2:D:141:CYS:CB	3.00	0.45
2:B:41:ARG:HG3	2:D:48:LEU:CD2	2.37	0.45
2:B:61:ILE:HG23	2:B:64:THR:HB	1.99	0.45
1:A:109:GLU:CG	1:A:132:ASN:HB2	2.41	0.45
1:C:132:ASN:CB	5:C:419:HOH:O	2.65	0.44
1:C:262:LYS:O	1:C:264:LEU:CD2	2.65	0.44
1:C:151:ARG:O	1:C:151:ARG:CZ	2.65	0.44
1:C:226:TYR:O	1:C:226:TYR:CD1	2.70	0.44
1:C:263:VAL:O	1:C:264:LEU:HD13	2.17	0.44
1:C:31:LYS:HG3	5:C:391:HOH:O	2.16	0.44
2:D:125:PHE:HD1	2:D:136:LEU:HB2	1.82	0.44
2:B:114:CYS:O	2:B:117:HIS:CE1	2.70	0.44
1:A:308:LEU:HD23	1:A:309:VAL:C	2.38	0.44
2:B:123:SER:O	2:B:124:SER:HB2	2.17	0.44
2:D:69:ASP:OD2	2:D:70:GLN:NE2	2.49	0.44
1:C:5:TYR:H	1:C:7:LYS:HG2	1.82	0.44
1:C:61:THR:O	1:C:64:HIS:HB2	2.16	0.44
2:D:75:ALA:CA	2:D:97:PRO:HB2	2.47	0.44
1:A:237:PRO:HA	1:A:240:TYR:CE1	2.52	0.44
2:D:105:ASN:C	2:D:106:VAL:HG22	2.37	0.44
2:B:12:ILE:CG1	2:B:13:LYS:N	2.80	0.44
1:A:39:LEU:O	1:A:68:ALA:N	2.50	0.44
2:D:9:VAL:O	2:D:9:VAL:HG13	2.18	0.44
1:C:151:ARG:HH21	1:C:151:ARG:HB3	1.82	0.44
2:D:58:LEU:C	2:D:59:ILE:HD12	2.37	0.44
1:A:166:GLY:O	1:A:168:THR:N	2.50	0.44
1:A:169:VAL:HG23	1:A:170:HIS:H	1.82	0.44
1:A:59:PHE:CD2	1:A:63:MET:HE2	2.51	0.44
1:C:39:LEU:C	1:C:41:HIS:H	2.20	0.44
1:C:80:SER:CA	1:C:84:LYS:HB2	2.47	0.44
1:C:152:LEU:HB2	1:C:179:PHE:CE2	2.53	0.44
1:C:295:ALA:O	1:C:298:ALA:N	2.42	0.44
2:D:72:ASP:HB3	2:D:100:PRO:CD	2.47	0.44
2:D:133:ASP:OD2	2:D:148:ASN:ND2	2.50	0.44
2:D:24:GLN:HE21	2:D:47:ASN:CG	2.21	0.44
2:D:24:GLN:NE2	2:D:47:ASN:OD1	2.50	0.44
1:A:3:PRO:HG2	1:A:22:LEU:CD2	2.47	0.44
1:A:113:ARG:HG2	1:A:113:ARG:NH2	2.31	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:66:LEU:HD13	2:D:83:VAL:CG2	2.47	0.44
2:D:66:LEU:HB3	2:D:67:SER:H	1.64	0.44
2:B:84:ASN:HB3	2:B:91:VAL:CG1	2.47	0.44
1:C:234:ARG:HD3	5:C:406:HOH:O	2.18	0.44
2:D:24:GLN:HG2	2:D:47:ASN:OD1	2.17	0.44
1:A:172:LEU:HG	1:A:176:LEU:HD11	1.99	0.44
1:A:243:VAL:HG13	1:A:244:LYS:N	2.25	0.44
1:C:131:SER:O	1:C:170:HIS:HE1	2.01	0.44
1:C:159:MET:HG2	1:C:172:LEU:CD2	2.48	0.44
1:C:44:ILE:HG22	1:C:70:VAL:HG13	2.00	0.44
2:B:34:LYS:C	2:B:36:THR:N	2.68	0.44
2:D:41:ARG:CB	2:D:62:GLU:HB3	2.48	0.44
1:A:88:LEU:N	2:B:119:GLU:OE1	2.49	0.44
1:A:145:ILE:O	1:A:149:GLN:HB2	2.18	0.44
2:B:140:TYR:HB2	5:B:221:HOH:O	2.17	0.44
1:C:38:LEU:C	1:C:38:LEU:HD13	2.38	0.44
1:C:161:GLY:HA2	5:C:338:HOH:O	2.18	0.44
1:C:227:MET:HE1	1:C:273:ILE:HD13	2.00	0.44
2:B:43:THR:CG2	2:D:44:ILE:O	2.66	0.44
1:A:195:PRO:HB2	1:A:198:ILE:CD1	2.48	0.44
