



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:35 am BST

PDB ID : 2G4C  
Title : Crystal Structure of human DNA polymerase gamma accessory subunit  
Authors : Fan, L.; Farr, C.L.; Kaguni, L.S.; Tainer, J.A.  
Deposited on : 2006-02-22  
Resolution : 3.15 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

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

with specific help available everywhere you see the ⓘ symbol.

---

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

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

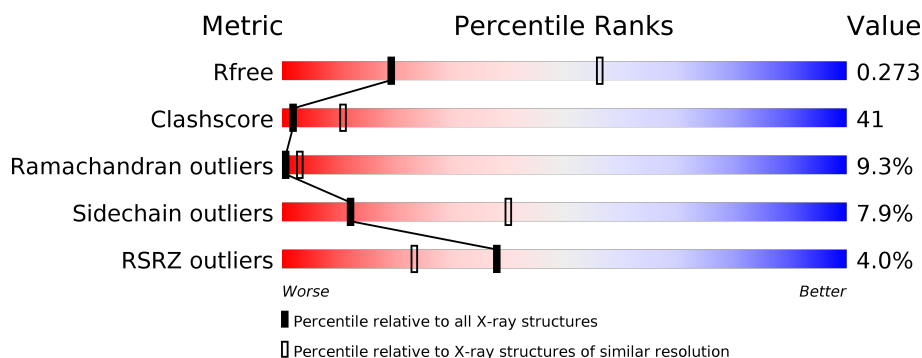
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	474	<div> <div>2%</div> <div> <div></div> <div>34%</div> <div>41%</div> <div>8%</div> <div>16%</div> </div> </div>
1	B	474	<div> <div>2%</div> <div> <div></div> <div>34%</div> <div>41%</div> <div>8%</div> <div>16%</div> </div> </div>
1	C	474	<div> <div>5%</div> <div> <div></div> <div>31%</div> <div>43%</div> <div>9%</div> <div>16%</div> </div> </div>
1	D	474	<div> <div>5%</div> <div> <div></div> <div>31%</div> <div>43%</div> <div>9%</div> <div>16%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12847 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 DNA polymerase gamma subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3202	2050	558	578	16			
1	B	397	Total	C	N	O	S	0	0	0
			3202	2050	558	578	16			
1	C	397	Total	C	N	O	S	0	0	0
			3206	2053	560	577	16			
1	D	397	Total	C	N	O	S	0	0	0
			3206	2053	560	577	16			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	INITIATING METHIONINE	UNP Q9UHN1
A	13	ARG	-	CLONING ARTIFACT	UNP Q9UHN1
A	14	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
A	15	SER	-	CLONING ARTIFACT	UNP Q9UHN1
A	16	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	17	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	18	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	19	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	20	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	21	HIS	-	EXPRESSION TAG	UNP Q9UHN1
A	22	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
A	23	SER	-	CLONING ARTIFACT	UNP Q9UHN1
A	24	THR	-	CLONING ARTIFACT	UNP Q9UHN1
A	25	MET	-	CLONING ARTIFACT	UNP Q9UHN1
A	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1
B	12	MET	-	INITIATING METHIONINE	UNP Q9UHN1
B	13	ARG	-	CLONING ARTIFACT	UNP Q9UHN1
B	14	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
B	15	SER	-	CLONING ARTIFACT	UNP Q9UHN1
B	16	HIS	-	EXPRESSION TAG	UNP Q9UHN1
B	17	HIS	-	EXPRESSION TAG	UNP Q9UHN1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	18	HIS	-	EXPRESSION TAG	UNP Q9UHN1
B	19	HIS	-	EXPRESSION TAG	UNP Q9UHN1
B	20	HIS	-	EXPRESSION TAG	UNP Q9UHN1
B	21	HIS	-	EXPRESSION TAG	UNP Q9UHN1
B	22	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
B	23	SER	-	CLONING ARTIFACT	UNP Q9UHN1
B	24	THR	-	CLONING ARTIFACT	UNP Q9UHN1
B	25	MET	-	CLONING ARTIFACT	UNP Q9UHN1
B	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1
C	12	MET	-	INITIATING METHIONINE	UNP Q9UHN1
C	13	ARG	-	CLONING ARTIFACT	UNP Q9UHN1
C	14	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
C	15	SER	-	CLONING ARTIFACT	UNP Q9UHN1
C	16	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	17	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	18	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	19	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	20	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	21	HIS	-	EXPRESSION TAG	UNP Q9UHN1
C	22	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
C	23	SER	-	CLONING ARTIFACT	UNP Q9UHN1
C	24	THR	-	CLONING ARTIFACT	UNP Q9UHN1
C	25	MET	-	CLONING ARTIFACT	UNP Q9UHN1
C	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1
D	12	MET	-	INITIATING METHIONINE	UNP Q9UHN1
D	13	ARG	-	CLONING ARTIFACT	UNP Q9UHN1
D	14	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
D	15	SER	-	CLONING ARTIFACT	UNP Q9UHN1
D	16	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	17	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	18	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	19	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	20	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	21	HIS	-	EXPRESSION TAG	UNP Q9UHN1
D	22	GLY	-	CLONING ARTIFACT	UNP Q9UHN1
D	23	SER	-	CLONING ARTIFACT	UNP Q9UHN1
D	24	THR	-	CLONING ARTIFACT	UNP Q9UHN1
D	25	MET	-	CLONING ARTIFACT	UNP Q9UHN1
D	169	THR	ALA	SEE REMARK 999	UNP Q9UHN1

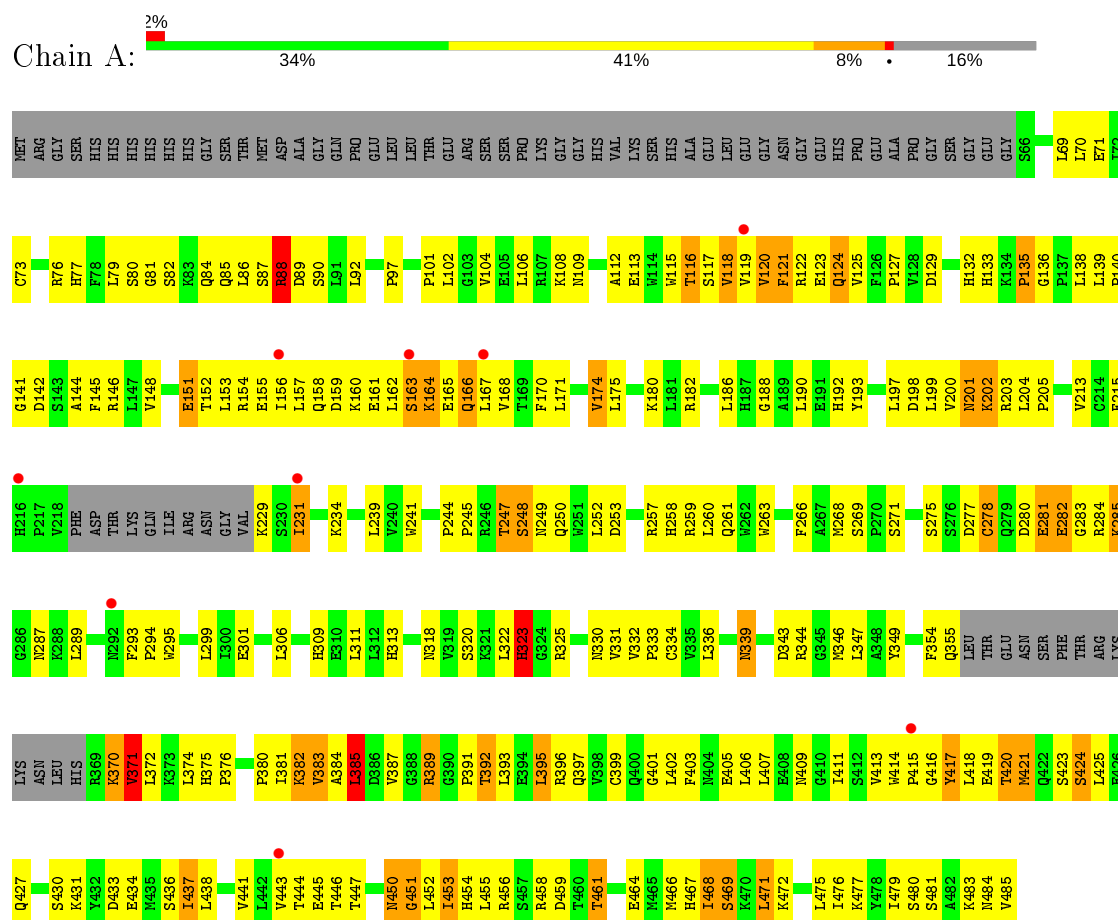
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total 12	O 12	0	0
2	B	5	Total 5	O 5	0	0
2	C	5	Total 5	O 5	0	0
2	D	9	Total 9	O 9	0	0

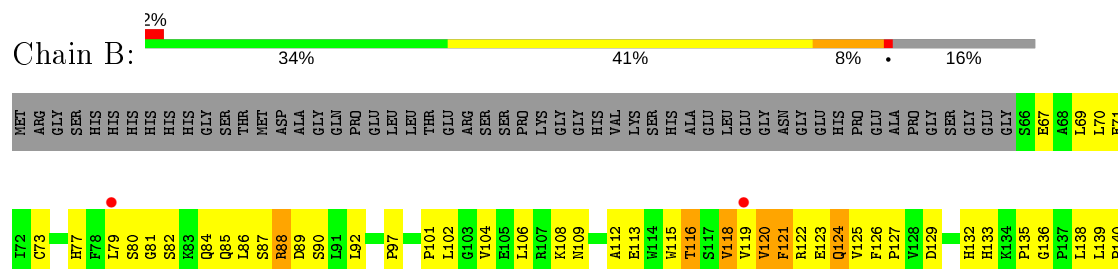
### 3 Residue-property plots

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

#### • Molecule 1: DNA polymerase gamma subunit 2



#### • Molecule 1: DNA polymerase gamma subunit 2









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.79Å 101.79Å 170.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.15 48.76 – 3.17	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.15) 95.9 (48.76-3.17)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.285 0.222 , 0.273	Depositor DCC
$R_{free}$ test set	1667 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	91.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 75.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l 0.054 for h,-h-k,-l 0.054 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12847	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.37% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.39	0/3278	0.74	3/4432 (0.1%)
1	B	0.39	0/3278	0.74	3/4432 (0.1%)
1	C	0.39	0/3283	0.66	1/4439 (0.0%)
1	D	0.39	0/3283	0.66	1/4439 (0.0%)
All	All	0.39	0/13122	0.70	8/17742 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	ARG	NE-CZ-NH1	-13.41	113.59	120.30
1	B	88	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	A	88	ARG	NE-CZ-NH2	13.12	126.86	120.30
1	B	88	ARG	NE-CZ-NH1	13.01	126.80	120.30
1	B	88	ARG	CD-NE-CZ	6.97	133.35	123.60
1	A	88	ARG	CD-NE-CZ	6.72	133.01	123.60
1	C	283	GLY	N-CA-C	-5.82	98.56	113.10
1	D	283	GLY	N-CA-C	-5.71	98.83	113.10

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	3202	0	3209	276	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3202	0	3209	267	0
1	C	3206	0	3211	289	0
1	D	3206	0	3211	277	0
2	A	12	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	9	0	0	0	0
All	All	12847	0	12840	1063	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 41.

