



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 08:18 PM EDT

PDB ID : 1R0B  
Title : Aspartate Transcarbamylase (ATCase) of Escherichia coli: A New Crystalline R State Bound to PALA, or to Product Analogues Phosphate and Citrate  
Authors : Huang, J.; Lipscomb, W.N.  
Deposited on : 2003-09-19  
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

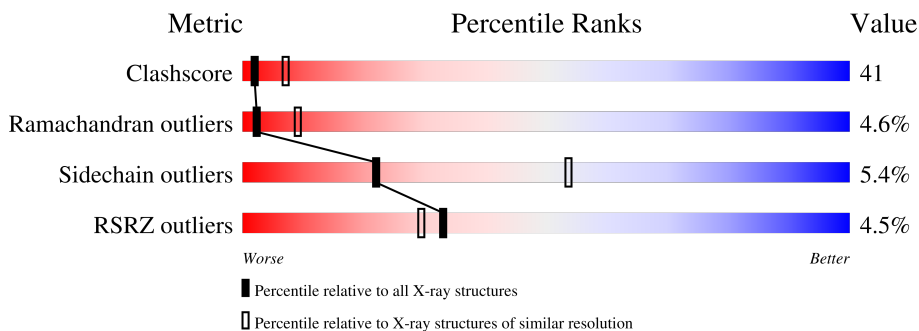
# 1 Overall quality at a glance i

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))
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	310	
1	B	310	
1	C	310	
1	D	310	
1	E	310	
1	F	310	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	153	
2	H	153	
2	I	153	
2	J	153	
2	K	153	
2	L	153	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	A	2001	-	-	X	-
3	FLC	B	2002	-	-	X	-
3	FLC	C	2003	-	-	X	-
3	FLC	D	2004	-	X	X	-
3	FLC	E	2005	-	-	X	-
4	PO4	A	3001	-	X	X	-
4	PO4	B	3002	-	X	-	-
4	PO4	C	3003	-	X	-	-
4	PO4	E	3005	-	X	-	-
4	PO4	F	3006	-	X	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 22698 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 Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2415	1527	423	456	9	0	0	0
1	B	310	2415	1527	423	456	9	0	0	0
1	C	310	2415	1527	423	456	9	0	0	0
1	D	310	2415	1527	423	456	9	0	0	0
1	E	310	2415	1527	423	456	9	0	0	0
1	F	310	2415	1527	423	456	9	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	153	1201	752	213	230	6	0	0	0
2	H	153	1201	752	213	230	6	0	0	0
2	I	153	1201	752	213	230	6	0	0	0
2	J	153	1201	752	213	230	6	0	0	0
2	K	153	1201	752	213	230	6	0	0	0
2	L	153	1201	752	213	230	6	0	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: C<sub>6</sub>H<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	E	1	Total O P 5 4 1	0	0
4	F	1	Total O P 5 4 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Zn 1 1	0	0
5	H	1	Total Zn 1 1	0	0
5	I	1	Total Zn 1 1	0	0
5	J	1	Total Zn 1 1	0	0
5	K	1	Total Zn 1 1	0	0
5	L	1	Total Zn 1 1	0	0

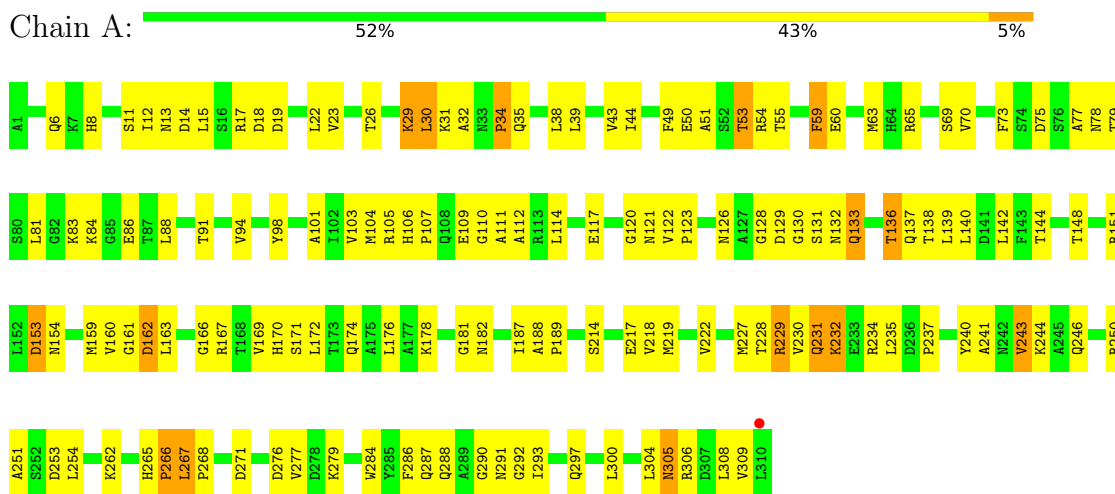
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	84	Total O 84 84	0	0
6	B	95	Total O 95 95	0	0
6	C	113	Total O 113 113	0	0
6	G	65	Total O 65 65	0	0
6	H	59	Total O 59 59	0	0
6	I	45	Total O 45 45	0	0
6	D	102	Total O 102 102	0	0
6	E	86	Total O 86 86	0	0
6	F	82	Total O 82 82	0	0
6	J	51	Total O 51 51	0	0
6	K	51	Total O 51 51	0	0
6	L	55	Total O 55 55	0	0

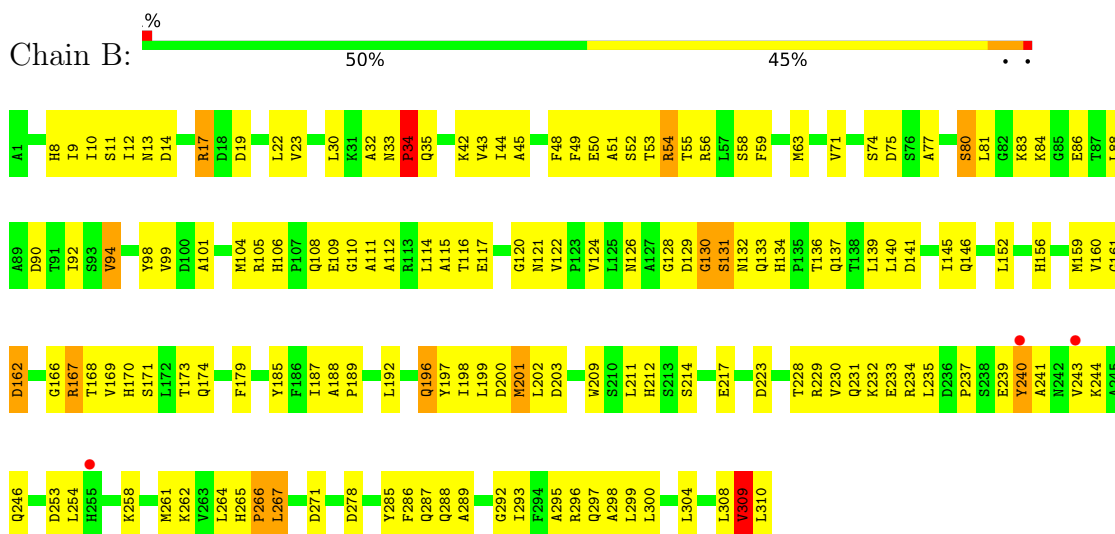
### 3 Residue-property plots

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: Aspartate carbamoyltransferase catalytic chain



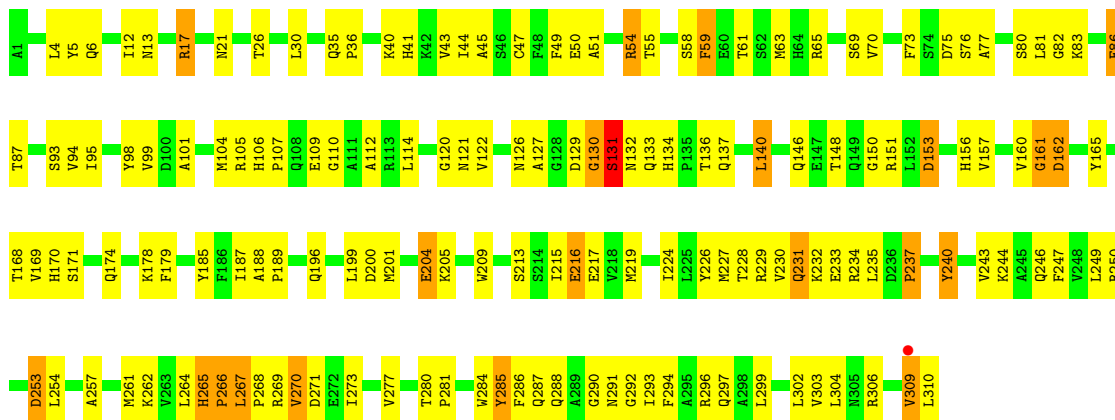
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



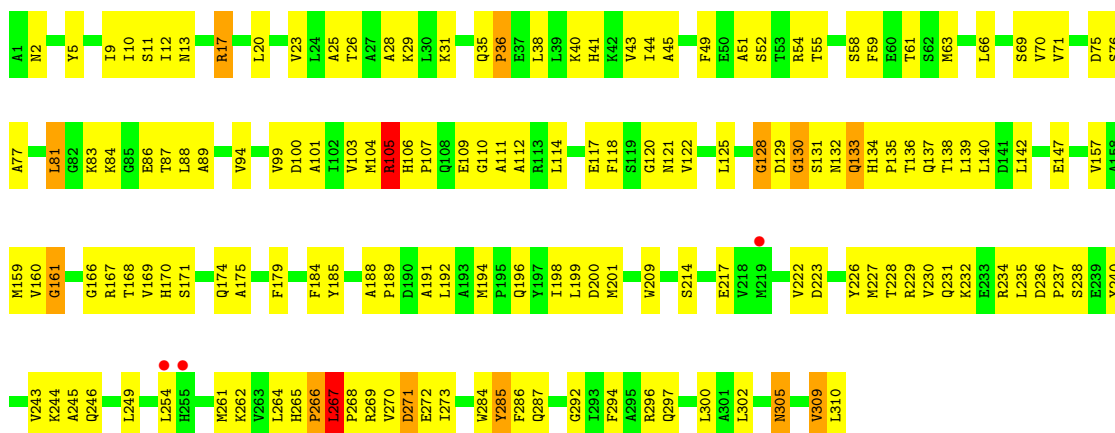
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



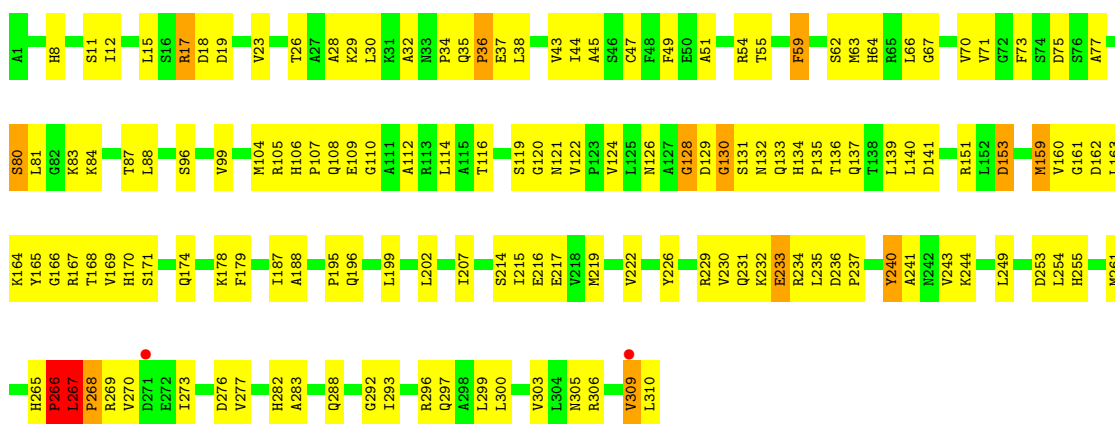




- Molecule 1: Aspartate carbamoyltransferase catalytic chain

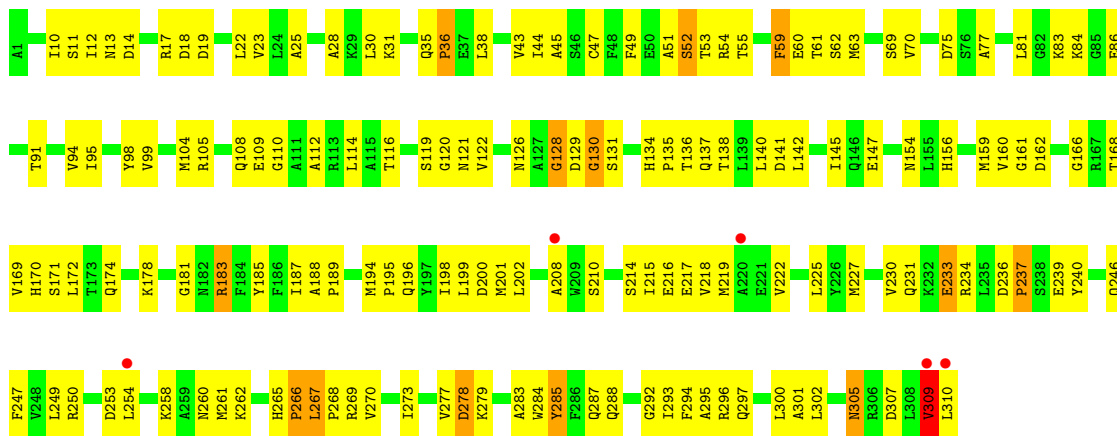


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

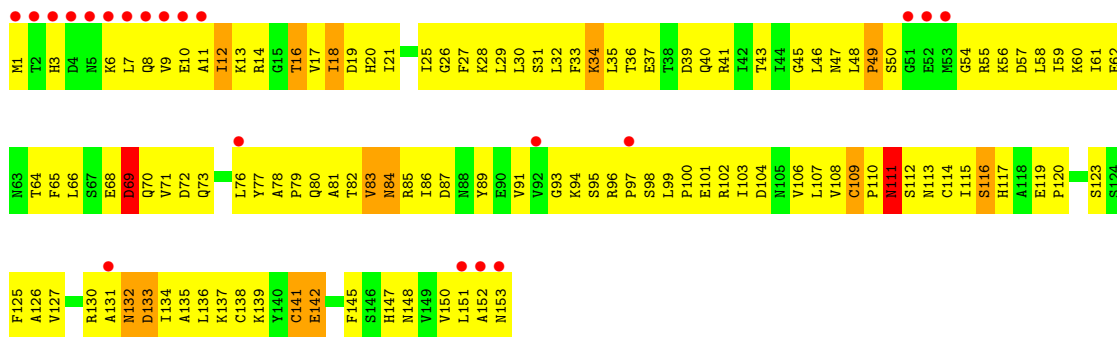


- Molecule 1: Aspartate carbamoyltransferase catalytic chain

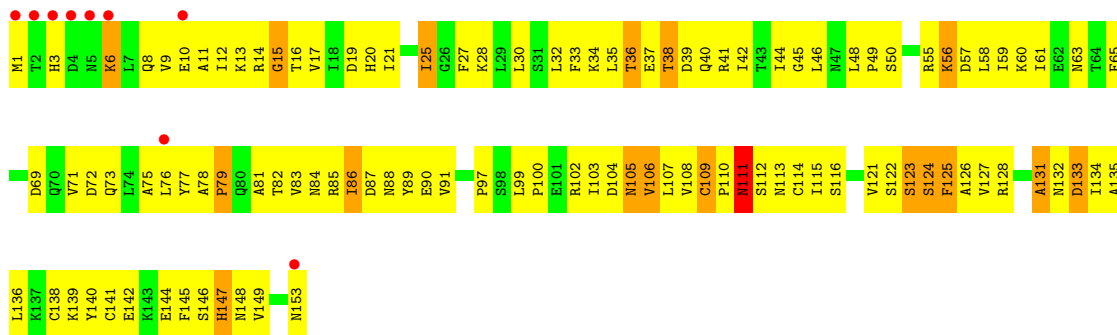




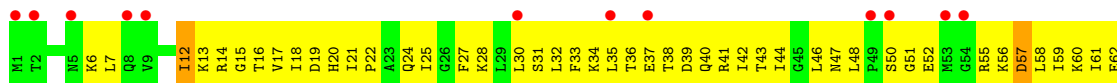
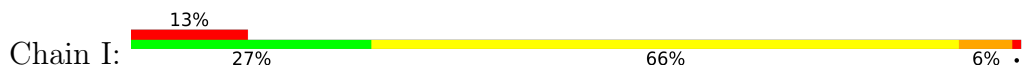
• Molecule 2: Aspartate carbamoyltransferase regulatory chain

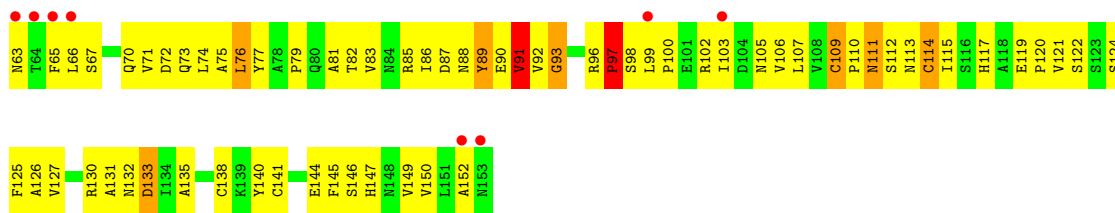


• Molecule 2: Aspartate carbamoyltransferase regulatory chain

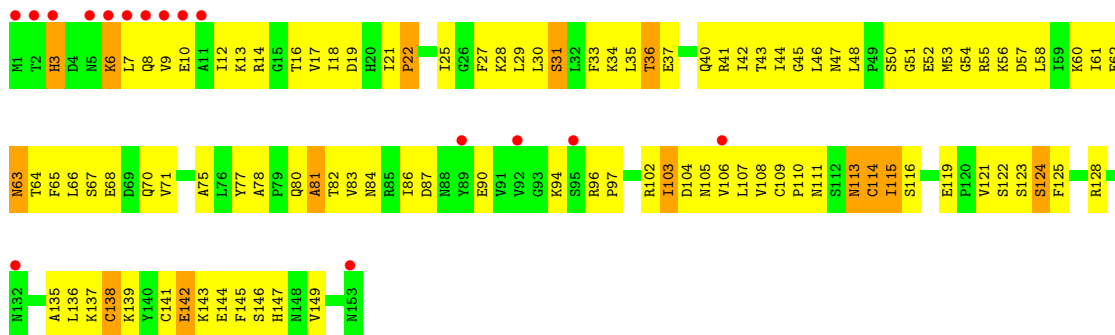


• Molecule 2: Aspartate carbamoyltransferase regulatory chain

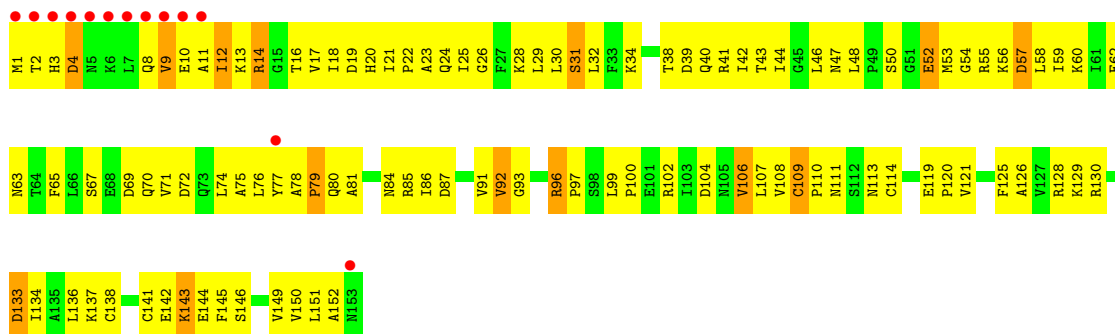




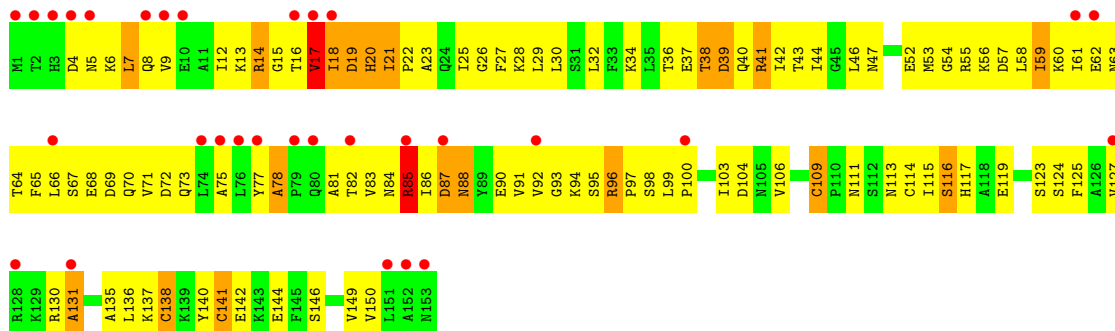
● Molecule 2: Aspartate carbamoyltransferase regulatory chain



● Molecule 2: Aspartate carbamoyltransferase regulatory chain



● Molecule 2: Aspartate carbamoyltransferase regulatory chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.69Å 155.40Å 194.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 42.82 – 2.86	Depositor EDS
% Data completeness (in resolution range)	72.5 (50.00-2.90) 70.5 (42.82-2.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 2.86Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.240 , 0.300 0.234 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtrriage
Anisotropy	0.405	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	22698	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, ZN, PO4

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	0.41	0/2461	0.75	3/3339 (0.1%)
1	B	0.38	0/2461	0.75	4/3339 (0.1%)
1	C	0.39	0/2461	0.72	4/3339 (0.1%)
1	D	0.37	0/2461	0.69	3/3339 (0.1%)
1	E	0.37	0/2461	0.69	3/3339 (0.1%)
1	F	0.34	0/2461	0.67	4/3339 (0.1%)
2	G	0.37	0/1219	0.66	0/1647
2	H	0.43	0/1219	0.79	0/1647
2	I	0.39	0/1219	0.70	0/1647
2	J	0.37	0/1219	0.73	1/1647 (0.1%)
2	K	0.39	0/1219	0.70	0/1647
2	L	0.39	0/1219	0.83	2/1647 (0.1%)
All	All	0.38	0/22080	0.72	24/29916 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	LEU	N-CA-C	9.60	136.91	111.00
1	F	267	LEU	N-CA-C	9.08	135.52	111.00
1	A	267	LEU	N-CA-C	9.05	135.44	111.00
1	B	267	LEU	N-CA-C	8.47	133.88	111.00
1	C	266	PRO	N-CA-C	-8.28	90.57	112.10
1	B	267	LEU	CA-CB-CG	-8.00	96.91	115.30
1	A	266	PRO	N-CA-C	-7.76	91.93	112.10
1	F	267	LEU	C-N-CD	7.29	143.70	128.40
1	D	267	LEU	N-CA-C	7.10	130.16	111.00
1	B	266	PRO	N-CA-C	-6.96	94.01	112.10
1	F	267	LEU	CA-CB-CG	-6.76	99.75	115.30
1	B	254	LEU	N-CA-C	6.71	129.11	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	3	HIS	N-CA-C	-6.60	93.18	111.00
1	F	266	PRO	N-CA-C	-6.44	95.36	112.10
2	L	141	CYS	CA-CB-SG	-6.29	102.69	114.00
1	C	267	LEU	C-N-CD	6.18	141.39	128.40
1	A	267	LEU	C-N-CD	6.11	141.24	128.40
1	E	266	PRO	C-N-CA	-5.88	107.01	121.70
2	L	21	ILE	CB-CA-C	-5.50	100.60	111.60
1	E	267	LEU	CA-CB-CG	-5.18	103.38	115.30
1	D	266	PRO	N-CA-C	-5.16	98.69	112.10
1	E	266	PRO	N-CA-C	-5.13	98.76	112.10
1	D	105	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	140	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2422	155	0
1	B	2415	0	2422	162	0
1	C	2415	0	2422	166	0
1	D	2415	0	2422	175	0
1	E	2415	0	2422	150	0
1	F	2415	0	2422	167	0
2	G	1201	0	1219	159	0
2	H	1201	0	1219	143	0
2	I	1201	0	1219	161	0
2	J	1201	0	1219	141	0
2	K	1201	0	1219	135	0
2	L	1201	0	1219	216	0
3	A	13	0	5	7	0
3	B	13	0	5	4	0
3	C	13	0	5	4	0
3	D	13	0	5	7	0
3	E	13	0	5	4	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	13	0	5	1	0
4	A	5	0	0	5	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
4	E	5	0	0	1	0
4	F	5	0	0	2	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
6	A	84	0	0	1	0
6	B	95	0	0	3	0
6	C	113	0	0	4	0
6	D	102	0	0	2	0
6	E	86	0	0	3	0
6	F	82	0	0	8	0
6	G	65	0	0	5	0
6	H	59	0	0	4	0
6	I	45	0	0	5	0
6	J	51	0	0	0	0
6	K	51	0	0	4	0
6	L	55	0	0	2	0
All	All	22698	0	21876	1795	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 (1795) 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:J:109:CYS:HB3	2:J:138:CYS:SG	1.64	1.36
1:F:114:LEU:HD22	2:L:115:ILE:CD1	1.62	1.28
2:L:21:ILE:HD12	2:L:21:ILE:O	1.35	1.25
2:J:114:CYS:SG	2:J:116:SER:HB3	1.81	1.20
2:L:21:ILE:HG22	2:L:56:LYS:HD3	1.25	1.19
2:K:12:ILE:HG22	2:K:13:LYS:H	1.01	1.14
1:F:140:LEU:HD22	1:F:292:GLY:HA2	1.29	1.14
2:L:22:PRO:HD2	2:L:57:ASP:HB3	1.25	1.13

