



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:24 PM GMT

PDB ID : 1TF7
Title : Crystal Structure of Circadian Clock Protein KaiC
Authors : Pattanayek, R.; Wang, J.; Mori, T.; Xu, Y.; Johnson, C.H.; Egli, M.
Deposited on : 2004-05-26
Resolution : 2.80 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

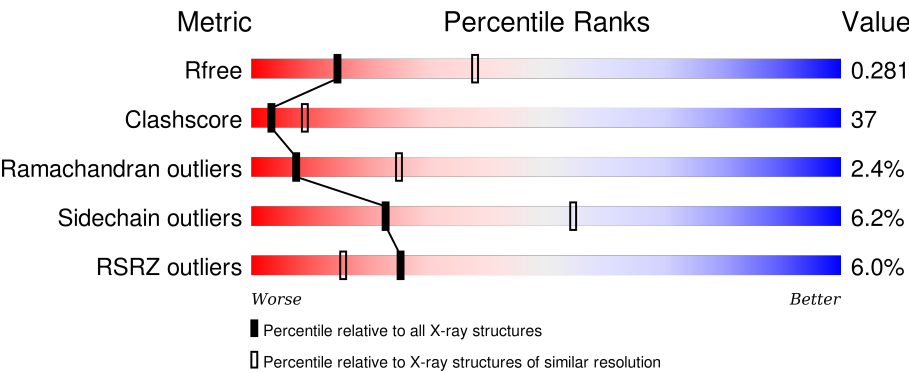
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	525	<div><div>8%</div><div><div></div><div>47%</div><div>40%</div><div>5%</div><div>8%</div></div></div>
1	B	525	<div><div>7%</div><div><div></div><div>46%</div><div>41%</div><div>5%</div><div>8%</div></div></div>
1	C	525	<div><div>5%</div><div><div></div><div>41%</div><div>44%</div><div>6%</div><div>8%</div></div></div>
1	D	525	<div><div>4%</div><div><div></div><div>47%</div><div>40%</div><div>5%</div><div>8%</div></div></div>
1	E	525	<div><div>5%</div><div><div></div><div>46%</div><div>41%</div><div>6%</div><div>8%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	525	<div><div></div><div>4%</div><div>43%</div><div>43%</div><div>6%</div><div>8%</div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 23333 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 KaiC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3815	2407	670	723	15			
1	B	484	Total	C	N	O	S	0	0	0
			3815	2407	670	723	15			
1	C	484	Total	C	N	O	S	0	0	0
			3815	2407	670	723	15			
1	D	484	Total	C	N	O	S	0	0	0
			3815	2407	670	723	15			
1	E	484	Total	C	N	O	S	0	0	0
			3815	2407	670	723	15			
1	F	484	Total	C	N	O	S	0	0	0
			3815	2407	670	723	15			

There are 36 discrepancies between the modelled and reference sequences:

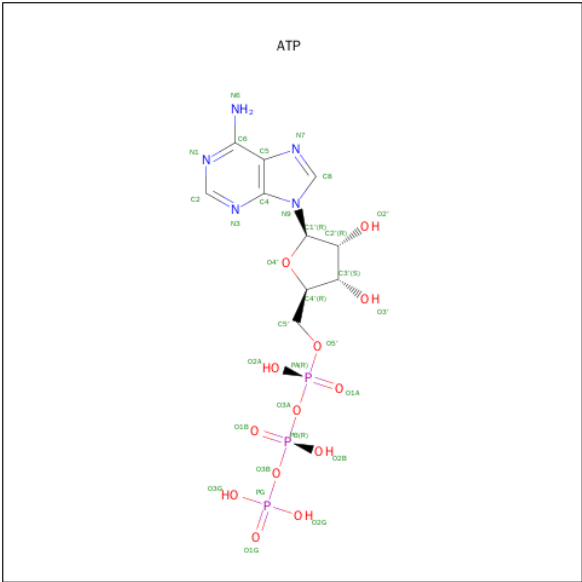
Chain	Residue	Modelled	Actual	Comment	Reference
A	520	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
A	521	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
A	522	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
A	523	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
A	524	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
A	525	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
B	520	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
B	521	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
B	522	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
B	523	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
B	524	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
B	525	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
C	520	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
C	521	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
C	522	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
C	523	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
C	524	HIS	-	EXPRESSION TAG	UNP Q9Z3H2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	525	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
D	520	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
D	521	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
D	522	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
D	523	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
D	524	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
D	525	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
E	520	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
E	521	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
E	522	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
E	523	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
E	524	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
E	525	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
F	520	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
F	521	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
F	522	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
F	523	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
F	524	HIS	-	EXPRESSION TAG	UNP Q9Z3H2
F	525	HIS	-	EXPRESSION TAG	UNP Q9Z3H2

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

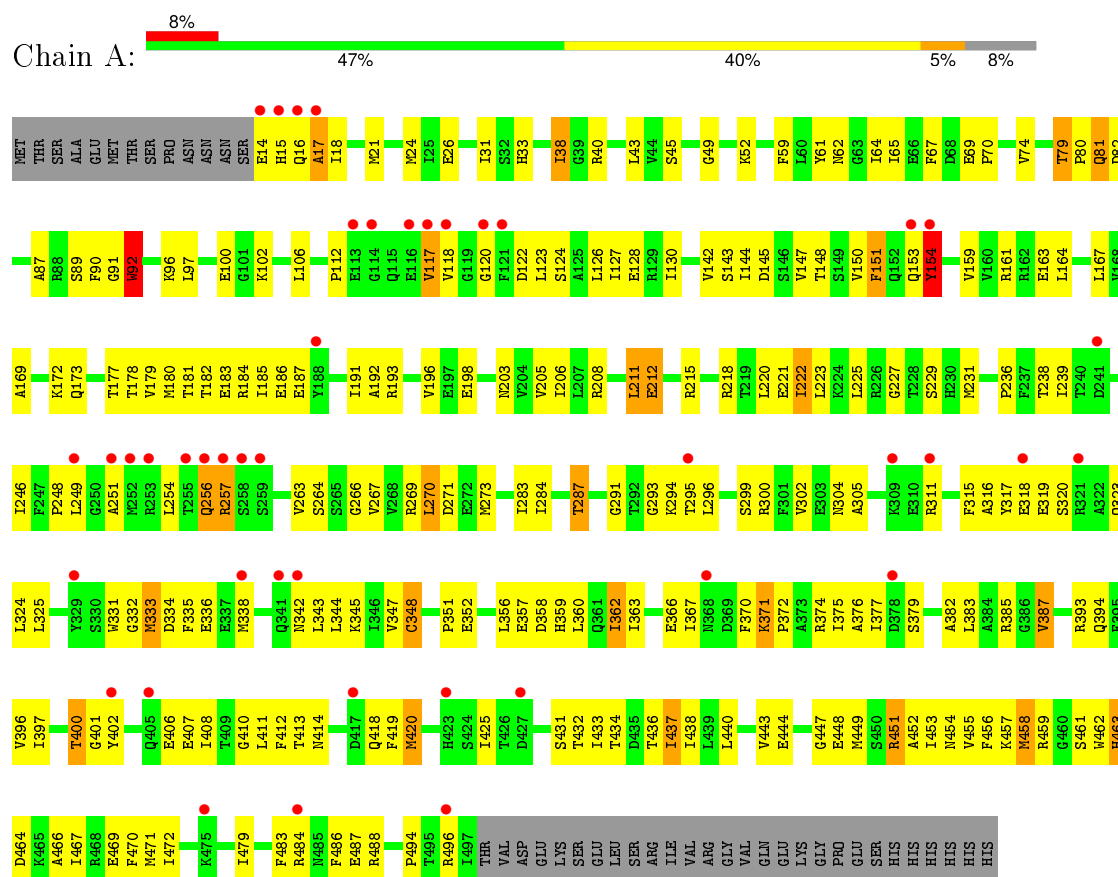
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	7	Total	O	0	0
			7	7		
3	C	7	Total	O	0	0
			7	7		
3	D	13	Total	O	0	0
			13	13		
3	E	12	Total	O	0	0
			12	12		
3	F	23	Total	O	0	0
			23	23		

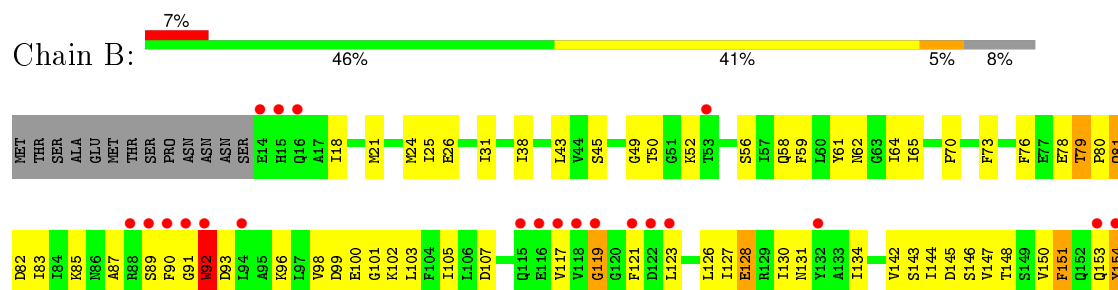
3 Residue-property plots

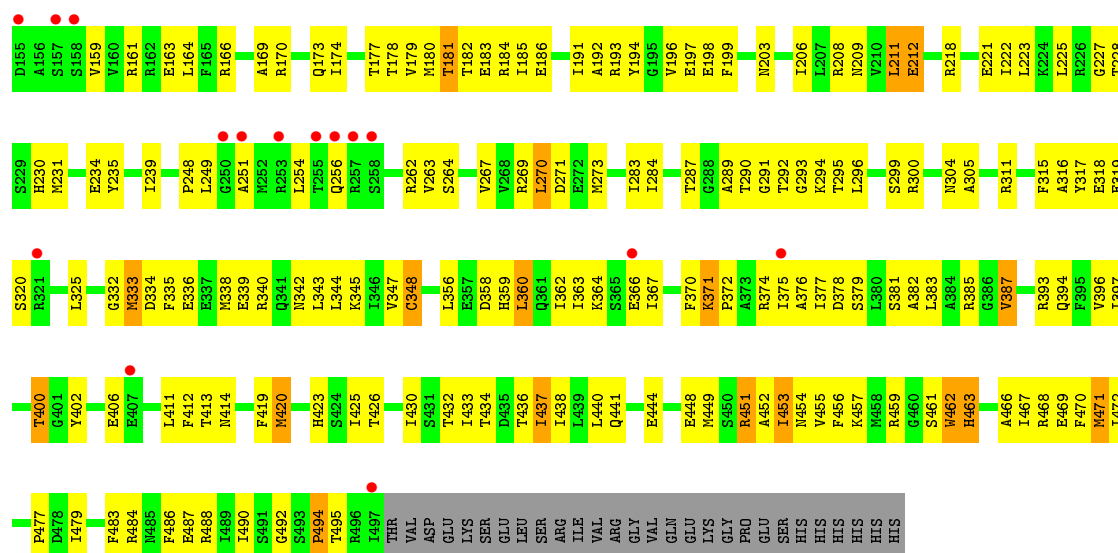
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: KaiC

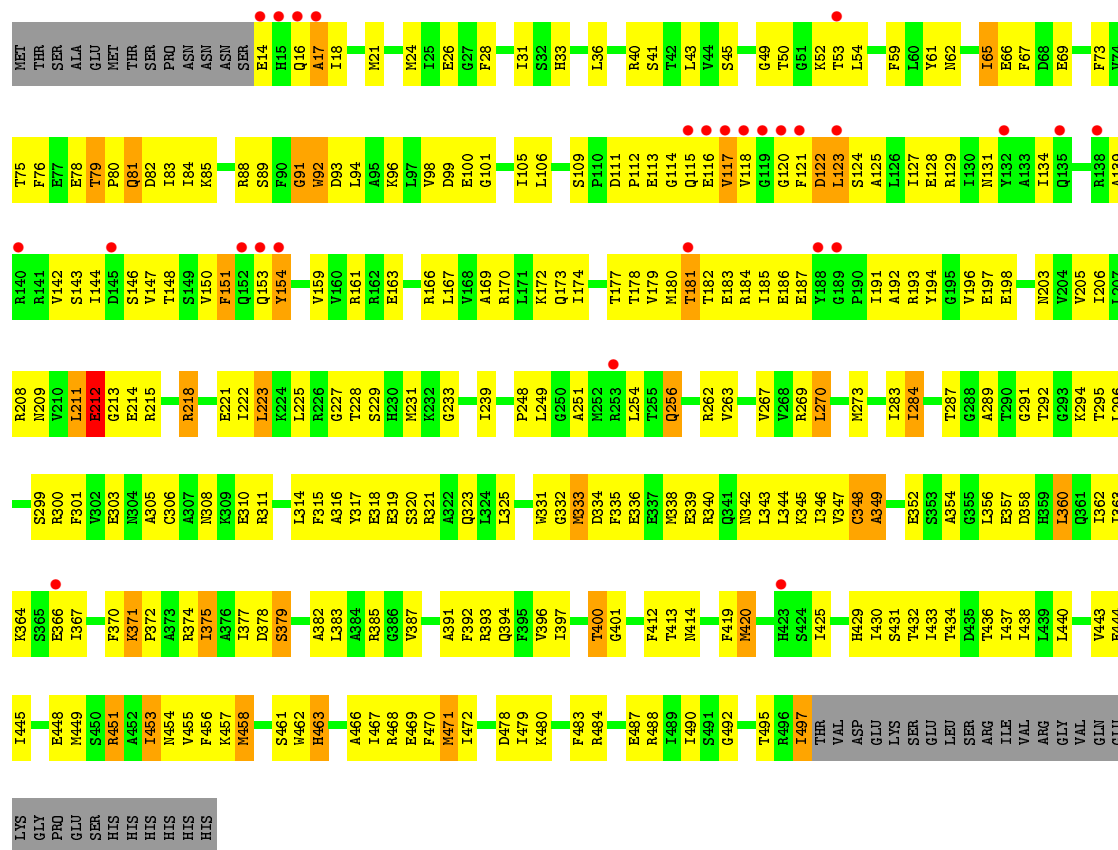


• Molecule 1: KaiC



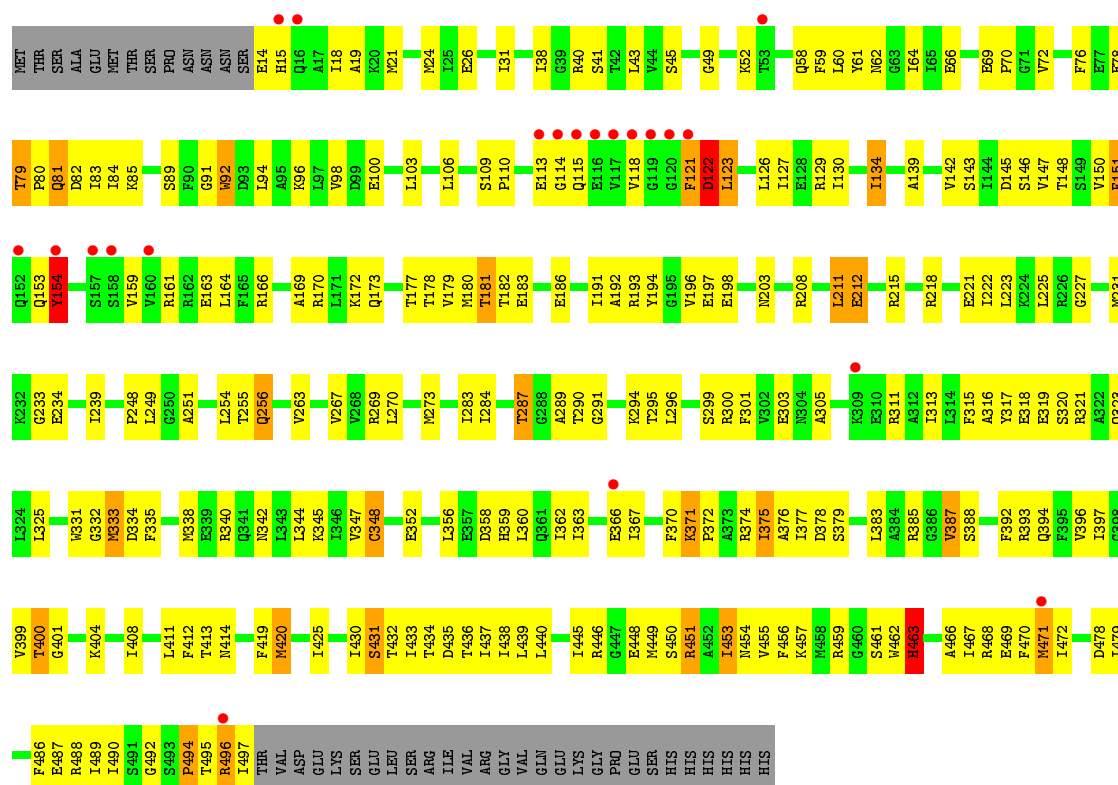


• Molecule 1: KaiC

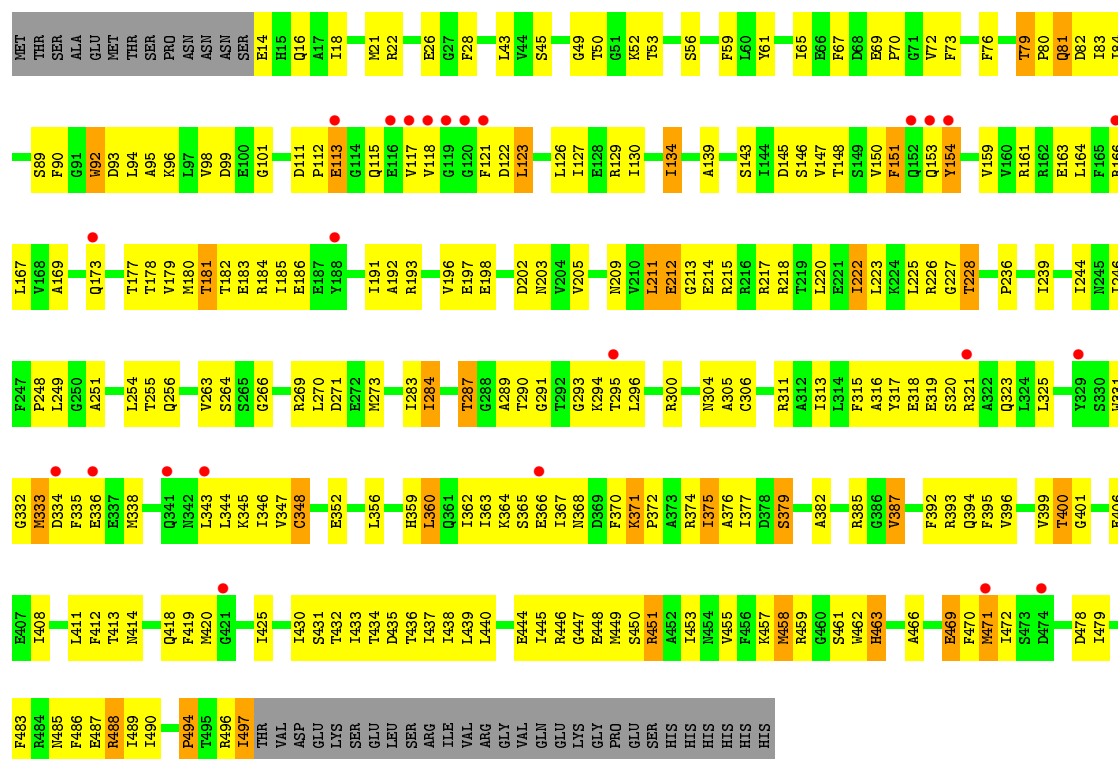


• Molecule 1: KaiC

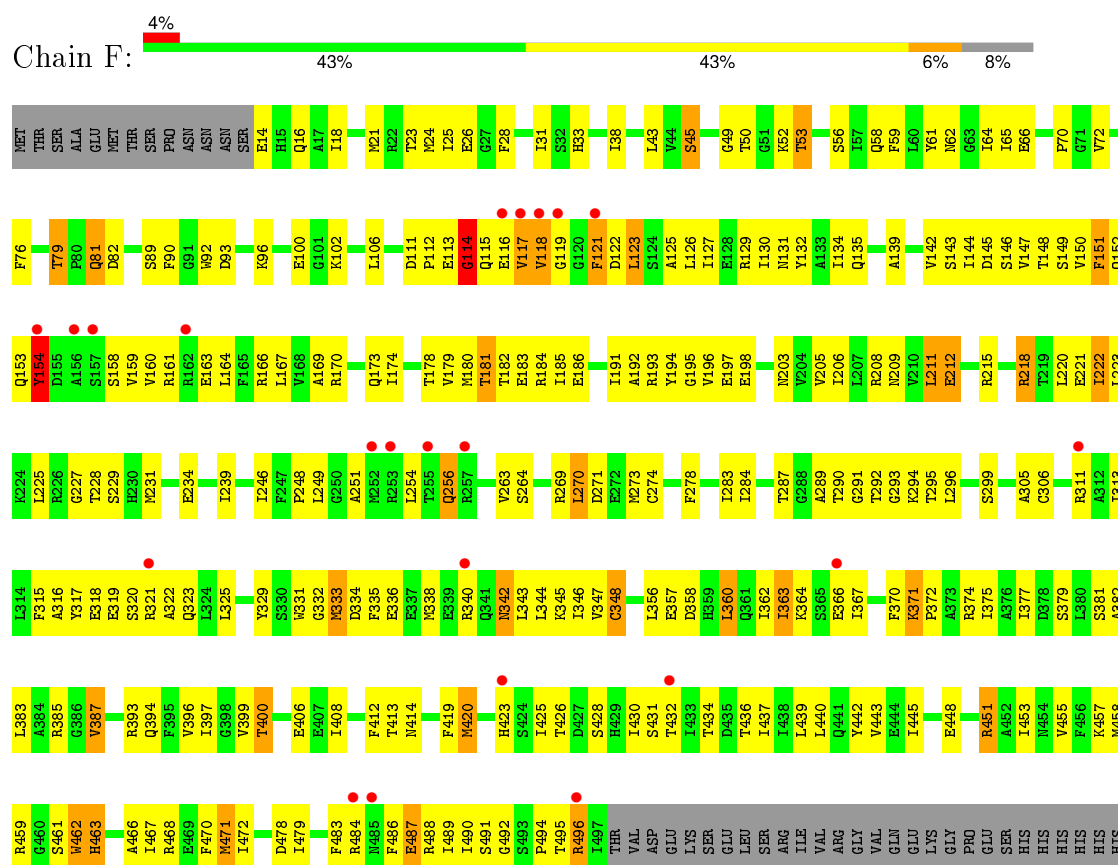




• Molecule 1: KaiC



• Molecule 1: KaiC



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.87Å 135.58Å 204.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.73 – 2.83	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 89.7 (29.73-2.83)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.85Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.280 0.241 , 0.281	Depositor DCC
R_{free} test set	4041 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.7	EDS
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 87615 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23333	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.47	3/3880 (0.1%)	0.66	3/5229 (0.1%)
1	B	0.40	1/3880 (0.0%)	0.62	0/5229
1	C	0.45	4/3880 (0.1%)	0.66	6/5229 (0.1%)
1	D	0.46	1/3880 (0.0%)	0.69	5/5229 (0.1%)
1	E	0.43	1/3880 (0.0%)	0.66	1/5229 (0.0%)
1	F	0.40	0/3880	0.64	1/5229 (0.0%)
All	All	0.44	10/23280 (0.0%)	0.66	16/31374 (0.1%)

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

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

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	TRP	CB-CG	11.02	1.70	1.50
1	A	92	TRP	CA-CB	9.65	1.75	1.53
1	D	91	GLY	C-O	-8.20	1.10	1.23
1	A	92	TRP	CA-C	6.83	1.70	1.52
1	C	91	GLY	CA-C	-6.37	1.41	1.51
1	C	92	TRP	N-CA	-5.54	1.35	1.46
1	B	92	TRP	CD2-CE3	-5.53	1.32	1.40
1	C	92	TRP	CG-CD1	-5.25	1.29	1.36
1	E	92	TRP	CD2-CE3	-5.24	1.32	1.40
1	C	92	TRP	CA-CB	-5.15	1.42	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	TRP	CB-CG-CD1	8.83	138.48	127.00
1	A	92	TRP	CB-CG-CD2	-7.66	116.64	126.60
1	D	91	GLY	CA-C-O	7.54	134.17	120.60
1	D	92	TRP	CB-CG-CD1	7.49	136.74	127.00
1	D	92	TRP	CA-CB-CG	7.19	127.37	113.70
1	D	92	TRP	CB-CG-CD2	-7.12	117.34	126.60
1	C	91	GLY	CA-C-O	6.73	132.72	120.60
1	C	213	GLY	N-CA-C	-6.58	96.64	113.10
1	E	213	GLY	N-CA-C	-6.37	97.17	113.10
1	D	92	TRP	N-CA-CB	-5.91	99.97	110.60
1	C	92	TRP	CB-CG-CD2	5.85	134.21	126.60
1	C	92	TRP	CG-CD1-NE1	5.39	115.49	110.10
1	F	114	GLY	N-CA-C	5.38	126.56	113.10
1	C	92	TRP	CB-CG-CD1	-5.22	120.21	127.00
1	A	92	TRP	CB-CA-C	5.16	120.72	110.40
1	C	92	TRP	CD1-CG-CD2	-5.04	102.27	106.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	257	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	3815	0	3814	287	0
1	B	3815	0	3814	288	0
1	C	3815	0	3814	302	0
1	D	3815	0	3814	318	0
1	E	3815	0	3814	287	0
1	F	3815	0	3814	340	0
2	A	62	0	24	8	0
2	B	62	0	24	10	0
2	C	62	0	24	8	0
2	D	62	0	24	7	0
2	E	62	0	24	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	62	0	24	8	0
3	A	9	0	0	0	0
3	B	7	0	0	0	0
3	C	7	0	0	2	0
3	D	13	0	0	1	0
3	E	12	0	0	2	0
3	F	23	0	0	5	0
All	All	23333	0	23028	1709	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 37.