All (1063) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:ASN:HD22	1:B:452:LEU:HD23	1.11	1.08
1:A:450:ASN:HD22	1:A:452:LEU:HD23	1.11	1.07
1:A:88:ARG:HD2	1:A:88:ARG:H	1.24	0.98
1:D:306:LEU:HB2	1:D:335:VAL:HG23	1.46	0.98
1:C:306:LEU:HB2	1:C:335:VAL:HG23	1.43	0.95
1:C:73:CYS:HB3	1:C:79:LEU:HD23	1.48	0.94
1:D:73:CYS:HB3	1:D:79:LEU:HD23	1.49	0.94
1:A:158:GLN:HG2	1:A:159:ASP:H	1.37	0.89
1:C:260:LEU:HD13	1:C:289:LEU:HD22	1.56	0.87
1:D:260:LEU:HD13	1:D:289:LEU:HD22	1.55	0.87
1:C:96:HIS:HB2	1:C:97:PRO:HD2	1.56	0.87
1:B:158:GLN:HG2	1:B:159:ASP:H	1.38	0.86
1:A:87:SER:HB2	1:A:90:SER:HB2	1.57	0.86
1:B:87:SER:HB2	1:B:90:SER:HB2	1.56	0.86
1:B:257:ARG:O	1:B:261:GLN:HG3	1.73	0.86
1:B:257:ARG:HB3	1:C:316:PRO:HG3	1.58	0.85
1:D:385:LEU:HB3	1:D:441:VAL:HG22	1.58	0.85
1:B:231:ILE:HD12	1:B:231:ILE:H	1.40	0.85
1:A:231:ILE:HD12	1:A:231:ILE:H	1.39	0.85
1:D:96:HIS:HB2	1:D:97:PRO:HD2	1.56	0.84
1:A:257:ARG:O	1:A:261:GLN:HG3	1.76	0.84
1:C:385:LEU:HB3	1:C:441:VAL:HG22	1.60	0.84
1:A:88:ARG:H	1:A:88:ARG:CD	1.91	0.84
1:C:77:HIS:O	1:C:102:LEU:HB2	1.78	0.83
1:B:450:ASN:HD22	1:B:452:LEU:CD2	1.91	0.83
1:A:201:ASN:HD22	1:A:203:ARG:HH22	1.23	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ASN:HD22	1:B:203:ARG:HH22	1.23	0.82
1:B:401:GLY:O	1:B:405:GLU:HB2	1.80	0.82
1:A:450:ASN:HD22	1:A:452:LEU:CD2	1.91	0.82
1:C:154:ARG:HH22	1:C:158:GLN:NE2	1.77	0.82
1:D:153:LEU:HD12	1:D:170:PHE:HE2	1.45	0.82
1:C:153:LEU:HD12	1:C:170:PHE:HE2	1.44	0.81
1:A:231:ILE:HD13	1:C:133:HIS:NE2	1.95	0.81
1:A:401:GLY:O	1:A:405:GLU:HB2	1.81	0.81
1:B:437:ILE:HG22	1:B:438:LEU:H	1.45	0.81
1:D:253:ASP:O	1:D:257:ARG:HG2	1.81	0.81
1:C:253:ASP:O	1:C:257:ARG:HG2	1.81	0.81
1:D:154:ARG:HH22	1:D:158:GLN:NE2	1.77	0.81
1:A:450:ASN:ND2	1:A:452:LEU:HD23	1.95	0.80
1:D:77:HIS:O	1:D:102:LEU:HB2	1.80	0.80
1:A:393:LEU:O	1:A:397:GLN:HG2	1.81	0.80
1:B:231:ILE:HD13	1:D:133:HIS:NE2	1.97	0.80
1:A:437:ILE:HG22	1:A:438:LEU:H	1.46	0.79
1:B:161:GLU:HG2	1:B:166:GLN:HG3	1.64	0.79
1:B:393:LEU:O	1:B:397:GLN:HG2	1.82	0.79
1:A:385:LEU:HD23	1:A:385:LEU:O	1.80	0.79
1:C:383:VAL:HG13	1:C:413:VAL:HG22	1.65	0.79
1:B:450:ASN:ND2	1:B:452:LEU:HD23	1.95	0.78
1:B:385:LEU:O	1:B:385:LEU:HD23	1.81	0.78
1:D:254:PHE:O	1:D:257:ARG:HG3	1.82	0.78
1:D:260:LEU:HD22	1:D:275:SER:HB3	1.66	0.78
1:A:161:GLU:HG2	1:A:166:GLN:HG3	1.64	0.78
1:C:254:PHE:O	1:C:257:ARG:HG3	1.83	0.77
1:C:260:LEU:HD22	1:C:275:SER:HB3	1.66	0.77
1:A:389:ARG:H	1:A:389:ARG:HD2	1.50	0.77
1:A:113:GLU:HG2	1:A:266:PHE:CZ	2.20	0.77
1:D:383:VAL:HG13	1:D:413:VAL:HG22	1.67	0.77
1:A:201:ASN:HD22	1:A:203:ARG:NH2	1.82	0.76
1:B:201:ASN:HD22	1:B:203:ARG:NH2	1.82	0.76
1:B:113:GLU:HG2	1:B:266:PHE:CZ	2.20	0.76
1:B:73:CYS:HB3	1:B:79:LEU:HD23	1.68	0.75
1:D:279:GLN:HB2	1:D:284:ARG:HG3	1.68	0.75
1:C:153:LEU:HD12	1:C:170:PHE:CE2	2.21	0.75
1:A:466:MET:HE1	1:A:471:LEU:HD13	1.69	0.75
1:C:279:GLN:HB2	1:C:284:ARG:HG3	1.68	0.75
1:B:455:LEU:HD23	1:B:455:LEU:H	1.52	0.75
1:A:73:CYS:HB3	1:A:79:LEU:HD23	1.68	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ARG:HD2	1:B:389:ARG:H	1.51	0.75
1:D:153:LEU:HD12	1:D:170:PHE:CE2	2.21	0.75
1:A:231:ILE:HD12	1:A:231:ILE:N	2.02	0.74
1:B:466:MET:HE1	1:B:471:LEU:HD13	1.70	0.74
1:B:254:PHE:CE1	1:C:316:PRO:HB3	2.23	0.74
1:A:455:LEU:HD23	1:A:455:LEU:H	1.53	0.73
1:A:129:ASP:HB2	1:C:104:VAL:HG22	1.71	0.73
1:B:231:ILE:HD12	1:B:231:ILE:N	2.03	0.73
1:B:441:VAL:HG11	1:B:471:LEU:HD21	1.71	0.73
1:D:204:LEU:HD21	1:D:324:GLY:HA3	1.72	0.72
1:B:437:ILE:HG22	1:B:438:LEU:N	2.05	0.72
1:A:139:LEU:HB2	1:A:140:PRO:HD2	1.71	0.72
1:B:200:VAL:O	1:B:202:LYS:N	2.23	0.72
1:B:280:ASP:HA	1:B:283:GLY:O	1.90	0.72
1:C:88:ARG:HD2	1:C:89:ASP:H	1.54	0.72
1:A:437:ILE:HG22	1:A:438:LEU:N	2.05	0.72
1:B:229:LYS:HB2	1:B:229:LYS:HZ2	1.55	0.71
1:A:441:VAL:HG11	1:A:471:LEU:HD21	1.72	0.71
1:B:323:HIS:HB2	1:B:331:VAL:C	2.11	0.71
1:D:76:ARG:NH2	1:D:431:LYS:HG3	2.05	0.71
1:D:254:PHE:HA	1:D:257:ARG:HD2	1.72	0.71
1:A:201:ASN:O	1:A:202:LYS:HB2	1.90	0.71
1:B:139:LEU:HB2	1:B:140:PRO:HD2	1.71	0.71
1:D:395:LEU:HD21	1:D:444:THR:HA	1.73	0.71
1:A:323:HIS:HB2	1:A:331:VAL:C	2.11	0.71
1:B:129:ASP:HB2	1:D:104:VAL:HG22	1.72	0.71
1:D:88:ARG:HD2	1:D:89:ASP:H	1.54	0.71
1:C:306:LEU:HB2	1:C:335:VAL:CG2	2.21	0.71
1:B:201:ASN:O	1:B:202:LYS:HB2	1.89	0.70
1:A:280:ASP:HA	1:A:283:GLY:O	1.91	0.70
1:C:395:LEU:HD21	1:C:444:THR:HA	1.72	0.70
1:C:76:ARG:NH2	1:C:431:LYS:HG3	2.06	0.70
1:D:76:ARG:HH21	1:D:431:LYS:HG3	1.56	0.70
1:B:204:LEU:HD13	1:B:333:PRO:HB3	1.72	0.70
1:C:204:LEU:HD21	1:C:324:GLY:HA3	1.74	0.70
1:C:146:ARG:HG2	1:C:146:ARG:HH11	1.57	0.69
1:A:186:LEU:HD11	1:A:306:LEU:HD11	1.75	0.69
1:B:409:ASN:ND2	1:B:472:LYS:HD2	2.07	0.69
1:A:200:VAL:O	1:A:202:LYS:N	2.24	0.69
1:A:174:VAL:HG12	1:A:175:LEU:N	2.09	0.68
1:D:260:LEU:HD13	1:D:289:LEU:CD2	2.23	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:LEU:HB2	1:D:335:VAL:CG2	2.23	0.68
1:D:451:GLY:C	1:D:452:LEU:HD22	2.14	0.68
1:A:284:ARG:O	1:A:285:LYS:HB2	1.92	0.68
1:B:277:ASP:O	1:B:278:CYS:HB3	1.93	0.68
1:B:186:LEU:HD11	1:B:306:LEU:HD11	1.76	0.68
1:C:254:PHE:HA	1:C:257:ARG:HD2	1.73	0.68
1:B:284:ARG:O	1:B:285:LYS:HB2	1.92	0.68
1:A:409:ASN:ND2	1:A:472:LYS:HD2	2.09	0.68
1:B:174:VAL:HG12	1:B:175:LEU:N	2.09	0.68
1:C:199:LEU:O	1:C:200:VAL:HG13	1.93	0.67
1:C:451:GLY:C	1:C:452:LEU:HD22	2.14	0.67
1:A:471:LEU:HD12	1:A:471:LEU:O	1.93	0.67
1:C:76:ARG:HG3	1:C:434:GLU:HB3	1.76	0.67
1:D:307:GLY:HA2	1:D:334:CYS:SG	2.34	0.67
1:C:76:ARG:HH21	1:C:431:LYS:HG3	1.59	0.67
1:D:281:GLU:HG2	1:D:282:GLU:H	1.60	0.67
1:D:69:LEU:HB2	1:D:354:PHE:CD2	2.30	0.67
1:A:204:LEU:HD13	1:A:333:PRO:HB3	1.74	0.67
1:B:471:LEU:O	1:B:471:LEU:HD12	1.94	0.67
1:B:81:GLY:HA3	1:B:97:PRO:HG3	1.77	0.67
1:C:260:LEU:HD13	1:C:289:LEU:CD2	2.25	0.67
1:C:69:LEU:HB2	1:C:354:PHE:CD2	2.29	0.67
1:D:146:ARG:HG2	1:D:146:ARG:HH11	1.60	0.67
1:A:277:ASP:O	1:A:278:CYS:HB3	1.94	0.66
1:B:372:LEU:HD13	1:B:434:GLU:O	1.95	0.66
1:D:202:LYS:O	1:D:325:ARG:N	2.27	0.66
1:A:82:SER:HB2	1:A:85:GLN:HG2	1.76	0.66
1:B:453:ILE:HG12	1:B:468:ILE:HB	1.78	0.66
1:D:370:LYS:O	1:D:371:VAL:HG12	1.95	0.66
1:D:456:ARG:HG2	1:D:457:SER:H	1.61	0.66
1:A:81:GLY:HA3	1:A:97:PRO:HG3	1.78	0.66
1:C:154:ARG:HH22	1:C:158:GLN:HE21	1.42	0.66
1:C:281:GLU:HG2	1:C:282:GLU:H	1.59	0.66
1:D:147:LEU:HD21	1:D:181:LEU:HD21	1.75	0.66
1:C:370:LYS:O	1:C:371:VAL:HG12	1.96	0.66
1:C:456:ARG:HG2	1:C:457:SER:H	1.60	0.65
1:B:145:PHE:HD1	1:D:149:SER:HA	1.61	0.65
1:B:371:VAL:HG23	1:B:433:ASP:HB3	1.78	0.65
1:D:154:ARG:HH22	1:D:158:GLN:HE21	1.42	0.65
1:A:157:LEU:HD21	1:C:171:LEU:HB3	1.79	0.65
1:D:76:ARG:HG3	1:D:434:GLU:HB3	1.78	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:SER:HB2	1:B:85:GLN:HG2	1.77	0.65
1:C:307:GLY:HA2	1:C:334:CYS:SG	2.37	0.65
1:B:323:HIS:HB3	1:B:332:VAL:HA	1.78	0.65
1:B:157:LEU:HD21	1:D:171:LEU:HB3	1.79	0.65
1:C:202:LYS:O	1:C:325:ARG:N	2.26	0.65
1:A:293:PHE:O	1:A:295:TRP:N	2.30	0.64
1:C:147:LEU:HD21	1:C:181:LEU:HD21	1.77	0.64
1:B:293:PHE:O	1:B:295:TRP:N	2.30	0.64
1:A:371:VAL:HG23	1:A:433:ASP:HB3	1.79	0.64
1:A:323:HIS:HB3	1:A:332:VAL:HA	1.79	0.64
1:C:455:LEU:HD12	1:C:455:LEU:C	2.18	0.64
1:D:256:LEU:HD22	1:D:287:ASN:CG	2.18	0.64
1:A:145:PHE:HD1	1:C:149:SER:HA	1.62	0.64
1:C:308:ASP:HB2	1:C:312:LEU:HD12	1.81	0.63
1:D:104:VAL:O	1:D:108:LYS:HB2	1.98	0.63
1:D:455:LEU:HD12	1:D:455:LEU:C	2.18	0.63
1:C:256:LEU:HD22	1:C:287:ASN:CG	2.19	0.63
1:D:199:LEU:O	1:D:200:VAL:HG13	1.98	0.63
1:D:116:THR:HA	1:D:120:VAL:HG23	1.80	0.63
1:B:163:SER:O	1:B:164:LYS:HG3	1.99	0.63
1:D:202:LYS:HD2	1:D:202:LYS:N	2.14	0.63
1:A:266:PHE:HA	1:A:375:HIS:HD2	1.62	0.62
1:A:163:SER:O	1:A:164:LYS:HG3	1.98	0.62
1:A:453:ILE:HG12	1:A:468:ILE:HB	1.81	0.62
1:A:133:HIS:CD2	1:C:231:ILE:HD12	2.33	0.62
1:A:372:LEU:HD13	1:A:434:GLU:O	1.99	0.62
1:C:116:THR:HA	1:C:120:VAL:HG23	1.81	0.62
1:C:243:THR:HB	1:C:244:PRO:HD2	1.81	0.62
1:D:385:LEU:CB	1:D:441:VAL:HG22	2.29	0.62
1:A:385:LEU:HB2	1:A:441:VAL:CG2	2.30	0.62
1:D:308:ASP:HB2	1:D:312:LEU:HD12	1.81	0.62
1:B:266:PHE:HA	1:B:375:HIS:HD2	1.65	0.62
1:C:231:ILE:CG2	1:C:232:GLY:N	2.63	0.62
1:A:375:HIS:ND1	1:A:376:PRO:HD2	2.14	0.62
1:C:202:LYS:HD2	1:C:202:LYS:N	2.14	0.62
1:C:427:GLN:O	1:C:431:LYS:HE3	2.00	0.62
1:A:395:LEU:HD11	1:A:443:VAL:O	2.00	0.62
1:D:331:VAL:HG22	1:D:332:VAL:N	2.15	0.62
1:A:284:ARG:O	1:A:285:LYS:CB	2.48	0.62
1:D:331:VAL:HG22	1:D:332:VAL:H	1.66	0.61
1:B:385:LEU:HA	1:B:441:VAL:O	1.99	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:PHE:HE1	1:B:415:PRO:HD3	1.65	0.61
1:B:395:LEU:HD11	1:B:443:VAL:O	2.00	0.61
1:B:344:ARG:HA	1:B:347:LEU:HD12	1.80	0.61
1:D:113:GLU:HG2	1:D:266:PHE:CZ	2.36	0.61
1:A:417:TYR:CD1	1:A:418:LEU:HG	2.35	0.61
1:C:307:GLY:O	1:C:335:VAL:HG22	2.01	0.61
1:D:372:LEU:HD22	1:D:434:GLU:O	2.00	0.61
1:D:88:ARG:CD	1:D:89:ASP:H	2.14	0.61
1:A:344:ARG:HA	1:A:347:LEU:HD12	1.81	0.61
1:C:372:LEU:HD22	1:C:434:GLU:O	2.01	0.61
1:A:129:ASP:HB2	1:C:104:VAL:CG2	2.31	0.60
1:B:284:ARG:O	1:B:285:LYS:CB	2.48	0.60
1:B:323:HIS:HB2	1:B:331:VAL:O	2.00	0.60
1:C:385:LEU:CB	1:C:441:VAL:HG22	2.29	0.60
1:B:385:LEU:HB2	1:B:441:VAL:CG2	2.32	0.60
1:A:430:SER:O	1:A:433:ASP:HB2	2.01	0.60
1:C:113:GLU:HG2	1:C:266:PHE:CZ	2.36	0.60
1:C:303:LEU:HG	1:C:338:VAL:HG13	1.83	0.60
1:D:150:ALA:O	1:D:154:ARG:HB2	2.02	0.60
1:B:229:LYS:HZ2	1:B:229:LYS:CB	2.14	0.60
1:A:174:VAL:HG11	1:C:153:LEU:HD21	1.84	0.60
