



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 08:27 AM EDT

PDB ID : 1JQJ  
Title : Mechanism of Processivity Clamp Opening by the Delta Subunit Wrench of the Clamp Loader Complex of E. coli DNA Polymerase III: Structure of the beta-delta complex  
Authors : Jeruzalmi, D.; Yurieva, O.; Zhao, Y.; Young, M.; Stewart, J.; Hingorani, M.; O'Donnell, M.; Kuriyan, J.  
Deposited on : 2001-08-07  
Resolution : 2.90 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 : 2.23.2  
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) : 2.23.2

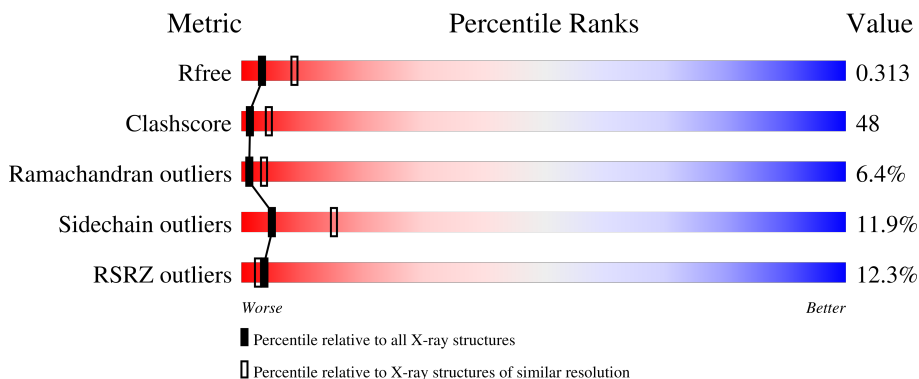
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 of 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	366	 9% 36% 54% 9%
1	B	366	 19% 36% 53% 10%
2	C	343	 7% 32% 50% 11%
2	D	343	 13% 35% 50% 9% 5%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10860 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 III, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	366	2837	1780	498	540	19	0	0	0
1	B	366	2837	1780	498	540	19	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	ALA	ILE	engineered mutation	UNP P0A988
A	273	ALA	LEU	engineered mutation	UNP P0A988
B	272	ALA	ILE	engineered mutation	UNP P0A988
B	273	ALA	LEU	engineered mutation	UNP P0A988

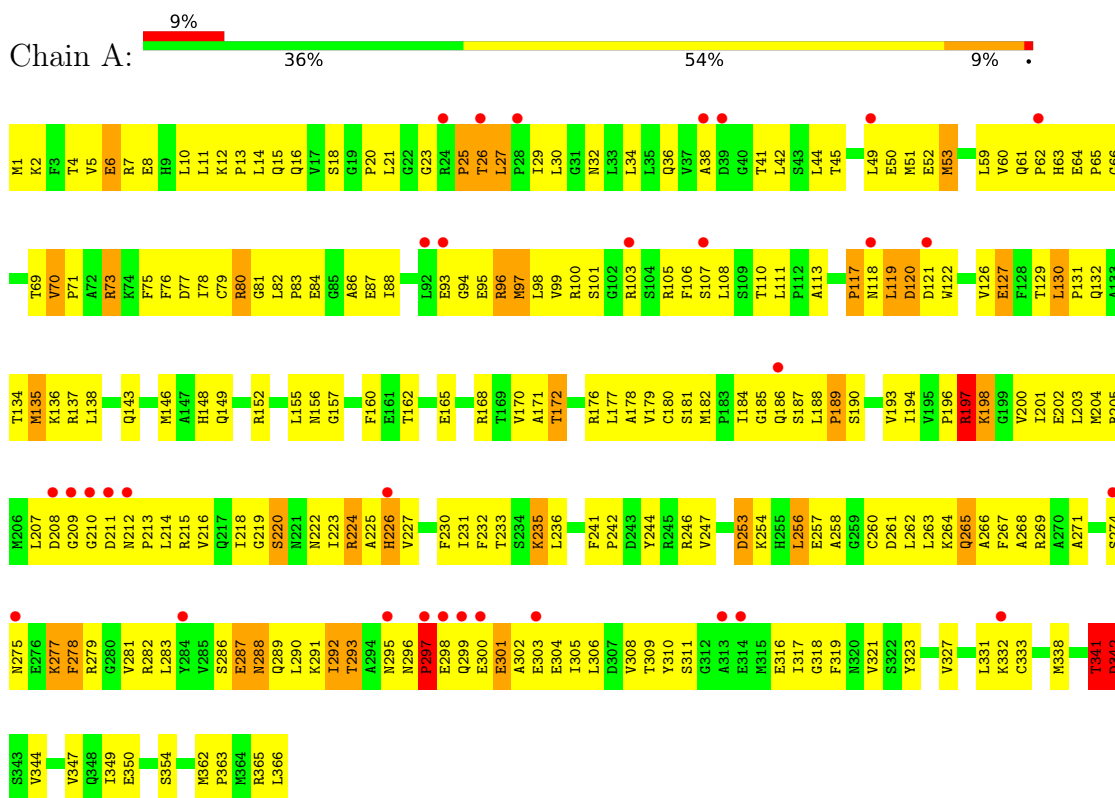
- Molecule 2 is a protein called DNA polymerase III, delta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	328	2606	1650	474	472	10	0	0	0
2	D	325	2580	1632	469	469	10	0	0	0

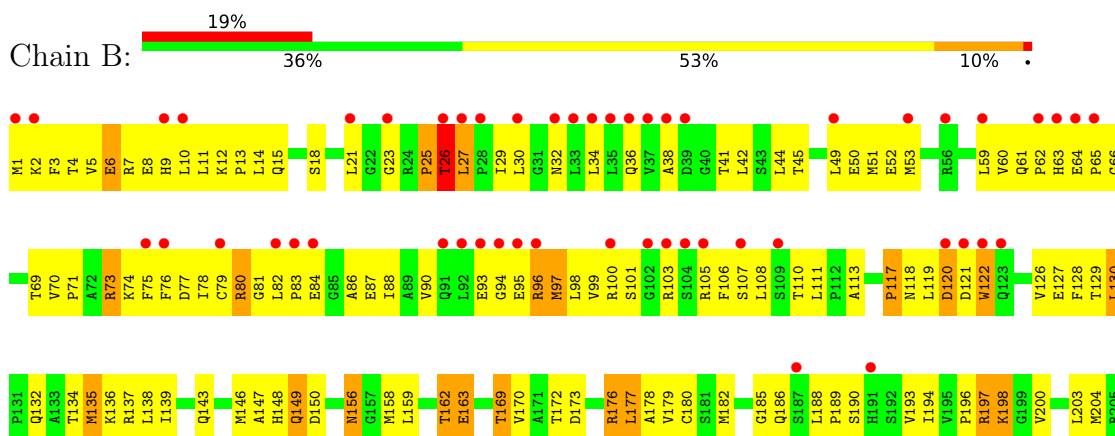
### 3 Residue-property plots

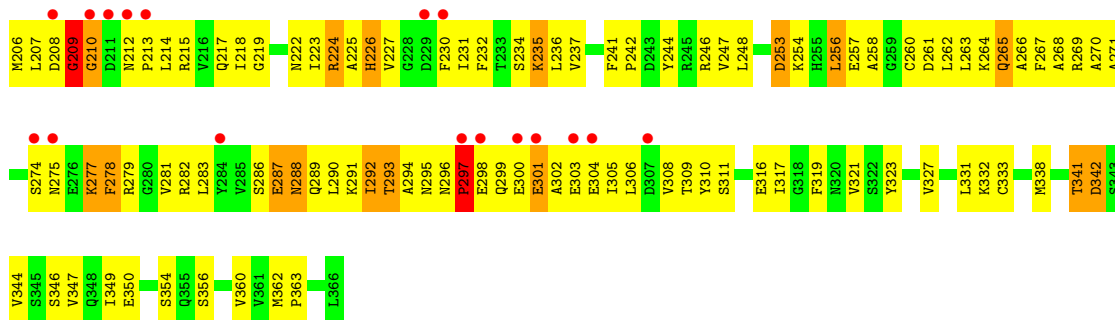
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

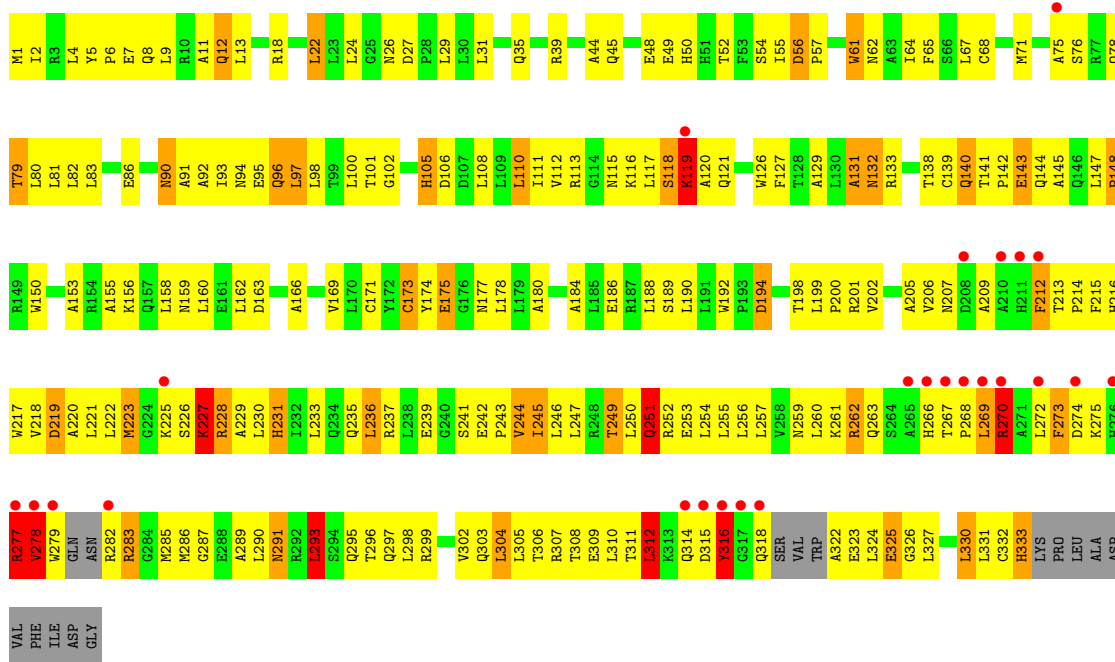


- Molecule 1: DNA polymerase III, beta chain

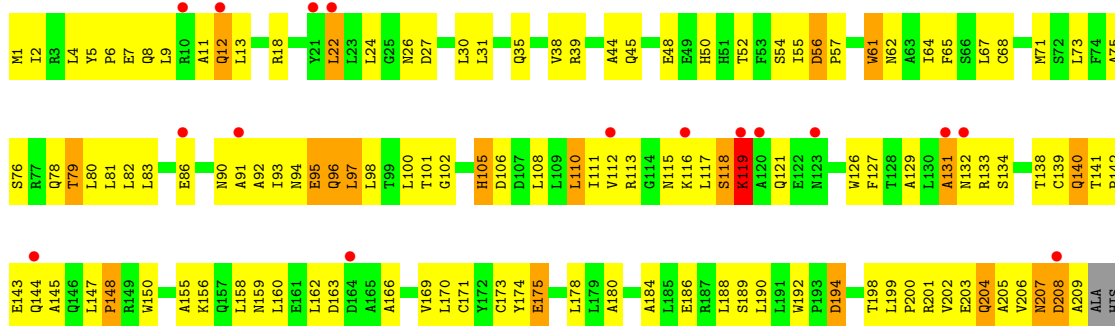
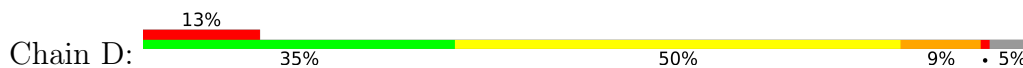


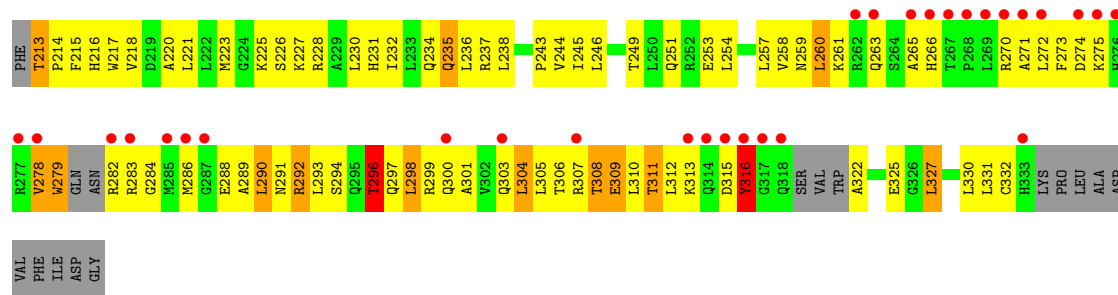


● Molecule 2: DNA polymerase III, delta subunit



● Molecule 2: DNA polymerase III, delta subunit





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.84Å 99.29Å 113.02Å 90.00° 119.17° 90.00°	Depositor
Resolution (Å)	500.00 – 2.90 19.89 – 2.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-2.90) 96.3 (19.89-2.87)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 2.88Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.266 , 0.308 0.276 , 0.313	Depositor DCC
$R_{free}$ test set	2188 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.3	Xtrriage
Anisotropy	0.414	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 64.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	10860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	0.46	0/2886	0.73	2/3907 (0.1%)
1	B	0.44	0/2886	0.72	2/3907 (0.1%)
2	C	0.63	3/2649 (0.1%)	0.97	11/3594 (0.3%)
2	D	0.35	0/2620	0.70	0/3553
All	All	0.48	3/11041 (0.0%)	0.78	15/14961 (0.1%)

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
1	B	0	1
2	C	0	2
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	269	LEU	C-N	-17.52	0.93	1.34
2	C	278	VAL	N-CA	13.96	1.74	1.46
2	C	270	ARG	CB-CG	-10.10	1.25	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	269	LEU	O-C-N	-20.83	89.37	122.70
2	C	269	LEU	C-N-CA	20.39	172.67	121.70
2	C	269	LEU	CA-C-N	13.67	147.26	117.20
2	C	278	VAL	N-CA-C	13.42	147.22	111.00
1	B	341	THR	C-N-CA	9.74	146.06	121.70
1	A	341	THR	C-N-CA	8.70	143.44	121.70

*Continued on next page...*



Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	ASP	N-CA-CB	7.25	123.65	110.60
2	C	270	ARG	CA-CB-CG	7.07	128.95	113.40
2	C	269	LEU	CA-CB-CG	6.55	130.36	115.30
2	C	293	LEU	CA-CB-CG	6.35	129.90	115.30
1	B	209	GLY	O-C-N	-6.21	112.64	123.20
2	C	278	VAL	N-CA-CB	-6.04	98.22	111.50
2	C	268	PRO	N-CA-C	5.80	127.18	112.10
2	C	212	PHE	N-CA-C	-5.23	96.89	111.00
2	C	267	THR	N-CA-C	-5.04	97.38	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	341	THR	Peptide
1	B	209	GLY	Mainchain
2	C	269	LEU	Peptide
2	C	277	ARG	Peptide

## 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	2837	0	2849	268	1
1	B	2837	0	2848	250	0
2	C	2606	0	2662	264	2
2	D	2580	0	2641	281	1
All	All	10860	0	11000	1048	2

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 48.