All (1709) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:TRP:CB	1:A:92:TRP:CA	1.75	1.58
1:A:257:ARG:NH2	1:A:407:GLU:HG2	1.50	1.26
1:F:313:ILE:HB	1:F:375:ILE:CD1	1.74	1.18
1:B:284:ILE:HD12	1:B:436:THR:HB	1.30	1.14
1:D:284:ILE:HD12	1:D:436:THR:HB	1.35	1.09
1:E:263:VAL:HG12	1:E:374:ARG:HH21	1.19	1.07
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.32	1.06
1:D:60:LEU:O	1:D:64:ILE:HD13	1.57	1.04
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.19	1.03
1:E:284:ILE:HD12	1:E:436:THR:HB	1.40	1.03
1:D:486:PHE:CB	1:D:489:ILE:HD11	1.89	1.03
1:C:284:ILE:HD12	1:C:436:THR:HB	1.34	1.03
1:C:205:VAL:HG22	1:C:222:ILE:HD13	1.38	1.02
1:E:123:LEU:HD13	1:E:166:ARG:HD2	1.41	1.01
1:A:257:ARG:NH2	1:A:407:GLU:CG	2.22	1.01
1:C:61:TYR:O	1:C:65:ILE:HD13	1.60	1.01
1:A:205:VAL:HG22	1:A:222:ILE:HD12	1.38	1.01
1:D:126:LEU:O	1:D:130:ILE:HD13	1.62	0.99
1:E:205:VAL:HG22	1:E:222:ILE:HD12	1.40	0.99
1:D:147:VAL:HG11	1:D:180:MET:HE3	1.41	0.99
1:B:263:VAL:HG12	1:B:374:ARG:HH21	1.27	0.99
1:F:205:VAL:HG22	1:F:222:ILE:HD12	1.44	0.99
1:A:379:SER:H	1:A:413:THR:HB	1.24	0.98
1:C:287:THR:HG23	1:C:414:ASN:HD22	1.28	0.97
1:D:486:PHE:HB3	1:D:489:ILE:HD11	1.46	0.96
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.32	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ALA:O	1:A:92:TRP:HB2	1.67	0.95
1:B:311:ARG:HD2	1:B:371:LYS:HD2	1.45	0.95
1:B:64:ILE:HD12	1:B:102:LYS:HB3	1.48	0.95
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.29	0.94
1:A:257:ARG:HH21	1:A:407:GLU:HG2	1.08	0.94
1:D:313:ILE:HD12	1:D:367:ILE:HD13	1.50	0.94
1:E:305:ALA:HB2	1:E:374:ARG:HD2	1.50	0.94
1:E:315:PHE:CE2	1:E:366:GLU:OE1	2.20	0.93
1:D:123:LEU:HD12	1:D:166:ARG:HD2	1.50	0.93
1:D:453:ILE:HG21	1:D:479:ILE:HD12	1.47	0.93
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.31	0.93
1:C:315:PHE:HE2	1:C:366:GLU:OE1	1.52	0.92
1:D:79:THR:HG22	1:D:82:ASP:H	1.32	0.92
1:F:313:ILE:HB	1:F:375:ILE:HD11	1.50	0.92
1:B:147:VAL:O	1:B:150:VAL:HG12	1.70	0.92
1:A:362:ILE:O	1:A:366:GLU:HG3	1.70	0.92
1:C:311:ARG:HD2	1:C:371:LYS:HD2	1.51	0.92
1:E:313:ILE:HD12	1:E:367:ILE:HD13	1.50	0.92
1:C:315:PHE:CE2	1:C:366:GLU:OE1	2.24	0.91
1:F:64:ILE:HD12	1:F:102:LYS:HB3	1.52	0.91
1:D:287:THR:HG23	1:D:414:ASN:HD22	1.36	0.91
1:B:64:ILE:HD11	1:B:70:PRO:HA	1.52	0.90
1:F:434:THR:HG23	1:F:437:ILE:HD11	1.52	0.90
1:D:146:SER:H	1:D:181:THR:HG22	1.36	0.90
1:F:106:LEU:HD11	1:F:129:ARG:CZ	2.02	0.90
1:E:315:PHE:HE2	1:E:366:GLU:OE1	1.55	0.89
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.54	0.89
1:A:147:VAL:O	1:A:150:VAL:HG12	1.72	0.89
1:F:315:PHE:CE2	1:F:366:GLU:OE1	2.24	0.89
1:B:305:ALA:HB2	1:B:374:ARG:HD2	1.53	0.89
1:F:379:SER:H	1:F:413:THR:HB	1.37	0.89
1:C:84:ILE:HD12	1:C:94:LEU:HB2	1.55	0.89
1:C:147:VAL:O	1:C:150:VAL:HG12	1.72	0.88
1:C:495:THR:HA	1:D:487:GLU:OE2	1.73	0.88
1:C:14:GLU:HG3	1:C:16:GLN:H	1.39	0.88
1:B:31:ILE:HG22	1:B:222:ILE:HD12	1.52	0.87
1:A:257:ARG:HH21	1:A:407:GLU:CG	1.85	0.87
1:E:147:VAL:O	1:E:150:VAL:HG12	1.75	0.86
1:F:123:LEU:HD12	1:F:166:ARG:HD2	1.56	0.86
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.55	0.86
1:D:18:ILE:H	1:D:18:ILE:HD12	1.39	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:VAL:HG11	1:C:180:MET:HE3	1.59	0.85
1:E:79:THR:CG2	1:E:81:GLN:HG2	2.06	0.85
1:E:287:THR:HG23	1:E:414:ASN:HD22	1.42	0.85
1:D:379:SER:H	1:D:413:THR:HB	1.42	0.85
1:E:147:VAL:HG11	1:E:180:MET:HE2	1.59	0.84
1:C:449:MET:CE	1:D:490:ILE:HD11	2.07	0.84
1:D:315:PHE:CE2	1:D:366:GLU:OE1	2.30	0.84
1:E:263:VAL:HG12	1:E:374:ARG:NH2	1.91	0.84
1:B:437:ILE:CD1	1:B:457:LYS:HE2	2.07	0.84
1:A:358:ASP:O	1:A:362:ILE:HD13	1.77	0.83
1:A:311:ARG:HD2	1:A:371:LYS:HD2	1.60	0.83
1:D:147:VAL:O	1:D:150:VAL:HG12	1.78	0.83
1:B:263:VAL:HG12	1:B:374:ARG:NH2	1.92	0.83
1:B:31:ILE:HD13	1:B:231:MET:SD	2.18	0.83
1:F:263:VAL:HG12	1:F:374:ARG:NH2	1.94	0.83
1:D:31:ILE:HG22	1:D:222:ILE:HD12	1.59	0.83
1:B:434:THR:HG23	1:B:437:ILE:HD11	1.60	0.83
1:D:446:ARG:N	1:D:496:ARG:HH12	1.75	0.83
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.09	0.83
1:E:446:ARG:HE	1:E:496:ARG:NH2	1.76	0.82
1:A:434:THR:HG23	1:A:437:ILE:HD11	1.61	0.82
1:D:446:ARG:H	1:D:496:ARG:HH12	1.26	0.82
1:F:147:VAL:O	1:F:150:VAL:HG12	1.79	0.82
1:A:315:PHE:CE2	1:A:366:GLU:OE1	2.32	0.82
1:D:311:ARG:HD2	1:D:371:LYS:HD2	1.61	0.82
1:E:79:THR:HG23	1:E:81:GLN:HG2	1.62	0.82
1:F:347:VAL:HG21	1:F:366:GLU:OE1	1.80	0.82
1:B:191:ILE:HD12	1:B:198:GLU:HG2	1.62	0.82
1:E:449:MET:HG2	1:F:467:ILE:HD11	1.62	0.82
1:C:488:ARG:NH2	1:D:488:ARG:HH21	1.78	0.81
1:F:25:ILE:HD12	1:F:58:GLN:HE21	1.42	0.81
1:B:311:ARG:HD2	1:B:371:LYS:CD	2.10	0.81
1:E:311:ARG:HD2	1:E:371:LYS:HD2	1.62	0.81
1:A:117:VAL:HA	1:A:154:TYR:OH	1.79	0.81
1:D:311:ARG:HD2	1:D:371:LYS:CD	2.11	0.81
1:C:392:PHE:HE2	1:C:430:ILE:HD11	1.45	0.81
1:D:486:PHE:HB2	1:D:489:ILE:HD11	1.60	0.81
1:C:311:ARG:HD2	1:C:371:LYS:CD	2.10	0.81
1:E:379:SER:H	1:E:413:THR:HB	1.43	0.81
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.92	0.81
1:E:283:ILE:HD12	1:E:412:PHE:HE1	1.45	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:VAL:HG11	1:B:180:MET:HE3	1.63	0.81
1:F:191:ILE:HB	1:F:198:GLU:CG	2.11	0.81
1:F:315:PHE:HE1	1:F:375:ILE:HD12	1.45	0.81
1:A:79:THR:HG22	1:A:82:ASP:H	1.46	0.81
1:B:436:THR:C	1:B:437:ILE:HD12	2.01	0.80
1:B:444:GLU:OE1	1:C:490:ILE:HD12	1.82	0.80
1:B:64:ILE:CD1	1:B:70:PRO:HA	2.11	0.80
1:F:313:ILE:HD12	1:F:367:ILE:HD13	1.63	0.80
1:F:64:ILE:HD11	1:F:70:PRO:HA	1.63	0.79
1:B:362:ILE:O	1:B:366:GLU:HG3	1.83	0.79
1:E:347:VAL:HG21	1:E:366:GLU:OE1	1.83	0.79
1:D:182:THR:HG21	1:D:192:ALA:HB1	1.65	0.79
1:F:287:THR:HG23	1:F:414:ASN:HD22	1.46	0.79
1:A:436:THR:C	1:A:437:ILE:HD12	2.03	0.78
1:C:347:VAL:HG21	1:C:366:GLU:OE1	1.83	0.78
1:C:263:VAL:HG12	1:C:374:ARG:HH21	1.48	0.78
1:B:45:SER:HB3	1:B:182:THR:HB	1.64	0.78
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.47	0.78
1:A:311:ARG:HD2	1:A:371:LYS:CD	2.13	0.78
1:A:263:VAL:HG12	1:A:374:ARG:NH2	1.97	0.78
1:F:79:THR:HG22	1:F:82:ASP:H	1.49	0.78
1:D:425:ILE:HD11	1:D:456:PHE:CE2	2.18	0.78
1:E:79:THR:HG22	1:E:82:ASP:H	1.48	0.78
1:C:73:PHE:HB3	1:C:105:ILE:HD13	1.66	0.78
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.63	0.77
1:E:49:GLY:HA2	2:E:5903:ATP:O2B	1.85	0.77
1:B:24:MET:HB2	1:B:62:ASN:HD22	1.47	0.77
1:D:263:VAL:HG12	1:D:374:ARG:HH21	1.50	0.77
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.63	0.77
1:F:436:THR:C	1:F:437:ILE:HD12	2.04	0.77
1:F:489:ILE:HA	1:F:494:PRO:HG3	1.65	0.77
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.67	0.77
1:D:287:THR:CG2	1:D:414:ASN:HD22	1.97	0.77
1:A:74:VAL:HB	1:A:144:ILE:HD12	1.67	0.77
1:B:284:ILE:HD12	1:B:436:THR:CB	2.13	0.77
1:F:25:ILE:HD12	1:F:58:GLN:NE2	1.99	0.77
1:B:420:MET:CE	1:C:490:ILE:HD13	2.15	0.77
1:D:495:THR:HA	1:E:487:GLU:OE2	1.85	0.77
1:D:489:ILE:HD13	1:D:494:PRO:HB3	1.65	0.76
1:D:367:ILE:HD12	1:D:375:ILE:HD11	1.66	0.76
1:F:313:ILE:HB	1:F:375:ILE:HD13	1.64	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ILE:HB	1:D:198:GLU:CG	2.16	0.76
1:B:73:PHE:HB3	1:B:105:ILE:HD13	1.65	0.76
1:A:347:VAL:HG21	1:A:366:GLU:OE1	1.85	0.76
1:C:362:ILE:O	1:C:366:GLU:HG3	1.86	0.76
1:C:305:ALA:HB2	1:C:374:ARG:HD2	1.68	0.76
1:A:315:PHE:HE2	1:A:366:GLU:OE1	1.66	0.76
1:C:449:MET:HE3	1:D:490:ILE:HD11	1.66	0.76
1:E:161:ARG:HB2	1:E:196:VAL:HG11	1.65	0.76
1:B:263:VAL:CG1	1:B:374:ARG:HH21	1.98	0.76
1:B:191:ILE:HB	1:B:198:GLU:CG	2.16	0.76
1:B:315:PHE:HE2	1:B:366:GLU:OE1	1.68	0.75
1:B:161:ARG:HB2	1:B:196:VAL:HG11	1.68	0.75
1:A:320:SER:HA	1:B:254:LEU:HG	1.67	0.75
1:A:315:PHE:CD2	1:A:363:ILE:HD12	2.20	0.75
1:C:344:LEU:HD22	1:C:345:LYS:N	2.01	0.75
1:A:92:TRP:CB	1:A:92:TRP:HA	2.11	0.75
1:D:305:ALA:HB2	1:D:374:ARG:HD2	1.69	0.75
1:D:347:VAL:HG21	1:D:366:GLU:OE1	1.87	0.75
1:E:72:VAL:HG21	1:E:134:ILE:HD12	1.69	0.75
1:C:367:ILE:HG12	1:C:375:ILE:HD11	1.67	0.74
1:F:53:THR:HG23	1:F:145:ASP:OD1	1.87	0.74
1:A:257:ARG:HH22	1:A:407:GLU:HG2	1.52	0.74
1:A:437:ILE:CD1	1:A:457:LYS:HE2	2.17	0.74
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.68	0.74
1:B:43:LEU:HD11	1:B:182:THR:OG1	1.87	0.74
1:B:441:GLN:HE22	1:B:490:ILE:HD13	1.51	0.74
1:D:79:THR:CG2	1:D:81:GLN:HG2	2.18	0.74
1:B:315:PHE:CE2	1:B:366:GLU:OE1	2.40	0.74
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.01	0.74
1:F:362:ILE:O	1:F:366:GLU:HG3	1.88	0.74
1:E:363:ILE:O	1:E:367:ILE:HG12	1.88	0.74
1:C:262:ARG:HH22	1:C:461:SER:HB2	1.52	0.74
1:A:299:SER:HB3	1:A:333:MET:HE1	1.69	0.74
1:C:284:ILE:HD11	3:C:3910:HOH:O	1.86	0.74
1:D:49:GLY:HA2	2:D:4903:ATP:O2B	1.87	0.73
1:B:377:ILE:HD13	1:B:412:PHE:CE2	2.22	0.73
1:B:347:VAL:HG21	1:B:366:GLU:OE1	1.88	0.73
1:D:284:ILE:HD12	1:D:436:THR:CB	2.17	0.73
1:F:486:PHE:CB	1:F:489:ILE:HD11	2.18	0.73
1:A:64:ILE:HD12	1:A:102:LYS:HB3	1.70	0.73
1:E:123:LEU:HD12	1:E:163:GLU:OE2	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:SER:HB3	1:D:333:MET:HE1	1.69	0.73
1:E:269:ARG:HG2	1:E:479:ILE:HB	1.71	0.73
1:E:263:VAL:CG1	1:E:374:ARG:HH21	2.00	0.73
1:B:287:THR:HG23	1:B:414:ASN:HD22	1.53	0.73
1:A:127:ILE:HD11	1:A:167:LEU:HD12	1.70	0.72
1:D:375:ILE:CD1	1:D:408:ILE:HG21	2.20	0.72
1:B:317:TYR:OH	1:B:363:ILE:HD11	1.89	0.72
1:E:191:ILE:HD12	1:E:198:GLU:HG2	1.71	0.72
1:F:315:PHE:HE2	1:F:366:GLU:OE1	1.68	0.72
1:B:49:GLY:HA2	2:B:2903:ATP:O2B	1.90	0.72
1:D:284:ILE:CD1	1:D:436:THR:HB	2.16	0.72
1:A:287:THR:CG2	1:A:414:ASN:HD22	2.02	0.72
1:D:263:VAL:HG12	1:D:374:ARG:NH2	2.05	0.72
1:E:311:ARG:HD2	1:E:371:LYS:CD	2.20	0.72
1:C:269:ARG:HG2	1:C:479:ILE:HB	1.72	0.72
1:D:392:PHE:HE2	1:D:430:ILE:HD11	1.52	0.72
1:F:363:ILE:O	1:F:367:ILE:HG12	1.90	0.72
1:F:118:VAL:HG12	1:F:153:GLN:HE22	1.54	0.72
1:D:315:PHE:HE2	1:D:366:GLU:OE1	1.69	0.71
1:B:127:ILE:HG21	1:B:170:ARG:HG3	1.72	0.71
1:B:420:MET:HE3	1:C:490:ILE:HD13	1.71	0.71
1:E:191:ILE:HB	1:E:198:GLU:CG	2.19	0.71
1:C:392:PHE:CE2	1:C:430:ILE:HD11	2.25	0.71
1:F:191:ILE:HG23	1:F:206:ILE:HD11	1.71	0.71
1:A:254:LEU:HG	1:F:320:SER:HA	1.72	0.71
1:C:487:GLU:HG3	1:C:497:ILE:HD11	1.72	0.71
1:F:344:LEU:HD22	1:F:345:LYS:N	2.06	0.71
1:E:367:ILE:HD12	1:E:375:ILE:HD11	1.73	0.71
1:C:440:LEU:CD2	1:C:453:ILE:HG12	2.20	0.71
1:E:446:ARG:HE	1:E:496:ARG:HH22	1.36	0.71
1:F:437:ILE:HD13	1:F:457:LYS:CE	2.20	0.71
1:C:85:LYS:NZ	1:D:14:GLU:HB3	2.05	0.71
1:A:437:ILE:HD13	1:A:457:LYS:CG	2.21	0.70
1:E:14:GLU:HG3	1:E:16:GLN:H	1.53	0.70
1:A:147:VAL:HG11	1:A:180:MET:CE	2.21	0.70
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.72	0.70
1:E:325:LEU:HD23	1:E:335:PHE:HB2	1.72	0.70
1:F:49:GLY:HA2	2:F:6903:ATP:O2B	1.92	0.70
1:E:284:ILE:HD11	3:E:5911:HOH:O	1.92	0.70
1:E:496:ARG:C	1:E:497:ILE:HD13	2.11	0.70
1:A:150:VAL:HG13	1:A:151:PHE:N	2.06	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:ARG:HB2	1:D:196:VAL:HG11	1.72	0.70
1:A:64:ILE:HD11	1:A:70:PRO:HA	1.72	0.70
1:B:218:ARG:NH1	1:B:239:ILE:HD12	2.07	0.70
1:B:123:LEU:HD12	1:B:166:ARG:HD2	1.74	0.70
1:F:299:SER:HB3	1:F:333:MET:HE1	1.74	0.70
1:A:377:ILE:HD13	1:A:412:PHE:CE2	2.26	0.69
1:F:79:THR:HG23	1:F:81:GLN:HG2	1.74	0.69
1:A:295:THR:HG21	1:A:319:GLU:OE2	1.92	0.69
1:C:123:LEU:HD12	1:C:163:GLU:OE2	1.92	0.69
1:C:299:SER:C	1:C:333:MET:HE1	2.13	0.69
1:C:379:SER:H	1:C:413:THR:HB	1.57	0.69
1:A:211:LEU:O	1:A:212:GLU:HB3	1.92	0.69
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.72	0.69
1:A:316:ALA:O	1:A:348:CYS:HA	1.92	0.69
1:F:325:LEU:HD23	1:F:335:PHE:HB2	1.74	0.69
1:A:448:GLU:HG2	1:B:466:ALA:HA	1.73	0.69
1:C:287:THR:HG21	1:C:425:ILE:O	1.91	0.69
1:C:150:VAL:HG13	1:C:151:PHE:N	2.07	0.69
1:B:287:THR:HG21	1:B:425:ILE:O	1.92	0.69
1:E:214:GLU:HB3	1:F:234:GLU:HB2	1.73	0.69
1:F:127:ILE:HD11	1:F:167:LEU:HA	1.75	0.69
1:E:447:GLY:O	1:F:467:ILE:HD13	1.93	0.69
1:B:182:THR:HG21	1:B:192:ALA:HB1	1.73	0.69
1:B:448:GLU:HG2	1:C:466:ALA:HA	1.75	0.69
1:A:24:MET:CB	1:A:62:ASN:HD22	2.05	0.69
1:D:375:ILE:HD12	1:D:408:ILE:HG21	1.75	0.69
1:D:72:VAL:HG21	1:D:134:ILE:HD12	1.75	0.68
1:C:377:ILE:HD12	1:C:412:PHE:CE2	2.29	0.68
1:E:93:ASP:OD2	1:E:96:LYS:HB2	1.92	0.68
1:E:61:TYR:CE2	1:E:65:ILE:HG13	2.29	0.68
1:B:79:THR:HG23	1:B:81:GLN:HG2	1.75	0.68
1:C:182:THR:HG21	1:C:192:ALA:HB1	1.76	0.68
1:B:283:ILE:HD13	1:B:400:THR:HG23	1.74	0.68
1:B:437:ILE:HD13	1:B:457:LYS:HE2	1.73	0.68
1:C:191:ILE:HB	1:C:198:GLU:CG	2.23	0.68
1:C:325:LEU:HD23	1:C:335:PHE:HB2	1.73	0.68
1:C:21:MET:HE2	1:C:177:THR:HG21	1.75	0.68
1:F:239:ILE:HB	3:F:6917:HOH:O	1.94	0.68
1:B:437:ILE:HD11	1:B:457:LYS:HE2	1.75	0.68
1:D:126:LEU:O	1:D:130:ILE:CD1	2.41	0.68
1:A:437:ILE:N	1:A:437:ILE:HD12	2.08	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:GLU:HB2	1:B:83:ILE:HD11	1.76	0.68
1:F:90:PHE:HB2	1:F:92:TRP:CE2	2.29	0.68
1:B:449:MET:CE	1:C:490:ILE:HD11	2.24	0.68
1:C:31:ILE:HD13	1:C:231:MET:SD	2.34	0.68
1:B:299:SER:HB3	1:B:333:MET:HE1	1.76	0.68
1:C:262:ARG:NH2	1:C:461:SER:HB2	2.10	0.67
1:E:182:THR:HG21	1:E:192:ALA:HB1	1.75	0.67
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.28	0.67
1:E:43:LEU:HD11	1:E:182:THR:OG1	1.94	0.67
1:B:85:LYS:NZ	1:C:14:GLU:HB3	2.10	0.67
1:E:123:LEU:O	1:E:127:ILE:HG12	1.94	0.67
1:D:370:PHE:O	1:D:371:LYS:HD3	1.95	0.67
1:F:486:PHE:HB2	1:F:489:ILE:HD11	1.76	0.67
1:A:182:THR:HG21	1:A:192:ALA:HB1	1.76	0.67
1:F:16:GLN:HE22	1:F:33:HIS:HB3	1.59	0.67
1:A:61:TYR:CE2	1:A:65:ILE:HG13	2.30	0.67
1:B:61:TYR:CE2	1:B:65:ILE:HG13	2.28	0.67
1:D:453:ILE:HD13	1:D:454:ASN:N	2.10	0.67
1:B:441:GLN:NE2	1:B:490:ILE:HD13	2.10	0.67
1:F:52:LYS:HE3	2:F:6903:ATP:O1B	1.94	0.67
1:D:377:ILE:HD12	1:D:412:PHE:CE2	2.29	0.67
1:A:370:PHE:O	1:A:371:LYS:HD3	1.95	0.67
1:F:144:ILE:CG2	1:F:147:VAL:HG12	2.25	0.67
1:E:487:GLU:O	1:E:488:ARG:HB2	1.95	0.66
1:F:79:THR:CG2	1:F:81:GLN:HG2	2.25	0.66
1:F:370:PHE:O	1:F:371:LYS:HG3	1.95	0.66
1:E:318:GLU:OE2	1:F:432:THR:CG2	2.43	0.66
1:E:323:GLN:NE2	1:F:459:ARG:HD3	2.10	0.66
1:A:92:TRP:HE3	1:A:92:TRP:CA	2.08	0.66
1:F:437:ILE:CD1	1:F:457:LYS:HE2	2.25	0.66
1:C:449:MET:HE1	1:D:490:ILE:HD11	1.76	0.66
1:E:148:THR:OG1	1:E:182:THR:HG23	1.96	0.66
1:D:150:VAL:HG13	1:D:151:PHE:N	2.10	0.66
1:B:24:MET:CB	1:B:62:ASN:HD22	2.07	0.66
1:A:49:GLY:HA2	2:A:1903:ATP:O2B	1.96	0.66
1:C:79:THR:HG23	1:C:81:GLN:HG2	1.76	0.66
1:B:483:PHE:HB3	1:B:486:PHE:HD1	1.60	0.66
1:D:43:LEU:HD11	1:D:182:THR:OG1	1.95	0.66
1:B:425:ILE:HD11	1:B:456:PHE:CE2	2.30	0.66
1:C:344:LEU:HD11	1:C:346:ILE:HD11	1.77	0.66
1:B:169:ALA:O	1:B:173:GLN:HG3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:TYR:O	1:C:65:ILE:CD1	2.39	0.66
1:C:425:ILE:HD11	1:C:456:PHE:CE2	2.30	0.66
1:D:114:GLY:O	1:D:115:GLN:HG3	1.96	0.66
1:C:321:ARG:HG2	1:C:348:CYS:SG	2.36	0.66
1:A:96:LYS:O	1:A:100:GLU:HG3	1.95	0.66
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.75	0.65
1:E:290:THR:HG22	2:E:5901:ATP:O1G	1.96	0.65
1:D:438:ILE:CD1	1:D:455:VAL:HG22	2.26	0.65
1:B:150:VAL:HG13	1:B:151:PHE:N	2.11	0.65
1:D:61:TYR:CE2	1:D:92:TRP:CD1	2.83	0.65
1:E:489:ILE:HA	1:E:494:PRO:HG3	1.77	0.65
1:B:453:ILE:HD13	1:B:454:ASN:N	2.11	0.65
1:B:147:VAL:HG11	1:B:180:MET:CE	2.26	0.65
1:D:85:LYS:NZ	1:E:14:GLU:HB3	2.11	0.65
1:C:159:VAL:O	1:C:163:GLU:HG2	1.96	0.65
1:C:453:ILE:HD13	1:C:454:ASN:N	2.11	0.65
1:D:325:LEU:HD23	1:D:335:PHE:HB2	1.79	0.65
1:B:52:LYS:N	2:B:2903:ATP:O1B	2.23	0.65
1:B:79:THR:CG2	1:B:81:GLN:HG2	2.25	0.65
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.32	0.65
1:E:283:ILE:HD12	1:E:412:PHE:CE1	2.29	0.65
1:E:317:TYR:OH	1:E:363:ILE:HD11	1.97	0.65
1:F:147:VAL:HG11	1:F:180:MET:HE2	1.79	0.65
1:B:449:MET:HE3	1:C:490:ILE:HD11	1.77	0.65
1:B:440:LEU:CD2	1:B:453:ILE:HG12	2.26	0.65
1:E:377:ILE:HD12	1:E:412:PHE:CE2	2.31	0.65
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.61	0.65
1:C:206:ILE:HD11	1:C:223:LEU:HB2	1.79	0.65
1:E:446:ARG:NE	1:E:496:ARG:HH22	1.94	0.65
1:D:147:VAL:HG11	1:D:180:MET:CE	2.24	0.65
1:D:362:ILE:O	1:D:366:GLU:HG3	1.97	0.65
1:C:320:SER:HA	1:D:254:LEU:HG	1.78	0.65
1:F:315:PHE:CE1	1:F:375:ILE:HD12	2.29	0.65
1:C:65:ILE:N	1:C:65:ILE:HD12	2.12	0.65
1:A:317:TYR:OH	1:A:363:ILE:HD11	1.97	0.64
1:B:437:ILE:HD13	1:B:457:LYS:CE	2.27	0.64
1:E:150:VAL:HG13	1:E:151:PHE:N	2.13	0.64
1:D:335:PHE:HA	1:D:338:MET:HG3	1.78	0.64
1:A:45:SER:HB3	1:A:182:THR:HB	1.79	0.64
1:B:18:ILE:HB	1:B:228:THR:HG23	1.80	0.64
1:E:344:LEU:HD22	1:E:345:LYS:N	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ILE:CD1	1:B:400:THR:HG23	2.27	0.64
1:C:314:LEU:HD23	1:C:346:ILE:HD12	1.79	0.64
1:A:218:ARG:CZ	1:A:239:ILE:HD12	2.27	0.64
1:E:147:VAL:HG11	1:E:180:MET:CE	2.26	0.64
1:F:218:ARG:HD2	3:F:6906:HOH:O	1.97	0.64
1:F:315:PHE:CE2	1:F:363:ILE:HD12	2.32	0.64
1:B:370:PHE:O	1:B:371:LYS:HD3	1.98	0.64
1:D:84:ILE:CD1	1:D:94:LEU:HB2	2.27	0.64
1:D:146:SER:H	1:D:181:THR:CG2	2.08	0.64
1:C:263:VAL:HG12	1:C:374:ARG:NH2	2.12	0.64
1:B:483:PHE:HB3	1:B:486:PHE:CD1	2.32	0.64
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.80	0.64
1:F:111:ASP:OD1	1:F:112:PRO:HD2	1.97	0.64
1:D:72:VAL:HG21	1:D:134:ILE:CD1	2.28	0.64
1:C:469:GLU:HG3	1:C:480:LYS:HE3	1.79	0.64
1:E:356:LEU:CD2	1:E:387:VAL:HG11	2.28	0.64
1:E:356:LEU:HD22	1:E:387:VAL:HG11	1.80	0.64
1:D:487:GLU:OE1	1:D:497:ILE:HD13	1.98	0.64
1:B:315:PHE:CD2	1:B:363:ILE:HD12	2.33	0.64
1:C:50:THR:HG22	1:C:209:ASN:HB2	1.80	0.64
1:E:191:ILE:CD1	1:E:198:GLU:HG2	2.27	0.64
1:C:121:PHE:O	1:C:125:ALA:HB3	1.97	0.64
1:E:287:THR:CG2	1:E:414:ASN:HD22	2.11	0.63
1:E:269:ARG:HB3	1:E:479:ILE:HD12	1.77	0.63
1:D:146:SER:N	1:D:181:THR:HG22	2.10	0.63
1:A:64:ILE:CD1	1:A:70:PRO:HA	2.28	0.63
1:C:218:ARG:NH1	1:C:239:ILE:HD12	2.13	0.63
1:B:344:LEU:HD22	1:B:345:LYS:N	2.14	0.63
1:C:296:LEU:CD2	1:C:472:ILE:HD12	2.28	0.63
1:D:451:ARG:HH11	1:D:451:ARG:HG2	1.63	0.63
1:C:444:GLU:OE1	1:D:490:ILE:HD12	1.98	0.63
1:F:117:VAL:HA	1:F:154:TYR:OH	1.98	0.63
1:C:471:MET:O	1:C:472:ILE:HD13	1.97	0.63
1:A:488:ARG:NE	1:F:488:ARG:HH12	1.96	0.63
1:F:315:PHE:CD2	1:F:363:ILE:HD12	2.33	0.63
1:D:218:ARG:CZ	1:D:239:ILE:HD12	2.28	0.63
1:F:377:ILE:HD12	1:F:412:PHE:CE2	2.34	0.63
1:E:79:THR:HG21	1:E:81:GLN:HG2	1.79	0.63
1:C:111:ASP:OD2	1:C:113:GLU:HG2	1.99	0.63
1:C:214:GLU:HB3	1:D:234:GLU:HB2	1.81	0.63
1:F:24:MET:HB2	1:F:62:ASN:HD22	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:THR:CG2	1:C:81:GLN:HG2	2.29	0.63
1:F:440:LEU:CD2	1:F:453:ILE:HG13	2.28	0.63
1:A:257:ARG:HH22	1:A:407:GLU:CG	2.09	0.63
1:C:218:ARG:CZ	1:C:239:ILE:HD12	2.29	0.63
1:E:382:ALA:O	1:E:385:ARG:HG3	1.98	0.63
1:F:396:VAL:O	1:F:400:THR:HB	1.99	0.63
1:D:488:ARG:NH1	1:E:488:ARG:HH21	1.97	0.62
1:C:344:LEU:HD22	1:C:345:LYS:H	1.63	0.62
1:C:314:LEU:HB3	1:C:346:ILE:HD13	1.81	0.62
1:C:182:THR:HG22	1:C:183:GLU:N	2.13	0.62
1:F:134:ILE:HD11	1:F:142:VAL:HG22	1.81	0.62
1:D:79:THR:HG23	1:D:81:GLN:HG2	1.80	0.62
1:A:49:GLY:CA	2:A:1903:ATP:O2B	2.47	0.62
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.80	0.62
1:D:393:ARG:O	1:D:397:ILE:HG12	1.99	0.62
1:C:431:SER:O	1:C:434:THR:HG22	1.99	0.62
1:D:295:THR:HG23	1:D:378:ASP:OD2	1.99	0.62
1:A:437:ILE:HD13	1:A:457:LYS:CE	2.28	0.62
1:E:191:ILE:HB	1:E:198:GLU:HG2	1.81	0.62
1:A:249:LEU:HD13	1:A:394:GLN:HG2	1.81	0.62
1:A:318:GLU:OE2	1:B:432:THR:CG2	2.47	0.62
1:B:273:MET:O	1:B:463:HIS:HA	1.99	0.62
1:E:248:PRO:HB2	1:E:251:ALA:HB3	1.81	0.62
1:B:437:ILE:HD12	1:B:437:ILE:N	2.14	0.62
1:E:377:ILE:HD12	1:E:412:PHE:HE2	1.65	0.62
1:F:64:ILE:CD1	1:F:70:PRO:HA	2.28	0.62
1:F:437:ILE:HD13	1:F:457:LYS:CG	2.28	0.62
1:B:437:ILE:HD13	1:B:457:LYS:CG	2.30	0.62
1:B:438:ILE:HG23	1:B:453:ILE:HD11	1.81	0.62
1:A:269:ARG:HG2	1:A:479:ILE:HB	1.81	0.62
1:E:284:ILE:HD12	1:E:436:THR:CB	2.23	0.62
1:D:151:PHE:C	1:D:153:GLN:H	2.00	0.62
1:D:182:THR:HG22	1:D:183:GLU:N	2.15	0.62
1:E:49:GLY:CA	2:E:5903:ATP:O2B	2.47	0.62
1:C:438:ILE:CD1	1:C:455:VAL:HG22	2.30	0.62
1:C:203:ASN:HB3	1:C:225:LEU:HD23	1.81	0.62
1:A:437:ILE:HD13	1:A:457:LYS:HG2	1.82	0.62
1:A:451:ARG:NH1	1:A:451:ARG:HG2	2.15	0.62
1:A:191:ILE:HB	1:A:198:GLU:CG	2.30	0.61
1:A:184:ARG:O	1:A:185:ILE:HD13	2.00	0.61
1:D:79:THR:HG21	1:D:81:GLN:HG2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:451:ARG:HH11	1:F:451:ARG:HG2	1.64	0.61
1:E:115:GLN:OE1	1:E:118:VAL:HG21	2.00	0.61
1:F:144:ILE:HG22	1:F:147:VAL:HG12	1.83	0.61
1:D:148:THR:CG2	1:D:193:ARG:HD2	2.30	0.61
1:B:123:LEU:O	1:B:123:LEU:HD13	2.01	0.61
1:F:370:PHE:C	1:F:371:LYS:HG3	2.20	0.61
1:B:379:SER:H	1:B:413:THR:HB	1.64	0.61
1:F:437:ILE:N	1:F:437:ILE:HD12	2.16	0.61
1:C:289:ALA:HB2	1:C:419:PHE:HA	1.80	0.61
1:C:148:THR:CG2	1:C:193:ARG:HD2	2.31	0.61
1:D:385:ARG:NH2	1:E:433:ILE:HD11	2.16	0.61
1:A:437:ILE:HD13	1:A:457:LYS:HE2	1.82	0.61
1:A:21:MET:HB2	1:A:38:ILE:CD1	2.30	0.61
1:F:437:ILE:HD13	1:F:457:LYS:HE2	1.83	0.61
1:D:321:ARG:HG2	1:D:348:CYS:SG	2.41	0.61
1:C:191:ILE:HB	1:C:198:GLU:HG2	1.83	0.61
1:F:377:ILE:HD11	1:F:399:VAL:HG11	1.83	0.61
1:B:145:ASP:OD2	1:B:181:THR:HG21	2.00	0.61
1:B:191:ILE:CD1	1:B:198:GLU:HG2	2.30	0.61
1:B:218:ARG:CZ	1:B:239:ILE:HD12	2.31	0.60
1:A:89:SER:HB2	1:B:227:GLY:O	2.00	0.60
1:A:92:TRP:CA	1:A:92:TRP:CE3	2.84	0.60
1:C:284:ILE:N	1:C:284:ILE:HD13	2.16	0.60
1:C:61:TYR:CE2	1:C:65:ILE:HG12	2.35	0.60
1:F:127:ILE:HD11	1:F:167:LEU:HD12	1.83	0.60
1:A:382:ALA:O	1:A:385:ARG:HG3	2.01	0.60
1:C:287:THR:CG2	1:C:414:ASN:HD22	2.06	0.60
1:D:315:PHE:CZ	1:D:363:ILE:HG23	2.36	0.60
1:E:79:THR:HG23	1:E:81:GLN:H	1.65	0.60
1:D:344:LEU:HD22	1:D:345:LYS:N	2.15	0.60
1:B:18:ILE:HB	1:B:228:THR:CG2	2.31	0.60
1:B:295:THR:HG21	1:B:319:GLU:OE2	2.01	0.60
1:F:486:PHE:CE2	1:F:496:ARG:HD2	2.36	0.60
1:D:49:GLY:CA	2:D:4903:ATP:O2B	2.49	0.60
1:B:123:LEU:O	1:B:127:ILE:HG13	2.00	0.60
1:E:359:HIS:O	1:E:363:ILE:HG12	2.01	0.60
1:F:461:SER:OG	1:F:462:TRP:N	2.34	0.60
1:F:159:VAL:O	1:F:163:GLU:HG2	2.01	0.60
1:D:440:LEU:CD2	1:D:453:ILE:HG12	2.32	0.60
1:D:79:THR:HG23	1:D:81:GLN:H	1.66	0.60
1:F:467:ILE:N	1:F:467:ILE:HD12	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLN:HG3	1:D:92:TRP:HZ2	1.66	0.60
1:D:486:PHE:CE2	1:D:496:ARG:HB3	2.37	0.60
1:E:362:ILE:O	1:E:366:GLU:HG3	2.02	0.60
1:F:122:ASP:OD2	1:F:123:LEU:N	2.35	0.60
1:C:420:MET:CE	1:D:490:ILE:HD13	2.32	0.60
1:D:194:TYR:O	1:D:196:VAL:HG23	2.01	0.60
1:B:78:GLU:CB	1:B:83:ILE:HD11	2.32	0.60
1:E:293:GLY:HA2	2:E:5901:ATP:O1A	2.02	0.60
1:E:451:ARG:HH11	1:E:451:ARG:HG2	1.67	0.60
1:C:28:PHE:CZ	1:C:222:ILE:HD11	2.36	0.60
1:D:392:PHE:CE2	1:D:430:ILE:HD11	2.34	0.60
1:A:14:GLU:HG3	1:A:16:GLN:OE1	2.01	0.60
1:E:159:VAL:O	1:E:163:GLU:HG2	2.02	0.60
1:A:344:LEU:HD22	1:A:345:LYS:N	2.17	0.60
1:E:461:SER:OG	1:E:462:TRP:N	2.33	0.60
1:D:489:ILE:HD13	1:D:494:PRO:CB	2.32	0.59
1:A:79:THR:HG23	1:A:81:GLN:H	1.67	0.59
1:F:382:ALA:O	1:F:385:ARG:HG3	2.02	0.59
1:F:293:GLY:HA2	2:F:6901:ATP:O1A	2.02	0.59
1:F:150:VAL:HG13	1:F:151:PHE:N	2.16	0.59
1:A:367:ILE:HG12	1:A:375:ILE:HD11	1.82	0.59
1:A:52:LYS:HE3	2:A:1903:ATP:O1B	2.02	0.59
1:A:433:ILE:HD11	1:F:385:ARG:NH2	2.17	0.59
1:E:396:VAL:O	1:E:400:THR:HB	2.02	0.59
1:F:484:ARG:HH11	1:F:484:ARG:HB3	1.68	0.59
1:A:208:ARG:NH2	1:A:221:GLU:OE2	2.35	0.59
1:C:205:VAL:CG2	1:C:222:ILE:HD13	2.24	0.59
1:F:437:ILE:CD1	1:F:457:LYS:CE	2.81	0.59
1:B:87:ALA:O	1:B:92:TRP:HB2	2.03	0.59
1:D:367:ILE:HG23	1:D:372:PRO:HD2	1.85	0.59
1:E:320:SER:HA	1:F:254:LEU:HG	1.83	0.59
1:F:311:ARG:HD2	1:F:371:LYS:HE2	1.84	0.59
1:B:269:ARG:HG2	1:B:479:ILE:HB	1.83	0.59
1:E:289:ALA:HB2	1:E:419:PHE:HA	1.84	0.59
1:B:437:ILE:HD13	1:B:457:LYS:HG2	1.84	0.59
1:C:400:THR:HG22	1:C:401:GLY:N	2.18	0.59
1:D:316:ALA:O	1:D:348:CYS:HA	2.02	0.59
1:F:146:SER:H	1:F:181:THR:HG22	1.67	0.59
1:F:49:GLY:CA	2:F:6903:ATP:O2B	2.50	0.59
1:B:453:ILE:HD13	1:B:454:ASN:H	1.66	0.59
1:B:444:GLU:HB2	1:C:490:ILE:CD1	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:THR:CG2	1:E:193:ARG:HD2	2.33	0.59
1:A:74:VAL:CB	1:A:144:ILE:HD12	2.33	0.59
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.37	0.59
1:D:431:SER:O	1:D:434:THR:HG22	2.02	0.59
1:E:372:PRO:HB2	1:E:375:ILE:HD11	1.84	0.58
1:C:84:ILE:CD1	1:C:94:LEU:HB2	2.29	0.58
1:A:437:ILE:HD11	1:A:457:LYS:HE2	1.84	0.58
1:E:273:MET:O	1:E:463:HIS:HA	2.02	0.58
1:D:400:THR:HG22	1:D:401:GLY:N	2.18	0.58
1:A:264:SER:HA	1:A:271:ASP:OD1	2.03	0.58
1:D:248:PRO:HB2	1:D:251:ALA:HB3	1.85	0.58
1:A:74:VAL:CG2	1:A:144:ILE:HD12	2.33	0.58
1:B:194:TYR:O	1:B:196:VAL:HG23	2.03	0.58
1:C:52:LYS:HE3	2:C:3903:ATP:O1B	2.02	0.58
1:E:22:ARG:HD3	3:E:5914:HOH:O	2.03	0.58
1:A:437:ILE:CD1	1:A:457:LYS:CE	2.81	0.58
1:C:24:MET:HB2	1:C:62:ASN:HD22	1.67	0.58
1:D:283:ILE:CD1	1:D:400:THR:HG23	2.33	0.58
1:C:273:MET:O	1:C:463:HIS:HA	2.04	0.58
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.85	0.58
1:B:50:THR:HG22	1:B:209:ASN:HB2	1.85	0.58
1:C:151:PHE:C	1:C:153:GLN:H	2.04	0.58
1:D:14:GLU:CD	1:D:15:HIS:H	2.07	0.58
1:A:379:SER:N	1:A:413:THR:HB	2.06	0.58
1:E:315:PHE:CD2	1:E:363:ILE:HD12	2.39	0.58
1:F:194:TYR:O	1:F:196:VAL:HG23	2.04	0.58
1:B:377:ILE:N	1:B:377:ILE:HD12	2.18	0.58
1:B:49:GLY:CA	2:B:2903:ATP:O2B	2.51	0.58
1:A:377:ILE:N	1:A:377:ILE:HD12	2.18	0.58
1:A:296:LEU:CD2	1:A:472:ILE:HD12	2.34	0.58
1:E:127:ILE:HD11	1:E:167:LEU:HD13	1.84	0.58
1:B:85:LYS:HZ3	1:C:14:GLU:HB3	1.68	0.58
1:B:269:ARG:HB3	1:B:479:ILE:HD12	1.84	0.58
1:F:131:ASN:O	1:F:135:GLN:HG3	2.04	0.58
1:B:451:ARG:HH11	1:B:451:ARG:HG2	1.68	0.58
1:A:396:VAL:O	1:A:400:THR:HB	2.03	0.58
1:C:315:PHE:CZ	1:C:363:ILE:HG23	2.38	0.58
1:F:79:THR:HG23	1:F:81:GLN:H	1.68	0.58
1:A:43:LEU:HD11	1:A:182:THR:OG1	2.04	0.58
1:F:316:ALA:O	1:F:348:CYS:HA	2.04	0.58
1:C:79:THR:HG22	1:C:82:ASP:H	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:470:PHE:CE1	1:E:472:ILE:HD11	2.38	0.58