1:A:129:ASP:O	1:A:129:ASP:OD2	2.35	0.44
1:C:237:PRO:CA	1:C:240:TYR:CE2	2.90	0.44
2:B:16:THR:CG2	2:B:17:VAL:N	2.81	0.44
2:B:50:SER:HA	2:B:56:LYS:CE	2.46	0.44
2:D:84:ASN:HD22	2:D:91:VAL:HG21	1.82	0.44
1:C:250:ARG:O	1:C:253:ASP:N	2.47	0.43
1:A:13:ASN:OD1	1:A:174:GLN:OE1	2.36	0.43
1:A:198:ILE:N	1:A:198:ILE:HD12	2.33	0.43
1:A:236:ALA:HB3	1:A:239:GLU:OE2	2.18	0.43
1:A:89:ALA:O	1:A:93:SER:N	2.45	0.43
2:B:17:VAL:CG1	2:B:58:LEU:HD21	2.48	0.43
1:C:274:ALA:H	1:C:277:VAL:HG21	1.83	0.43
1:A:46:SER:H	1:A:72:GLY:HA3	1.83	0.43
1:A:143:PHE:C	1:A:143:PHE:CD1	2.91	0.43
1:C:227:MET:O	1:C:266:PRO:CD	2.62	0.43
1:C:284:TRP:O	1:C:284:TRP:CD1	2.71	0.43
1:C:4:LEU:HD23	1:C:4:LEU:O	2.18	0.43
2:D:124:SER:CB	2:D:139:LYS:HD3	2.48	0.43
1:A:148:THR:OG1	1:A:149:GLN:HG2	2.17	0.43
1:A:280:THR:HA	5:A:1411:HOH:O	2.18	0.43
1:A:87:THR:HB	2:B:119:GLU:OE2	2.18	0.43
1:A:94:VAL:CG2	1:A:95:ILE:N	2.82	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:150:GLY:O	1:C:151:ARG:C	2.57	0.43
2:B:39:ASP:CG	2:D:55:ARG:NH1	2.71	0.43
2:D:41:ARG:NH2	2:D:60:LYS:HD3	2.34	0.43
1:A:173:THR:HG21	1:A:194:MET:CE	2.48	0.43
2:B:100:PRO:O	2:B:127:VAL:HB	2.18	0.43
1:A:21:ASN:N	1:A:21:ASN:OD1	2.49	0.43
1:C:112:ALA:O	1:C:116:THR:HG23	2.18	0.43
1:C:46:SER:C	1:C:72:GLY:HA3	2.39	0.43
1:A:17:ARG:HG2	1:A:179:PHE:CE1	2.53	0.43
1:A:133:GLN:HG3	2:B:142:GLU:OE1	2.19	0.43
1:C:16:SER:O	1:C:19:ASP:OD2	2.37	0.43
1:A:220:ALA:HB2	1:A:256:ASN:HD22	1.83	0.43
1:C:97:THR:O	1:C:98:TYR:C	2.57	0.43
1:C:126:ASN:HD21	1:C:128:GLY:C	2.21	0.43
1:C:157:VAL:HA	1:C:224:ILE:O	2.19	0.43
1:C:218:VAL:CG1	1:C:218:VAL:O	2.62	0.43
1:C:267:LEU:HD13	1:C:268:PRO:HA	2.01	0.43
1:C:66:LEU:HD12	1:C:300:LEU:HB2	2.00	0.43
1:C:66:LEU:HD21	1:C:297:GLN:HB3	1.99	0.43
1:A:102:ILE:O	1:A:124:VAL:HA	2.19	0.43
1:A:81:LEU:HD12	1:A:88:LEU:HA	2.01	0.43
2:B:19:ASP:HA	2:B:58:LEU:HG	2.00	0.43
1:A:181:GLY:O	1:A:182:ASN:CG	2.57	0.43
1:C:306:ARG:HB2	1:C:306:ARG:HH21	1.82	0.43
1:C:114:LEU:CD1	1:C:114:LEU:C	2.83	0.43
1:C:151:ARG:HG2	1:C:153:ASP:H	1.84	0.43
1:A:284:TRP:O	1:A:284:TRP:CD1	2.71	0.43
2:D:9:VAL:C	2:D:11:ALA:N	2.71	0.43
1:C:12:ILE:O	1:C:12:ILE:HG22	2.18	0.43
1:C:59:PHE:HE1	1:C:296:ARG:NH2	2.16	0.43
2:D:126:ALA:O	2:D:136:LEU:CB	2.66	0.43
2:D:132:ASN:CG	2:D:133:ASP:H	2.21	0.43
1:A:110:GLY:C	1:A:112:ALA:N	2.70	0.43
1:A:167:ARG:HG3	1:A:168:THR:H	1.82	0.43
1:C:137:GLN:HG3	5:C:325:HOH:O	2.18	0.43