1:B:451:GLY:C	1:B:452:LEU:HD22	2.22	0.60
1:B:466:MET:CE	1:B:471:LEU:HD22	2.32	0.60
1:C:88:ARG:CD	1:C:89:ASP:H	2.14	0.60
1:B:133:HIS:CD2	1:D:231:ILE:HD12	2.36	0.60
1:D:427:GLN:O	1:D:431:LYS:HE3	2.01	0.60
1:A:420:THR:HG23	1:A:421:MET:H	1.67	0.60
1:A:445:GLU:C	1:A:447:THR:H	2.05	0.60
1:B:417:TYR:CD1	1:B:418:LEU:HG	2.36	0.60
1:C:104:VAL:O	1:C:108:LYS:HB2	2.00	0.60
1:A:385:LEU:HA	1:A:441:VAL:O	2.01	0.60
1:C:135:PRO:O	1:C:138:LEU:HD21	2.02	0.60
1:C:155:GLU:O	1:C:156:ILE:HG13	2.02	0.60
1:D:307:GLY:O	1:D:335:VAL:HG22	2.01	0.60
1:A:266:PHE:HA	1:A:375:HIS:CD2	2.37	0.59
1:C:456:ARG:CG	1:C:457:SER:H	2.15	0.59
1:A:466:MET:CE	1:A:471:LEU:HD22	2.32	0.59
1:B:129:ASP:HB2	1:D:104:VAL:CG2	2.32	0.59
1:A:420:THR:HG23	1:A:421:MET:N	2.17	0.59
1:C:445:GLU:C	1:C:447:THR:H	2.05	0.59
1:D:467:HIS:C	1:D:469:SER:H	2.05	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:THR:HG22	1:A:393:LEU:N	2.16	0.59
1:B:420:THR:HG23	1:B:421:MET:H	1.67	0.59
1:C:383:VAL:CG1	1:C:413:VAL:HG22	2.32	0.59
1:D:243:THR:HB	1:D:244:PRO:HD2	1.83	0.59
1:D:456:ARG:CG	1:D:457:SER:H	2.15	0.59
1:B:392:THR:HG22	1:B:393:LEU:N	2.16	0.59
1:C:331:VAL:HG22	1:C:332:VAL:N	2.16	0.59
1:C:331:VAL:HG22	1:C:332:VAL:H	1.67	0.59
1:C:150:ALA:O	1:C:154:ARG:HB2	2.02	0.59
1:D:204:LEU:HD13	1:D:333:PRO:HB3	1.85	0.59
1:D:303:LEU:HG	1:D:338:VAL:HG13	1.85	0.59
1:B:430:SER:O	1:B:433:ASP:HB2	2.02	0.59
1:B:445:GLU:C	1:B:447:THR:H	2.05	0.59
1:C:96:HIS:HB2	1:C:97:PRO:CD	2.30	0.59
1:A:451:GLY:C	1:A:452:LEU:HD22	2.22	0.58
1:B:266:PHE:HA	1:B:375:HIS:CD2	2.38	0.58
1:C:275:SER:O	1:C:276:SER:HB3	2.02	0.58
1:C:467:HIS:C	1:C:469:SER:H	2.05	0.58
1:B:375:HIS:ND1	1:B:376:PRO:HD2	2.17	0.58
1:D:135:PRO:O	1:D:138:LEU:HD21	2.04	0.58
1:D:254:PHE:HA	1:D:257:ARG:CD	2.32	0.58
1:B:293:PHE:C	1:B:295:TRP:H	2.06	0.58
1:C:479:ILE:C	1:C:481:SER:H	2.06	0.58
1:D:479:ILE:C	1:D:481:SER:H	2.06	0.58
1:B:420:THR:HG23	1:B:421:MET:N	2.17	0.58
1:B:371:VAL:HG23	1:B:433:ASP:CB	2.34	0.58
1:D:445:GLU:C	1:D:447:THR:H	2.05	0.58
1:B:165:GLU:HA	1:B:165:GLU:OE1	2.03	0.58
1:A:293:PHE:C	1:A:295:TRP:H	2.06	0.58
1:A:395:LEU:HD21	1:A:444:THR:C	2.24	0.58
1:D:155:GLU:O	1:D:156:ILE:HG13	2.02	0.58
1:D:471:LEU:O	1:D:475:LEU:HG	2.04	0.58
1:A:152:THR:O	1:A:156:ILE:HG13	2.04	0.58
1:B:370:LYS:O	1:B:371:VAL:HG12	2.04	0.58
1:C:204:LEU:HD13	1:C:333:PRO:HB3	1.86	0.58
1:D:231:ILE:CG2	1:D:232:GLY:N	2.67	0.58
1:D:275:SER:O	1:D:276:SER:HB3	2.03	0.58
1:C:231:ILE:HG22	1:C:232:GLY:N	2.16	0.58
1:C:106:LEU:HD23	1:C:346:MET:SD	2.44	0.58
1:B:452:LEU:CD1	1:B:467:HIS:HA	2.34	0.58
1:C:254:PHE:HA	1:C:257:ARG:CD	2.33	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ARG:NH1	1:A:330:ASN:HD21	2.02	0.58
1:A:403:PHE:HE1	1:A:415:PRO:HD3	1.67	0.58
1:C:471:LEU:O	1:C:475:LEU:HG	2.04	0.58
1:D:146:ARG:HB3	1:D:178:SER:OG	2.03	0.58
1:A:452:LEU:CD1	1:A:467:HIS:HA	2.34	0.57
1:C:116:THR:HA	1:C:120:VAL:CG2	2.34	0.57
1:C:284:ARG:O	1:C:285:LYS:HB2	2.04	0.57
1:B:260:LEU:HD13	1:B:289:LEU:HD12	1.86	0.57
1:C:371:VAL:HG23	1:C:433:ASP:HB3	1.86	0.57
1:D:82:SER:C	1:D:84:GLN:H	2.07	0.57
1:A:162:LEU:C	1:A:164:LYS:H	2.07	0.57
1:A:323:HIS:HB2	1:A:331:VAL:O	2.03	0.57
1:C:121:PHE:O	1:C:122:ARG:C	2.42	0.57
1:D:462:MET:O	1:D:463:LYS:HG3	2.04	0.57
1:B:269:SER:C	1:B:271:SER:H	2.07	0.57
1:A:371:VAL:HG23	1:A:433:ASP:CB	2.35	0.57
1:B:152:THR:O	1:B:156:ILE:HG13	2.04	0.57
1:B:467:HIS:O	1:B:469:SER:N	2.38	0.57
1:C:385:LEU:O	1:C:385:LEU:HD12	2.04	0.57
1:C:462:MET:O	1:C:463:LYS:HG3	2.05	0.57
1:A:165:GLU:HA	1:A:165:GLU:OE1	2.04	0.57
1:A:403:PHE:O	1:A:407:LEU:HG	2.04	0.57
1:B:257:ARG:HG3	1:B:257:ARG:HH21	1.70	0.57
1:B:385:LEU:HB2	1:B:441:VAL:HG23	1.86	0.57
1:D:121:PHE:O	1:D:122:ARG:C	2.43	0.57
1:D:284:ARG:O	1:D:285:LYS:HB2	2.05	0.57
1:D:371:VAL:HG23	1:D:433:ASP:HB3	1.86	0.57
1:A:452:LEU:HD13	1:A:467:HIS:HA	1.86	0.57
1:B:372:LEU:HB2	1:B:436:SER:HB2	1.86	0.57
1:B:453:ILE:CG1	1:B:468:ILE:HB	2.34	0.57
1:D:447:THR:HG21	1:D:453:ILE:CG2	2.35	0.57
1:B:325:ARG:NH1	1:B:330:ASN:HD21	2.02	0.57
1:A:186:LEU:HD23	1:A:190:LEU:HG	1.87	0.57
1:B:395:LEU:HD21	1:B:444:THR:C	2.25	0.57
1:D:167:LEU:O	1:D:168:VAL:HB	2.05	0.57
1:A:370:LYS:O	1:A:371:VAL:HG12	2.05	0.56
1:C:190:LEU:C	1:C:192:HIS:H	2.08	0.56
1:C:422:GLN:HG3	1:C:423:SER:N	2.20	0.56
1:D:116:THR:HA	1:D:120:VAL:CG2	2.34	0.56
1:A:148:VAL:HG21	1:C:148:VAL:HG21	1.87	0.56
1:A:281:GLU:O	1:A:282:GLU:HG3	2.04	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:CYS:SG	1:D:350:LEU:HD22	2.46	0.56
1:D:383:VAL:CG1	1:D:413:VAL:HG22	2.34	0.56
1:D:422:GLN:HG3	1:D:423:SER:N	2.20	0.56
1:C:441:VAL:HG11	1:C:471:LEU:HD21	1.88	0.56
1:B:77:HIS:CD2	1:D:199:LEU:HD22	2.41	0.56
1:D:385:LEU:O	1:D:385:LEU:HD12	2.05	0.56
1:A:421:MET:HG3	1:A:423:SER:H	1.70	0.56
1:A:403:PHE:HZ	1:C:123:GLU:HG2	1.69	0.56
1:C:82:SER:C	1:C:84:GLN:H	2.07	0.56
1:D:106:LEU:HD23	1:D:346:MET:SD	2.45	0.56
1:B:403:PHE:HZ	1:D:123:GLU:HG2	1.69	0.56
1:A:257:ARG:HG3	1:A:257:ARG:HH21	1.71	0.56
1:B:323:HIS:HB3	1:B:332:VAL:CA	2.35	0.56
1:C:151:GLU:OE1	1:C:151:GLU:N	2.38	0.56
1:C:212:GLY:O	1:C:236:GLU:N	2.34	0.56
1:C:447:THR:HG21	1:C:453:ILE:CG2	2.35	0.56
1:D:151:GLU:OE1	1:D:151:GLU:N	2.38	0.56
1:D:455:LEU:HD12	1:D:455:LEU:O	2.06	0.56
1:A:413:VAL:HG12	1:A:414:TRP:N	2.21	0.56
1:B:162:LEU:C	1:B:164:LYS:H	2.08	0.56
1:B:413:VAL:HG12	1:B:414:TRP:N	2.20	0.56
1:B:403:PHE:O	1:B:407:LEU:HG	2.06	0.56
1:D:190:LEU:C	1:D:192:HIS:H	2.07	0.56
1:D:423:SER:O	1:D:424:SER:HB3	2.06	0.56
1:A:467:HIS:O	1:A:469:SER:N	2.38	0.56
1:C:281:GLU:HG2	1:C:282:GLU:N	2.20	0.56
1:C:455:LEU:HD12	1:C:455:LEU:O	2.05	0.56
1:A:158:GLN:HG2	1:A:159:ASP:N	2.16	0.56
1:A:399:CYS:HB3	1:A:417:TYR:CD2	2.41	0.56
1:A:385:LEU:HB2	1:A:441:VAL:HG23	1.86	0.56
1:B:186:LEU:HD23	1:B:190:LEU:HG	1.88	0.56
1:B:259:ARG:HE	1:B:301:GLU:CD	2.08	0.56
1:C:420:THR:HG23	1:C:421:MET:N	2.21	0.56
1:C:427:GLN:O	1:C:431:LYS:HB2	2.06	0.56
1:A:471:LEU:HD12	1:A:475:LEU:HG	1.88	0.56
1:C:214:CYS:HB2	1:C:216:HIS:HE1	1.71	0.56
1:C:76:ARG:HG3	1:C:434:GLU:CB	2.36	0.56
1:A:323:HIS:HB3	1:A:332:VAL:CA	2.35	0.55
1:B:162:LEU:O	1:B:164:LYS:N	2.37	0.55
1:B:260:LEU:HD13	1:B:289:LEU:CD1	2.36	0.55
1:C:167:LEU:O	1:C:168:VAL:HB	2.05	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:GLU:HG2	1:D:282:GLU:N	2.20	0.55
1:D:82:SER:O	1:D:84:GLN:N	2.37	0.55
1:A:77:HIS:CD2	1:C:199:LEU:HD22	2.41	0.55
1:B:452:LEU:HD13	1:B:467:HIS:HA	1.87	0.55
1:B:455:LEU:CD2	1:B:455:LEU:H	2.19	0.55
1:D:420:THR:HG23	1:D:421:MET:N	2.21	0.55
1:D:73:CYS:CB	1:D:79:LEU:HD23	2.31	0.55
1:A:156:ILE:HG23	1:A:167:LEU:HD11	1.88	0.55
1:A:480:SER:O	1:A:483:LYS:HB3	2.07	0.55
1:D:152:THR:HG22	1:D:170:PHE:HE1	1.70	0.55
1:D:214:CYS:HB2	1:D:216:HIS:HE1	1.71	0.55
1:A:434:GLU:C	1:A:436:SER:H	2.09	0.55
1:A:453:ILE:CG1	1:A:468:ILE:HB	2.35	0.55
1:C:119:VAL:O	1:C:121:PHE:N	2.40	0.55
1:D:422:GLN:HG3	1:D:423:SER:H	1.71	0.55
1:D:427:GLN:O	1:D:431:LYS:HB2	2.05	0.55
1:C:423:SER:O	1:C:424:SER:HB3	2.06	0.55
1:D:231:ILE:HG22	1:D:232:GLY:N	2.21	0.55
1:D:441:VAL:HG11	1:D:471:LEU:HD21	1.88	0.55
1:B:399:CYS:HB3	1:B:417:TYR:CD2	2.41	0.55
1:C:384:ALA:O	1:C:385:LEU:HB3	2.07	0.55
1:A:138:LEU:HD21	1:A:180:LYS:HD3	1.87	0.55
1:A:259:ARG:HE	1:A:301:GLU:CD	2.10	0.55
1:C:152:THR:HG22	1:C:170:PHE:HE1	1.70	0.55
1:A:372:LEU:HB2	1:A:436:SER:HB2	1.87	0.55
1:B:434:GLU:C	1:B:436:SER:H	2.10	0.55
1:B:281:GLU:O	1:B:282:GLU:HG3	2.06	0.55
1:B:421:MET:HG3	1:B:423:SER:H	1.71	0.55
1:B:471:LEU:HD12	1:B:475:LEU:HG	1.87	0.55
1:C:346:MET:O	1:C:350:LEU:HD12	2.06	0.55
1:B:162:LEU:HD22	1:B:166:GLN:HG2	1.89	0.55
1:D:119:VAL:O	1:D:121:PHE:N	2.39	0.55
1:A:162:LEU:HD22	1:A:166:GLN:HG2	1.89	0.54
1:B:403:PHE:CE1	1:B:415:PRO:HD3	2.42	0.54
1:C:422:GLN:HG3	1:C:423:SER:H	1.70	0.54
1:A:260:LEU:HD13	1:A:289:LEU:HD12	1.89	0.54
1:A:447:THR:HG23	1:A:452:LEU:O	2.07	0.54
1:B:383:VAL:HG22	1:B:384:ALA:O	2.08	0.54
1:C:149:SER:O	1:C:153:LEU:HB2	2.07	0.54
1:D:472:LYS:HD3	1:D:473:ASP:N	2.23	0.54
1:A:186:LEU:O	1:A:186:LEU:HD23	2.06	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:THR:HG23	1:B:452:LEU:O	2.08	0.54
1:C:76:ARG:HD2	1:C:435:MET:HG3	1.90	0.54
1:A:455:LEU:CD2	1:A:455:LEU:H	2.20	0.54
1:A:198:ASP:O	1:A:200:VAL:N	2.41	0.54
1:A:269:SER:C	1:A:271:SER:H	2.09	0.54
1:A:383:VAL:HG22	1:A:384:ALA:O	2.08	0.54
1:B:116:THR:HA	1:B:120:VAL:CG2	2.38	0.54
1:B:252:LEU:HD11	1:B:287:ASN:HD21	1.73	0.54
1:C:146:ARG:HB3	1:C:178:SER:OG	2.07	0.54
1:D:149:SER:O	1:D:153:LEU:HB2	2.07	0.54
1:D:76:ARG:HG3	1:D:434:GLU:CB	2.37	0.54
1:B:148:VAL:HG21	1:D:148:VAL:HG21	1.90	0.54
1:C:182:ARG:HH11	1:C:182:ARG:HG2	1.72	0.54
1:B:198:ASP:O	1:B:200:VAL:N	2.41	0.54
1:A:320:SER:HA	1:A:323:HIS:NE2	2.23	0.54
1:C:122:ARG:HH11	1:C:122:ARG:HB3	1.73	0.54
1:C:472:LYS:HD3	1:C:473:ASP:N	2.23	0.54
1:D:122:ARG:HB3	1:D:122:ARG:HH11	1.73	0.54
1:A:193:TYR:CZ	1:A:197:LEU:HD22	2.43	0.54
1:C:264:ARG:HG2	1:C:264:ARG:HH11	1.73	0.54
1:D:189:ALA:O	1:D:192:HIS:HB2	2.07	0.54
1:D:323:HIS:HA	1:D:331:VAL:O	2.08	0.54
1:A:162:LEU:HB2	1:A:166:GLN:CG	2.37	0.53
1:B:174:VAL:HG11	1:D:153:LEU:HD21	1.89	0.53
1:B:437:ILE:CG2	1:B:438:LEU:H	2.16	0.53
1:B:162:LEU:HB2	1:B:166:GLN:CG	2.38	0.53
1:C:323:HIS:HA	1:C:331:VAL:O	2.07	0.53
1:C:73:CYS:SG	1:C:350:LEU:HD22	2.48	0.53
1:B:320:SER:HA	1:B:323:HIS:NE2	2.23	0.53
1:C:252:LEU:HA	1:C:336:LEU:HD11	1.90	0.53
1:A:437:ILE:CG2	1:A:438:LEU:H	2.17	0.53