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:LEU:HD22	1:C:292:GLY:HA2	1.30	1.11
2:L:14:ARG:HG2	2:L:88:ASN:HA	1.29	1.11
2:J:6:LYS:HB2	2:J:9:VAL:HB	1.30	1.11
2:I:109:CYS:SG	2:I:114:CYS:CB	2.39	1.11
2:G:34:LYS:HB3	2:G:37:GLU:HG3	1.30	1.10
1:F:114:LEU:HD22	2:L:115:ILE:HD13	1.28	1.09
1:F:114:LEU:CD2	2:L:115:ILE:HD11	1.82	1.09
2:J:109:CYS:CB	2:J:138:CYS:SG	2.29	1.09
2:K:72:ASP:HB3	2:K:100:PRO:HG3	1.33	1.09
1:A:94:VAL:HG11	1:C:54:ARG:HH12	1.08	1.08
2:L:82:THR:HG22	2:L:83:VAL:H	0.93	1.08
2:L:72:ASP:HB3	2:L:100:PRO:HG2	1.33	1.07
2:L:83:VAL:HG11	2:L:94:LYS:HB2	1.31	1.07
2:K:12:ILE:HG23	2:K:62:GLU:HG2	1.37	1.06
1:F:114:LEU:CD2	2:L:115:ILE:CD1	2.33	1.06
2:G:12:ILE:HG22	2:G:13:LYS:H	1.13	1.06
2:J:104:ASP:HB3	2:J:124:SER:HA	1.38	1.05
2:J:114:CYS:SG	2:J:116:SER:CB	2.45	1.05
1:C:243:VAL:HG13	1:C:244:LYS:HD2	1.40	1.04
2:G:76:LEU:HD11	2:G:103:ILE:HG21	1.39	1.03
1:A:44:ILE:HD12	1:A:63:MET:HG2	1.40	1.03
2:L:82:THR:HG22	2:L:83:VAL:N	1.75	1.02
1:A:94:VAL:HG11	1:C:54:ARG:NH1	1.72	1.02
2:L:82:THR:CG2	2:L:83:VAL:H	1.72	1.00
1:B:243:VAL:HG13	1:B:244:LYS:HD2	1.42	1.00
2:G:103:ILE:HD12	2:G:107:LEU:HD11	1.44	1.00
2:K:30:LEU:HD21	2:K:44:ILE:HG12	1.46	0.98
2:K:14:ARG:H	2:K:87:ASP:HA	1.26	0.98
2:K:38:THR:HG22	2:K:40:GLN:H	1.24	0.98
1:F:114:LEU:HD22	2:L:115:ILE:HD11	1.41	0.97
2:L:83:VAL:HG13	2:L:95:SER:H	1.24	0.96
1:B:109:GLU:HG3	1:B:130:GLY:O	1.66	0.96
1:F:265:HIS:H	1:F:288:GLN:HE22	1.09	0.96
2:L:21:ILE:O	2:L:21:ILE:CD1	2.14	0.95
1:C:104:MET:HE1	1:C:112:ALA:HA	1.49	0.94
2:I:109:CYS:HB2	2:I:138:CYS:SG	2.04	0.94
2:L:42:ILE:HG22	2:L:44:ILE:HG13	1.48	0.94
2:I:13:LYS:HB2	2:I:89:TYR:CE1	2.02	0.94
2:K:12:ILE:HG22	2:K:13:LYS:N	1.82	0.94
1:E:243:VAL:HG13	1:E:244:LYS:HD2	1.50	0.94
2:L:16:THR:HB	2:L:60:LYS:HB3	1.46	0.94