1:A:372:PRO:O	1:A:408:ILE:HD12	2.03	0.58
1:F:90:PHE:O	1:F:92:TRP:CD1	2.56	0.58
1:E:67:PHE:HB2	1:E:69:GLU:HG3	1.86	0.58
1:F:486:PHE:HB3	1:F:489:ILE:HD11	1.86	0.57
1:D:161:ARG:HD2	1:D:196:VAL:HG13	1.86	0.57
1:B:461:SER:OG	1:B:462:TRP:N	2.37	0.57
1:C:221:GLU:HG3	1:C:233:GLY:O	2.03	0.57
1:C:142:VAL:O	1:C:178:THR:HA	2.03	0.57
1:A:315:PHE:CE2	1:A:363:ILE:HD12	2.39	0.57
1:D:367:ILE:HD12	1:D:372:PRO:HG2	1.85	0.57
1:F:147:VAL:HG11	1:F:180:MET:CE	2.34	0.57
1:F:484:ARG:HB3	1:F:484:ARG:NH1	2.18	0.57
1:A:126:LEU:HG	1:A:130:ILE:CD1	2.34	0.57
1:D:150:VAL:O	1:D:153:GLN:HG3	2.03	0.57
1:F:287:THR:CG2	1:F:414:ASN:HD22	2.17	0.57
1:C:88:ARG:NE	1:D:15:HIS:HA	2.18	0.57
1:B:438:ILE:CD1	1:B:455:VAL:HG22	2.34	0.57
1:E:169:ALA:O	1:E:173:GLN:HG3	2.03	0.57
1:D:470:PHE:CB	1:D:479:ILE:HD13	2.34	0.57
1:F:191:ILE:HB	1:F:198:GLU:CD	2.24	0.57
1:E:28:PHE:HE1	1:E:222:ILE:HD11	1.68	0.57
1:A:273:MET:O	1:A:463:HIS:HA	2.03	0.57
1:E:437:ILE:CD1	1:E:457:LYS:HE2	2.34	0.57
1:F:150:VAL:O	1:F:153:GLN:HG3	2.05	0.57
1:A:161:ARG:HD2	1:A:196:VAL:HG13	1.87	0.57
1:F:134:ILE:HD11	1:F:142:VAL:CG2	2.34	0.57
1:A:191:ILE:HG23	1:A:206:ILE:CD1	2.35	0.57
1:D:363:ILE:O	1:D:367:ILE:HG12	2.05	0.57
1:E:18:ILE:HD11	1:E:227:GLY:C	2.25	0.57
1:F:169:ALA:O	1:F:173:GLN:HG3	2.05	0.57
1:E:453:ILE:HB	1:E:470:PHE:CD2	2.40	0.57
1:F:14:GLU:HG2	3:F:6924:HOH:O	2.03	0.57
1:F:372:PRO:O	1:F:408:ILE:HD12	2.04	0.57
1:A:14:GLU:HG3	1:A:15:HIS:H	1.68	0.57
1:C:484:ARG:HB3	1:C:484:ARG:NH1	2.19	0.57
1:E:370:PHE:O	1:E:371:LYS:HD3	2.04	0.57
1:C:94:LEU:O	1:C:98:VAL:HG23	2.05	0.57
1:C:148:THR:HG21	1:C:193:ARG:HD2	1.87	0.57
1:E:50:THR:HG22	1:E:209:ASN:HB2	1.86	0.57
1:B:89:SER:HB2	1:C:227:GLY:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ARG:HD3	1:F:323:GLN:NE2	2.20	0.57
1:A:436:THR:HG23	1:A:458:MET:HG2	1.87	0.56
1:E:76:PHE:HZ	1:E:126:LEU:HD21	1.69	0.56
1:F:420:MET:HE3	1:F:492:GLY:HA3	1.86	0.56
1:C:461:SER:OG	1:C:462:TRP:N	2.36	0.56
1:B:249:LEU:HD13	1:B:394:GLN:HG2	1.86	0.56
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.40	0.56
1:B:296:LEU:CD2	1:B:472:ILE:HD12	2.35	0.56
1:A:311:ARG:HA	1:A:343:LEU:O	2.05	0.56
1:C:147:VAL:HG11	1:C:180:MET:CE	2.34	0.56
1:D:31:ILE:HD13	1:D:231:MET:SD	2.46	0.56
1:C:440:LEU:HD21	1:C:453:ILE:HG12	1.87	0.56
1:D:24:MET:HG3	1:D:66:GLU:HG3	1.87	0.56
1:F:231:MET:CE	1:F:251:ALA:HB2	2.34	0.56
1:B:320:SER:HA	1:C:254:LEU:HG	1.87	0.56
1:C:150:VAL:HG13	1:C:151:PHE:H	1.70	0.56
1:B:367:ILE:HG12	1:B:375:ILE:HD11	1.86	0.56
1:E:203:ASN:HB3	1:E:225:LEU:HD23	1.86	0.56
1:A:287:THR:HG21	1:A:425:ILE:O	2.06	0.56
1:B:178:THR:HG22	1:B:179:VAL:N	2.20	0.56
1:A:124:SER:O	1:A:128:GLU:HG3	2.05	0.56
1:A:127:ILE:HD11	1:A:167:LEU:CD1	2.34	0.56
1:F:273:MET:O	1:F:463:HIS:HA	2.05	0.56
1:D:487:GLU:OE1	1:D:497:ILE:HG21	2.04	0.56
1:D:21:MET:HE1	1:D:177:THR:HB	1.88	0.56
1:D:453:ILE:HD13	1:D:454:ASN:H	1.69	0.56
1:D:80:PRO:HD2	1:D:81:GLN:NE2	2.21	0.56
1:F:377:ILE:HD12	1:F:412:PHE:HE2	1.70	0.56
1:D:317:TYR:CE2	1:D:383:LEU:HD21	2.40	0.56
1:C:377:ILE:HD12	1:C:412:PHE:HE2	1.69	0.56
1:C:218:ARG:HB3	3:C:3906:HOH:O	2.05	0.56
1:B:438:ILE:HD13	1:B:455:VAL:HA	1.88	0.56
1:D:435:ASP:HA	1:D:459:ARG:HD2	1.86	0.56
1:A:362:ILE:HG22	1:A:366:GLU:OE2	2.06	0.56
1:A:151:PHE:C	1:A:153:GLN:H	2.09	0.56
1:D:320:SER:HA	1:E:254:LEU:HG	1.88	0.56
1:B:56:SER:HB2	1:B:143:SER:HB3	1.87	0.55
1:A:92:TRP:HE3	1:A:92:TRP:N	2.03	0.55
1:A:466:ALA:HA	1:F:448:GLU:HG2	1.87	0.55
1:F:96:LYS:O	1:F:100:GLU:HG3	2.07	0.55
1:B:79:THR:CG2	1:B:82:ASP:H	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:THR:HG21	1:D:425:ILE:O	2.06	0.55
1:A:437:ILE:N	1:A:437:ILE:CD1	2.69	0.55
1:F:338:MET:HB3	1:F:344:LEU:HB3	1.88	0.55
1:C:79:THR:CG2	1:C:82:ASP:H	2.18	0.55
1:F:356:LEU:CD2	1:F:387:VAL:HG11	2.36	0.55
1:D:318:GLU:OE2	1:E:432:THR:CG2	2.54	0.55
1:B:117:VAL:HG12	1:B:117:VAL:O	2.07	0.55
1:A:150:VAL:CG1	1:A:151:PHE:N	2.69	0.55
1:C:150:VAL:O	1:C:153:GLN:HG3	2.06	0.55
1:F:393:ARG:O	1:F:397:ILE:HG12	2.07	0.55
1:E:244:ILE:HG22	1:E:246:ILE:HD11	1.89	0.55
1:D:40:ARG:HG2	1:D:172:LYS:HE3	1.88	0.55
1:B:148:THR:CG2	1:B:193:ARG:HD2	2.36	0.55
1:B:191:ILE:HB	1:B:198:GLU:CD	2.27	0.55
1:C:269:ARG:HB3	1:C:479:ILE:HD13	1.89	0.55
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.87	0.55
1:D:432:THR:HG22	1:D:432:THR:O	2.05	0.55
1:B:316:ALA:O	1:B:348:CYS:HA	2.06	0.55
1:B:437:ILE:CD1	1:B:437:ILE:N	2.68	0.55
1:B:164:LEU:HD11	1:B:197:GLU:HG3	1.88	0.55
1:F:249:LEU:HD13	1:F:394:GLN:HG2	1.88	0.55
1:C:347:VAL:O	1:C:348:CYS:HB2	2.06	0.55
1:F:284:ILE:N	1:F:284:ILE:HD12	2.22	0.55
1:A:363:ILE:O	1:A:367:ILE:HG13	2.06	0.55
1:E:375:ILE:CD1	1:E:408:ILE:HG21	2.37	0.55
1:B:318:GLU:OE2	1:C:432:THR:CG2	2.55	0.55
1:F:123:LEU:O	1:F:123:LEU:HD13	2.07	0.55
1:B:45:SER:CB	1:B:182:THR:HB	2.37	0.55
1:A:266:GLY:HA3	1:A:300:ARG:O	2.07	0.55
1:A:294:LYS:N	2:A:1901:ATP:O1B	2.40	0.54
1:E:496:ARG:O	1:E:497:ILE:HD13	2.06	0.54
1:C:287:THR:HG23	1:C:414:ASN:ND2	2.11	0.54
1:B:85:LYS:HE3	1:C:17:ALA:O	2.07	0.54
1:A:438:ILE:CD1	1:A:455:VAL:HG22	2.37	0.54
1:F:313:ILE:CB	1:F:375:ILE:HD11	2.33	0.54
1:B:283:ILE:C	1:B:284:ILE:HD13	2.27	0.54
1:B:52:LYS:HE3	2:B:2903:ATP:O1B	2.07	0.54
1:C:122:ASP:O	1:C:123:LEU:C	2.45	0.54
1:E:318:GLU:OE2	1:F:432:THR:HG23	2.06	0.54
1:D:96:LYS:O	1:D:100:GLU:HG3	2.07	0.54
1:E:367:ILE:HD12	1:E:375:ILE:CD1	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:PHE:O	1:F:125:ALA:N	2.37	0.54
1:D:356:LEU:HD13	1:D:387:VAL:HG21	1.89	0.54
1:D:249:LEU:HD13	1:D:394:GLN:HG2	1.89	0.54
1:B:433:ILE:O	1:B:433:ILE:HG22	2.07	0.54
1:A:284:ILE:N	1:A:284:ILE:HD12	2.22	0.54
1:A:295:THR:HB	2:A:1901:ATP:PA	2.48	0.54
1:E:446:ARG:NE	1:E:496:ARG:NH2	2.51	0.54
1:D:84:ILE:HD12	1:D:94:LEU:HB2	1.87	0.54
1:B:150:VAL:O	1:B:153:GLN:HG3	2.06	0.54
1:D:311:ARG:HD2	1:D:371:LYS:HD3	1.87	0.54
1:F:191:ILE:HG23	1:F:206:ILE:CD1	2.35	0.54
1:C:448:GLU:HG2	1:D:466:ALA:HA	1.90	0.54
1:D:52:LYS:HE3	2:D:4903:ATP:O1B	2.08	0.54
1:A:440:LEU:HD23	1:A:453:ILE:HG13	1.89	0.54
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.89	0.54
1:C:451:ARG:HH11	1:C:451:ARG:HG2	1.73	0.54
1:F:317:TYR:OH	1:F:363:ILE:HD11	2.07	0.54
1:D:367:ILE:O	1:D:372:PRO:HD3	2.08	0.54
1:C:370:PHE:O	1:C:371:LYS:HD3	2.08	0.54
1:D:299:SER:CB	1:D:333:MET:HE1	2.38	0.54
1:F:90:PHE:O	1:F:92:TRP:NE1	2.41	0.54
1:A:191:ILE:HG23	1:A:206:ILE:HD11	1.88	0.54
1:A:21:MET:HE1	1:A:59:PHE:HZ	1.72	0.54
1:D:486:PHE:HB3	1:D:489:ILE:CD1	2.31	0.54
1:E:489:ILE:HD13	1:E:494:PRO:CG	2.37	0.54
1:E:440:LEU:CD2	1:E:453:ILE:HG13	2.37	0.54
1:D:437:ILE:CD1	1:D:457:LYS:HE2	2.38	0.54
1:D:80:PRO:O	1:D:84:ILE:HG12	2.08	0.54
1:C:80:PRO:O	1:C:84:ILE:HG12	2.08	0.54
1:F:151:PHE:C	1:F:153:GLN:H	2.11	0.54
1:C:150:VAL:CG1	1:C:151:PHE:N	2.70	0.54
1:E:153:GLN:O	1:F:158:SER:HB2	2.07	0.54
1:D:148:THR:HG21	1:D:193:ARG:HD2	1.90	0.54
1:D:332:GLY:O	1:D:333:MET:O	2.26	0.54
1:A:400:THR:HG22	1:A:401:GLY:N	2.22	0.54
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.88	0.54
1:B:150:VAL:HG13	1:B:151:PHE:H	1.73	0.54
1:B:363:ILE:O	1:B:367:ILE:HG13	2.08	0.54
1:D:377:ILE:HD12	1:D:412:PHE:HE2	1.71	0.54
1:E:294:LYS:N	2:E:5901:ATP:O1B	2.41	0.54
1:F:377:ILE:CD1	1:F:399:VAL:HG11	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ASP:C	1:C:113:GLU:H	2.12	0.54
1:C:185:ILE:N	1:C:185:ILE:HD12	2.22	0.54
1:F:185:ILE:N	1:F:185:ILE:HD12	2.23	0.54
1:A:273:MET:O	1:A:464:ASP:N	2.36	0.53
1:E:356:LEU:HD13	1:E:387:VAL:HG21	1.89	0.53
1:F:93:ASP:OD2	1:F:96:LYS:HB2	2.08	0.53
1:A:169:ALA:O	1:A:173:GLN:HG3	2.08	0.53
1:B:437:ILE:CD1	1:B:457:LYS:CE	2.83	0.53
1:F:208:ARG:NH2	1:F:221:GLU:OE2	2.41	0.53
1:D:79:THR:CG2	1:D:82:ASP:H	2.14	0.53
1:F:347:VAL:O	1:F:348:CYS:HB2	2.08	0.53
1:A:150:VAL:HG13	1:A:151:PHE:H	1.70	0.53
1:C:419:PHE:O	1:C:420:MET:HB2	2.08	0.53
1:F:218:ARG:HB3	3:F:6920:HOH:O	2.08	0.53
1:E:266:GLY:HA2	1:E:304:ASN:HD22	1.73	0.53
1:A:461:SER:OG	1:A:462:TRP:N	2.41	0.53
1:F:317:TYR:CD2	1:F:383:LEU:HD21	2.44	0.53
1:D:453:ILE:CG2	1:D:479:ILE:HD12	2.29	0.53
1:C:89:SER:HB2	1:D:227:GLY:O	2.08	0.53
1:E:448:GLU:HG2	1:F:466:ALA:HA	1.90	0.53
1:F:24:MET:HG3	1:F:66:GLU:HG3	1.90	0.53
1:A:440:LEU:CD2	1:A:453:ILE:HG13	2.38	0.53
1:E:295:THR:HG21	1:E:319:GLU:OE2	2.08	0.53
1:E:418:GLN:HB2	1:F:423:HIS:O	2.08	0.53
1:C:248:PRO:HB2	1:C:251:ALA:HB3	1.89	0.53
1:E:372:PRO:HB2	1:E:375:ILE:CD1	2.39	0.53
1:C:470:PHE:HB2	1:C:478:ASP:O	2.08	0.53
1:C:169:ALA:O	1:C:173:GLN:HG3	2.08	0.53
1:F:149:SER:HA	1:F:152:GLN:HB2	1.90	0.53
1:E:347:VAL:O	1:E:348:CYS:HB2	2.08	0.53
1:D:438:ILE:HG23	1:D:453:ILE:HD11	1.89	0.53
1:F:182:THR:HG22	1:F:183:GLU:N	2.21	0.53
1:A:74:VAL:HG22	1:A:106:LEU:HD23	1.91	0.53
1:D:299:SER:C	1:D:333:MET:HE1	2.29	0.53
1:C:85:LYS:HZ3	1:D:14:GLU:HB3	1.72	0.53
1:F:420:MET:HA	3:F:6916:HOH:O	2.07	0.53
1:E:146:SER:H	1:E:181:THR:HG22	1.74	0.53
1:B:362:ILE:HG22	1:B:366:GLU:OE2	2.09	0.53
1:E:76:PHE:CZ	1:E:126:LEU:HD21	2.44	0.53
1:A:438:ILE:HD13	1:A:455:VAL:HA	1.91	0.53
1:D:375:ILE:HD13	1:D:408:ILE:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ASP:HA	1:F:125:ALA:HB3	1.91	0.53
1:E:447:GLY:C	1:F:467:ILE:HD13	2.28	0.53
1:C:334:ASP:OD1	1:C:336:GLU:HB2	2.09	0.53
1:B:159:VAL:O	1:B:163:GLU:HG2	2.08	0.53
1:E:18:ILE:HG13	1:E:228:THR:HG23	1.91	0.53
1:E:202:ASP:HA	1:E:226:ARG:HD2	1.90	0.53
1:A:254:LEU:HD23	1:F:348:CYS:HB3	1.91	0.53
1:D:396:VAL:O	1:D:400:THR:HB	2.09	0.53
1:F:264:SER:O	1:F:374:ARG:NH2	2.41	0.52
1:A:21:MET:HE2	1:A:177:THR:HG21	1.90	0.52
1:F:164:LEU:HD11	1:F:197:GLU:HG3	1.90	0.52
1:A:90:PHE:O	1:A:92:TRP:CE3	2.62	0.52
1:F:317:TYR:CE2	1:F:383:LEU:HD21	2.43	0.52
1:D:269:ARG:HG2	1:D:479:ILE:HB	1.89	0.52
1:A:91:GLY:C	1:A:92:TRP:HE3	2.13	0.52
1:B:311:ARG:HA	1:B:343:LEU:O	2.10	0.52
1:C:479:ILE:HD12	1:C:479:ILE:N	2.25	0.52
1:D:294:LYS:N	2:D:4901:ATP:O1B	2.42	0.52
1:E:80:PRO:HD2	1:E:81:GLN:NE2	2.24	0.52
1:E:70:PRO:HB2	1:E:139:ALA:HA	1.92	0.52
1:F:25:ILE:HD13	1:F:62:ASN:ND2	2.25	0.52
1:A:14:GLU:CG	1:A:15:HIS:H	2.21	0.52
1:D:446:ARG:H	1:D:496:ARG:NH1	2.03	0.52
1:B:64:ILE:HD11	1:B:102:LYS:O	2.09	0.52
1:D:347:VAL:O	1:D:348:CYS:HB2	2.10	0.52
1:F:25:ILE:HD12	1:F:58:GLN:HG2	1.92	0.52
1:C:65:ILE:N	1:C:65:ILE:CD1	2.70	0.52
1:D:84:ILE:HD13	1:D:94:LEU:HB2	1.90	0.52
1:F:184:ARG:HG2	1:F:191:ILE:O	2.10	0.52
1:C:206:ILE:HD12	1:C:206:ILE:N	2.24	0.52
1:F:440:LEU:HD23	1:F:453:ILE:HG13	1.90	0.52
1:B:248:PRO:HB2	1:B:251:ALA:HB3	1.92	0.52
1:E:444:GLU:OE1	1:F:490:ILE:HG12	2.09	0.52
1:E:431:SER:O	1:E:434:THR:HG22	2.09	0.52
1:B:206:ILE:N	1:B:206:ILE:HD12	2.25	0.52
1:D:495:THR:O	1:D:497:ILE:HG23	2.10	0.52
1:F:126:LEU:HG	1:F:130:ILE:HD11	1.92	0.52
1:F:406:GLU:HB3	1:F:408:ILE:HG12	1.92	0.52
1:B:290:THR:HG22	2:B:2901:ATP:O1G	2.10	0.52
1:A:371:LYS:N	1:A:372:PRO:HD3	2.25	0.52
1:E:348:CYS:HB3	1:F:254:LEU:HD23	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:ILE:HD12	1:F:139:ALA:HB3	1.91	0.52
1:A:318:GLU:OE2	1:B:432:THR:HG23	2.09	0.52
1:A:126:LEU:HG	1:A:130:ILE:HD11	1.92	0.52
1:D:89:SER:HB2	1:E:227:GLY:O	2.09	0.52
1:C:117:VAL:HG12	1:C:117:VAL:O	2.10	0.52
1:B:356:LEU:HD22	1:B:387:VAL:HG11	1.90	0.52
1:D:472:ILE:N	1:D:472:ILE:HD12	2.24	0.52
1:C:311:ARG:HA	1:C:343:LEU:O	2.10	0.52
1:F:115:GLN:HG3	1:F:116:GLU:N	2.25	0.52
1:A:18:ILE:HD12	1:A:18:ILE:N	2.25	0.52
1:D:267:VAL:CG2	1:D:300:ARG:HG2	2.40	0.52
1:F:315:PHE:CZ	1:F:363:ILE:HG23	2.44	0.51
1:D:440:LEU:HD21	1:D:453:ILE:HG12	1.92	0.51
1:C:371:LYS:HD3	1:C:371:LYS:O	2.10	0.51
1:C:318:GLU:OE2	1:D:432:THR:CG2	2.58	0.51
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.91	0.51
1:D:489:ILE:HA	1:D:494:PRO:HG3	1.92	0.51
1:D:489:ILE:HD13	1:D:494:PRO:CG	2.40	0.51
1:C:49:GLY:HA2	2:C:3903:ATP:O2B	2.10	0.51
1:C:81:GLN:CD	1:C:81:GLN:H	2.13	0.51
1:C:81:GLN:H	1:C:81:GLN:NE2	2.07	0.51
1:E:356:LEU:CD1	1:E:387:VAL:HG21	2.40	0.51
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.91	0.51
1:D:21:MET:HE3	1:D:59:PHE:CZ	2.45	0.51
1:B:433:ILE:HD12	1:B:433:ILE:N	2.25	0.51
1:B:325:LEU:HD23	1:B:335:PHE:HB2	1.92	0.51
1:F:56:SER:HB2	1:F:143:SER:HB2	1.91	0.51
1:D:287:THR:HG23	1:D:414:ASN:ND2	2.17	0.51
1:F:14:GLU:HG3	1:F:16:GLN:HG3	1.93	0.51
1:E:323:GLN:HE21	1:F:459:ARG:HD3	1.74	0.51
1:E:438:ILE:CD1	1:E:455:VAL:HG22	2.41	0.51
1:D:106:LEU:HD11	1:D:129:ARG:NH2	2.25	0.51
1:D:367:ILE:CD1	1:D:372:PRO:HG2	2.40	0.51
1:E:347:VAL:HG12	1:E:348:CYS:N	2.23	0.51
1:C:438:ILE:HD13	1:C:455:VAL:HA	1.93	0.51
1:B:90:PHE:O	1:B:92:TRP:CZ3	2.63	0.51
1:E:300:ARG:HA	1:E:333:MET:HE3	1.93	0.51
1:D:170:ARG:HD2	1:D:173:GLN:OE1	2.10	0.51
1:E:496:ARG:HG3	1:E:497:ILE:H	1.75	0.51
1:D:150:VAL:CG1	1:D:151:PHE:N	2.72	0.51
1:E:316:ALA:O	1:E:348:CYS:HA	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:PHE:C	1:E:153:GLN:H	2.14	0.51
1:F:489:ILE:HD13	1:F:494:PRO:CG	2.41	0.51
1:F:479:ILE:N	1:F:479:ILE:HD12	2.26	0.51
1:A:488:ARG:HE	1:F:488:ARG:HH12	1.56	0.51
1:A:21:MET:HB2	1:A:38:ILE:HD11	1.93	0.51
1:E:123:LEU:C	1:E:127:ILE:HG12	2.31	0.51
1:D:18:ILE:CD1	1:D:18:ILE:H	2.17	0.51
1:C:420:MET:HE3	1:D:490:ILE:HD13	1.91	0.51
1:F:287:THR:HG21	1:F:425:ILE:O	2.10	0.51
1:E:126:LEU:O	1:E:129:ARG:HB2	2.11	0.51
1:C:111:ASP:O	1:C:113:GLU:N	2.41	0.51
1:F:291:GLY:N	2:F:6901:ATP:O2B	2.44	0.51
1:E:264:SER:O	1:E:374:ARG:NH2	2.44	0.51
1:C:191:ILE:H	1:C:191:ILE:HD12	1.75	0.51
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.92	0.51
1:A:449:MET:HG2	1:B:467:ILE:HD11	1.92	0.51
1:B:467:ILE:N	1:B:467:ILE:HD12	2.26	0.51
1:A:432:THR:CG2	1:F:318:GLU:OE2	2.59	0.51
1:A:150:VAL:CG1	1:A:151:PHE:H	2.23	0.51
1:F:118:VAL:CG1	1:F:153:GLN:HE22	2.23	0.51
1:B:444:GLU:HB2	1:C:490:ILE:HD11	1.93	0.51
1:D:311:ARG:HD3	1:D:370:PHE:CE1	2.46	0.51
1:D:311:ARG:HD3	1:D:370:PHE:CZ	2.45	0.51
1:F:218:ARG:CZ	1:F:239:ILE:HD12	2.41	0.51
1:D:290:THR:HG22	2:D:4901:ATP:O1G	2.11	0.51
1:B:264:SER:HB3	1:B:304:ASN:HD21	1.75	0.51
1:D:362:ILE:HG22	1:D:366:GLU:OE2	2.11	0.51
1:B:31:ILE:HA	1:B:231:MET:SD	2.51	0.51
1:F:79:THR:CG2	1:F:82:ASP:H	2.22	0.51
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.41	0.51
1:A:182:THR:HG22	1:A:183:GLU:N	2.26	0.51
1:C:344:LEU:HD11	1:C:346:ILE:CD1	2.41	0.51
1:C:182:THR:CG2	1:C:183:GLU:N	2.74	0.51
1:B:299:SER:C	1:B:333:MET:HE1	2.32	0.51
1:E:72:VAL:HG21	1:E:134:ILE:CD1	2.38	0.50
1:E:486:PHE:HB2	1:E:489:ILE:HD11	1.93	0.50
1:E:360:LEU:CD2	1:E:364:LYS:HE3	2.41	0.50
1:A:484:ARG:HB3	1:A:484:ARG:NH1	2.25	0.50
1:B:130:ILE:O	1:B:134:ILE:HG13	2.11	0.50
1:E:284:ILE:N	1:E:284:ILE:HD13	2.26	0.50
1:B:150:VAL:CG1	1:B:151:PHE:N	2.74	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:ILE:HG21	1:F:147:VAL:HG12	1.93	0.50
1:C:31:ILE:HD11	1:C:248:PRO:HB3	1.94	0.50
1:A:21:MET:HE3	1:A:59:PHE:CE1	2.47	0.50
1:B:294:LYS:N	2:B:2901:ATP:O1B	2.44	0.50
1:D:127:ILE:HD13	1:D:170:ARG:HG3	1.93	0.50
1:D:60:LEU:O	1:D:64:ILE:CD1	2.46	0.50
1:C:332:GLY:O	1:C:333:MET:O	2.30	0.50
1:E:472:ILE:HD12	1:E:472:ILE:N	2.26	0.50
1:C:114:GLY:O	1:C:115:GLN:HB3	2.11	0.50
1:A:92:TRP:HA	1:A:92:TRP:CE3	2.47	0.50
1:C:43:LEU:HD11	1:C:182:THR:OG1	2.11	0.50
1:D:169:ALA:O	1:D:173:GLN:HG3	2.10	0.50
1:E:218:ARG:CZ	1:E:239:ILE:HD12	2.42	0.50
1:E:283:ILE:C	1:E:284:ILE:HD13	2.31	0.50
1:E:315:PHE:CZ	1:E:363:ILE:HG23	2.46	0.50
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.93	0.50
1:C:49:GLY:O	1:C:218:ARG:NH2	2.43	0.50
1:F:72:VAL:HG21	1:F:134:ILE:HD13	1.93	0.50
1:B:99:ASP:C	1:B:101:GLY:H	2.14	0.50
1:F:50:THR:HG22	1:F:209:ASN:HB2	1.92	0.50
1:E:296:LEU:HD13	1:E:331:TRP:CD2	2.47	0.50
1:B:371:LYS:N	1:B:372:PRO:HD3	2.27	0.50
1:A:64:ILE:HD11	1:A:102:LYS:O	2.12	0.50
1:D:338:MET:HB3	1:D:344:LEU:HB3	1.93	0.50
1:B:92:TRP:CE3	1:B:92:TRP:CA	2.94	0.50
1:D:283:ILE:HD13	1:D:400:THR:HG23	1.94	0.50
1:E:332:GLY:O	1:E:333:MET:O	2.30	0.50
1:A:348:CYS:HB3	1:B:254:LEU:HD23	1.93	0.50
1:D:150:VAL:HG13	1:D:151:PHE:H	1.76	0.50
1:B:184:ARG:HG2	1:B:191:ILE:O	2.11	0.50
1:B:420:MET:SD	1:C:490:ILE:HD13	2.52	0.50
1:D:430:ILE:HA	1:D:433:ILE:HD13	1.94	0.50
1:B:123:LEU:HG	1:B:163:GLU:OE2	2.12	0.50
1:F:90:PHE:CB	1:F:92:TRP:CE2	2.94	0.50
1:C:396:VAL:O	1:C:400:THR:HB	2.12	0.50
1:F:28:PHE:HE1	1:F:222:ILE:HD11	1.77	0.50
1:B:123:LEU:CD1	1:B:166:ARG:HD2	2.40	0.50
1:F:218:ARG:NH1	1:F:239:ILE:HD12	2.27	0.50
1:E:89:SER:HB2	1:F:227:GLY:O	2.12	0.50
1:B:211:LEU:O	1:B:212:GLU:HB3	2.11	0.50
1:D:64:ILE:HD12	1:D:64:ILE:N	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:439:LEU:HD12	1:D:440:LEU:N	2.27	0.50
1:D:451:ARG:HG2	1:D:451:ARG:NH1	2.25	0.50
1:C:348:CYS:O	1:C:349:ALA:HB2	2.12	0.50
1:C:420:MET:SD	1:D:490:ILE:HD13	2.52	0.50
1:D:49:GLY:O	1:D:218:ARG:NH2	2.45	0.50
1:D:344:LEU:HD13	1:D:344:LEU:C	2.32	0.50
1:F:439:LEU:HD12	1:F:440:LEU:N	2.26	0.50
1:C:134:ILE:HG23	1:C:139:ALA:HB3	1.94	0.50
1:D:420:MET:HE3	1:D:492:GLY:HA3	1.94	0.49
1:B:185:ILE:HD11	1:B:193:ARG:NH1	2.27	0.49
1:A:451:ARG:N	1:A:451:ARG:HD2	2.27	0.49
1:D:85:LYS:HZ3	1:E:14:GLU:HB3	1.75	0.49
1:A:283:ILE:HD12	1:A:412:PHE:HE1	1.77	0.49
1:C:332:GLY:O	1:C:333:MET:C	2.50	0.49
1:A:142:VAL:O	1:A:178:THR:HA	2.12	0.49
1:C:150:VAL:CG1	1:C:151:PHE:H	2.24	0.49
1:E:52:LYS:HD3	1:E:182:THR:O	2.12	0.49
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.41	0.49
1:C:120:GLY:C	1:C:122:ASP:H	2.16	0.49
1:F:283:ILE:HG23	1:F:412:PHE:HE1	1.75	0.49
1:F:360:LEU:CD2	1:F:364:LYS:HE3	2.42	0.49
1:E:255:THR:HG22	1:E:255:THR:O	2.12	0.49
1:B:492:GLY:O	1:B:494:PRO:HD3	2.13	0.49
1:A:90:PHE:O	1:A:92:TRP:CZ3	2.65	0.49
1:E:375:ILE:HD12	1:E:408:ILE:HG21	1.93	0.49
1:E:448:GLU:HA	1:F:467:ILE:CD1	2.43	0.49
1:F:496:ARG:HD3	1:F:496:ARG:N	2.27	0.49
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.94	0.49
1:B:264:SER:HA	1:B:271:ASP:OD1	2.12	0.49
1:E:130:ILE:O	1:E:134:ILE:HD13	2.11	0.49
1:D:203:ASN:HB3	1:D:225:LEU:HD23	1.95	0.49
1:C:91:GLY:O	1:C:92:TRP:HE3	1.94	0.49
1:C:352:GLU:OE2	1:C:385:ARG:HD2	2.13	0.49
1:B:151:PHE:C	1:B:153:GLN:H	2.14	0.49
1:F:483:PHE:HB3	1:F:486:PHE:CD1	2.47	0.49
1:D:433:ILE:HD12	1:D:433:ILE:N	2.28	0.49
1:F:16:GLN:NE2	1:F:33:HIS:HB3	2.27	0.49
1:E:496:ARG:HG3	1:E:497:ILE:N	2.28	0.49
1:B:296:LEU:HD21	1:B:477:PRO:HD3	1.94	0.49
1:C:323:GLN:NE2	1:D:459:ARG:HD3	2.27	0.49
1:E:360:LEU:HD21	1:E:364:LYS:HE3	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:LEU:HD11	1:C:129:ARG:NH2	2.27	0.49
1:B:334:ASP:OD1	1:B:336:GLU:HB2	2.12	0.49
1:B:334:ASP:O	1:B:338:MET:HG2	2.13	0.49
1:E:436:THR:HG23	1:E:458:MET:HG2	1.93	0.49
1:C:28:PHE:CE1	1:C:222:ILE:HD11	2.48	0.49
1:E:28:PHE:CE1	1:E:222:ILE:HD11	2.47	0.49
1:D:451:ARG:NH1	1:D:472:ILE:HD13	2.28	0.49
1:D:94:LEU:O	1:D:98:VAL:HG23	2.11	0.49
1:E:52:LYS:HE3	2:E:5903:ATP:O1B	2.12	0.49
1:D:191:ILE:HB	1:D:198:GLU:HG2	1.90	0.49
1:B:441:GLN:HE22	1:B:490:ILE:HA	1.78	0.49
1:E:150:VAL:HG13	1:E:151:PHE:H	1.78	0.49
1:C:203:ASN:HB3	1:C:225:LEU:CD2	2.43	0.49
1:B:146:SER:H	1:B:181:THR:CG2	2.26	0.49
1:A:338:MET:HB3	1:A:344:LEU:HB3	1.94	0.49
1:D:370:PHE:O	1:D:371:LYS:CD	2.61	0.49
1:C:440:LEU:HD23	1:C:453:ILE:HG12	1.93	0.49
1:C:469:GLU:CG	1:C:480:LYS:HE3	2.43	0.49
1:A:269:ARG:HB3	1:A:479:ILE:HD12	1.94	0.49
1:F:451:ARG:NH1	1:F:472:ILE:HD12	2.27	0.49
1:B:91:GLY:C	1:B:92:TRP:HE3	2.16	0.49
1:D:445:ILE:HD12	1:D:450:SER:OG	2.13	0.49
1:F:115:GLN:CG	1:F:116:GLU:H	2.26	0.48
1:B:182:THR:HG22	1:B:183:GLU:N	2.28	0.48
1:F:182:THR:HG21	1:F:192:ALA:CB	2.40	0.48
1:C:453:ILE:HD13	1:C:454:ASN:H	1.78	0.48
1:C:300:ARG:N	1:C:333:MET:HE1	2.28	0.48
1:C:191:ILE:HD12	1:C:191:ILE:N	2.28	0.48
1:C:356:LEU:HD22	1:C:387:VAL:HG11	1.94	0.48
1:D:468:ARG:HH11	1:D:468:ARG:HG2	1.78	0.48
1:D:182:THR:HG21	1:D:192:ALA:CB	2.40	0.48
1:E:72:VAL:CG2	1:E:134:ILE:HD12	2.41	0.48
1:E:344:LEU:HD22	1:E:345:LYS:H	1.78	0.48
1:F:453:ILE:HB	1:F:470:PHE:CD2	2.49	0.48
1:B:145:ASP:HA	1:B:181:THR:HB	1.95	0.48
1:A:344:LEU:HD22	1:A:345:LYS:H	1.77	0.48
1:B:430:ILE:HA	1:B:433:ILE:HD13	1.94	0.48
1:F:211:LEU:O	1:F:212:GLU:HB3	2.12	0.48
1:D:151:PHE:C	1:D:153:GLN:N	2.67	0.48
1:F:64:ILE:HD11	1:F:102:LYS:O	2.14	0.48
1:A:434:THR:HG23	1:A:437:ILE:CD1	2.36	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:THR:HB	1:F:25:ILE:HG12	1.95	0.48
1:D:255:THR:HG22	1:D:255:THR:O	2.14	0.48
1:E:306:CYS:SG	1:E:344:LEU:HB2	2.53	0.48
1:B:262:ARG:NH2	1:B:461:SER:HB2	2.28	0.48
1:D:267:VAL:HG22	1:D:300:ARG:HG2	1.96	0.48
1:D:468:ARG:NH1	1:D:468:ARG:HG2	2.29	0.48
1:F:182:THR:CG2	1:F:183:GLU:N	2.75	0.48
1:A:144:ILE:N	1:A:144:ILE:HD13	2.29	0.48
1:C:49:GLY:CA	2:C:3903:ATP:O2B	2.61	0.48
1:E:291:GLY:N	2:E:5901:ATP:O2B	2.46	0.48
1:F:134:ILE:CD1	1:F:139:ALA:HB3	2.42	0.48
1:A:21:MET:CE	1:A:59:PHE:HZ	2.27	0.48
1:A:419:PHE:O	1:A:420:MET:HB2	2.13	0.48
1:F:274:CYS:HG	1:F:278:PHE:HE2	1.60	0.48
1:A:454:ASN:CG	1:A:467:ILE:HD13	2.33	0.48
1:E:123:LEU:HD23	1:E:127:ILE:HD11	1.95	0.48
1:E:150:VAL:CG1	1:E:151:PHE:N	2.75	0.48
1:E:182:THR:HG22	1:E:183:GLU:N	2.28	0.48
1:D:332:GLY:O	1:D:333:MET:C	2.51	0.48
1:C:469:GLU:HB3	1:C:483:PHE:CZ	2.48	0.48
1:D:356:LEU:CD2	1:D:387:VAL:HG11	2.44	0.48
1:D:130:ILE:HD12	1:D:130:ILE:N	2.28	0.48
1:D:367:ILE:HD12	1:D:375:ILE:CD1	2.41	0.48
1:B:148:THR:HG21	1:B:193:ARG:HD2	1.96	0.48
1:F:437:ILE:CD1	1:F:437:ILE:N	2.77	0.48
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.39	0.48
1:A:487:GLU:OE1	1:F:495:THR:HA	2.14	0.48
1:E:134:ILE:N	1:E:134:ILE:HD13	2.29	0.48
1:C:438:ILE:HG23	1:C:453:ILE:HD11	1.95	0.48
1:B:79:THR:HG22	1:B:82:ASP:H	1.78	0.48
1:F:371:LYS:N	1:F:372:PRO:HD3	2.29	0.48
1:C:296:LEU:HD13	1:C:331:TRP:CD2	2.49	0.48
1:A:14:GLU:HG3	1:A:15:HIS:N	2.29	0.48
1:B:208:ARG:NH2	1:B:221:GLU:OE2	2.47	0.48
1:B:93:ASP:OD2	1:B:96:LYS:HB2	2.13	0.48
1:E:99:ASP:C	1:E:101:GLY:H	2.17	0.48
1:A:347:VAL:O	1:A:348:CYS:HB2	2.14	0.48
1:E:321:ARG:HG2	1:E:348:CYS:SG	2.54	0.48
1:D:263:VAL:CG1	1:D:374:ARG:HH21	2.21	0.48
1:C:325:LEU:HD23	1:C:335:PHE:CB	2.43	0.48
1:C:21:MET:HE2	1:C:177:THR:CG2	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:GLU:HG3	1:D:233:GLY:O	2.13	0.48
1:D:289:ALA:HB2	1:D:419:PHE:HA	1.96	0.48
1:C:283:ILE:C	1:C:284:ILE:HD13	2.33	0.48
1:C:334:ASP:O	1:C:338:MET:HG2	2.14	0.48
1:F:291:GLY:HA3	1:F:442:TYR:OH	2.14	0.48
1:B:87:ALA:HB1	1:B:92:TRP:HB2	1.96	0.48
1:C:294:LYS:N	2:C:3901:ATP:O1B	2.47	0.48
1:F:21:MET:HE3	1:F:59:PHE:CE1	2.49	0.48
1:C:433:ILE:HD12	1:C:433:ILE:N	2.29	0.48
1:D:372:PRO:HB2	1:D:375:ILE:CD1	2.44	0.48
1:F:116:GLU:O	1:F:117:VAL:HB	2.14	0.48
1:F:191:ILE:HB	1:F:198:GLU:HG3	1.94	0.48
1:F:61:TYR:CE2	1:F:65:ILE:HG13	2.48	0.48
1:A:89:SER:CB	1:B:227:GLY:O	2.61	0.48
1:C:185:ILE:HA	3:D:4912:HOH:O	2.13	0.48
1:C:393:ARG:O	1:C:397:ILE:HG12	2.14	0.48
1:D:372:PRO:HB2	1:D:375:ILE:HD11	1.96	0.47
1:B:150:VAL:CG1	1:B:151:PHE:H	2.27	0.47
1:F:106:LEU:CD1	1:F:129:ARG:CZ	2.84	0.47
1:F:127:ILE:CD1	1:F:167:LEU:HD12	2.43	0.47
1:C:471:MET:HG3	1:C:478:ASP:HB3	1.95	0.47
1:A:145:ASP:OD2	1:A:181:THR:HG21	2.14	0.47
1:C:371:LYS:N	1:C:372:PRO:HD3	2.29	0.47
1:C:144:ILE:CG2	1:C:147:VAL:HG12	2.44	0.47
1:C:18:ILE:HB	1:C:228:THR:HG23	1.96	0.47
1:D:148:THR:OG1	1:D:182:THR:HG23	2.14	0.47
1:B:197:GLU:CD	1:B:197:GLU:H	2.18	0.47
1:F:299:SER:CB	1:F:333:MET:HE1	2.43	0.47
1:E:451:ARG:NH1	1:E:472:ILE:HD13	2.28	0.47
1:C:73:PHE:HB3	1:C:105:ILE:CD1	2.41	0.47
1:E:148:THR:HG21	1:E:183:GLU:CG	2.45	0.47
1:F:311:ARG:HA	1:F:343:LEU:O	2.14	0.47
1:A:488:ARG:NH1	1:B:488:ARG:HH21	2.11	0.47
1:E:146:SER:H	1:E:181:THR:CG2	2.27	0.47
1:A:402:TYR:O	1:A:406:GLU:HB2	2.13	0.47
1:F:170:ARG:HD2	1:F:173:GLN:OE1	2.14	0.47
1:F:178:THR:HG22	1:F:179:VAL:N	2.29	0.47
1:F:294:LYS:N	2:F:6901:ATP:O1B	2.47	0.47
1:A:459:ARG:HD3	1:F:323:GLN:HE21	1.79	0.47
1:C:357:GLU:HG3	1:C:358:ASP:N	2.29	0.47
1:C:468:ARG:HG2	1:C:468:ARG:HH11	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:GLU:HB3	1:A:408:ILE:HG12	1.97	0.47
1:B:396:VAL:O	1:B:400:THR:HB	2.14	0.47
1:F:437:ILE:HD11	1:F:457:LYS:HE2	1.96	0.47
1:C:84:ILE:HD12	1:C:94:LEU:CB	2.38	0.47
1:D:18:ILE:HD13	1:D:227:GLY:O	2.14	0.47
1:F:445:ILE:CD1	1:F:483:PHE:CE2	2.97	0.47
1:E:14:GLU:HG3	1:E:16:GLN:HB2	1.95	0.47
1:A:433:ILE:HD11	1:F:385:ARG:CZ	2.44	0.47
1:F:356:LEU:HD21	1:F:387:VAL:HG11	1.97	0.47
1:F:334:ASP:OD1	1:F:336:GLU:HB2	2.15	0.47
1:E:73:PHE:CE2	1:E:83:ILE:HD13	2.49	0.47
1:D:142:VAL:O	1:D:178:THR:HA	2.13	0.47
1:E:311:ARG:HA	1:E:343:LEU:O	2.15	0.47
1:C:17:ALA:C	1:C:18:ILE:HD12	2.34	0.47
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.96	0.47
1:E:14:GLU:HG3	1:E:16:GLN:N	2.24	0.47
1:B:344:LEU:HD22	1:B:345:LYS:H	1.79	0.47
1:B:262:ARG:HH22	1:B:461:SER:HB2	1.79	0.47
1:E:143:SER:HA	1:E:179:VAL:O	2.15	0.47
1:E:313:ILE:HD12	1:E:367:ILE:CD1	2.35	0.47
1:E:287:THR:HG21	1:E:425:ILE:O	2.15	0.47
1:F:45:SER:HB2	1:F:182:THR:HB	1.95	0.47
1:A:143:SER:C	1:A:144:ILE:HD13	2.35	0.47
1:C:122:ASP:O	1:C:124:SER:N	2.47	0.47
1:C:45:SER:CB	1:C:182:THR:HB	2.44	0.47
1:E:439:LEU:HD12	1:E:440:LEU:N	2.29	0.47
1:A:16:GLN:O	1:A:17:ALA:O	2.32	0.47
1:F:295:THR:HB	2:F:6901:ATP:PA	2.54	0.47
1:F:18:ILE:HG12	1:F:228:THR:HG23	1.96	0.47
1:C:363:ILE:O	1:C:367:ILE:HG13	2.14	0.47
1:D:31:ILE:HD11	1:D:248:PRO:HB3	1.96	0.47
1:D:191:ILE:HD12	1:D:191:ILE:N	2.30	0.47
1:F:146:SER:H	1:F:181:THR:CG2	2.27	0.47
1:C:487:GLU:CG	1:C:497:ILE:HD11	2.44	0.47
1:A:211:LEU:HD12	1:A:215:ARG:O	2.15	0.47
1:B:203:ASN:HB3	1:B:225:LEU:HD23	1.97	0.47
1:D:197:GLU:CD	1:D:197:GLU:H	2.16	0.47
1:E:127:ILE:CD1	1:E:167:LEU:HD13	2.45	0.47
1:D:371:LYS:HE2	1:D:371:LYS:O	2.15	0.47
1:A:64:ILE:HD13	1:A:69:GLU:O	2.15	0.47
1:D:433:ILE:HG22	1:D:433:ILE:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:NH1	1:A:239:ILE:HD12	2.29	0.47
1:C:267:VAL:HB	1:C:270:LEU:HB2	1.97	0.47
1:F:76:PHE:HZ	1:F:126:LEU:HD21	1.80	0.47