All (1048) 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)
2:C:278:VAL:N	2:C:278:VAL:CA	1.74	1.51

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:304:LEU:HA	2:D:307:ARG:HD2	1.15	1.11
2:D:304:LEU:CA	2:D:307:ARG:HD2	1.85	1.04
1:A:1:MET:HB3	1:A:66:GLY:HA3	1.39	1.04
1:B:266:ALA:HB1	1:B:292:ILE:HG21	1.40	1.02
1:A:266:ALA:HB1	1:A:292:ILE:HG21	1.38	1.01
2:D:96:GLN:HA	2:D:96:GLN:HE21	1.25	1.00
2:D:304:LEU:HA	2:D:307:ARG:CD	1.91	1.00
1:B:1:MET:HB3	1:B:66:GLY:HA3	1.40	0.99
2:C:166:ALA:HB1	2:C:202:VAL:HG21	1.44	0.99
2:C:96:GLN:HA	2:C:96:GLN:HE21	1.27	0.96
1:B:246:ARG:NH1	1:B:246:ARG:HB3	1.83	0.94
2:C:90:ASN:ND2	2:C:91:ALA:H	1.65	0.94
1:A:126:VAL:CG1	1:A:218:ILE:HB	1.96	0.94
1:A:246:ARG:HB3	1:A:246:ARG:NH1	1.83	0.93
1:B:283:LEU:HD22	1:B:290:LEU:HD11	1.50	0.93
2:D:90:ASN:ND2	2:D:91:ALA:H	1.67	0.93
2:D:300:GLN:HE21	2:D:307:ARG:HH22	1.13	0.92
2:D:292:ARG:HB2	2:D:292:ARG:NH1	1.84	0.92
1:A:165:GLU:HG2	1:A:187:SER:HA	1.49	0.91
2:D:90:ASN:HB3	2:D:93:ILE:HG12	1.50	0.91
2:D:304:LEU:HD11	2:D:327:LEU:HD22	1.51	0.91
1:B:208:ASP:O	1:B:210:GLY:N	2.03	0.90
1:A:246:ARG:HB3	1:A:246:ARG:HH11	1.36	0.90
2:C:140:GLN:HE21	2:C:140:GLN:HA	1.37	0.90
1:B:246:ARG:HB3	1:B:246:ARG:HH11	1.36	0.89
2:D:311:THR:HG22	2:D:315:ASP:HB2	1.52	0.88
1:A:283:LEU:HD22	1:A:290:LEU:HD11	1.52	0.88
2:D:227:LYS:H	2:D:227:LYS:HD2	1.38	0.88
2:C:311:THR:HA	2:C:315:ASP:OD2	1.74	0.88
2:C:90:ASN:HB3	2:C:93:ILE:HG12	1.54	0.88
2:D:1:MET:HB2	2:D:131:ALA:O	1.74	0.88
2:C:225:LYS:O	2:C:229:ALA:HB2	1.74	0.87
2:C:1:MET:HB2	2:C:131:ALA:O	1.75	0.87
1:B:197:ARG:HG2	1:B:198:LYS:HE2	1.56	0.87
2:C:163:ASP:OD1	2:C:198:THR:HA	1.75	0.87
2:D:163:ASP:OD1	2:D:198:THR:HA	1.74	0.87
2:C:86:GLU:CD	2:C:86:GLU:H	1.78	0.87
1:A:226:HIS:CD2	1:A:226:HIS:H	1.91	0.87
2:D:39:ARG:HE	2:D:79:THR:HG21	1.39	0.87
2:D:86:GLU:H	2:D:86:GLU:CD	1.77	0.86
1:B:170:VAL:HG12	1:B:179:VAL:HG13	1.54	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:39:ARG:HE	2:C:79:THR:HG21	1.41	0.85
2:C:225:LYS:HE2	2:C:228:ARG:HB2	1.58	0.84
1:A:177:LEU:HD21	1:A:179:VAL:HG23	1.59	0.84
2:D:118:SER:HB2	2:D:121:GLN:HE21	1.43	0.83
1:A:226:HIS:H	1:A:226:HIS:HD2	1.26	0.83
2:C:118:SER:HB2	2:C:121:GLN:HE21	1.42	0.83
2:D:225:LYS:HB3	2:D:227:LYS:HD3	1.61	0.83
2:D:292:ARG:HB2	2:D:292:ARG:HH11	1.41	0.83
2:C:270:ARG:O	2:C:274:ASP:OD2	1.97	0.83
1:A:126:VAL:HG12	1:A:218:ILE:HB	1.62	0.82
2:C:140:GLN:HA	2:C:140:GLN:NE2	1.93	0.82
2:C:50:HIS:ND1	2:C:79:THR:HB	1.95	0.82
2:D:225:LYS:HB2	2:D:228:ARG:HE	1.45	0.82
2:C:306:THR:O	2:C:310:LEU:HG	1.80	0.81
2:C:307:ARG:HA	2:C:310:LEU:HD12	1.63	0.81
2:C:22:LEU:HD12	2:C:112:VAL:HB	1.62	0.81
1:B:2:LYS:HG2	1:B:64:GLU:HB2	1.63	0.81
2:C:141:THR:HG22	2:C:142:PRO:O	1.81	0.81
2:D:39:ARG:HH21	2:D:79:THR:HG22	1.45	0.80
2:D:50:HIS:ND1	2:D:79:THR:HB	1.97	0.80
2:D:308:THR:HA	2:D:311:THR:OG1	1.82	0.80
1:A:222:ASN:HD21	1:A:235:LYS:NZ	1.79	0.79
2:D:223:MET:CE	2:D:289:ALA:HA	2.12	0.79
2:D:56:ASP:HB2	2:D:57:PRO:HD2	1.64	0.79
1:A:2:LYS:HG2	1:A:64:GLU:HB2	1.63	0.79
2:C:39:ARG:HH21	2:C:79:THR:HG22	1.47	0.78
1:A:130:LEU:HD21	1:A:135:MET:HB2	1.65	0.78
1:A:122:TRP:HZ3	1:A:219:GLY:HA3	1.46	0.78
2:C:296:THR:HG23	2:C:299:ARG:HH12	1.47	0.78
2:D:141:THR:HG22	2:D:142:PRO:O	1.82	0.78
1:A:100:ARG:HG2	1:A:105:ARG:HB3	1.66	0.78
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.64	0.78
1:A:256:LEU:HD13	1:A:308:VAL:HG21	1.65	0.78
1:A:165:GLU:OE2	1:B:60:VAL:HB	1.84	0.78
2:C:282:ARG:O	2:C:285:MET:N	2.15	0.77
1:A:262:LEU:HG	1:A:306:LEU:HD21	1.66	0.77
1:B:218:ILE:HG22	1:B:219:GLY:H	1.49	0.77
2:C:56:ASP:HB2	2:C:57:PRO:HD2	1.66	0.77
1:A:156:ASN:O	1:A:197:ARG:HG2	1.85	0.77
1:A:224:ARG:HD2	1:A:226:HIS:NE2	2.00	0.77
2:C:202:VAL:O	2:C:206:VAL:HG23	1.85	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:277:ARG:C	2:C:278:VAL:CA	2.53	0.77
1:B:100:ARG:HG2	1:B:105:ARG:HB3	1.65	0.77
1:B:214:LEU:CD1	1:B:225:ALA:HB1	2.15	0.77
2:D:22:LEU:HD12	2:D:112:VAL:HB	1.67	0.77
2:C:278:VAL:H	2:C:278:VAL:HG13	1.50	0.76
1:A:222:ASN:HD21	1:A:235:LYS:HZ1	1.30	0.76
2:D:199:LEU:HB3	2:D:200:PRO:HD3	1.68	0.76
1:A:152:ARG:HD3	2:C:48:GLU:HG3	1.69	0.75
2:C:199:LEU:HB3	2:C:200:PRO:HD3	1.68	0.75
1:A:122:TRP:CZ3	1:A:219:GLY:HA3	2.21	0.75
2:D:221:LEU:C	2:D:223:MET:H	1.90	0.75
2:C:242:GLU:O	2:C:245:ILE:HG22	1.87	0.75
2:D:293:LEU:HD23	2:D:294:SER:N	2.02	0.75
1:B:279:ARG:HD2	1:B:297:PRO:HG2	1.69	0.74
1:A:118:ASN:O	1:A:120:ASP:N	2.20	0.74
2:D:140:GLN:NE2	2:D:140:GLN:HA	2.02	0.74
1:B:308:VAL:HG22	1:B:309:THR:N	2.03	0.74
2:D:140:GLN:HA	2:D:140:GLN:HE21	1.53	0.74
2:D:249:THR:O	2:D:253:GLU:HG2	1.87	0.74
2:C:287:GLY:O	2:C:291:ASN:HB2	1.88	0.74
1:A:129:THR:H	1:A:186:GLN:HE22	1.34	0.74
1:B:256:LEU:HD13	1:B:308:VAL:HG21	1.68	0.74
2:D:199:LEU:O	2:D:203:GLU:HG2	1.87	0.74
2:D:254:LEU:HD21	2:D:301:ALA:HB3	1.69	0.74
1:A:69:THR:HB	1:A:111:LEU:O	1.88	0.73
2:D:225:LYS:HD3	2:D:228:ARG:HH21	1.53	0.73
2:D:300:GLN:NE2	2:D:307:ARG:HH22	1.85	0.73
2:C:173:CYS:HB3	2:C:212:PHE:HE1	1.53	0.73
1:B:176:ARG:HH11	1:B:176:ARG:HG2	1.53	0.73
1:B:289:GLN:OE1	1:B:291:LYS:HE3	1.88	0.73
2:C:278:VAL:N	2:C:278:VAL:CB	2.50	0.73
1:B:281:VAL:HG23	1:B:321:VAL:HG22	1.71	0.73
1:B:282:ARG:HB2	1:B:295:ASN:HB2	1.71	0.73
1:A:308:VAL:HG22	1:A:309:THR:N	2.04	0.73
1:B:262:LEU:HG	1:B:306:LEU:HD21	1.71	0.73
2:C:118:SER:HB2	2:C:121:GLN:NE2	2.03	0.73
1:A:177:LEU:HD13	1:A:247:VAL:HG21	1.71	0.73
1:A:281:VAL:HG23	1:A:321:VAL:HG22	1.69	0.73
2:D:118:SER:OG	2:D:121:GLN:HG2	1.89	0.73
2:D:221:LEU:HD23	2:D:221:LEU:O	1.89	0.73
1:B:218:ILE:HG22	1:B:219:GLY:N	2.04	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:SER:HB2	2:D:121:GLN:NE2	2.03	0.72
2:C:118:SER:OG	2:C:121:GLN:HG2	1.89	0.72
2:C:81:LEU:HD12	2:C:111:ILE:HB	1.69	0.72
1:A:289:GLN:OE1	1:A:291:LYS:HE3	1.88	0.72
1:A:282:ARG:HB2	1:A:295:ASN:HB2	1.70	0.72
2:C:80:LEU:HD23	2:C:110:LEU:HD12	1.72	0.72
2:D:299:ARG:NH1	2:D:299:ARG:HB3	2.04	0.72
1:A:279:ARG:HD2	1:A:297:PRO:HG2	1.71	0.72
2:D:80:LEU:HD23	2:D:110:LEU:HD12	1.70	0.71
1:B:293:THR:HB	1:B:303:GLU:HB3	1.71	0.71
1:A:293:THR:HB	1:A:303:GLU:HB3	1.72	0.71
2:D:260:LEU:HD23	2:D:272:LEU:HD23	1.72	0.71
2:D:303:GLN:O	2:D:307:ARG:HG3	1.91	0.71
1:B:208:ASP:O	1:B:208:ASP:OD1	2.09	0.71
1:A:308:VAL:HG22	1:A:309:THR:H	1.56	0.70
1:A:82:LEU:HB3	1:A:83:PRO:HD2	1.74	0.70
2:D:223:MET:HE1	2:D:289:ALA:HA	1.74	0.70
1:B:308:VAL:HG22	1:B:309:THR:H	1.57	0.70
1:A:23:GLY:C	1:A:25:PRO:HD3	2.12	0.70
2:C:26:ASN:H	2:C:140:GLN:HE22	1.37	0.70
2:C:257:LEU:HD23	2:C:260:LEU:HD12	1.73	0.69
2:D:166:ALA:HB1	2:D:202:VAL:HG21	1.74	0.69
1:A:363:PRO:HG2	2:C:71:MET:HE1	1.74	0.69
1:B:277:LYS:HE3	2:D:62:ASN:HD21	1.56	0.69
2:C:278:VAL:N	2:C:278:VAL:HA	2.01	0.69
1:B:69:THR:HB	1:B:111:LEU:O	1.91	0.69
1:A:143:GLN:O	1:A:146:MET:HG2	1.91	0.69
1:B:23:GLY:C	1:B:25:PRO:HD3	2.12	0.69
2:C:96:GLN:HE21	2:C:96:GLN:CA	2.03	0.69
2:C:260:LEU:HB3	2:C:290:LEU:HD11	1.73	0.69
2:D:253:GLU:HB3	2:D:286:MET:CE	2.22	0.69
1:A:226:HIS:CD2	1:A:226:HIS:N	2.60	0.69
1:B:12:LYS:HB2	1:B:13:PRO:HD3	1.75	0.69
1:B:103:ARG:HH11	1:B:105:ARG:NH1	1.92	0.69
2:C:90:ASN:ND2	2:C:91:ALA:N	2.41	0.68
2:C:251:GLN:HB2	2:C:305:LEU:HD21	1.74	0.68
2:D:97:LEU:O	2:D:101:THR:HG23	1.93	0.68
1:B:82:LEU:HB3	1:B:83:PRO:HD2	1.75	0.68
1:B:138:LEU:HD21	1:B:182:MET:HG2	1.74	0.68
1:A:103:ARG:HH11	1:A:105:ARG:NH1	1.92	0.68
2:C:225:LYS:HE2	2:C:228:ARG:CB	2.23	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:ASN:H	2:D:140:GLN:HE22	1.42	0.68
2:C:140:GLN:HE21	2:C:140:GLN:CA	2.03	0.68
1:B:2:LYS:HE2	1:B:64:GLU:HG3	1.76	0.67
2:D:35:GLN:O	2:D:39:ARG:HG3	1.94	0.67
1:A:2:LYS:HE2	1:A:64:GLU:HG3	1.75	0.67
2:D:81:LEU:HD12	2:D:111:ILE:HB	1.75	0.67
2:C:247:LEU:HD11	2:C:308:THR:HG22	1.76	0.67
2:D:306:THR:O	2:D:310:LEU:HG	1.93	0.67
1:A:230:PHE:C	1:A:231:ILE:HD12	2.15	0.67
2:C:1:MET:HE3	2:C:131:ALA:HA	1.76	0.67
1:B:196:PRO:O	1:B:200:VAL:HG23	1.94	0.67
2:D:223:MET:SD	2:D:292:ARG:HB3	2.34	0.67
2:D:300:GLN:HE21	2:D:307:ARG:NH2	1.91	0.67
2:C:225:LYS:O	2:C:229:ALA:CB	2.42	0.67
1:A:12:LYS:HB2	1:A:13:PRO:HD3	1.75	0.67
2:D:96:GLN:HE21	2:D:96:GLN:CA	2.01	0.67
1:A:148:HIS:ND1	1:A:149:GLN:HG3	2.10	0.67
1:A:16:GLN:HG2	1:A:230:PHE:CD2	2.29	0.67
1:A:130:LEU:HD22	1:A:131:PRO:O	1.95	0.67
2:D:273:PHE:CZ	2:D:283:ARG:HG3	2.30	0.67
1:B:317:ILE:HD11	1:B:363:PRO:HB3	1.77	0.66
2:C:133:ARG:O	2:C:133:ARG:HG2	1.95	0.66
2:D:96:GLN:HA	2:D:96:GLN:NE2	2.07	0.66
1:B:83:PRO:HG2	1:B:86:ALA:HB2	1.78	0.66
2:C:65:PHE:HE2	2:C:100:LEU:HB2	1.59	0.66
2:C:166:ALA:HB1	2:C:202:VAL:CG2	2.22	0.66
1:B:38:ALA:O	1:B:41:THR:HG22	1.96	0.66
1:B:118:ASN:O	1:B:120:ASP:N	2.29	0.66
2:C:278:VAL:N	2:C:278:VAL:CG1	2.58	0.66
2:D:39:ARG:NE	2:D:79:THR:HG21	2.11	0.66
1:A:288:ASN:N	1:A:288:ASN:HD22	1.92	0.66
2:C:217:TRP:NE1	2:C:233:LEU:HD13	2.10	0.66
1:A:317:ILE:HD11	1:A:363:PRO:HB3	1.78	0.66
1:B:230:PHE:O	1:B:231:ILE:HD12	1.96	0.66
2:C:186:GLU:O	2:C:189:SER:HB3	1.96	0.65
2:D:186:GLU:O	2:D:189:SER:HB3	1.96	0.65
1:B:176:ARG:HG2	1:B:176:ARG:NH1	2.11	0.65
2:D:174:TYR:CD2	2:D:180:ALA:HB1	2.32	0.65
1:B:194:ILE:CG2	1:B:237:VAL:HB	2.26	0.65
2:C:97:LEU:O	2:C:101:THR:HG23	1.95	0.65
2:C:174:TYR:CD2	2:C:180:ALA:HB1	2.32	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:ALA:O	2:C:148:PRO:HD2	1.96	0.65
2:C:96:GLN:HA	2:C:96:GLN:NE2	2.08	0.65
1:B:51:MET:CE	1:B:198:LYS:HB3	2.27	0.65
2:C:247:LEU:CD1	2:C:309:GLU:HB3	2.27	0.65
2:D:65:PHE:HE2	2:D:100:LEU:HB2	1.60	0.65
2:D:204:GLN:HG2	2:D:204:GLN:O	1.97	0.65
1:A:83:PRO:HG2	1:A:86:ALA:HB2	1.77	0.65
1:A:184:ILE:HG13	1:A:186:GLN:H	1.61	0.65
1:B:51:MET:HE2	1:B:198:LYS:HB3	1.79	0.65
2:C:26:ASN:H	2:C:140:GLN:NE2	1.94	0.65
1:A:288:ASN:HD22	1:A:288:ASN:H	1.46	0.64
2:D:203:GLU:C	2:D:205:ALA:H	2.00	0.64
2:D:304:LEU:HA	2:D:307:ARG:CG	2.27	0.64
1:A:53:MET:HE1	1:A:230:PHE:HB3	1.80	0.64
1:A:60:VAL:HG23	1:A:61:GLN:HG3	1.80	0.64
2:D:225:LYS:CB	2:D:227:LYS:HD3	2.27	0.64
1:B:51:MET:HB2	1:B:232:PHE:HE1	1.62	0.64
2:C:225:LYS:HE2	2:C:228:ARG:HG3	1.80	0.64
2:D:253:GLU:HB3	2:D:286:MET:HE1	1.78	0.64
1:B:34:LEU:HB3	1:B:45:THR:HB	1.80	0.64
2:D:133:ARG:O	2:D:133:ARG:HG2	1.96	0.64
2:C:173:CYS:HB3	2:C:212:PHE:CE1	2.33	0.64
2:C:214:PRO:HB3	2:C:246:LEU:CD2	2.27	0.64
2:C:260:LEU:CB	2:C:290:LEU:HD11	2.28	0.64
2:D:90:ASN:ND2	2:D:91:ALA:N	2.44	0.64
2:D:234:GLN:O	2:D:238:LEU:HG	1.98	0.64
1:B:137:ARG:HH22	1:B:356:SER:HB2	1.62	0.63
1:A:38:ALA:O	1:A:41:THR:HG22	1.98	0.63
2:D:86:GLU:CD	2:D:86:GLU:N	2.52	0.63
2:C:11:ALA:C	2:C:13:LEU:H	2.01	0.63
2:D:2:ILE:HD12	2:D:2:ILE:N	2.14	0.63
1:B:103:ARG:NH1	1:B:105:ARG:HH12	1.97	0.63
2:D:26:ASN:H	2:D:140:GLN:NE2	1.97	0.63
1:B:172:THR:HB	1:B:177:LEU:HD12	1.80	0.63
2:C:35:GLN:O	2:C:39:ARG:HG3	1.98	0.63
2:C:278:VAL:N	2:C:278:VAL:HG13	2.13	0.63
1:B:60:VAL:HG23	1:B:61:GLN:HG3	1.79	0.63
1:B:193:VAL:HB	1:B:236:LEU:HD13	1.80	0.63
2:C:2:ILE:N	2:C:2:ILE:HD12	2.13	0.63
2:C:247:LEU:HD12	2:C:309:GLU:HB3	1.80	0.63
2:C:192:TRP:CE2	2:C:201:ARG:HD3	2.33	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:306:THR:O	2:D:309:GLU:HG3	1.99	0.62
2:D:227:LYS:H	2:D:227:LYS:CD	2.10	0.62
1:B:132:GLN:NE2	1:B:227:VAL:HG13	2.14	0.62
1:B:288:ASN:N	1:B:288:ASN:HD22	1.96	0.62
2:D:225:LYS:HB2	2:D:228:ARG:NE	2.13	0.62
2:D:272:LEU:HA	2:D:275:LYS:HB2	1.82	0.62
1:B:23:GLY:O	1:B:25:PRO:HD3	1.99	0.62
1:B:170:VAL:CG1	1:B:179:VAL:HG13	2.29	0.62
2:C:39:ARG:NE	2:C:79:THR:HG21	2.11	0.62
2:D:278:VAL:HG13	2:D:282:ARG:NH1	2.15	0.62
2:D:207:ASN:HD22	2:D:208:ASP:H	1.47	0.62