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:105:ASN:H	2:J:123:SER:HB3	1.34	0.93
1:C:257:ALA:HB1	1:C:261:MET:CE	1.98	0.93
1:D:243:VAL:HG13	1:D:244:LYS:HD2	1.48	0.93
2:G:34:LYS:HB3	2:G:37:GLU:CG	1.99	0.92
2:H:138:CYS:HB2	2:H:141:CYS:SG	2.09	0.92
1:D:140:LEU:HD22	1:D:292:GLY:HA2	1.50	0.91
2:G:12:ILE:H	2:G:60:LYS:HZ3	1.18	0.91
2:H:17:VAL:HG22	2:H:60:LYS:HG2	1.50	0.91
2:H:138:CYS:CB	2:H:141:CYS:SG	2.59	0.91
2:L:96:ARG:O	2:L:96:ARG:HG2	1.70	0.90
2:G:68:GLU:HA	2:G:71:VAL:HG12	1.54	0.90
2:I:109:CYS:SG	2:I:111:ASN:HB3	2.11	0.90
2:L:70:GLN:HA	2:L:73:GLN:NE2	1.85	0.90
2:I:42:ILE:HD11	2:L:46:LEU:HD12	1.54	0.90
1:F:44:ILE:HD12	1:F:63:MET:HG2	1.52	0.90
2:G:111:ASN:ND2	2:G:113:ASN:H	1.71	0.89
1:B:108:GLN:HB2	2:H:115:ILE:HG13	1.53	0.89
2:G:13:LYS:HD3	2:G:89:TYR:CE1	2.07	0.89
2:H:114:CYS:SG	2:H:140:TYR:HB2	2.12	0.89
1:A:170:HIS:O	1:A:174:GLN:HG3	1.73	0.88
1:C:30:LEU:HD21	1:C:309:VAL:HG21	1.55	0.88
1:D:54:ARG:HD3	1:D:267:LEU:HB2	1.54	0.88
2:L:21:ILE:CG2	2:L:56:LYS:HD3	2.03	0.88
2:L:14:ARG:HD3	2:L:65:PHE:HZ	1.38	0.88
2:L:78:ALA:HB1	2:L:81:ALA:HB2	1.54	0.88
1:A:59:PHE:HE1	1:A:136:THR:HG21	1.37	0.88
2:G:54:GLY:HA2	6:G:1026:HOH:O	1.72	0.87
1:A:109:GLU:HG3	1:A:130:GLY:O	1.73	0.87
2:H:41:ARG:CZ	2:K:8:GLN:HE21	1.86	0.87
2:G:48:LEU:HD23	2:J:41:ARG:HD2	1.57	0.86
2:G:114:CYS:SG	2:G:116:SER:OG	2.34	0.86
2:L:21:ILE:HG22	2:L:56:LYS:CD	2.05	0.86
1:B:35:GLN:HE22	1:B:309:VAL:HG23	1.40	0.85
2:G:152:ALA:HB3	6:G:1058:HOH:O	1.76	0.85
2:K:14:ARG:HH11	2:K:14:ARG:HB3	1.41	0.85
2:G:17:VAL:HG22	2:G:60:LYS:HE3	1.58	0.85
1:F:126:ASN:HD21	1:F:129:ASP:HB2	1.39	0.85
2:L:25:ILE:HG22	2:L:29:LEU:HG	1.55	0.85
2:G:12:ILE:HG22	2:G:13:LYS:N	1.92	0.85
1:B:261:MET:HG2	1:B:262:LYS:N	1.91	0.85
2:L:18:ILE:HG22	2:L:19:ASP:H	1.41	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:HD13	1:A:304:LEU:HD12	1.58	0.85
1:B:161:GLY:HA3	1:B:228:THR:OG1	1.76	0.84
1:C:140:LEU:CD2	1:C:292:GLY:HA2	2.07	0.84
1:E:45:ALA:HB2	1:E:99:VAL:HG11	1.58	0.84
1:F:268:PRO:HD3	6:F:3075:HOH:O	1.76	0.84
1:A:88:LEU:HD23	1:A:114:LEU:HD23	1.59	0.84
2:I:15:GLY:HA2	2:I:63:ASN:H	1.42	0.84
2:L:14:ARG:HH21	2:L:88:ASN:HD22	1.25	0.84
2:G:12:ILE:N	2:G:60:LYS:HZ3	1.76	0.84
2:H:19:ASP:HA	2:H:58:LEU:HD23	1.60	0.84
1:C:161:GLY:HA3	1:C:228:THR:OG1	1.76	0.84
2:I:109:CYS:SG	2:I:114:CYS:HB3	2.11	0.84
1:D:105:ARG:HD2	1:D:128:GLY:HA3	1.60	0.84
1:B:132:ASN:O	1:B:167:ARG:HB2	1.77	0.83
1:E:108:GLN:HB2	2:K:113:ASN:O	1.76	0.83
2:K:12:ILE:CG2	2:K:13:LYS:H	1.86	0.83
1:B:200:ASP:HB3	2:H:128:ARG:HH22	1.44	0.83
1:F:81:LEU:HD12	1:F:86:GLU:O	1.79	0.83
2:L:83:VAL:HG11	2:L:94:LYS:CB	2.08	0.83
1:A:54:ARG:HH21	1:A:268:PRO:HG3	1.44	0.83
2:I:46:LEU:HB2	2:L:42:ILE:HG13	1.60	0.83
2:J:12:ILE:HG22	2:J:13:LYS:H	1.43	0.83
1:E:266:PRO:HB3	3:E:2005:FCL:HG1	1.59	0.83
1:B:140:LEU:HD22	1:B:292:GLY:HA2	1.61	0.82
1:D:132:ASN:O	1:D:167:ARG:HB2	1.79	0.82
2:K:14:ARG:HB3	2:K:14:ARG:NH1	1.93	0.82
2:L:14:ARG:CG	2:L:88:ASN:HA	2.09	0.82
2:J:48:LEU:HD12	2:J:58:LEU:HG	1.62	0.82
2:I:107:LEU:HA	2:I:152:ALA:HB2	1.61	0.82
2:I:55:ARG:HH11	2:L:39:ASP:HB3	1.45	0.81
1:D:120:GLY:O	1:D:122:VAL:HG23	1.79	0.81
1:B:59:PHE:CD1	1:B:296:ARG:HD3	2.15	0.81
2:G:141:CYS:O	2:G:141:CYS:SG	2.38	0.81
2:H:35:LEU:HD13	2:H:61:ILE:HD11	1.61	0.81
2:G:83:VAL:HG22	2:G:84:ASN:H	1.45	0.81
2:G:32:LEU:HD13	2:G:152:ALA:HB1	1.61	0.81
1:F:45:ALA:HB2	1:F:99:VAL:HG11	1.61	0.81
1:F:59:PHE:HE1	1:F:136:THR:HG21	1.46	0.81
1:C:17:ARG:HG2	1:C:17:ARG:HH11	1.45	0.80
2:L:22:PRO:HD2	2:L:57:ASP:CB	2.09	0.80
1:A:109:GLU:HB3	2:G:141:CYS:HB2	1.64	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:HIS:O	1:D:174:GLN:HG3	1.81	0.80
1:C:257:ALA:CB	1:C:261:MET:CE	2.59	0.80
2:G:17:VAL:HG13	2:G:60:LYS:HG2	1.63	0.80
1:E:237:PRO:HA	1:E:240:TYR:CE2	2.17	0.80
1:F:114:LEU:CD2	2:L:115:ILE:HD13	2.05	0.80
2:L:15:GLY:O	2:L:86:ILE:HB	1.82	0.80
2:I:13:LYS:HG3	2:I:88:ASN:HA	1.63	0.79
1:F:59:PHE:CD1	1:F:296:ARG:HD3	2.17	0.79
2:K:12:ILE:HD11	2:K:60:LYS:HB2	1.63	0.79
2:I:44:ILE:HB	2:L:44:ILE:CG2	2.13	0.79
1:B:174:GLN:HA	1:B:201:MET:CE	2.13	0.79
1:F:63:MET:HG3	1:F:300:LEU:HD11	1.65	0.79
1:D:267:LEU:HD12	1:F:94:VAL:HG12	1.64	0.79
2:L:17:VAL:HG23	2:L:86:ILE:HD12	1.64	0.79
1:F:265:HIS:H	1:F:288:GLN:NE2	1.81	0.78
1:C:160:VAL:HB	1:C:227:MET:HG2	1.65	0.78
2:H:109:CYS:SG	2:H:111:ASN:HB3	2.22	0.78
1:E:229:ARG:HH11	1:E:232:LYS:HE2	1.45	0.78
2:L:114:CYS:SG	2:L:116:SER:OG	2.40	0.78
1:A:114:LEU:HD22	2:G:115:ILE:HG21	1.64	0.78
1:E:59:PHE:HE1	1:E:136:THR:HG21	1.48	0.78
1:B:45:ALA:HB2	1:B:99:VAL:HG11	1.63	0.78
2:I:12:ILE:HD12	2:I:61:ILE:O	1.84	0.78
2:J:104:ASP:CB	2:J:124:SER:HA	2.13	0.78
2:L:71:VAL:HG21	2:L:85:ARG:HE	1.49	0.78
1:B:239:GLU:C	1:B:241:ALA:H	1.86	0.78
1:F:131:SER:HB2	1:F:234:ARG:HD3	1.64	0.78
2:J:43:THR:HB	2:J:60:LYS:HB2	1.64	0.78
2:H:85:ARG:C	2:H:86:ILE:HG12	2.03	0.78
1:F:55:THR:O	1:F:59:PHE:HB2	1.83	0.77
2:J:67:SER:H	2:J:70:GLN:HE21	1.30	0.77
2:I:87:ASP:OD2	2:I:92:VAL:HG21	1.85	0.77
1:C:109:GLU:HG3	1:C:130:GLY:O	1.85	0.77
1:A:81:LEU:HD12	1:A:86:GLU:O	1.84	0.77
1:E:35:GLN:NE2	1:E:309:VAL:HG23	2.00	0.77
1:A:237:PRO:HA	1:A:240:TYR:CE2	2.18	0.77
2:I:86:ILE:HG23	2:I:91:VAL:HA	1.66	0.77
1:D:214:SER:OG	1:D:217:GLU:HG3	1.84	0.77
1:C:106:HIS:ND1	1:C:107:PRO:HD2	1.99	0.76
1:C:120:GLY:O	1:C:122:VAL:HG23	1.84	0.76
2:H:27:PHE:HZ	2:K:31:SER:HB2	1.49	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:PHE:HE1	1:D:136:THR:HG21	1.48	0.76
1:E:44:ILE:HD12	1:E:63:MET:HG2	1.66	0.76
1:F:265:HIS:ND1	1:F:266:PRO:O	2.17	0.76
1:B:106:HIS:CE1	2:H:115:ILE:HD11	2.21	0.76
2:J:21:ILE:O	2:J:56:LYS:HA	1.86	0.76
2:L:86:ILE:HD13	2:L:92:VAL:HA	1.68	0.76
1:B:131:SER:HB3	1:B:234:ARG:HD3	1.65	0.76
1:B:267:LEU:HD13	1:B:289:ALA:HB2	1.68	0.76
2:G:70:GLN:O	2:G:73:GLN:HG2	1.85	0.76
2:L:86:ILE:HG23	2:L:93:GLY:N	2.01	0.76
1:C:257:ALA:HB1	1:C:261:MET:HE2	1.67	0.76
2:L:83:VAL:CG1	2:L:95:SER:H	1.98	0.76
1:C:43:VAL:HG22	1:C:69:SER:HB2	1.66	0.76
2:K:84:ASN:HB3	2:K:91:VAL:HG13	1.68	0.76
2:I:19:ASP:HB2	2:I:56:LYS:HZ1	1.49	0.76
2:I:138:CYS:HB2	2:I:141:CYS:SG	2.25	0.76
1:C:59:PHE:CD1	1:C:296:ARG:HD3	2.21	0.75
1:F:225:LEU:HD21	1:F:227:MET:CE	2.17	0.75
1:D:94:VAL:CG1	1:E:267:LEU:HD22	2.16	0.75
2:L:14:ARG:HD3	2:L:65:PHE:CZ	2.20	0.75
1:B:59:PHE:HE1	1:B:136:THR:HG21	1.50	0.75
2:J:34:LYS:HB3	2:J:37:GLU:HG2	1.69	0.75
1:E:137:GLN:HG2	1:E:168:THR:HG22	1.68	0.75
1:C:137:GLN:HG2	1:C:168:THR:HG22	1.69	0.75
2:G:85:ARG:HB3	2:G:93:GLY:H	1.50	0.75
2:J:41:ARG:HB3	2:J:62:GLU:OE1	1.85	0.75
2:L:18:ILE:HG22	2:L:19:ASP:N	2.01	0.75
1:D:237:PRO:HA	1:D:240:TYR:CE1	2.22	0.75
1:E:44:ILE:HB	1:E:63:MET:CE	2.16	0.75
1:B:111:ALA:HB2	2:H:115:ILE:HD12	1.68	0.74
2:L:62:GLU:HA	6:L:1049:HOH:O	1.85	0.74
1:C:109:GLU:HA	1:C:129:ASP:OD1	1.86	0.74
1:B:48:PHE:CE2	1:B:56:ARG:HB2	2.23	0.74
1:D:109:GLU:OE2	1:D:131:SER:HB3	1.88	0.74
2:G:16:THR:HB	2:G:65:PHE:HD2	1.53	0.74
1:D:189:PRO:HB3	1:D:246:GLN:HE22	1.53	0.74
1:A:29:LYS:O	1:A:32:ALA:N	2.21	0.74
1:D:63:MET:HE2	1:D:70:VAL:HG22	1.68	0.74
2:I:18:ILE:HG12	2:I:83:VAL:HG23	1.70	0.74
2:I:19:ASP:HB2	2:I:56:LYS:NZ	2.02	0.74
1:A:109:GLU:OE1	2:G:113:ASN:HB3	1.88	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:14:ARG:HB3	2:H:63:ASN:HD22	1.52	0.73
2:I:40:GLN:HG3	2:I:62:GLU:HB2	1.68	0.73
2:L:46:LEU:HD23	2:L:57:ASP:OD1	1.88	0.73
2:L:86:ILE:HG23	2:L:93:GLY:H	1.53	0.73
1:E:170:HIS:O	1:E:174:GLN:HG3	1.88	0.73
1:F:126:ASN:ND2	1:F:129:ASP:HB2	2.03	0.73
2:J:34:LYS:HB3	2:J:37:GLU:CG	2.18	0.73
2:L:14:ARG:CD	2:L:65:PHE:HZ	2.00	0.73
2:L:83:VAL:HG12	2:L:84:ASN:N	2.03	0.73
1:A:140:LEU:HD22	1:A:292:GLY:HA2	1.70	0.73
2:I:132:ASN:O	2:I:133:ASP:HB2	1.87	0.73
2:J:141:CYS:O	2:J:141:CYS:SG	2.46	0.73
1:B:214:SER:OG	1:B:217:GLU:HG3	1.88	0.73
1:B:293:ILE:O	1:B:297:GLN:HB2	1.89	0.73
2:K:102:ARG:HB3	2:K:102:ARG:NH1	2.04	0.73
1:D:35:GLN:NE2	1:D:309:VAL:HG23	2.04	0.73
2:J:17:VAL:HG11	2:J:86:ILE:HD12	1.71	0.73
2:K:12:ILE:CG2	2:K:62:GLU:HG2	2.17	0.73
1:A:53:THR:N	4:A:3001:PO4:O1	2.22	0.73
1:B:131:SER:HB3	1:B:234:ARG:CD	2.18	0.73
1:F:10:ILE:HD12	1:F:112:ALA:HB1	1.71	0.73
2:J:110:PRO:HD2	2:J:145:PHE:CE2	2.24	0.73
1:B:267:LEU:CD1	1:B:289:ALA:HB2	2.19	0.72
1:F:54:ARG:HD3	1:F:267:LEU:HB2	1.71	0.72
2:G:76:LEU:HD11	2:G:103:ILE:HD13	1.70	0.72
2:G:111:ASN:HD22	2:G:113:ASN:H	1.37	0.72
1:F:237:PRO:HA	1:F:240:TYR:CE2	2.24	0.72
2:J:14:ARG:HG3	2:J:14:ARG:O	1.89	0.72
2:L:61:ILE:CG2	2:L:64:THR:HB	2.19	0.72
2:L:86:ILE:HG21	2:L:91:VAL:O	1.89	0.72
2:L:86:ILE:HG22	2:L:87:ASP:N	2.05	0.72
1:C:65:ARG:HH11	1:C:293:ILE:HG21	1.54	0.72
2:G:19:ASP:HA	2:G:58:LEU:CD1	2.20	0.72
1:D:120:GLY:O	1:D:122:VAL:N	2.23	0.72
2:L:12:ILE:HD11	2:L:15:GLY:HA2	1.70	0.72
2:I:110:PRO:HD2	2:I:145:PHE:CE2	2.25	0.72
2:L:16:THR:HA	2:L:86:ILE:HG13	1.72	0.72
1:B:35:GLN:NE2	1:B:309:VAL:HG23	2.04	0.72
1:C:65:ARG:NH1	1:C:293:ILE:HG21	2.04	0.72
1:C:237:PRO:HA	1:C:240:TYR:CE2	2.25	0.72
1:E:59:PHE:CE1	1:E:136:THR:HG21	2.25	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:GLY:O	1:E:122:VAL:HG23	1.89	0.72
1:C:54:ARG:CZ	1:C:267:LEU:HB3	2.19	0.71
1:C:104:MET:CE	1:C:112:ALA:HA	2.19	0.71
2:K:18:ILE:O	2:K:58:LEU:HD12	1.89	0.71
2:L:23:ALA:N	2:L:25:ILE:HG12	2.04	0.71
1:C:114:LEU:HD13	2:I:121:VAL:HG11	1.72	0.71
1:C:17:ARG:HG2	1:C:17:ARG:NH1	2.00	0.71
2:I:56:LYS:HE3	2:I:58:LEU:HG	1.72	0.71
1:C:106:HIS:HD2	6:C:3063:HOH:O	1.72	0.71
1:C:188:ALA:HA	1:C:247:PHE:HE2	1.55	0.71
1:C:189:PRO:HB3	1:C:246:GLN:OE1	1.90	0.71
2:G:12:ILE:H	2:G:60:LYS:NZ	1.89	0.71
2:G:76:LEU:CD1	2:G:103:ILE:HD13	2.19	0.71
1:D:45:ALA:HB2	1:D:99:VAL:HG11	1.72	0.71
1:A:138:THR:O	1:A:142:LEU:HG	1.90	0.71
1:E:109:GLU:HG3	1:E:130:GLY:O	1.91	0.71
2:K:26:GLY:O	2:K:30:LEU:HB2	1.91	0.71
2:I:30:LEU:HD23	2:I:35:LEU:HD12	1.70	0.71
1:D:40:LYS:HG2	1:D:41:HIS:CD2	2.26	0.71
2:L:71:VAL:HG12	2:L:97:PRO:HG2	1.73	0.71
2:I:82:THR:HG22	2:I:96:ARG:HB3	1.73	0.71
2:I:107:LEU:HD23	2:I:152:ALA:HB2	1.72	0.71
2:J:30:LEU:HD11	2:J:44:ILE:HD13	1.73	0.71
1:C:59:PHE:HE1	1:C:136:THR:HG21	1.56	0.70
2:K:114:CYS:SG	2:K:141:CYS:HB3	2.31	0.70
1:F:225:LEU:HD21	1:F:227:MET:HE1	1.73	0.70
2:I:107:LEU:HA	2:I:152:ALA:CB	2.21	0.70
2:L:16:THR:HG21	2:L:84:ASN:HA	1.74	0.70
1:E:214:SER:OG	1:E:217:GLU:HG3	1.91	0.70
2:K:129:LYS:HA	2:K:134:ILE:HG22	1.74	0.70
1:C:293:ILE:O	1:C:297:GLN:HB2	1.91	0.70
1:F:293:ILE:O	1:F:297:GLN:HB2	1.92	0.70
1:D:189:PRO:HB3	1:D:246:GLN:NE2	2.07	0.70
2:L:17:VAL:C	2:L:18:ILE:HG12	2.12	0.70
1:B:239:GLU:O	1:B:241:ALA:N	2.25	0.70
1:C:284:TRP:HA	1:C:287:GLN:OE1	1.92	0.70
2:H:19:ASP:HA	2:H:58:LEU:CD2	2.21	0.70
2:K:130:ARG:HB2	2:K:133:ASP:O	1.91	0.70
2:L:18:ILE:HG13	2:L:83:VAL:HB	1.72	0.70
1:E:114:LEU:HD21	2:K:119:GLU:HG3	1.74	0.69
2:H:110:PRO:HD2	2:H:145:PHE:CE2	2.27	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:LYS:HE2	6:F:3069:HOH:O	1.91	0.69
2:L:115:ILE:HD11	2:L:119:GLU:HG3	1.75	0.69
2:G:103:ILE:CD1	2:G:107:LEU:HD11	2.21	0.69
2:J:104:ASP:HB2	2:J:123:SER:O	1.92	0.69
2:J:46:LEU:HD22	2:J:57:ASP:OD2	1.92	0.69
1:B:90:ASP:O	1:B:94:VAL:HG22	1.92	0.69
2:G:12:ILE:CG2	2:G:13:LYS:H	1.98	0.69
2:L:75:ALA:HB1	2:L:98:SER:O	1.93	0.69
2:G:27:PHE:HZ	2:J:31:SER:HB3	1.58	0.69
2:I:75:ALA:O	2:I:79:PRO:HG3	1.93	0.69
1:B:156:HIS:HD2	1:B:185:TYR:OH	1.76	0.69
1:B:174:GLN:HA	1:B:201:MET:HE1	1.75	0.69
1:C:257:ALA:CB	1:C:261:MET:HE1	2.23	0.69
2:G:46:LEU:HA	2:G:57:ASP:OD1	1.92	0.69
1:D:44:ILE:HD12	1:D:63:MET:HG2	1.74	0.69
1:D:199:LEU:HD13	1:D:209:TRP:CH2	2.27	0.69
2:K:53:MET:HG2	2:K:54:GLY:H	1.58	0.69
1:A:32:ALA:O	1:A:34:PRO:HD3	1.92	0.68
2:K:43:THR:HB	2:K:60:LYS:CG	2.23	0.68
1:B:267:LEU:HD21	1:B:285:TYR:O	1.93	0.68
2:I:111:ASN:ND2	2:I:113:ASN:H	1.91	0.68
1:A:54:ARG:HB2	4:A:3001:PO4:O3	1.93	0.68
1:D:59:PHE:CD1	1:D:296:ARG:HD3	2.28	0.68
2:J:146:SER:O	2:J:149:VAL:HG22	1.93	0.68
2:K:52:GLU:HG3	6:K:1034:HOH:O	1.92	0.68
2:L:109:CYS:SG	2:L:138:CYS:HB2	2.33	0.68
1:A:214:SER:OG	1:A:217:GLU:HG3	1.94	0.68
1:E:66:LEU:HD21	1:E:297:GLN:HE21	1.57	0.68
1:B:75:ASP:OD2	1:B:77:ALA:HB3	1.94	0.68
1:F:189:PRO:HG3	1:F:246:GLN:OE1	1.94	0.68
1:B:159:MET:CE	1:B:173:THR:OG1	2.42	0.68
1:C:264:LEU:O	1:C:265:HIS:HB2	1.94	0.68
2:I:76:LEU:HD13	2:I:103:ILE:HD11	1.74	0.68
2:I:109:CYS:SG	2:I:114:CYS:HB2	2.23	0.68
1:D:94:VAL:HG11	1:E:267:LEU:HD22	1.74	0.68
2:J:12:ILE:HG22	2:J:13:LYS:N	2.08	0.68
1:B:232:LYS:HA	1:B:235:LEU:HD12	1.76	0.68
2:J:53:MET:HG3	2:J:54:GLY:H	1.58	0.68
2:I:30:LEU:HD21	2:I:59:ILE:HD13	1.76	0.67
1:D:267:LEU:CD1	1:F:94:VAL:HG12	2.23	0.67
1:F:284:TRP:HA	1:F:287:GLN:OE1	1.94	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:HA	2:G:115:ILE:HD12	1.76	0.67
2:I:44:ILE:O	2:L:44:ILE:HB	1.95	0.67
2:I:92:VAL:HG12	2:I:93:GLY:N	2.10	0.67
2:I:107:LEU:HD23	2:I:152:ALA:CB	2.25	0.67
2:G:41:ARG:HD3	2:G:62:GLU:OE1	1.94	0.67
2:G:78:ALA:HB1	2:G:81:ALA:HB2	1.75	0.67
1:B:12:ILE:HG13	1:B:171:SER:HB3	1.76	0.67
1:D:69:SER:HA	6:D:3063:HOH:O	1.93	0.67
1:E:270:VAL:O	1:E:270:VAL:HG12	1.94	0.67
1:F:35:GLN:HE22	1:F:309:VAL:HG23	1.60	0.67
2:J:14:ARG:O	2:J:63:ASN:HA	1.94	0.67
2:L:57:ASP:OD2	2:L:58:LEU:N	2.27	0.67
2:G:138:CYS:HB3	2:G:141:CYS:O	1.94	0.67
2:I:106:VAL:O	2:I:152:ALA:HB1	1.95	0.67
1:E:83:LYS:HG3	1:F:51:ALA:HB2	1.76	0.67
2:J:18:ILE:HG22	2:J:21:ILE:HD11	1.76	0.67
2:J:114:CYS:SG	2:J:116:SER:HB2	2.32	0.67
1:A:55:THR:O	1:A:59:PHE:HB2	1.94	0.67
1:B:209:TRP:HZ3	1:B:211:LEU:HD21	1.60	0.67
2:I:107:LEU:HD22	2:I:150:VAL:HG12	1.75	0.67
1:D:188:ALA:HB1	1:D:189:PRO:HD2	1.75	0.67
2:J:51:GLY:C	2:J:53:MET:H	1.98	0.67
1:B:54:ARG:NH2	1:C:80:SER:OG	2.28	0.67
2:I:38:THR:O	2:L:47:ASN:ND2	2.27	0.67
2:I:88:ASN:C	2:I:90:GLU:H	1.97	0.66
1:E:49:PHE:HE2	1:E:81:LEU:HD22	1.60	0.66
1:A:240:TYR:O	1:A:243:VAL:HG23	1.95	0.66
1:B:168:THR:HG21	1:B:266:PRO:HB3	1.77	0.66
1:A:104:MET:HE1	1:A:112:ALA:HA	1.77	0.66
2:I:105:ASN:OD1	2:I:122:SER:HB3	1.96	0.66
1:D:51:ALA:HB2	1:F:83:LYS:HG3	1.75	0.66
1:B:106:HIS:HE1	1:B:108:GLN:HG2	1.60	0.66
1:B:265:HIS:ND1	1:B:266:PRO:O	2.19	0.66
2:L:14:ARG:HH21	2:L:88:ASN:ND2	1.92	0.66
1:F:63:MET:HG3	1:F:300:LEU:CD1	2.26	0.66
1:F:170:HIS:O	1:F:174:GLN:HG3	1.96	0.66
2:J:103:ILE:HD11	2:J:107:LEU:HG	1.78	0.66
1:A:75:ASP:OD2	1:A:77:ALA:HB3	1.96	0.66
1:A:219:MET:CE	1:A:254:LEU:HD23	2.25	0.66
1:B:170:HIS:O	1:B:174:GLN:HG3	1.96	0.66
1:C:55:THR:O	1:C:59:PHE:HB2	1.96	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:HIS:C	1:E:266:PRO:O	2.30	0.66
2:K:99:LEU:HD12	2:K:129:LYS:HE2	1.78	0.66
2:G:134:ILE:HB	2:G:147:HIS:HD2	1.60	0.66
2:I:109:CYS:CB	2:I:138:CYS:SG	2.84	0.66
1:C:81:LEU:HD13	1:C:86:GLU:O	1.96	0.66
1:F:59:PHE:CE1	1:F:136:THR:HG21	2.31	0.66
2:H:86:ILE:HG23	2:H:91:VAL:HA	1.77	0.65
1:E:132:ASN:O	1:E:167:ARG:HB2	1.96	0.65
1:E:299:LEU:O	1:E:303:VAL:HG23	1.96	0.65
2:L:22:PRO:HD3	2:L:57:ASP:O	1.95	0.65
1:B:237:PRO:HA	1:B:240:TYR:CD1	2.31	0.65
1:F:159:MET:HE3	1:F:172:LEU:HD23	1.79	0.65
2:J:105:ASN:OD1	2:J:122:SER:HB3	1.97	0.65
1:A:60:GLU:HG2	1:A:70:VAL:HG11	1.78	0.65
1:B:111:ALA:CB	2:H:115:ILE:HD12	2.27	0.65
1:B:166:GLY:O	1:B:169:VAL:HG22	1.97	0.65
2:H:14:ARG:HB3	2:H:63:ASN:ND2	2.11	0.65
2:H:46:LEU:HA	2:H:57:ASP:OD1	1.96	0.65
1:E:55:THR:O	1:E:59:PHE:HB2	1.97	0.65
1:B:203:ASP:HB3	6:B:3061:HOH:O	1.95	0.65
2:G:71:VAL:HG22	2:G:97:PRO:HG3	1.78	0.65
2:I:28:LYS:HE3	2:I:77:TYR:HE2	1.62	0.65
2:L:23:ALA:H	2:L:25:ILE:HG12	1.61	0.65
1:C:75:ASP:OD2	1:C:77:ALA:HB3	1.97	0.65
1:A:44:ILE:HB	1:A:63:MET:CE	2.27	0.65
2:J:136:LEU:O	2:J:144:GLU:HA	1.97	0.65
1:F:154:ASN:HA	1:F:181:GLY:O	1.97	0.64
2:J:30:LEU:CD1	2:J:44:ILE:HD13	2.27	0.64
2:J:53:MET:CG	2:J:54:GLY:H	2.09	0.64
1:A:84:LYS:NZ	3:C:2003:FLC:OHB	2.30	0.64
1:B:54:ARG:NH2	1:C:86:GLU:OE1	2.29	0.64
1:B:106:HIS:CE1	1:B:108:GLN:HG2	2.32	0.64
1:B:126:ASN:HD21	1:B:129:ASP:HB2	1.61	0.64
1:D:105:ARG:NH2	3:D:2004:FLC:OB2	2.30	0.64
1:F:75:ASP:OD2	1:F:77:ALA:HB3	1.97	0.64
1:B:58:SER:HB3	1:C:98:TYR:CZ	2.32	0.64
1:C:35:GLN:NE2	1:C:309:VAL:HG23	2.13	0.64
2:L:17:VAL:O	2:L:18:ILE:HG12	1.98	0.64
2:L:115:ILE:C	2:L:117:HIS:H	2.01	0.64
1:A:109:GLU:CB	2:G:141:CYS:HB2	2.27	0.64
2:I:88:ASN:O	2:I:90:GLU:N	2.30	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:ASP:HB3	6:E:3077:HOH:O	1.97	0.64
1:A:104:MET:CE	1:A:112:ALA:HA	2.28	0.64
1:B:54:ARG:HD3	1:B:267:LEU:CB	2.27	0.64
1:C:49:PHE:HE2	1:C:81:LEU:HD23	1.61	0.64
2:G:94:LYS:HE2	2:G:96:ARG:HH21	1.62	0.64
1:E:44:ILE:HB	1:E:63:MET:HE3	1.79	0.64
1:F:94:VAL:HG23	1:F:95:ILE:N	2.13	0.64
2:H:39:ASP:HB3	2:K:55:ARG:NH1	2.13	0.64
2:J:6:LYS:O	2:J:6:LYS:HG3	1.98	0.63
1:A:63:MET:HE1	1:A:70:VAL:HG22	1.80	0.63
2:I:30:LEU:CD2	2:I:35:LEU:HD12	2.27	0.63
2:I:55:ARG:HH11	2:L:39:ASP:CB	2.12	0.63
2:L:22:PRO:HB3	2:L:25:ILE:HB	1.80	0.63
1:E:26:THR:HG22	1:E:30:LEU:HD12	1.80	0.63
1:E:63:MET:HE1	1:E:70:VAL:HG22	1.79	0.63
1:E:132:ASN:ND2	1:E:133:GLN:H	1.97	0.63
1:B:109:GLU:HB3	2:H:141:CYS:HA	1.78	0.63
2:I:42:ILE:HD12	2:I:44:ILE:HD11	1.80	0.63
1:F:134:HIS:CE1	1:F:137:GLN:HB2	2.33	0.63
2:J:137:LYS:HA	2:J:143:LYS:O	1.97	0.63
2:K:12:ILE:HG13	2:K:60:LYS:HE2	1.79	0.63
2:K:137:LYS:HD3	2:K:144:GLU:HG3	1.81	0.63
1:A:69:SER:HA	6:A:3041:HOH:O	1.97	0.63
2:G:30:LEU:HD21	2:G:59:ILE:HD13	1.81	0.63
1:F:91:THR:O	1:F:94:VAL:HG22	1.98	0.63
1:D:63:MET:HG3	1:D:300:LEU:CD1	2.27	0.63
1:E:166:GLY:O	1:E:169:VAL:HG22	1.97	0.63
2:K:75:ALA:O	2:K:79:PRO:HG3	1.98	0.63
2:G:25:ILE:HG22	2:G:29:LEU:HG	1.81	0.63
2:I:76:LEU:HD13	2:I:103:ILE:CD1	2.28	0.63
1:F:140:LEU:HD23	1:F:295:ALA:HB3	1.81	0.63
2:L:12:ILE:CD1	2:L:15:GLY:HA2	2.29	0.63
1:B:174:GLN:HA	1:B:201:MET:HE2	1.80	0.63
1:E:44:ILE:HB	1:E:63:MET:HE2	1.79	0.63
1:A:43:VAL:HG11	1:C:61:THR:HG23	1.81	0.63
1:A:50:GLU:HB3	1:A:105:ARG:HG2	1.80	0.63
1:B:23:VAL:HG11	1:B:139:LEU:HD13	1.80	0.63
1:F:114:LEU:HD23	2:L:115:ILE:HD11	1.77	0.63
2:K:30:LEU:CD2	2:K:44:ILE:HG12	2.25	0.63
2:I:30:LEU:HD21	2:I:59:ILE:HG21	1.82	0.62
2:I:46:LEU:HB2	2:L:42:ILE:CG1	2.29	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:PHE:CE2	1:D:103:VAL:HG21	2.34	0.62
1:D:66:LEU:HD21	1:D:297:GLN:HG2	1.81	0.62
2:I:110:PRO:HD2	2:I:145:PHE:CD2	2.34	0.62
1:E:126:ASN:HD21	1:E:129:ASP:HB2	1.63	0.62
1:A:54:ARG:NH2	1:A:268:PRO:HG3	2.13	0.62
1:A:132:ASN:O	1:A:167:ARG:HB2	1.99	0.62
1:D:129:ASP:OD1	1:D:129:ASP:O	2.17	0.62
1:F:218:VAL:O	1:F:222:VAL:HG13	1.99	0.62
2:K:2:THR:O	2:K:4:ASP:N	2.32	0.62
2:G:71:VAL:HG13	2:G:72:ASP:N	2.13	0.62
2:H:134:ILE:HD12	2:H:134:ILE:N	2.14	0.62
2:I:51:GLY:HA2	6:I:1014:HOH:O	1.99	0.62
1:F:219:MET:HE3	1:F:254:LEU:HD23	1.81	0.62
1:B:189:PRO:HB3	1:B:246:GLN:OE1	2.00	0.62
1:E:114:LEU:CD2	2:K:119:GLU:HG3	2.28	0.62
1:A:29:LYS:O	1:A:31:LYS:N	2.33	0.62
1:B:308:LEU:O	1:B:310:LEU:N	2.32	0.62
2:G:12:ILE:HD13	2:G:62:GLU:OE1	2.00	0.62
2:J:30:LEU:HA	2:J:35:LEU:HD12	1.80	0.62
2:K:29:LEU:HD21	2:K:77:TYR:HB2	1.82	0.62
2:L:18:ILE:CG2	2:L:19:ASP:H	2.12	0.62
2:L:83:VAL:CG1	2:L:94:LYS:HB2	2.20	0.62
2:H:116:SER:HA	2:H:121:VAL:HG21	1.82	0.62
2:H:14:ARG:HG3	2:H:65:PHE:CZ	2.34	0.62
1:B:108:GLN:CB	2:H:115:ILE:HG13	2.29	0.62
1:C:257:ALA:CB	1:C:261:MET:HE2	2.25	0.62
2:H:111:ASN:C	2:H:113:ASN:H	2.04	0.62
2:K:16:THR:HG22	2:K:17:VAL:N	2.15	0.62
2:I:100:PRO:O	2:I:127:VAL:HB	1.99	0.61
1:D:227:MET:HE1	1:D:272:GLU:O	2.00	0.61
2:L:86:ILE:HG21	2:L:92:VAL:HA	1.82	0.61
1:C:229:ARG:HB3	3:C:2003:FLC:OA2	2.00	0.61
2:J:104:ASP:O	2:J:105:ASN:HB2	1.99	0.61
2:H:86:ILE:HG22	2:H:90:GLU:C	2.21	0.61
2:I:70:GLN:HB2	6:I:1007:HOH:O	2.00	0.61
1:D:261:MET:HG2	1:D:262:LYS:N	2.15	0.61
1:F:44:ILE:HB	1:F:63:MET:CE	2.29	0.61
1:F:47:CYS:O	1:F:104:MET:HA	2.00	0.61
1:B:162:ASP:HB2	1:B:192:LEU:HD13	1.82	0.61
2:H:12:ILE:HG22	2:H:13:LYS:N	2.15	0.61
2:H:109:CYS:N	2:H:125:PHE:HZ	1.98	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:VAL:HG11	1:E:139:LEU:HD13	1.81	0.61
1:F:214:SER:OG	1:F:217:GLU:HG3	2.00	0.61
1:C:12:ILE:HG13	1:C:171:SER:HB3	1.83	0.61
1:C:265:HIS:ND1	1:C:267:LEU:HD12	2.16	0.61
1:E:105:ARG:HG3	1:E:128:GLY:HA3	1.82	0.61
2:L:58:LEU:O	2:L:59:ILE:HG13	2.00	0.61
1:C:49:PHE:CE2	1:C:81:LEU:HD23	2.36	0.61
1:D:132:ASN:O	1:D:167:ARG:CB	2.48	0.61
1:F:31:LYS:HE2	1:F:294:PHE:CE2	2.35	0.61
2:L:21:ILE:O	2:L:21:ILE:CG1	2.46	0.61
2:L:28:LYS:HE2	2:L:32:LEU:HD11	1.82	0.61
1:A:109:GLU:OE2	1:A:131:SER:HB3	2.00	0.61
1:A:279:LYS:O	1:A:279:LYS:HG2	2.00	0.61
1:B:54:ARG:HD3	1:B:267:LEU:HB3	1.83	0.61
2:G:68:GLU:O	2:G:70:GLN:N	2.34	0.61
2:G:30:LEU:HA	2:G:35:LEU:HD12	1.83	0.61
1:D:167:ARG:HE	3:D:2004:FLC:HA1	1.65	0.61
1:E:77:ALA:O	1:E:83:LYS:HE2	2.01	0.61
1:F:196:GLN:HG3	1:F:200:ASP:OD2	2.01	0.61
2:K:9:VAL:HG11	2:K:58:LEU:HD23	1.83	0.61
1:B:231:GLN:HE22	3:B:2002:FLC:HA1	1.66	0.61
1:C:26:THR:HG23	1:C:309:VAL:CG1	2.31	0.60
1:F:12:ILE:HG13	1:F:171:SER:HB3	1.82	0.60
1:F:110:GLY:HA3	2:L:140:TYR:HB3	1.82	0.60
2:G:111:ASN:HD22	2:G:111:ASN:C	2.02	0.60
1:A:39:LEU:CD1	1:A:304:LEU:HD12	2.29	0.60
3:A:2001:FLC:OG1	4:A:3001:PO4:P	2.60	0.60
1:C:267:LEU:HD13	1:C:285:TYR:HB2	1.84	0.60
2:G:101:GLU:O	2:G:127:VAL:HG23	2.01	0.60
1:A:107:PRO:O	1:A:130:GLY:HA3	2.01	0.60
2:H:15:GLY:HA3	2:H:61:ILE:O	2.02	0.60
2:H:111:ASN:HB2	2:H:145:PHE:HZ	1.66	0.60
2:I:92:VAL:HG12	2:I:93:GLY:H	1.66	0.60
1:E:11:SER:CB	1:E:133:GLN:HG3	2.32	0.60
2:J:102:ARG:HB2	2:J:125:PHE:O	2.01	0.60
1:B:160:VAL:O	1:B:160:VAL:HG12	2.00	0.60
2:J:111:ASN:C	2:J:113:ASN:H	2.05	0.60
1:B:44:ILE:HG21	1:B:63:MET:CE	2.32	0.60
1:B:54:ARG:HD2	4:B:3002:PO4:O3	2.02	0.60
1:E:63:MET:CE	1:E:70:VAL:HG22	2.32	0.60
1:B:159:MET:HE1	1:B:173:THR:OG1	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ASP:HB3	2:H:128:ARG:NH2	2.17	0.60
2:I:13:LYS:HE3	2:I:88:ASN:CG	2.22	0.60
1:D:196:GLN:HG3	1:D:200:ASP:OD2	2.01	0.60
1:F:43:VAL:HG22	1:F:69:SER:HB2	1.83	0.60
1:F:52:SER:HB2	1:F:105:ARG:NH1	2.17	0.60
1:A:101:ALA:HB2	1:A:304:LEU:HD21	1.83	0.59
1:A:111:ALA:HA	2:G:115:ILE:CD1	2.32	0.59
1:C:264:LEU:HB3	1:C:288:GLN:NE2	2.17	0.59
1:D:160:VAL:O	1:D:161:GLY:O	2.20	0.59
1:E:105:ARG:CZ	1:E:167:ARG:NH2	2.65	0.59
2:K:125:PHE:HB3	2:K:136:LEU:HB3	1.83	0.59
2:L:14:ARG:HH11	2:L:65:PHE:HZ	1.48	0.59
1:B:45:ALA:HA	1:B:71:VAL:O	2.02	0.59
1:D:43:VAL:HG22	1:D:69:SER:HB2	1.82	0.59
2:L:12:ILE:HD13	2:L:62:GLU:HA	1.84	0.59
2:G:21:ILE:HB	2:G:57:ASP:HB2	1.84	0.59
2:G:76:LEU:CD1	2:G:103:ILE:HG21	2.24	0.59
1:D:52:SER:OG	1:D:105:ARG:NH1	2.34	0.59
1:F:114:LEU:HD23	2:L:115:ILE:CD1	2.30	0.59
2:H:13:LYS:HD3	2:H:13:LYS:C	2.23	0.59
2:H:27:PHE:CZ	2:K:31:SER:HB2	2.34	0.59
2:L:86:ILE:HG22	2:L:87:ASP:H	1.68	0.59
1:B:308:LEU:O	1:B:310:LEU:HG	2.02	0.59
2:I:71:VAL:O	2:I:74:LEU:HG	2.02	0.59
2:J:141:CYS:O	2:J:143:LYS:N	2.36	0.59
2:L:34:LYS:HB3	2:L:37:GLU:OE1	2.03	0.59
1:A:131:SER:HB2	1:A:234:ARG:HD3	1.84	0.59
2:G:69:ASP:HB3	6:G:1041:HOH:O	2.01	0.59
2:H:30:LEU:CD1	2:H:44:ILE:HD13	2.32	0.59
2:H:136:LEU:O	2:H:144:GLU:HA	2.03	0.59
1:D:31:LYS:HG3	1:D:294:PHE:CE1	2.38	0.59
1:D:81:LEU:HD12	1:D:86:GLU:O	2.02	0.59
2:J:17:VAL:CG1	2:J:86:ILE:HD12	2.32	0.59
2:J:94:LYS:CE	2:J:96:ARG:HG3	2.32	0.59
2:K:102:ARG:HB3	2:K:102:ARG:CZ	2.32	0.59
2:G:16:THR:HG22	2:G:64:THR:O	2.03	0.59
1:E:12:ILE:HG13	1:E:171:SER:HB3	1.85	0.59
1:F:53:THR:N	4:F:3006:PO4:O3	2.33	0.59
2:L:115:ILE:O	2:L:117:HIS:N	2.36	0.59
1:A:267:LEU:O	1:A:267:LEU:HG	2.03	0.59
1:C:226:TYR:OH	1:C:266:PRO:HG3	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LEU:HD12	1:F:94:VAL:CG1	2.33	0.59
2:K:14:ARG:HA	2:K:87:ASP:OD2	2.02	0.59
2:G:49:PRO:HA	2:G:55:ARG:HG2	1.83	0.59
1:E:229:ARG:NH1	1:E:232:LYS:HE2	2.17	0.59
2:J:41:ARG:O	2:J:62:GLU:HB3	2.02	0.59
1:A:79:THR:OG1	1:A:81:LEU:HB3	2.03	0.58
1:E:232:LYS:HA	1:E:235:LEU:HD12	1.85	0.58
2:J:94:LYS:HE2	2:J:96:ARG:HG3	1.85	0.58
2:L:83:VAL:HG22	2:L:95:SER:O	2.03	0.58
1:B:120:GLY:O	1:B:122:VAL:HG23	2.03	0.58
1:C:237:PRO:HA	1:C:240:TYR:CD2	2.38	0.58
1:C:265:HIS:O	1:C:266:PRO:C	2.39	0.58
1:E:140:LEU:HD13	1:E:292:GLY:HA2	1.86	0.58
1:F:217:GLU:HG2	6:F:3047:HOH:O	2.03	0.58
1:D:10:ILE:HD12	1:D:112:ALA:HB1	1.84	0.58
1:A:44:ILE:HG23	1:A:101:ALA:HB3	1.84	0.58
1:B:81:LEU:HD13	1:B:86:GLU:O	2.04	0.58
1:D:84:LYS:NZ	3:E:2005:FLC:OHB	2.36	0.58
1:C:216:GLU:H	1:C:216:GLU:CD	2.06	0.58
1:B:110:GLY:HA3	2:H:140:TYR:HB3	1.86	0.58
1:B:111:ALA:HB2	2:H:115:ILE:CD1	2.34	0.58
1:E:110:GLY:N	1:E:129:ASP:OD1	2.37	0.58
1:E:265:HIS:O	1:E:266:PRO:O	2.22	0.58
1:F:120:GLY:O	1:F:122:VAL:HG23	2.03	0.58
2:J:16:THR:HG23	2:J:64:THR:O	2.03	0.58
2:L:17:VAL:HA	2:L:60:LYS:HE2	1.85	0.58
2:G:26:GLY:O	2:G:30:LEU:HG	2.04	0.58
2:H:49:PRO:HG3	2:H:55:ARG:NH1	2.19	0.58
1:D:2:ASN:HB3	1:D:5:TYR:HB2	1.85	0.58
1:F:267:LEU:N	6:F:3075:HOH:O	2.36	0.58
2:I:146:SER:O	2:I:149:VAL:HG22	2.04	0.58
2:L:137:LYS:HG3	2:L:137:LYS:O	2.03	0.58
1:A:35:GLN:NE2	1:A:309:VAL:HG23	2.19	0.58
2:I:19:ASP:O	2:I:21:ILE:HD12	2.04	0.58
1:D:12:ILE:HG21	1:D:175:ALA:HB2	1.86	0.58
1:E:38:LEU:HD11	1:E:305:ASN:ND2	2.19	0.58
2:J:25:ILE:O	2:J:29:LEU:HG	2.04	0.58
1:A:26:THR:HG23	1:A:309:VAL:CG1	2.34	0.57
1:A:293:ILE:HG22	1:A:297:GLN:OE1	2.04	0.57
1:B:132:ASN:O	1:B:167:ARG:CB	2.52	0.57
2:G:115:ILE:O	2:G:117:HIS:N	2.37	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:86:ILE:HG23	2:I:91:VAL:CA	2.33	0.57
1:D:227:MET:CE	1:D:272:GLU:O	2.51	0.57
1:A:231:GLN:O	1:A:235:LEU:HG	2.05	0.57
1:A:290:GLY:C	1:A:292:GLY:H	2.07	0.57
1:B:81:LEU:CD1	1:B:86:GLU:O	2.52	0.57
1:F:278:ASP:OD1	1:F:278:ASP:N	2.37	0.57
1:A:44:ILE:HB	1:A:63:MET:HE3	1.86	0.57
1:D:189:PRO:HG2	1:D:192:LEU:HB2	1.86	0.57
2:L:113:ASN:O	2:L:113:ASN:OD1	2.21	0.57