1:C:45:ALA:CB	1:C:72:GLY:H	2.31	0.43
2:D:111:ASN:O	2:D:113:ASN:N	2.52	0.43
1:A:205:LYS:O	1:A:207:ILE:HG12	2.18	0.43
2:D:105:ASN:C	2:D:106:VAL:CG2	2.87	0.43
1:C:244:LYS:HE3	5:C:376:HOH:O	2.19	0.43
1:C:169:VAL:C	1:C:172:LEU:HD13	2.39	0.43
1:C:250:ARG:C	1:C:252:SER:N	2.71	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:76:LEU:HA	2:D:134:ILE:HG13	2.01	0.43
1:A:2:ASN:OD1	1:A:5:TYR:N	2.52	0.43
2:B:150:VAL:HG12	2:B:150:VAL:O	2.18	0.43
1:C:130:GLY:O	1:C:167:ARG:HD3	2.20	0.42
1:C:235:LEU:N	1:C:235:LEU:HD23	2.33	0.42
2:D:28:LYS:O	2:D:32:LEU:N	2.52	0.42
2:D:56:LYS:CD	2:D:57:ASP:N	2.74	0.42
1:A:187:ILE:N	1:A:187:ILE:CD1	2.75	0.42
1:A:5:TYR:CG	1:A:306:ARG:HA	2.54	0.42
1:A:183:ARG:CZ	1:A:208:ALA:HB3	2.49	0.42
1:A:309:VAL:HG23	1:A:310:LEU:N	2.34	0.42
2:B:25:ILE:HG22	2:B:25:ILE:O	2.19	0.42
2:D:9:VAL:O	2:D:11:ALA:N	2.52	0.42
2:B:107:LEU:HB2	2:B:125:PHE:CE1	2.54	0.42
1:C:252:SER:O	1:C:255:HIS:CE1	2.73	0.42
1:C:261:MET:SD	1:C:262:LYS:N	2.92	0.42
1:C:4:LEU:HB3	1:C:22:LEU:HD23	2.01	0.42
2:D:99:LEU:CD2	2:D:129:LYS:NZ	2.82	0.42
1:A:205:LYS:C	1:A:207:ILE:N	2.70	0.42
1:A:26:THR:CG2	1:A:302:LEU:HD21	2.50	0.42
1:A:119:SER:HG	1:A:120:GLY:N	2.17	0.42
2:B:115:ILE:HA	5:B:173:HOH:O	2.19	0.42
1:A:204:GLU:C	1:A:206:GLY:N	2.72	0.42
2:D:103:ILE:HG13	2:D:126:ALA:N	2.34	0.42
1:A:265:HIS:HA	1:A:266:PRO:HD2	1.75	0.42
1:A:73:PHE:CD2	1:A:79:THR:HG21	2.55	0.42
1:A:261:MET:SD	1:A:262:LYS:N	2.92	0.42
2:B:12:ILE:CG1	2:B:13:LYS:H	2.31	0.42
2:B:24:GLN:NE2	2:D:38:THR:O	2.52	0.42
1:C:139:LEU:O	1:C:142:LEU:N	2.52	0.42
1:C:262:LYS:HB2	5:C:377:HOH:O	2.19	0.42
1:C:263:VAL:O	1:C:284:TRP:N	2.42	0.42
2:D:137:LYS:HB2	2:D:144:GLU:CD	2.39	0.42
2:D:12:ILE:HG23	2:D:41:ARG:HH21	1.83	0.42
2:D:26:GLY:O	2:D:30:LEU:CD2	2.68	0.42
2:D:79:PRO:HG2	2:D:80:GLN:H	1.84	0.42
1:A:174:GLN:HA	1:A:201:MET:HE1	2.02	0.42
1:A:149:GLN:O	1:A:150:GLY:C	2.58	0.42
1:A:23:VAL:HG22	1:A:302:LEU:HD11	2.01	0.42
1:A:104:MET:O	1:A:127:ALA:N	2.47	0.42
1:A:92:ILE:O	1:A:93:SER:C	2.58	0.42
1:C:45:ALA:HB3	1:C:102:ILE:HG22	2.00	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:132:ASN:CA	1:C:170:HIS:ND1	2.76	0.42
2:B:42:ILE:HG12	2:B:61:ILE:HG13	2.01	0.42
2:D:37:GLU:HB3	5:D:173:HOH:O	2.18	0.42
1:A:187:ILE:HA	5:A:1327:HOH:O	2.19	0.42
1:A:22:LEU:HD12	5:A:1421:HOH:O	2.20	0.42
2:D:16:THR:CB	2:D:65:PHE:HA	2.50	0.42
1:C:104:MET:HG3	1:C:126:ASN:OD1	2.20	0.42