1:B:156:ILE:HG23	1:B:167:LEU:HD11	1.89	0.53
1:C:189:ALA:O	1:C:192:HIS:HB2	2.08	0.53
1:A:260:LEU:HD13	1:A:289:LEU:CD1	2.39	0.53
1:B:423:SER:O	1:B:424:SER:HB3	2.09	0.53
1:D:411:ILE:HD11	1:D:476:ILE:HG13	1.90	0.53
1:A:116:THR:HA	1:A:120:VAL:CG2	2.39	0.53
1:B:193:TYR:CZ	1:B:197:LEU:HD22	2.44	0.53
1:C:186:LEU:HD12	1:C:240:VAL:HG22	1.91	0.53
1:D:252:LEU:HA	1:D:336:LEU:HD11	1.91	0.53
1:A:423:SER:O	1:A:424:SER:HB3	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ALA:O	1:D:385:LEU:HB3	2.08	0.53
1:D:182:ARG:HG2	1:D:182:ARG:HH11	1.74	0.53
1:A:313:HIS:O	1:A:313:HIS:CD2	2.62	0.52
1:A:403:PHE:CE1	1:A:415:PRO:HD3	2.44	0.52
1:B:480:SER:O	1:B:483:LYS:HB3	2.09	0.52
1:C:411:ILE:HD11	1:C:476:ILE:HG13	1.91	0.52
1:B:382:LYS:O	1:B:438:LEU:HB2	2.09	0.52
1:C:73:CYS:CB	1:C:79:LEU:HD23	2.30	0.52
1:D:212:GLY:O	1:D:236:GLU:N	2.36	0.52
1:D:76:ARG:O	1:D:102:LEU:HD22	2.09	0.52
1:A:382:LYS:O	1:A:438:LEU:HB2	2.10	0.52
1:C:76:ARG:O	1:C:102:LEU:HD22	2.10	0.52
1:D:154:ARG:NH1	1:D:158:GLN:HB2	2.24	0.52
1:D:281:GLU:CG	1:D:282:GLU:H	2.20	0.52
1:A:468:ILE:HG23	1:A:468:ILE:O	2.10	0.52
1:A:375:HIS:ND1	1:A:376:PRO:N	2.58	0.52
1:A:384:ALA:O	1:A:385:LEU:HB3	2.09	0.52
1:A:252:LEU:HD11	1:A:287:ASN:HD21	1.75	0.52
1:A:116:THR:HA	1:A:120:VAL:HG23	1.91	0.52
1:A:122:ARG:HG3	1:A:122:ARG:O	2.10	0.52
1:D:264:ARG:HH11	1:D:264:ARG:HG2	1.73	0.52
1:B:186:LEU:HD23	1:B:186:LEU:O	2.09	0.52
1:B:437:ILE:CG2	1:B:438:LEU:N	2.73	0.52
1:C:154:ARG:NH1	1:C:158:GLN:HB2	2.24	0.52
1:D:122:ARG:NH1	1:D:122:ARG:HB3	2.25	0.52
1:C:135:PRO:O	1:C:138:LEU:CD2	2.58	0.52
1:C:266:PHE:HE1	1:C:377:CYS:HG	1.55	0.52
1:B:263:TRP:O	1:B:349:TYR:OH	2.28	0.51
1:C:122:ARG:NH1	1:C:122:ARG:HB3	2.25	0.51
1:C:133:HIS:CG	1:C:133:HIS:O	2.64	0.51
1:B:258:HIS:HB2	1:C:316:PRO:HB2	1.92	0.51
1:C:313:HIS:O	1:C:316:PRO:HD3	2.10	0.51
1:D:92:LEU:HD11	1:D:295:TRP:HZ2	1.76	0.51
1:C:456:ARG:HG2	1:C:457:SER:N	2.24	0.51
1:A:387:VAL:HB	1:A:395:LEU:HD12	1.92	0.51
1:B:116:THR:HA	1:B:120:VAL:HG23	1.91	0.51
1:B:414:TRP:CD1	1:B:414:TRP:O	2.63	0.51
1:D:128:VAL:HG12	1:D:209:ALA:O	2.10	0.51
1:B:159:ASP:C	1:B:161:GLU:H	2.13	0.51
1:D:371:VAL:HG13	1:D:371:VAL:O	2.09	0.51
1:A:159:ASP:C	1:A:161:GLU:H	2.14	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:HIS:ND1	1:A:376:PRO:CD	2.73	0.51
1:D:384:ALA:HB2	1:D:437:ILE:HD13	1.93	0.51
1:B:313:HIS:CD2	1:B:313:HIS:O	2.63	0.51
1:C:182:ARG:HG2	1:C:182:ARG:NH1	2.25	0.51
1:D:279:GLN:OE1	1:D:284:ARG:HD3	2.11	0.51
1:D:456:ARG:HG2	1:D:457:SER:N	2.24	0.51
1:B:323:HIS:CB	1:B:331:VAL:C	2.79	0.51
1:B:443:VAL:HG22	1:B:453:ILE:HG21	1.93	0.51
1:B:138:LEU:HD21	1:B:180:LYS:HD3	1.92	0.51
1:B:387:VAL:HB	1:B:395:LEU:HD12	1.93	0.51
1:C:279:GLN:OE1	1:C:284:ARG:HD3	2.11	0.51
1:B:393:LEU:HD23	1:B:393:LEU:O	2.11	0.51
1:C:154:ARG:HD3	1:C:154:ARG:C	2.31	0.51
1:D:384:ALA:HB3	1:D:440:THR:HG23	1.93	0.51
1:C:152:THR:HG22	1:C:170:PHE:CE1	2.46	0.51
1:D:76:ARG:HD2	1:D:435:MET:HG3	1.93	0.51
1:D:186:LEU:HD12	1:D:240:VAL:HG22	1.92	0.50
1:D:346:MET:O	1:D:350:LEU:HD12	2.10	0.50
1:A:323:HIS:CB	1:A:331:VAL:C	2.79	0.50
1:A:437:ILE:CG2	1:A:438:LEU:N	2.74	0.50
1:B:106:LEU:O	1:B:106:LEU:HD12	2.11	0.50
1:C:252:LEU:CA	1:C:336:LEU:HD11	2.41	0.50
1:C:453:ILE:HG23	1:C:468:ILE:HB	1.93	0.50
1:C:92:LEU:HD11	1:C:295:TRP:HZ2	1.77	0.50
1:D:468:ILE:O	1:D:468:ILE:HG12	2.11	0.50
1:B:406:LEU:HB3	1:B:411:ILE:HB	1.92	0.50
1:B:416:GLY:C	1:B:418:LEU:H	2.14	0.50
1:B:115:TRP:CZ2	1:B:119:VAL:HG11	2.46	0.50
1:C:384:ALA:HB2	1:C:437:ILE:HD13	1.94	0.50
1:D:96:HIS:HB2	1:D:97:PRO:CD	2.29	0.50
1:C:371:VAL:HG13	1:C:371:VAL:O	2.10	0.50
1:C:468:ILE:O	1:C:468:ILE:HG12	2.11	0.50
1:D:154:ARG:C	1:D:154:ARG:HD3	2.32	0.50
1:D:69:LEU:HD21	1:D:351:TYR:HA	1.92	0.50
1:D:453:ILE:HG23	1:D:468:ILE:HB	1.94	0.50
1:A:393:LEU:O	1:A:393:LEU:HD23	2.12	0.50
1:B:122:ARG:O	1:B:122:ARG:HG3	2.11	0.50
1:D:133:HIS:O	1:D:133:HIS:CG	2.65	0.50
1:A:158:GLN:O	1:A:160:LYS:N	2.38	0.50
1:A:414:TRP:O	1:A:414:TRP:CD1	2.65	0.50
1:A:416:GLY:C	1:A:418:LEU:H	2.14	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LEU:HD12	1:A:475:LEU:HD12	1.94	0.50
1:B:468:ILE:HG23	1:B:468:ILE:O	2.12	0.50
1:D:152:THR:HG22	1:D:170:PHE:CE1	2.45	0.50
1:D:182:ARG:NH1	1:D:182:ARG:HG2	2.26	0.50
1:A:118:VAL:HG21	1:A:239:LEU:HD22	1.93	0.50
1:A:407:LEU:C	1:A:409:ASN:H	2.14	0.50
1:A:406:LEU:HB3	1:A:411:ILE:HB	1.93	0.50
1:B:384:ALA:HB2	1:B:437:ILE:HD13	1.94	0.50
1:D:135:PRO:O	1:D:138:LEU:CD2	2.60	0.50
1:D:254:PHE:HD1	1:D:257:ARG:HD2	1.76	0.50
1:D:313:HIS:O	1:D:316:PRO:HD3	2.12	0.50
1:D:375:HIS:ND1	1:D:376:PRO:HD2	2.26	0.50
1:A:162:LEU:O	1:A:164:LYS:N	2.36	0.50
1:B:269:SER:C	1:B:271:SER:N	2.66	0.50
1:C:384:ALA:HB3	1:C:440:THR:HG23	1.93	0.50
1:D:252:LEU:CA	1:D:336:LEU:HD11	2.42	0.50
1:A:106:LEU:HD12	1:A:106:LEU:O	2.12	0.49
1:B:168:VAL:O	1:B:168:VAL:HG12	2.11	0.49
1:C:254:PHE:HD1	1:C:257:ARG:HD2	1.77	0.49
1:A:384:ALA:HB2	1:A:437:ILE:HD13	1.94	0.49
1:B:104:VAL:HG11	1:D:127:PRO:HB2	1.93	0.49
1:B:213:VAL:HG21	1:D:132:HIS:CE1	2.47	0.49
1:B:277:ASP:O	1:B:278:CYS:CB	2.60	0.49
1:B:375:HIS:ND1	1:B:376:PRO:N	2.60	0.49
1:D:120:VAL:O	1:D:120:VAL:HG12	2.11	0.49
1:D:404:ASN:O	1:D:408:GLU:HG3	2.11	0.49
1:A:109:ASN:O	1:A:112:ALA:HB3	2.12	0.49
1:A:443:VAL:HG22	1:A:453:ILE:HG21	1.94	0.49
1:C:420:THR:OG1	1:C:421:MET:N	2.45	0.49
1:C:69:LEU:HD21	1:C:351:TYR:HA	1.93	0.49
1:D:154:ARG:NH2	1:D:158:GLN:HE21	2.10	0.49
1:A:154:ARG:C	1:A:156:ILE:H	2.15	0.49
1:B:407:LEU:C	1:B:409:ASN:H	2.14	0.49
1:B:213:VAL:HG21	1:D:132:HIS:HE1	1.78	0.49
1:A:133:HIS:HB2	1:A:180:LYS:O	2.12	0.49
1:B:375:HIS:ND1	1:B:376:PRO:CD	2.76	0.49
1:B:406:LEU:HD12	1:B:475:LEU:HD12	1.94	0.49
1:D:118:VAL:CG2	1:D:118:VAL:O	2.61	0.49
1:D:78:PHE:HB3	1:D:79:LEU:HD22	1.94	0.49
1:B:156:ILE:HD13	1:B:170:PHE:CE2	2.48	0.49
1:B:269:SER:O	1:B:271:SER:N	2.45	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:HIS:HB3	1:B:101:PRO:HD2	1.95	0.49
1:C:92:LEU:C	1:C:94:GLY:N	2.66	0.49
1:C:92:LEU:C	1:C:94:GLY:H	2.16	0.49
1:B:384:ALA:O	1:B:385:LEU:HB3	2.12	0.49
1:B:477:LYS:O	1:B:481:SER:N	2.45	0.49
1:C:381:ILE:HG21	1:C:414:TRP:HB2	1.95	0.49
1:C:82:SER:O	1:C:84:GLN:N	2.37	0.49
1:A:468:ILE:HG12	1:A:468:ILE:O	2.11	0.49
1:A:162:LEU:HD23	1:A:165:GLU:HB2	1.95	0.49
1:A:213:VAL:HG21	1:C:132:HIS:CE1	2.48	0.49
1:A:260:LEU:HD22	1:A:275:SER:HB3	1.94	0.49
1:A:77:HIS:HB3	1:A:101:PRO:HD2	1.95	0.49
1:C:391:PRO:HG2	1:C:395:LEU:HB2	1.95	0.49
1:C:402:LEU:O	1:C:406:LEU:HB2	2.13	0.49
1:D:420:THR:OG1	1:D:421:MET:N	2.46	0.49
1:A:168:VAL:O	1:A:168:VAL:HG12	2.12	0.48
1:A:263:TRP:O	1:A:349:TYR:OH	2.29	0.48
1:A:269:SER:C	1:A:271:SER:N	2.66	0.48
1:A:323:HIS:HA	1:A:333:PRO:HD3	1.94	0.48
1:D:381:ILE:HG21	1:D:414:TRP:HB2	1.95	0.48
1:A:423:SER:O	1:A:427:GLN:HB2	2.13	0.48
1:B:154:ARG:C	1:B:156:ILE:H	2.15	0.48
1:B:133:HIS:HB2	1:B:180:LYS:O	2.13	0.48
1:B:323:HIS:HA	1:B:333:PRO:HD3	1.94	0.48
1:B:423:SER:O	1:B:427:GLN:HB2	2.13	0.48
1:A:104:VAL:HG11	1:C:127:PRO:HB2	1.94	0.48
1:C:447:THR:HG21	1:C:453:ILE:HG23	1.95	0.48
1:C:146:ARG:HG2	1:C:146:ARG:NH1	2.25	0.48
1:C:154:ARG:NH2	1:C:158:GLN:HE21	2.10	0.48
1:D:281:GLU:C	1:D:283:GLY:H	2.17	0.48
1:D:467:HIS:O	1:D:469:SER:N	2.46	0.48
1:B:468:ILE:O	1:B:468:ILE:HG12	2.13	0.48
1:C:266:PHE:HB3	1:C:378:LEU:HD22	1.95	0.48
1:C:281:GLU:CG	1:C:282:GLU:H	2.20	0.48
1:C:404:ASN:O	1:C:408:GLU:HG3	2.13	0.48
1:A:269:SER:O	1:A:271:SER:N	2.47	0.48
1:A:434:GLU:C	1:A:436:SER:N	2.66	0.48
1:B:389:ARG:N	1:B:389:ARG:HD2	2.26	0.48
1:D:280:ASP:CG	1:D:284:ARG:HH21	2.16	0.48
1:C:78:PHE:HB3	1:C:79:LEU:HD22	1.95	0.48
1:A:120:VAL:O	1:A:121:PHE:C	2.52	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:SER:O	1:A:86:LEU:HD21	2.13	0.48
1:B:109:ASN:O	1:B:112:ALA:HB3	2.14	0.48
1:C:186:LEU:HD13	1:C:337:SER:OG	2.13	0.48
1:C:67:GLU:N	1:C:67:GLU:CD	2.67	0.48
1:D:453:ILE:HD11	1:D:466:MET:HB3	1.95	0.48
1:D:92:LEU:C	1:D:94:GLY:H	2.16	0.48
1:A:156:ILE:HD13	1:A:170:PHE:CE2	2.48	0.48
1:B:374:LEU:HB2	1:B:436:SER:OG	2.13	0.48
1:B:419:GLU:HG2	1:B:420:THR:HG22	1.96	0.48
1:B:80:SER:O	1:B:86:LEU:HD21	2.14	0.48
1:C:118:VAL:O	1:C:118:VAL:CG2	2.62	0.48
1:A:157:LEU:HD21	1:C:171:LEU:CB	2.42	0.48
1:C:369:ARG:HH11	1:C:369:ARG:HG3	1.79	0.48
1:D:416:GLY:C	1:D:418:LEU:H	2.17	0.48
1:A:188:GLY:O	1:A:192:HIS:HD2	1.96	0.48
1:C:280:ASP:CG	1:C:284:ARG:HH21	2.17	0.48
1:B:434:GLU:C	1:B:436:SER:N	2.67	0.48
1:A:419:GLU:HG2	1:A:420:THR:HG22	1.96	0.47
1:B:118:VAL:HG21	1:B:239:LEU:HD22	1.95	0.47
1:B:260:LEU:HD22	1:B:275:SER:HB3	1.95	0.47
1:C:416:GLY:C	1:C:418:LEU:H	2.18	0.47
1:D:391:PRO:HG2	1:D:395:LEU:HB2	1.96	0.47
1:D:67:GLU:CD	1:D:67:GLU:N	2.67	0.47
1:D:92:LEU:C	1:D:94:GLY:N	2.65	0.47
1:A:343:ASP:O	1:A:346:MET:HB2	2.14	0.47
1:A:381:ILE:O	1:A:437:ILE:HG23	2.13	0.47
1:D:447:THR:HG21	1:D:453:ILE:HG22	1.96	0.47
1:D:447:THR:HG21	1:D:453:ILE:HG23	1.95	0.47
1:B:146:ARG:HG2	1:B:146:ARG:HH11	1.79	0.47
1:B:188:GLY:O	1:B:192:HIS:HD2	1.96	0.47
1:B:389:ARG:CD	1:B:389:ARG:H	2.24	0.47
1:B:419:GLU:HG3	1:D:201:ASN:ND2	2.29	0.47
1:D:146:ARG:HG2	1:D:146:ARG:NH1	2.27	0.47
1:D:254:PHE:HA	1:D:257:ARG:CG	2.44	0.47
1:D:186:LEU:HD13	1:D:337:SER:OG	2.15	0.47
1:A:115:TRP:CZ2	1:A:119:VAL:HG11	2.49	0.47
1:A:146:ARG:HH11	1:A:146:ARG:HG2	1.80	0.47
1:C:120:VAL:HG12	1:C:120:VAL:O	2.14	0.47
1:C:214:CYS:HB2	1:C:216:HIS:CE1	2.50	0.47
1:C:467:HIS:O	1:C:469:SER:N	2.46	0.47