1:F:110:GLY:N	1:F:129:ASP:OD1	2.37	0.57
1:F:140:LEU:CD2	1:F:292:GLY:HA2	2.19	0.57
2:K:24:GLN:HA	6:K:1008:HOH:O	2.03	0.57
2:H:106:VAL:HG12	2:H:107:LEU:HD23	1.84	0.57
2:H:138:CYS:HB3	2:H:142:GLU:H	1.69	0.57
1:D:159:MET:HA	1:D:226:TYR:O	2.05	0.57
1:D:229:ARG:NH2	1:F:84:LYS:HD3	2.20	0.57
1:E:88:LEU:H	2:K:119:GLU:CD	2.08	0.57
1:F:166:GLY:O	1:F:169:VAL:HG22	2.04	0.57
1:A:63:MET:HE1	1:A:70:VAL:HG13	1.86	0.57
2:I:19:ASP:HB3	2:I:58:LEU:HD21	1.86	0.57
2:L:18:ILE:CG1	2:L:83:VAL:HB	2.34	0.57
2:L:114:CYS:CB	2:L:141:CYS:SG	2.85	0.57
1:A:29:LYS:O	1:A:30:LEU:C	2.43	0.57
1:B:200:ASP:CB	2:H:128:ARG:HH22	2.16	0.57
2:L:14:ARG:HE	2:L:88:ASN:ND2	2.02	0.57
1:C:35:GLN:NE2	1:C:309:VAL:CG2	2.67	0.57
2:G:18:ILE:HA	2:G:83:VAL:HA	1.86	0.57
2:G:91:VAL:HG22	6:G:1046:HOH:O	2.03	0.57
2:I:55:ARG:NH1	2:L:39:ASP:HB3	2.18	0.57
1:D:75:ASP:OD2	1:D:77:ALA:HB3	2.04	0.57
1:D:132:ASN:CG	1:D:133:GLN:H	2.08	0.57
1:E:306:ARG:NH1	1:E:306:ARG:HB2	2.20	0.57
2:K:138:CYS:HB2	2:K:142:GLU:H	1.69	0.57
2:G:106:VAL:HG23	2:G:107:LEU:CD2	2.35	0.57
2:L:83:VAL:HG13	2:L:95:SER:O	2.05	0.57
1:C:267:LEU:O	1:C:267:LEU:HG	2.04	0.57
1:D:109:GLU:HA	1:D:129:ASP:OD1	2.05	0.57
1:E:80:SER:HB3	1:E:84:LYS:HD2	1.86	0.57
1:E:266:PRO:HB2	3:E:2005:FLL:HA2	1.86	0.57
1:D:134:HIS:NE2	3:D:2004:FLL:OB1	2.38	0.56
1:F:63:MET:HE1	1:F:70:VAL:HG13	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ILE:HG21	1:B:299:LEU:HD21	1.88	0.56
2:G:109:CYS:SG	2:G:111:ASN:HB3	2.45	0.56
2:J:103:ILE:HD11	2:J:107:LEU:CG	2.35	0.56
2:L:13:LYS:O	2:L:14:ARG:HB2	2.04	0.56
1:B:117:GLU:OE1	2:H:139:LYS:NZ	2.36	0.56
1:B:261:MET:HG2	1:B:262:LYS:H	1.70	0.56
1:C:54:ARG:NH1	1:C:267:LEU:HB3	2.20	0.56
2:H:86:ILE:HG22	2:H:90:GLU:O	2.04	0.56
2:H:131:ALA:O	2:H:132:ASN:HB3	2.04	0.56
1:D:88:LEU:HD23	1:D:114:LEU:HD23	1.87	0.56
1:D:94:VAL:HG21	1:E:54:ARG:HH11	1.71	0.56
1:B:19:ASP:O	1:B:22:LEU:HB3	2.05	0.56
1:B:198:ILE:O	1:B:202:LEU:HG	2.05	0.56
1:A:126:ASN:HD21	1:A:129:ASP:HB2	1.69	0.56
1:D:230:VAL:O	1:D:232:LYS:N	2.38	0.56
1:A:110:GLY:N	1:A:129:ASP:OD1	2.33	0.56
1:C:106:HIS:ND1	1:C:107:PRO:CD	2.69	0.56
1:C:131:SER:HB3	1:C:234:ARG:HD3	1.87	0.56
2:K:8:GLN:O	2:K:9:VAL:HG13	2.05	0.56
2:L:130:ARG:HG2	2:L:130:ARG:HH11	1.71	0.56
1:C:188:ALA:HA	1:C:247:PHE:CE2	2.39	0.56
2:G:110:PRO:HD2	2:G:145:PHE:CD2	2.41	0.56
1:E:106:HIS:ND1	1:E:107:PRO:HD2	2.20	0.56
1:B:239:GLU:C	1:B:241:ALA:N	2.54	0.56
2:G:103:ILE:HD11	2:G:136:LEU:HD13	1.87	0.56
1:D:105:ARG:NE	1:D:167:ARG:HH22	2.04	0.56
2:H:139:LYS:O	2:H:139:LYS:HG2	2.05	0.56
1:D:109:GLU:HG3	1:D:130:GLY:O	2.06	0.56
1:E:29:LYS:HD3	1:E:310:LEU:O	2.06	0.56
1:A:219:MET:HE1	1:A:254:LEU:HD23	1.87	0.55
1:C:59:PHE:CE1	1:C:136:THR:HG21	2.39	0.55
1:C:174:GLN:HA	1:C:201:MET:HE1	1.87	0.55
2:I:50:SER:HB3	2:I:56:LYS:HE2	1.86	0.55
2:I:111:ASN:O	2:I:117:HIS:CD2	2.59	0.55
1:D:167:ARG:HH21	3:D:2004:FLC:CBC	2.18	0.55
1:E:26:THR:HG23	1:E:309:VAL:HG11	1.89	0.55
2:K:78:ALA:C	2:K:80:GLN:H	2.09	0.55
2:K:138:CYS:HB2	2:K:142:GLU:N	2.20	0.55
2:H:30:LEU:HD21	2:H:59:ILE:HG23	1.86	0.55
2:H:46:LEU:HB2	2:K:42:ILE:HB	1.87	0.55
1:E:17:ARG:HD2	1:E:179:PHE:CE1	2.40	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:GLN:HE22	1:E:309:VAL:HG23	1.70	0.55
1:F:174:GLN:HA	1:F:201:MET:HE3	1.87	0.55
1:A:219:MET:HE3	1:A:254:LEU:HD23	1.87	0.55
3:A:2001:FLC:OG1	4:A:3001:PO4:O4	2.24	0.55
1:C:131:SER:CB	1:C:234:ARG:HD3	2.36	0.55
2:L:75:ALA:CB	2:L:98:SER:O	2.54	0.55
1:A:11:SER:HB3	1:A:14:ASP:OD2	2.06	0.55
1:B:101:ALA:HB2	1:B:304:LEU:HD21	1.89	0.55
1:C:188:ALA:HB1	1:C:189:PRO:HD2	1.88	0.55
1:C:264:LEU:HB3	1:C:288:GLN:HE22	1.72	0.55
2:I:20:HIS:HA	2:I:56:LYS:HD2	1.88	0.55
1:D:63:MET:HG3	1:D:300:LEU:HD11	1.87	0.55
1:B:116:THR:HG22	1:B:124:VAL:HB	1.88	0.55
1:D:120:GLY:C	1:D:122:VAL:H	2.09	0.55
2:L:14:ARG:CD	2:L:65:PHE:CZ	2.86	0.55
1:C:129:ASP:O	1:C:130:GLY:C	2.42	0.55
2:H:115:ILE:HG22	2:H:115:ILE:O	2.06	0.55
2:I:42:ILE:HG13	2:I:42:ILE:O	2.05	0.55
2:I:44:ILE:HB	2:L:44:ILE:CB	2.37	0.55
1:D:55:THR:O	1:D:59:PHE:HB2	2.07	0.55
1:D:63:MET:HE2	1:D:70:VAL:CG2	2.37	0.55
2:K:107:LEU:HD13	2:K:150:VAL:HG11	1.87	0.55
2:G:48:LEU:CD2	2:J:41:ARG:HD2	2.33	0.55
2:J:47:ASN:HB3	2:J:55:ARG:CD	2.37	0.55
2:L:43:THR:O	2:L:59:ILE:HG12	2.06	0.55
1:A:166:GLY:O	1:A:169:VAL:HG22	2.06	0.55
1:C:234:ARG:HG2	1:C:234:ARG:HH11	1.72	0.55
1:C:267:LEU:O	1:C:269:ARG:N	2.40	0.55
1:E:237:PRO:HA	1:E:240:TYR:CD2	2.42	0.55
1:B:264:LEU:HB3	1:B:288:GLN:NE2	2.22	0.55
1:F:11:SER:HB3	1:F:14:ASP:OD2	2.07	0.55
1:F:77:ALA:O	1:F:83:LYS:HE2	2.06	0.55
1:F:137:GLN:HG2	1:F:168:THR:HG22	1.88	0.55
2:J:104:ASP:HB2	2:J:123:SER:C	2.27	0.55
2:G:71:VAL:CG1	2:G:72:ASP:N	2.70	0.55
2:G:102:ARG:HD3	6:G:1003:HOH:O	2.06	0.55
2:K:111:ASN:ND2	2:K:143:LYS:HE2	2.22	0.55
1:B:50:GLU:HB3	1:B:105:ARG:HG2	1.89	0.54
1:C:170:HIS:O	1:C:174:GLN:HG3	2.06	0.54
1:B:265:HIS:C	1:B:266:PRO:O	2.38	0.54
1:C:140:LEU:HD22	1:C:292:GLY:CA	2.21	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:100:PRO:O	2:G:127:VAL:HB	2.07	0.54
2:H:102:ARG:HB3	2:H:126:ALA:HA	1.89	0.54
2:J:115:ILE:HD11	2:J:119:GLU:HG3	1.88	0.54
2:K:25:ILE:HG22	2:K:29:LEU:HG	1.89	0.54
1:C:299:LEU:O	1:C:303:VAL:HG23	2.08	0.54
2:I:38:THR:HG22	2:I:40:GLN:CB	2.36	0.54
1:D:17:ARG:HG2	1:D:17:ARG:HH11	1.72	0.54
1:D:45:ALA:HA	1:D:71:VAL:O	2.07	0.54
1:D:134:HIS:CE1	1:D:137:GLN:HB2	2.42	0.54
1:E:267:LEU:O	1:E:268:PRO:C	2.42	0.54
2:L:12:ILE:HD13	2:L:62:GLU:HB2	1.87	0.54
2:L:16:THR:O	2:L:60:LYS:HD3	2.07	0.54
2:L:99:LEU:HG	2:L:127:VAL:HG11	1.87	0.54
1:B:114:LEU:HD13	2:H:121:VAL:HG12	1.89	0.54
2:G:68:GLU:C	2:G:70:GLN:N	2.61	0.54
2:I:44:ILE:HB	2:L:44:ILE:HB	1.89	0.54
1:D:168:THR:HG21	1:D:266:PRO:HG2	1.89	0.54
1:E:105:ARG:NH2	1:E:167:ARG:HH21	2.04	0.54
1:F:285:TYR:O	1:F:288:GLN:HG2	2.07	0.54
2:J:67:SER:H	2:J:70:GLN:NE2	2.03	0.54
1:B:161:GLY:CA	1:B:228:THR:OG1	2.52	0.54
1:C:109:GLU:O	2:I:115:ILE:HB	2.07	0.54
1:C:114:LEU:CD1	2:I:121:VAL:HG11	2.37	0.54
2:I:18:ILE:HG22	2:I:21:ILE:HD11	1.89	0.54
1:D:26:THR:HG23	1:D:309:VAL:CG1	2.37	0.54
1:D:29:LYS:HD3	1:D:310:LEU:O	2.08	0.54
1:D:267:LEU:HD21	1:D:285:TYR:CB	2.37	0.54
2:L:20:HIS:HE1	2:L:84:ASN:HD21	1.55	0.54
1:D:199:LEU:HD22	1:D:209:TRP:CZ3	2.43	0.54
1:F:44:ILE:HB	1:F:63:MET:HE3	1.90	0.54
1:B:137:GLN:HG2	1:B:168:THR:HG22	1.89	0.54
2:H:76:LEU:HD12	2:H:103:ILE:HD11	1.89	0.54
1:F:138:THR:O	1:F:142:LEU:HG	2.07	0.54
1:F:225:LEU:CD2	1:F:227:MET:CE	2.86	0.54
2:L:146:SER:OG	2:L:149:VAL:HG23	2.08	0.54
1:C:265:HIS:ND1	1:C:266:PRO:O	2.41	0.54
2:G:68:GLU:C	2:G:70:GLN:H	2.11	0.54
2:H:111:ASN:O	2:H:113:ASN:N	2.38	0.54
2:L:41:ARG:C	2:L:42:ILE:HG12	2.28	0.54
2:G:46:LEU:HD13	2:J:36:THR:HG23	1.90	0.54
2:G:106:VAL:HG23	2:G:107:LEU:HD23	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:27:PHE:CB	2:L:36:THR:HG21	2.38	0.54
1:A:12:ILE:HG13	1:A:171:SER:HB3	1.90	0.54
1:B:108:GLN:HB2	2:H:115:ILE:CG1	2.33	0.54
1:C:204:GLU:HG2	1:C:205:LYS:N	2.22	0.54
2:G:14:ARG:HA	2:G:86:ILE:O	2.08	0.54
2:I:44:ILE:HB	2:L:44:ILE:HG22	1.90	0.54
1:D:83:LYS:HG3	1:E:51:ALA:HB2	1.89	0.54
1:E:140:LEU:HD13	1:E:292:GLY:CA	2.38	0.54
2:K:9:VAL:HG11	2:K:58:LEU:CD2	2.38	0.54
2:L:83:VAL:HG12	2:L:84:ASN:H	1.71	0.54
2:L:91:VAL:HG12	2:L:92:VAL:N	2.22	0.54
1:B:10:ILE:HD12	1:B:112:ALA:HB1	1.89	0.53
1:C:49:PHE:CZ	1:C:73:PHE:HZ	2.25	0.53
1:D:110:GLY:O	2:J:115:ILE:HG21	2.08	0.53
1:E:140:LEU:HD11	1:E:288:GLN:O	2.08	0.53
2:L:86:ILE:CG2	2:L:87:ASP:N	2.71	0.53
2:L:150:VAL:O	2:L:150:VAL:HG12	2.08	0.53
1:B:58:SER:HB3	1:C:98:TYR:CE1	2.44	0.53
1:D:77:ALA:O	1:D:83:LYS:HE2	2.08	0.53
1:F:301:ALA:O	1:F:305:ASN:HB2	2.09	0.53
2:K:17:VAL:HG21	2:K:86:ILE:CD1	2.37	0.53
2:K:41:ARG:HD3	2:K:62:GLU:OE2	2.08	0.53
1:B:198:ILE:O	1:B:201:MET:HG2	2.09	0.53
1:E:59:PHE:CD1	1:E:296:ARG:HD3	2.43	0.53
2:K:104:ASP:O	2:K:106:VAL:HG23	2.08	0.53
1:A:162:ASP:C	1:A:162:ASP:OD1	2.46	0.53
1:D:63:MET:CE	1:D:70:VAL:HG22	2.38	0.53
1:D:161:GLY:HA3	1:D:228:THR:O	2.08	0.53
1:E:216:GLU:HG3	1:E:219:MET:CB	2.38	0.53
1:F:198:ILE:O	1:F:202:LEU:HG	2.07	0.53
1:F:267:LEU:O	1:F:269:ARG:N	2.40	0.53
1:A:229:ARG:HD3	3:A:2001:FLL:OA1	2.09	0.53
2:G:119:GLU:HB3	2:G:120:PRO:CD	2.38	0.53
2:H:30:LEU:HD11	2:H:44:ILE:HD13	1.90	0.53
2:I:12:ILE:HD13	2:I:61:ILE:N	2.24	0.53
1:D:35:GLN:HE22	1:D:309:VAL:HG23	1.72	0.53
1:C:137:GLN:HG2	1:C:168:THR:CG2	2.39	0.53
1:D:267:LEU:O	1:D:269:ARG:N	2.41	0.53
1:B:44:ILE:CG2	1:B:63:MET:HE1	2.38	0.53
2:H:12:ILE:CG2	2:H:13:LYS:N	2.71	0.53
2:J:40:GLN:HG2	2:J:63:ASN:HB3	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:111:ASN:HD22	2:J:114:CYS:N	2.07	0.53
2:L:86:ILE:CG2	2:L:93:GLY:H	2.21	0.53
1:A:117:GLU:OE1	2:G:139:LYS:HE2	2.08	0.53
1:A:250:ARG:HG2	1:A:250:ARG:HH11	1.73	0.53
2:I:22:PRO:HB2	2:I:25:ILE:HG13	1.89	0.53
1:F:160:VAL:HG22	1:F:187:ILE:HB	1.91	0.53
2:J:114:CYS:O	2:J:116:SER:N	2.42	0.53
2:L:83:VAL:CG1	2:L:84:ASN:N	2.71	0.53
1:B:126:ASN:ND2	1:B:129:ASP:HB2	2.24	0.53
2:I:43:THR:HB	2:I:60:LYS:HB2	1.90	0.53
1:E:63:MET:HE1	1:E:70:VAL:HG13	1.90	0.53
1:F:23:VAL:HA	1:F:302:LEU:HD11	1.91	0.53
1:F:174:GLN:HG2	1:F:201:MET:HE1	1.91	0.53
1:B:44:ILE:HG21	1:B:63:MET:HE1	1.91	0.53
2:I:28:LYS:HE3	2:I:77:TYR:CE2	2.44	0.53
2:I:38:THR:HG22	2:I:40:GLN:HB3	1.90	0.53
2:K:43:THR:HB	2:K:60:LYS:HG2	1.91	0.53
2:L:18:ILE:HD12	2:L:94:LYS:HE3	1.91	0.53
1:B:104:MET:HE1	1:B:115:ALA:HB3	1.91	0.52
1:C:247:PHE:HB2	6:C:3043:HOH:O	2.08	0.52
1:C:267:LEU:O	1:C:268:PRO:C	2.44	0.52
1:C:290:GLY:C	1:C:292:GLY:N	2.62	0.52
2:G:103:ILE:HG13	2:G:103:ILE:O	2.10	0.52
2:H:17:VAL:HG23	2:H:86:ILE:HD11	1.89	0.52
2:I:111:ASN:HB3	2:I:114:CYS:HB2	1.91	0.52
1:E:160:VAL:HG13	1:E:187:ILE:HB	1.91	0.52
2:K:78:ALA:O	2:K:80:GLN:N	2.38	0.52
2:K:86:ILE:C	2:K:87:ASP:OD1	2.48	0.52
1:A:44:ILE:HB	1:A:63:MET:HE2	1.90	0.52
1:A:187:ILE:O	1:A:188:ALA:HB2	2.10	0.52
2:I:12:ILE:CD1	2:I:61:ILE:H	2.22	0.52
2:I:88:ASN:C	2:I:90:GLU:N	2.61	0.52
1:D:52:SER:HA	4:D:3004:PO4:O1	2.08	0.52
2:K:38:THR:HG22	2:K:39:ASP:N	2.24	0.52
2:L:104:ASP:O	2:L:106:VAL:HG23	2.09	0.52
1:A:131:SER:O	1:A:131:SER:OG	2.28	0.52
1:B:55:THR:O	1:B:59:PHE:HB2	2.10	0.52
1:B:141:ASP:O	1:B:145:ILE:HG13	2.09	0.52
1:B:188:ALA:HB1	1:B:189:PRO:HD2	1.92	0.52
1:B:265:HIS:O	1:B:266:PRO:C	2.42	0.52
1:B:295:ALA:O	1:B:298:ALA:HB3	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:VAL:O	1:C:232:LYS:N	2.38	0.52
1:D:49:PHE:HB2	1:D:107:PRO:HD3	1.91	0.52
2:J:105:ASN:N	2:J:123:SER:HB3	2.16	0.52
1:A:53:THR:CG2	1:A:54:ARG:N	2.72	0.52
1:A:189:PRO:HB3	1:A:246:GLN:NE2	2.24	0.52
2:G:9:VAL:HG12	2:G:10:GLU:H	1.75	0.52
2:G:28:LYS:HZ3	2:G:77:TYR:HE2	1.57	0.52
1:C:50:GLU:HB2	1:C:107:PRO:HG3	1.91	0.52
1:C:87:THR:HB	2:I:119:GLU:OE2	2.10	0.52
2:H:25:ILE:O	2:H:28:LYS:HB3	2.10	0.52
1:F:104:MET:HE1	1:F:112:ALA:HA	1.91	0.52
2:J:51:GLY:O	2:J:53:MET:N	2.41	0.52
2:L:16:THR:CG2	2:L:84:ASN:HA	2.38	0.52
2:L:67:SER:C	2:L:69:ASP:H	2.12	0.52
1:C:290:GLY:C	1:C:292:GLY:H	2.12	0.52
2:I:37:GLU:HG2	2:I:37:GLU:O	2.09	0.52
1:F:234:ARG:HH11	1:F:234:ARG:HG2	1.74	0.52
2:L:77:TYR:O	2:L:78:ALA:HB2	2.10	0.52
1:A:65:ARG:NH1	1:B:43:VAL:HG23	2.25	0.52
1:B:8:HIS:O	1:B:9:ILE:HD13	2.09	0.52
1:D:54:ARG:HH11	1:F:94:VAL:HG11	1.75	0.52
1:A:106:HIS:ND1	1:A:107:PRO:HD2	2.25	0.52
1:A:218:VAL:O	1:A:222:VAL:HG13	2.10	0.52
1:D:94:VAL:HG13	1:E:267:LEU:HD22	1.88	0.52
1:E:63:MET:HG3	1:E:300:LEU:CD1	2.40	0.52
1:E:202:LEU:HB3	1:E:207:ILE:HB	1.92	0.52
2:L:90:GLU:HG3	2:L:90:GLU:O	2.10	0.52
1:B:54:ARG:HD3	1:B:267:LEU:HB2	1.91	0.52
1:E:130:GLY:O	1:E:131:SER:HB3	2.10	0.52
1:C:136:THR:HB	1:C:296:ARG:HE	1.74	0.51
1:C:160:VAL:HB	1:C:227:MET:CG	2.38	0.51
2:G:1:MET:HG2	2:G:89:TYR:HB3	1.91	0.51
2:G:101:GLU:O	2:G:127:VAL:N	2.37	0.51
2:G:152:ALA:O	2:G:153:ASN:OXT	2.28	0.51
2:H:33:PHE:O	2:H:34:LYS:C	2.49	0.51
2:H:146:SER:C	2:H:148:ASN:H	2.12	0.51
1:D:31:LYS:HE2	1:D:294:PHE:CE2	2.45	0.51
1:C:126:ASN:HD21	1:C:129:ASP:HB2	1.76	0.51
2:H:19:ASP:OD1	2:H:20:HIS:N	2.43	0.51
2:H:45:GLY:O	2:H:46:LEU:HD23	2.10	0.51
2:H:107:LEU:O	2:H:108:VAL:HG13	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:108:VAL:CG2	2:H:153:ASN:HB3	2.41	0.51
2:L:16:THR:HA	2:L:86:ILE:CG1	2.37	0.51
2:L:111:ASN:HB3	2:L:114:CYS:CB	2.40	0.51
2:H:9:VAL:O	2:H:10:GLU:HG3	2.11	0.51
2:I:92:VAL:O	2:I:93:GLY:O	2.28	0.51
1:D:117:GLU:OE1	2:J:139:LYS:HE2	2.10	0.51
1:E:132:ASN:O	1:E:167:ARG:CB	2.57	0.51
1:F:183:ARG:NH1	1:F:185:TYR:HE1	2.08	0.51
1:B:140:LEU:CD2	1:B:292:GLY:HA2	2.38	0.51
1:C:44:ILE:HG21	1:C:63:MET:HE2	1.92	0.51
1:C:199:LEU:HD13	1:C:209:TRP:CH2	2.44	0.51
2:I:111:ASN:O	2:I:117:HIS:HD2	1.94	0.51
1:E:63:MET:HG3	1:E:300:LEU:HD11	1.92	0.51
2:L:20:HIS:HA	2:L:82:THR:OG1	2.11	0.51
1:A:120:GLY:O	1:A:121:ASN:HB2	2.10	0.51
1:B:214:SER:HG	1:B:217:GLU:HG3	1.76	0.51
1:B:286:PHE:CE1	1:C:93:SER:HB2	2.45	0.51
1:B:309:VAL:O	1:B:309:VAL:HG22	2.09	0.51
2:G:17:VAL:CG2	2:G:60:LYS:HE3	2.36	0.51
2:G:147:HIS:O	2:G:150:VAL:HG22	2.10	0.51
2:I:130:ARG:HD3	2:I:133:ASP:HB3	1.92	0.51
1:D:114:LEU:HD12	2:J:121:VAL:HG11	1.93	0.51
2:G:66:LEU:HB3	2:G:70:GLN:NE2	2.25	0.51
2:G:131:ALA:O	2:G:132:ASN:CB	2.59	0.51
2:H:108:VAL:HG21	2:H:153:ASN:HB3	1.91	0.51
2:I:7:LEU:HD13	2:I:50:SER:HA	1.92	0.51
1:F:195:PRO:O	1:F:199:LEU:HG	2.10	0.51
2:L:16:THR:HG23	2:L:84:ASN:C	2.31	0.51
1:A:241:ALA:HB2	1:E:241:ALA:CB	2.40	0.51
1:B:129:ASP:O	1:B:130:GLY:C	2.48	0.51
1:C:105:ARG:HB2	1:C:127:ALA:HB3	1.92	0.51
2:I:130:ARG:HG3	2:I:131:ALA:N	2.26	0.51
1:E:222:VAL:HG23	1:E:261:MET:SD	2.51	0.51
1:F:129:ASP:O	1:F:130:GLY:C	2.49	0.51
2:K:146:SER:O	2:K:150:VAL:HG23	2.11	0.51
2:L:91:VAL:CG1	2:L:92:VAL:N	2.73	0.51
1:A:132:ASN:O	1:A:133:GLN:O	2.28	0.51
1:C:47:CYS:O	1:C:104:MET:HA	2.09	0.51
1:C:134:HIS:CE1	1:C:137:GLN:HB2	2.46	0.51
1:C:162:ASP:C	1:C:162:ASP:OD1	2.49	0.51
1:F:35:GLN:NE2	1:F:309:VAL:HG23	2.23	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:ARG:HH22	1:F:210:SER:HB3	1.76	0.51
2:J:47:ASN:HB3	2:J:55:ARG:HD2	1.93	0.51
2:L:111:ASN:HB3	2:L:114:CYS:HB2	1.92	0.51
1:A:51:ALA:HB2	1:B:83:LYS:HG3	1.92	0.51
1:A:237:PRO:HA	1:A:240:TYR:CD2	2.46	0.51
2:G:125:PHE:HA	2:G:137:LYS:O	2.10	0.51
2:J:135:ALA:O	2:J:136:LEU:HD23	2.11	0.51
2:L:55:ARG:HG2	2:L:56:LYS:N	2.25	0.51
1:E:17:ARG:HG2	1:E:17:ARG:HH11	1.75	0.51
2:J:17:VAL:CG2	2:J:84:ASN:HB2	2.41	0.51
2:J:75:ALA:HB2	2:J:97:PRO:HB3	1.92	0.51
2:J:109:CYS:CA	2:J:125:PHE:HZ	2.24	0.51
2:L:20:HIS:HE1	2:L:84:ASN:ND2	2.09	0.51
2:G:83:VAL:HG12	2:G:95:SER:O	2.11	0.50
1:E:243:VAL:CG1	1:E:244:LYS:HD2	2.33	0.50
1:F:160:VAL:HG12	1:F:161:GLY:N	2.26	0.50
2:J:14:ARG:O	2:J:14:ARG:CG	2.57	0.50
2:K:1:MET:HB2	2:K:11:ALA:CB	2.42	0.50
2:K:16:THR:HG22	2:K:17:VAL:H	1.74	0.50
1:C:157:VAL:HG13	1:C:224:ILE:HB	1.94	0.50
2:H:6:LYS:HE3	2:K:10:GLU:OE2	2.09	0.50
1:D:17:ARG:HG2	1:D:17:ARG:NH1	2.26	0.50
1:D:54:ARG:CD	1:D:267:LEU:HB2	2.34	0.50
1:E:137:GLN:NE2	1:E:140:LEU:HD23	2.26	0.50
2:L:12:ILE:HD13	2:L:62:GLU:CB	2.41	0.50
2:L:18:ILE:HD11	2:L:94:LYS:HB3	1.93	0.50
1:A:49:PHE:HE2	1:A:81:LEU:HD22	1.77	0.50
1:A:267:LEU:HD21	1:A:286:PHE:CE1	2.46	0.50
1:C:81:LEU:HD12	1:C:81:LEU:O	2.11	0.50
2:G:66:LEU:HD13	2:G:70:GLN:OE1	2.11	0.50
2:G:147:HIS:ND1	2:G:148:ASN:N	2.60	0.50
2:H:21:ILE:CG2	2:H:25:ILE:HG22	2.41	0.50
2:H:72:ASP:HB3	2:H:100:PRO:HG3	1.93	0.50
1:E:129:ASP:HB3	1:E:132:ASN:HB3	1.94	0.50
2:J:7:LEU:O	2:J:8:GLN:HB2	2.11	0.50
1:A:241:ALA:HB2	1:E:241:ALA:HB2	1.92	0.50
1:C:17:ARG:O	1:C:17:ARG:HG3	2.11	0.50
2:H:14:ARG:HA	2:H:86:ILE:O	2.11	0.50
1:A:268:PRO:HD3	3:A:2001:FLC:HG2	1.93	0.50
1:B:32:ALA:C	1:B:34:PRO:HD3	2.31	0.50
1:C:165:TYR:O	1:C:231:GLN:HG3	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:ALA:HB1	1:C:261:MET:SD	2.51	0.50
2:L:78:ALA:CB	2:L:81:ALA:HB2	2.35	0.50
2:H:105:ASN:OD1	2:H:122:SER:HB3	2.12	0.50
1:E:26:THR:HG23	1:E:309:VAL:CG1	2.41	0.50
1:B:77:ALA:O	1:B:83:LYS:HE2	2.11	0.50
2:G:8:GLN:HE21	2:J:10:GLU:HA	1.76	0.50
2:G:46:LEU:HD13	2:J:36:THR:CG2	2.42	0.50
2:G:50:SER:O	2:G:54:GLY:O	2.30	0.50
1:F:225:LEU:CD2	1:F:227:MET:HE2	2.41	0.50
2:K:77:TYR:C	2:K:79:PRO:HD3	2.32	0.50
2:L:21:ILE:HG21	2:L:56:LYS:CE	2.42	0.50
1:A:265:HIS:HD2	1:A:267:LEU:HD12	1.77	0.50
1:B:196:GLN:O	1:B:199:LEU:N	2.45	0.50
1:C:187:ILE:O	1:C:188:ALA:HB2	2.12	0.50
2:G:76:LEU:HD13	2:G:103:ILE:HD13	1.93	0.50
1:D:132:ASN:CG	1:D:133:GLN:N	2.64	0.50
2:L:5:ASN:C	2:L:6:LYS:HG3	2.33	0.50
2:L:70:GLN:HA	2:L:73:GLN:HE21	1.71	0.50
1:A:265:HIS:O	1:A:266:PRO:C	2.49	0.50
2:G:48:LEU:HB2	2:G:56:LYS:O	2.10	0.50
2:G:110:PRO:HD2	2:G:145:PHE:CE2	2.46	0.50
2:H:50:SER:HB2	2:H:56:LYS:CG	2.42	0.50
2:H:77:TYR:C	2:H:79:PRO:HD3	2.32	0.50
2:H:135:ALA:O	2:H:136:LEU:HD23	2.12	0.50
1:E:87:THR:HB	2:K:119:GLU:OE1	2.11	0.50
1:F:22:LEU:O	1:F:25:ALA:HB3	2.10	0.50
1:F:233:GLU:HG3	1:F:234:ARG:HG3	1.92	0.50
2:J:45:GLY:O	2:J:46:LEU:HD23	2.11	0.50
2:G:49:PRO:CD	2:J:41:ARG:HD3	2.42	0.49
1:E:132:ASN:CG	1:E:133:GLN:H	2.15	0.49
1:A:268:PRO:CD	3:A:2001:FLC:HG2	2.42	0.49
2:H:50:SER:HB2	2:H:56:LYS:HG2	1.93	0.49
2:I:30:LEU:HD21	2:I:59:ILE:CG2	2.41	0.49
1:D:44:ILE:HB	1:D:63:MET:CE	2.42	0.49
1:D:120:GLY:C	1:D:122:VAL:N	2.65	0.49
2:L:21:ILE:CG2	2:L:56:LYS:CD	2.79	0.49
2:L:115:ILE:C	2:L:117:HIS:N	2.65	0.49
1:A:159:MET:HE2	1:A:169:VAL:HG12	1.94	0.49
1:B:229:ARG:HG2	1:B:230:VAL:O	2.12	0.49
2:J:51:GLY:C	2:J:53:MET:N	2.66	0.49
2:L:72:ASP:CB	2:L:100:PRO:HG2	2.23	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:VAL:HG11	1:A:139:LEU:HD13	1.94	0.49
2:I:67:SER:O	2:I:71:VAL:HG13	2.13	0.49
2:I:91:VAL:HB	6:I:1041:HOH:O	2.12	0.49
1:D:104:MET:HE1	1:D:112:ALA:HA	1.93	0.49
1:E:59:PHE:O	1:E:62:SER:HB2	2.12	0.49
1:E:116:THR:HG22	1:E:124:VAL:HB	1.93	0.49
2:J:66:LEU:HA	2:J:70:GLN:NE2	2.27	0.49
2:J:111:ASN:C	2:J:113:ASN:N	2.66	0.49
2:L:21:ILE:HG22	2:L:56:LYS:HB3	1.94	0.49
2:J:16:THR:CG2	2:J:65:PHE:HA	2.43	0.49
2:K:69:ASP:HA	2:K:72:ASP:HB2	1.95	0.49
2:K:76:LEU:CD2	2:K:134:ILE:HD11	2.42	0.49
1:B:237:PRO:HA	1:B:240:TYR:CE1	2.46	0.49
2:H:21:ILE:HB	2:H:57:ASP:HB2	1.95	0.49
1:D:114:LEU:CD1	2:J:121:VAL:HG11	2.42	0.49
1:D:245:ALA:HB3	1:D:271:ASP:OD1	2.12	0.49
1:E:35:GLN:N	1:E:36:PRO:HD3	2.27	0.49
1:F:49:PHE:CE2	1:F:81:LEU:HD22	2.47	0.49
2:J:121:VAL:HG23	2:J:121:VAL:O	2.11	0.49
2:K:12:ILE:CD1	2:K:60:LYS:HB2	2.39	0.49
2:L:18:ILE:HG13	2:L:83:VAL:CB	2.42	0.49
1:B:201:MET:CG	1:B:202:LEU:N	2.76	0.49
2:H:71:VAL:HG13	2:H:97:PRO:HG3	1.95	0.49
2:I:124:SER:C	2:I:125:PHE:CD1	2.86	0.49
1:D:266:PRO:O	1:D:268:PRO:HD2	2.13	0.49
1:E:159:MET:HB3	1:E:226:TYR:HB3	1.94	0.49
1:A:39:LEU:HD13	1:A:304:LEU:CD1	2.39	0.49
1:A:148:THR:HG21	1:A:262:LYS:HG3	1.94	0.49
1:A:161:GLY:HA3	1:A:228:THR:OG1	2.13	0.49
2:H:6:LYS:HG2	2:H:6:LYS:O	2.11	0.49
1:D:35:GLN:N	1:D:36:PRO:HD3	2.28	0.49
1:E:38:LEU:CD1	1:E:305:ASN:ND2	2.76	0.49
1:F:94:VAL:CG2	1:F:95:ILE:N	2.75	0.49
2:L:86:ILE:CG2	2:L:87:ASP:H	2.25	0.49
1:A:38:LEU:HD11	1:A:305:ASN:ND2	2.27	0.49
1:B:52:SER:HB2	1:B:105:ARG:NH1	2.28	0.49
2:H:114:CYS:C	2:H:116:SER:N	2.66	0.49
2:H:149:VAL:CG1	6:H:1039:HOH:O	2.61	0.49
1:E:236:ASP:OD1	1:E:237:PRO:HD2	2.13	0.49
1:F:183:ARG:HG2	1:F:208:ALA:HB3	1.95	0.49
1:F:258:LYS:HE2	1:F:260:ASN:OD1	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:43:THR:O	2:K:60:LYS:HG2	2.12	0.49
2:L:20:HIS:N	2:L:82:THR:HG21	2.28	0.49
2:I:55:ARG:NH1	2:L:39:ASP:CB	2.75	0.49
1:D:159:MET:HE2	1:D:169:VAL:HG12	1.94	0.49
1:D:240:TYR:HB3	6:D:3030:HOH:O	2.13	0.49
2:J:53:MET:CG	2:J:54:GLY:N	2.74	0.49
1:B:49:PHE:HE2	1:B:81:LEU:HD23	1.76	0.48
1:B:146:GLN:O	1:B:146:GLN:HG2	2.13	0.48
2:G:47:ASN:O	2:G:49:PRO:HD3	2.13	0.48
2:H:35:LEU:C	2:H:37:GLU:H	2.16	0.48
2:I:24:GLN:OE1	2:L:36:THR:HG22	2.13	0.48
1:D:58:SER:HB3	1:F:98:TYR:CZ	2.48	0.48
1:E:12:ILE:CG1	1:E:171:SER:HB3	2.42	0.48
1:E:17:ARG:HG2	1:E:17:ARG:NH1	2.27	0.48
1:E:49:PHE:CE2	1:E:81:LEU:HD22	2.46	0.48
2:G:83:VAL:HG22	2:G:84:ASN:N	2.21	0.48
2:G:130:ARG:HD2	2:G:133:ASP:OD2	2.13	0.48
2:H:40:GLN:OE1	2:H:63:ASN:HB2	2.12	0.48
1:D:2:ASN:HD21	1:D:302:LEU:HB3	1.78	0.48
1:E:81:LEU:HG	1:E:81:LEU:O	2.11	0.48
1:F:35:GLN:N	1:F:36:PRO:HD3	2.27	0.48
2:G:45:GLY:O	2:G:57:ASP:HA	2.13	0.48
2:G:68:GLU:O	2:G:71:VAL:N	2.47	0.48
1:D:117:GLU:OE1	2:J:139:LYS:CE	2.60	0.48
1:D:192:LEU:HD21	1:D:235:LEU:HD21	1.95	0.48
1:D:269:ARG:HH11	1:D:273:ILE:HG22	1.78	0.48
1:F:140:LEU:HD11	1:F:296:ARG:NH1	2.27	0.48
1:A:59:PHE:CE2	1:A:103:VAL:HG21	2.48	0.48
2:G:111:ASN:HD21	2:G:113:ASN:CB	2.26	0.48
2:G:132:ASN:O	2:G:133:ASP:HB3	2.12	0.48
1:E:15:LEU:O	1:E:178:LYS:HE3	2.12	0.48
1:F:279:LYS:HG2	1:F:279:LYS:O	2.13	0.48
2:J:25:ILE:HD13	2:J:77:TYR:HB3	1.95	0.48
2:J:123:SER:O	2:J:124:SER:HB2	2.14	0.48
2:L:14:ARG:HE	2:L:88:ASN:CG	2.16	0.48
1:A:8:HIS:HE1	1:A:122:VAL:O	1.96	0.48
2:H:149:VAL:O	2:H:149:VAL:HG12	2.14	0.48
1:E:249:LEU:HD23	1:E:273:ILE:HG23	1.95	0.48
2:K:48:LEU:O	2:K:55:ARG:HA	2.13	0.48
2:L:14:ARG:HA	2:L:88:ASN:O	2.14	0.48
1:A:266:PRO:HB3	3:A:2001:FLC:HG1	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:126:ALA:O	2:G:136:LEU:HA	2.14	0.48
2:H:136:LEU:N	2:H:145:PHE:O	2.39	0.48
2:I:92:VAL:CG1	2:I:93:GLY:N	2.77	0.48
2:L:70:GLN:O	2:L:73:GLN:HB2	2.12	0.48
2:G:61:ILE:HG22	2:G:64:THR:HB	1.95	0.48
1:D:166:GLY:O	1:D:169:VAL:HG22	2.13	0.48
1:D:167:ARG:NE	3:D:2004:FCL:HA1	2.29	0.48
2:H:12:ILE:HG12	2:H:60:LYS:HD3	1.96	0.48
1:F:134:HIS:N	1:F:135:PRO:HD3	2.28	0.48
1:F:237:PRO:HA	1:F:240:TYR:CD2	2.48	0.48
1:F:249:LEU:HD11	1:F:254:LEU:HD21	1.94	0.48
1:A:59:PHE:CE1	1:A:136:THR:HG21	2.30	0.48
1:A:227:MET:O	1:A:265:HIS:ND1	2.41	0.48
1:A:251:ALA:N	1:A:276:ASP:OD1	2.43	0.48
1:B:12:ILE:N	1:B:133:GLN:OE1	2.45	0.48
2:G:48:LEU:HD23	2:J:41:ARG:CD	2.38	0.48
2:H:73:GLN:OE1	2:H:103:ILE:HG23	2.13	0.48
2:H:111:ASN:HB2	2:H:145:PHE:CZ	2.48	0.48
1:D:129:ASP:O	1:D:132:ASN:HB3	2.13	0.48
1:D:271:ASP:C	1:D:273:ILE:N	2.67	0.48
1:F:112:ALA:O	1:F:116:THR:HG23	2.14	0.48
2:J:114:CYS:SG	2:J:114:CYS:O	2.72	0.48
2:J:145:PHE:HB3	2:J:149:VAL:CG2	2.44	0.48
2:L:14:ARG:N	2:L:88:ASN:O	2.46	0.48
1:A:15:LEU:O	1:A:178:LYS:HE3	2.14	0.48
1:A:49:PHE:CZ	1:A:73:PHE:HZ	2.31	0.48
2:H:123:SER:OG	2:H:125:PHE:HE1	1.96	0.48
1:F:38:LEU:HD11	1:F:305:ASN:ND2	2.29	0.48
2:K:81:ALA:O	2:K:97:PRO:HD3	2.14	0.48
2:H:14:ARG:HG3	2:H:65:PHE:HZ	1.75	0.47
1:D:59:PHE:CE2	1:D:103:VAL:CG2	2.97	0.47
1:E:187:ILE:O	1:E:188:ALA:HB2	2.14	0.47
2:G:39:ASP:O	2:J:55:ARG:NH1	2.47	0.47
2:H:146:SER:OG	2:H:148:ASN:ND2	2.47	0.47
2:I:42:ILE:CD1	2:I:44:ILE:HD11	2.44	0.47
2:I:72:ASP:HB3	2:I:98:SER:O	2.14	0.47
2:J:114:CYS:O	2:J:115:ILE:C	2.52	0.47
2:K:138:CYS:CB	2:K:142:GLU:H	2.27	0.47
1:B:63:MET:HG2	1:B:300:LEU:HD11	1.96	0.47
1:B:110:GLY:N	1:B:129:ASP:OD1	2.43	0.47
1:B:287:GLN:HA	6:C:3061:HOH:O	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:MET:SD	1:F:195:PRO:HD2	2.54	0.47
2:J:67:SER:O	2:J:68:GLU:C	2.52	0.47
1:C:94:VAL:HG23	1:C:95:ILE:N	2.30	0.47
2:I:19:ASP:O	2:I:81:ALA:HB1	2.14	0.47
2:I:46:LEU:HD12	2:L:42:ILE:HG21	1.97	0.47
2:I:103:ILE:HG13	2:I:127:VAL:CG2	2.44	0.47
2:J:109:CYS:N	2:J:125:PHE:HZ	2.11	0.47
1:B:11:SER:O	1:B:14:ASP:N	2.33	0.47
2:H:32:LEU:HD21	2:H:77:TYR:CE1	2.50	0.47
1:D:38:LEU:HD11	1:D:305:ASN:ND2	2.30	0.47
1:F:49:PHE:HE2	1:F:81:LEU:HD22	1.79	0.47
2:K:78:ALA:HB1	2:K:81:ALA:HB2	1.96	0.47
2:K:107:LEU:HD22	2:K:151:LEU:O	2.15	0.47
2:L:13:LYS:O	2:L:14:ARG:CB	2.62	0.47
1:B:131:SER:HB3	1:B:234:ARG:HD2	1.97	0.47
1:C:130:GLY:O	1:C:132:ASN:N	2.47	0.47
2:G:16:THR:HB	2:G:65:PHE:CD2	2.41	0.47
2:G:111:ASN:HD22	2:G:112:SER:N	2.13	0.47
2:I:30:LEU:CD2	2:I:59:ILE:HD13	2.44	0.47
2:I:102:ARG:HG2	2:I:126:ALA:HA	1.95	0.47
1:E:75:ASP:OD2	1:E:77:ALA:HB3	2.14	0.47
1:E:237:PRO:HA	1:E:240:TYR:CZ	2.49	0.47
1:F:19:ASP:O	1:F:22:LEU:HB3	2.14	0.47
1:F:267:LEU:HD21	1:F:285:TYR:HB2	1.96	0.47
1:A:161:GLY:O	1:A:163:LEU:HG	2.15	0.47
1:A:265:HIS:C	1:A:266:PRO:O	2.49	0.47
1:C:213:SER:HB2	6:C:3092:HOH:O	2.14	0.47
2:H:44:ILE:HB	2:K:44:ILE:HB	1.96	0.47
2:H:102:ARG:CB	2:H:126:ALA:HA	2.45	0.47
2:I:15:GLY:HA2	2:I:63:ASN:N	2.21	0.47
2:I:130:ARG:HG2	2:I:133:ASP:O	2.14	0.47
1:D:201:MET:O	1:D:201:MET:HG2	2.14	0.47
1:E:66:LEU:HD21	1:E:297:GLN:NE2	2.26	0.47
1:E:164:LYS:HD3	1:E:165:TYR:CE2	2.50	0.47
2:K:8:GLN:HG3	2:K:48:LEU:HD22	1.96	0.47
1:A:172:LEU:HG	1:A:176:LEU:HD12	1.97	0.47
1:C:40:LYS:HG2	1:C:41:HIS:CD2	2.50	0.47
1:C:161:GLY:CA	1:C:228:THR:OG1	2.58	0.47
2:G:68:GLU:OE1	2:G:68:GLU:N	2.36	0.47
2:H:12:ILE:HD11	2:H:60:LYS:HB3	1.97	0.47
1:D:135:PRO:O	1:D:138:THR:HB	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:12:ILE:HD13	2:L:62:GLU:CA	2.45	0.47
1:A:63:MET:HG3	1:A:300:LEU:CD1	2.45	0.47
2:I:20:HIS:O	2:I:81:ALA:HB2	2.15	0.47
2:K:9:VAL:HG23	2:K:9:VAL:O	2.15	0.47
2:L:137:LYS:HB3	2:L:144:GLU:HG2	1.97	0.47
1:C:17:ARG:HD2	1:C:179:PHE:CE1	2.50	0.47
1:C:45:ALA:HB2	1:C:99:VAL:HG11	1.97	0.47
1:C:146:GLN:O	1:C:150:GLY:N	2.48	0.47
2:G:31:SER:HB3	2:J:27:PHE:HZ	1.80	0.47
2:H:146:SER:C	2:H:148:ASN:N	2.67	0.47
1:D:81:LEU:HA	1:D:86:GLU:HB3	1.96	0.47
2:K:14:ARG:HH11	2:K:14:ARG:CB	2.21	0.47
2:L:135:ALA:HA	2:L:146:SER:HA	1.96	0.47
1:C:232:LYS:HA	1:C:235:LEU:HD12	1.96	0.46
2:G:43:THR:HB	2:G:60:LYS:HB2	1.96	0.46
2:H:48:LEU:O	2:H:55:ARG:HA	2.15	0.46
2:H:123:SER:O	2:H:124:SER:HB2	2.15	0.46
1:F:140:LEU:HD11	1:F:296:ARG:HH12	1.80	0.46
2:J:42:ILE:CG2	2:J:43:THR:N	2.78	0.46
1:A:30:LEU:C	1:A:32:ALA:H	2.18	0.46
1:B:54:ARG:CD	1:B:267:LEU:HB2	2.45	0.46
2:G:1:MET:HG3	2:G:1:MET:O	2.15	0.46
1:D:63:MET:CE	1:D:70:VAL:HG13	2.46	0.46
1:F:292:GLY:O	1:F:296:ARG:HG3	2.15	0.46
2:J:103:ILE:HD11	2:J:107:LEU:CD1	2.45	0.46