2:D:288:GLU:HG2	2:D:292:ARG:NH1	2.15	0.62
2:D:257:LEU:HA	2:D:290:LEU:HD21	1.82	0.62
1:A:103:ARG:NH1	1:A:105:ARG:HH12	1.97	0.62
2:C:177:ASN:HD22	2:C:241:SER:HB2	1.64	0.62
2:D:145:ALA:O	2:D:148:PRO:HD2	1.99	0.61
1:A:23:GLY:O	1:A:25:PRO:HD3	2.00	0.61
1:A:7:ARG:HG2	1:A:7:ARG:O	2.01	0.61
2:D:221:LEU:HD21	2:D:331:LEU:HD12	1.83	0.61
2:D:312:LEU:O	2:D:316:TYR:HD2	1.83	0.61
1:B:73:ARG:HE	1:B:73:ARG:HA	1.65	0.61
1:B:82:LEU:HD13	1:B:101:SER:CB	2.31	0.61
1:B:292:ILE:C	1:B:292:ILE:HD13	2.20	0.61
2:C:225:LYS:HG3	2:C:228:ARG:HG3	1.81	0.61
2:D:203:GLU:O	2:D:205:ALA:N	2.34	0.61
1:A:292:ILE:HD13	1:A:292:ILE:C	2.21	0.61
2:D:221:LEU:C	2:D:223:MET:N	2.54	0.61
2:D:330:LEU:HD13	2:D:330:LEU:O	2.00	0.61
2:C:150:TRP:CH2	2:C:178:LEU:HD12	2.36	0.61
2:C:273:PHE:HZ	2:C:286:MET:HB2	1.66	0.61
1:A:73:ARG:HE	1:A:73:ARG:HA	1.66	0.61
1:B:208:ASP:C	1:B:210:GLY:H	2.00	0.61
2:D:313:LYS:HA	2:D:316:TYR:CD2	2.36	0.61
1:A:111:LEU:N	1:A:111:LEU:HD12	2.16	0.61
2:D:101:THR:HG21	2:D:126:TRP:HB2	1.82	0.61
1:A:224:ARG:HD2	1:A:226:HIS:CD2	2.36	0.60
2:C:101:THR:HG21	2:C:126:TRP:HB2	1.82	0.60
1:A:137:ARG:NH1	1:A:180:CYS:SG	2.74	0.60
1:A:215:ARG:NH2	1:A:226:HIS:ND1	2.48	0.60
2:C:231:HIS:C	2:C:231:HIS:CD2	2.75	0.60
2:D:140:GLN:HE21	2:D:140:GLN:CA	2.13	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:296:THR:HA	2:D:299:ARG:HH12	1.67	0.60
1:B:209:GLY:O	1:B:210:GLY:O	2.19	0.60
2:C:256:LEU:HA	2:C:259:ASN:ND2	2.16	0.60
2:C:86:GLU:CD	2:C:86:GLU:N	2.52	0.60
1:A:257:GLU:O	1:A:308:VAL:HG23	2.01	0.60
1:B:7:ARG:O	1:B:7:ARG:HG2	2.02	0.60
1:B:136:LYS:HG3	1:B:204:MET:HE1	1.83	0.60
2:D:169:VAL:HG21	2:D:199:LEU:HD11	1.82	0.60
1:A:1:MET:HB3	1:A:66:GLY:CA	2.25	0.60
1:A:53:MET:CE	1:A:230:PHE:HB3	2.32	0.60
1:A:82:LEU:HD13	1:A:101:SER:CB	2.32	0.60
1:A:60:VAL:HG23	1:A:61:GLN:H	1.66	0.60
2:C:1:MET:CB	2:C:131:ALA:O	2.50	0.60
2:D:11:ALA:C	2:D:13:LEU:H	2.04	0.60
2:D:150:TRP:CH2	2:D:178:LEU:HD12	2.37	0.60
2:C:169:VAL:HG21	2:C:199:LEU:HD11	1.82	0.60
2:D:309:GLU:OE1	2:D:310:LEU:HD23	2.02	0.60
1:A:203:LEU:HD12	1:A:203:LEU:O	2.01	0.59
2:D:243:PRO:HA	2:D:246:LEU:HD12	1.84	0.59
1:B:230:PHE:C	1:B:231:ILE:HD12	2.21	0.59
2:C:255:LEU:HD23	2:C:259:ASN:HD21	1.67	0.59
1:A:203:LEU:O	1:A:207:LEU:HG	2.01	0.59
1:A:286:SER:O	1:A:287:GLU:C	2.40	0.59
1:A:34:LEU:HB3	1:A:45:THR:HB	1.83	0.59
2:C:217:TRP:CE2	2:C:233:LEU:HD13	2.37	0.59
2:C:226:SER:O	2:C:230:LEU:HD13	2.03	0.59
1:A:349:ILE:HD12	1:A:349:ILE:N	2.17	0.59
1:B:269:ARG:HD2	1:B:304:GLU:OE1	2.03	0.59
1:B:288:ASN:HD22	1:B:288:ASN:H	1.49	0.59
2:C:27:ASP:OD2	2:C:178:LEU:HD23	2.01	0.59
2:D:90:ASN:O	2:D:94:ASN:ND2	2.34	0.59
1:A:14:LEU:HD21	1:A:76:PHE:HA	1.85	0.59
1:B:185:GLY:O	1:B:186:GLN:HG3	2.03	0.59
2:C:225:LYS:CE	2:C:228:ARG:HB2	2.31	0.59
2:C:306:THR:HG22	2:C:310:LEU:HD11	1.83	0.59
1:A:260:CYS:O	1:A:264:LYS:HG3	2.03	0.59
1:B:60:VAL:HG23	1:B:61:GLN:H	1.67	0.59
1:B:223:ILE:HG22	1:B:236:LEU:HD21	1.85	0.59
1:B:257:GLU:O	1:B:308:VAL:HG23	2.03	0.59
1:A:27:LEU:HG	1:A:30:LEU:HD12	1.85	0.59
1:A:36:GLN:O	1:A:42:LEU:HD12	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:LEU:HD21	2:D:12:GLN:HB2	1.85	0.59
2:D:207:ASN:HD22	2:D:208:ASP:N	2.00	0.59
1:A:32:ASN:HB3	1:A:69:THR:HG22	1.84	0.58
1:A:362:MET:CE	2:C:71:MET:HB3	2.33	0.58
1:B:32:ASN:HB3	1:B:69:THR:HG22	1.84	0.58
2:C:311:THR:O	2:C:315:ASP:N	2.36	0.58
2:D:39:ARG:HH21	2:D:79:THR:CG2	2.13	0.58
1:A:168:ARG:HG3	1:A:168:ARG:O	2.03	0.58
1:B:128:PHE:HE2	1:B:218:ILE:HD11	1.67	0.58
1:B:214:LEU:HD11	1:B:225:ALA:CB	2.32	0.58
2:C:118:SER:CB	2:C:121:GLN:HE21	2.15	0.58
2:C:296:THR:CG2	2:C:299:ARG:HH12	2.16	0.58
2:D:327:LEU:O	2:D:331:LEU:HG	2.02	0.58
1:A:165:GLU:HG2	1:A:187:SER:CA	2.31	0.58
1:B:14:LEU:HD21	1:B:76:PHE:HA	1.84	0.58
1:A:63:HIS:O	1:A:64:GLU:HG2	2.04	0.58
1:B:103:ARG:HH11	1:B:105:ARG:HH12	1.50	0.58
1:A:88:ILE:HD12	1:A:88:ILE:N	2.19	0.58
1:B:150:ASP:O	1:B:156:ASN:ND2	2.36	0.58
2:D:293:LEU:HD22	2:D:298:LEU:HD13	1.85	0.58
1:A:196:PRO:O	1:A:200:VAL:HG23	2.04	0.58
1:B:129:THR:H	1:B:186:GLN:HE22	1.52	0.58
2:D:1:MET:HE3	2:D:131:ALA:HA	1.83	0.58
2:D:118:SER:CB	2:D:121:GLN:HE21	2.16	0.58
2:C:90:ASN:O	2:C:94:ASN:ND2	2.37	0.57
2:C:255:LEU:CD2	2:C:259:ASN:HD21	2.17	0.57
1:A:103:ARG:HH11	1:A:105:ARG:HH12	1.50	0.57
1:A:129:THR:O	1:A:130:LEU:HB3	2.04	0.57
1:B:27:LEU:HG	1:B:30:LEU:HD12	1.86	0.57
2:C:31:LEU:HD23	2:C:139:CYS:SG	2.44	0.57
1:A:93:GLU:O	1:A:95:GLU:N	2.37	0.57
1:B:36:GLN:O	1:B:42:LEU:HD12	2.04	0.57
1:B:111:LEU:HD12	1:B:111:LEU:N	2.20	0.57
2:D:257:LEU:HD21	2:D:286:MET:HB3	1.85	0.57
1:A:269:ARG:HD2	1:A:304:GLU:OE1	2.04	0.57
2:C:39:ARG:HH21	2:C:79:THR:CG2	2.16	0.57
2:D:2:ILE:HD11	2:D:18:ARG:NH2	2.18	0.57
2:D:279:TRP:HE3	2:D:279:TRP:H	1.51	0.57
2:D:309:GLU:O	2:D:313:LYS:HE2	2.05	0.57
1:B:137:ARG:NH1	1:B:180:CYS:SG	2.78	0.57
1:B:170:VAL:HA	1:B:178:ALA:O	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:222:LEU:HD12	2:C:285:MET:HE3	1.87	0.57
2:D:299:ARG:HB3	2:D:299:ARG:CZ	2.35	0.57
1:A:53:MET:SD	1:A:230:PHE:HB3	2.45	0.57
1:B:299:GLN:OE1	1:B:301:GLU:HG2	2.05	0.57
1:A:362:MET:HE2	2:C:71:MET:HB3	1.86	0.57
1:B:231:ILE:O	1:B:231:ILE:HG22	2.02	0.57
2:C:304:LEU:HB3	2:C:327:LEU:HD21	1.87	0.57
2:D:278:VAL:HG12	2:D:278:VAL:O	2.05	0.57
2:D:304:LEU:C	2:D:304:LEU:HD12	2.25	0.57
1:B:138:LEU:CD2	1:B:182:MET:HG2	2.35	0.57
2:C:282:ARG:O	2:C:283:ARG:C	2.42	0.57
1:B:88:ILE:N	1:B:88:ILE:HD12	2.19	0.56
2:D:226:SER:HB3	2:D:332:CYS:SG	2.44	0.56
2:D:227:LYS:HD2	2:D:227:LYS:N	2.13	0.56
2:D:230:LEU:HD11	2:D:325:GLU:CG	2.35	0.56
1:B:136:LYS:HG3	1:B:204:MET:CE	2.35	0.56
1:B:349:ILE:N	1:B:349:ILE:HD12	2.19	0.56
2:C:22:LEU:CD1	2:C:112:VAL:HB	2.34	0.56
1:B:63:HIS:O	1:B:64:GLU:HG2	2.05	0.56
1:B:286:SER:O	1:B:287:GLU:C	2.42	0.56
2:D:7:GLU:OE2	2:D:7:GLU:N	2.37	0.56
1:A:299:GLN:OE1	1:A:301:GLU:HG2	2.05	0.56
1:B:93:GLU:O	1:B:95:GLU:N	2.36	0.56
1:B:122:TRP:CE2	1:B:222:ASN:HB2	2.41	0.56
2:C:81:LEU:CD1	2:C:111:ILE:HB	2.36	0.56
2:C:215:PHE:O	2:C:219:ASP:HB2	2.06	0.56
2:D:259:ASN:C	2:D:261:LYS:H	2.09	0.56
2:C:192:TRP:HB3	2:C:201:ARG:NH1	2.20	0.55
2:C:220:ALA:HB1	2:C:229:ALA:HB2	1.87	0.55
2:C:235:GLN:O	2:C:239:GLU:HG3	2.06	0.55
2:D:297:GLN:CD	2:D:297:GLN:H	2.09	0.55
2:C:4:LEU:HD21	2:C:12:GLN:HB2	1.89	0.55
2:C:263:GLN:HB3	2:C:266:HIS:HB3	1.88	0.55
2:D:31:LEU:HD23	2:D:139:CYS:SG	2.46	0.55
1:A:365:ARG:HH21	2:C:105:HIS:CE1	2.25	0.55
2:C:2:ILE:HD11	2:C:18:ARG:NH2	2.22	0.55
2:C:273:PHE:CZ	2:C:286:MET:HB2	2.42	0.55
1:B:127:GLU:HB3	1:B:217:GLN:HG2	1.88	0.55
1:B:223:ILE:CG2	1:B:236:LEU:HD21	2.36	0.55
2:C:173:CYS:CB	2:C:212:PHE:HE1	2.18	0.55
1:B:1:MET:HA	1:B:65:PRO:O	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:307:ARG:O	2:C:311:THR:HG23	2.07	0.55
1:A:277:LYS:HE3	2:C:62:ASN:ND2	2.22	0.55
2:D:236:LEU:HD13	2:D:246:LEU:HD21	1.87	0.55
1:A:214:LEU:HD12	1:A:215:ARG:N	2.22	0.55
2:D:22:LEU:CD1	2:D:112:VAL:HB	2.35	0.55
1:A:129:THR:HG22	1:A:130:LEU:N	2.22	0.55
1:B:277:LYS:HE3	2:D:62:ASN:ND2	2.21	0.55
2:D:184:ALA:O	2:D:188:LEU:HD12	2.07	0.55
2:D:230:LEU:HD11	2:D:325:GLU:HG3	1.89	0.55
2:D:231:HIS:CE1	2:D:235:GLN:HE21	2.25	0.55
2:D:293:LEU:HD23	2:D:294:SER:H	1.72	0.55
2:C:314:GLN:HA	2:C:316:TYR:HE2	1.72	0.54
1:A:127:GLU:HA	1:A:216:VAL:O	2.08	0.54
2:D:272:LEU:HD12	2:D:275:LYS:CB	2.38	0.54
1:B:138:LEU:HD23	1:B:180:CYS:SG	2.47	0.54
2:C:243:PRO:C	2:C:245:ILE:H	2.09	0.54
2:C:309:GLU:HA	2:C:312:LEU:HD21	1.90	0.54
1:A:222:ASN:ND2	1:A:235:LYS:NZ	2.52	0.54
1:A:265:GLN:O	1:A:266:ALA:C	2.46	0.54
1:B:129:THR:HG22	1:B:130:LEU:N	2.21	0.54
1:B:172:THR:OG1	1:B:177:LEU:HB2	2.07	0.54
2:C:68:CYS:O	2:C:105:HIS:HE1	1.90	0.54
2:C:218:VAL:HG11	2:C:253:GLU:HG3	1.90	0.54
2:D:207:ASN:HD22	2:D:207:ASN:N	2.06	0.54
2:D:1:MET:CB	2:D:131:ALA:O	2.50	0.54
2:D:244:VAL:HG22	2:D:312:LEU:HD22	1.87	0.54
2:C:11:ALA:O	2:C:13:LEU:N	2.38	0.54
2:C:212:PHE:HB3	2:C:215:PHE:CD1	2.42	0.54
2:D:251:GLN:HB2	2:D:305:LEU:HD22	1.89	0.54
2:D:272:LEU:HD12	2:D:275:LYS:HB3	1.90	0.54
1:B:2:LYS:CG	1:B:64:GLU:HB2	2.35	0.54
2:C:214:PRO:HB3	2:C:246:LEU:HD23	1.87	0.54
1:A:197:ARG:O	1:A:201:ILE:HG12	2.08	0.54
1:B:50:GLU:OE2	1:B:198:LYS:HD2	2.08	0.54
2:D:198:THR:OG1	2:D:201:ARG:HG3	2.07	0.54
2:C:52:THR:HG23	2:C:81:LEU:HD23	1.89	0.54
1:A:135:MET:O	1:A:135:MET:SD	2.66	0.54
1:A:278:PHE:O	1:A:278:PHE:CD1	2.61	0.54
1:B:194:ILE:HG22	1:B:237:VAL:HB	1.90	0.54
1:A:170:VAL:HG22	1:A:241:PHE:CE2	2.43	0.53
1:B:226:HIS:N	1:B:226:HIS:CD2	2.75	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:231:HIS:NE2	2:C:235:GLN:CD	2.61	0.53
1:B:222:ASN:OD1	1:B:235:LYS:NZ	2.40	0.53
2:C:225:LYS:HE2	2:C:228:ARG:CG	2.38	0.53
2:D:293:LEU:HD13	2:D:298:LEU:HD13	1.90	0.53
2:D:307:ARG:O	2:D:311:THR:OG1	2.25	0.53
1:A:130:LEU:HD21	1:A:135:MET:CB	2.38	0.53
2:C:184:ALA:O	2:C:188:LEU:HD12	2.08	0.53
2:C:255:LEU:HD23	2:C:255:LEU:C	2.29	0.53
2:C:305:LEU:C	2:C:305:LEU:HD23	2.28	0.53
2:C:325:GLU:N	2:C:325:GLU:OE1	2.42	0.53
2:D:52:THR:HG23	2:D:81:LEU:HD23	1.91	0.53
2:D:254:LEU:HD11	2:D:298:LEU:HD12	1.89	0.53
1:A:136:LYS:HG3	1:A:204:MET:HE1	1.90	0.53
1:A:177:LEU:HD21	1:A:179:VAL:CG2	2.35	0.53
1:B:139:ILE:O	1:B:143:GLN:HB2	2.08	0.53
1:A:171:ALA:C	1:A:172:THR:HG22	2.27	0.53
1:B:293:THR:HB	1:B:303:GLU:CB	2.39	0.53
1:A:204:MET:HE3	1:A:204:MET:O	2.08	0.53
2:C:166:ALA:HB2	2:C:199:LEU:HA	1.91	0.53
2:D:221:LEU:O	2:D:223:MET:N	2.30	0.53
2:D:260:LEU:HD13	2:D:290:LEU:HD11	1.91	0.53
1:A:135:MET:CE	1:A:160:PHE:HE2	2.22	0.53
2:C:192:TRP:CD2	2:C:201:ARG:HD3	2.43	0.53
1:A:129:THR:HG22	1:A:130:LEU:H	1.74	0.53
1:A:170:VAL:HG22	1:A:241:PHE:HE2	1.74	0.53
1:A:256:LEU:CD1	1:A:308:VAL:HG21	2.38	0.53
1:A:268:ALA:O	1:A:271:ALA:HB3	2.07	0.53
1:A:278:PHE:O	1:A:278:PHE:HD1	1.91	0.53
1:A:319:PHE:HZ	1:A:347:VAL:HG21	1.74	0.53
2:D:305:LEU:HD23	2:D:305:LEU:O	2.08	0.53
1:A:2:LYS:CG	1:A:64:GLU:HB2	2.33	0.53
2:D:260:LEU:HB3	2:D:290:LEU:CD1	2.39	0.53
1:B:319:PHE:HZ	1:B:347:VAL:HG21	1.73	0.52
2:C:225:LYS:CG	2:C:228:ARG:HG3	2.39	0.52
2:C:256:LEU:HA	2:C:259:ASN:HD22	1.72	0.52
2:D:312:LEU:O	2:D:316:TYR:CD2	2.63	0.52
1:A:293:THR:HB	1:A:303:GLU:CB	2.39	0.52
1:A:308:VAL:CG2	1:A:309:THR:H	2.21	0.52
1:A:308:VAL:CG2	1:A:309:THR:N	2.72	0.52
1:B:271:ALA:HB2	1:B:321:VAL:HG11	1.91	0.52
2:C:100:LEU:C	2:C:102:GLY:H	2.13	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:214:PRO:HB3	2:D:246:LEU:HD23	1.91	0.52
1:A:1:MET:HA	1:A:65:PRO:O	2.08	0.52
1:A:170:VAL:CG2	1:A:241:PHE:HE2	2.23	0.52
1:A:197:ARG:NH1	1:A:197:ARG:HB3	2.24	0.52
1:B:1:MET:HB3	1:B:66:GLY:CA	2.28	0.52
1:A:310:TYR:CG	1:A:311:SER:N	2.78	0.52
1:B:258:ALA:HB3	1:B:263:LEU:HD11	1.92	0.52
1:B:308:VAL:CG2	1:B:309:THR:N	2.71	0.52
2:D:300:GLN:O	2:D:303:GLN:HB2	2.09	0.52
1:B:196:PRO:HG3	1:B:237:VAL:HG23	1.92	0.52
1:B:260:CYS:O	1:B:264:LYS:HG3	2.09	0.52
2:C:92:ALA:O	2:C:95:GLU:HB2	2.09	0.52
2:D:296:THR:HB	2:D:297:GLN:NE2	2.24	0.52
1:B:298:GLU:O	1:B:299:GLN:HB2	2.09	0.52
2:C:293:LEU:HD23	2:C:297:GLN:OE1	2.09	0.52
2:D:56:ASP:HB2	2:D:57:PRO:CD	2.38	0.52
1:B:218:ILE:N	1:B:218:ILE:HD12	2.25	0.52
1:B:232:PHE:CZ	1:B:234:SER:HB2	2.45	0.52
1:B:265:GLN:O	1:B:266:ALA:C	2.48	0.52
1:A:246:ARG:HH11	1:A:246:ARG:CB	2.16	0.52
1:A:258:ALA:HB3	1:A:263:LEU:HD11	1.92	0.52
1:B:173:ASP:OD1	1:B:176:ARG:HD2	2.10	0.52
1:B:218:ILE:HD12	1:B:218:ILE:H	1.74	0.52
2:C:90:ASN:HD22	2:C:91:ALA:H	1.55	0.52
2:D:207:ASN:N	2:D:207:ASN:ND2	2.58	0.52
1:A:136:LYS:HG3	1:A:204:MET:CE	2.40	0.51
1:A:197:ARG:HB2	1:A:198:LYS:HE2	1.91	0.51