1:F:150:VAL:CG1	1:F:151:PHE:N	2.78	0.47
1:B:191:ILE:HB	1:B:198:GLU:HG2	1.97	0.47
1:F:25:ILE:CD1	1:F:58:GLN:HG2	2.45	0.47
1:E:440:LEU:HD23	1:E:453:ILE:HG13	1.97	0.47
1:A:334:ASP:OD1	1:A:336:GLU:HB2	2.14	0.47
1:B:96:LYS:O	1:B:100:GLU:HG3	2.13	0.47
1:C:131:ASN:OD1	1:C:174:ILE:HD12	2.15	0.47
1:D:488:ARG:HH12	1:E:488:ARG:HH21	1.61	0.46
1:E:123:LEU:HD21	1:E:167:LEU:HB2	1.96	0.46
1:C:123:LEU:HD13	1:C:166:ARG:HD2	1.96	0.46
1:B:249:LEU:CD1	1:B:394:GLN:HG2	2.45	0.46
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.79	0.46
1:D:461:SER:OG	1:D:462:TRP:N	2.47	0.46
1:F:21:MET:HB2	1:F:38:ILE:HG12	1.97	0.46
1:D:143:SER:HA	1:D:179:VAL:O	2.15	0.46
1:C:146:SER:H	1:C:181:THR:HG22	1.79	0.46
1:E:90:PHE:HB2	1:E:92:TRP:CE2	2.50	0.46
1:A:362:ILE:CD1	1:A:362:ILE:N	2.78	0.46
1:E:161:ARG:CB	1:E:196:VAL:HG11	2.38	0.46
1:A:332:GLY:O	1:A:333:MET:C	2.53	0.46
1:D:14:GLU:CG	1:D:15:HIS:H	2.28	0.46
1:B:451:ARG:NH1	1:B:451:ARG:HG2	2.30	0.46
1:E:435:ASP:HA	1:E:459:ARG:HD2	1.97	0.46
1:E:21:MET:HE3	1:E:59:PHE:CE1	2.51	0.46
1:C:93:ASP:OD2	1:C:96:LYS:HB2	2.15	0.46
1:E:486:PHE:CB	1:E:489:ILE:HD11	2.45	0.46
1:A:21:MET:CE	1:A:59:PHE:CZ	2.97	0.46
1:B:92:TRP:HE3	1:B:92:TRP:CA	2.27	0.46
1:B:142:VAL:O	1:B:178:THR:HA	2.16	0.46
1:E:145:ASP:OD2	1:E:181:THR:HG21	2.16	0.46
1:C:393:ARG:HH21	1:C:429:HIS:HB2	1.80	0.46
1:F:18:ILE:CG1	1:F:228:THR:HG23	2.45	0.46
1:A:91:GLY:C	1:A:92:TRP:CE3	2.89	0.46
1:D:64:ILE:CD1	1:D:64:ILE:N	2.78	0.46
1:B:449:MET:CE	1:C:467:ILE:HD11	2.45	0.46
1:F:127:ILE:HD12	1:F:170:ARG:HB2	1.97	0.46
1:A:249:LEU:CD1	1:A:394:GLN:HG2	2.44	0.46
1:F:451:ARG:NH1	1:F:451:ARG:HG2	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:MET:CB	1:C:62:ASN:HD22	2.29	0.46
1:B:340:ARG:C	1:B:342:ASN:H	2.18	0.46
1:F:428:SER:OG	1:F:430:ILE:HG12	2.16	0.46
1:A:376:ALA:HA	1:A:411:LEU:O	2.16	0.46
1:F:321:ARG:O	1:F:325:LEU:HD12	2.15	0.46
1:D:64:ILE:HD12	1:D:69:GLU:O	2.15	0.46
1:E:153:GLN:C	1:F:158:SER:HB2	2.36	0.46
1:D:301:PHE:CZ	1:D:374:ARG:HD3	2.50	0.46
1:C:314:LEU:HB3	1:C:346:ILE:CD1	2.46	0.46
1:A:126:LEU:O	1:A:130:ILE:HG13	2.15	0.46
1:B:130:ILE:HG22	1:B:134:ILE:HD11	1.98	0.46
1:D:178:THR:HG22	1:D:179:VAL:N	2.31	0.46
1:B:264:SER:HB3	1:B:304:ASN:ND2	2.31	0.46
1:D:470:PHE:CE1	1:D:472:ILE:HD11	2.50	0.46
1:F:106:LEU:CD1	1:F:129:ARG:NH2	2.78	0.46
1:B:182:THR:HG21	1:B:192:ALA:CB	2.43	0.46
1:C:335:PHE:O	1:C:339:GLU:HG3	2.15	0.46
1:B:381:SER:HB3	1:B:414:ASN:OD1	2.16	0.46
1:A:325:LEU:HD23	1:A:335:PHE:CB	2.45	0.46
1:F:356:LEU:HD13	1:F:387:VAL:HG21	1.98	0.46
1:E:246:ILE:HD12	1:E:246:ILE:N	2.31	0.46
1:B:131:ASN:OD1	1:B:174:ILE:HD12	2.16	0.46
1:B:393:ARG:O	1:B:397:ILE:HG12	2.16	0.46
1:C:36:LEU:HD12	1:C:59:PHE:CE1	2.51	0.46
1:F:313:ILE:CB	1:F:375:ILE:CD1	2.69	0.46
1:A:183:GLU:HB2	1:B:199:PHE:CE1	2.50	0.46
1:B:332:GLY:O	1:B:333:MET:C	2.54	0.46
1:F:371:LYS:HE3	1:F:371:LYS:O	2.15	0.46
1:C:81:GLN:CD	1:C:81:GLN:N	2.69	0.46
1:F:321:ARG:HG2	1:F:348:CYS:SG	2.56	0.46
1:D:150:VAL:CG1	1:D:151:PHE:H	2.29	0.46
1:F:115:GLN:HG3	1:F:116:GLU:H	1.80	0.46
1:F:344:LEU:HD22	1:F:345:LYS:H	1.77	0.46
1:D:203:ASN:HB3	1:D:225:LEU:CD2	2.45	0.46
1:D:211:LEU:O	1:D:215:ARG:O	2.32	0.46
1:B:360:LEU:CD2	1:B:364:LYS:HE3	2.46	0.46
1:D:340:ARG:C	1:D:342:ASN:H	2.19	0.46
1:B:284:ILE:N	1:B:284:ILE:HD13	2.31	0.46
1:D:495:THR:HG23	1:E:487:GLU:OE2	2.16	0.46
1:E:325:LEU:HD23	1:E:335:PHE:CB	2.43	0.46
1:D:182:THR:CG2	1:D:183:GLU:N	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ARG:HD3	1:D:15:HIS:C	2.37	0.46
1:B:430:ILE:HG22	1:B:430:ILE:O	2.16	0.46
1:A:231:MET:CE	1:A:251:ALA:HB2	2.46	0.46
1:A:31:ILE:CD1	1:A:246:ILE:HG21	2.46	0.46
1:C:291:GLY:N	2:C:3901:ATP:O2B	2.49	0.46
1:C:78:GLU:HB2	1:C:83:ILE:HD11	1.97	0.46
1:A:311:ARG:HD2	1:A:371:LYS:HD3	1.96	0.46
1:B:161:ARG:CB	1:B:196:VAL:HG11	2.42	0.46
1:B:49:GLY:O	1:B:218:ARG:NH2	2.48	0.46
1:C:148:THR:OG1	1:C:182:THR:HG23	2.16	0.46
1:E:344:LEU:C	1:E:344:LEU:HD13	2.36	0.46
1:F:72:VAL:CG2	1:F:134:ILE:HD13	2.46	0.46
1:F:289:ALA:HB2	1:F:419:PHE:HA	1.98	0.46
1:E:126:LEU:O	1:E:130:ILE:HG13	2.16	0.45
1:F:145:ASP:OD2	1:F:181:THR:HG21	2.16	0.45
1:B:377:ILE:HD13	1:B:412:PHE:CD2	2.50	0.45
1:B:92:TRP:N	1:B:92:TRP:HE3	2.13	0.45
1:D:273:MET:O	1:D:463:HIS:HA	2.15	0.45
1:E:21:MET:CE	1:E:59:PHE:CZ	2.99	0.45
1:D:70:PRO:HB2	1:D:139:ALA:HA	1.97	0.45
1:D:106:LEU:CD1	1:D:129:ARG:NH2	2.79	0.45
1:C:362:ILE:HG22	1:C:366:GLU:OE2	2.16	0.45
1:F:129:ARG:O	1:F:132:TYR:HB3	2.16	0.45
1:A:150:VAL:O	1:A:153:GLN:HG3	2.16	0.45
1:D:76:PHE:O	1:D:109:SER:HA	2.15	0.45
1:A:375:ILE:O	1:A:410:GLY:HA2	2.15	0.45
1:F:443:VAL:HG12	1:F:445:ILE:HG13	1.97	0.45
1:D:377:ILE:HD11	1:D:399:VAL:HG11	1.99	0.45
1:B:295:THR:HB	2:B:2901:ATP:PA	2.56	0.45
1:D:387:VAL:HG12	1:D:388:SER:N	2.30	0.45
1:D:448:GLU:HG2	1:E:466:ALA:HA	1.97	0.45
1:A:45:SER:CB	1:A:182:THR:HB	2.46	0.45
1:F:61:TYR:CE1	1:F:92:TRP:HB3	2.52	0.45
1:F:484:ARG:CB	1:F:484:ARG:NH1	2.79	0.45
1:F:356:LEU:HD22	1:F:387:VAL:HG11	1.98	0.45
1:B:126:LEU:C	1:B:128:GLU:N	2.70	0.45
1:E:487:GLU:HB2	1:E:497:ILE:HD11	1.99	0.45
1:F:24:MET:HB2	1:F:62:ASN:ND2	2.30	0.45
1:B:79:THR:O	1:B:83:ILE:HG12	2.17	0.45
1:B:90:PHE:O	1:B:92:TRP:CE3	2.69	0.45
1:C:208:ARG:NH2	1:C:221:GLU:OE2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:SER:N	1:E:181:THR:HG22	2.32	0.45
1:A:418:GLN:HB2	1:B:423:HIS:O	2.16	0.45
1:E:406:GLU:O	1:E:408:ILE:HG13	2.15	0.45
1:D:425:ILE:HD11	1:D:456:PHE:CD2	2.52	0.45
1:B:449:MET:HE1	1:C:490:ILE:HD11	1.95	0.45
1:B:359:HIS:O	1:B:363:ILE:HG12	2.17	0.45
1:C:305:ALA:HB2	1:C:374:ARG:CD	2.43	0.45
1:F:486:PHE:HE2	1:F:496:ARG:CD	2.27	0.45
1:F:292:THR:HB	1:F:440:LEU:HB3	1.98	0.45
1:A:191:ILE:HB	1:A:198:GLU:HG2	1.98	0.45
1:D:21:MET:CE	1:D:59:PHE:HZ	2.30	0.45
1:C:295:THR:HG21	1:C:319:GLU:OE2	2.16	0.45
1:A:323:GLN:NE2	1:B:459:ARG:HD3	2.31	0.45
1:E:469:GLU:HB3	1:E:483:PHE:CZ	2.52	0.45
1:D:492:GLY:O	1:D:494:PRO:HD3	2.17	0.45
1:A:80:PRO:HD2	1:A:81:GLN:NE2	2.31	0.45
1:B:317:TYR:CE2	1:B:383:LEU:HD21	2.52	0.45
1:B:161:ARG:HD2	1:B:196:VAL:HG13	1.97	0.45
1:C:451:ARG:NH1	1:C:451:ARG:HG2	2.31	0.45
1:F:357:GLU:HG3	1:F:358:ASP:N	2.32	0.45
1:B:484:ARG:NH1	1:B:484:ARG:HB3	2.32	0.45
1:E:371:LYS:N	1:E:372:PRO:HD3	2.31	0.45
1:A:332:GLY:O	1:A:333:MET:O	2.35	0.45
1:F:33:HIS:HD2	1:F:229:SER:OG	1.99	0.45
1:B:452:ALA:HA	1:B:469:GLU:HA	1.99	0.45
1:E:338:MET:HB3	1:E:344:LEU:HB3	1.98	0.45
1:D:352:GLU:OE2	1:D:385:ARG:HD2	2.17	0.45
1:C:249:LEU:HD13	1:C:394:GLN:HG2	1.99	0.45
1:E:211:LEU:O	1:E:212:GLU:HB3	2.16	0.45
1:A:351:PRO:HB3	1:A:383:LEU:HD23	1.98	0.45
1:D:371:LYS:HD3	1:D:371:LYS:O	2.16	0.45
1:F:479:ILE:H	1:F:479:ILE:HD12	1.82	0.45
1:B:469:GLU:HB3	1:B:483:PHE:CZ	2.52	0.45
1:A:18:ILE:HD13	1:A:227:GLY:O	2.17	0.45
1:F:290:THR:HG22	2:F:6901:ATP:O1G	2.17	0.45
1:E:332:GLY:O	1:E:333:MET:C	2.55	0.45
1:D:164:LEU:HD11	1:D:197:GLU:HG3	1.99	0.45
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.47	0.45
1:C:443:VAL:HG12	1:C:445:ILE:HG13	1.99	0.45
1:C:437:ILE:CD1	1:C:457:LYS:HE2	2.47	0.45
1:A:118:VAL:HG12	1:A:122:ASP:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:ARG:HH22	1:D:488:ARG:HH21	1.61	0.45
1:F:467:ILE:N	1:F:467:ILE:CD1	2.80	0.45
1:B:317:TYR:CD2	1:B:383:LEU:HD21	2.51	0.45
1:D:45:SER:HB3	1:D:182:THR:HB	1.98	0.45
1:D:218:ARG:NH1	1:D:239:ILE:HD12	2.33	0.45
1:C:124:SER:O	1:C:128:GLU:HG3	2.17	0.45
1:A:211:LEU:O	1:A:212:GLU:CB	2.64	0.45
1:D:295:THR:HG21	1:D:319:GLU:OE2	2.17	0.45
1:A:352:GLU:OE2	1:A:385:ARG:HD2	2.17	0.45
1:C:24:MET:HG3	1:C:66:GLU:HG3	1.99	0.45
1:C:178:THR:HG22	1:C:179:VAL:N	2.32	0.45
1:B:402:TYR:O	1:B:406:GLU:HB2	2.17	0.45
1:A:256:GLN:O	1:F:322:ALA:HB3	2.17	0.45
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.98	0.45
1:C:33:HIS:HD2	1:C:229:SER:OG	2.00	0.45
1:A:362:ILE:O	1:A:366:GLU:CG	2.53	0.44
1:A:315:PHE:CZ	1:A:363:ILE:HG23	2.52	0.44
1:B:92:TRP:CE3	1:B:92:TRP:N	2.86	0.44
1:C:187:GLU:O	1:C:208:ARG:HD3	2.18	0.44
1:D:21:MET:HE3	1:D:59:PHE:CE1	2.52	0.44
1:F:215:ARG:NE	1:F:215:ARG:HA	2.31	0.44
1:E:334:ASP:OD1	1:E:336:GLU:HB2	2.17	0.44
1:E:485:ASN:HD22	1:E:496:ARG:HD3	1.82	0.44
1:E:487:GLU:O	1:E:488:ARG:CB	2.64	0.44
1:C:316:ALA:O	1:C:348:CYS:HA	2.17	0.44
1:F:23:THR:O	1:F:24:MET:HB2	2.17	0.44
1:B:419:PHE:O	1:B:420:MET:HB2	2.17	0.44
1:C:40:ARG:HG2	1:C:172:LYS:HE3	1.99	0.44
1:A:433:ILE:HG22	1:A:433:ILE:O	2.17	0.44
1:A:356:LEU:HD22	1:A:387:VAL:HG11	1.98	0.44
1:F:21:MET:CE	1:F:59:PHE:CZ	2.99	0.44
1:C:468:ARG:HG2	1:C:468:ARG:NH1	2.31	0.44
1:D:212:GLU:O	1:D:212:GLU:HG2	2.17	0.44
1:F:363:ILE:N	1:F:363:ILE:HD13	2.32	0.44
1:E:79:THR:CG2	1:E:82:ASP:H	2.26	0.44
1:B:192:ALA:HB3	1:B:197:GLU:OE2	2.18	0.44
1:E:193:ARG:NH2	1:F:195:GLY:O	2.29	0.44
1:B:81:GLN:CD	1:B:81:GLN:H	2.20	0.44
1:F:111:ASP:OD2	1:F:113:GLU:HG3	2.17	0.44
1:C:211:LEU:O	1:C:212:GLU:HB3	2.17	0.44
1:E:455:VAL:HG11	1:E:463:HIS:HB2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:LEU:HD21	1:F:364:LYS:HE3	1.99	0.44
1:C:449:MET:CE	1:D:467:ILE:HD11	2.48	0.44
1:D:231:MET:CE	1:D:251:ALA:HB2	2.48	0.44
1:E:148:THR:HG21	1:E:193:ARG:HD2	1.99	0.44
1:A:227:GLY:O	1:F:89:SER:HB2	2.18	0.44
1:F:21:MET:HE1	1:F:59:PHE:HZ	1.82	0.44
1:E:205:VAL:CG2	1:E:222:ILE:HD12	2.28	0.44
1:D:79:THR:HG23	1:D:81:GLN:N	2.31	0.44
1:F:76:PHE:HZ	1:F:126:LEU:CD2	2.30	0.44
1:C:45:SER:HB3	1:C:182:THR:HB	1.99	0.44
1:C:146:SER:H	1:C:181:THR:CG2	2.31	0.44
1:E:81:GLN:NE2	1:E:81:GLN:H	2.16	0.44
1:F:489:ILE:HD13	1:F:494:PRO:HG2	2.00	0.44
1:C:335:PHE:HA	1:C:338:MET:HG3	2.00	0.44
1:B:21:MET:HE3	1:B:59:PHE:CE1	2.53	0.44
1:C:249:LEU:CD1	1:C:394:GLN:HG2	2.48	0.44
1:D:449:MET:HE3	1:E:490:ILE:HD11	2.00	0.44
1:D:64:ILE:CD1	1:D:64:ILE:H	2.31	0.44
1:C:65:ILE:H	1:C:65:ILE:CD1	2.31	0.44
1:C:151:PHE:C	1:C:153:GLN:N	2.71	0.44
1:D:31:ILE:HA	1:D:231:MET:SD	2.58	0.44
1:F:43:LEU:HD11	1:F:182:THR:OG1	2.17	0.44
1:B:495:THR:HG23	1:C:487:GLU:OE2	2.18	0.44
1:D:21:MET:CE	1:D:59:PHE:CZ	3.01	0.44
1:A:453:ILE:HB	1:A:470:PHE:CD2	2.52	0.44
1:E:364:LYS:O	1:E:368:ASN:ND2	2.51	0.44
1:B:98:VAL:HA	1:B:103:LEU:O	2.17	0.44
1:D:358:ASP:O	1:D:362:ILE:HG12	2.18	0.44
1:D:122:ASP:HB3	1:D:123:LEU:H	1.43	0.44
1:D:98:VAL:HA	1:D:103:LEU:O	2.18	0.44
1:C:88:ARG:HG2	1:C:88:ARG:HH11	1.83	0.44
1:E:451:ARG:HG2	1:E:451:ARG:NH1	2.32	0.44
1:C:143:SER:HA	1:C:179:VAL:O	2.18	0.44
1:E:56:SER:HB2	1:E:143:SER:HB2	1.99	0.44
1:B:119:GLY:C	1:B:121:PHE:H	2.21	0.44
1:A:357:GLU:HG3	1:A:358:ASP:N	2.32	0.43
1:D:106:LEU:CD1	1:D:129:ARG:HH21	2.31	0.43
1:A:14:GLU:CG	1:A:15:HIS:N	2.81	0.43
1:D:356:LEU:HD22	1:D:387:VAL:HG11	2.00	0.43
1:D:211:LEU:HD12	1:D:215:ARG:O	2.18	0.43
1:C:78:GLU:CB	1:C:83:ILE:HD11	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:ASP:O	1:E:113:GLU:N	2.51	0.43
1:A:375:ILE:HD12	1:A:408:ILE:HG21	2.00	0.43
1:A:220:LEU:HD21	1:A:222:ILE:CD1	2.47	0.43
1:F:381:SER:HB3	1:F:414:ASN:OD1	2.18	0.43
1:C:387:VAL:CG1	1:C:391:ALA:HB3	2.48	0.43
1:F:340:ARG:C	1:F:342:ASN:H	2.22	0.43
1:B:484:ARG:HH11	1:B:484:ARG:HB3	1.83	0.43
1:C:317:TYR:CE2	1:C:383:LEU:HD21	2.54	0.43
1:D:106:LEU:HD21	1:D:130:ILE:HD12	2.01	0.43
1:B:305:ALA:HB2	1:B:374:ARG:CD	2.38	0.43
1:D:440:LEU:HD23	1:D:453:ILE:HG12	2.00	0.43
1:D:470:PHE:HB3	1:D:479:ILE:HD13	2.00	0.43
1:D:81:GLN:CD	1:D:81:GLN:H	2.22	0.43
1:D:14:GLU:CG	1:D:15:HIS:N	2.80	0.43
1:A:296:LEU:HD23	1:A:472:ILE:HD12	1.99	0.43
1:B:291:GLY:N	2:B:2901:ATP:O2B	2.51	0.43
1:D:291:GLY:N	2:D:4901:ATP:O2B	2.50	0.43
1:E:18:ILE:HD11	1:E:228:THR:N	2.33	0.43
1:D:21:MET:HE2	1:D:177:THR:HG21	1.99	0.43
1:E:211:LEU:HD12	1:E:215:ARG:O	2.18	0.43
1:E:376:ALA:HA	1:E:411:LEU:O	2.17	0.43
1:A:293:GLY:HA2	2:A:1901:ATP:O1A	2.18	0.43
1:A:431:SER:O	1:A:434:THR:HG22	2.19	0.43
1:A:436:THR:CG2	1:A:458:MET:HG2	2.48	0.43
1:F:332:GLY:O	1:F:333:MET:C	2.56	0.43
1:B:79:THR:HG21	1:B:81:GLN:HG2	2.01	0.43
1:E:81:GLN:CD	1:E:81:GLN:H	2.20	0.43
1:C:338:MET:HB3	1:C:344:LEU:HB3	2.01	0.43
1:B:80:PRO:HD2	1:B:81:GLN:NE2	2.33	0.43
1:B:81:GLN:H	1:B:81:GLN:NE2	2.16	0.43
1:A:65:ILE:O	1:A:65:ILE:HG22	2.17	0.43
1:B:440:LEU:HD21	1:B:453:ILE:HG12	2.00	0.43
1:C:215:ARG:HA	1:C:215:ARG:NE	2.32	0.43
1:E:385:ARG:HA	1:F:393:ARG:HH12	1.83	0.43
1:B:432:THR:HG22	1:B:432:THR:O	2.17	0.43
1:A:87:ALA:HB1	1:A:92:TRP:CB	2.49	0.43
1:F:126:LEU:HG	1:F:130:ILE:CD1	2.47	0.43
1:F:191:ILE:CB	1:F:198:GLU:CG	2.90	0.43
1:E:45:SER:CB	1:E:182:THR:HB	2.48	0.43
1:D:344:LEU:HD22	1:D:345:LYS:H	1.80	0.43
1:E:396:VAL:HG11	1:E:430:ILE:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:LEU:O	1:F:273:MET:HB2	2.19	0.43
1:D:317:TYR:CD2	1:D:383:LEU:HD21	2.53	0.43
1:B:56:SER:O	1:B:59:PHE:HB3	2.18	0.43
1:E:249:LEU:HD13	1:E:394:GLN:HG2	2.01	0.43
1:A:291:GLY:N	2:A:1901:ATP:O2B	2.51	0.43
1:F:81:GLN:N	1:F:81:GLN:CD	2.72	0.43
1:A:184:ARG:O	1:B:199:PHE:HZ	2.02	0.43
1:A:334:ASP:O	1:A:338:MET:HG2	2.19	0.43
1:A:459:ARG:HH11	1:F:323:GLN:HE22	1.65	0.43
1:F:419:PHE:O	1:F:420:MET:HB2	2.18	0.43
1:D:387:VAL:CG1	1:D:388:SER:N	2.82	0.43
1:E:21:MET:HE1	1:E:177:THR:HB	2.01	0.43
1:C:118:VAL:O	1:C:118:VAL:HG12	2.19	0.43
1:F:468:ARG:NH1	1:F:468:ARG:HG2	2.34	0.43
1:F:264:SER:HA	1:F:271:ASP:OD1	2.18	0.43
1:F:148:THR:HG21	1:F:183:GLU:HG3	2.00	0.43
1:E:184:ARG:HG2	1:E:191:ILE:O	2.19	0.43
1:B:378:ASP:O	1:B:379:SER:HB3	2.18	0.43
1:A:178:THR:HG22	1:A:179:VAL:N	2.34	0.43
1:C:340:ARG:C	1:C:342:ASN:H	2.22	0.43
1:D:256:GLN:HG3	1:D:404:LYS:HD3	2.00	0.43
1:F:431:SER:HA	1:F:434:THR:HG22	1.99	0.43
1:E:150:VAL:CG1	1:E:151:PHE:H	2.32	0.43
1:A:299:SER:C	1:A:333:MET:HE1	2.39	0.43
1:D:134:ILE:HD13	1:D:134:ILE:N	2.34	0.43
1:A:344:LEU:HD13	1:A:344:LEU:C	2.38	0.43
1:A:447:GLY:C	1:B:467:ILE:HD13	2.39	0.43
1:C:67:PHE:HB2	1:C:69:GLU:HG3	1.99	0.43
1:A:362:ILE:CG2	1:A:366:GLU:OE2	2.67	0.43
1:A:406:GLU:O	1:A:407:GLU:HB2	2.19	0.43
1:F:28:PHE:CE1	1:F:222:ILE:HD11	2.53	0.43
1:C:311:ARG:HD2	1:C:371:LYS:HD3	1.96	0.43
1:E:447:GLY:O	1:F:467:ILE:CD1	2.65	0.43
1:A:215:ARG:NH2	1:B:234:GLU:O	2.52	0.43
1:D:61:TYR:CE2	1:D:92:TRP:HD1	2.37	0.43
1:A:218:ARG:O	1:A:236:PRO:HA	2.19	0.43
1:B:462:TRP:O	1:B:463:HIS:O	2.35	0.43
1:C:484:ARG:HH11	1:C:484:ARG:HB3	1.82	0.43
1:C:360:LEU:CD2	1:C:364:LYS:HE3	2.49	0.43
1:F:180:MET:HB3	1:F:180:MET:HE2	1.84	0.42
1:F:25:ILE:HD12	1:F:58:GLN:CG	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:ILE:HB	1:F:198:GLU:HG2	1.95	0.42
1:C:301:PHE:O	1:C:374:ARG:NH1	2.50	0.42
1:C:184:ARG:HG2	1:C:191:ILE:O	2.18	0.42
1:E:294:LYS:HB2	2:E:5901:ATP:O1B	2.19	0.42
1:E:356:LEU:HD21	1:E:387:VAL:HG11	1.99	0.42
1:F:142:VAL:O	1:F:178:THR:HA	2.19	0.42
1:A:393:ARG:O	1:A:397:ILE:HG12	2.18	0.42
1:D:359:HIS:O	1:D:363:ILE:HG13	2.18	0.42
1:A:425:ILE:HD11	1:A:456:PHE:CE2	2.54	0.42
1:F:106:LEU:HD11	1:F:129:ARG:NH2	2.33	0.42
1:F:425:ILE:HG22	1:F:426:THR:HG23	2.01	0.42
1:E:203:ASN:HB3	1:E:225:LEU:CD2	2.47	0.42
1:A:359:HIS:O	1:A:363:ILE:HG12	2.18	0.42
1:A:317:TYR:CD2	1:A:383:LEU:HD21	2.54	0.42
1:F:325:LEU:HD23	1:F:335:PHE:CB	2.45	0.42
1:E:446:ARG:HH21	1:E:496:ARG:NH2	2.16	0.42
1:B:264:SER:O	1:B:374:ARG:NH2	2.51	0.42
1:E:191:ILE:CB	1:E:198:GLU:HG2	2.47	0.42
1:C:292:THR:HB	1:C:440:LEU:HB3	2.01	0.42
1:C:123:LEU:CD2	1:C:167:LEU:HB2	2.49	0.42
1:C:52:LYS:N	2:C:3903:ATP:O1B	2.49	0.42
1:D:377:ILE:CD1	1:D:399:VAL:HG11	2.50	0.42
1:F:111:ASP:OD1	1:F:112:PRO:CD	2.66	0.42
1:E:400:THR:HG22	1:E:401:GLY:N	2.33	0.42
1:B:21:MET:HB2	1:B:38:ILE:HG12	2.02	0.42
1:D:437:ILE:HD11	1:D:457:LYS:HE2	2.00	0.42
1:E:53:THR:HG23	1:E:145:ASP:OD1	2.18	0.42
1:C:356:LEU:CD2	1:C:387:VAL:HG11	2.50	0.42
1:C:308:ASN:O	1:C:310:GLU:HG3	2.20	0.42
1:C:75:THR:HG23	1:C:75:THR:O	2.19	0.42
1:A:304:ASN:HB3	1:A:374:ARG:HH12	1.84	0.42
1:D:123:LEU:HA	1:D:123:LEU:HD22	1.84	0.42
1:F:437:ILE:HD13	1:F:457:LYS:HG2	2.00	0.42
1:F:121:PHE:HA	1:F:121:PHE:HD2	1.74	0.42
1:F:115:GLN:CG	1:F:116:GLU:N	2.82	0.42
1:E:148:THR:HG21	1:E:183:GLU:HG3	2.02	0.42
1:D:334:ASP:O	1:D:338:MET:HG2	2.19	0.42
1:C:214:GLU:C	1:C:215:ARG:HE	2.23	0.42
1:F:295:THR:HG21	1:F:319:GLU:OE2	2.19	0.42
1:B:471:MET:O	1:B:472:ILE:HD13	2.19	0.42
1:F:211:LEU:HD12	1:F:215:ARG:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:LYS:O	1:C:100:GLU:HG3	2.19	0.42
1:E:164:LEU:HD11	1:E:197:GLU:HG3	2.02	0.42
1:F:119:GLY:HA2	1:F:122:ASP:OD1	2.19	0.42
1:F:122:ASP:O	1:F:126:LEU:N	2.33	0.42
1:B:289:ALA:HB2	1:B:419:PHE:HA	2.01	0.42
1:D:45:SER:CB	1:D:182:THR:HB	2.50	0.42
1:C:123:LEU:O	1:C:124:SER:C	2.57	0.42
1:A:17:ALA:C	1:A:18:ILE:HD12	2.40	0.42
1:B:21:MET:HE2	1:B:177:THR:HG21	2.02	0.42
1:A:454:ASN:HB2	1:A:467:ILE:HD13	2.02	0.42
1:D:323:GLN:NE2	1:E:459:ARG:HD3	2.34	0.42
1:A:33:HIS:HD2	1:A:229:SER:OG	2.02	0.42
1:B:107:ASP:C	1:B:107:ASP:OD1	2.58	0.42
1:A:291:GLY:O	2:A:1901:ATP:H4'	2.19	0.42
1:E:321:ARG:O	1:E:325:LEU:HD12	2.19	0.42
1:D:145:ASP:OD2	1:D:181:THR:HG21	2.20	0.42
1:C:420:MET:HE2	1:C:492:GLY:HA3	2.01	0.42
1:B:315:PHE:CD2	1:B:363:ILE:CD1	3.03	0.42
1:B:73:PHE:HB3	1:B:105:ILE:CD1	2.42	0.42
1:A:52:LYS:HD3	1:A:182:THR:O	2.20	0.42
1:D:412:PHE:CD1	1:D:412:PHE:N	2.88	0.42
1:C:41:SER:HA	1:C:178:THR:O	2.19	0.42
1:B:336:GLU:OE1	1:B:336:GLU:HA	2.20	0.42
1:D:296:LEU:HD13	1:D:331:TRP:CD2	2.55	0.42
1:D:362:ILE:CG2	1:D:366:GLU:OE2	2.67	0.42
1:F:306:CYS:SG	1:F:344:LEU:HB2	2.60	0.42
1:A:377:ILE:HD13	1:A:412:PHE:CD2	2.53	0.42
1:B:292:THR:HB	1:B:440:LEU:HB3	2.01	0.42
1:A:488:ARG:NE	1:F:488:ARG:NH1	2.66	0.42
1:E:396:VAL:HG11	1:E:430:ILE:CG2	2.49	0.42
1:D:387:VAL:HG12	1:D:388:SER:O	2.19	0.42
1:C:116:GLU:O	1:C:117:VAL:HB	2.19	0.42
1:B:487:GLU:O	1:B:494:PRO:HA	2.20	0.42
1:F:431:SER:O	1:F:434:THR:HG22	2.19	0.42
1:E:81:GLN:CD	1:E:81:GLN:N	2.72	0.42
1:C:449:MET:HE3	1:D:467:ILE:HD11	2.02	0.42
1:B:146:SER:H	1:B:181:THR:HG22	1.84	0.42
1:F:356:LEU:CD1	1:F:387:VAL:HG21	2.50	0.42
1:E:244:ILE:HG22	1:E:246:ILE:CD1	2.50	0.42
1:A:159:VAL:O	1:A:163:GLU:HG2	2.19	0.42
1:A:443:VAL:CG1	1:A:494:PRO:HG2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:ILE:CD1	1:C:400:THR:HG23	2.50	0.42
1:B:45:SER:HA	1:B:182:THR:O	2.19	0.42
1:D:208:ARG:O	1:D:218:ARG:HA	2.20	0.42
1:E:438:ILE:HD13	1:E:455:VAL:HA	2.02	0.42
1:D:41:SER:HA	1:D:178:THR:O	2.20	0.42
1:D:109:SER:HA	1:D:110:PRO:HD3	1.88	0.42
1:C:161:ARG:HB2	1:C:196:VAL:HG11	2.01	0.42
1:D:303:GLU:O	1:D:303:GLU:HG2	2.19	0.42
1:D:19:ALA:CB	1:D:38:ILE:HD12	2.49	0.42
1:C:61:TYR:C	1:C:65:ILE:HD13	2.33	0.42
1:B:358:ASP:O	1:B:362:ILE:HG12	2.19	0.42
1:E:333:MET:HB2	1:E:333:MET:HE2	1.87	0.42
1:F:336:GLU:HB3	1:F:340:ARG:NH2	2.35	0.42
1:B:267:VAL:HB	1:B:270:LEU:HB2	2.01	0.42
1:C:197:GLU:OE2	1:C:197:GLU:N	2.36	0.42
1:D:489:ILE:CD1	1:D:494:PRO:HB3	2.43	0.41
1:A:437:ILE:HD13	1:A:457:LYS:HG3	2.01	0.41
1:C:123:LEU:HD11	1:C:163:GLU:O	2.20	0.41
1:E:344:LEU:HD11	1:E:346:ILE:HG13	2.01	0.41
1:F:440:LEU:HD21	1:F:453:ILE:HG13	2.01	0.41
1:B:126:LEU:C	1:B:128:GLU:H	2.23	0.41
1:D:78:GLU:OE1	1:D:83:ILE:HD13	2.19	0.41
1:E:84:ILE:HG21	1:E:95:ALA:HB2	2.02	0.41
1:A:316:ALA:CB	1:A:324:LEU:HD11	2.50	0.41
1:E:371:LYS:HD3	1:E:371:LYS:O	2.20	0.41
1:E:52:LYS:N	2:E:5903:ATP:O1B	2.48	0.41
1:E:134:ILE:N	1:E:134:ILE:CD1	2.83	0.41
1:F:329:TYR:HA	1:F:332:GLY:O	2.20	0.41
1:E:21:MET:CE	1:E:59:PHE:HZ	2.34	0.41
1:B:360:LEU:HD21	1:B:364:LYS:HE3	2.03	0.41
1:D:376:ALA:HA	1:D:411:LEU:O	2.20	0.41
1:F:151:PHE:CZ	1:F:160:VAL:HG13	2.55	0.41
1:C:52:LYS:HD3	1:C:182:THR:O	2.20	0.41
1:A:302:VAL:HG13	1:A:344:LEU:HD23	2.03	0.41
1:A:433:ILE:CD1	1:F:385:ARG:NH2	2.83	0.41
1:C:170:ARG:O	1:C:174:ILE:HG12	2.21	0.41
1:B:85:LYS:HZ2	1:C:14:GLU:HB3	1.82	0.41
1:E:193:ARG:HH11	1:E:193:ARG:HG2	1.85	0.41
1:F:161:ARG:CB	1:F:196:VAL:HG11	2.42	0.41
1:C:123:LEU:HD11	1:C:163:GLU:CA	2.51	0.41
1:C:123:LEU:HD22	1:C:167:LEU:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:GLU:O	1:F:114:GLY:O	2.39	0.41
1:F:487:GLU:O	1:F:488:ARG:HB2	2.19	0.41
2:B:2901:ATP:H3'	1:C:458:MET:O	2.20	0.41
1:F:131:ASN:OD1	1:F:174:ILE:HD12	2.21	0.41
1:B:178:THR:CG2	1:B:179:VAL:N	2.84	0.41
1:C:295:THR:HB	2:C:3901:ATP:PA	2.61	0.41
1:E:469:GLU:CB	1:E:483:PHE:CZ	3.03	0.41
1:E:377:ILE:HD11	1:E:399:VAL:HG11	2.03	0.41
1:A:451:ARG:CG	1:A:451:ARG:NH1	2.78	0.41
1:D:72:VAL:CG2	1:D:134:ILE:HD12	2.46	0.41
1:F:468:ARG:HH11	1:F:468:ARG:HG2	1.85	0.41
1:A:40:ARG:HG2	1:A:172:LYS:HE3	2.03	0.41
1:B:25:ILE:HG23	1:B:58:GLN:NE2	2.35	0.41
1:C:194:TYR:CD1	1:C:194:TYR:N	2.89	0.41
1:A:87:ALA:HB1	1:A:92:TRP:HB3	2.02	0.41
1:E:372:PRO:CB	1:E:375:ILE:HD11	2.48	0.41
1:B:449:MET:HE3	1:C:467:ILE:HD11	2.01	0.41
1:C:306:CYS:SG	1:C:344:LEU:HB2	2.61	0.41
1:E:352:GLU:OE2	1:E:385:ARG:HD2	2.20	0.41
1:B:91:GLY:C	1:B:92:TRP:CE3	2.94	0.41
1:D:249:LEU:CD1	1:D:394:GLN:HG2	2.51	0.41
1:D:79:THR:HG22	1:D:82:ASP:N	2.16	0.41
1:A:299:SER:CB	1:A:333:MET:HE1	2.43	0.41
1:B:300:ARG:HA	1:B:333:MET:HE3	2.03	0.41
1:D:61:TYR:CZ	1:D:92:TRP:CD1	3.08	0.41
1:A:483:PHE:HB3	1:A:486:PHE:HD1	1.85	0.41
1:B:356:LEU:HD13	1:B:387:VAL:HG21	2.02	0.41
1:E:178:THR:HG22	1:E:179:VAL:N	2.35	0.41
1:E:249:LEU:CD1	1:E:394:GLN:HG2	2.50	0.41
1:F:31:ILE:CD1	1:F:246:ILE:HG21	2.51	0.41
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.56	0.41
1:D:488:ARG:HH12	1:E:488:ARG:NH2	2.18	0.41
1:F:118:VAL:O	1:F:118:VAL:HG22	2.20	0.41
1:F:148:THR:HG21	1:F:183:GLU:CG	2.51	0.41
1:A:182:THR:CG2	1:A:183:GLU:N	2.84	0.41
1:B:425:ILE:HG22	1:B:426:THR:HG23	2.03	0.41
1:C:296:LEU:HD23	1:C:472:ILE:HD12	2.02	0.41
1:C:211:LEU:HD12	1:C:215:ARG:O	2.21	0.41
1:C:382:ALA:O	1:C:385:ARG:HG3	2.21	0.41
1:F:375:ILE:HD13	1:F:375:ILE:HA	1.98	0.41
1:D:495:THR:O	1:D:495:THR:HG22	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ILE:HD13	1:E:127:ILE:N	2.35	0.41
1:B:148:THR:HA	1:B:151:PHE:CE1	2.56	0.41
1:A:153:GLN:O	1:A:154:TYR:CB	2.69	0.41
1:C:144:ILE:HG21	1:C:147:VAL:HG12	2.02	0.41
1:F:117:VAL:O	1:F:118:VAL:HB	2.21	0.41
1:E:379:SER:N	1:E:413:THR:HB	2.23	0.41
1:A:487:GLU:HG2	1:F:496:ARG:CZ	2.51	0.41
1:A:64:ILE:HG21	1:A:97:LEU:HD22	2.02	0.41
1:B:127:ILE:HG22	1:B:127:ILE:O	2.20	0.41
1:C:438:ILE:HD12	1:C:455:VAL:HG22	2.03	0.41
1:F:269:ARG:HB3	1:F:479:ILE:HD13	2.02	0.41
1:F:92:TRP:CD1	1:F:92:TRP:N	2.86	0.41
1:F:90:PHE:CB	1:F:92:TRP:CZ2	3.04	0.41
1:B:470:PHE:HE1	1:B:472:ILE:HD11	1.85	0.41
1:D:432:THR:O	1:D:432:THR:CG2	2.69	0.41
1:C:432:THR:HG22	1:C:432:THR:O	2.20	0.41
1:E:365:SER:HA	1:E:368:ASN:HD22	1.86	0.41
1:D:273:MET:CE	1:D:468:ARG:HD2	2.51	0.41
1:F:21:MET:CE	1:F:59:PHE:CE1	3.04	0.41
1:B:225:LEU:HD12	1:B:230:HIS:HB3	2.03	0.41
1:D:159:VAL:O	1:D:163:GLU:HG2	2.21	0.41
1:F:220:LEU:C	1:F:220:LEU:HD23	2.41	0.41
1:B:376:ALA:HA	1:B:411:LEU:O	2.21	0.41
1:E:217:ARG:HH21	1:E:236:PRO:HB3	1.86	0.41
1:D:496:ARG:HG2	1:E:487:GLU:OE1	2.20	0.41
1:F:221:GLU:C	1:F:222:ILE:HD13	2.41	0.41
1:F:123:LEU:HA	1:F:123:LEU:HD22	1.82	0.41
1:E:79:THR:HG23	1:E:81:GLN:CG	2.41	0.41
1:F:287:THR:HA	1:F:414:ASN:O	2.21	0.41
1:A:183:GLU:OE2	1:B:161:ARG:NH1	2.46	0.41
1:E:191:ILE:CG2	1:E:198:GLU:HG3	2.51	0.41
1:B:293:GLY:HA2	2:B:2901:ATP:O1A	2.21	0.41
1:E:437:ILE:HD12	1:E:457:LYS:HE2	2.01	0.41
1:D:24:MET:HB2	1:D:62:ASN:HD22	1.86	0.41
1:B:126:LEU:HG	1:B:130:ILE:CD1	2.51	0.41
1:C:161:ARG:HD2	1:C:196:VAL:HG13	2.03	0.41
1:E:220:LEU:HD21	1:E:222:ILE:CD1	2.51	0.40
1:C:123:LEU:HB3	1:C:127:ILE:HD11	2.03	0.40
1:A:187:GLU:O	1:A:208:ARG:HD3	2.20	0.40
1:B:335:PHE:O	1:B:339:GLU:HG3	2.21	0.40
2:C:3901:ATP:C2	1:D:462:TRP:HA	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:357:GLU:HG3	1:F:358:ASP:H	1.86	0.40
1:E:445:ILE:HD12	1:E:450:SER:OG	2.21	0.40
1:D:471:MET:HG3	1:D:478:ASP:HB3	2.04	0.40
1:C:76:PHE:O	1:C:109:SER:HA	2.21	0.40
1:C:53:THR:O	1:C:54:LEU:C	2.60	0.40
1:D:419:PHE:O	1:D:420:MET:HB2	2.21	0.40
1:D:191:ILE:HB	1:D:198:GLU:CD	2.40	0.40
1:E:184:ARG:O	1:E:185:ILE:HD13	2.21	0.40
1:C:378:ASP:O	1:C:379:SER:HB3	2.22	0.40
1:D:325:LEU:HD23	1:D:335:PHE:CB	2.48	0.40
1:E:146:SER:HA	1:E:181:THR:HG22	2.03	0.40
1:C:354:ALA:HB1	1:C:358:ASP:HB2	2.04	0.40
1:B:382:ALA:O	1:B:385:ARG:HG3	2.22	0.40
1:B:76:PHE:HE1	1:B:144:ILE:CG2	2.33	0.40
1:A:319:GLU:O	1:B:254:LEU:HD21	2.21	0.40
1:A:220:LEU:HD21	1:A:222:ILE:HD11	2.02	0.40
1:D:153:GLN:O	1:D:154:TYR:CB	2.69	0.40
1:B:273:MET:CE	1:B:468:ARG:HD2	2.51	0.40
1:D:385:ARG:HG2	1:E:393:ARG:NH1	2.36	0.40
1:A:444:GLU:O	1:A:494:PRO:HD2	2.21	0.40
1:A:452:ALA:HA	1:A:469:GLU:HA	2.03	0.40
1:E:94:LEU:O	1:E:98:VAL:HG23	2.21	0.40
1:F:256:GLN:H	1:F:256:GLN:HG2	1.69	0.40
1:A:164:LEU:HA	1:A:164:LEU:HD23	1.83	0.40
1:D:121:PHE:N	1:D:121:PHE:CD1	2.89	0.40
1:A:90:PHE:HB2	1:A:92:TRP:CG	2.57	0.40
1:E:264:SER:HA	1:E:271:ASP:OD1	2.22	0.40
1:A:283:ILE:HG23	1:A:412:PHE:CE1	2.56	0.40
1:B:299:SER:CB	1:B:333:MET:HE1	2.49	0.40
1:D:61:TYR:CD2	1:D:92:TRP:CD1	3.10	0.40
2:D:4901:ATP:C2	1:E:462:TRP:HA	2.56	0.40
1:B:433:ILE:CG2	1:B:433:ILE:O	2.69	0.40
1:E:392:PHE:O	1:E:395:PHE:HB3	2.22	0.40
1:B:31:ILE:HD12	1:B:235:TYR:CD1	2.56	0.40
1:F:79:THR:HG21	1:F:81:GLN:HG2	2.01	0.40
1:F:161:ARG:HB2	1:F:196:VAL:CG1	2.43	0.40
1:D:385:ARG:NH2	1:E:433:ILE:CD1	2.83	0.40
1:B:92:TRP:CE3	1:B:92:TRP:HA	2.57	0.40
1:B:21:MET:HE3	1:B:59:PHE:CZ	2.56	0.40
1:B:99:ASP:C	1:B:101:GLY:N	2.74	0.40
1:E:471:MET:HG3	1:E:478:ASP:HB3	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:GLN:H	1:C:256:GLN:HG2	1.70	0.40
1:C:99:ASP:C	1:C:101:GLY:H	2.25	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	482/525 (92%)	438 (91%)	33 (7%)	11 (2%)	8	26
1	B	482/525 (92%)	432 (90%)	41 (8%)	9 (2%)	10	32
1	C	482/525 (92%)	431 (89%)	37 (8%)	14 (3%)	6	19
1	D	482/525 (92%)	439 (91%)	32 (7%)	11 (2%)	8	26
1	E	482/525 (92%)	434 (90%)	33 (7%)	15 (3%)	5	17
1	F	482/525 (92%)	436 (90%)	36 (8%)	10 (2%)	9	29
All	All	2892/3150 (92%)	2610 (90%)	212 (7%)	70 (2%)	7	25