1:C:196:GLN:HG3	1:C:200:ASP:OD2	2.16	0.46
1:C:227:MET:CE	1:C:249:LEU:HD22	2.44	0.46
2:G:131:ALA:O	2:G:132:ASN:HB3	2.15	0.46
2:I:31:SER:CB	2:L:27:PHE:HZ	2.28	0.46
1:D:138:THR:O	1:D:142:LEU:HG	2.16	0.46
1:D:234:ARG:HG2	1:D:234:ARG:HH11	1.81	0.46
1:E:170:HIS:NE2	1:E:195:PRO:HG2	2.31	0.46
2:K:8:GLN:OE1	2:K:8:GLN:HA	2.14	0.46
2:L:82:THR:CG2	2:L:83:VAL:N	2.47	0.46
2:I:102:ARG:HA	2:I:125:PHE:O	2.16	0.46
1:D:49:PHE:CE2	1:D:81:LEU:HD22	2.50	0.46
1:D:267:LEU:HD21	1:D:285:TYR:HB3	1.96	0.46
1:E:216:GLU:HA	1:E:219:MET:HB2	1.96	0.46
2:J:53:MET:HG3	2:J:54:GLY:N	2.29	0.46
2:G:33:PHE:CE2	2:G:73:GLN:HG3	2.50	0.46
2:H:78:ALA:HB1	2:H:81:ALA:HB2	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:PHE:HE2	1:D:81:LEU:HD22	1.79	0.46
1:E:161:GLY:O	1:E:163:LEU:HG	2.15	0.46
1:F:108:GLN:HA	2:L:113:ASN:OD1	2.16	0.46
1:F:277:VAL:O	1:F:283:ALA:HB2	2.16	0.46
2:K:17:VAL:HG21	2:K:86:ILE:HD12	1.97	0.46
2:K:109:CYS:HB2	2:K:138:CYS:SG	2.54	0.46
2:I:13:LYS:HB2	2:I:89:TYR:CZ	2.49	0.46
2:J:111:ASN:ND2	2:J:114:CYS:N	2.63	0.46
2:K:125:PHE:HA	2:K:137:LYS:O	2.16	0.46
1:A:63:MET:CE	1:A:70:VAL:HG22	2.43	0.46
1:A:132:ASN:CG	1:A:133:GLN:H	2.19	0.46
1:B:49:PHE:HE2	1:B:81:LEU:CD2	2.29	0.46
1:B:162:ASP:C	1:B:162:ASP:OD1	2.54	0.46
1:D:105:ARG:CZ	3:D:2004:FLC:OB2	2.64	0.46
1:D:167:ARG:HE	3:D:2004:FLC:CA	2.28	0.46
2:K:19:ASP:OD1	2:K:20:HIS:N	2.49	0.46
2:L:14:ARG:NH2	2:L:88:ASN:HD22	2.04	0.46
1:A:26:THR:HG23	1:A:309:VAL:HG11	1.97	0.46
1:C:109:GLU:OE1	2:I:113:ASN:HB3	2.15	0.46
2:G:94:LYS:O	2:G:94:LYS:HG2	2.16	0.46
2:H:1:MET:O	2:H:3:HIS:N	2.47	0.46
2:H:19:ASP:HB3	2:H:82:THR:CG2	2.46	0.46
2:H:87:ASP:O	2:H:88:ASN:C	2.54	0.46
2:H:114:CYS:HB3	2:H:116:SER:OG	2.15	0.46
2:I:109:CYS:O	2:I:117:HIS:NE2	2.49	0.46
1:D:59:PHE:CE1	1:D:136:THR:HG21	2.38	0.46
1:D:236:ASP:OD1	1:D:237:PRO:HD2	2.15	0.46
1:D:264:LEU:O	1:D:265:HIS:HB2	2.15	0.46
1:E:129:ASP:O	1:E:130:GLY:C	2.53	0.46
1:F:183:ARG:NH1	1:F:185:TYR:CE1	2.83	0.46
2:J:111:ASN:HD21	2:J:113:ASN:HB3	1.80	0.46
2:L:8:GLN:CD	2:L:58:LEU:HD11	2.36	0.46
2:L:98:SER:C	2:L:100:PRO:HD3	2.37	0.46
2:L:115:ILE:CD1	2:L:119:GLU:HG3	2.45	0.46
1:A:98:TYR:CZ	1:C:58:SER:HB3	2.51	0.46
1:B:53:THR:HB	1:B:54:ARG:HH21	1.81	0.46
1:C:250:ARG:O	1:C:253:ASP:HB2	2.16	0.46
1:C:309:VAL:O	1:C:310:LEU:HB3	2.16	0.46
2:H:146:SER:O	2:H:148:ASN:N	2.49	0.46
2:I:132:ASN:O	2:I:133:ASP:CB	2.59	0.46
1:D:104:MET:CE	1:D:112:ALA:HA	2.45	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:PHE:CZ	1:E:73:PHE:HZ	2.33	0.46
1:E:104:MET:CE	1:E:112:ALA:HA	2.45	0.46
2:K:23:ALA:O	2:K:24:GLN:HB2	2.15	0.46
2:K:50:SER:HB3	2:K:53:MET:C	2.36	0.46
1:C:132:ASN:CG	1:C:133:GLN:N	2.69	0.46
1:F:156:HIS:HD2	1:F:185:TYR:OH	1.99	0.46
1:A:290:GLY:C	1:A:292:GLY:N	2.70	0.45
2:H:48:LEU:CD2	2:K:41:ARG:HE	2.28	0.45
1:F:25:ALA:O	1:F:28:ALA:HB3	2.16	0.45
2:J:94:LYS:HE3	2:J:96:ARG:HG3	1.98	0.45
2:K:109:CYS:SG	2:K:109:CYS:O	2.73	0.45
1:A:11:SER:CB	1:A:133:GLN:HG3	2.45	0.45
2:H:35:LEU:O	2:H:37:GLU:N	2.49	0.45
1:E:106:HIS:CE1	1:E:107:PRO:HD2	2.51	0.45
1:B:53:THR:HB	1:C:80:SER:OG	2.17	0.45
1:B:132:ASN:CG	1:B:133:GLN:H	2.19	0.45
1:C:5:TYR:O	1:C:6:GLN:HB2	2.17	0.45
2:G:119:GLU:HB3	2:G:120:PRO:HD2	1.98	0.45
2:I:42:ILE:HG22	2:I:61:ILE:HG23	1.98	0.45
2:I:107:LEU:HD22	2:I:150:VAL:CG1	2.44	0.45
1:D:100:ASP:O	1:D:101:ALA:HB2	2.16	0.45
2:K:96:ARG:HH11	2:K:96:ARG:HG3	1.80	0.45
2:G:111:ASN:ND2	2:G:113:ASN:N	2.53	0.45
2:G:134:ILE:HB	2:G:147:HIS:CD2	2.47	0.45
2:H:65:PHE:CD2	2:H:85:ARG:HD3	2.52	0.45
2:I:109:CYS:C	2:I:111:ASN:H	2.19	0.45
1:D:63:MET:HG3	1:D:300:LEU:HD13	1.97	0.45
1:D:270:VAL:O	1:D:271:ASP:CG	2.54	0.45
1:A:234:ARG:HG2	1:A:234:ARG:HH11	1.80	0.45
1:C:215:ILE:O	1:C:217:GLU:N	2.50	0.45
2:G:71:VAL:CG1	2:G:72:ASP:H	2.29	0.45
2:I:28:LYS:O	2:I:32:LEU:HB2	2.16	0.45
2:I:92:VAL:CG1	2:I:93:GLY:H	2.29	0.45
2:J:18:ILE:CG2	2:J:21:ILE:HD11	2.44	0.45
2:K:48:LEU:O	2:K:56:LYS:N	2.49	0.45
1:B:146:GLN:HB2	1:B:152:LEU:HG	1.99	0.45
1:C:110:GLY:HA3	2:I:140:TYR:O	2.16	0.45
1:C:148:THR:HG21	1:C:262:LYS:HG3	1.99	0.45
1:C:280:THR:HA	1:C:281:PRO:HD3	1.80	0.45
1:E:43:VAL:O	1:E:99:VAL:HB	2.17	0.45
2:K:16:THR:OG1	2:K:65:PHE:HA	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:21:ILE:HB	2:K:57:ASP:O	2.16	0.45
1:B:33:ASN:N	1:B:34:PRO:HD3	2.32	0.45
2:H:131:ALA:O	2:H:132:ASN:CB	2.65	0.45
1:E:47:CYS:O	1:E:104:MET:HA	2.16	0.45
1:F:120:GLY:O	1:F:121:ASN:HB2	2.17	0.45
1:F:141:ASP:O	1:F:145:ILE:HG13	2.16	0.45
1:F:154:ASN:HB3	6:F:3088:HOH:O	2.16	0.45
2:K:92:VAL:HB	2:K:93:GLY:H	1.49	0.45
1:A:54:ARG:NE	4:A:3001:PO4:O3	2.50	0.45
1:A:132:ASN:O	1:A:133:GLN:C	2.53	0.45
1:A:284:TRP:HA	1:A:287:GLN:OE1	2.17	0.45
1:B:278:ASP:HB3	6:B:3077:HOH:O	2.16	0.45
1:C:81:LEU:O	1:C:81:LEU:CG	2.65	0.45
1:C:246:GLN:HG2	1:C:246:GLN:O	2.16	0.45
2:I:17:VAL:HG22	2:I:60:LYS:HD3	1.98	0.45
2:I:48:LEU:O	2:I:56:LYS:HG2	2.17	0.45
1:D:160:VAL:HB	1:D:227:MET:HG2	1.99	0.45
1:E:254:LEU:HD13	1:E:282:HIS:CD2	2.50	0.45
2:J:12:ILE:CG2	2:J:13:LYS:N	2.79	0.45
2:J:21:ILE:HA	2:J:22:PRO:HD3	1.83	0.45
2:K:86:ILE:O	2:K:87:ASP:OD1	2.35	0.45
2:K:107:LEU:HD13	2:K:150:VAL:CG1	2.46	0.45
2:L:71:VAL:HG11	2:L:85:ARG:HH21	1.81	0.45
2:L:109:CYS:HB2	2:L:138:CYS:SG	2.56	0.45
1:A:137:GLN:HA	1:A:140:LEU:HG	1.98	0.45
2:G:32:LEU:HD12	2:G:32:LEU:O	2.16	0.45
2:H:110:PRO:HD2	2:H:145:PHE:CD2	2.51	0.45
1:D:105:ARG:CD	1:D:128:GLY:HA3	2.41	0.45
1:F:30:LEU:HD22	1:F:297:GLN:HE21	1.81	0.45
2:J:12:ILE:HD12	2:J:41:ARG:NH2	2.32	0.45
2:K:78:ALA:N	2:K:79:PRO:HD3	2.32	0.45
2:L:26:GLY:O	2:L:30:LEU:HG	2.17	0.45
1:A:31:LYS:CG	1:A:31:LYS:O	2.64	0.45
1:A:250:ARG:HG2	1:A:250:ARG:NH1	2.32	0.45
1:B:114:LEU:CD1	2:H:121:VAL:HG12	2.47	0.45
2:I:30:LEU:HD13	2:I:44:ILE:HG12	1.99	0.45
2:I:107:LEU:HB3	2:I:150:VAL:CG1	2.47	0.45
1:D:11:SER:HB2	2:J:142:GLU:OE2	2.17	0.45
1:D:51:ALA:CB	1:F:83:LYS:HG3	2.46	0.45
1:D:75:ASP:OD1	1:D:77:ALA:CB	2.65	0.45
1:D:286:PHE:O	1:D:287:GLN:C	2.54	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:ALA:HB2	6:E:3024:HOH:O	2.16	0.45
1:E:196:GLN:O	1:E:199:LEU:N	2.50	0.45
1:F:215:ILE:C	1:F:217:GLU:H	2.19	0.45
1:F:227:MET:HE3	1:F:249:LEU:HB2	1.97	0.45
2:L:103:ILE:O	2:L:124:SER:HA	2.17	0.45
1:A:11:SER:HA	1:A:133:GLN:HG3	1.99	0.44
1:B:264:LEU:HB3	1:B:288:GLN:HE22	1.81	0.44
2:H:114:CYS:C	2:H:116:SER:H	2.18	0.44
2:I:42:ILE:HD11	2:L:46:LEU:CD1	2.36	0.44
1:D:129:ASP:O	1:D:130:GLY:C	2.56	0.44
2:J:16:THR:HG21	2:J:65:PHE:HA	1.99	0.44
2:J:40:GLN:HG2	2:J:62:GLU:O	2.16	0.44
2:J:47:ASN:O	2:J:55:ARG:HD3	2.17	0.44
2:J:128:ARG:HH11	2:J:128:ARG:HG3	1.82	0.44
2:J:137:LYS:HG2	2:J:144:GLU:HB3	2.00	0.44
2:L:130:ARG:HG2	2:L:131:ALA:H	1.82	0.44
1:A:54:ARG:HG2	1:B:98:TYR:OH	2.16	0.44
1:A:132:ASN:O	1:A:167:ARG:CB	2.65	0.44
1:B:211:LEU:O	1:B:212:HIS:CG	2.70	0.44
1:C:229:ARG:NE	3:C:2003:FLC:OA1	2.49	0.44
1:C:277:VAL:O	1:C:277:VAL:HG12	2.17	0.44
2:I:19:ASP:C	2:I:21:ILE:HD12	2.37	0.44
1:D:194:MET:SD	1:D:198:ILE:HG21	2.57	0.44
1:D:223:ASP:O	1:D:261:MET:HA	2.18	0.44
1:E:109:GLU:OE1	2:K:111:ASN:ND2	2.40	0.44
2:K:30:LEU:HD13	2:K:59:ILE:HD13	1.99	0.44
2:L:42:ILE:HG22	2:L:44:ILE:CG1	2.33	0.44
1:A:290:GLY:O	1:A:292:GLY:N	2.51	0.44
1:B:88:LEU:O	1:B:92:ILE:HG12	2.17	0.44
1:B:133:GLN:NE2	1:B:174:GLN:OE1	2.50	0.44
2:G:94:LYS:CE	2:G:96:ARG:HH21	2.28	0.44
2:H:41:ARG:NE	2:K:8:GLN:HE21	2.11	0.44
2:I:83:VAL:HG13	2:I:83:VAL:O	2.18	0.44
2:I:111:ASN:O	2:I:114:CYS:HB3	2.17	0.44
2:K:34:LYS:HA	6:K:1011:HOH:O	2.16	0.44
2:L:86:ILE:HD13	2:L:92:VAL:CA	2.43	0.44
1:C:58:SER:OG	1:C:296:ARG:NH1	2.51	0.44
2:G:34:LYS:HB3	2:G:37:GLU:HG2	1.96	0.44
2:G:56:LYS:HD2	2:G:56:LYS:C	2.37	0.44
2:H:104:ASP:O	2:H:106:VAL:N	2.51	0.44
2:H:134:ILE:HB	2:H:147:HIS:CD2	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:6:LYS:O	2:I:6:LYS:HG2	2.16	0.44
1:D:138:THR:OG1	1:D:171:SER:HB2	2.17	0.44
1:F:138:THR:OG1	1:F:171:SER:HB2	2.17	0.44
2:L:61:ILE:HD13	6:L:1047:HOH:O	2.18	0.44
1:A:54:ARG:CZ	1:A:267:LEU:HB3	2.48	0.44
1:B:17:ARG:HG2	1:B:17:ARG:HH11	1.83	0.44
1:C:153:ASP:OD1	1:C:153:ASP:N	2.50	0.44
1:D:76:SER:HB2	1:D:81:LEU:HD23	1.99	0.44
1:E:277:VAL:O	1:E:283:ALA:HB2	2.18	0.44
1:F:44:ILE:HB	1:F:63:MET:HE2	1.99	0.44
1:A:132:ASN:CG	1:A:133:GLN:N	2.71	0.44
1:B:187:ILE:O	1:B:188:ALA:HB2	2.18	0.44
1:B:229:ARG:HB3	3:B:2002:FLC:OA2	2.16	0.44
1:C:291:ASN:HA	1:C:294:PHE:HD2	1.83	0.44
2:G:49:PRO:HD2	2:J:41:ARG:HD3	1.98	0.44
2:H:42:ILE:HA	2:H:60:LYS:O	2.18	0.44
2:H:125:PHE:N	2:H:125:PHE:CD1	2.86	0.44
1:D:265:HIS:O	1:D:267:LEU:N	2.51	0.44
1:E:151:ARG:HD2	1:E:153:ASP:O	2.17	0.44
1:F:268:PRO:CD	6:F:3075:HOH:O	2.50	0.44
2:J:86:ILE:CG2	2:J:87:ASP:N	2.80	0.44
2:J:145:PHE:HB3	2:J:149:VAL:HG21	1.99	0.44
1:C:284:TRP:O	1:C:288:GLN:HB3	2.18	0.44
2:G:11:ALA:HA	2:G:60:LYS:NZ	2.33	0.44
2:I:16:THR:N	2:I:61:ILE:O	2.44	0.44
2:I:32:LEU:C	2:I:34:LYS:H	2.21	0.44
1:D:284:TRP:HA	1:D:287:GLN:OE1	2.18	0.44
1:B:160:VAL:HG13	1:B:187:ILE:HB	2.00	0.44
2:G:70:GLN:O	2:G:73:GLN:CG	2.60	0.44
2:G:115:ILE:C	2:G:117:HIS:N	2.71	0.44
2:I:41:ARG:HB3	2:I:62:GLU:CD	2.37	0.44
1:D:25:ALA:O	1:D:28:ALA:HB3	2.17	0.44
1:E:32:ALA:O	1:E:34:PRO:HD3	2.16	0.44
1:E:66:LEU:HG	1:E:297:GLN:HG3	1.99	0.44
1:F:63:MET:HE1	1:F:70:VAL:HG22	1.99	0.44
1:F:160:VAL:HG22	1:F:187:ILE:HD12	1.99	0.44
2:J:25:ILE:O	2:J:25:ILE:CG2	2.66	0.44
2:J:57:ASP:C	2:J:58:LEU:HD23	2.38	0.44
2:K:32:LEU:HD11	2:K:106:VAL:CG1	2.47	0.44
2:K:109:CYS:SG	2:K:114:CYS:CB	3.05	0.44
2:L:18:ILE:CB	2:L:83:VAL:HB	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:PHE:CE2	1:B:81:LEU:HD23	2.53	0.44
1:B:166:GLY:O	1:B:168:THR:N	2.51	0.44
1:C:120:GLY:O	1:C:121:ASN:CG	2.57	0.44
1:C:229:ARG:NH2	3:C:2003:FLC:OA1	2.48	0.44
2:H:36:THR:HG22	2:K:46:LEU:CD1	2.47	0.44
2:I:13:LYS:O	2:I:14:ARG:HB3	2.18	0.44
2:I:21:ILE:HB	2:I:57:ASP:O	2.17	0.44
2:I:111:ASN:C	2:I:111:ASN:HD22	2.20	0.44
1:F:54:ARG:N	4:F:3006:PO4:O3	2.51	0.44
1:F:61:THR:O	1:F:62:SER:C	2.56	0.44
1:F:265:HIS:N	1:F:288:GLN:HE22	1.93	0.44
2:K:134:ILE:HG13	2:K:134:ILE:O	2.17	0.44
2:K:137:LYS:HE2	2:K:142:GLU:C	2.38	0.44
2:L:38:THR:HG22	2:L:40:GLN:HG3	2.00	0.44
2:L:125:PHE:HB3	2:L:136:LEU:HB3	2.00	0.44
1:A:189:PRO:HB3	1:A:246:GLN:HE22	1.82	0.43
2:G:83:VAL:O	2:G:84:ASN:HB2	2.18	0.43
2:I:12:ILE:HD11	2:I:17:VAL:CG2	2.48	0.43
2:I:40:GLN:HG3	2:I:62:GLU:CB	2.43	0.43
1:E:49:PHE:CD1	1:E:49:PHE:N	2.85	0.43
2:L:14:ARG:HA	2:L:88:ASN:C	2.39	0.43
1:A:31:LYS:O	1:A:31:LYS:HG2	2.18	0.43
1:C:30:LEU:CD2	1:C:309:VAL:HG21	2.39	0.43
2:G:130:ARG:O	2:G:133:ASP:O	2.36	0.43
2:G:138:CYS:CB	2:G:141:CYS:O	2.64	0.43
1:D:273:ILE:HD13	1:D:285:TYR:CE2	2.53	0.43
2:L:20:HIS:CE1	2:L:84:ASN:HD21	2.36	0.43
2:L:21:ILE:CG2	2:L:56:LYS:CE	2.95	0.43
2:L:52:GLU:O	2:L:53:MET:HG3	2.18	0.43
2:L:71:VAL:HG21	2:L:85:ARG:NE	2.25	0.43
1:A:267:LEU:O	1:A:267:LEU:CG	2.66	0.43
1:A:308:LEU:O	1:A:309:VAL:C	2.57	0.43
1:C:114:LEU:CD1	2:I:121:VAL:CG1	2.97	0.43
2:G:20:HIS:C	2:G:21:ILE:HG13	2.37	0.43
2:G:46:LEU:HB2	2:J:42:ILE:HB	1.99	0.43
2:G:98:SER:O	2:G:99:LEU:C	2.56	0.43
2:H:79:PRO:HG2	6:H:1035:HOH:O	2.16	0.43
1:E:37:GLU:HA	1:E:37:GLU:OE2	2.18	0.43
1:E:134:HIS:CE1	1:E:137:GLN:HB2	2.53	0.43
1:F:59:PHE:O	1:F:62:SER:HB2	2.18	0.43
2:L:55:ARG:O	2:L:56:LYS:HG2	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:115:ILE:HG23	2:L:116:SER:N	2.32	0.43
1:A:277:VAL:O	1:A:277:VAL:HG12	2.17	0.43
2:I:27:PHE:HB3	2:L:36:THR:HG21	2.00	0.43
2:I:47:ASN:O	2:I:48:LEU:HD23	2.18	0.43
2:I:66:LEU:HB3	2:I:70:GLN:HB3	2.00	0.43
2:I:81:ALA:O	2:I:97:PRO:HD2	2.18	0.43
2:I:135:ALA:HB1	2:I:144:GLU:CD	2.38	0.43
1:D:109:GLU:OE1	2:J:113:ASN:HB3	2.19	0.43
2:J:33:PHE:O	2:J:34:LYS:C	2.55	0.43
2:J:47:ASN:HB3	2:J:55:ARG:HD3	2.00	0.43
2:J:114:CYS:HB2	2:J:141:CYS:HB3	2.00	0.43
2:L:125:PHE:CD1	2:L:125:PHE:N	2.86	0.43
1:A:83:LYS:HG3	1:C:51:ALA:HB2	2.00	0.43
1:A:151:ARG:HD2	1:A:153:ASP:O	2.19	0.43
1:A:230:VAL:O	1:A:232:LYS:N	2.52	0.43
2:G:83:VAL:HG13	2:G:84:ASN:N	2.33	0.43
1:D:191:ALA:O	1:D:192:LEU:HD23	2.18	0.43
1:F:261:MET:HG2	1:F:262:LYS:N	2.34	0.43
1:F:266:PRO:C	6:F:3075:HOH:O	2.56	0.43
2:K:108:VAL:O	2:K:110:PRO:HD3	2.19	0.43
2:L:12:ILE:CG1	2:L:62:GLU:HB2	2.47	0.43
2:L:38:THR:C	2:L:40:GLN:H	2.21	0.43
1:A:176:LEU:O	1:A:182:ASN:ND2	2.50	0.43
1:C:267:LEU:O	1:C:267:LEU:CG	2.66	0.43
2:G:3:HIS:CD2	2:G:6:LYS:HA	2.54	0.43
2:H:134:ILE:N	2:H:134:ILE:CD1	2.82	0.43
2:I:63:ASN:CB	6:I:1042:HOH:O	2.67	0.43
1:D:9:ILE:HB	1:D:125:LEU:HD22	2.00	0.43
1:E:216:GLU:OE2	1:E:255:HIS:NE2	2.51	0.43
1:F:188:ALA:HA	1:F:247:PHE:HE2	1.83	0.43
2:J:25:ILE:HG12	2:J:28:LYS:HD2	2.01	0.43
2:K:38:THR:HG22	2:K:40:GLN:N	2.09	0.43
2:L:16:THR:O	2:L:17:VAL:HG22	2.19	0.43
2:L:83:VAL:CG1	2:L:84:ASN:H	2.30	0.43
2:L:149:VAL:O	2:L:149:VAL:HG12	2.19	0.43
1:C:26:THR:HG23	1:C:309:VAL:HG11	2.01	0.43
2:G:7:LEU:HG	2:G:9:VAL:HG23	1.99	0.43
2:G:70:GLN:O	2:G:73:GLN:NE2	2.51	0.43
1:F:174:GLN:HA	1:F:201:MET:CE	2.48	0.43
2:K:28:LYS:HD2	2:K:28:LYS:HA	1.92	0.43
2:K:110:PRO:HD2	2:K:145:PHE:HD1	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:138:CYS:CB	2:K:141:CYS:SG	3.01	0.43
1:A:144:THR:HG21	1:A:288:GLN:HB2	2.01	0.43
1:B:223:ASP:O	1:B:261:MET:HA	2.19	0.43
1:C:151:ARG:HD2	1:C:153:ASP:O	2.19	0.43
1:C:156:HIS:HD2	1:C:185:TYR:OH	2.02	0.43
1:C:291:ASN:HA	1:C:294:PHE:CD2	2.54	0.43
2:H:106:VAL:C	2:H:107:LEU:HD23	2.39	0.43
2:I:12:ILE:CD1	2:I:61:ILE:N	2.82	0.43
1:D:129:ASP:CG	1:D:132:ASN:HD22	2.22	0.43
1:D:267:LEU:CD1	1:F:94:VAL:CG1	2.95	0.43
1:D:270:VAL:H	1:D:272:GLU:CD	2.21	0.43
1:E:229:ARG:HB3	3:E:2005:FLC:OA2	2.19	0.43
1:E:267:LEU:O	1:E:269:ARG:N	2.51	0.43
1:F:105:ARG:HG3	1:F:128:GLY:HA3	2.01	0.43
2:L:83:VAL:HA	2:L:95:SER:O	2.19	0.43
2:L:109:CYS:O	2:L:117:HIS:NE2	2.52	0.43
2:G:33:PHE:O	2:G:34:LYS:C	2.57	0.43
2:H:25:ILE:O	2:H:25:ILE:HG23	2.18	0.43
2:K:85:ARG:O	2:K:87:ASP:OD1	2.36	0.43
2:L:61:ILE:HG22	2:L:64:THR:HB	1.98	0.43
1:C:306:ARG:HB2	1:C:306:ARG:NH1	2.34	0.43
2:H:99:LEU:HA	2:H:100:PRO:HD3	1.87	0.43
1:D:61:THR:HG23	1:F:43:VAL:HG11	2.01	0.43
1:F:215:ILE:O	1:F:217:GLU:N	2.52	0.43
1:F:250:ARG:HB3	6:F:3008:HOH:O	2.18	0.43
2:J:35:LEU:HD22	2:J:61:ILE:CD1	2.49	0.43
2:J:106:VAL:HG23	2:J:107:LEU:HG	2.00	0.43
2:J:114:CYS:C	2:J:116:SER:N	2.71	0.43
2:K:28:LYS:HG2	6:K:1007:HOH:O	2.19	0.43
2:K:67:SER:O	2:K:70:GLN:N	2.48	0.43
1:A:63:MET:HE1	1:A:70:VAL:CG2	2.49	0.42
1:A:246:GLN:O	1:A:246:GLN:CG	2.67	0.42
2:G:70:GLN:HA	2:G:73:GLN:CD	2.39	0.42
2:G:134:ILE:CG2	2:G:135:ALA:N	2.81	0.42
2:H:16:THR:CG2	2:H:83:VAL:HG13	2.49	0.42
1:E:34:PRO:C	1:E:36:PRO:HD3	2.39	0.42
1:E:162:ASP:C	1:E:162:ASP:OD1	2.56	0.42
1:F:109:GLU:HA	1:F:129:ASP:OD1	2.19	0.42
2:J:14:ARG:HD2	2:J:65:PHE:HZ	1.83	0.42
2:J:25:ILE:CG2	2:J:77:TYR:HB3	2.48	0.42
2:K:50:SER:HB3	2:K:53:MET:O	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:16:THR:HG22	2:L:17:VAL:N	2.33	0.42
1:A:63:MET:HG3	1:A:300:LEU:HD11	2.01	0.42
1:B:17:ARG:HD2	1:B:179:PHE:CE1	2.54	0.42
1:C:240:TYR:O	1:C:243:VAL:HG12	2.19	0.42
2:H:76:LEU:HD12	2:H:103:ILE:CD1	2.48	0.42
2:H:149:VAL:HG12	6:H:1039:HOH:O	2.18	0.42
1:F:140:LEU:HD23	1:F:295:ALA:CB	2.48	0.42
2:K:107:LEU:HA	2:K:152:ALA:HA	2.01	0.42
2:L:14:ARG:CA	2:L:88:ASN:O	2.68	0.42
2:L:38:THR:O	2:L:40:GLN:N	2.49	0.42
2:H:38:THR:O	2:K:47:ASN:ND2	2.51	0.42
2:H:122:SER:HB2	6:H:1006:HOH:O	2.19	0.42
1:D:63:MET:HE2	1:D:70:VAL:HG13	2.00	0.42
2:K:16:THR:CG2	2:K:17:VAL:N	2.82	0.42
1:A:91:THR:O	1:A:94:VAL:HG22	2.19	0.42
1:A:243:VAL:HG12	1:A:244:LYS:N	2.34	0.42
2:G:14:ARG:HG2	2:G:87:ASP:CB	2.49	0.42
1:D:66:LEU:HD21	1:D:297:GLN:CG	2.47	0.42
1:D:185:TYR:CE2	1:D:222:VAL:HG12	2.55	0.42
1:E:19:ASP:O	1:E:23:VAL:HG23	2.19	0.42
2:J:80:GLN:O	2:J:81:ALA:C	2.58	0.42
2:K:22:PRO:HG3	2:K:80:GLN:NE2	2.35	0.42
2:L:18:ILE:HG13	2:L:83:VAL:CG1	2.49	0.42
1:A:306:ARG:NH1	1:A:306:ARG:HB2	2.34	0.42
1:B:51:ALA:HB2	1:C:83:LYS:HG3	2.01	0.42
1:B:231:GLN:HE22	3:B:2002:FLC:CA	2.30	0.42
1:B:232:LYS:HA	1:B:235:LEU:CD1	2.48	0.42
2:H:111:ASN:C	2:H:113:ASN:N	2.70	0.42
1:D:267:LEU:O	1:D:268:PRO:C	2.57	0.42
1:D:267:LEU:HD11	1:D:286:PHE:HA	2.02	0.42
1:E:55:THR:HB	4:E:3005:PO4:O1	2.20	0.42
1:E:267:LEU:HD12	1:E:267:LEU:HA	1.74	0.42
1:F:75:ASP:C	1:F:77:ALA:H	2.23	0.42
1:F:159:MET:HE1	1:F:172:LEU:HB3	2.01	0.42
1:F:309:VAL:CG2	1:F:310:LEU:N	2.81	0.42
2:J:80:GLN:O	2:J:82:THR:N	2.52	0.42
2:K:99:LEU:HA	2:K:100:PRO:HD3	1.91	0.42
1:B:81:LEU:HD12	1:B:86:GLU:O	2.19	0.42
1:B:229:ARG:NE	3:B:2002:FLC:OA1	2.46	0.42
2:I:33:PHE:CE2	2:I:73:GLN:HB3	2.53	0.42
2:I:111:ASN:HD22	2:I:112:SER:N	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:GLN:NE2	6:E:3073:HOH:O	2.53	0.42
1:F:168:THR:HG21	3:F:2006:FCL:HG1	2.02	0.42
2:J:78:ALA:HB1	2:J:81:ALA:HB2	2.02	0.42
1:A:162:ASP:HB3	1:A:230:VAL:HA	2.01	0.42
1:B:42:LYS:NZ	6:B:3014:HOH:O	2.52	0.42
1:C:120:GLY:O	1:C:121:ASN:OD1	2.37	0.42
1:D:106:HIS:HA	1:D:107:PRO:HD3	1.82	0.42
1:D:269:ARG:HH11	1:D:273:ILE:CG2	2.32	0.42
2:K:53:MET:CG	2:K:54:GLY:H	2.30	0.42
2:L:14:ARG:HA	2:L:88:ASN:CA	2.49	0.42
2:L:20:HIS:HA	2:L:82:THR:HG21	2.01	0.42
1:B:88:LEU:O	1:B:88:LEU:HG	2.19	0.42
1:C:285:TYR:CE1	1:C:286:PHE:CE2	3.07	0.42
2:G:111:ASN:ND2	2:G:111:ASN:C	2.69	0.42
1:E:233:GLU:HG2	1:E:234:ARG:HG3	2.01	0.42
1:F:162:ASP:HB2	1:F:230:VAL:HA	2.01	0.42
2:J:34:LYS:HB3	2:J:37:GLU:HG3	1.97	0.42
2:K:54:GLY:O	2:K:55:ARG:C	2.58	0.42
1:A:122:VAL:HA	1:A:123:PRO:HD3	1.77	0.42
1:C:270:VAL:O	1:C:271:ASP:CG	2.58	0.42
2:G:82:THR:HG23	2:G:96:ARG:HG2	2.01	0.42
2:G:108:VAL:HB	2:G:151:LEU:HB3	2.02	0.42
2:H:133:ASP:C	2:H:134:ILE:HD12	2.39	0.42
1:E:64:HIS:O	1:E:67:GLY:N	2.38	0.42
2:K:1:MET:HB2	2:K:11:ALA:HB2	2.02	0.42
2:K:108:VAL:O	2:K:108:VAL:HG23	2.20	0.42
1:B:114:LEU:HD13	2:H:121:VAL:CG1	2.48	0.42
1:B:233:GLU:HG2	1:B:234:ARG:HG3	2.02	0.42
2:I:20:HIS:H	2:I:56:LYS:HD2	1.84	0.42
1:E:106:HIS:CE1	1:E:108:GLN:HG2	2.55	0.42
2:J:128:ARG:HG3	2:J:128:ARG:NH1	2.35	0.42
2:K:12:ILE:CG1	2:K:60:LYS:HE2	2.48	0.42
2:K:32:LEU:HD21	2:K:77:TYR:OH	2.20	0.42
2:K:78:ALA:C	2:K:80:GLN:N	2.73	0.42
1:C:35:GLN:HE22	1:C:309:VAL:HG23	1.85	0.41
1:C:265:HIS:CD2	1:C:273:ILE:HD11	2.55	0.41
2:H:109:CYS:HA	2:H:110:PRO:HD3	1.59	0.41
2:H:114:CYS:O	2:H:116:SER:N	2.47	0.41
2:I:30:LEU:CD1	2:I:44:ILE:HG12	2.49	0.41
2:I:130:ARG:CG	2:I:131:ALA:N	2.81	0.41
1:D:17:ARG:HD2	1:D:179:PHE:CE1	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:LEU:HD11	1:D:254:LEU:CD2	2.50	0.41
1:D:270:VAL:N	1:D:272:GLU:OE2	2.51	0.41
1:E:105:ARG:NH2	1:E:167:ARG:NH2	2.69	0.41
2:J:65:PHE:C	2:J:66:LEU:HD23	2.40	0.41
1:E:114:LEU:CD1	2:K:121:VAL:HG11	2.50	0.41
1:E:215:ILE:HD13	1:E:249:LEU:HD13	2.03	0.41
1:E:306:ARG:CB	1:E:306:ARG:HH11	2.33	0.41
1:F:109:GLU:OE2	1:F:131:SER:HB3	2.20	0.41
2:L:130:ARG:HG2	2:L:130:ARG:NH1	2.34	0.41
1:C:101:ALA:HB2	1:C:304:LEU:HD21	2.02	0.41
1:C:219:MET:CE	1:C:254:LEU:HD23	2.50	0.41
2:G:19:ASP:HA	2:G:58:LEU:HD13	2.01	0.41
2:G:138:CYS:HB3	2:G:141:CYS:C	2.40	0.41
1:D:132:ASN:O	1:D:133:GLN:O	2.39	0.41
1:E:151:ARG:HG2	1:E:151:ARG:HH11	1.85	0.41
1:F:60:GLU:HG2	1:F:70:VAL:HG11	2.02	0.41
2:J:12:ILE:CG2	2:J:13:LYS:H	2.22	0.41
2:J:47:ASN:HB3	2:J:55:ARG:HH11	1.85	0.41
2:G:3:HIS:NE2	2:G:6:LYS:HA	2.36	0.41
2:H:111:ASN:HD21	2:H:113:ASN:HB3	1.85	0.41
6:I:1037:HOH:O	2:L:7:LEU:HD11	2.19	0.41
1:E:8:HIS:CD2	1:E:116:THR:HB	2.55	0.41
2:L:16:THR:HB	2:L:60:LYS:CB	2.34	0.41
1:A:154:ASN:HA	1:A:181:GLY:O	2.21	0.41
1:A:231:GLN:HE22	3:A:2001:FLC:CAC	2.33	0.41
1:B:17:ARG:HG2	1:B:17:ARG:NH1	2.36	0.41
1:B:131:SER:HA	1:B:167:ARG:HB3	2.01	0.41
2:G:49:PRO:HD3	2:J:41:ARG:HD3	2.02	0.41
2:I:40:GLN:HG3	2:I:62:GLU:OE1	2.20	0.41
1:E:45:ALA:HA	1:E:71:VAL:O	2.20	0.41
1:E:132:ASN:CG	1:E:133:GLN:N	2.74	0.41
1:F:91:THR:HG22	1:F:95:ILE:HD12	2.03	0.41
2:K:29:LEU:HD13	2:K:74:LEU:HD22	2.03	0.41
2:L:68:GLU:HG2	2:L:85:ARG:NH1	2.35	0.41
1:B:49:PHE:CD1	1:B:49:PHE:N	2.88	0.41
2:G:40:GLN:O	2:J:47:ASN:HB2	2.20	0.41
1:D:26:THR:HG23	1:D:309:VAL:HG11	2.01	0.41
1:E:234:ARG:HH11	1:E:234:ARG:HG2	1.86	0.41
1:F:174:GLN:O	1:F:178:LYS:HG3	2.21	0.41
1:F:227:MET:HB2	1:F:273:ILE:HD11	2.02	0.41
2:L:16:THR:HG21	2:L:84:ASN:CA	2.48	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:20:HIS:CA	2:L:82:THR:HG21	2.50	0.41
1:A:219:MET:HE3	1:A:254:LEU:HA	2.03	0.41
1:A:265:HIS:CD2	1:A:266:PRO:O	2.74	0.41
1:C:81:LEU:O	1:C:81:LEU:HG	2.21	0.41
1:C:246:GLN:O	1:C:246:GLN:CG	2.68	0.41
2:G:94:LYS:HE2	2:G:96:ARG:NH2	2.33	0.41
2:I:15:GLY:CA	2:I:63:ASN:H	2.24	0.41
2:I:63:ASN:O	2:I:63:ASN:CG	2.58	0.41
2:I:121:VAL:O	2:I:121:VAL:HG23	2.20	0.41
1:D:106:HIS:HB3	1:D:111:ALA:HB3	2.02	0.41
1:D:157:VAL:O	1:D:184:PHE:HA	2.21	0.41
1:F:94:VAL:HG23	1:F:95:ILE:HG13	2.02	0.41
1:F:119:SER:O	1:F:119:SER:OG	2.37	0.41
2:K:96:ARG:HA	2:K:97:PRO:HD3	1.87	0.41
2:L:57:ASP:OD2	2:L:57:ASP:C	2.58	0.41
1:A:160:VAL:HG22	1:A:187:ILE:HD12	2.02	0.41
1:C:174:GLN:O	1:C:178:LYS:HG3	2.21	0.41
2:H:30:LEU:HD13	2:H:44:ILE:HD13	2.03	0.41
2:H:114:CYS:HB3	2:H:116:SER:CB	2.51	0.41
2:I:33:PHE:HE2	2:I:73:GLN:HB3	1.84	0.41
2:I:65:PHE:CD2	2:I:85:ARG:HG3	2.55	0.41
1:D:38:LEU:CD1	1:D:305:ASN:ND2	2.83	0.41
1:D:199:LEU:HD22	1:D:209:TRP:CH2	2.55	0.41
1:F:140:LEU:CD2	1:F:295:ALA:HB3	2.49	0.41
1:F:267:LEU:O	1:F:268:PRO:C	2.54	0.41
2:K:58:LEU:HG	2:K:59:ILE:N	2.36	0.41
2:K:106:VAL:O	2:K:106:VAL:HG12	2.19	0.41
1:A:49:PHE:CE2	1:A:81:LEU:HD22	2.56	0.41
1:B:48:PHE:CD2	1:B:56:ARG:HB2	2.55	0.41
1:B:63:MET:CG	1:B:300:LEU:HD11	2.51	0.41
1:B:80:SER:HB3	1:B:84:LYS:HD2	2.03	0.41
1:C:63:MET:SD	1:C:70:VAL:HG22	2.61	0.41
1:C:237:PRO:HA	1:C:240:TYR:CZ	2.56	0.41
2:G:59:ILE:HG22	2:G:60:LYS:N	2.36	0.41
2:G:79:PRO:O	2:G:80:GLN:HB2	2.20	0.41
2:G:91:VAL:O	2:G:91:VAL:HG23	2.21	0.41
2:H:72:ASP:O	2:H:75:ALA:CB	2.69	0.41
2:H:89:TYR:O	2:H:89:TYR:CD1	2.73	0.41
2:I:59:ILE:HG22	2:I:61:ILE:HD11	2.02	0.41
2:I:115:ILE:C	2:I:117:HIS:H	2.24	0.41
1:D:89:ALA:HB1	1:D:118:PHE:CZ	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:GLN:O	1:D:199:LEU:N	2.53	0.41
1:E:230:VAL:O	1:E:232:LYS:N	2.51	0.41
1:F:109:GLU:OE1	2:L:113:ASN:O	2.39	0.41
1:F:227:MET:HG3	1:F:273:ILE:HD11	2.03	0.41
2:L:16:THR:C	2:L:17:VAL:HG22	2.41	0.41
2:L:114:CYS:O	2:L:115:ILE:C	2.59	0.41
2:L:130:ARG:HG2	2:L:131:ALA:N	2.36	0.41
1:B:136:THR:HB	1:B:296:ARG:HE	1.86	0.41
1:C:21:ASN:HD22	1:C:21:ASN:HA	1.65	0.41
2:G:10:GLU:HG2	2:G:11:ALA:N	2.36	0.41
2:G:40:GLN:HG3	2:G:64:THR:OG1	2.21	0.41
2:H:113:ASN:O	2:H:114:CYS:C	2.59	0.41
1:D:75:ASP:CG	1:D:77:ALA:HB3	2.41	0.41
1:F:219:MET:CE	1:F:254:LEU:HD23	2.50	0.41
1:F:227:MET:CB	1:F:273:ILE:HD11	2.51	0.41
1:F:236:ASP:O	1:F:239:GLU:N	2.49	0.41
2:J:110:PRO:HD2	2:J:145:PHE:CD2	2.56	0.41
1:A:78:ASN:CG	1:C:75:ASP:HB2	2.41	0.40
1:C:106:HIS:CE1	1:C:107:PRO:HD2	2.53	0.40
1:C:277:VAL:O	1:C:280:THR:OG1	2.29	0.40
2:H:8:GLN:O	2:H:9:VAL:HG23	2.20	0.40
2:H:138:CYS:HB3	2:H:142:GLU:N	2.33	0.40
2:I:48:LEU:HD23	2:I:48:LEU:HA	1.86	0.40
2:I:99:LEU:HD23	2:I:99:LEU:HA	1.88	0.40
1:D:110:GLY:C	2:J:115:ILE:HG21	2.40	0.40
2:J:103:ILE:HD11	2:J:107:LEU:HD11	2.03	0.40
2:K:102:ARG:NH1	2:K:102:ARG:CB	2.80	0.40
2:K:119:GLU:HA	2:K:120:PRO:HD3	1.87	0.40
2:L:20:HIS:CE1	2:L:84:ASN:OD1	2.74	0.40
1:A:98:TYR:OH	1:C:54:ARG:HB3	2.21	0.40
1:A:109:GLU:CG	1:A:130:GLY:O	2.58	0.40
1:B:134:HIS:CE1	1:B:137:GLN:HB2	2.57	0.40
1:C:234:ARG:HG2	1:C:234:ARG:NH1	2.34	0.40
1:D:17:ARG:O	1:D:20:LEU:HB2	2.21	0.40
1:D:23:VAL:HG11	1:D:139:LEU:HD13	2.03	0.40
1:E:137:GLN:O	1:E:141:ASP:OD2	2.38	0.40
1:F:215:ILE:C	1:F:217:GLU:N	2.74	0.40
2:J:111:ASN:HD22	2:J:114:CYS:H	1.67	0.40
2:K:53:MET:HG2	2:K:54:GLY:N	2.30	0.40
2:L:83:VAL:HG13	2:L:95:SER:N	2.09	0.40
2:L:85:ARG:O	2:L:85:ARG:HG3	2.22	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:109:CYS:CB	2:L:138:CYS:SG	3.01	0.40
1:A:19:ASP:O	1:A:22:LEU:HB3	2.21	0.40
1:D:129:ASP:OD1	1:D:132:ASN:HB3	2.21	0.40
1:E:54:ARG:HD3	1:E:267:LEU:HB2	2.04	0.40
1:E:96:SER:CB	1:E:119:SER:HA	2.51	0.40
1:E:120:GLY:O	1:E:121:ASN:C	2.60	0.40
1:E:240:TYR:O	1:E:243:VAL:HG12	2.21	0.40
1:F:38:LEU:HD11	1:F:305:ASN:HD21	1.87	0.40
2:K:126:ALA:O	2:K:136:LEU:HA	2.21	0.40
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.87	0.40
2:H:42:ILE:HG22	2:H:44:ILE:HG13	2.04	0.40
2:H:75:ALA:HB3	2:H:100:PRO:HD3	2.03	0.40
2:I:39:ASP:HB3	2:L:55:ARG:HH12	1.87	0.40
1:D:69:SER:HB3	1:E:64:HIS:CG	2.57	0.40
2:L:66:LEU:HD23	2:L:66:LEU:HA	1.84	0.40
1:C:4:LEU:HD12	1:C:302:LEU:HD13	2.03	0.40
1:C:49:PHE:CD2	1:C:76:SER:HB3	2.57	0.40
2:G:65:PHE:CZ	2:G:85:ARG:NE	2.87	0.40
2:G:102:ARG:HA	2:G:125:PHE:O	2.21	0.40
2:I:14:ARG:H	2:I:88:ASN:H	1.70	0.40
2:I:36:THR:O	2:I:38:THR:N	2.52	0.40
2:J:71:VAL:HG13	2:J:83:VAL:HG21	2.02	0.40
2:K:40:GLN:OE1	2:K:63:ASN:HB2	2.21	0.40
2:L:62:GLU:CG	2:L:63:ASN:N	2.85	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	308/310 (99%)	260 (84%)	38 (12%)	10 (3%)	<b>4</b> <b>16</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	308/310 (99%)	257 (83%)	39 (13%)	12 (4%)	3	12
1	C	308/310 (99%)	260 (84%)	37 (12%)	11 (4%)	3	14
1	D	308/310 (99%)	265 (86%)	32 (10%)	11 (4%)	3	14
1	E	308/310 (99%)	262 (85%)	36 (12%)	10 (3%)	4	16
1	F	308/310 (99%)	263 (85%)	36 (12%)	9 (3%)	4	18
2	G	151/153 (99%)	105 (70%)	33 (22%)	13 (9%)	1	2
2	H	151/153 (99%)	104 (69%)	34 (22%)	13 (9%)	1	2
2	I	151/153 (99%)	112 (74%)	33 (22%)	6 (4%)	3	11
2	J	151/153 (99%)	104 (69%)	38 (25%)	9 (6%)	1	4
2	K	151/153 (99%)	125 (83%)	20 (13%)	6 (4%)	3	11
2	L	151/153 (99%)	94 (62%)	40 (26%)	17 (11%)	0	1
All	All	2754/2778 (99%)	2211 (80%)	416 (15%)	127 (5%)	2	9

