



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:49 am BST

PDB ID : 2NVT  
Title : RNA Polymerase II Elongation Complex in 150 mM Mg+2 with GMPCPP  
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.  
Deposited on : 2006-11-13  
Resolution : 3.36 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

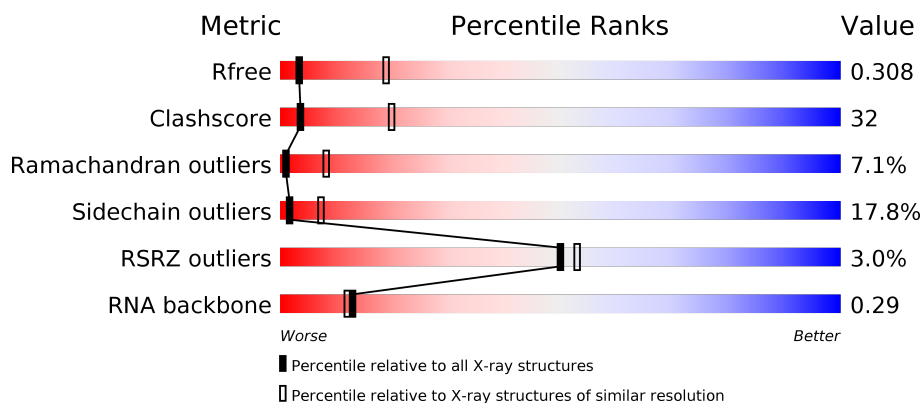
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.36 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	10	
2	T	21	
3	N	7	
4	A	1733	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	B	1224	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>2%37%39%13%9%</div></div>
6	C	318	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>%39%39%6%16%</div></div>
7	E	215	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>5%56%34%9%</div></div>
8	F	155	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>36%16%45%</div></div>
9	H	146	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>3%43%38%8%9%</div></div>
10	I	122	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>53%35%8%</div></div>
11	J	70	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>43%33%14%7%</div></div>
12	K	120	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>54%37%5%</div></div>
13	L	70	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>7%23%29%13%34%</div></div>

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29168 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 RNA chain called 5'-R(\*AP\*AP\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			214	97	44	64	9			

- Molecule 2 is a DNA chain called 5'-D(P\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*AP\*CP\*GP\*CP\*CP\*TP\*GP\*GP\*TP\*CP\*TP\*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	21	Total	C	N	O	P	0	0	0
			426	204	72	129	21			

- Molecule 3 is a DNA chain called 5'-D(\*GP\*TP\*AP\*CP\*TP\*TP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	7	Total	C	N	O	P	0	0	0
			141	69	24	42	6			

- Molecule 4 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1411	Total	C	N	O	S	0	0	0
			11090	6993	1942	2094	61			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1114	Total	C	N	O	S	0	0	0
			8861	5610	1549	1647	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	85	Total	C	N	O	S	0	0	0
			688	439	116	130	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

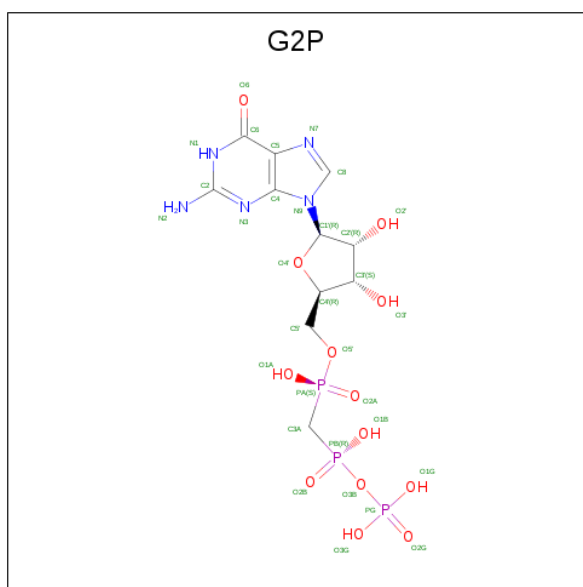
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypep-

tide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 14 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula:  $C_{11}H_{18}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	T	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	1	Total	Zn	0	0
			1	1		
15	B	1	Total	Zn	0	0
			1	1		
15	I	2	Total	Zn	0	0
			2	2		
15	C	1	Total	Zn	0	0
			1	1		
15	A	2	Total	Zn	0	0
			2	2		
15	L	1	Total	Zn	0	0
			1	1		

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	2	Total	Mg	0	0
			2	2		

### 3 Residue-property plots [i](#)

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

- Molecule 1: 5'-R(\*AP\*AP\*GP\*AP\*CP\*CP\*AP\*GP\*GP\*C)-3'

Chain R: 



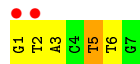
- Molecule 2: 5'-D(P\*CP\*AP\*AP\*GP\*TP\*AP\*CP\*TP\*TP\*AP\*CP\*GP\*CP\*CP\*TP\*GP\*GP\*TP\*CP\*TP\*T)-3'

Chain T: 



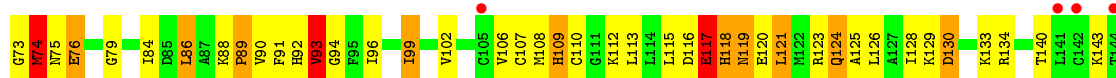
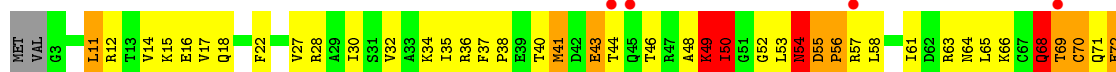
- Molecule 3: 5'-D(\*GP\*TP\*AP\*CP\*TP\*TP\*G)-3'

Chain N: 