1:B:268:ALA:O	1:B:271:ALA:HB3	2.10	0.51
2:C:263:GLN:CB	2:C:266:HIS:HB3	2.40	0.51
2:C:314:GLN:HA	2:C:316:TYR:CE2	2.45	0.51
1:A:177:LEU:C	1:A:177:LEU:HD23	2.31	0.51
1:B:256:LEU:CD1	1:B:308:VAL:HG21	2.39	0.51
2:D:228:ARG:O	2:D:231:HIS:HB3	2.11	0.51
1:A:77:ASP:O	1:A:81:GLY:N	2.42	0.51
1:B:50:GLU:OE1	1:B:51:MET:HE2	2.10	0.51
2:C:255:LEU:HD23	2:C:255:LEU:O	2.09	0.51
2:D:1:MET:HE2	2:D:22:LEU:HD23	1.91	0.51
2:D:158:LEU:O	2:D:160:LEU:HD13	2.09	0.51
2:D:260:LEU:HB3	2:D:290:LEU:HD13	1.92	0.51
1:A:119:LEU:O	1:A:120:ASP:C	2.49	0.51
1:A:277:LYS:HE3	2:C:62:ASN:HD21	1.75	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:THR:HG22	1:A:342:ASP:HB2	1.93	0.51
2:C:250:LEU:C	2:C:252:ARG:H	2.13	0.51
1:B:362:MET:HG2	2:D:73:LEU:HG	1.93	0.51
2:D:166:ALA:HB2	2:D:199:LEU:HA	1.91	0.51
1:A:184:ILE:HG13	1:A:185:GLY:N	2.26	0.51
1:A:363:PRO:HG2	2:C:71:MET:CE	2.41	0.51
1:B:97:MET:HB3	1:B:108:LEU:HB2	1.92	0.51
2:C:115:ASN:O	2:C:116:LYS:C	2.49	0.51
2:C:247:LEU:HD22	2:C:305:LEU:HG	1.93	0.51
2:C:261:LYS:C	2:C:263:GLN:H	2.12	0.51
2:D:293:LEU:CD2	2:D:298:LEU:HB2	2.41	0.51
1:A:61:GLN:HB3	1:A:62:PRO:HD2	1.93	0.51
1:B:77:ASP:O	1:B:81:GLY:N	2.43	0.51
2:C:26:ASN:N	2:C:140:GLN:HE22	2.07	0.51
1:A:177:LEU:CD2	1:A:179:VAL:HG23	2.38	0.51
1:B:305:ILE:CG2	1:B:306:LEU:N	2.74	0.51
1:B:308:VAL:CG2	1:B:309:THR:H	2.21	0.51
2:C:256:LEU:O	2:C:260:LEU:HG	2.11	0.51
2:D:92:ALA:O	2:D:95:GLU:HB2	2.11	0.51
2:D:150:TRP:CZ2	2:D:178:LEU:HD12	2.46	0.51
2:D:217:TRP:CE2	2:D:221:LEU:HD12	2.45	0.51
1:A:138:LEU:HD21	1:A:182:MET:HG2	1.93	0.51
2:C:97:LEU:HD23	2:C:126:TRP:CD2	2.46	0.51
2:C:158:LEU:O	2:C:160:LEU:HD13	2.11	0.51
1:A:14:LEU:CD2	1:A:76:PHE:HA	2.41	0.50
1:B:51:MET:HB2	1:B:232:PHE:CE1	2.44	0.50
1:B:61:GLN:HB3	1:B:62:PRO:HD2	1.92	0.50
1:B:278:PHE:O	1:B:278:PHE:CD1	2.64	0.50
2:D:97:LEU:HD23	2:D:126:TRP:CD2	2.46	0.50
1:A:70:VAL:HG21	1:A:75:PHE:CD2	2.46	0.50
1:B:14:LEU:CD2	1:B:76:PHE:HA	2.41	0.50
1:B:130:LEU:HD21	1:B:135:MET:HG2	1.93	0.50
2:C:245:ILE:HG23	2:C:246:LEU:N	2.25	0.50
2:D:55:ILE:HD12	2:D:61:TRP:CH2	2.46	0.50
2:D:81:LEU:CD1	2:D:111:ILE:HB	2.42	0.50
2:D:100:LEU:C	2:D:102:GLY:H	2.12	0.50
2:D:313:LYS:HA	2:D:316:TYR:CE2	2.46	0.50
2:C:91:ALA:O	2:C:95:GLU:OE1	2.30	0.50
1:A:271:ALA:HB2	1:A:321:VAL:HG11	1.93	0.50
1:A:298:GLU:O	1:A:299:GLN:HB2	2.09	0.50
1:B:83:PRO:HG2	1:B:86:ALA:CB	2.41	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:296:THR:HA	2:C:299:ARG:NH1	2.26	0.50
2:D:91:ALA:O	2:D:95:GLU:OE1	2.30	0.50
1:B:278:PHE:O	1:B:278:PHE:HD1	1.95	0.50
1:B:310:TYR:CG	1:B:311:SER:N	2.80	0.50
1:B:341:THR:HG22	1:B:342:ASP:N	2.26	0.50
1:A:16:GLN:NE2	1:A:230:PHE:CD1	2.74	0.50
1:A:122:TRP:CD1	1:A:122:TRP:N	2.79	0.50
2:D:44:ALA:O	2:D:45:GLN:HG3	2.11	0.50
2:D:126:TRP:CG	2:D:127:PHE:N	2.80	0.50
2:D:254:LEU:O	2:D:258:VAL:HG23	2.11	0.50
1:A:281:VAL:HG12	1:A:282:ARG:N	2.27	0.50
1:B:60:VAL:HG23	1:B:61:GLN:N	2.27	0.50
1:B:147:ALA:HB2	1:B:173:ASP:HA	1.94	0.50
1:B:281:VAL:HG12	1:B:282:ARG:N	2.27	0.50
2:C:221:LEU:HD12	2:C:250:LEU:HD13	1.93	0.50
2:D:313:LYS:O	2:D:316:TYR:CE2	2.64	0.50
1:A:83:PRO:HG2	1:A:86:ALA:CB	2.41	0.50
2:C:31:LEU:HD23	2:C:139:CYS:CB	2.42	0.50
1:A:51:MET:HE1	1:A:198:LYS:HB3	1.94	0.49
2:D:215:PHE:CE2	2:D:249:THR:HG23	2.47	0.49
2:D:253:GLU:HB3	2:D:286:MET:SD	2.52	0.49
1:A:197:ARG:HB3	1:A:197:ARG:CZ	2.42	0.49
1:B:261:ASP:OD2	1:B:262:LEU:N	2.45	0.49
2:C:126:TRP:CG	2:C:127:PHE:N	2.80	0.49
1:A:97:MET:HB3	1:A:108:LEU:HB2	1.94	0.49
1:A:266:ALA:HB1	1:A:292:ILE:CG2	2.28	0.49
1:B:27:LEU:HD12	1:B:29:ILE:HG22	1.94	0.49
1:B:80:ARG:HE	1:B:80:ARG:C	2.16	0.49
2:C:150:TRP:CZ2	2:C:178:LEU:HD12	2.46	0.49
2:C:332:CYS:O	2:C:333:HIS:C	2.50	0.49
1:A:278:PHE:CD1	1:A:278:PHE:C	2.86	0.49
1:A:168:ARG:HE	1:A:181:SER:HG	1.57	0.49
1:A:323:TYR:O	1:A:327:VAL:HG23	2.13	0.49
2:C:55:ILE:HD12	2:C:61:TRP:CH2	2.46	0.49
2:D:278:VAL:CG1	2:D:282:ARG:HH11	2.25	0.49
1:A:20:PRO:HB3	1:A:202:GLU:HG2	1.95	0.49
1:A:60:VAL:HG23	1:A:61:GLN:N	2.26	0.49
1:A:184:ILE:HD12	1:A:188:LEU:HD11	1.95	0.49
1:A:256:LEU:C	1:A:256:LEU:HD12	2.33	0.49
1:B:70:VAL:HG21	1:B:75:PHE:CD2	2.48	0.49
2:D:68:CYS:O	2:D:105:HIS:HE1	1.95	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:LEU:HB3	2:C:148:PRO:HD3	1.95	0.49
2:D:217:TRP:NE1	2:D:221:LEU:HD12	2.28	0.49
2:D:279:TRP:O	2:D:282:ARG:N	2.46	0.49
1:A:269:ARG:HH11	1:A:269:ARG:HG2	1.78	0.49
1:A:288:ASN:H	1:A:310:TYR:HB3	1.77	0.49
2:D:11:ALA:O	2:D:13:LEU:N	2.44	0.49
1:A:70:VAL:HA	1:A:110:THR:HG22	1.95	0.49
1:A:162:THR:O	1:A:190:SER:HA	2.13	0.49
1:B:203:LEU:O	1:B:207:LEU:HG	2.13	0.49
2:C:222:LEU:HD12	2:C:285:MET:CE	2.42	0.49
2:D:297:GLN:O	2:D:299:ARG:N	2.46	0.49
2:C:309:GLU:HA	2:C:312:LEU:CD2	2.43	0.49
2:D:147:LEU:HB3	2:D:148:PRO:HD3	1.94	0.49
2:D:322:ALA:O	2:D:325:GLU:HB3	2.12	0.49
1:A:34:LEU:HD11	1:A:113:ALA:HB1	1.95	0.48
2:C:7:GLU:OE2	2:C:7:GLU:N	2.40	0.48
2:C:31:LEU:HD23	2:C:139:CYS:HB2	1.95	0.48
2:D:225:LYS:HD3	2:D:228:ARG:NH2	2.26	0.48
1:A:130:LEU:CD2	1:A:135:MET:HB2	2.40	0.48
1:B:93:GLU:OE1	1:B:98:LEU:HD21	2.13	0.48
2:D:48:GLU:HG2	2:D:76:SER:CB	2.43	0.48
2:D:254:LEU:HD21	2:D:301:ALA:CB	2.42	0.48
2:D:273:PHE:HB3	2:D:279:TRP:CD1	2.47	0.48
1:A:130:LEU:HD13	1:A:130:LEU:O	2.13	0.48
1:A:184:ILE:HD11	1:A:188:LEU:HG	1.95	0.48
1:B:70:VAL:HG11	1:B:97:MET:SD	2.53	0.48
1:A:20:PRO:HD3	1:A:202:GLU:OE2	2.12	0.48
1:A:261:ASP:OD2	1:A:262:LEU:N	2.47	0.48
1:B:70:VAL:HA	1:B:110:THR:HG22	1.96	0.48
1:B:147:ALA:HB1	1:B:150:ASP:HB2	1.95	0.48
2:C:64:ILE:O	2:C:67:LEU:HB3	2.13	0.48
2:C:243:PRO:O	2:C:245:ILE:N	2.46	0.48
2:D:100:LEU:C	2:D:102:GLY:N	2.67	0.48
2:D:206:VAL:O	2:D:209:ALA:HB3	2.14	0.48
2:D:221:LEU:O	2:D:221:LEU:CD2	2.58	0.48
2:D:304:LEU:CB	2:D:307:ARG:HD2	2.41	0.48
1:A:80:ARG:C	1:A:80:ARG:HE	2.17	0.48
1:B:32:ASN:HB3	1:B:69:THR:CG2	2.43	0.48
2:D:142:PRO:HD2	2:D:178:LEU:HD21	1.95	0.48
1:A:194:ILE:HD11	1:A:241:PHE:HB2	1.95	0.48
1:B:246:ARG:HH11	1:B:246:ARG:CB	2.16	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:207:ASN:ND2	2:D:207:ASN:H	2.12	0.48
1:B:197:ARG:CG	1:B:198:LYS:N	2.75	0.48
2:C:142:PRO:HD2	2:C:178:LEU:HD21	1.96	0.48
2:C:225:LYS:O	2:C:225:LYS:HG2	2.14	0.48
2:C:245:ILE:C	2:C:245:ILE:HD13	2.34	0.48
2:D:115:ASN:O	2:D:116:LYS:C	2.52	0.48
1:A:29:ILE:HD12	1:A:69:THR:HG21	1.96	0.48
1:B:265:GLN:NE2	1:B:269:ARG:NH2	2.62	0.48
2:D:207:ASN:C	2:D:209:ALA:H	2.17	0.48
1:B:29:ILE:HD12	1:B:69:THR:HG21	1.95	0.48
1:B:224:ARG:HD2	1:B:226:HIS:NE2	2.28	0.48
2:D:78:GLN:HG3	2:D:108:LEU:HD13	1.95	0.48
2:D:304:LEU:HA	2:D:307:ARG:HB2	1.96	0.48
1:A:32:ASN:HB3	1:A:69:THR:CG2	2.44	0.48
1:B:162:THR:O	1:B:163:GLU:HB3	2.14	0.48
2:C:100:LEU:C	2:C:102:GLY:N	2.65	0.48
1:A:11:LEU:HD23	1:A:11:LEU:O	2.13	0.47
1:B:278:PHE:CD1	1:B:278:PHE:C	2.86	0.47
1:A:170:VAL:HB	1:A:179:VAL:HG22	1.96	0.47
1:A:288:ASN:N	1:A:288:ASN:ND2	2.61	0.47
1:A:349:ILE:HG22	1:A:350:GLU:N	2.29	0.47
2:C:56:ASP:HB2	2:C:57:PRO:CD	2.41	0.47
1:A:305:ILE:CG2	1:A:306:LEU:N	2.76	0.47
1:A:316:GLU:O	1:A:316:GLU:HG3	2.14	0.47
1:B:11:LEU:O	1:B:11:LEU:HD23	2.14	0.47
1:B:27:LEU:HD12	1:B:29:ILE:CG2	2.45	0.47
2:C:177:ASN:HB2	2:C:241:SER:HA	1.97	0.47
2:C:257:LEU:O	2:C:290:LEU:HD21	2.14	0.47
1:B:256:LEU:HD12	1:B:256:LEU:C	2.35	0.47
2:C:277:ARG:O	2:C:278:VAL:HA	2.15	0.47
1:B:135:MET:HG3	1:B:214:LEU:HD23	1.94	0.47
2:C:31:LEU:CD1	2:C:113:ARG:HE	2.27	0.47
2:C:305:LEU:HB2	2:C:327:LEU:HD11	1.97	0.47
2:D:254:LEU:CD1	2:D:298:LEU:HD12	2.44	0.47
1:A:51:MET:CE	1:A:198:LYS:HB3	2.44	0.47
1:B:204:MET:HE2	1:B:204:MET:O	2.14	0.47
1:B:288:ASN:H	1:B:310:TYR:HB3	1.78	0.47
1:B:341:THR:HG22	1:B:342:ASP:HB2	1.97	0.47
2:C:243:PRO:C	2:C:245:ILE:N	2.67	0.47
1:B:214:LEU:HD12	1:B:215:ARG:N	2.29	0.47
2:C:236:LEU:O	2:C:241:SER:HB3	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:MET:HE2	2:D:289:ALA:HA	1.94	0.47
2:C:101:THR:CG2	2:C:126:TRP:HB2	2.45	0.47
2:D:231:HIS:HE1	2:D:235:GLN:HE21	1.62	0.47
2:D:306:THR:HA	2:D:309:GLU:HG2	1.95	0.47
1:B:269:ARG:HG2	1:B:269:ARG:HH11	1.80	0.47
2:C:78:GLN:HG3	2:C:108:LEU:HD13	1.96	0.47
2:D:95:GLU:O	2:D:98:LEU:HB3	2.15	0.47
2:D:283:ARG:O	2:D:283:ARG:HG2	2.15	0.47
1:A:126:VAL:HG22	1:A:127:GLU:N	2.30	0.47
2:C:48:GLU:HG2	2:C:76:SER:CB	2.44	0.47
2:D:31:LEU:HD23	2:D:139:CYS:CB	2.45	0.47
2:D:289:ALA:C	2:D:291:ASN:H	2.17	0.47
1:A:44:LEU:HD12	1:A:44:LEU:N	2.30	0.46
1:B:34:LEU:HD11	1:B:113:ALA:HB1	1.96	0.46
1:B:256:LEU:HD12	1:B:257:GLU:N	2.30	0.46
2:C:273:PHE:CE2	2:C:283:ARG:HA	2.50	0.46
2:D:101:THR:CG2	2:D:126:TRP:HB2	2.45	0.46
2:D:117:LEU:HD23	2:D:117:LEU:HA	1.75	0.46
2:D:203:GLU:C	2:D:205:ALA:N	2.68	0.46
2:D:214:PRO:CB	2:D:246:LEU:HD23	2.45	0.46
1:A:256:LEU:HD12	1:A:257:GLU:N	2.30	0.46
1:A:265:GLN:NE2	1:A:269:ARG:NH2	2.63	0.46
1:B:253:ASP:OD2	1:B:254:LYS:HG3	2.15	0.46
1:B:283:LEU:O	1:B:316:GLU:HA	2.15	0.46
1:B:316:GLU:HG3	1:B:316:GLU:O	2.15	0.46
2:C:1:MET:HE2	2:C:22:LEU:HD23	1.97	0.46
2:C:308:THR:O	2:C:312:LEU:HD22	2.16	0.46
2:D:54:SER:HA	2:D:83:LEU:HB2	1.98	0.46
2:D:64:ILE:O	2:D:67:LEU:HB3	2.15	0.46
2:D:309:GLU:O	2:D:313:LYS:HG2	2.15	0.46
1:A:253:ASP:OD2	1:A:254:LYS:HG3	2.15	0.46
2:C:44:ALA:O	2:C:45:GLN:HG3	2.15	0.46
2:D:278:VAL:CG1	2:D:282:ARG:NH1	2.78	0.46
1:A:53:MET:HE1	1:A:230:PHE:CB	2.44	0.46
1:B:323:TYR:O	1:B:327:VAL:HG23	2.16	0.46
2:C:205:ALA:O	2:C:209:ALA:HB3	2.16	0.46
2:C:231:HIS:C	2:C:231:HIS:HD2	2.18	0.46
1:B:122:TRP:HZ3	1:B:219:GLY:HA3	1.79	0.46
2:C:95:GLU:O	2:C:98:LEU:HB3	2.16	0.46
2:C:119:LYS:H	2:C:119:LYS:HG2	1.53	0.46
2:D:9:LEU:HG	2:D:13:LEU:HD22	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:300:GLN:HG3	2:D:303:GLN:NE2	2.31	0.46
1:A:96:ARG:NH1	1:A:107:SER:OG	2.49	0.46
2:D:198:THR:O	2:D:202:VAL:HG23	2.16	0.46
1:A:4:THR:HG22	1:A:61:GLN:NE2	2.31	0.46
1:A:283:LEU:O	1:A:316:GLU:HA	2.16	0.46
1:B:212:ASN:O	1:B:214:LEU:N	2.49	0.46
2:D:100:LEU:C	2:D:100:LEU:HD23	2.37	0.46
2:D:217:TRP:HA	2:D:232:ILE:CD1	2.46	0.46
1:A:168:ARG:NE	1:A:181:SER:OG	2.46	0.46
1:B:82:LEU:HD13	1:B:101:SER:HB2	1.97	0.46
1:B:295:ASN:ND2	1:B:297:PRO:HD3	2.31	0.46
1:B:349:ILE:HG22	1:B:350:GLU:N	2.31	0.46
2:C:105:HIS:CD2	2:C:106:ASP:H	2.34	0.46
2:D:48:GLU:HG2	2:D:76:SER:HB2	1.98	0.46
1:A:227:VAL:HG12	1:A:227:VAL:O	2.15	0.45
1:A:344:VAL:HA	2:C:71:MET:HE1	1.98	0.45
2:C:97:LEU:HD23	2:C:126:TRP:CE2	2.51	0.45
2:D:150:TRP:CZ3	2:D:178:LEU:HD12	2.51	0.45
2:D:292:ARG:HB2	2:D:292:ARG:CZ	2.44	0.45
1:A:349:ILE:O	1:A:350:GLU:HB3	2.16	0.45
1:B:143:GLN:HG2	1:B:143:GLN:O	2.17	0.45
2:C:54:SER:HA	2:C:83:LEU:HB2	1.98	0.45
1:A:8:GLU:C	1:A:10:LEU:H	2.19	0.45
2:C:39:ARG:NH2	2:C:79:THR:HG22	2.25	0.45
2:C:226:SER:O	2:C:229:ALA:HB3	2.17	0.45
2:D:202:VAL:O	2:D:205:ALA:HB3	2.17	0.45
2:D:311:THR:HG22	2:D:315:ASP:CB	2.35	0.45
1:A:82:LEU:HD13	1:A:101:SER:HB2	1.97	0.45
1:A:152:ARG:NH2	2:C:49:GLU:HG3	2.32	0.45
1:A:331:LEU:C	1:A:333:CYS:H	2.19	0.45
1:B:162:THR:O	1:B:190:SER:HA	2.16	0.45
1:B:349:ILE:O	1:B:350:GLU:HB3	2.16	0.45
2:C:126:TRP:O	2:C:129:ALA:HB3	2.16	0.45
2:C:270:ARG:O	2:C:274:ASP:CG	2.54	0.45
2:D:31:LEU:HD23	2:D:139:CYS:HB2	1.98	0.45
2:D:170:LEU:HG	2:D:202:VAL:HG11	1.98	0.45
1:A:78:ILE:O	1:A:82:LEU:HG	2.16	0.45
1:A:295:ASN:ND2	1:A:297:PRO:HD3	2.32	0.45
1:B:122:TRP:CZ3	1:B:219:GLY:HA3	2.52	0.45
1:B:194:ILE:HG21	1:B:237:VAL:HB	1.97	0.45
2:C:141:THR:C	2:C:142:PRO:O	2.53	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:ASN:N	2:D:140:GLN:HE22	2.10	0.45
2:D:97:LEU:HD23	2:D:126:TRP:CE2	2.51	0.45
1:A:93:GLU:OE1	1:A:98:LEU:HD21	2.16	0.45
2:C:9:LEU:HG	2:C:13:LEU:HD22	1.99	0.45