1:C:167:ARG:HH11	1:C:234:ARG:HH22	1.68	0.42
1:C:285:TYR:CA	1:C:288:GLN:OE1	2.60	0.42
2:D:107:LEU:CD1	2:D:151:LEU:HD21	2.47	0.42
2:B:28:LYS:C	2:B:30:LEU:N	2.72	0.42
1:A:196:GLN:C	1:A:198:ILE:N	2.72	0.42
2:B:76:LEU:N	2:B:76:LEU:HD23	2.09	0.42
1:A:109:GLU:CB	2:B:114:CYS:HA	2.49	0.42
2:B:140:TYR:N	5:B:221:HOH:O	2.52	0.42
1:A:255:HIS:HB3	5:A:1396:HOH:O	2.19	0.42
2:D:126:ALA:O	2:D:127:VAL:CG1	2.62	0.42
2:B:75:ALA:HB2	2:B:98:SER:O	2.20	0.42
1:A:186:PHE:C	1:A:187:ILE:HD12	2.40	0.42
1:A:131:SER:N	1:A:234:ARG:NE	2.67	0.42
1:C:165:TYR:CE2	1:C:192:LEU:HD21	2.55	0.42
2:D:96:ARG:NH2	2:D:97:PRO:CD	2.81	0.42
1:A:217:GLU:C	1:A:219:MET:H	2.22	0.42
1:A:264:LEU:CD2	1:A:288:GLN:HB2	2.50	0.42
1:A:89:ALA:O	1:A:93:SER:OG	2.38	0.42
1:C:127:ALA:HB1	1:C:136:THR:HG1	1.85	0.42
1:C:280:THR:O	1:C:282:HIS:N	2.53	0.42
1:C:45:ALA:N	1:C:99:VAL:HG11	2.35	0.42
2:B:39:ASP:CA	2:D:55:ARG:NH2	2.81	0.42
1:A:55:THR:HG21	1:A:105:ARG:NH1	2.33	0.42
2:D:16:THR:HB	2:D:65:PHE:HA	2.02	0.42
2:B:129:LYS:CE	2:B:129:LYS:C	2.86	0.42
2:D:18:ILE:HG22	2:D:21:ILE:HD11	2.02	0.42
1:C:172:LEU:O	1:C:174:GLN:N	2.43	0.42
2:B:44:ILE:CG2	2:D:44:ILE:HB	2.27	0.42
1:A:214:SER:HB3	1:A:217:GLU:HG3	2.02	0.42
1:A:109:GLU:OE2	1:A:132:ASN:CB	2.68	0.42
1:A:55:THR:HB	4:A:1311:PCT:O1	2.19	0.42
1:C:48:PHE:CE2	1:C:51:ALA:HA	2.55	0.42
2:B:134:ILE:O	2:B:147:HIS:HB3	2.20	0.42
2:B:136:LEU:O	2:B:145:PHE:N	2.53	0.42
2:B:94:LYS:HD2	2:B:94:LYS:HA	1.81	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:13:ASN:HB2	1:C:174:GLN:CD	2.41	0.41
1:C:59:PHE:O	1:C:60:GLU:C	2.58	0.41
2:D:111:ASN:C	2:D:113:ASN:N	2.73	0.41
1:A:280:THR:CB	1:A:281:PRO:CD	2.87	0.41
1:C:178:LYS:HA	5:C:367:HOH:O	2.21	0.41
1:C:223:ASP:C	1:C:224:ILE:HG13	2.41	0.41
1:C:292:GLY:O	1:C:296:ARG:HB2	2.20	0.41
1:C:61:THR:HG21	5:C:351:HOH:O	2.17	0.41
1:A:202:LEU:H	1:A:202:LEU:HG	1.54	0.41
2:B:76:LEU:HG	2:B:77:TYR:CD2	2.55	0.41
1:A:10:ILE:CG1	1:A:11:SER:H	2.32	0.41
1:A:136:THR:HB	1:A:296:ARG:HH11	1.84	0.41
1:C:260:ASN:O	5:C:331:HOH:O	2.21	0.41
1:C:26:THR:HG22	1:C:30:LEU:HG	2.01	0.41
2:D:143:LYS:HB3	2:D:145:PHE:CZ	2.55	0.41
2:D:28:LYS:C	2:D:30:LEU:N	2.73	0.41
1:A:277:VAL:O	1:A:283:ALA:HB2	2.19	0.41
2:D:86:ILE:CG2	2:D:90:GLU:N	2.84	0.41
2:B:104:ASP:HB2	5:B:172:HOH:O	2.19	0.41
1:C:59:PHE:CE2	1:C:300:LEU:HD21	2.55	0.41
1:C:6:GLN:H	1:C:303:VAL:HG13	1.86	0.41
2:D:56:LYS:HD2	2:D:57:ASP:H	1.77	0.41
1:A:189:PRO:CG	1:A:192:LEU:HD12	2.30	0.41