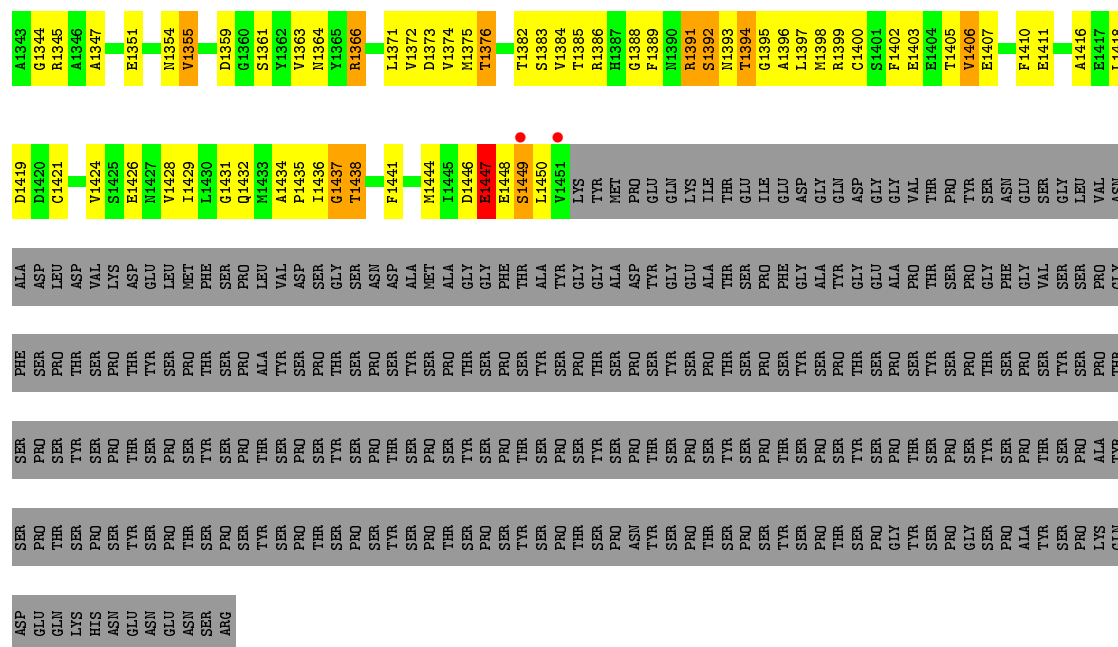
- Molecule 4: DNA-directed RNA polymerase II largest subunit

Chain A: 

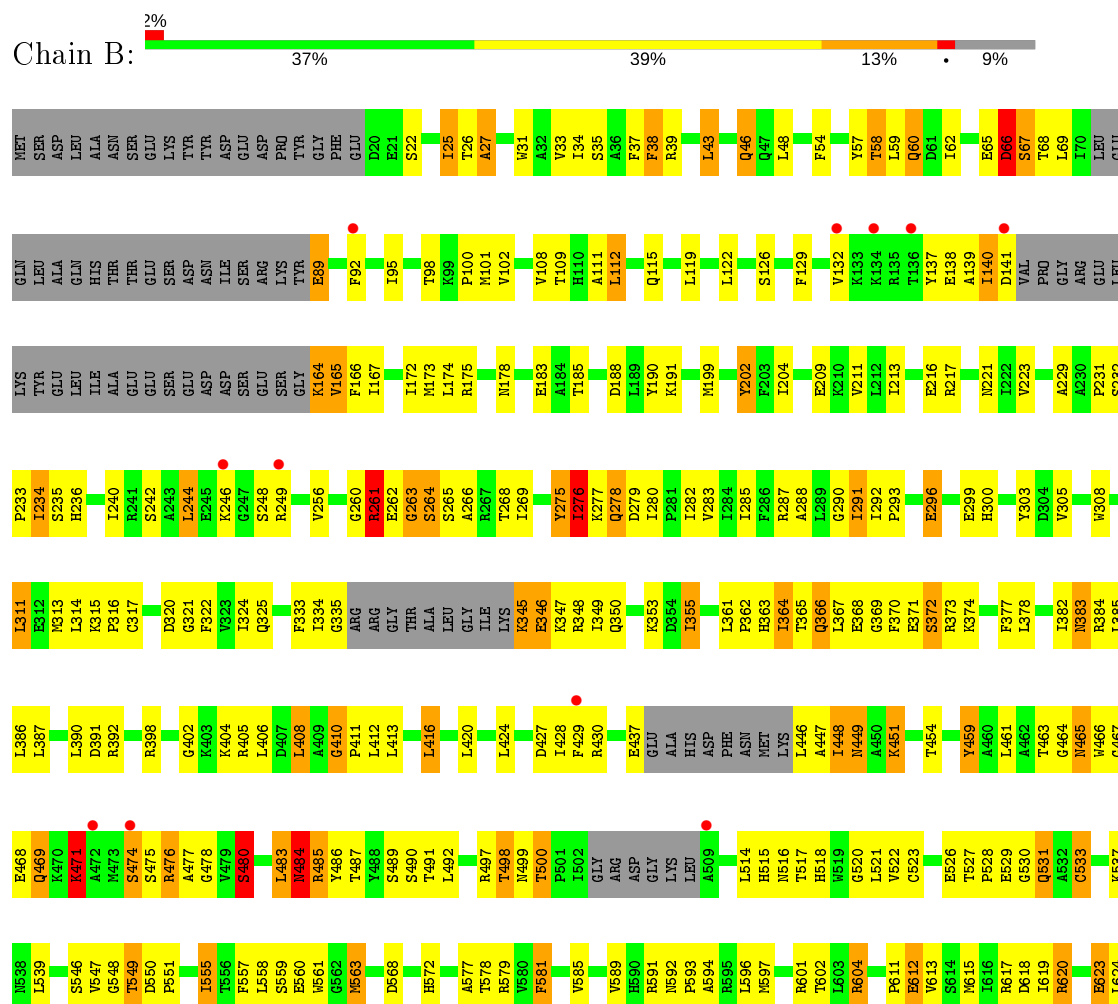






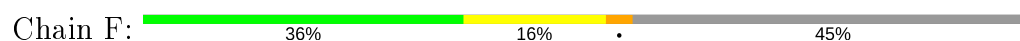


- Molecule 5: DNA-directed RNA polymerase II 140 kDa polypeptide



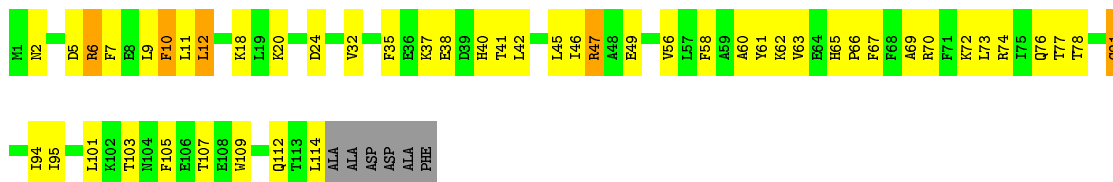


- Chain E: 