1:D:351:TYR:O	1:D:353:SER:N	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASN:HD21	1:A:285:LYS:HE2	1.79	0.47
1:B:106:LEU:HG	1:B:346:MET:SD	2.54	0.47
1:D:392:THR:HG22	1:D:396:ARG:HD3	1.97	0.47
1:A:381:ILE:HG13	1:A:437:ILE:HG12	1.96	0.47
1:B:158:GLN:O	1:B:160:LYS:N	2.38	0.47
1:C:281:GLU:C	1:C:283:GLY:H	2.17	0.47
1:C:447:THR:HG21	1:C:453:ILE:HG22	1.97	0.47
1:B:213:VAL:HA	1:B:234:LYS:O	2.15	0.47
1:B:204:LEU:CD1	1:B:333:PRO:HB3	2.42	0.47
1:B:451:GLY:O	1:B:452:LEU:HD13	2.15	0.47
1:A:419:GLU:HG3	1:C:201:ASN:ND2	2.29	0.47
1:A:477:LYS:O	1:A:481:SER:N	2.44	0.47
1:B:249:ASN:HD21	1:B:285:LYS:HE2	1.79	0.47
1:C:453:ILE:HD11	1:C:466:MET:HB3	1.97	0.47
1:D:369:ARG:HG3	1:D:369:ARG:HH11	1.80	0.47
1:A:158:GLN:C	1:A:160:LYS:H	2.19	0.47
1:B:158:GLN:HG2	1:B:159:ASP:N	2.17	0.47
1:C:405:GLU:O	1:C:409:ASN:ND2	2.47	0.47
1:B:104:VAL:HG22	1:D:129:ASP:HB2	1.96	0.47
1:B:343:ASP:O	1:B:346:MET:HB2	2.15	0.47
1:D:289:LEU:HD12	1:D:301:GLU:HG2	1.97	0.47
1:A:76:ARG:HD3	1:A:76:ARG:HA	1.72	0.46
1:B:145:PHE:CD1	1:D:149:SER:HA	2.47	0.46
1:D:392:THR:C	1:D:394:GLU:H	2.19	0.46
1:D:405:GLU:O	1:D:409:ASN:ND2	2.47	0.46
1:D:448:LEU:O	1:D:448:LEU:HD23	2.15	0.46
1:B:120:VAL:O	1:B:121:PHE:C	2.54	0.46
1:B:396:ARG:HA	1:B:399:CYS:SG	2.55	0.46
1:D:266:PHE:HB3	1:D:378:LEU:HD22	1.97	0.46
1:A:451:GLY:O	1:A:452:LEU:HD13	2.15	0.46
1:B:381:ILE:O	1:B:437:ILE:HG23	2.14	0.46
1:B:481:SER:C	1:B:483:LYS:N	2.69	0.46
1:C:254:PHE:HA	1:C:257:ARG:CG	2.44	0.46
1:C:289:LEU:HD12	1:C:301:GLU:HG2	1.96	0.46
1:D:389:ARG:HD2	1:D:389:ARG:H	1.81	0.46
1:A:399:CYS:HB3	1:A:417:TYR:CE2	2.51	0.46
1:C:128:VAL:HG12	1:C:209:ALA:O	2.16	0.46
1:C:448:LEU:HD23	1:C:448:LEU:O	2.15	0.46
1:D:384:ALA:HB2	1:D:437:ILE:CD1	2.45	0.46
1:A:396:ARG:HA	1:A:399:CYS:SG	2.55	0.46
1:A:145:PHE:CD1	1:C:149:SER:HA	2.48	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:ARG:HD2	1:C:389:ARG:H	1.81	0.46
1:D:162:LEU:HB2	1:D:166:GLN:NE2	2.30	0.46
1:D:118:VAL:CG2	1:D:239:LEU:HD22	2.45	0.46
1:D:317:GLY:O	1:D:319:VAL:N	2.48	0.46
1:A:148:VAL:HG21	1:C:148:VAL:CG2	2.45	0.46
1:B:402:LEU:HA	1:B:405:GLU:HB3	1.97	0.46
1:B:399:CYS:HB3	1:B:417:TYR:CE2	2.50	0.46
1:B:381:ILE:HG13	1:B:437:ILE:HG12	1.97	0.46
1:C:384:ALA:HB2	1:C:437:ILE:CD1	2.46	0.46
1:B:157:LEU:HD21	1:D:171:LEU:CB	2.43	0.46
1:A:250:GLN:HA	1:A:253:ASP:OD2	2.16	0.46
1:A:277:ASP:O	1:A:278:CYS:CB	2.60	0.46
1:A:484:ASN:O	1:A:485:VAL:C	2.54	0.46
1:B:162:LEU:HD23	1:B:165:GLU:HB2	1.98	0.46
1:B:323:HIS:HB3	1:B:332:VAL:N	2.30	0.46
1:C:353:SER:O	1:C:372:LEU:HA	2.15	0.46
1:D:211:ILE:HA	1:D:237:ALA:HA	1.98	0.46
1:D:353:SER:O	1:D:372:LEU:HA	2.16	0.46
1:A:323:HIS:HB3	1:A:332:VAL:N	2.30	0.46
1:C:308:ASP:HB2	1:C:312:LEU:CD1	2.45	0.46
1:C:392:THR:HG22	1:C:396:ARG:HD3	1.97	0.46
1:C:445:GLU:C	1:C:447:THR:N	2.69	0.46
1:D:147:LEU:HD21	1:D:181:LEU:CD2	2.46	0.46
1:D:242:PHE:CE1	1:D:335:VAL:HG12	2.51	0.46
1:D:453:ILE:C	1:D:453:ILE:HD12	2.36	0.46
1:D:69:LEU:CD2	1:D:351:TYR:HA	2.45	0.46
1:B:293:PHE:C	1:B:295:TRP:N	2.69	0.46
1:C:467:HIS:C	1:C:469:SER:N	2.69	0.46
1:A:402:LEU:HA	1:A:405:GLU:HB3	1.98	0.45
1:B:402:LEU:O	1:B:405:GLU:N	2.50	0.45
1:C:392:THR:C	1:C:394:GLU:H	2.18	0.45
1:C:162:LEU:HB2	1:C:166:GLN:NE2	2.31	0.45
1:C:211:ILE:HA	1:C:237:ALA:HA	1.98	0.45
1:C:317:GLY:O	1:C:319:VAL:N	2.48	0.45
1:C:351:TYR:O	1:C:353:SER:N	2.49	0.45
1:A:252:LEU:C	1:A:252:LEU:HD13	2.36	0.45
1:B:119:VAL:HG22	1:B:125:VAL:HG11	1.98	0.45
1:B:484:ASN:O	1:B:485:VAL:C	2.55	0.45
1:C:199:LEU:O	1:C:200:VAL:CG1	2.64	0.45
1:D:256:LEU:HD22	1:D:287:ASN:OD1	2.15	0.45
1:D:467:HIS:C	1:D:469:SER:N	2.69	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ILE:HG12	1:D:434:GLU:OE1	2.17	0.45
1:A:402:LEU:HA	1:A:402:LEU:HD23	1.78	0.45
1:A:420:THR:CG2	1:A:421:MET:H	2.27	0.45
1:B:122:ARG:O	1:B:124:GLN:HG3	2.15	0.45
1:B:402:LEU:O	1:B:403:PHE:C	2.54	0.45
1:B:437:ILE:O	1:B:458:ARG:HD3	2.16	0.45
1:B:69:LEU:C	1:B:71:GLU:H	2.20	0.45
1:C:118:VAL:CG2	1:C:239:LEU:HD22	2.47	0.45
1:A:104:VAL:HG22	1:C:129:ASP:HB2	1.97	0.45
1:C:299:LEU:HD21	1:C:302:THR:HG22	1.98	0.45
1:C:69:LEU:HD13	1:C:354:PHE:CG	2.52	0.45
1:A:402:LEU:O	1:A:403:PHE:C	2.55	0.45
1:B:247:THR:O	1:B:250:GLN:HB3	2.17	0.45
1:B:403:PHE:HZ	1:D:123:GLU:CG	2.30	0.45
1:D:375:HIS:CG	1:D:376:PRO:HD2	2.51	0.45
1:A:213:VAL:HA	1:A:234:LYS:O	2.17	0.45
1:A:374:LEU:HB2	1:A:436:SER:OG	2.16	0.45
1:A:402:LEU:O	1:A:405:GLU:N	2.50	0.45
1:A:445:GLU:C	1:A:447:THR:N	2.70	0.45
1:B:250:GLN:HA	1:B:253:ASP:OD2	2.16	0.45
1:B:472:LYS:O	1:B:476:ILE:HG13	2.17	0.45
1:C:205:PRO:HB3	1:C:243:THR:HG22	1.98	0.45
1:C:453:ILE:C	1:C:453:ILE:HD12	2.36	0.45
1:A:106:LEU:HG	1:A:346:MET:SD	2.56	0.45
1:A:472:LYS:O	1:A:476:ILE:HG13	2.17	0.45
1:A:69:LEU:C	1:A:71:GLU:H	2.20	0.45
1:B:382:LYS:HG3	1:B:479:ILE:HD11	1.98	0.45
1:D:146:ARG:HA	1:D:179:GLY:O	2.17	0.45
1:D:270:PRO:C	1:D:272:ASN:H	2.20	0.45
1:B:132:HIS:CE1	1:D:213:VAL:HG21	2.52	0.45
1:D:247:THR:HG22	1:D:250:GLN:CB	2.47	0.45
1:A:403:PHE:HZ	1:C:123:GLU:CG	2.30	0.45
1:C:69:LEU:CD2	1:C:351:TYR:HA	2.47	0.45
1:A:132:HIS:CE1	1:C:213:VAL:HG21	2.51	0.44
1:D:154:ARG:CZ	1:D:158:GLN:HB2	2.48	0.44
1:C:247:THR:HG22	1:C:250:GLN:CB	2.47	0.44
1:D:445:GLU:C	1:D:447:THR:N	2.70	0.44
1:A:395:LEU:HD11	1:A:443:VAL:C	2.38	0.44
1:A:382:LYS:HG3	1:A:479:ILE:HD11	1.99	0.44
1:A:481:SER:C	1:A:483:LYS:N	2.69	0.44
1:A:88:ARG:N	1:A:88:ARG:CD	2.68	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:PHE:CE1	1:C:335:VAL:HG12	2.52	0.44
1:C:375:HIS:ND1	1:C:376:PRO:HD2	2.32	0.44
1:D:320:SER:HA	1:D:323:HIS:CD2	2.52	0.44
1:D:71:GLU:O	1:D:74:GLN:HB3	2.17	0.44
1:D:82:SER:HB3	1:D:85:GLN:HG2	1.99	0.44
1:C:154:ARG:CZ	1:C:158:GLN:HB2	2.48	0.44
1:C:71:GLU:O	1:C:74:GLN:HB3	2.18	0.44
1:C:72:ILE:HG12	1:C:434:GLU:OE1	2.16	0.44
1:D:260:LEU:CD2	1:D:275:SER:HB3	2.43	0.44
1:B:441:VAL:HG12	1:B:455:LEU:HB3	1.99	0.44
1:A:204:LEU:CD1	1:A:333:PRO:HB3	2.44	0.44
1:A:459:ASP:C	1:A:461:THR:H	2.21	0.44
1:B:154:ARG:O	1:B:156:ILE:N	2.50	0.44
1:C:155:GLU:C	1:C:156:ILE:HG13	2.37	0.44
1:D:288:LYS:HG2	1:D:302:THR:HG22	2.00	0.44
1:D:69:LEU:HD13	1:D:354:PHE:CG	2.53	0.44
1:A:119:VAL:HG22	1:A:125:VAL:HG11	2.00	0.44
1:A:215:PHE:CD1	1:A:215:PHE:N	2.86	0.44
1:C:141:GLY:O	1:C:142:ASP:CB	2.65	0.44
1:C:270:PRO:C	1:C:272:ASN:H	2.21	0.44
1:C:70:LEU:HD13	1:C:70:LEU:O	2.17	0.44
1:D:141:GLY:O	1:D:142:ASP:CB	2.65	0.44
1:D:205:PRO:HB3	1:D:243:THR:HG22	1.99	0.44
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.18	0.44
1:A:293:PHE:C	1:A:295:TRP:N	2.69	0.44
1:A:431:LYS:O	1:A:434:GLU:HB2	2.18	0.44
1:B:252:LEU:C	1:B:252:LEU:HD13	2.37	0.44
1:B:92:LEU:HD22	1:B:344:ARG:NE	2.33	0.44
1:C:256:LEU:HD22	1:C:287:ASN:OD1	2.18	0.44
1:C:420:THR:HG23	1:C:421:MET:H	1.82	0.44
1:D:214:CYS:HB2	1:D:216:HIS:CE1	2.50	0.44
1:A:154:ARG:O	1:A:156:ILE:N	2.51	0.44
1:D:155:GLU:C	1:D:156:ILE:HG13	2.38	0.44
1:A:174:VAL:CG1	1:C:153:LEU:HD21	2.47	0.43
1:B:151:GLU:OE1	1:B:151:GLU:HA	2.18	0.43
1:C:320:SER:HA	1:C:323:HIS:CD2	2.53	0.43
1:D:299:LEU:HD21	1:D:302:THR:HG22	1.99	0.43
1:D:308:ASP:HB2	1:D:312:LEU:CD1	2.46	0.43
1:D:399:CYS:HB3	1:D:417:TYR:CD2	2.53	0.43
1:D:82:SER:C	1:D:84:GLN:N	2.72	0.43
1:D:71:GLU:HG2	1:D:83:LYS:NZ	2.32	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:HIS:CE1	1:A:376:PRO:HD2	2.53	0.43
1:A:452:LEU:N	1:A:452:LEU:HD22	2.33	0.43
1:B:148:VAL:HG21	1:D:148:VAL:CG2	2.48	0.43
1:B:455:LEU:HD23	1:B:455:LEU:N	2.24	0.43
1:C:82:SER:HB3	1:C:85:GLN:HG2	1.99	0.43
1:A:174:VAL:CG1	1:A:175:LEU:N	2.79	0.43
1:B:153:LEU:HA	1:B:156:ILE:HD12	2.00	0.43
1:C:71:GLU:HG2	1:C:83:LYS:NZ	2.33	0.43
1:D:420:THR:HG23	1:D:421:MET:H	1.82	0.43
1:A:122:ARG:O	1:A:124:GLN:HG3	2.18	0.43
1:A:407:LEU:C	1:A:409:ASN:N	2.71	0.43
1:B:395:LEU:HD11	1:B:443:VAL:C	2.38	0.43
1:B:424:SER:HB3	1:B:427:GLN:HB2	1.99	0.43
1:B:450:ASN:CG	1:B:451:GLY:H	2.21	0.43
1:D:402:LEU:O	1:D:406:LEU:HB2	2.18	0.43
1:A:153:LEU:HA	1:A:156:ILE:HD12	2.01	0.43
1:A:247:THR:O	1:A:250:GLN:HB3	2.18	0.43
1:A:389:ARG:H	1:A:389:ARG:CD	2.23	0.43
1:A:424:SER:HB3	1:A:427:GLN:HB2	1.99	0.43
1:C:146:ARG:HA	1:C:179:GLY:O	2.18	0.43
1:D:190:LEU:C	1:D:192:HIS:N	2.71	0.43
1:A:437:ILE:O	1:A:458:ARG:HD3	2.18	0.43
1:B:162:LEU:HB2	1:B:166:GLN:HB2	2.00	0.43
1:C:188:GLY:O	1:C:192:HIS:HD2	2.02	0.43
1:C:415:PRO:HB2	1:C:418:LEU:HD13	2.01	0.43
1:D:424:SER:OG	1:D:425:LEU:N	2.51	0.43
1:D:429:TYR:HD2	1:D:429:TYR:HA	1.73	0.43
1:A:133:HIS:O	1:A:135:PRO:HD3	2.18	0.43
1:A:162:LEU:HB2	1:A:166:GLN:HB2	1.99	0.43
1:A:385:LEU:O	1:A:385:LEU:CD2	2.60	0.43
1:B:407:LEU:C	1:B:409:ASN:N	2.71	0.43
1:B:431:LYS:O	1:B:434:GLU:HB2	2.19	0.43
1:C:205:PRO:CB	1:C:243:THR:HG22	2.48	0.43
1:C:375:HIS:CG	1:C:376:PRO:HD2	2.53	0.43
1:C:456:ARG:CG	1:C:457:SER:N	2.81	0.43
1:D:371:VAL:CG1	1:D:371:VAL:O	2.67	0.43
1:D:418:LEU:HD12	1:D:418:LEU:N	2.33	0.43
1:A:459:ASP:C	1:A:461:THR:N	2.72	0.43
1:B:322:LEU:O	1:B:323:HIS:O	2.36	0.43
1:B:245:PRO:HG3	1:B:334:CYS:SG	2.59	0.43
1:B:481:SER:C	1:B:483:LYS:H	2.21	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:SER:C	1:C:84:GLN:N	2.71	0.43
1:B:445:GLU:C	1:B:447:THR:N	2.70	0.43
1:B:454:HIS:ND1	1:B:454:HIS:N	2.67	0.43
1:C:288:LYS:HG2	1:C:302:THR:HG22	2.01	0.43
1:C:424:SER:OG	1:C:425:LEU:N	2.51	0.43
1:A:313:HIS:O	1:A:313:HIS:HD2	2.02	0.43
1:C:147:LEU:HD21	1:C:181:LEU:CD2	2.48	0.43
1:C:399:CYS:HB3	1:C:417:TYR:CD2	2.54	0.43
1:D:182:ARG:NE	1:D:213:VAL:O	2.48	0.43