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	30	LEU
1	A	133	GLN
1	A	243	VAL
1	B	131	SER
1	B	240	TYR
1	B	271	ASP
1	B	309	VAL
1	C	131	SER
2	G	142	GLU
2	H	36	THR
2	H	105	ASN
2	H	131	ALA
2	I	89	TYR
2	I	93	GLY
2	I	97	PRO
1	D	121	ASN
1	D	130	GLY
1	D	133	GLN
1	D	161	GLY
1	E	231	GLN
1	F	130	GLY

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	81	ALA
2	J	142	GLU
2	K	92	VAL
2	L	14	ARG
2	L	41	ARG
2	L	85	ARG
2	L	116	SER
1	A	231	GLN
1	A	291	ASN
1	B	130	GLY
1	C	216	GLU
1	C	231	GLN
1	C	270	VAL
1	C	309	VAL
2	G	34	LYS
2	G	69	ASP
2	G	83	VAL
2	G	116	SER
2	H	6	LYS
2	H	15	GLY
1	D	231	GLN
1	D	238	SER
1	E	130	GLY
1	F	231	GLN
1	F	309	VAL
2	J	52	GLU
2	J	115	ILE
2	L	7	LEU
2	L	17	VAL
2	L	38	THR
2	L	39	ASP
1	A	6	GLN
1	A	34	PRO
1	A	271	ASP
1	B	121	ASN
1	B	167	ARG
2	G	133	ASP
2	H	106	VAL
2	H	111	ASN
2	H	112	SER
2	H	123	SER
2	H	124	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	91	VAL
1	D	36	PRO
1	D	267	LEU
1	E	36	PRO
1	E	266	PRO
1	F	36	PRO
1	F	216	GLU
2	J	6	LYS
2	K	3	HIS
2	L	9	VAL
2	L	19	ASP
2	L	59	ILE
2	L	78	ALA
1	A	128	GLY
1	B	30	LEU
1	B	34	PRO
1	B	128	GLY
1	B	197	TYR
1	C	36	PRO
2	G	84	ASN
2	G	123	SER
2	G	132	ASN
2	H	147	HIS
1	D	271	ASP
1	E	240	TYR
1	E	268	PRO
1	E	293	ILE
2	J	3	HIS
2	J	90	GLU
2	L	123	SER
2	L	142	GLU
1	B	258	LYS
2	G	18	ILE
2	H	11	ALA
2	I	133	ASP
1	D	87	THR
1	F	52	SER
1	F	233	GLU
2	J	124	SER
2	L	54	GLY
2	L	88	ASN
2	L	131	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	161	GLY
1	C	240	TYR
2	G	111	ASN
2	I	120	PRO
1	D	128	GLY
1	C	82	GLY
1	C	265	HIS
2	G	49	PRO
1	E	135	PRO
2	J	22	PRO
2	K	9	VAL
2	K	106	VAL
2	H	79	PRO
2	K	12	ILE
1	C	130	GLY
2	G	12	ILE
1	F	128	GLY
1	F	270	VAL
2	K	79	PRO
1	E	128	GLY
1	E	267	LEU