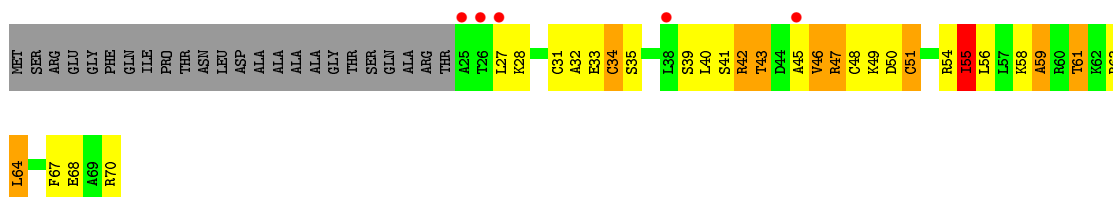
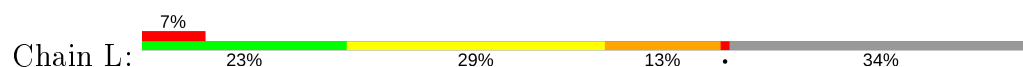




- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.87Å 222.82Å 195.80Å 90.00° 102.39° 90.00°	Depositor
Resolution (Å)	40.00 – 3.36 39.86 – 3.36	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.36) 97.1 (39.86-3.36)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.230 , 0.283 0.257 , 0.308	Depositor DCC
$R_{free}$ test set	4911 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.0	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	29168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, G2P

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	R	1.40	3/240 (1.2%)	2.56	27/373 (7.2%)
2	T	1.19	0/475	2.56	38/730 (5.2%)
3	N	0.91	0/157	1.68	6/241 (2.5%)
4	A	0.68	2/11288 (0.0%)	0.82	6/15263 (0.0%)
5	B	0.82	7/9033 (0.1%)	0.91	16/12181 (0.1%)
6	C	0.76	1/2139 (0.0%)	0.89	1/2899 (0.0%)
7	E	0.51	0/1788	0.69	1/2406 (0.0%)
8	F	0.54	0/700	0.75	0/945
9	H	0.56	0/1086	0.77	0/1470
10	I	0.59	0/989	0.73	1/1331 (0.1%)
11	J	0.90	0/541	0.91	0/727
12	K	0.65	0/937	0.76	0/1265
13	L	0.66	0/365	0.93	0/485
All	All	0.74	13/29738 (0.0%)	0.94	96/40316 (0.2%)

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
4	A	0	5
5	B	0	6
9	H	0	1
All	All	0	12

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1222	ARG	CZ-NH1	7.73	1.43	1.33
1	R	10	C	C2-N3	7.26	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	10	C	C2'-C1'	6.83	1.60	1.53
1	R	10	C	N3-C4	6.79	1.38	1.33
4	A	1020	CYS	CB-SG	-6.59	1.71	1.82
5	B	1086	PHE	C-O	6.30	1.35	1.23
6	C	94	LYS	CE-NZ	6.00	1.64	1.49
5	B	529	GLU	CG-CD	5.78	1.60	1.51
4	A	404	TYR	CE2-CZ	5.72	1.46	1.38
5	B	752	ALA	CA-CB	5.68	1.64	1.52
5	B	1029	CYS	CB-SG	-5.34	1.73	1.81
5	B	757	PRO	CB-CG	5.11	1.75	1.50
5	B	833	TYR	CE1-CZ	5.08	1.45	1.38

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	22	DT	C4-C5-C7	-16.64	109.02	119.00
2	T	27	DT	C6-C5-C7	-12.28	115.53	122.90
2	T	13	DA	O4'-C1'-N9	11.91	116.34	108.00
2	T	20	DC	O4'-C4'-C3'	-11.64	99.01	106.00
2	T	22	DT	C5-C4-O4	-11.59	116.79	124.90
2	T	22	DT	N3-C4-O4	11.51	126.80	119.90
2	T	22	DT	O4'-C4'-C3'	-11.09	99.34	106.00
2	T	19	DG	O4'-C1'-N9	11.08	115.76	108.00
1	R	10	C	N3-C4-N4	10.18	125.13	118.00
2	T	11	DG	O4'-C1'-N9	10.17	115.12	108.00
2	T	21	DC	N3-C4-C5	9.68	125.77	121.90
1	R	10	C	P-O5'-C5'	-9.17	106.23	120.90
2	T	16	DT	O4'-C4'-C3'	-8.85	100.69	106.00
1	R	10	C	C5-C4-N4	-8.77	114.06	120.20
5	B	983	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	R	8	G	C1'-O4'-C4'	-8.60	103.02	109.90
1	R	10	C	N1-C2-O2	-8.43	113.84	118.90
1	R	10	C	C5'-C4'-C3'	-8.42	102.53	116.00
2	T	22	DT	C6-C5-C7	-7.94	118.14	122.90
5	B	1100	ASP	CB-CG-OD2	7.78	125.30	118.30
3	N	2	DT	C6-C5-C7	-7.77	118.24	122.90
2	T	21	DC	N1-C2-O2	7.73	123.54	118.90
2	T	20	DC	N3-C4-N4	-7.64	112.65	118.00
2	T	18	DC	N1-C2-O2	7.63	123.48	118.90
1	R	10	C	O5'-P-OP2	-7.60	98.86	105.70
2	T	20	DC	N1-C2-O2	7.39	123.34	118.90
1	R	10	C	O4'-C1'-N1	-7.39	102.29	108.20