2:B:60:LYS:HG3	5:B:186:HOH:O	2.19	0.41
1:C:4:LEU:HA	1:C:7:LYS:HG3	2.01	0.41
2:D:134:ILE:H	2:D:147:HIS:CE1	2.39	0.41
1:A:229:ARG:HD2	1:A:270:VAL:HG23	2.02	0.41
1:A:219:MET:HE2	1:A:257:ALA:HA	2.02	0.41
1:C:274:ALA:O	1:C:277:VAL:CG2	2.67	0.41
1:C:183:ARG:HG2	1:C:208:ALA:CB	2.51	0.41
1:C:204:GLU:HG2	1:C:205:LYS:HZ2	1.85	0.41
1:C:187:ILE:HG21	1:C:215:ILE:HD11	2.02	0.41
1:C:229:ARG:HH12	1:C:233:GLU:CG	2.34	0.41
1:C:60:GLU:O	1:C:70:VAL:HG21	2.20	0.41
1:C:65:ARG:CZ	5:C:351:HOH:O	2.69	0.41
2:D:125:PHE:HB3	2:D:126:ALA:H	1.55	0.41
2:D:141:CYS:C	2:D:143:LYS:N	2.73	0.41
2:D:68:GLU:O	2:D:72:ASP:OD2	2.38	0.41
2:D:99:LEU:CD2	2:D:129:LYS:HZ2	2.33	0.41
2:B:38:THR:O	2:B:38:THR:HG23	2.21	0.41
1:A:197:TYR:CE1	1:A:198:ILE:HD11	2.56	0.41
1:A:26:THR:CB	1:A:302:LEU:HD21	2.50	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4:LEU:HD23	1:A:7:LYS:HD2	2.02	0.41
1:A:176:LEU:CD1	1:A:184:PHE:CZ	3.03	0.41
2:D:67:SER:O	2:D:71:VAL:CG2	2.68	0.41
2:D:93:GLY:C	2:D:95:SER:H	2.24	0.41
1:C:109:GLU:C	1:C:111:ALA:H	2.24	0.41
1:C:12:ILE:C	1:C:174:GLN:HE22	2.20	0.41
1:C:186:PHE:HE1	1:C:209:TRP:HB2	1.86	0.41
1:C:88:LEU:HD22	1:C:106:HIS:NE2	2.36	0.41
1:A:196:GLN:HA	1:A:199:LEU:HB2	2.02	0.41
1:A:114:LEU:CD2	2:B:115:ILE:HG23	2.50	0.41
1:C:50:GLU:HB3	1:C:51:ALA:H	1.65	0.41
1:A:146:GLN:HE21	1:A:152:LEU:N	2.19	0.41
1:C:110:GLY:N	1:C:129:ASP:OD1	2.49	0.41
1:C:157:VAL:CG1	1:C:158:ALA:H	2.12	0.41
2:B:30:LEU:HA	2:B:35:LEU:HD12	2.01	0.41
2:D:30:LEU:HB3	2:D:36:THR:OG1	2.21	0.41
2:B:58:LEU:HD23	2:B:59:ILE:O	2.21	0.41
1:A:41:HIS:O	1:A:42:LYS:O	2.39	0.41
1:C:186:PHE:O	1:C:187:ILE:HG13	2.21	0.41
1:C:163:LEU:CD1	1:C:188:ALA:HB2	2.51	0.41
1:C:44:ILE:HG13	1:C:101:ALA:CB	2.42	0.41
1:C:92:ILE:HD13	1:C:95:ILE:HD12	2.02	0.41
2:D:111:ASN:C	2:D:113:ASN:H	2.23	0.41
1:C:116:THR:HG22	1:C:124:VAL:HG11	2.03	0.41
1:C:126:ASN:C	1:C:126:ASN:ND2	2.74	0.41
1:C:54:ARG:NH1	1:C:268:PRO:HD3	2.35	0.41
1:C:26:THR:HA	1:C:29:LYS:HD2	2.02	0.41
1:A:110:GLY:C	1:A:112:ALA:H	2.24	0.41
1:A:56:ARG:HG2	1:A:60:GLU:OE2	2.21	0.41
1:A:10:ILE:HD12	1:A:113:ARG:HD2	2.02	0.41
1:A:126:ASN:HD22	1:A:135:PRO:HD2	1.86	0.41
2:D:41:ARG:CB	2:D:62:GLU:CB	2.93	0.41
2:D:105:ASN:HA	2:D:123:SER:C	2.42	0.41
1:C:214:SER:HB2	1:C:216:GLU:CD	2.40	0.41
2:B:23:ALA:C	2:B:25:ILE:H	2.23	0.41
1:C:92:ILE:CD1	1:C:115:ALA:HB1	2.52	0.40
1:C:9:ILE:HB	1:C:125:LEU:HG	2.02	0.40