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ALA
1	A	117	VAL
1	A	154	TYR
1	A	211	LEU
1	A	333	MET
1	A	463	HIS
1	B	154	TYR
1	B	333	MET
1	B	463	HIS
1	C	17	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	117	VAL
1	C	122	ASP
1	C	123	LEU
1	C	154	TYR
1	C	333	MET
1	C	463	HIS
1	D	113	GLU
1	D	122	ASP
1	D	154	TYR
1	D	333	MET
1	E	122	ASP
1	E	154	TYR
1	E	211	LEU
1	E	333	MET
1	E	463	HIS
1	F	114	GLY
1	F	118	VAL
1	F	154	TYR
1	F	333	MET
1	F	463	HIS
1	B	119	GLY
1	B	211	LEU
1	D	463	HIS
1	E	113	GLU
1	E	123	LEU
1	E	387	VAL
1	E	420	MET
1	F	211	LEU
1	A	120	GLY
1	A	387	VAL
1	A	420	MET
1	B	420	MET
1	C	112	PRO
1	C	211	LEU
1	C	349	ALA
1	D	211	LEU
1	D	420	MET
1	E	488	ARG
1	F	117	VAL
1	F	420	MET
1	C	420	MET
1	E	494	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	348	CYS
1	B	348	CYS
1	B	494	PRO
1	C	348	CYS
1	C	379	SER
1	D	118	VAL
1	D	387	VAL
1	E	117	VAL
1	E	348	CYS
1	E	379	SER
1	C	212	GLU
1	D	348	CYS
1	D	494	PRO
1	F	348	CYS
1	A	112	PRO
1	E	112	PRO
1	F	387	VAL
1	B	387	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/450 (92%)	386 (94%)	26 (6%)	22	53
1	B	412/450 (92%)	391 (95%)	21 (5%)	29	63
1	C	412/450 (92%)	388 (94%)	24 (6%)	25	57
1	D	412/450 (92%)	385 (93%)	27 (7%)	21	51
1	E	412/450 (92%)	386 (94%)	26 (6%)	22	53
1	F	412/450 (92%)	383 (93%)	29 (7%)	19	47
All	All	2472/2700 (92%)	2319 (94%)	153 (6%)	23	54