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	9	G	O5'-P-OP1	7.38	119.56	110.70
2	T	20	DC	N3-C4-C5	7.36	124.85	121.90
2	T	25	DT	O4'-C1'-N1	7.33	113.13	108.00
5	B	998	ASP	CB-CG-OD1	7.29	124.86	118.30
2	T	16	DT	O4'-C1'-N1	6.96	112.88	108.00
3	N	6	DT	O4'-C1'-N1	6.94	112.86	108.00
1	R	7	A	O4'-C1'-N9	-6.91	102.67	108.20
5	B	539	LEU	CA-CB-CG	6.87	131.11	115.30
5	B	1030	LEU	CA-CB-CG	6.76	130.85	115.30
1	R	10	C	C5'-C4'-O4'	6.70	117.14	109.10
2	T	21	DC	O4'-C1'-N1	-6.67	103.33	108.00
2	T	16	DT	C1'-O4'-C4'	-6.65	103.45	110.10
2	T	22	DT	C5'-C4'-O4'	-6.64	96.69	109.30
1	R	2	A	C4'-C3'-C2'	-6.61	95.99	102.60
2	T	16	DT	C4'-C3'-C2'	-6.60	97.16	103.10
2	T	21	DC	P-O3'-C3'	6.53	127.53	119.70
1	R	2	A	C1'-O4'-C4'	-6.51	104.69	109.90
1	R	8	G	N9-C1'-C2'	-6.46	104.89	112.00
1	R	9	G	OP1-P-OP2	-6.39	110.02	119.60
1	R	10	C	OP1-P-OP2	-6.36	110.06	119.60
5	B	1222	ARG	NE-CZ-NH2	-6.33	117.14	120.30
10	I	53	GLY	N-CA-C	6.33	128.92	113.10
5	B	966	VAL	CB-CA-C	-6.20	99.61	111.40
2	T	18	DC	N3-C2-O2	-6.18	117.57	121.90
2	T	15	DT	P-O3'-C3'	6.12	127.04	119.70
2	T	21	DC	O5'-P-OP2	-6.10	100.21	105.70
5	B	998	ASP	CB-CG-OD2	-6.10	112.81	118.30
2	T	21	DC	O4'-C1'-C2'	6.09	110.77	105.90
5	B	710	LEU	CA-CB-CG	6.07	129.27	115.30
1	R	7	A	C4'-C3'-C2'	-6.06	96.54	102.60
1	R	10	C	C3'-C2'-C1'	6.06	106.35	101.50
1	R	8	G	C4'-C3'-C2'	-5.98	96.62	102.60
5	B	1101	ASP	CB-CG-OD1	-5.98	112.92	118.30
5	B	883	LEU	CA-CB-CG	5.90	128.87	115.30
1	R	5	C	C6-N1-C2	-5.90	117.94	120.30
4	A	239	LEU	CA-CB-CG	5.89	128.84	115.30
5	B	1010	LEU	CB-CG-CD1	-5.82	101.11	111.00
1	R	9	G	OP2-P-O3'	5.80	117.96	105.20
4	A	509	LEU	CA-CB-CG	5.78	128.60	115.30
2	T	21	DC	C1'-O4'-C4'	-5.75	104.35	110.10
2	T	24	DG	O4'-C1'-N9	5.74	112.02	108.00
1	R	7	A	C5-C6-N1	5.68	120.54	117.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	5	DT	O4'-C1'-N1	5.66	111.96	108.00
2	T	11	DG	C1'-O4'-C4'	-5.61	104.49	110.10
3	N	2	DT	P-O3'-C3'	5.60	126.42	119.70
1	R	10	C	N3-C2-O2	5.60	125.82	121.90
2	T	11	DG	O4'-C1'-C2'	-5.56	101.45	105.90
2	T	13	DA	O4'-C1'-C2'	-5.52	101.49	105.90
4	A	208	LEU	CA-CB-CG	5.49	127.92	115.30
2	T	21	DC	C6-N1-C2	5.48	122.49	120.30
1	R	8	G	O4'-C4'-C3'	-5.48	98.52	104.00
2	T	12	DT	P-O3'-C3'	5.45	126.24	119.70
5	B	711	GLU	N-CA-C	5.44	125.69	111.00
2	T	19	DG	N3-C2-N2	-5.39	116.12	119.90
4	A	629	LEU	CA-CB-CG	5.36	127.62	115.30
5	B	483	LEU	CB-CG-CD1	5.32	120.03	111.00
2	T	8	DC	P-O3'-C3'	5.29	126.04	119.70
7	E	175	LEU	CA-CB-CG	5.29	127.46	115.30
3	N	5	DT	P-O3'-C3'	5.27	126.02	119.70
1	R	9	G	C5'-C4'-O4'	5.24	115.38	109.10
1	R	8	G	C2-N3-C4	5.23	114.52	111.90
1	R	8	G	C5-C6-N1	5.18	114.09	111.50
5	B	883	LEU	CB-CG-CD2	5.15	119.75	111.00
3	N	1	DG	O4'-C1'-N9	5.13	111.59	108.00
5	B	819	ALA	N-CA-C	-5.11	97.22	111.00
2	T	22	DT	C5'-C4'-C3'	5.10	123.28	114.10
6	C	66	ARG	NE-CZ-NH2	-5.04	117.78	120.30
4	A	710	LEU	CA-CB-CG	5.04	126.88	115.30
4	A	489	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	115	LEU	Peptide
4	A	117	GLU	Peptide
4	A	342	GLY	Peptide
4	A	482	PHE	Peptide
4	A	484	GLY	Peptide
5	B	1053	GLU	Peptide
5	B	1085	ILE	Peptide
5	B	140	ILE	Peptide
5	B	828	ALA	Peptide
5	B	976	ILE	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
5	B	989	THR	Peptide
9	H	91	ASP	Peptide

## 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	R	214	0	111	18	0
2	T	426	0	239	23	0
3	N	141	0	82	2	0
4	A	11090	0	11173	784	1
5	B	8861	0	8884	722	0
6	C	2101	0	2056	149	1
7	E	1752	0	1776	74	0
8	F	688	0	707	26	0
9	H	1068	0	1040	54	0
10	I	971	0	927	36	0
11	J	532	0	542	71	0
12	K	919	0	929	65	0
13	L	363	0	386	27	0
14	T	32	0	14	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	A	2	0	0	0	0
All	All	29168	0	28866	1832	1

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 32.