1:D:318:ASN:HD22	1:D:318:ASN:HA	1.55	0.43
1:D:415:PRO:HB2	1:D:418:LEU:HD13	2.01	0.43
1:D:455:LEU:C	1:D:455:LEU:CD1	2.86	0.43
1:A:122:ARG:HD3	1:A:124:GLN:NE2	2.34	0.42
1:A:241:TRP:HB3	1:A:336:LEU:HB3	2.00	0.42
1:B:144:ALA:O	1:B:146:ARG:NH1	2.52	0.42
1:B:402:LEU:HD23	1:B:402:LEU:HA	1.79	0.42
1:A:213:VAL:HG21	1:C:132:HIS:HE1	1.82	0.42
1:C:313:HIS:CD2	1:C:313:HIS:O	2.72	0.42
1:C:432:TYR:CD1	1:C:437:ILE:HD12	2.54	0.42
1:A:92:LEU:HD22	1:A:344:ARG:NE	2.34	0.42
1:B:431:LYS:NZ	1:B:431:LYS:HB2	2.34	0.42
1:C:479:ILE:O	1:C:483:LYS:HB2	2.18	0.42
1:C:308:ASP:O	1:C:312:LEU:HD12	2.19	0.42
1:D:479:ILE:O	1:D:483:LYS:HB2	2.18	0.42
1:A:73:CYS:CB	1:A:79:LEU:HD23	2.42	0.42
1:B:413:VAL:CG1	1:B:414:TRP:N	2.81	0.42
1:B:452:LEU:N	1:B:452:LEU:HD22	2.34	0.42
1:C:289:LEU:HD12	1:C:301:GLU:CG	2.50	0.42
1:C:455:LEU:CD1	1:C:455:LEU:C	2.86	0.42
1:D:118:VAL:O	1:D:118:VAL:HG23	2.19	0.42
1:D:197:LEU:HD12	1:D:197:LEU:HA	1.86	0.42
1:D:477:LYS:HA	1:D:477:LYS:HD3	1.94	0.42
1:A:141:GLY:O	1:A:142:ASP:HB2	2.19	0.42
1:A:245:PRO:O	1:A:248:SER:HB3	2.19	0.42
1:D:205:PRO:CB	1:D:243:THR:HG22	2.49	0.42
1:A:104:VAL:O	1:A:108:LYS:HB2	2.20	0.42
1:A:281:GLU:OE2	1:A:282:GLU:HB2	2.20	0.42
1:A:450:ASN:CG	1:A:451:GLY:H	2.21	0.42
1:B:141:GLY:O	1:B:142:ASP:HB2	2.18	0.42
1:B:153:LEU:O	1:B:156:ILE:HB	2.19	0.42
1:B:417:TYR:O	1:B:417:TYR:HD1	2.03	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ARG:HG2	1:B:456:ARG:NH1	2.35	0.42
1:C:182:ARG:NE	1:C:213:VAL:O	2.49	0.42
1:C:318:ASN:HA	1:C:318:ASN:HD22	1.54	0.42
1:D:118:VAL:HG21	1:D:239:LEU:HD22	2.01	0.42
1:D:313:HIS:O	1:D:313:HIS:CD2	2.72	0.42
1:A:153:LEU:O	1:A:156:ILE:HB	2.20	0.42
1:A:322:LEU:O	1:A:323:HIS:O	2.38	0.42
1:A:325:ARG:NH1	1:A:330:ASN:ND2	2.67	0.42
1:A:387:VAL:CB	1:A:395:LEU:HD12	2.49	0.42
1:B:158:GLN:C	1:B:160:LYS:H	2.18	0.42
1:B:231:ILE:HD13	1:D:133:HIS:CD2	2.55	0.42
1:C:231:ILE:CG2	1:C:232:GLY:H	2.32	0.42
1:C:215:PHE:CD2	1:C:233:GLU:HG2	2.55	0.42
1:C:278:CYS:O	1:C:285:LYS:HA	2.19	0.42
1:C:96:HIS:CB	1:C:97:PRO:HD2	2.37	0.42
1:A:301:GLU:HG3	1:A:339:ASN:O	2.20	0.42
1:B:126:PHE:CE2	1:B:199:LEU:HD21	2.55	0.42
1:B:162:LEU:C	1:B:164:LYS:N	2.73	0.42
1:B:215:PHE:CD1	1:B:215:PHE:N	2.88	0.42
1:B:459:ASP:C	1:B:461:THR:H	2.22	0.42
1:C:418:LEU:N	1:C:418:LEU:HD12	2.34	0.42
1:C:423:SER:O	1:C:427:GLN:HB2	2.19	0.42
1:D:204:LEU:CD2	1:D:324:GLY:HA3	2.47	0.42
1:A:245:PRO:HG3	1:A:334:CYS:SG	2.59	0.42
1:A:441:VAL:HG12	1:A:455:LEU:HB3	2.02	0.42
1:A:456:ARG:HG2	1:A:456:ARG:NH1	2.35	0.42
1:B:281:GLU:OE2	1:B:282:GLU:HB2	2.20	0.42
1:B:421:MET:C	1:B:423:SER:N	2.73	0.42
1:B:445:GLU:O	1:B:447:THR:N	2.53	0.42
1:C:154:ARG:HG2	1:C:154:ARG:HH11	1.85	0.42
1:C:268:MET:O	1:C:270:PRO:HD2	2.20	0.42
1:C:401:GLY:O	1:C:405:GLU:HB2	2.20	0.42
1:C:411:ILE:O	1:C:413:VAL:HG23	2.20	0.42
1:C:479:ILE:C	1:C:481:SER:N	2.73	0.42
1:D:308:ASP:N	1:D:308:ASP:OD2	2.52	0.42
1:D:266:PHE:HE1	1:D:377:CYS:HG	1.67	0.42
1:D:456:ARG:CG	1:D:457:SER:N	2.81	0.42
1:D:479:ILE:C	1:D:481:SER:N	2.73	0.42
1:D:82:SER:H	1:D:85:GLN:CG	2.33	0.42
1:A:144:ALA:O	1:A:146:ARG:NH1	2.53	0.42
1:A:229:LYS:CB	1:A:229:LYS:NZ	2.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:SER:HA	1:B:323:HIS:CE1	2.55	0.42
1:B:387:VAL:CB	1:B:395:LEU:HD12	2.49	0.42
1:B:421:MET:C	1:B:423:SER:H	2.23	0.42
1:B:459:ASP:C	1:B:461:THR:N	2.73	0.42
1:B:73:CYS:CB	1:B:79:LEU:HD23	2.42	0.42
1:C:260:LEU:CD2	1:C:275:SER:HB3	2.44	0.42
1:C:82:SER:H	1:C:85:GLN:CG	2.33	0.42
1:A:454:HIS:N	1:A:454:HIS:ND1	2.68	0.41
1:A:481:SER:C	1:A:483:LYS:H	2.21	0.41
1:B:245:PRO:O	1:B:248:SER:HB3	2.20	0.41
1:B:325:ARG:NH1	1:B:330:ASN:ND2	2.67	0.41
1:C:371:VAL:CG1	1:C:371:VAL:O	2.68	0.41
1:C:375:HIS:CE1	1:C:377:CYS:SG	3.13	0.41
1:C:386:ASP:OD1	1:C:386:ASP:N	2.53	0.41
1:C:455:LEU:HD13	1:C:456:ARG:O	2.19	0.41
1:D:460:THR:O	1:D:462:MET:N	2.52	0.41
1:A:417:TYR:HD1	1:A:417:TYR:O	2.03	0.41
1:B:122:ARG:HD3	1:B:124:GLN:NE2	2.35	0.41
1:B:420:THR:CG2	1:B:421:MET:N	2.81	0.41
1:C:175:LEU:HD22	1:C:175:LEU:N	2.35	0.41
1:D:175:LEU:N	1:D:175:LEU:HD22	2.35	0.41
1:D:186:LEU:HD12	1:D:240:VAL:CG2	2.51	0.41
1:D:278:CYS:O	1:D:285:LYS:HA	2.19	0.41
1:D:423:SER:O	1:D:427:GLN:HB2	2.19	0.41
1:D:435:MET:O	1:D:436:SER:OG	2.34	0.41
1:D:70:LEU:O	1:D:70:LEU:HD13	2.20	0.41
1:A:115:TRP:CZ2	1:A:127:PRO:HB3	2.55	0.41
1:A:117:SER:OG	1:A:258:HIS:CE1	2.73	0.41
1:A:354:PHE:CG	1:A:355:GLN:N	2.86	0.41
1:C:197:LEU:HD12	1:C:197:LEU:HA	1.88	0.41
1:C:252:LEU:N	1:C:336:LEU:HD11	2.35	0.41
1:D:386:ASP:OD1	1:D:386:ASP:N	2.54	0.41
1:D:483:LYS:HD2	1:D:484:ASN:OD1	2.20	0.41
1:A:162:LEU:HB2	1:A:166:GLN:CB	2.50	0.41
1:B:347:LEU:O	1:B:348:ALA:C	2.58	0.41
1:C:243:THR:O	1:C:333:PRO:HA	2.20	0.41
1:C:308:ASP:OD2	1:C:308:ASP:N	2.53	0.41
1:C:429:TYR:HD2	1:C:429:TYR:HA	1.73	0.41
1:C:457:SER:HB2	1:C:462:MET:HG2	2.02	0.41
1:D:411:ILE:O	1:D:413:VAL:HG23	2.20	0.41
1:A:289:LEU:HD13	1:A:289:LEU:HA	1.91	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:LEU:HD12	1:A:471:LEU:C	2.40	0.41
1:A:453:ILE:HD11	1:A:471:LEU:HD22	2.03	0.41
1:B:471:LEU:C	1:B:471:LEU:HD12	2.40	0.41
1:A:148:VAL:CG2	1:C:148:VAL:CG2	2.98	0.41
1:C:476:ILE:O	1:C:476:ILE:HG22	2.21	0.41
1:D:215:PHE:N	1:D:215:PHE:CD1	2.89	0.41
1:D:289:LEU:HD12	1:D:301:GLU:CG	2.51	0.41
1:D:455:LEU:HD13	1:D:456:ARG:O	2.20	0.41
1:B:154:ARG:C	1:B:156:ILE:N	2.74	0.41
1:B:421:MET:HG3	1:B:423:SER:N	2.36	0.41
1:C:141:GLY:O	1:C:142:ASP:HB3	2.21	0.41
1:D:146:ARG:HD2	1:D:178:SER:OG	2.20	0.41
1:D:414:TRP:HA	1:D:415:PRO:HD2	1.80	0.41
1:A:156:ILE:CG2	1:A:167:LEU:HD11	2.51	0.41
1:A:383:VAL:HG13	1:A:383:VAL:O	2.21	0.41
1:B:160:LYS:HA	1:B:163:SER:OG	2.21	0.41
1:B:455:LEU:HD13	1:B:466:MET:HE2	2.01	0.41
1:C:186:LEU:HD12	1:C:240:VAL:CG2	2.51	0.41
1:C:254:PHE:O	1:C:257:ARG:CG	2.61	0.41
1:C:193:TYR:OH	1:C:333:PRO:HG3	2.20	0.41
1:C:483:LYS:HD2	1:C:484:ASN:OD1	2.21	0.41
1:D:119:VAL:HG13	1:D:125:VAL:CG1	2.51	0.41
1:D:161:GLU:O	1:D:163:SER:N	2.47	0.41
1:D:202:LYS:CD	1:D:202:LYS:N	2.84	0.41
1:D:401:GLY:O	1:D:405:GLU:HB2	2.20	0.41
1:A:374:LEU:O	1:A:375:HIS:C	2.59	0.41
1:A:413:VAL:CG1	1:A:414:TRP:N	2.82	0.41
1:C:118:VAL:O	1:C:118:VAL:HG23	2.21	0.41
1:C:190:LEU:C	1:C:192:HIS:N	2.72	0.41
1:C:186:LEU:HD21	1:C:306:LEU:HD11	2.02	0.41
1:C:460:THR:O	1:C:462:MET:N	2.53	0.41
1:D:476:ILE:O	1:D:476:ILE:HG22	2.21	0.41
1:A:385:LEU:HD21	1:A:417:TYR:CD2	2.56	0.41
1:A:389:ARG:HD2	1:A:389:ARG:N	2.25	0.41
1:B:385:LEU:CD2	1:B:385:LEU:O	2.61	0.41
1:D:381:ILE:HG22	1:D:437:ILE:HG23	2.02	0.41
1:D:457:SER:HB2	1:D:462:MET:HG2	2.02	0.41
1:A:421:MET:C	1:A:423:SER:N	2.73	0.41
1:C:167:LEU:N	1:C:167:LEU:HD22	2.36	0.41
1:C:435:MET:O	1:C:436:SER:OG	2.36	0.41
1:D:154:ARG:HH11	1:D:154:ARG:HG2	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:PHE:O	1:D:257:ARG:CG	2.62	0.41
1:D:264:ARG:HG2	1:D:264:ARG:NH1	2.35	0.41
1:D:78:PHE:CZ	1:D:102:LEU:HD23	2.56	0.41
1:A:145:PHE:CE2	1:A:231:ILE:HG13	2.56	0.41
1:A:421:MET:C	1:A:423:SER:H	2.23	0.41
1:B:104:VAL:O	1:B:108:LYS:HB2	2.21	0.41
1:B:113:GLU:HG2	1:B:266:PHE:HZ	1.79	0.41
1:C:135:PRO:HB2	1:C:136:GLY:H	1.70	0.41
1:C:200:VAL:O	1:C:201:ASN:C	2.60	0.41
1:D:141:GLY:O	1:D:142:ASP:HB3	2.20	0.41
1:D:381:ILE:O	1:D:381:ILE:HG22	2.21	0.41
1:A:201:ASN:HB2	1:A:203:ARG:NH2	2.36	0.40
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.73	0.40
1:B:145:PHE:CE2	1:B:231:ILE:HG13	2.56	0.40
1:B:313:HIS:O	1:B:313:HIS:HD2	2.04	0.40
1:C:134:LYS:HA	1:C:135:PRO:HD2	1.95	0.40
1:D:429:TYR:O	1:D:433:ASP:OD2	2.39	0.40
1:A:323:HIS:O	1:A:323:HIS:HD2	2.03	0.40
1:B:453:ILE:HD11	1:B:471:LEU:HD22	2.03	0.40
1:C:277:ASP:OD2	1:C:277:ASP:N	2.54	0.40
1:C:432:TYR:HD2	1:C:440:THR:HG21	1.87	0.40
1:D:164:LYS:HB2	1:D:165:GLU:H	1.66	0.40
1:D:215:PHE:CD2	1:D:233:GLU:HG2	2.56	0.40
1:D:331:VAL:CG2	1:D:332:VAL:N	2.83	0.40
1:D:352:ASP:CG	1:D:352:ASP:O	2.59	0.40
1:A:421:MET:HG3	1:A:423:SER:N	2.35	0.40
1:A:431:LYS:HB2	1:A:431:LYS:NZ	2.36	0.40
1:C:122:ARG:O	1:C:122:ARG:HG3	2.21	0.40
1:C:136:GLY:O	1:C:138:LEU:HD22	2.22	0.40
1:C:186:LEU:HD21	1:C:306:LEU:CD1	2.52	0.40
1:C:185:LEU:HD13	1:C:210:GLN:HG2	2.03	0.40
1:C:264:ARG:NH1	1:C:264:ARG:HG2	2.35	0.40
1:D:420:THR:CG2	1:D:421:MET:H	2.34	0.40
1:D:432:TYR:CD1	1:D:437:ILE:HD12	2.56	0.40
1:A:154:ARG:C	1:A:156:ILE:N	2.74	0.40
1:A:313:HIS:CD2	1:A:313:HIS:C	2.95	0.40
1:A:385:LEU:HB2	1:A:441:VAL:HG22	2.02	0.40
1:B:162:LEU:HB2	1:B:166:GLN:CB	2.51	0.40
1:B:323:HIS:HD2	1:B:323:HIS:O	2.04	0.40
1:C:138:LEU:HD13	1:C:138:LEU:HA	1.91	0.40
1:C:148:VAL:HG11	1:C:153:LEU:HD13	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:PRO:HA	1:C:245:PRO:HD3	1.91	0.40
1:C:352:ASP:O	1:C:352:ASP:CG	2.60	0.40
1:C:69:LEU:HD13	1:C:354:PHE:HB2	2.02	0.40
1:C:70:LEU:HD22	1:C:70:LEU:HA	1.94	0.40
1:D:247:THR:HG22	1:D:250:GLN:HB3	2.03	0.40
1:A:244:PRO:HA	1:A:245:PRO:HD3	1.87	0.40
1:A:380:PRO:HG2	1:A:381:ILE:H	1.86	0.40
1:B:115:TRP:CZ2	1:B:127:PRO:HB3	2.57	0.40
1:B:354:PHE:CG	1:B:355:GLN:N	2.86	0.40
1:C:145:PHE:O	1:C:180:LYS:HA	2.22	0.40
1:D:193:TYR:OH	1:D:333:PRO:HG3	2.22	0.40
1:D:451:GLY:O	1:D:452:LEU:HD13	2.22	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	391/474 (82%)	284 (73%)	66 (17%)	41 (10%)	0	2
1	B	391/474 (82%)	284 (73%)	64 (16%)	43 (11%)	0	2
1	C	391/474 (82%)	288 (74%)	72 (18%)	31 (8%)	1	5
1	D	391/474 (82%)	288 (74%)	73 (19%)	30 (8%)	1	5
All	All	1564/1896 (82%)	1144 (73%)	275 (18%)	145 (9%)	0	3