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	38	ILE
1	A	79	THR
1	A	81	GLN
1	A	92	TRP
1	A	123	LEU
1	A	151	PHE
1	A	154	TYR
1	A	186	GLU
1	A	212	GLU
1	A	222	ILE
1	A	223	LEU
1	A	238	THR
1	A	256	GLN
1	A	270	LEU
1	A	287	THR
1	A	342	ASN
1	A	360	LEU
1	A	362	ILE
1	A	371	LYS
1	A	400	THR
1	A	437	ILE
1	A	451	ARG
1	A	458	MET
1	A	471	MET
1	A	496	ARG
1	B	26	GLU
1	B	79	THR
1	B	81	GLN
1	B	92	TRP
1	B	128	GLU
1	B	151	PHE
1	B	154	TYR
1	B	181	THR
1	B	186	GLU
1	B	212	GLU
1	B	223	LEU
1	B	256	GLN
1	B	270	LEU
1	B	360	LEU
1	B	371	LYS
1	B	400	THR
1	B	437	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	451	ARG
1	B	453	ILE
1	B	462	TRP
1	B	471	MET
1	C	26	GLU
1	C	65	ILE
1	C	79	THR
1	C	81	GLN
1	C	151	PHE
1	C	154	TYR
1	C	181	THR
1	C	186	GLU
1	C	212	GLU
1	C	218	ARG
1	C	223	LEU
1	C	256	GLN
1	C	270	LEU
1	C	284	ILE
1	C	303	GLU
1	C	360	LEU
1	C	371	LYS
1	C	375	ILE
1	C	400	THR
1	C	451	ARG
1	C	453	ILE
1	C	458	MET
1	C	471	MET
1	C	497	ILE
1	D	26	GLU
1	D	79	THR
1	D	81	GLN
1	D	121	PHE
1	D	122	ASP
1	D	123	LEU
1	D	134	ILE
1	D	151	PHE
1	D	154	TYR
1	D	181	THR
1	D	186	GLU
1	D	212	GLU
1	D	223	LEU
1	D	256	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	270	LEU
1	D	287	THR
1	D	360	LEU
1	D	371	LYS
1	D	375	ILE
1	D	400	THR
1	D	431	SER
1	D	451	ARG
1	D	453	ILE
1	D	463	HIS
1	D	469	GLU
1	D	471	MET
1	D	496	ARG
1	E	26	GLU
1	E	79	THR
1	E	81	GLN
1	E	121	PHE
1	E	134	ILE
1	E	151	PHE
1	E	154	TYR
1	E	181	THR
1	E	186	GLU
1	E	212	GLU
1	E	222	ILE
1	E	223	LEU
1	E	228	THR
1	E	256	GLN
1	E	270	LEU
1	E	284	ILE
1	E	287	THR
1	E	360	LEU
1	E	371	LYS
1	E	375	ILE
1	E	400	THR
1	E	451	ARG
1	E	458	MET
1	E	469	GLU
1	E	471	MET
1	E	497	ILE
1	F	26	GLU
1	F	45	SER
1	F	53	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	79	THR
1	F	81	GLN
1	F	121	PHE
1	F	123	LEU
1	F	151	PHE
1	F	154	TYR
1	F	181	THR
1	F	186	GLU
1	F	212	GLU
1	F	218	ARG
1	F	222	ILE
1	F	223	LEU
1	F	256	GLN
1	F	270	LEU
1	F	342	ASN
1	F	360	LEU
1	F	363	ILE
1	F	371	LYS
1	F	400	THR
1	F	451	ARG
1	F	458	MET
1	F	462	TRP
1	F	471	MET
1	F	487	GLU
1	F	491	SER
1	F	496	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	62	ASN
1	A	81	GLN
1	A	209	ASN
1	A	361	GLN
1	A	368	ASN
1	A	414	ASN
1	A	441	GLN
1	B	16	GLN
1	B	62	ASN
1	B	81	GLN
1	B	209	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	368	ASN
1	B	414	ASN
1	B	441	GLN
1	C	33	HIS
1	C	62	ASN
1	C	81	GLN
1	C	209	ASN
1	C	368	ASN
1	C	414	ASN
1	D	33	HIS
1	D	81	GLN
1	D	209	ASN
1	D	361	GLN
1	D	368	ASN
1	D	414	ASN
1	E	33	HIS
1	E	81	GLN
1	E	209	ASN
1	E	304	ASN
1	E	361	GLN
1	E	368	ASN
1	E	414	ASN
1	E	441	GLN
1	E	454	ASN
1	F	16	GLN
1	F	33	HIS
1	F	62	ASN
1	F	81	GLN
1	F	153	GLN
1	F	209	ASN
1	F	361	GLN
1	F	368	ASN
1	F	414	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