1:C:12:ILE:CD1	1:C:135:PRO:HA	2.32	0.40
1:C:261:MET:O	1:C:282:HIS:ND1	2.54	0.40
2:D:141:CYS:C	2:D:143:LYS:H	2.25	0.40
2:D:75:ALA:N	2:D:97:PRO:HB2	2.36	0.40
2:B:34:LYS:HD3	2:B:37:GLU:OE2	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:195:PRO:O	1:A:198:ILE:HD13	2.22	0.40
1:A:266:PRO:O	1:A:267:LEU:O	2.38	0.40
2:B:138:CYS:CB	5:B:221:HOH:O	2.69	0.40
1:A:176:LEU:HB2	1:A:184:PHE:CZ	2.55	0.40
1:C:48:PHE:HB3	1:C:74:SER:O	2.20	0.40
1:A:146:GLN:NE2	1:A:152:LEU:N	2.68	0.40
2:D:22:PRO:HB2	2:D:25:ILE:HG13	2.03	0.40
1:A:100:ASP:HB2	5:A:1410:HOH:O	2.21	0.40
1:C:132:ASN:O	1:C:170:HIS:ND1	2.54	0.40
1:C:197:TYR:CE1	2:D:143:LYS:HA	2.56	0.40
1:C:219:MET:CB	1:C:256:ASN:ND2	2.72	0.40
1:A:298:ALA:O	1:A:302:LEU:CD2	2.69	0.40
1:A:55:THR:HG21	1:A:105:ARG:NE	2.35	0.40
2:D:65:PHE:HB3	2:D:66:LEU:H	1.67	0.40
1:A:262:LYS:HG2	1:A:282:HIS:HA	2.03	0.40
1:C:39:LEU:N	1:C:39:LEU:HD12	2.36	0.40
2:D:86:ILE:HG13	2:D:91:VAL:HG22	2.02	0.40
1:A:250:ARG:NH2	1:A:276:ASP:OD2	2.54	0.40
5:B:165:HOH:O	2:D:49:PRO:HG2	2.21	0.40
1:C:135:PRO:HG2	1:C:136:THR:N	2.35	0.40
1:C:189:PRO:HD2	1:C:192:LEU:HD12	2.02	0.40
1:C:250:ARG:O	1:C:252:SER:N	2.54	0.40
1:C:264:LEU:CA	1:C:288:GLN:OE1	2.70	0.40
1:C:271:ASP:O	1:C:272:GLU:C	2.59	0.40
1:A:33:ASN:HA	1:A:34:PRO:HD3	1.74	0.40
1:C:164:LYS:HG3	1:C:195:PRO:HD3	2.02	0.40
2:D:34:LYS:HD3	2:D:37:GLU:CD	2.42	0.40
1:A:160:VAL:O	1:A:227:MET:HA	2.21	0.40
1:A:229:ARG:HA	1:A:272:GLU:OE2	2.21	0.40
1:A:12:ILE:HD11	1:A:135:PRO:HA	2.04	0.40
1:A:277:VAL:HG12	1:A:285:TYR:OH	2.21	0.40
1:C:31:LYS:NZ	1:C:143:PHE:CE2	2.80	0.40
1:C:246:GLN:HA	5:C:314:HOH:O	2.20	0.40
2:B:46:LEU:HD12	2:D:42:ILE:CD1	2.52	0.40
2:D:30:LEU:N	2:D:30:LEU:HD13	2.34	0.40
2:B:117:HIS:N	2:B:117:HIS:ND1	2.69	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	308/310 (99%)	200 (65%)	73 (24%)	35 (11%)	1	1
1	C	308/310 (99%)	187 (61%)	70 (23%)	51 (17%)	0	0
2	B	144/153 (94%)	82 (57%)	44 (31%)	18 (12%)	1	1
2	D	144/153 (94%)	88 (61%)	34 (24%)	22 (15%)	0	1
All	All	904/926 (98%)	557 (62%)	221 (24%)	126 (14%)	0	1

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	21	ASN
1	A	192	LEU
1	A	231	GLN
1	A	244	LYS
1	A	302	LEU
2	B	10	GLU
2	B	85	ARG
2	B	106	VAL
2	B	142	GLU
1	C	32	ALA
1	C	37	GLU
1	C	68	ALA
1	C	97	THR
1	C	98	TYR
1	C	190	ASP
1	C	209	TRP
1	C	213	SER
1	C	231	GLN
1	C	235	LEU
1	C	258	LYS
1	C	283	ALA
1	C	293	ILE
1	C	295	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	296	ARG