2:D:126:TRP:O	2:D:129:ALA:HB3	2.16	0.45
2:D:221:LEU:HD21	2:D:331:LEU:HB2	1.99	0.45
1:B:218:ILE:CG2	1:B:219:GLY:N	2.76	0.45
2:C:68:CYS:O	2:C:105:HIS:CE1	2.69	0.45
1:B:8:GLU:C	1:B:10:LEU:H	2.20	0.45
2:C:11:ALA:C	2:C:13:LEU:N	2.69	0.45
2:C:100:LEU:C	2:C:100:LEU:HD23	2.37	0.45
2:C:255:LEU:HD23	2:C:259:ASN:ND2	2.32	0.45
1:A:70:VAL:HG11	1:A:97:MET:SD	2.57	0.45
1:A:262:LEU:HD12	1:A:262:LEU:HA	1.82	0.45
2:C:214:PRO:HB3	2:C:246:LEU:HD22	1.98	0.45
2:C:283:ARG:O	2:C:287:GLY:N	2.48	0.45
2:D:31:LEU:CD1	2:D:113:ARG:HE	2.30	0.45
2:D:67:LEU:HD11	2:D:78:GLN:NE2	2.32	0.45
2:D:270:ARG:HA	2:D:273:PHE:CE1	2.52	0.45
2:D:293:LEU:HD22	2:D:298:LEU:HB2	1.99	0.45
2:D:313:LYS:C	2:D:316:TYR:CE2	2.90	0.45
1:A:27:LEU:HD12	1:A:29:ILE:CG2	2.47	0.44
1:B:78:ILE:O	1:B:82:LEU:HG	2.17	0.44
2:C:31:LEU:HD13	2:C:113:ARG:CG	2.47	0.44
2:C:171:CYS:O	2:C:175:GLU:HB2	2.17	0.44
2:C:249:THR:OG1	2:C:250:LEU:N	2.49	0.44
2:D:119:LYS:H	2:D:119:LYS:HG2	1.43	0.44
1:A:70:VAL:HG23	1:A:71:PRO:O	2.18	0.44
1:A:155:LEU:C	1:A:157:GLY:H	2.21	0.44
1:A:267:PHE:HZ	1:A:283:LEU:HD11	1.81	0.44
1:A:349:ILE:N	1:A:349:ILE:CD1	2.80	0.44
1:B:44:LEU:N	1:B:44:LEU:HD12	2.32	0.44
2:C:150:TRP:CZ3	2:C:178:LEU:HD12	2.52	0.44
2:D:4:LEU:HG	2:D:8:GLN:HB2	1.99	0.44
1:A:271:ALA:O	1:A:274:SER:HB3	2.17	0.44
1:A:279:ARG:HD2	1:A:297:PRO:CG	2.44	0.44
1:B:106:PHE:CD1	1:B:106:PHE:N	2.86	0.44
1:B:214:LEU:HD13	1:B:225:ALA:HB1	1.94	0.44
1:B:224:ARG:HB2	1:B:232:PHE:O	2.17	0.44
1:B:331:LEU:C	1:B:333:CYS:H	2.21	0.44
2:D:205:ALA:O	2:D:209:ALA:HB2	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD21	1:B:117:PRO:HB2	1.98	0.44
1:B:279:ARG:HD2	1:B:297:PRO:CG	2.42	0.44
1:B:295:ASN:CG	1:B:297:PRO:HD3	2.38	0.44
2:C:295:GLN:HA	2:C:298:LEU:HB2	1.99	0.44
1:A:111:LEU:HD12	1:A:111:LEU:H	1.82	0.44
1:A:177:LEU:HD23	1:A:178:ALA:N	2.33	0.44
1:B:18:SER:HA	1:B:21:LEU:HG	1.99	0.44
2:C:55:ILE:HD11	2:C:82:LEU:HG	1.99	0.44
2:C:110:LEU:HG	2:C:111:ILE:N	2.33	0.44
1:A:52:GLU:O	1:A:52:GLU:HG3	2.17	0.44
1:A:95:GLU:O	1:A:96:ARG:HD3	2.18	0.44
1:A:106:PHE:CD1	1:A:106:PHE:N	2.86	0.44
1:B:10:LEU:C	1:B:13:PRO:HD2	2.38	0.44
1:B:305:ILE:HG22	1:B:306:LEU:N	2.33	0.44
2:C:27:ASP:OD1	2:C:27:ASP:C	2.55	0.44
2:C:143:GLU:O	2:C:147:LEU:N	2.50	0.44
2:D:35:GLN:NE2	2:D:81:LEU:HD22	2.32	0.44
2:D:171:CYS:O	2:D:175:GLU:HB2	2.18	0.44
1:A:295:ASN:CG	1:A:297:PRO:HD3	2.38	0.44
1:B:52:GLU:HG3	1:B:52:GLU:O	2.17	0.44
1:B:78:ILE:HG22	1:B:79:CYS:N	2.32	0.44
1:B:158:MET:SD	1:B:169:THR:HG21	2.57	0.44
1:B:271:ALA:O	1:B:274:SER:HB3	2.17	0.44
2:D:31:LEU:HD13	2:D:113:ARG:CG	2.48	0.44
2:D:303:GLN:O	2:D:307:ARG:N	2.51	0.44
1:B:223:ILE:CG1	1:B:224:ARG:N	2.81	0.44
2:D:199:LEU:HB3	2:D:200:PRO:CD	2.45	0.44
1:A:11:LEU:HD23	1:A:11:LEU:C	2.39	0.44
1:B:122:TRP:CD1	1:B:122:TRP:N	2.67	0.44
2:C:199:LEU:HB3	2:C:200:PRO:CD	2.45	0.44
2:C:247:LEU:HD21	2:C:324:LEU:HD21	2.00	0.44
2:D:156:LYS:C	2:D:158:LEU:H	2.20	0.44
1:A:42:LEU:HB2	1:A:59:LEU:HD11	2.00	0.43
1:A:78:ILE:HG22	1:A:79:CYS:N	2.32	0.43
2:D:225:LYS:HG3	2:D:227:LYS:HZ3	1.82	0.43
2:D:330:LEU:HD13	2:D:330:LEU:C	2.38	0.43
1:A:49:LEU:HD21	1:A:117:PRO:HB2	1.99	0.43
1:A:51:MET:HB2	1:A:232:PHE:CE1	2.53	0.43
1:A:135:MET:HG3	1:A:214:LEU:HD23	2.00	0.43
1:A:210:GLY:C	1:A:212:ASN:H	2.22	0.43
2:C:247:LEU:HD13	2:C:309:GLU:HB3	1.98	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:ILE:HD11	2:D:82:LEU:HG	2.00	0.43
1:A:11:LEU:O	1:A:15:GLN:HB2	2.19	0.43
1:A:214:LEU:CD1	1:A:225:ALA:HB1	2.48	0.43
1:B:70:VAL:HG23	1:B:71:PRO:O	2.19	0.43
1:B:96:ARG:NH1	1:B:107:SER:OG	2.51	0.43
2:C:326:GLY:O	2:C:330:LEU:HB2	2.19	0.43
2:D:271:ALA:C	2:D:273:PHE:N	2.72	0.43
1:A:27:LEU:HD12	1:A:29:ILE:HG22	1.99	0.43
1:B:128:PHE:CE2	1:B:218:ILE:HD11	2.48	0.43
1:B:296:ASN:HB3	1:B:299:GLN:HB3	2.01	0.43
1:B:301:GLU:HB2	1:B:302:ALA:H	1.50	0.43
2:C:48:GLU:HG2	2:C:76:SER:HB2	2.00	0.43
2:D:68:CYS:O	2:D:105:HIS:CE1	2.71	0.43
2:D:90:ASN:HB3	2:D:93:ILE:CG1	2.36	0.43
2:D:90:ASN:HD22	2:D:91:ALA:H	1.58	0.43
1:A:135:MET:HE3	1:A:160:PHE:HE2	1.84	0.43
1:A:215:ARG:NH2	1:A:226:HIS:CE1	2.87	0.43
1:A:292:ILE:HD13	1:A:292:ILE:O	2.19	0.43
1:B:132:GLN:NE2	1:B:227:VAL:CG1	2.80	0.43
1:B:224:ARG:HD2	1:B:226:HIS:CD2	2.53	0.43
2:C:156:LYS:C	2:C:158:LEU:H	2.20	0.43
1:A:138:LEU:HG	1:A:182:MET:HG3	2.00	0.43
1:B:4:THR:HG22	1:B:61:GLN:NE2	2.33	0.43
2:D:236:LEU:HD13	2:D:246:LEU:CD2	2.49	0.43
1:A:4:THR:HG22	1:A:61:GLN:HE22	1.84	0.43
1:A:184:ILE:HD11	1:A:186:GLN:O	2.18	0.43
1:B:11:LEU:HD23	1:B:11:LEU:C	2.39	0.43
1:B:73:ARG:NH2	1:B:76:PHE:HD2	2.17	0.43
1:B:288:ASN:N	1:B:288:ASN:ND2	2.64	0.43
2:C:5:TYR:N	2:C:8:GLN:OE1	2.51	0.43
2:C:133:ARG:O	2:C:133:ARG:CG	2.65	0.43
2:D:39:ARG:NH2	2:D:79:THR:HG22	2.23	0.43
2:D:110:LEU:HG	2:D:111:ILE:N	2.34	0.43
2:D:217:TRP:HA	2:D:232:ILE:HD12	1.99	0.43
2:D:235:GLN:OE1	2:D:235:GLN:HA	2.18	0.43
1:A:10:LEU:C	1:A:13:PRO:HD2	2.39	0.43
1:B:3:PHE:HB2	1:B:59:LEU:HD13	2.00	0.43
1:B:97:MET:HA	1:B:97:MET:CE	2.48	0.43
1:A:51:MET:HB2	1:A:233:THR:O	2.19	0.43
2:D:304:LEU:CD1	2:D:327:LEU:HD22	2.34	0.43
1:A:51:MET:HE1	1:A:198:LYS:CB	2.48	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:138:THR:O	2:C:138:THR:HG22	2.19	0.43
2:C:272:LEU:HD12	2:C:275:LYS:HG3	2.00	0.43
1:A:18:SER:HA	1:A:21:LEU:HG	2.00	0.42
1:A:73:ARG:NH2	1:A:76:PHE:HD2	2.17	0.42
1:A:296:ASN:HB3	1:A:299:GLN:HB3	1.99	0.42
1:B:300:GLU:OE1	1:B:300:GLU:N	2.51	0.42
2:C:277:ARG:C	2:C:278:VAL:HA	2.31	0.42
2:D:159:ASN:O	2:D:160:LEU:HD12	2.18	0.42
1:B:163:GLU:HG3	1:B:163:GLU:O	2.19	0.42
1:B:344:VAL:HA	2:D:71:MET:HE3	2.01	0.42
2:C:225:LYS:CG	2:C:228:ARG:CG	2.98	0.42
2:C:235:GLN:O	2:C:237:ARG:N	2.51	0.42
2:C:298:LEU:O	2:C:302:VAL:HG23	2.19	0.42
2:D:5:TYR:O	2:D:8:GLN:N	2.52	0.42
2:D:13:LEU:HD21	2:D:38:VAL:HA	2.01	0.42
2:D:213:THR:HG21	2:D:216:HIS:ND1	2.34	0.42
1:B:95:GLU:O	1:B:96:ARG:HD3	2.20	0.42
1:B:148:HIS:ND1	1:B:149:GLN:CG	2.83	0.42
2:C:159:ASN:O	2:C:160:LEU:HD12	2.18	0.42
2:C:118:SER:O	2:C:120:ALA:N	2.53	0.42
2:C:250:LEU:C	2:C:252:ARG:N	2.72	0.42
1:A:32:ASN:ND2	1:A:70:VAL:C	2.73	0.42
1:A:50:GLU:OE1	1:A:198:LYS:HB2	2.19	0.42
1:A:126:VAL:HG11	1:A:218:ILE:HB	1.93	0.42
2:D:133:ARG:O	2:D:133:ARG:CG	2.66	0.42
2:D:223:MET:HG2	2:D:331:LEU:O	2.18	0.42
1:A:51:MET:SD	1:A:232:PHE:HE1	2.43	0.42
1:A:318:GLY:H	1:A:366:LEU:HD11	1.85	0.42
1:B:148:HIS:ND1	1:B:149:GLN:HG2	2.35	0.42
1:B:170:VAL:HG23	1:B:241:PHE:CE2	2.55	0.42
1:B:292:ILE:HD13	1:B:292:ILE:O	2.19	0.42
2:D:312:LEU:O	2:D:312:LEU:HG	2.18	0.42
1:A:103:ARG:O	1:A:105:ARG:HG2	2.20	0.42
1:A:168:ARG:O	1:A:168:ARG:CG	2.68	0.42
1:A:301:GLU:HB2	1:A:302:ALA:H	1.51	0.42
1:B:51:MET:HE1	1:B:198:LYS:HB3	2.00	0.42
1:B:99:VAL:HG12	1:B:100:ARG:N	2.34	0.42
2:C:90:ASN:HD22	2:C:91:ALA:N	2.15	0.42
1:A:132:GLN:OE1	1:A:209:GLY:N	2.52	0.42
1:A:304:GLU:C	1:A:305:ILE:HD12	2.40	0.42
1:B:11:LEU:O	1:B:15:GLN:HB2	2.20	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:MET:HG3	2:C:285:MET:HG2	2.01	0.42
2:D:203:GLU:O	2:D:207:ASN:ND2	2.52	0.42
2:D:237:ARG:HE	2:D:237:ARG:HB3	1.70	0.42
1:A:219:GLY:O	1:A:220:SER:C	2.58	0.42
1:B:224:ARG:NH1	1:B:226:HIS:CE1	2.88	0.42
1:B:267:PHE:HZ	1:B:283:LEU:HD11	1.84	0.42
2:C:5:TYR:O	2:C:8:GLN:N	2.53	0.42
1:A:69:THR:OG1	1:A:113:ALA:HA	2.20	0.42
1:A:193:VAL:HB	1:A:236:LEU:HD13	2.02	0.42
1:B:134:THR:C	1:B:136:LYS:N	2.74	0.42
1:B:288:ASN:ND2	1:B:310:TYR:H	2.17	0.42
2:C:279:TRP:CE2	2:C:283:ARG:HD2	2.55	0.42
2:D:271:ALA:C	2:D:273:PHE:H	2.22	0.42
2:D:275:LYS:O	2:D:275:LYS:HD3	2.20	0.42
1:A:12:LYS:HA	1:A:12:LYS:HD3	1.76	0.41
1:A:97:MET:CE	1:A:97:MET:HA	2.50	0.41
1:B:256:LEU:HG	1:B:338:MET:HB3	2.01	0.41
1:B:270:ALA:O	1:B:294:ALA:HB2	2.20	0.41
2:C:140:GLN:NE2	2:C:140:GLN:CA	2.66	0.41
2:C:261:LYS:NZ	2:C:290:LEU:O	2.51	0.41
2:D:312:LEU:HA	2:D:316:TYR:HA	2.02	0.41
1:A:27:LEU:HG	1:A:30:LEU:CD1	2.49	0.41
1:B:159:LEU:HD13	1:B:241:PHE:CD2	2.54	0.41
2:C:117:LEU:HA	2:C:117:LEU:HD23	1.77	0.41
2:C:322:ALA:C	2:C:324:LEU:H	2.23	0.41
2:D:30:LEU:HB2	2:D:139:CYS:HB3	2.01	0.41
2:D:218:VAL:C	2:D:220:ALA:H	2.23	0.41
1:A:188:LEU:HB3	1:A:189:PRO:HD2	2.02	0.41
1:A:262:LEU:HG	1:A:306:LEU:CD2	2.44	0.41
1:B:103:ARG:O	1:B:105:ARG:HG2	2.20	0.41
2:C:96:GLN:CA	2:C:96:GLN:NE2	2.74	0.41
2:D:192:TRP:C	2:D:194:ASP:N	2.74	0.41
1:A:61:GLN:HB3	1:A:62:PRO:CD	2.51	0.41
1:A:73:ARG:HA	1:A:73:ARG:NE	2.33	0.41
1:A:137:ARG:HG3	1:A:137:ARG:HH11	1.85	0.41
1:A:300:GLU:N	1:A:300:GLU:OE1	2.53	0.41
1:B:129:THR:CG2	1:B:130:LEU:N	2.84	0.41
1:B:292:ILE:O	1:B:292:ILE:HG23	2.21	0.41
1:B:347:VAL:O	1:B:360:VAL:HA	2.20	0.41
2:C:331:LEU:HD13	2:C:331:LEU:HA	1.93	0.41
2:D:263:GLN:C	2:D:265:ALA:H	2.23	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:HIS:CD2	1:B:9:HIS:N	2.88	0.41
1:B:26:THR:HB	1:B:27:LEU:H	1.33	0.41
1:B:227:VAL:HG12	1:B:227:VAL:O	2.21	0.41
2:C:227:LYS:HD2	2:C:227:LYS:H	1.85	0.41
2:C:252:ARG:O	2:C:253:GLU:C	2.59	0.41
2:D:155:ALA:O	2:D:158:LEU:HB2	2.21	0.41
2:D:214:PRO:HB3	2:D:246:LEU:CD2	2.50	0.41
2:D:245:ILE:HD12	2:D:245:ILE:N	2.36	0.41
2:D:300:GLN:HG2	2:D:307:ARG:NH2	2.35	0.41
1:A:29:ILE:CD1	1:A:69:THR:HG21	2.51	0.41
1:A:256:LEU:HG	1:A:338:MET:HB3	2.02	0.41
2:C:192:TRP:C	2:C:194:ASP:N	2.74	0.41
2:D:18:ARG:HG2	2:D:134:SER:HA	2.02	0.41
1:A:99:VAL:HG12	1:A:100:ARG:N	2.36	0.41
1:A:288:ASN:ND2	1:A:310:TYR:H	2.18	0.41
1:B:61:GLN:HB3	1:B:62:PRO:CD	2.50	0.41
1:B:159:LEU:HB3	1:B:170:VAL:HG22	2.03	0.41
2:C:27:ASP:OD1	2:C:29:LEU:N	2.51	0.41
2:C:260:LEU:HB2	2:C:290:LEU:HD11	2.02	0.41
2:D:27:ASP:OD1	2:D:27:ASP:C	2.59	0.41
2:D:304:LEU:HA	2:D:307:ARG:CB	2.50	0.41
1:A:64:GLU:HA	1:A:65:PRO:HD3	1.91	0.41
1:B:134:THR:C	1:B:136:LYS:H	2.23	0.41
1:B:206:MET:O	1:B:207:LEU:C	2.59	0.41
2:C:4:LEU:HG	2:C:8:GLN:HB2	2.01	0.41
1:B:29:ILE:CD1	1:B:69:THR:HG21	2.51	0.41
1:B:51:MET:HE2	1:B:198:LYS:CB	2.49	0.41
1:B:188:LEU:HB3	1:B:189:PRO:HD2	2.02	0.41
2:C:2:ILE:HD11	2:C:18:ARG:CZ	2.51	0.41
2:C:192:TRP:HB3	2:C:201:ARG:HH12	1.86	0.41
2:D:11:ALA:C	2:D:13:LEU:N	2.72	0.41
2:D:299:ARG:HB3	2:D:299:ARG:HH11	1.84	0.41
2:D:304:LEU:O	2:D:307:ARG:HB2	2.21	0.41
1:A:292:ILE:O	1:A:292:ILE:HG23	2.22	0.41
1:B:32:ASN:ND2	1:B:70:VAL:C	2.74	0.41
2:C:244:VAL:HG12	2:C:244:VAL:O	2.21	0.41
2:D:138:THR:O	2:D:138:THR:HG22	2.20	0.41
2:D:251:GLN:HB2	2:D:305:LEU:CD2	2.51	0.41
1:A:168:ARG:HB2	1:A:180:CYS:O	2.20	0.40
1:B:69:THR:OG1	1:B:113:ALA:HA	2.21	0.40
2:C:4:LEU:HD11	2:C:12:GLN:HG3	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:52:THR:CG2	2:C:81:LEU:HD23	2.50	0.40
1:A:305:ILE:HG22	1:A:306:LEU:N	2.36	0.40
1:B:247:VAL:O	1:B:248:LEU:C	2.60	0.40
2:D:259:ASN:C	2:D:261:LYS:N	2.75	0.40
1:A:214:LEU:HD13	1:A:225:ALA:HB1	2.03	0.40
1:B:2:LYS:HA	1:B:90:VAL:O	2.22	0.40
2:C:2:ILE:N	2:C:2:ILE:CD1	2.83	0.40
2:C:117:LEU:O	2:C:118:SER:C	2.60	0.40
1:A:7:ARG:O	1:A:7:ARG:CG	2.68	0.40
1:A:130:LEU:HD23	1:A:134:THR:CG2	2.51	0.40
2:C:31:LEU:CD2	2:C:139:CYS:HB2	2.51	0.40
2:C:213:THR:O	2:C:216:HIS:HB2	2.22	0.40
2:C:245:ILE:HD13	2:C:245:ILE:O	2.20	0.40
2:D:106:ASP:C	2:D:108:LEU:H	2.25	0.40
2:D:299:ARG:HE	2:D:303:GLN:HE21	1.69	0.40
1:A:231:ILE:HD12	1:A:231:ILE:N	2.36	0.40
1:B:42:LEU:HB2	1:B:59:LEU:HD11	2.04	0.40
2:C:153:ALA:O	2:C:156:LYS:N	2.55	0.40
2:C:155:ALA:O	2:C:158:LEU:HB2	2.20	0.40
2:C:250:LEU:O	2:C:254:LEU:HB2	2.21	0.40
2:C:257:LEU:O	2:C:261:LYS:HB2	2.21	0.40
2:D:27:ASP:O	2:D:31:LEU:HG	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:315:ASP:OD2	2:D:315:ASP:OD2[2_647]	1.79	0.41
1:A:279:ARG:NH1	2:C:132:ASN:OD1[2_656]	1.81	0.39