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PHE
1	A	199	LEU
1	A	202	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	282	GLU
1	A	309	HIS
1	A	323	HIS
1	A	370	LYS
1	A	450	ASN
1	A	461	THR
1	A	464	GLU
1	A	468	ILE
1	A	469	SER
1	B	121	PHE
1	B	199	LEU
1	B	202	LYS
1	B	282	GLU
1	B	309	HIS
1	B	323	HIS
1	B	370	LYS
1	B	450	ASN
1	B	461	THR
1	B	464	GLU
1	B	468	ILE
1	B	469	SER
1	C	168	VAL
1	C	200	VAL
1	C	318	ASN
1	D	168	VAL
1	D	200	VAL
1	D	318	ASN
1	D	462	MET
1	A	136	GLY
1	A	163	SER
1	A	278	CYS
1	A	285	LYS
1	A	294	PRO
1	A	371	VAL
1	A	382	LYS
1	A	391	PRO
1	A	392	THR
1	A	424	SER
1	A	425	LEU
1	B	136	GLY
1	B	163	SER
1	B	248	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	278	CYS
1	B	285	LYS
1	B	294	PRO
1	B	371	VAL
1	B	382	LYS
1	B	391	PRO
1	B	392	THR
1	B	424	SER
1	B	425	LEU
1	C	120	VAL
1	C	135	PRO
1	C	156	ILE
1	C	161	GLU
1	C	309	HIS
1	C	370	LYS
1	C	371	VAL
1	C	461	THR
1	C	462	MET
1	C	468	ILE
1	D	120	VAL
1	D	135	PRO
1	D	156	ILE
1	D	161	GLU
1	D	309	HIS
1	D	370	LYS
1	D	371	VAL
1	D	417	TYR
1	D	461	THR
1	D	468	ILE
1	A	135	PRO
1	A	155	GLU
1	A	171	LEU
1	A	248	SER
1	A	446	THR
1	B	155	GLU
1	B	171	LEU
1	B	446	THR
1	C	83	LYS
1	C	122	ARG
1	C	276	SER
1	C	278	CYS
1	C	352	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	385	LEU
1	C	417	TYR
1	C	451	GLY
1	D	83	LYS
1	D	122	ARG
1	D	276	SER
1	D	278	CYS
1	D	352	ASP
1	D	385	LEU
1	D	451	GLY
1	A	120	VAL
1	A	151	GLU
1	A	385	LEU
1	A	417	TYR
1	B	120	VAL
1	B	123	GLU
1	B	135	PRO
1	B	151	GLU
1	C	136	GLY
1	C	393	LEU
1	C	424	SER
1	C	446	THR
1	D	393	LEU
1	D	424	SER
1	D	446	THR
1	A	123	GLU
1	A	420	THR
1	A	421	MET
1	B	174	VAL
1	B	201	ASN
1	B	385	LEU
1	B	417	TYR
1	B	420	THR
1	C	142	ASP
1	C	285	LYS
1	C	321	LYS
1	C	480	SER
1	D	142	ASP
1	D	285	LYS
1	D	480	SER
1	A	164	LYS
1	A	174	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	201	ASN
1	A	383	VAL
1	A	437	ILE
1	A	451	GLY
1	B	149	SER
1	B	164	LYS
1	B	383	VAL
1	B	421	MET
1	B	437	ILE
1	B	451	GLY
1	C	123	GLU
1	C	166	GLN
1	D	136	GLY
1	D	166	GLN
1	D	321	LYS
1	B	270	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	356/419 (85%)	331 (93%)	25 (7%)	15	45
1	B	356/419 (85%)	330 (93%)	26 (7%)	14	43
1	C	356/419 (85%)	325 (91%)	31 (9%)	10	34
1	D	356/419 (85%)	325 (91%)	31 (9%)	10	34
All	All	1424/1676 (85%)	1311 (92%)	113 (8%)	12	40