2	D	75	ALA
2	D	105	ASN
2	D	106	VAL
2	D	115	ILE
2	D	127	VAL
1	A	37	GLU
1	A	38	LEU
1	A	42	LYS
1	A	89	ALA
1	A	93	SER
1	A	132	ASN
1	A	150	GLY
1	A	197	TYR
1	A	201	MET
1	A	252	SER
1	A	267	LEU
1	A	309	VAL
2	B	41	ARG
2	B	67	SER
2	B	77	TYR
2	B	101	GLU
2	B	105	ASN
2	B	118	ALA
1	C	14	ASP
1	C	42	LYS
1	C	113	ARG
1	C	153	ASP
1	C	154	ASN
1	C	166	GLY
1	C	193	ALA
1	C	238	SER
1	C	255	HIS
1	C	306	ARG
2	D	29	LEU
2	D	114	CYS
2	D	123	SER
2	D	135	ALA
2	D	142	GLU
1	A	16	SER
1	A	52	SER
1	A	78	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	205	LYS
1	A	283	ALA
2	B	9	VAL
2	B	47	ASN
2	B	63	ASN
2	B	88	ASN
1	C	18	ASP
1	C	40	LYS
1	C	54	ARG
1	C	55	THR
1	C	135	PRO
1	C	151	ARG
1	C	157	VAL
1	C	158	ALA
1	C	172	LEU
1	C	194	MET
1	C	292	GLY
2	D	10	GLU
2	D	112	SER
2	D	131	ALA
2	D	147	HIS
1	A	167	ARG
1	A	219	MET
1	A	255	HIS
2	B	124	SER
1	C	67	GLY
1	C	246	GLN
2	D	42	ILE
2	D	67	SER
2	D	116	SER
1	A	3	PRO
1	A	271	ASP
2	B	73	GLN
2	B	130	ARG
1	C	36	PRO
1	C	71	VAL
1	C	83	LYS
1	C	84	LYS
1	C	242	ASN
1	C	302	LEU
2	D	95	SER
1	A	144	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	168	THR
1	A	218	VAL
1	C	66	LEU
1	C	76	SER
1	C	267	LEU
2	D	12	ILE
1	A	206	GLY
1	A	222	VAL
2	D	45	GLY
2	D	134	ILE
1	A	293	ILE
1	C	10	ILE
1	A	189	PRO
2	B	92	VAL
1	C	270	VAL
2	D	121	VAL
1	C	187	ILE
1	C	207	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/260 (100%)	209 (80%)	51 (20%)	2	6
1	C	260/260 (100%)	218 (84%)	42 (16%)	3	10
2	B	129/137 (94%)	112 (87%)	17 (13%)	6	16
2	D	129/137 (94%)	112 (87%)	17 (13%)	6	16
All	All	778/794 (98%)	651 (84%)	127 (16%)	3	10

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	18	ASP
1	A	19	ASP
1	A	21	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	35	GLN
1	A	37	GLU
1	A	47	CYS
1	A	59	PHE
1	A	62	SER
1	A	70	VAL
1	A	74	SER
1	A	79	THR
1	A	91	THR
1	A	92	ILE
1	A	97	THR
1	A	100	ASP
1	A	104	MET
1	A	109	GLU
1	A	113	ARG
1	A	114	LEU
1	A	125	LEU
1	A	134	HIS
1	A	137	GLN
1	A	143	PHE
1	A	144	THR
1	A	145	ILE
1	A	146	GLN
1	A	152	LEU
1	A	156	HIS
1	A	176	LEU
1	A	180	ASP
1	A	194	MET
1	A	196	GLN
1	A	219	MET
1	A	225	LEU
1	A	233	GLU
1	A	250	ARG
1	A	253	ASP
1	A	255	HIS
1	A	267	LEU
1	A	269	ARG
1	A	275	THR
1	A	278	ASP
1	A	282	HIS
1	A	285	TYR
1	A	287	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	291	ASN
1	A	302	LEU
1	A	303	VAL
1	A	305	ASN
1	A	306	ARG
2	B	36	THR
2	B	37	GLU
2	B	38	THR
2	B	44	ILE