All (1832) 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)
4:A:336:ILE:CD1	4:A:1405:THR:CG2	1.78	1.57
5:B:976:ILE:HD11	5:B:991:GLY:C	1.14	1.48
4:A:341:MET:SD	4:A:1428:VAL:HG12	1.62	1.39
4:A:336:ILE:CD1	4:A:1405:THR:HG21	0.93	1.39
5:B:757:PRO:CG	5:B:757:PRO:CB	1.75	1.38
4:A:336:ILE:HD13	4:A:1405:THR:CG2	1.47	1.34
5:B:839:MET:CE	5:B:990:ILE:HG12	1.55	1.34
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	1.41	1.33
4:A:343:LYS:NZ	5:B:1156:ASP:OD2	1.58	1.32
4:A:117:GLU:N	4:A:118:HIS:HB2	1.41	1.31
5:B:976:ILE:HD11	5:B:991:GLY:O	1.28	1.28
4:A:341:MET:SD	4:A:1428:VAL:CG1	2.20	1.27
4:A:117:GLU:H	4:A:118:HIS:CB	1.46	1.26
4:A:343:LYS:NZ	5:B:1197:PRO:HB3	1.49	1.26
4:A:341:MET:CE	4:A:1428:VAL:HB	1.69	1.22
5:B:647:GLY:HA3	5:B:648:HIS:CB	1.70	1.21
5:B:1122:ARG:HH11	5:B:1122:ARG:HG2	1.05	1.20
5:B:976:ILE:CD1	5:B:991:GLY:C	2.09	1.19
5:B:1122:ARG:HH11	5:B:1122:ARG:CG	1.54	1.18
4:A:336:ILE:HD12	4:A:1405:THR:CG2	1.71	1.17
5:B:976:ILE:HD12	5:B:992:ILE:HA	1.20	1.16
10:I:117:LYS:HB3	10:I:118:ARG:HA	1.17	1.16
4:A:343:LYS:CE	5:B:1156:ASP:OD2	1.94	1.15
5:B:839:MET:HE1	5:B:990:ILE:CG1	1.76	1.15
5:B:839:MET:CG	5:B:989:THR:O	1.95	1.14
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	1.83	1.13
4:A:443:LEU:HD21	4:A:455:MET:HG3	1.17	1.11
5:B:976:ILE:HD11	5:B:992:ILE:N	1.63	1.11
5:B:1094:ARG:HG2	5:B:1094:ARG:HH11	1.16	1.11
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	0.94	1.09
9:H:82:PRO:HB2	9:H:83:GLN:HA	1.23	1.09
6:C:57:VAL:HG11	11:J:60:PHE:HB3	1.24	1.09
4:A:567:LYS:HB3	9:H:96:VAL:H	1.13	1.09
5:B:807:ARG:HG3	5:B:807:ARG:HH11	1.15	1.09
4:A:341:MET:HE1	4:A:1428:VAL:CB	1.81	1.08
5:B:345:LYS:N	5:B:346:GLU:HA	1.67	1.08
5:B:976:ILE:CD1	5:B:991:GLY:O	2.00	1.08
5:B:976:ILE:CD1	5:B:992:ILE:HA	1.83	1.07
4:A:565:ILE:HG23	4:A:567:LYS:HE3	1.35	1.07
4:A:1364:ASN:HD22	4:A:1366:ARG:CG	1.69	1.05
5:B:879:ARG:NH1	5:B:882:THR:HG22	1.69	1.04
4:A:55:ASP:H	4:A:56:PRO:HD2	1.18	1.04