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	84	GLN
1	A	88	ARG
1	A	89	ASP
1	A	102	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	116	THR
1	A	118	VAL
1	A	124	GLN
1	A	166	GLN
1	A	182	ARG
1	A	205	PRO
1	A	231	ILE
1	A	247	THR
1	A	268	MET
1	A	281	GLU
1	A	299	LEU
1	A	318	ASN
1	A	323	HIS
1	A	339	ASN
1	A	371	VAL
1	A	385	LEU
1	A	389	ARG
1	A	395	LEU
1	A	453	ILE
1	A	471	LEU
1	B	67	GLU
1	B	70	LEU
1	B	84	GLN
1	B	88	ARG
1	B	89	ASP
1	B	102	LEU
1	B	116	THR
1	B	118	VAL
1	B	124	GLN
1	B	166	GLN
1	B	182	ARG
1	B	205	PRO
1	B	231	ILE
1	B	247	THR
1	B	268	MET
1	B	281	GLU
1	B	299	LEU
1	B	318	ASN
1	B	323	HIS
1	B	339	ASN
1	B	371	VAL
1	B	385	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	389	ARG
1	B	395	LEU
1	B	453	ILE
1	B	471	LEU
1	C	67	GLU
1	C	70	LEU
1	C	88	ARG
1	C	91	LEU
1	C	116	THR
1	C	118	VAL
1	C	122	ARG
1	C	138	LEU
1	C	154	ARG
1	C	155	GLU
1	C	182	ARG
1	C	238	SER
1	C	241	TRP
1	C	247	THR
1	C	257	ARG
1	C	277	ASP
1	C	310	GLU
1	C	311	LEU
1	C	312	LEU
1	C	314	MET
1	C	318	ASN
1	C	376	PRO
1	C	386	ASP
1	C	389	ARG
1	C	406	LEU
1	C	426	GLU
1	C	429	TYR
1	C	440	THR
1	C	441	VAL
1	C	472	LYS
1	C	483	LYS
1	D	67	GLU
1	D	70	LEU
1	D	88	ARG
1	D	91	LEU
1	D	116	THR
1	D	118	VAL
1	D	122	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	138	LEU
1	D	154	ARG
1	D	155	GLU
1	D	182	ARG
1	D	238	SER
1	D	241	TRP
1	D	247	THR
1	D	257	ARG
1	D	277	ASP
1	D	310	GLU
1	D	311	LEU
1	D	312	LEU
1	D	314	MET
1	D	318	ASN
1	D	376	PRO
1	D	386	ASP
1	D	389	ARG
1	D	406	LEU
1	D	426	GLU
1	D	429	TYR
1	D	440	THR
1	D	441	VAL
1	D	472	LYS
1	D	483	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	96	HIS
1	A	124	GLN
1	A	166	GLN
1	A	187	HIS
1	A	192	HIS
1	A	201	ASN
1	A	249	ASN
1	A	258	HIS
1	A	287	ASN
1	A	313	HIS
1	A	318	ASN
1	A	323	HIS
1	A	400	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	409	ASN
1	A	427	GLN
1	B	84	GLN
1	B	96	HIS
1	B	124	GLN
1	B	166	GLN
1	B	187	HIS
1	B	192	HIS
1	B	201	ASN
1	B	249	ASN
1	B	258	HIS
1	B	287	ASN
1	B	313	HIS
1	B	318	ASN
1	B	323	HIS
1	B	400	GLN
1	B	409	ASN
1	B	427	GLN
1	C	124	GLN
1	C	158	GLN
1	C	192	HIS
1	C	201	ASN
1	C	216	HIS
1	C	292	ASN
1	C	318	ASN
1	C	400	GLN
1	D	158	GLN
1	D	192	HIS
1	D	201	ASN
1	D	216	HIS
1	D	292	ASN
1	D	313	HIS
1	D	318	ASN
1	D	400	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	397/474 (83%)	0.19	9 (2%) 60 46	23, 73, 155, 193	0
1	B	397/474 (83%)	0.20	9 (2%) 60 46	26, 74, 161, 194	0
1	C	397/474 (83%)	0.28	24 (6%) 21 11	28, 80, 163, 202	0
1	D	397/474 (83%)	0.25	22 (5%) 25 13	26, 78, 169, 202	0
All	All	1588/1896 (83%)	0.23	64 (4%) 38 23	23, 77, 162, 202	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	161	GLU	5.3
1	B	406	LEU	4.2
1	D	443	VAL	4.1
1	C	439	PHE	4.0
1	C	281	GLU	3.8
1	D	448	LEU	3.8
1	C	393	LEU	3.7
1	C	229	LYS	3.7
1	A	163	SER	3.5
1	B	394	GLU	3.5
1	B	467	HIS	3.5
1	C	467	HIS	3.5
1	D	156	ILE	3.5
1	C	346	MET	3.5
1	C	460	THR	3.4
1	A	156	ILE	3.3
1	B	79	LEU	3.3
1	A	167	LEU	3.1
1	D	159	ASP	3.1
1	A	415	PRO	3.1
1	D	161	GLU	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	86	LEU	3.0
1	B	119	VAL	2.9
1	C	175	LEU	2.9
1	A	216	HIS	2.9
1	D	157	LEU	2.9
1	C	146	ARG	2.8
1	C	321	LYS	2.8
1	B	388	GLY	2.8
1	D	68	ALA	2.8
1	B	423	SER	2.8
1	C	381	ILE	2.7
1	A	231	ILE	2.7
1	D	86	LEU	2.6
1	D	445	GLU	2.5
1	C	204	LEU	2.4
1	C	485	VAL	2.4
1	D	160	LYS	2.4
1	B	282	GLU	2.3
1	D	402	LEU	2.3
1	C	162	LEU	2.3
1	A	119	VAL	2.3
1	D	170	PHE	2.3
1	C	241	TRP	2.3
1	D	332	VAL	2.3
1	D	439	PHE	2.3
1	D	391	PRO	2.2
1	D	167	LEU	2.2
1	D	387	VAL	2.2
1	C	336	LEU	2.2
1	D	158	GLN	2.2
1	D	234	LYS	2.2
1	D	485	VAL	2.2
1	D	438	LEU	2.2
1	C	396	ARG	2.2
1	A	443	VAL	2.2
1	C	156	ILE	2.1
1	A	292	ASN	2.1
1	D	136	GLY	2.1
1	C	141	GLY	2.1
1	C	428	LEU	2.0
1	B	167	LEU	2.0
1	C	413	VAL	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	170	PHE	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.