## 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	364/366 (100%)	281 (77%)	62 (17%)	21 (6%)	1	5
1	B	364/366 (100%)	284 (78%)	59 (16%)	21 (6%)	1	5
2	C	322/343 (94%)	234 (73%)	62 (19%)	26 (8%)	1	2
2	D	317/343 (92%)	229 (72%)	69 (22%)	19 (6%)	1	4
All	All	1367/1418 (96%)	1028 (75%)	252 (18%)	87 (6%)	1	4

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	26	THR
1	A	119	LEU
1	B	6	GLU
1	B	26	THR
1	B	119	LEU
1	B	209	GLY
2	C	119	LYS
2	C	131	ALA
2	C	144	GLN
2	C	207	ASN
2	C	270	ARG
2	C	316	TYR
2	D	119	LYS
2	D	131	ALA
2	D	204	GLN
2	D	296	THR
2	D	316	TYR
1	A	94	GLY
1	A	197	ARG
1	A	211	ASP
1	A	220	SER
1	A	277	LYS
1	B	94	GLY
1	B	126	VAL
1	B	156	ASN
1	B	277	LYS
2	C	277	ARG
2	C	278	VAL
2	C	289	ALA
2	C	323	GLU
2	D	75	ALA
2	D	144	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	298	LEU
1	A	121	ASP
1	A	208	ASP
1	A	213	PRO
1	A	287	GLU
1	A	297	PRO
1	A	332	LYS
1	B	25	PRO
1	B	213	PRO
1	B	287	GLU
1	B	297	PRO
1	B	346	SER
2	C	12	GLN
2	C	75	ALA
2	C	227	LYS
2	C	236	LEU
2	C	244	VAL
2	C	283	ARG
2	C	291	ASN
2	D	12	GLN
2	D	61	TRP
2	D	266	HIS
2	D	290	LEU
1	A	25	PRO
1	A	205	ARG
1	B	332	LYS
2	C	105	HIS
2	C	223	MET
2	D	105	HIS
2	D	260	LEU
1	A	84	GLU
1	A	189	PRO
1	A	265	GLN
1	B	84	GLU
1	B	163	GLU
1	B	242	PRO
2	C	61	TRP
2	C	175	GLU
2	C	262	ARG
2	C	312	LEU
2	D	175	GLU
2	D	284	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	117	PRO
1	B	74	LYS
1	B	117	PRO
1	B	265	GLN
2	C	251	GLN
2	C	6	PRO
2	C	56	ASP
2	D	56	ASP
1	A	242	PRO
2	D	6	PRO
1	B	210	GLY
2	D	278	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	311/311 (100%)	276 (89%)	35 (11%)	6 18
1	B	311/311 (100%)	273 (88%)	38 (12%)	5 15
2	C	278/291 (96%)	242 (87%)	36 (13%)	4 13
2	D	276/291 (95%)	245 (89%)	31 (11%)	6 18
All	All	1176/1204 (98%)	1036 (88%)	140 (12%)	5 15