2	B	46	LEU
2	B	47	ASN
2	B	53	MET
2	B	70	GLN
2	B	76	LEU
2	B	102	ARG
2	B	106	VAL
2	B	113	ASN
2	B	117	HIS
2	B	129	LYS
2	B	134	ILE
2	B	151	LEU
2	B	153	ASN
1	C	14	ASP
1	C	15	LEU
1	C	18	ASP
1	C	23	VAL
1	C	37	GLU
1	C	38	LEU
1	C	48	PHE
1	C	49	PHE
1	C	56	ARG
1	C	59	PHE
1	C	70	VAL
1	C	98	TYR
1	C	100	ASP
1	C	102	ILE
1	C	106	HIS
1	C	109	GLU
1	C	121	ASN
1	C	140	LEU
1	C	146	GLN
1	C	147	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	149	GLN
1	C	151	ARG
1	C	152	LEU
1	C	174	GLN
1	C	180	ASP
1	C	183	ARG
1	C	196	GLN
1	C	202	LEU
1	C	204	GLU
1	C	205	LYS
1	C	216	GLU
1	C	233	GLU
1	C	235	LEU
1	C	242	ASN
1	C	243	VAL
1	C	247	PHE
1	C	278	ASP
1	C	293	ILE
1	C	294	PHE
1	C	306	ARG
1	C	308	LEU
1	C	310	LEU
2	D	12	ILE
2	D	27	PHE
2	D	30	LEU
2	D	36	THR
2	D	39	ASP
2	D	44	ILE
2	D	52	GLU
2	D	57	ASP
2	D	58	LEU
2	D	72	ASP
2	D	76	LEU
2	D	77	TYR
2	D	99	LEU
2	D	106	VAL
2	D	114	CYS
2	D	125	PHE
2	D	136	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	35	GLN
1	A	78	ASN
1	A	126	ASN
1	A	146	GLN
1	A	149	GLN
1	A	231	GLN
1	A	242	ASN
1	A	287	GLN
1	A	291	ASN
2	B	63	ASN
2	B	70	GLN
2	B	105	ASN
2	B	132	ASN
1	C	33	ASN
1	C	64	HIS
1	C	121	ASN
1	C	231	GLN
1	C	256	ASN
1	C	287	GLN
2	D	24	GLN
2	D	63	ASN
2	D	111	ASN
2	D	132	ASN
2	D	148	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z  > 2$
4	PCT	A	1311	-	7,7,7	2.85	3 (42%)	10,10,10	0.92	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PCT	A	1311	-	-	0/5/5/5	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1311	PCT	P-O1P	4.96	1.61	1.50
4	A	1311	PCT	P-O2P	-3.90	1.47	1.54
4	A	1311	PCT	P-O3P	3.54	1.61	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	310/310 (100%)	-0.60	0 100 100	13, 49, 72, 89	0
1	C	310/310 (100%)	-0.46	3 (0%) 79 86	60, 90, 112, 137	0
2	B	146/153 (95%)	-0.44	2 (1%) 72 80	41, 78, 98, 102	0
2	D	146/153 (95%)	-0.18	6 (4%) 35 43	84, 104, 121, 127	0
All	All	912/926 (98%)	-0.46	11 (1%) 75 83	13, 82, 115, 137	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	18	ILE	5.7
2	D	58	LEU	5.3
2	D	59	ILE	4.5
1	C	173	THR	4.2
2	B	9	VAL	3.1
2	D	56	LYS	3.0
1	C	186	PHE	2.8
2	D	21	ILE	2.6
1	C	40	LYS	2.4
2	B	59	ILE	2.0
2	D	107	LEU	2.0

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	B	154	1/1	0.16	1.20	45,45,45,45	0
4	PCT	A	1311	8/8	0.15	0.45	32,36,38,39	0
3	ZN	D	154	1/1	0.07	-1.21	47,47,47,47	0

## 6.5 Other polymers

There are no such residues in this entry.