### 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	261/261 (100%)	249 (95%)	12 (5%)	27	60
1	B	261/261 (100%)	249 (95%)	12 (5%)	27	60
1	C	261/261 (100%)	247 (95%)	14 (5%)	22	54
1	D	261/261 (100%)	253 (97%)	8 (3%)	40	74
1	E	261/261 (100%)	251 (96%)	10 (4%)	33	67
1	F	261/261 (100%)	248 (95%)	13 (5%)	24	57
2	G	137/137 (100%)	129 (94%)	8 (6%)	20	50
2	H	137/137 (100%)	126 (92%)	11 (8%)	12	33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	137/137 (100%)	127 (93%)	10 (7%)	14	38
2	J	137/137 (100%)	126 (92%)	11 (8%)	12	33
2	K	137/137 (100%)	125 (91%)	12 (9%)	10	30
2	L	137/137 (100%)	128 (93%)	9 (7%)	16	44
All	All	2388/2388 (100%)	2258 (95%)	130 (5%)	22	54

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	17	ARG
1	A	18	ASP
1	A	53	THR
1	A	59	PHE
1	A	136	THR
1	A	153	ASP
1	A	162	ASP
1	A	229	ARG
1	A	232	LYS
1	A	253	ASP
1	A	305	ASN
1	B	13	ASN
1	B	17	ARG
1	B	34	PRO
1	B	54	ARG
1	B	74	SER
1	B	80	SER
1	B	94	VAL
1	B	162	ASP
1	B	196	GLN
1	B	201	MET
1	B	253	ASP
1	B	309	VAL
1	C	13	ASN
1	C	17	ARG
1	C	54	ARG
1	C	59	PHE
1	C	86	GLU
1	C	131	SER
1	C	153	ASP
1	C	162	ASP