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	6	GLU
1	A	26	THR
1	A	27	LEU
1	A	53	MET
1	A	70	VAL
1	A	73	ARG
1	A	80	ARG
1	A	87	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	96	ARG
1	A	97	MET
1	A	120	ASP
1	A	127	GLU
1	A	130	LEU
1	A	135	MET
1	A	172	THR
1	A	176	ARG
1	A	197	ARG
1	A	198	LYS
1	A	223	ILE
1	A	224	ARG
1	A	226	HIS
1	A	235	LYS
1	A	244	TYR
1	A	253	ASP
1	A	256	LEU
1	A	275	ASN
1	A	278	PHE
1	A	288	ASN
1	A	292	ILE
1	A	293	THR
1	A	297	PRO
1	A	301	GLU
1	A	342	ASP
1	A	354	SER
1	B	5	VAL
1	B	6	GLU
1	B	26	THR
1	B	27	LEU
1	B	53	MET
1	B	73	ARG
1	B	80	ARG
1	B	87	GLU
1	B	96	ARG
1	B	97	MET
1	B	120	ASP
1	B	121	ASP
1	B	122	TRP
1	B	130	LEU
1	B	135	MET
1	B	146	MET

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	149	GLN
1	B	162	THR
1	B	169	THR
1	B	176	ARG
1	B	177	LEU
1	B	197	ARG
1	B	198	LYS
1	B	224	ARG
1	B	226	HIS
1	B	235	LYS
1	B	244	TYR
1	B	253	ASP
1	B	256	LEU
1	B	275	ASN
1	B	278	PHE
1	B	288	ASN
1	B	292	ILE
1	B	293	THR
1	B	297	PRO
1	B	301	GLU
1	B	342	ASP
1	B	354	SER
2	C	22	LEU
2	C	24	LEU
2	C	79	THR
2	C	90	ASN
2	C	96	GLN
2	C	97	LEU
2	C	110	LEU
2	C	118	SER
2	C	119	LYS
2	C	132	ASN
2	C	140	GLN
2	C	143	GLU
2	C	148	PRO
2	C	162	LEU
2	C	173	CYS
2	C	190	LEU
2	C	194	ASP
2	C	219	ASP
2	C	227	LYS
2	C	228	ARG