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:647:GLY:HA3	5:B:648:HIS:HB3	1.38	1.03
4:A:336:ILE:HD12	4:A:1405:THR:HG21	1.32	1.03
4:A:336:ILE:HD11	4:A:1405:THR:HG21	1.36	1.03
5:B:446:LEU:HG	5:B:447:ALA:H	1.21	1.02
4:A:343:LYS:CD	5:B:1156:ASP:OD2	2.06	1.02
5:B:994:TYR:HB2	5:B:999:MET:CE	1.87	1.02
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.42	1.02
4:A:341:MET:CE	4:A:1428:VAL:CB	2.36	1.02
4:A:443:LEU:HD21	4:A:455:MET:CG	1.89	1.02
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.41	1.02
4:A:440:ASP:OD2	4:A:441:PRO:HD2	1.58	1.01
4:A:443:LEU:CD2	4:A:455:MET:HG3	1.91	1.01
4:A:48:ALA:HB1	4:A:49:LYS:HB3	1.41	1.01
6:C:57:VAL:HG11	11:J:60:PHE:CB	1.91	1.00
4:A:372:LYS:HA	4:A:435:HIS:CD2	1.96	1.00
4:A:49:LYS:HD2	4:A:55:ASP:OD2	1.61	1.00
11:J:7:CYS:HB2	11:J:49:MET:HG2	1.42	1.00
4:A:760:GLN:HA	4:A:760:GLN:HE21	1.23	1.00
4:A:490:HIS:HB3	5:B:1150:ARG:NH1	1.76	0.99
4:A:447:GLN:HB3	4:A:448:PRO:HA	1.45	0.98
5:B:167:ILE:O	5:B:167:ILE:HG22	1.62	0.98
5:B:879:ARG:CZ	5:B:879:ARG:HA	1.93	0.98
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	0.96	0.97
5:B:822:ASN:HD22	11:J:52:THR:CG2	1.77	0.97
4:A:311:GLN:HB3	4:A:312:PRO:HD2	1.44	0.97
4:A:343:LYS:HD3	5:B:1156:ASP:OD2	1.64	0.97
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.29	0.96
4:A:853:ASP:OD1	4:A:855:THR:HG22	1.65	0.96
6:C:142:VAL:H	11:J:16:ASP:HB3	1.30	0.96
5:B:1094:ARG:CG	5:B:1094:ARG:HH11	1.79	0.96
4:A:96:ILE:HG21	4:A:176:LYS:HE3	1.47	0.95
4:A:218:ASP:H	4:A:219:PHE:HB3	1.31	0.95
4:A:1015:VAL:HG12	4:A:1019:CYS:SG	2.06	0.95
5:B:977:GLY:O	5:B:989:THR:HG22	1.68	0.94
4:A:666:ILE:HD12	5:B:1026:LEU:HB2	1.46	0.94
5:B:778:MET:CE	5:B:1094:ARG:NH1	2.29	0.94
5:B:647:GLY:HA3	5:B:648:HIS:HB2	1.46	0.94
4:A:336:ILE:HG13	4:A:337:ARG:H	1.33	0.93
4:A:341:MET:CE	4:A:1428:VAL:CG1	2.47	0.93
4:A:351:THR:HG22	4:A:352:VAL:N	1.81	0.93
5:B:976:ILE:HD12	5:B:992:ILE:CA	1.98	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:276:LEU:HD11	4:A:292:ALA:HB1	1.48	0.93
4:A:48:ALA:CB	4:A:49:LYS:HB3	1.97	0.93
5:B:702:LEU:HD21	5:B:735:ALA:HB1	1.49	0.93
4:A:341:MET:HE1	4:A:1428:VAL:HB	0.96	0.92
4:A:336:ILE:HD12	4:A:1405:THR:HG23	1.47	0.92
5:B:976:ILE:CD1	5:B:992:ILE:CA	2.47	0.92
5:B:1122:ARG:NH1	5:B:1122:ARG:HG2	1.68	0.92
4:A:901:LEU:HA	4:A:907:THR:HG22	1.51	0.91
4:A:901:LEU:H	4:A:926:GLN:HE21	1.14	0.91
5:B:31:TRP:HA	5:B:34:ILE:HD12	1.50	0.91
5:B:976:ILE:HG23	5:B:976:ILE:O	1.71	0.91
4:A:472:LEU:O	4:A:475:THR:HB	1.71	0.91
4:A:14:VAL:H	4:A:1432:GLN:HE22	1.19	0.91
5:B:778:MET:HE1	5:B:1094:ARG:NH1	1.86	0.91
10:I:117:LYS:CB	10:I:118:ARG:HA	2.00	0.90
5:B:1106:ARG:HD2	5:B:1126:GLY:O	1.70	0.90
4:A:809:THR:HG22	4:A:810:PRO:HD2	1.52	0.90
5:B:1029:CYS:SG	5:B:1088:GLY:HA3	2.12	0.90
6:C:57:VAL:CG1	11:J:60:PHE:HB3	2.01	0.90
4:A:351:THR:HG23	5:B:1103:ILE:HD13	1.51	0.90
4:A:48:ALA:CA	4:A:49:LYS:HB3	2.01	0.90
5:B:980:PHE:CE1	5:B:990:ILE:HD11	2.06	0.90
5:B:1094:ARG:HG2	5:B:1094:ARG:NH1	1.76	0.90
4:A:868:TYR:HE1	4:A:1064:VAL:CG1	1.82	0.89
5:B:879:ARG:HA	5:B:879:ARG:NE	1.84	0.89
5:B:994:TYR:HB2	5:B:999:MET:HE1	1.51	0.89
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.52	0.89
4:A:351:THR:HG22	4:A:352:VAL:H	1.34	0.88
4:A:364:VAL:HG12	4:A:459:ARG:O	1.72	0.88
5:B:843:GLN:OE1	5:B:843:GLN:HA	1.71	0.88
4:A:323:LYS:NZ	4:A:324:SER:H	1.71	0.88
4:A:269:ILE:HG22	4:A:299:HIS:HB2	1.54	0.88
11:J:19:GLU:HA	11:J:19:GLU:OE1	1.73	0.88
5:B:994:TYR:HB2	5:B:999:MET:HE3	1.56	0.88
4:A:803:SER:OG	4:A:806:ARG:HB2	1.74	0.86
5:B:822:ASN:HD22	11:J:52:THR:HG21	1.39	0.86
4:A:37:PHE:HB2	4:A:52:GLY:HA3	1.56	0.86
9:H:2:SER:HB2	9:H:3:ASN:HB2	1.57	0.86
5:B:839:MET:HG3	5:B:989:THR:O	1.75	0.86
4:A:372:LYS:HA	4:A:435:HIS:HD2	1.39	0.86