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	169	VAL
1	C	204	GLU
1	C	233	GLU
1	C	237	PRO
1	C	253	ASP
1	C	285	TYR
2	G	16	THR
2	G	36	THR
2	G	69	ASP
2	G	104	ASP
2	G	109	CYS
2	G	111	ASN
2	G	141	CYS
2	G	142	GLU
2	H	25	ILE
2	H	38	THR
2	H	56	LYS
2	H	69	ASP
2	H	84	ASN
2	H	86	ILE
2	H	109	CYS
2	H	111	ASN
2	H	125	PHE
2	H	127	VAL
2	H	133	ASP
2	I	12	ILE
2	I	52	GLU
2	I	57	ASP
2	I	76	LEU
2	I	91	VAL
2	I	97	PRO
2	I	109	CYS
2	I	111	ASN
2	I	114	CYS
2	I	147	HIS
1	D	13	ASN
1	D	17	ARG
1	D	81	LEU
1	D	105	ARG
1	D	147	GLU
1	D	285	TYR
1	D	305	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	309	VAL
1	E	17	ARG
1	E	18	ASP
1	E	59	PHE
1	E	80	SER
1	E	153	ASP
1	E	159	MET
1	E	233	GLU
1	E	253	ASP
1	E	266	PRO
1	E	309	VAL
1	F	13	ASN
1	F	17	ARG
1	F	18	ASP
1	F	59	PHE
1	F	147	GLU
1	F	183	ARG
1	F	237	PRO
1	F	253	ASP
1	F	278	ASP
1	F	285	TYR
1	F	305	ASN
1	F	307	ASP
1	F	309	VAL
2	J	19	ASP
2	J	31	SER
2	J	36	THR
2	J	50	SER
2	J	63	ASN
2	J	103	ILE
2	J	108	VAL
2	J	113	ASN
2	J	114	CYS
2	J	138	CYS
2	J	147	HIS
2	K	4	ASP
2	K	14	ARG
2	K	31	SER
2	K	52	GLU
2	K	57	ASP
2	K	71	VAL
2	K	96	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	K	109	CYS
2	K	128	ARG
2	K	133	ASP
2	K	143	LYS
2	K	149	VAL
2	L	4	ASP
2	L	17	VAL
2	L	18	ILE
2	L	20	HIS
2	L	85	ARG
2	L	87	ASP
2	L	96	ARG
2	L	109	CYS
2	L	138	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	21	ASN
1	A	41	HIS
1	A	132	ASN
1	A	156	HIS
1	A	231	GLN
1	A	246	GLN
1	A	291	ASN
1	A	305	ASN
1	B	13	ASN
1	B	21	ASN
1	B	35	GLN
1	B	41	HIS
1	B	108	GLN
1	B	156	HIS
1	B	231	GLN
1	B	291	ASN
1	B	305	ASN
1	C	13	ASN
1	C	21	ASN
1	C	35	GLN
1	C	41	HIS
1	C	132	ASN
1	C	156	HIS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	231	GLN
1	C	291	ASN
1	C	305	ASN
2	G	8	GLN
2	G	111	ASN
2	G	148	ASN
2	H	20	HIS
2	H	63	ASN
2	H	111	ASN
2	H	147	HIS
2	H	148	ASN
2	I	70	GLN
2	I	84	ASN
2	I	111	ASN
2	I	117	HIS
2	I	147	HIS
1	D	13	ASN
1	D	21	ASN
1	D	35	GLN
1	D	41	HIS
1	D	64	HIS
1	D	132	ASN
1	D	246	GLN
1	D	291	ASN
1	D	297	GLN
1	D	305	ASN
1	E	13	ASN
1	E	21	ASN
1	E	35	GLN
1	E	41	HIS
1	E	108	GLN
1	E	126	ASN
1	E	132	ASN
1	E	137	GLN
1	E	246	GLN
1	E	291	ASN
1	E	297	GLN
1	E	305	ASN
1	F	13	ASN
1	F	21	ASN
1	F	35	GLN
1	F	41	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	126	ASN
1	F	156	HIS
1	F	170	HIS
1	F	242	ASN
1	F	288	GLN
1	F	291	ASN
1	F	297	GLN
1	F	305	ASN
2	J	3	HIS
2	J	70	GLN
2	J	84	ASN
2	J	111	ASN
2	J	113	ASN
2	J	153	ASN
2	K	8	GLN
2	K	20	HIS
2	K	80	GLN
2	K	147	HIS
2	L	20	HIS
2	L	84	ASN
2	L	88	ASN
2	L	105	ASN

### 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](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	B	3002	-	4,4,4	2.20	2 (50%)	6,6,6	2.06	2 (33%)
3	FLC	F	2006	-	12,12,12	3.26	6 (50%)	17,17,17	1.62	5 (29%)
3	FLC	A	2001	-	12,12,12	4.48	5 (41%)	17,17,17	1.41	3 (17%)
3	FLC	E	2005	-	12,12,12	4.21	3 (25%)	17,17,17	1.52	4 (23%)
4	PO4	D	3004	-	4,4,4	1.92	1 (25%)	6,6,6	1.86	2 (33%)
4	PO4	F	3006	-	4,4,4	2.06	1 (25%)	6,6,6	1.93	3 (50%)
3	FLC	B	2002	-	12,12,12	2.92	5 (41%)	17,17,17	1.24	2 (11%)
4	PO4	E	3005	-	4,4,4	2.10	1 (25%)	6,6,6	2.00	3 (50%)
3	FLC	C	2003	-	12,12,12	4.81	7 (58%)	17,17,17	1.58	3 (17%)
4	PO4	A	3001	-	4,4,4	1.70	1 (25%)	6,6,6	2.22	4 (66%)
4	PO4	C	3003	-	4,4,4	2.20	1 (25%)	6,6,6	1.79	3 (50%)
3	FLC	D	2004	-	12,12,12	3.96	7 (58%)	17,17,17	1.28	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	F	2006	-	-	4/16/16/16	-
3	FLC	A	2001	-	-	9/16/16/16	-
3	FLC	E	2005	-	-	8/16/16/16	-
3	FLC	B	2002	-	-	7/16/16/16	-
3	FLC	C	2003	-	-	5/16/16/16	-
3	FLC	D	2004	-	-	9/16/16/16	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2003	FLC	CB-CBC	12.51	1.66	1.53
3	A	2001	FLC	CB-CBC	9.80	1.63	1.53
3	E	2005	FLC	CB-CBC	8.68	1.62	1.53

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2003	FLC	CG-CB	8.39	1.64	1.53
3	A	2001	FLC	CA-CB	8.13	1.63	1.53
3	E	2005	FLC	CA-CB	8.06	1.63	1.53
3	D	2004	FLC	CB-CBC	7.91	1.61	1.53
3	A	2001	FLC	CG-CB	7.50	1.63	1.53
3	E	2005	FLC	CG-CB	7.43	1.63	1.53
3	D	2004	FLC	CA-CB	7.37	1.63	1.53
3	F	2006	FLC	CA-CB	7.15	1.62	1.53
3	F	2006	FLC	CG-CB	6.59	1.62	1.53
3	D	2004	FLC	CG-CB	6.49	1.61	1.53
3	B	2002	FLC	CB-CBC	6.00	1.59	1.53
3	C	2003	FLC	CA-CB	5.45	1.60	1.53
3	B	2002	FLC	CG-CB	5.26	1.60	1.53
3	B	2002	FLC	CA-CB	4.39	1.59	1.53
4	C	3003	PO4	P-O1	4.19	1.60	1.50
4	E	3005	PO4	P-O1	4.15	1.60	1.50
4	F	3006	PO4	P-O1	4.07	1.60	1.50
4	D	3004	PO4	P-O1	3.53	1.59	1.50
3	F	2006	FLC	CB-CBC	3.39	1.56	1.53
4	B	3002	PO4	P-O1	3.36	1.58	1.50
4	A	3001	PO4	P-O1	3.21	1.58	1.50
3	A	2001	FLC	OG2-CGC	-2.57	1.22	1.30
4	B	3002	PO4	P-O3	2.57	1.62	1.54
3	B	2002	FLC	OG2-CGC	-2.55	1.22	1.30
3	C	2003	FLC	CG-CGC	2.43	1.58	1.50
3	A	2001	FLC	CA-CAC	2.42	1.58	1.50
3	F	2006	FLC	CG-CGC	2.39	1.58	1.50
3	D	2004	FLC	OA2-CAC	-2.36	1.22	1.30
3	F	2006	FLC	OG2-CGC	-2.18	1.23	1.30
3	C	2003	FLC	OA2-CAC	-2.17	1.23	1.30
3	F	2006	FLC	OA2-CAC	-2.14	1.23	1.30
3	D	2004	FLC	OG2-CGC	-2.09	1.23	1.30
3	C	2003	FLC	CA-CAC	2.07	1.57	1.50
3	D	2004	FLC	CA-CAC	2.07	1.57	1.50
3	D	2004	FLC	OHB-CB	2.06	1.47	1.43
3	B	2002	FLC	CG-CGC	2.06	1.57	1.50
3	C	2003	FLC	OG2-CGC	-2.04	1.23	1.30

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2006	FLC	CB-CA-CAC	3.47	122.23	113.81

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	PO4	O4-P-O1	-3.25	99.00	110.89
3	C	2003	FLC	CG-CB-CBC	3.22	117.02	110.11
3	D	2004	FLC	OHB-CB-CG	-3.17	101.99	109.40
4	E	3005	PO4	O3-P-O1	-3.06	99.71	110.89
4	B	3002	PO4	O3-P-O1	-3.04	99.77	110.89
3	B	2002	FLC	OHB-CB-CG	-3.01	102.36	109.40
3	C	2003	FLC	OHB-CB-CG	-2.92	102.57	109.40
3	A	2001	FLC	CG-CB-CBC	2.91	116.35	110.11
4	A	3001	PO4	O3-P-O1	-2.80	100.65	110.89
4	D	3004	PO4	O4-P-O1	-2.75	100.85	110.89
3	C	2003	FLC	OB2-CBC-CB	2.72	117.77	113.05
4	B	3002	PO4	O4-P-O1	-2.67	101.13	110.89
3	E	2005	FLC	CG-CB-CBC	2.62	115.74	110.11
3	D	2004	FLC	CB-CA-CAC	2.61	120.14	113.81
4	F	3006	PO4	O3-P-O1	-2.61	101.35	110.89
3	E	2005	FLC	CB-CA-CAC	2.60	120.10	113.81
3	A	2001	FLC	CB-CA-CAC	2.53	119.93	113.81
3	E	2005	FLC	OHB-CB-CG	-2.49	103.58	109.40
4	F	3006	PO4	O4-P-O1	-2.49	101.79	110.89
3	F	2006	FLC	OB1-CBC-CB	-2.43	118.81	122.25
4	C	3003	PO4	O3-P-O1	-2.38	102.18	110.89
4	E	3005	PO4	O4-P-O1	-2.38	102.19	110.89
4	C	3003	PO4	O4-P-O1	-2.37	102.22	110.89
4	F	3006	PO4	O4-P-O2	2.34	115.47	107.97
4	D	3004	PO4	O3-P-O1	-2.27	102.58	110.89
3	F	2006	FLC	OHB-CB-CG	-2.22	104.20	109.40
3	A	2001	FLC	OHB-CB-CBC	-2.20	105.77	108.86
3	E	2005	FLC	OB2-CBC-CB	2.19	116.84	113.05
3	F	2006	FLC	CA-CB-CBC	-2.15	105.48	110.11
4	E	3005	PO4	O4-P-O2	2.15	114.86	107.97
3	B	2002	FLC	CG-CB-CBC	2.12	114.66	110.11
4	A	3001	PO4	O4-P-O2	2.10	114.71	107.97
4	A	3001	PO4	O2-P-O1	2.06	118.44	110.89
3	F	2006	FLC	CG-CB-CBC	2.02	114.45	110.11
4	C	3003	PO4	O4-P-O2	2.02	114.46	107.97

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	FLC	CAC-CA-CB-CBC
3	A	2001	FLC	CAC-CA-CB-CG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	2001	FLC	CAC-CA-CB-OHB
3	A	2001	FLC	CG-CB-CBC-OB1
3	A	2001	FLC	CG-CB-CBC-OB2
3	A	2001	FLC	OHB-CB-CBC-OB1
3	A	2001	FLC	OHB-CB-CBC-OB2
3	B	2002	FLC	CAC-CA-CB-CBC
3	B	2002	FLC	CAC-CA-CB-CG
3	B	2002	FLC	CAC-CA-CB-OHB
3	B	2002	FLC	CG-CB-CBC-OB1
3	B	2002	FLC	OHB-CB-CBC-OB1
3	B	2002	FLC	OHB-CB-CBC-OB2
3	C	2003	FLC	CG-CB-CBC-OB1
3	C	2003	FLC	CG-CB-CBC-OB2
3	C	2003	FLC	OHB-CB-CBC-OB1
3	C	2003	FLC	OHB-CB-CBC-OB2
3	D	2004	FLC	CAC-CA-CB-CBC
3	D	2004	FLC	CAC-CA-CB-CG
3	D	2004	FLC	CAC-CA-CB-OHB
3	D	2004	FLC	OHB-CB-CBC-OB1
3	D	2004	FLC	OHB-CB-CBC-OB2
3	E	2005	FLC	CAC-CA-CB-CBC
3	E	2005	FLC	CAC-CA-CB-CG
3	E	2005	FLC	CAC-CA-CB-OHB
3	F	2006	FLC	CG-CB-CBC-OB2
3	F	2006	FLC	OHB-CB-CBC-OB1
3	F	2006	FLC	OHB-CB-CBC-OB2
3	B	2002	FLC	CG-CB-CBC-OB2
3	D	2004	FLC	CA-CB-CBC-OB2
3	F	2006	FLC	CG-CB-CBC-OB1
3	A	2001	FLC	CBC-CB-CG-CGC
3	D	2004	FLC	CG-CB-CBC-OB1
3	D	2004	FLC	CG-CB-CBC-OB2
3	E	2005	FLC	CA-CB-CBC-OB1
3	E	2005	FLC	CA-CB-CBC-OB2
3	E	2005	FLC	CG-CB-CBC-OB1
3	E	2005	FLC	CG-CB-CBC-OB2
3	E	2005	FLC	CBC-CB-CG-CGC
3	D	2004	FLC	CA-CB-CBC-OB1
3	A	2001	FLC	OHB-CB-CG-CGC
3	C	2003	FLC	CAC-CA-CB-CG

There are no ring outliers.

11 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	3002	PO4	1	0
3	F	2006	FLC	1	0
3	A	2001	FLC	7	0
3	E	2005	FLC	4	0
4	D	3004	PO4	1	0
4	F	3006	PO4	2	0
3	B	2002	FLC	4	0
4	E	3005	PO4	1	0
3	C	2003	FLC	4	0
4	A	3001	PO4	5	0
3	D	2004	FLC	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	310/310 (100%)	-0.36	1 (0%) 94 94	15, 42, 66, 78	0
1	B	310/310 (100%)	-0.13	3 (0%) 82 82	20, 60, 91, 113	0
1	C	310/310 (100%)	-0.30	1 (0%) 94 94	19, 46, 69, 97	0
1	D	310/310 (100%)	-0.19	3 (0%) 82 82	31, 59, 83, 109	0
1	E	310/310 (100%)	-0.19	2 (0%) 89 89	34, 54, 85, 103	0
1	F	310/310 (100%)	-0.12	5 (1%) 72 71	36, 66, 91, 118	0
2	G	153/153 (100%)	0.57	21 (13%) 3 2	45, 92, 161, 182	0
2	H	153/153 (100%)	0.05	9 (5%) 22 18	40, 63, 133, 171	0
2	I	153/153 (100%)	0.61	20 (13%) 3 2	57, 99, 144, 161	0
2	J	153/153 (100%)	0.60	16 (10%) 6 5	49, 89, 164, 192	0
2	K	153/153 (100%)	0.31	13 (8%) 10 8	34, 63, 149, 181	0
2	L	153/153 (100%)	1.08	31 (20%) 1 0	62, 126, 163, 170	0
All	All	2778/2778 (100%)	0.03	125 (4%) 33 29	15, 61, 130, 192	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	3	HIS	11.6
2	J	1	MET	10.7
2	G	1	MET	10.0
2	J	7	LEU	9.7
2	K	4	ASP	9.1
2	L	17	VAL	8.3
2	J	2	THR	7.7
2	J	9	VAL	7.5
2	K	2	THR	7.3
2	I	153	ASN	7.3
2	G	2	THR	7.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	I	2	THR	6.8
2	H	4	ASP	6.8
2	J	6	LYS	6.5
2	L	8	GLN	6.4
2	J	10	GLU	6.4
2	G	5	ASN	6.3
2	K	9	VAL	6.3
2	I	152	ALA	6.1
2	G	3	HIS	5.9
2	G	9	VAL	5.9
2	L	79	PRO	5.7
2	G	153	ASN	5.6
2	K	6	LYS	5.6
2	K	5	ASN	5.6
2	G	11	ALA	5.4
2	H	1	MET	5.4
2	J	95	SER	5.4
1	F	310	LEU	5.3
2	L	10	GLU	5.2
2	H	10	GLU	5.0
2	K	153	ASN	4.9
2	K	8	GLN	4.8
2	J	11	ALA	4.6
2	K	10	GLU	4.6
1	C	309	VAL	4.5
2	G	10	GLU	4.5
2	L	75	ALA	4.5
2	L	16	THR	4.5
2	I	49	PRO	4.4
2	L	80	GLN	4.4
2	H	6	LYS	4.4
2	I	1	MET	4.2
2	J	8	GLN	4.1
2	L	76	LEU	4.1
2	H	5	ASN	4.0
2	G	8	GLN	4.0
2	G	152	ALA	4.0
2	K	1	MET	4.0
2	G	53	MET	3.9
2	I	63	ASN	3.8
2	L	9	VAL	3.8
2	I	50	SER	3.7

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	153	ASN	3.7
2	G	4	ASP	3.6
2	L	87	ASP	3.6
1	A	310	LEU	3.6
2	L	151	LEU	3.6
2	L	152	ALA	3.6
2	I	30	LEU	3.5
2	J	5	ASN	3.5
2	I	8	GLN	3.5
2	G	51	GLY	3.4
1	B	255	HIS	3.4
2	L	131	ALA	3.4
2	G	151	LEU	3.3
2	L	5	ASN	3.2
2	H	2	THR	3.2
2	I	66	LEU	3.2
2	K	7	LEU	3.2
2	L	18	ILE	3.1
2	L	85	ARG	3.1
1	E	271	ASP	3.1
1	F	208	ALA	3.1
2	I	9	VAL	3.1
2	L	3	HIS	3.1
2	H	3	HIS	3.0
2	L	1	MET	3.0
1	D	255	HIS	3.0
2	L	153	ASN	3.0
2	I	54	GLY	3.0
2	I	64	THR	2.9
2	L	61	ILE	2.8
2	L	77	TYR	2.8
1	D	254	LEU	2.8
2	L	4	ASP	2.8
2	G	7	LEU	2.8
2	G	92	VAL	2.8
2	L	74	LEU	2.8
2	I	99	LEU	2.7
1	E	309	VAL	2.7
2	L	92	VAL	2.7
2	J	132	ASN	2.6
2	L	82	THR	2.6
2	I	35	LEU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	J	153	ASN	2.6
2	L	128	ARG	2.5
2	L	66	LEU	2.5
2	J	3	HIS	2.4
2	L	62	GLU	2.4
1	B	240	TYR	2.4
2	J	92	VAL	2.4
2	J	106	VAL	2.4
2	G	97	PRO	2.3
2	K	11	ALA	2.3
2	G	52	GLU	2.3
2	I	5	ASN	2.3
2	H	76	LEU	2.3
2	G	6	LYS	2.3
2	I	103	ILE	2.3
2	K	77	TYR	2.3
1	F	254	LEU	2.3
2	G	76	LEU	2.2
2	L	127	VAL	2.2
2	G	131	ALA	2.2
1	F	309	VAL	2.2
2	L	2	THR	2.1
1	F	220	ALA	2.1
2	I	37	GLU	2.1
2	L	100	PRO	2.1
1	D	219	MET	2.1
2	I	53	MET	2.1
2	I	65	PHE	2.1
2	J	89	TYR	2.0
1	B	243	VAL	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	ZN	J	1004	1/1	0.81	0.09	52,52,52,52	0
5	ZN	I	1003	1/1	0.87	0.17	67,67,67,67	0
3	FLC	D	2004	13/13	0.88	0.23	63,65,68,70	0
3	FLC	C	2003	13/13	0.91	0.23	46,50,55,55	0
3	FLC	A	2001	13/13	0.91	0.23	34,48,52,55	0
3	FLC	B	2002	13/13	0.92	0.26	65,68,69,71	0
3	FLC	E	2005	13/13	0.93	0.23	68,70,72,72	0
3	FLC	F	2006	13/13	0.93	0.24	61,64,67,68	0
5	ZN	K	1005	1/1	0.93	0.15	64,64,64,64	0
4	PO4	F	3006	5/5	0.96	0.22	49,49,51,51	0
4	PO4	E	3005	5/5	0.97	0.23	41,41,42,43	0
5	ZN	L	1006	1/1	0.97	0.14	63,63,63,63	0
4	PO4	A	3001	5/5	0.98	0.20	26,26,30,32	0
4	PO4	B	3002	5/5	0.98	0.28	37,37,40,41	0
4	PO4	C	3003	5/5	0.98	0.23	38,39,41,41	0
5	ZN	G	1001	1/1	0.99	0.11	57,57,57,57	0
5	ZN	H	1002	1/1	0.99	0.14	56,56,56,56	0
4	PO4	D	3004	5/5	0.99	0.19	29,30,33,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.