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	C	231	HIS
2	C	245	ILE
2	C	249	THR
2	C	251	GLN
2	C	262	ARG
2	C	270	ARG
2	C	273	PHE
2	C	293	LEU
2	C	303	GLN
2	C	304	LEU
2	C	312	LEU
2	C	316	TYR
2	C	318	GLN
2	C	325	GLU
2	C	330	LEU
2	C	333	HIS
2	D	22	LEU
2	D	24	LEU
2	D	79	THR
2	D	95	GLU
2	D	96	GLN
2	D	97	LEU
2	D	110	LEU
2	D	118	SER
2	D	119	LYS
2	D	132	ASN
2	D	140	GLN
2	D	143	GLU
2	D	148	PRO
2	D	162	LEU
2	D	173	CYS
2	D	190	LEU
2	D	194	ASP
2	D	207	ASN
2	D	208	ASP
2	D	213	THR
2	D	235	GLN
2	D	274	ASP
2	D	279	TRP
2	D	292	ARG
2	D	296	THR
2	D	304	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	308	THR
2	D	309	GLU
2	D	311	THR
2	D	316	TYR
2	D	327	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	32	ASN
1	A	61	GLN
1	A	186	GLN
1	A	222	ASN
1	A	255	HIS
1	A	265	GLN
1	A	288	ASN
1	A	329	ASN
1	B	9	HIS
1	B	32	ASN
1	B	61	GLN
1	B	186	GLN
1	B	226	HIS
1	B	255	HIS
1	B	265	GLN
1	B	288	ASN
1	B	329	ASN
2	C	32	GLN
2	C	78	GLN
2	C	90	ASN
2	C	94	ASN
2	C	96	GLN
2	C	105	HIS
2	C	140	GLN
2	C	207	ASN
2	C	216	HIS
2	C	251	GLN
2	C	259	ASN
2	C	303	GLN
2	D	62	ASN
2	D	78	GLN
2	D	90	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	94	ASN
2	D	96	GLN
2	D	105	HIS
2	D	140	GLN
2	D	207	ASN
2	D	231	HIS
2	D	251	GLN
2	D	300	GLN
2	D	303	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	269:LEU	C	270:ARG	N	0.93

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	366/366 (100%)	0.53	32 (8%) 10 7	26, 72, 106, 122	0
1	B	366/366 (100%)	0.85	68 (18%) 1 0	30, 81, 135, 149	0
2	C	328/343 (95%)	0.28	25 (7%) 13 10	21, 60, 132, 168	0
2	D	325/343 (94%)	0.66	46 (14%) 2 2	22, 82, 142, 160	0
All	All	1385/1418 (97%)	0.59	171 (12%) 4 3	21, 73, 132, 168	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	131	ALA	9.3
1	A	297	PRO	8.2
2	D	314	GLN	7.5
2	C	277	ARG	6.9
1	B	104	SER	6.5
1	B	94	GLY	6.3
1	B	102	GLY	6.1
2	D	268	PRO	5.9
1	A	298	GLU	5.9
2	C	279	TRP	5.9
2	D	267	THR	5.9
1	B	211	ASP	5.8
2	C	314	GLN	5.6
2	D	270	ARG	5.6
2	C	278	VAL	5.5
2	C	212	PHE	5.2
2	D	263	GLN	5.0
2	C	317	GLY	5.0
2	D	262	ARG	5.0
1	B	28	PRO	5.0
2	C	267	THR	4.9

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	275	LYS	4.9
2	D	278	VAL	4.8
1	A	300	GLU	4.8
1	B	275	ASN	4.7
2	D	269	LEU	4.6
1	A	209	GLY	4.5
2	D	276	HIS	4.5
1	B	93	GLU	4.4
1	B	103	ARG	4.4
2	D	272	LEU	4.4
2	C	266	HIS	4.2
2	D	266	HIS	4.2
2	D	282	ARG	4.2
2	C	225	LYS	4.2
2	D	315	ASP	4.1
2	D	285	MET	4.0
2	C	316	TYR	4.0
1	A	211	ASP	4.0
1	B	121	ASP	4.0
1	B	297	PRO	3.9
1	B	59	LEU	3.9
1	A	274	SER	3.9
2	D	313	LYS	3.9
2	C	274	ASP	3.9
1	A	103	ARG	3.8
1	A	210	GLY	3.8
2	C	276	HIS	3.8
2	C	270	ARG	3.8
1	B	298	GLU	3.7
1	A	314	GLU	3.7
1	B	213	PRO	3.7
1	B	38	ALA	3.6
1	B	35	LEU	3.6
1	B	105	ARG	3.5
1	B	82	LEU	3.5
1	B	79	CYS	3.5
1	B	300	GLU	3.4
1	B	26	THR	3.4
1	B	39	ASP	3.4
1	A	313	ALA	3.4
1	A	299	GLN	3.3
1	B	210	GLY	3.3

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	303	GLU	3.3
2	D	317	GLY	3.3
1	B	109	SER	3.2
1	B	284	TYR	3.2
2	C	211	HIS	3.2
2	D	271	ALA	3.2
2	D	123	ASN	3.2
2	D	116	LYS	3.1
1	B	30	LEU	3.1
1	A	26	THR	3.1
1	B	56	ARG	3.1
1	B	36	GLN	3.1
1	B	65	PRO	3.1
1	B	32	ASN	3.1
2	C	315	ASP	3.1
2	C	269	LEU	3.1
1	A	208	ASP	3.1
1	B	53	MET	3.1
1	B	229	ASP	3.1
1	B	64	GLU	3.0
1	A	284	TYR	3.0
1	B	33	LEU	3.0
2	C	119	LYS	3.0
1	A	93	GLU	2.9
2	D	287	GLY	2.9
1	B	212	ASN	2.9
1	B	95	GLU	2.9
2	D	307	ARG	2.9
2	D	303	GLN	2.9
2	D	91	ALA	2.9
2	D	132	ASN	2.8
1	B	49	LEU	2.8
2	C	75	ALA	2.7
2	D	316	TYR	2.7
2	D	277	ARG	2.7
1	A	28	PRO	2.7
1	B	303	GLU	2.7
1	B	62	PRO	2.7
1	B	83	PRO	2.7
2	D	274	ASP	2.6
1	B	2	LYS	2.6
1	B	123	GLN	2.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	274	SER	2.6
1	A	295	ASN	2.6
1	B	1	MET	2.6
1	B	23	GLY	2.6
1	B	75	PHE	2.6
2	D	120	ALA	2.6
1	A	226	HIS	2.6
1	B	27	LEU	2.5
1	B	21	LEU	2.5
1	B	92	LEU	2.5
2	C	272	LEU	2.5
2	D	112	VAL	2.5
1	A	107	SER	2.5
2	D	318	GLN	2.5
1	A	92	LEU	2.5
2	D	119	LYS	2.5
1	A	121	ASP	2.4
1	A	332	LYS	2.4
1	A	38	ALA	2.4
2	D	283	ARG	2.4
2	D	86	GLU	2.4
1	A	275	ASN	2.4
2	C	318	GLN	2.3
2	D	286	MET	2.3
2	C	265	ALA	2.3
1	B	301	GLU	2.3
1	B	191	HIS	2.3
1	A	24	ARG	2.3
1	B	10	LEU	2.3
1	A	49	LEU	2.3
1	A	39	ASP	2.2
2	D	144	GLN	2.2
1	B	107	SER	2.2
1	B	208	ASP	2.2
1	B	76	PHE	2.2
1	B	304	GLU	2.2
1	B	307	ASP	2.2
2	D	333	HIS	2.2
1	B	187	SER	2.2
1	A	212	ASN	2.1
2	D	12	GLN	2.1
2	D	265	ALA	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	9	HIS	2.1
1	B	37	VAL	2.1
2	C	210	ALA	2.1
1	B	91	GLN	2.1
2	D	164	ASP	2.1
1	A	118	ASN	2.1
1	A	62	PRO	2.1
2	D	10	ARG	2.1
1	B	120	ASP	2.1
1	B	122	TRP	2.1
1	B	230	PHE	2.1
2	D	300	GLN	2.1
1	B	100	ARG	2.1
2	C	268	PRO	2.1
2	D	208	ASP	2.0
1	A	186	GLN	2.0
2	C	282	ARG	2.0
1	B	84	GLU	2.0
1	B	34	LEU	2.0
1	B	63	HIS	2.0
2	C	208	ASP	2.0
2	D	21	TYR	2.0
1	B	96	ARG	2.0
2	D	22	LEU	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 monosaccharides 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.