4:A:367:PRO:HD3	4:A:467:THR:O	1.75	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:466:SER:O	5:B:1103:ILE:HD12	1.75	0.85
5:B:839:MET:HG2	5:B:989:THR:O	1.76	0.85
5:B:999:MET:HG2	5:B:1008:PRO:HD2	1.58	0.85
4:A:48:ALA:HA	4:A:49:LYS:CB	2.06	0.85
5:B:778:MET:O	5:B:819:ALA:HB1	1.75	0.85
5:B:969:ARG:HH11	5:B:969:ARG:HB3	1.42	0.85
4:A:214:ILE:HG22	4:A:215:SER:H	1.41	0.85
4:A:754:SER:H	4:A:757:ASN:ND2	1.74	0.84
4:A:343:LYS:HZ1	5:B:1197:PRO:HB3	1.41	0.84
5:B:976:ILE:CD1	5:B:992:ILE:N	2.34	0.84
4:A:323:LYS:HZ3	4:A:324:SER:H	1.26	0.84
5:B:839:MET:HE1	5:B:990:ILE:HG12	0.85	0.84
5:B:69:LEU:O	5:B:89:GLU:HG2	1.78	0.84
4:A:444:PHE:HE2	4:A:470:LEU:CD2	1.90	0.84
4:A:814:PHE:O	4:A:817:ALA:HB3	1.78	0.83
5:B:1150:ARG:O	5:B:1150:ARG:HG3	1.77	0.83
5:B:879:ARG:HH12	5:B:882:THR:HG22	1.41	0.83
5:B:913:GLY:HA2	5:B:938:SER:OG	1.77	0.83
4:A:117:GLU:H	4:A:118:HIS:HB2	0.69	0.83
5:B:390:LEU:HD13	5:B:392:ARG:HH21	1.44	0.83
4:A:839:ARG:HH11	4:A:839:ARG:CG	1.92	0.82
5:B:263:GLY:HA2	5:B:264:SER:O	1.80	0.82
4:A:79:GLY:O	4:A:243:PRO:HG3	1.79	0.82
4:A:901:LEU:H	4:A:926:GLN:NE2	1.77	0.82
9:H:2:SER:CB	9:H:3:ASN:HB2	2.09	0.82
12:K:37:LYS:HA	12:K:69:ALA:HB1	1.59	0.82
5:B:647:GLY:CA	5:B:648:HIS:CB	2.57	0.82
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.12	0.82
5:B:345:LYS:N	5:B:346:GLU:CA	2.43	0.81
4:A:313:GLN:HG2	4:A:322:VAL:HG22	1.61	0.81
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.63	0.81
4:A:215:SER:HB3	4:A:218:ASP:HB2	1.63	0.81
4:A:14:VAL:H	4:A:1432:GLN:NE2	1.77	0.81
4:A:353:ILE:HD13	4:A:487:MET:HE2	1.61	0.81
5:B:980:PHE:CE1	5:B:990:ILE:CD1	2.63	0.81
4:A:754:SER:H	4:A:757:ASN:HD22	1.29	0.81
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.14	0.81
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.61	0.81
4:A:353:ILE:HG23	4:A:487:MET:HG3	1.61	0.80
5:B:484:ASN:ND2	5:B:490:SER:OG	2.12	0.80
4:A:567:LYS:CB	4:A:568:PRO:HD2	2.11	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:805:THR:HG21	5:B:815:ARG:HH21	1.46	0.80
4:A:340:LEU:HD21	5:B:1199:ALA:C	2.02	0.80
4:A:353:ILE:CG2	4:A:487:MET:HG3	2.11	0.80
5:B:1163:CYS:HB3	5:B:1167:GLY:H	1.44	0.80
5:B:839:MET:CE	5:B:990:ILE:CG1	2.46	0.80
5:B:842:ASN:HD22	5:B:845:SER:HB3	1.47	0.80
4:A:336:ILE:HG13	4:A:337:ARG:N	1.95	0.80
4:A:351:THR:HG21	4:A:466:SER:O	1.81	0.80
4:A:407:ARG:HD2	4:A:413:ILE:HD11	1.63	0.80
6:C:6:PRO:HB3	6:C:25:VAL:HG22	1.62	0.79
5:B:448:ILE:HG23	5:B:449:ASN:H	1.47	0.79
4:A:55:ASP:N	4:A:56:PRO:HD2	1.96	0.79
5:B:1122:ARG:CG	5:B:1122:ARG:NH1	2.26	0.79
4:A:336:ILE:HD11	4:A:1405:THR:CG2	1.99	0.79
5:B:655:LYS:O	5:B:658:ILE:HG22	1.82	0.79
4:A:364:VAL:O	4:A:364:VAL:HG13	1.82	0.79
5:B:778:MET:CE	5:B:1094:ARG:HH11	1.94	0.79
7:E:130:ALA:HA	7:E:131:THR:OG1	1.83	0.79
5:B:408:LEU:O	5:B:412:LEU:HG	1.83	0.79
6:C:33:LEU:HD23	6:C:37:MET:HE3	1.65	0.79
4:A:1063:MET:SD	4:A:1436:ILE:HG13	2.23	0.79
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.64	0.79
5:B:464:GLY:HA3	5:B:478:GLY:HA2	1.65	0.78
9:H:82:PRO:CB	9:H:83:GLN:HA	2.10	0.78
5:B:521:LEU:HD22	5:B:633:VAL:HG12	1.64	0.78
4:A:535:THR:HG21	4:A:617:VAL:H	1.47	0.78
7:E:179:GLN:HB2	7:E:182:ASP:HB2	1.65	0.78
5:B:167:ILE:CG2	5:B:167:ILE:O	2.30	0.78
11:J:7:CYS:HB2	11:J:49:MET:CG	2.14	0.78
2:T:8:DC:H4'	2:T:9:DA:O5'	1.82	0.78
4:A:913:LEU:HD12	4:A:914:GLU:H	1.49	0.78
4:A:500:GLU:OE2	5:B:1145:SER:HB2	1.83	0.77
5:B:807:ARG:CG	5:B:807:ARG:HH11	1.97	0.77
5:B:647:GLY:CA	5:B:648:HIS:HB3	2.13	0.77
5:B:765:PRO:O	5:B:767:ASN:N	2.18	0.77
8:F:103:MET:O	8:F:104:ASN:HB2	1.83	0.77
4:A:341:MET:CE	4:A:1428:VAL:HG11	2.14	0.77
4:A:341:MET:SD	4:A:1428:VAL:HG11	2.24	0.77
4:A:543:LEU:HG	4:A:547:LEU:HD11	1.66	0.77
6:C:215:GLU:H	6:C:216:GLY:HA3	1.46	0.77
11:J:48:ARG:HG2	11:J:48:ARG:HH11	1.49	0.77