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$
2	ATP	A	1901	-	24,33,33	1.37	4 (16%)	31,52,52	2.86	8 (25%)
2	ATP	A	1903	-	24,33,33	1.29	3 (12%)	31,52,52	2.56	6 (19%)
2	ATP	B	2901	-	24,33,33	1.36	4 (16%)	31,52,52	2.95	7 (22%)
2	ATP	B	2903	-	24,33,33	1.30	3 (12%)	31,52,52	2.58	6 (19%)
2	ATP	C	3901	-	24,33,33	1.41	4 (16%)	31,52,52	2.82	6 (19%)
2	ATP	C	3903	-	24,33,33	1.08	1 (4%)	31,52,52	2.60	5 (16%)
2	ATP	D	4901	-	24,33,33	1.43	4 (16%)	31,52,52	2.90	8 (25%)
2	ATP	D	4903	-	24,33,33	1.28	2 (8%)	31,52,52	2.66	5 (16%)
2	ATP	E	5901	-	24,33,33	1.41	4 (16%)	31,52,52	2.91	9 (29%)
2	ATP	E	5903	-	24,33,33	1.18	1 (4%)	31,52,52	2.58	5 (16%)
2	ATP	F	6901	-	24,33,33	1.42	4 (16%)	31,52,52	2.88	10 (32%)
2	ATP	F	6903	-	24,33,33	1.22	2 (8%)	31,52,52	2.57	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	A	1901	-	-	0/18/38/38	0/3/3/3
2	ATP	A	1903	-	-	0/18/38/38	0/3/3/3
2	ATP	B	2901	-	-	0/18/38/38	0/3/3/3
2	ATP	B	2903	-	-	0/18/38/38	0/3/3/3
2	ATP	C	3901	-	-	0/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	C	3903	-	-	0/18/38/38	0/3/3/3
2	ATP	D	4901	-	-	0/18/38/38	0/3/3/3
2	ATP	D	4903	-	-	0/18/38/38	0/3/3/3
2	ATP	E	5901	-	-	0/18/38/38	0/3/3/3
2	ATP	E	5903	-	-	0/18/38/38	0/3/3/3
2	ATP	F	6901	-	-	0/18/38/38	0/3/3/3
2	ATP	F	6903	-	-	0/18/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4901	ATP	O2'-C2'	-2.53	1.36	1.43
2	E	5901	ATP	O2'-C2'	-2.32	1.37	1.43
2	C	3901	ATP	O2'-C2'	-2.26	1.37	1.43
2	B	2901	ATP	O2'-C2'	-2.16	1.37	1.43
2	A	1901	ATP	O2'-C2'	-2.13	1.37	1.43
2	F	6901	ATP	O2'-C2'	-2.12	1.37	1.43
2	D	4903	ATP	O4'-C4'	-2.06	1.40	1.45
2	A	1903	ATP	O4'-C1'	2.00	1.43	1.41
2	B	2903	ATP	C2-N1	2.28	1.38	1.33
2	F	6903	ATP	C2-N1	2.29	1.38	1.33
2	E	5901	ATP	O4'-C1'	2.38	1.44	1.41
2	B	2903	ATP	O4'-C1'	2.42	1.44	1.41
2	A	1903	ATP	C2-N1	2.52	1.38	1.33
2	B	2901	ATP	O4'-C1'	2.63	1.44	1.41
2	D	4901	ATP	C2-N1	2.65	1.38	1.33
2	A	1901	ATP	C2-N1	2.71	1.39	1.33
2	C	3901	ATP	C2-N1	2.75	1.39	1.33
2	E	5901	ATP	C2-N1	2.78	1.39	1.33
2	C	3901	ATP	O4'-C1'	2.84	1.44	1.41
2	D	4901	ATP	O4'-C1'	2.85	1.44	1.41
2	F	6901	ATP	C2-N1	2.89	1.39	1.33
2	F	6901	ATP	O4'-C1'	2.93	1.44	1.41
2	A	1901	ATP	O4'-C1'	3.00	1.45	1.41
2	B	2901	ATP	C2-N1	3.02	1.39	1.33
2	B	2901	ATP	C2-N3	3.21	1.37	1.32
2	C	3903	ATP	C2-N3	3.33	1.38	1.32
2	E	5903	ATP	C2-N3	3.39	1.38	1.32
2	A	1901	ATP	C2-N3	3.41	1.38	1.32
2	D	4901	ATP	C2-N3	3.51	1.38	1.32
2	F	6901	ATP	C2-N3	3.61	1.38	1.32
2	D	4903	ATP	C2-N3	3.64	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3901	ATP	C2-N3	3.71	1.38	1.32
2	A	1903	ATP	C2-N3	3.72	1.38	1.32
2	F	6903	ATP	C2-N3	3.75	1.38	1.32
2	E	5901	ATP	C2-N3	3.89	1.39	1.32
2	B	2903	ATP	C2-N3	4.04	1.39	1.32

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2901	ATP	N3-C2-N1	-12.15	119.59	128.89
2	E	5901	ATP	N3-C2-N1	-11.82	119.85	128.89
2	D	4901	ATP	N3-C2-N1	-11.75	119.90	128.89
2	D	4903	ATP	N3-C2-N1	-11.70	119.93	128.89
2	C	3903	ATP	N3-C2-N1	-11.65	119.97	128.89
2	A	1901	ATP	N3-C2-N1	-11.60	120.01	128.89
2	F	6901	ATP	N3-C2-N1	-11.56	120.05	128.89
2	C	3901	ATP	N3-C2-N1	-11.51	120.08	128.89
2	E	5903	ATP	N3-C2-N1	-11.40	120.17	128.89
2	A	1903	ATP	N3-C2-N1	-11.36	120.20	128.89
2	B	2903	ATP	N3-C2-N1	-11.23	120.30	128.89
2	F	6903	ATP	N3-C2-N1	-11.04	120.44	128.89
2	F	6903	ATP	C4-C5-N7	-4.92	104.95	109.48
2	B	2903	ATP	C4-C5-N7	-4.87	105.00	109.48
2	D	4903	ATP	C4-C5-N7	-4.74	105.12	109.48
2	E	5903	ATP	C4-C5-N7	-4.63	105.22	109.48
2	A	1903	ATP	C4-C5-N7	-4.61	105.24	109.48
2	F	6901	ATP	C4-C5-N7	-4.61	105.24	109.48
2	E	5901	ATP	C4-C5-N7	-4.58	105.26	109.48
2	C	3901	ATP	C4-C5-N7	-4.55	105.29	109.48
2	D	4901	ATP	C4-C5-N7	-4.43	105.41	109.48
2	C	3903	ATP	C4-C5-N7	-4.39	105.44	109.48
2	A	1901	ATP	C4-C5-N7	-4.38	105.45	109.48
2	B	2901	ATP	C4-C5-N7	-4.29	105.53	109.48
2	B	2903	ATP	N6-C6-N1	-2.73	113.33	119.20
2	B	2901	ATP	O5'-PA-O1A	-2.72	99.08	109.62
2	E	5901	ATP	O5'-PA-O1A	-2.62	99.43	109.62
2	D	4901	ATP	O5'-PA-O1A	-2.61	99.49	109.62
2	F	6901	ATP	O5'-PA-O1A	-2.44	100.13	109.62
2	A	1901	ATP	O5'-PA-O1A	-2.44	100.13	109.62
2	F	6903	ATP	N6-C6-N1	-2.39	114.07	119.20
2	C	3901	ATP	O5'-PA-O1A	-2.39	100.36	109.62
2	A	1903	ATP	N6-C6-N1	-2.38	114.10	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	6901	ATP	C1'-N9-C4	-2.36	123.38	126.94
2	E	5903	ATP	N6-C6-N1	-2.35	114.17	119.20
2	B	2901	ATP	C1'-N9-C4	-2.33	123.42	126.94
2	B	2903	ATP	PB-O3B-PG	-2.30	124.96	132.67
2	D	4903	ATP	N6-C6-N1	-2.25	114.38	119.20
2	A	1901	ATP	PB-O3B-PG	-2.24	125.14	132.67
2	F	6901	ATP	PB-O3B-PG	-2.23	125.19	132.67
2	A	1901	ATP	C1'-N9-C4	-2.20	123.62	126.94
2	D	4901	ATP	PB-O3B-PG	-2.14	125.50	132.67
2	E	5901	ATP	C1'-N9-C4	-2.13	123.72	126.94
2	F	6901	ATP	N6-C6-N1	-2.11	114.67	119.20
2	D	4901	ATP	C1'-N9-C4	-2.09	123.79	126.94
2	C	3903	ATP	N6-C6-N1	-2.08	114.73	119.20
2	A	1903	ATP	PB-O3B-PG	-2.07	125.72	132.67
2	E	5901	ATP	N6-C6-N1	-2.07	114.77	119.20
2	E	5901	ATP	PB-O3B-PG	-2.02	125.89	132.67
2	F	6901	ATP	C2'-C1'-N9	2.02	117.38	114.29
2	E	5901	ATP	O2B-PB-O3B	2.22	115.16	105.09
2	A	1901	ATP	O2B-PB-O3B	2.30	115.54	105.09
2	F	6901	ATP	O2B-PB-O3B	2.33	115.66	105.09
2	D	4901	ATP	O2B-PB-O3B	2.36	115.82	105.09
2	B	2903	ATP	C2'-C1'-N9	2.37	117.92	114.29
2	C	3901	ATP	O2B-PB-O3B	2.41	116.04	105.09
2	A	1903	ATP	O3A-PA-O5'	2.46	109.47	102.94
2	B	2901	ATP	O2B-PB-O3B	2.51	116.46	105.09
2	E	5903	ATP	C2'-C1'-N9	2.74	118.48	114.29
2	E	5903	ATP	O3A-PA-O5'	2.83	110.44	102.94
2	A	1903	ATP	C2'-C1'-N9	2.84	118.63	114.29
2	C	3903	ATP	O3A-PA-O5'	2.91	110.66	102.94
2	B	2903	ATP	O3A-PA-O5'	2.99	110.88	102.94
2	D	4903	ATP	O3A-PA-O5'	3.05	111.03	102.94
2	F	6903	ATP	O3A-PA-O5'	3.08	111.12	102.94
2	C	3903	ATP	C2'-C1'-N9	3.19	119.17	114.29
2	A	1901	ATP	PA-O3A-PB	3.29	141.98	132.73
2	F	6901	ATP	PA-O3A-PB	3.30	142.00	132.73
2	E	5901	ATP	PA-O3A-PB	3.35	142.14	132.73
2	C	3901	ATP	PA-O3A-PB	3.40	142.28	132.73
2	F	6903	ATP	C2'-C1'-N9	3.40	119.49	114.29
2	D	4901	ATP	PA-O3A-PB	3.42	142.34	132.73
2	B	2901	ATP	PA-O3A-PB	3.45	142.43	132.73
2	D	4903	ATP	C2'-C1'-N9	3.67	119.90	114.29
2	A	1901	ATP	O3A-PA-O5'	5.95	118.73	102.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3901	ATP	O3A-PA-O5'	5.99	118.83	102.94
2	B	2901	ATP	O3A-PA-O5'	6.01	118.89	102.94
2	E	5901	ATP	O3A-PA-O5'	6.06	119.00	102.94
2	F	6901	ATP	O3A-PA-O5'	6.09	119.08	102.94
2	D	4901	ATP	O3A-PA-O5'	6.18	119.34	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1901	ATP	5	0
2	A	1903	ATP	3	0
2	B	2901	ATP	6	0
2	B	2903	ATP	4	0
2	C	3901	ATP	4	0
2	C	3903	ATP	4	0
2	D	4901	ATP	4	0
2	D	4903	ATP	3	0
2	E	5901	ATP	5	0
2	E	5903	ATP	4	0
2	F	6901	ATP	5	0
2	F	6903	ATP	3	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	484/525 (92%)	0.32	43 (8%) 12 6	31, 77, 129, 156	0
1	B	484/525 (92%)	0.40	36 (7%) 17 9	42, 83, 129, 161	0
1	C	484/525 (92%)	0.20	27 (5%) 28 18	34, 74, 125, 161	0
1	D	484/525 (92%)	-0.02	21 (4%) 39 27	28, 59, 110, 161	0
1	E	484/525 (92%)	-0.02	24 (4%) 32 21	21, 61, 108, 156	0
1	F	484/525 (92%)	0.06	22 (4%) 37 26	21, 69, 116, 159	0
All	All	2904/3150 (92%)	0.16	173 (5%) 25 15	21, 71, 122, 161	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	118	VAL	10.1
1	B	117	VAL	8.7
1	B	116	GLU	8.5
1	B	118	VAL	8.3
1	D	117	VAL	8.0
1	F	117	VAL	7.9
1	F	154	TYR	7.5
1	A	121	PHE	6.9
1	D	118	VAL	6.9
1	D	121	PHE	6.8
1	C	117	VAL	6.7
1	D	120	GLY	6.7
1	C	120	GLY	6.3
1	B	121	PHE	6.3
1	D	119	GLY	6.0
1	A	257	ARG	5.9
1	A	258	SER	5.7
1	B	15	HIS	5.6
1	C	17	ALA	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	119	GLY	5.0
1	D	113	GLU	4.9
1	E	117	VAL	4.9
1	B	154	TYR	4.8
1	B	115	GLN	4.7
1	A	154	TYR	4.7
1	E	154	TYR	4.5
1	D	158	SER	4.4
1	B	258	SER	4.2
1	B	255	THR	4.2
1	F	366	GLU	4.1
1	F	257	ARG	4.1
1	A	253	ARG	4.0
1	A	475	LYS	4.0
1	A	295	THR	4.0
1	F	116	GLU	4.0
1	E	118	VAL	3.9
1	D	15	HIS	3.9
1	B	158	SER	3.9
1	C	15	HIS	3.9
1	D	154	TYR	3.8
1	B	119	GLY	3.8
1	B	366	GLU	3.8
1	E	329	TYR	3.7
1	B	16	GLN	3.7
1	C	423	HIS	3.7
1	E	366	GLU	3.6
1	C	153	GLN	3.6
1	A	329	TYR	3.5
1	B	122	ASP	3.5
1	F	496	ARG	3.5
1	D	471	MET	3.5
1	B	157	SER	3.5
1	C	152	GLN	3.5
1	A	120	GLY	3.5
1	C	154	TYR	3.5
1	C	116	GLU	3.5
1	A	342	ASN	3.5
1	F	118	VAL	3.5
1	A	251	ALA	3.5
1	E	152	GLN	3.4
1	A	16	GLN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	153	GLN	3.4
1	C	115	GLN	3.4
1	A	311	ARG	3.3
1	F	255	THR	3.3
1	F	311	ARG	3.3
1	F	485	ASN	3.2
1	C	366	GLU	3.2
1	A	417	ASP	3.2
1	C	123	LEU	3.2
1	A	256	GLN	3.1
1	B	321	ARG	3.1
1	F	253	ARG	3.1
1	A	496	ARG	3.1
1	F	484	ARG	3.1
1	A	341	GLN	3.1
1	B	257	ARG	3.1
1	A	309	LYS	3.0
1	D	160	VAL	3.0
1	C	140	ARG	3.0
1	F	157	SER	3.0
1	A	17	ALA	2.9
1	F	156	ALA	2.9
1	A	113	GLU	2.9
1	D	116	GLU	2.9
1	B	253	ARG	2.9
1	B	88	ARG	2.9
1	F	321	ARG	2.8
1	A	114	GLY	2.8
1	A	153	GLN	2.8
1	C	145	ASP	2.8
1	C	16	GLN	2.8
1	A	241	ASP	2.8
1	C	53	THR	2.8
1	E	188	TYR	2.8
1	A	368	ASN	2.7
1	A	318	GLU	2.7
1	E	120	GLY	2.7
1	A	14	GLU	2.6
1	A	402	TYR	2.6
1	B	53	THR	2.6
1	F	121	PHE	2.6
1	B	251	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	119	GLY	2.6
1	B	497	ILE	2.6
1	E	341	GLN	2.6
1	B	90	PHE	2.5
1	E	321	ARG	2.5
1	A	249	LEU	2.5
1	A	252	MET	2.5
1	D	16	GLN	2.5
1	D	366	GLU	2.5
1	C	121	PHE	2.5
1	E	334	ASP	2.5
1	B	92	TRP	2.4
1	A	15	HIS	2.4
1	E	113	GLU	2.4
1	F	423	HIS	2.4
1	D	496	ARG	2.4
1	E	119	GLY	2.4
1	A	378	ASP	2.4
1	A	116	GLU	2.4
1	E	295	THR	2.4
1	A	405	GLN	2.4
1	B	89	SER	2.4
1	C	135	GLN	2.3
1	B	250	GLY	2.3
1	A	117	VAL	2.3
1	A	423	HIS	2.3
1	A	118	VAL	2.3
1	A	255	THR	2.3
1	A	338	MET	2.3
1	D	114	GLY	2.3
1	A	427	ASP	2.3
1	E	116	GLU	2.3
1	C	138	ARG	2.3
1	B	155	ASP	2.2
1	B	256	GLN	2.2
1	E	343	LEU	2.2
1	A	321	ARG	2.2
1	B	375	ILE	2.2
1	A	484	ARG	2.2
1	E	474	ASP	2.2
1	F	252	MET	2.2
1	B	14	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	336	GLU	2.2
1	C	189	GLY	2.2
1	E	421	GLY	2.2
1	B	123	LEU	2.2
1	C	188	TYR	2.2
1	B	153	GLN	2.2
1	D	157	SER	2.1
1	E	166	ARG	2.1
1	B	94	LEU	2.1
1	F	432	THR	2.1
1	E	121	PHE	2.1
1	F	162	ARG	2.1
1	B	91	GLY	2.1
1	B	407	GLU	2.1
1	F	340	ARG	2.1
1	C	132	TYR	2.1
1	A	188	TYR	2.1
1	D	152	GLN	2.1
1	D	309	LYS	2.1
1	C	253	ARG	2.1
1	C	181	THR	2.1
1	C	14	GLU	2.1
1	A	259	SER	2.1
1	E	471	MET	2.0
1	D	53	THR	2.0
1	B	132	TYR	2.0
1	E	173	GLN	2.0
1	D	115	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
2	ATP	D	4903	31/31	0.90	0.28	1.98	43,54,77,81	0
2	ATP	E	5903	31/31	0.94	0.25	1.43	43,54,77,81	0
2	ATP	F	6903	31/31	0.91	0.23	1.27	43,55,77,80	0
2	ATP	F	6901	31/31	0.87	0.27	1.00	75,90,115,121	0
2	ATP	D	4901	31/31	0.93	0.24	0.95	54,66,90,105	0
2	ATP	B	2901	31/31	0.90	0.24	0.94	62,74,110,116	0
2	ATP	C	3901	31/31	0.92	0.21	0.67	48,56,97,110	0
2	ATP	A	1903	31/31	0.84	0.25	0.65	43,55,77,81	0
2	ATP	A	1901	31/31	0.86	0.29	0.31	76,89,103,113	0
2	ATP	C	3903	31/31	0.88	0.23	0.21	43,55,77,81	0
2	ATP	B	2903	31/31	0.84	0.21	-0.08	44,55,77,81	0
2	ATP	E	5901	31/31	0.90	0.23	-0.10	62,78,101,114	0

6.5 Other polymers

There are no such residues in this entry.