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:65:HIS:CD2	12:K:66:PRO:HD2	2.20	0.77
4:A:565:ILE:CG2	4:A:567:LYS:HE3	2.12	0.77
4:A:22:PHE:HB2	5:B:121:ASN:OD1	1.85	0.77
5:B:654:ARG:H	5:B:657:HIS:HD2	1.33	0.77
6:C:123:ASN:ND2	6:C:125:MET:HG3	2.00	0.77
6:C:33:LEU:HD23	6:C:37:MET:CE	2.15	0.77
4:A:214:ILE:HG22	4:A:215:SER:N	2.00	0.77
4:A:48:ALA:CA	4:A:49:LYS:CB	2.60	0.77
4:A:341:MET:SD	4:A:1429:ILE:HG13	2.25	0.77
4:A:41:MET:HG2	4:A:41:MET:O	1.85	0.77
4:A:129:LYS:O	4:A:130:ASP:HB2	1.83	0.76
4:A:760:GLN:CA	4:A:760:GLN:HE21	1.96	0.76
5:B:805:THR:HG21	5:B:815:ARG:NH2	2.00	0.76
4:A:830:LYS:O	4:A:834:THR:HG23	1.84	0.76
4:A:1101:LEU:O	4:A:1105:LEU:HD12	1.84	0.76
5:B:822:ASN:HD22	11:J:52:THR:HG23	1.50	0.76
2:T:27:DT:H2''	2:T:28:DT:O5'	1.85	0.76
4:A:465:TYR:HE1	12:K:67:PHE:CE2	2.03	0.76
5:B:390:LEU:HD13	5:B:392:ARG:NH2	2.00	0.76
12:K:58:PHE:HE2	12:K:74:ARG:HE	1.32	0.76
4:A:311:GLN:HB3	4:A:312:PRO:CD	2.15	0.75
5:B:841:MET:HE1	5:B:990:ILE:HD11	1.66	0.75
4:A:1123:GLY:HA3	4:A:1124:HIS:HB2	1.69	0.75
4:A:336:ILE:CG1	4:A:337:ARG:H	1.97	0.75
5:B:710:LEU:O	5:B:711:GLU:HB3	1.85	0.75
4:A:436:ILE:HD11	4:A:491:VAL:HG11	1.68	0.75
10:I:65:ASP:OD1	10:I:66:PRO:HD2	1.86	0.75
5:B:1054:GLY:O	5:B:1055:ILE:C	2.25	0.75
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.69	0.75
5:B:839:MET:HG3	5:B:990:ILE:HA	1.68	0.75
6:C:73:GLN:HE21	6:C:74:SER:N	1.84	0.75
4:A:1156:PRO:O	4:A:1158:PRO:HD3	1.87	0.74
5:B:483:LEU:O	5:B:484:ASN:HB3	1.87	0.74
5:B:956:THR:HB	13:L:46:VAL:HG21	1.68	0.74
4:A:902:LEU:HG	4:A:926:GLN:HG3	1.69	0.74
5:B:486:TYR:HE1	5:B:794:ASN:HB2	1.52	0.74
5:B:840:ILE:HG21	5:B:1011:ILE:HD12	1.68	0.74
5:B:822:ASN:ND2	11:J:52:THR:CG2	2.50	0.74
5:B:986:GLN:NE2	5:B:1022:THR:HG21	2.03	0.74
4:A:1364:ASN:ND2	4:A:1366:ARG:CG	2.32	0.74
4:A:343:LYS:HZ2	5:B:1156:ASP:CG	1.89	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:654:ARG:H	5:B:657:HIS:CD2	2.05	0.74
5:B:900:ALA:CB	13:L:61:THR:HG23	2.18	0.74
4:A:84:ILE:CD1	4:A:270:LEU:HD12	2.18	0.74
6:C:167:HIS:CE1	13:L:70:ARG:HA	2.23	0.73
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.69	0.73
11:J:48:ARG:CG	11:J:48:ARG:HH11	2.01	0.73
4:A:341:MET:HE3	4:A:1428:VAL:HG11	1.68	0.73
5:B:515:HIS:HD2	5:B:517:THR:H	1.36	0.73
4:A:106:VAL:HG12	4:A:107:CYS:N	2.03	0.73
4:A:116:ASP:HB3	4:A:117:GLU:HB2	1.69	0.73
7:E:55:ARG:HD2	7:E:83:CYS:O	1.88	0.73
6:C:14:SER:O	6:C:240:VAL:HG21	1.88	0.73
4:A:1199:ARG:O	4:A:1203:ASN:ND2	2.20	0.72
11:J:57:ILE:HA	11:J:60:PHE:HD2	1.54	0.72
4:A:482:PHE:C	4:A:484:GLY:H	1.91	0.72
5:B:886:LYS:HB3	5:B:887:HIS:HA	1.68	0.72
5:B:911:ILE:HD11	5:B:941:LEU:HD12	1.70	0.72
4:A:598:LEU:HD11	9:H:39:THR:HG21	1.71	0.72
4:A:18:GLN:HG2	4:A:1418:LEU:HD12	1.69	0.72
5:B:25:ILE:CD1	5:B:653:VAL:HB	2.20	0.72
1:R:9:G:H2'	1:R:10:C:C6	2.25	0.72
4:A:326:ARG:HG2	4:A:1406:VAL:HG21	1.72	0.72
4:A:886:ILE:HD11	4:A:943:LEU:CB	2.19	0.72
5:B:291:ILE:N	5:B:291:ILE:HD12	2.04	0.72
5:B:880:THR:O	5:B:882:THR:N	2.23	0.72
4:A:645:LEU:HD11	4:A:649:ILE:HD11	1.70	0.72
4:A:1015:VAL:HG12	4:A:1019:CYS:HG	1.52	0.71
4:A:343:LYS:NZ	5:B:1197:PRO:CB	2.43	0.71
4:A:377:PRO:HB2	4:A:431:LYS:HE3	1.70	0.71
5:B:446:LEU:HG	5:B:447:ALA:N	2.03	0.71
4:A:399:HIS:HD2	4:A:400:PRO:HG3	1.53	0.71
4:A:839:ARG:HG2	4:A:839:ARG:HH11	1.54	0.71
4:A:341:MET:SD	4:A:1428:VAL:CB	2.77	0.71
5:B:555:ILE:HA	5:B:558:LEU:HD12	1.71	0.71
5:B:822:ASN:ND2	11:J:52:THR:HG23	2.05	0.71
4:A:1116:LEU:HD13	4:A:1329:THR:HB	1.71	0.71
4:A:269:ILE:CG2	4:A:299:HIS:HB2	2.20	0.71
4:A:779:PHE:CZ	5:B:517:THR:HA	2.26	0.71
5:B:990:ILE:HG22	5:B:991:GLY:H	1.56	0.71
4:A:482:PHE:O	5:B:989:THR:OG1	2.07	0.71
5:B:807:ARG:HG3	5:B:807:ARG:NH1	1.92	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:976:ILE:HD11	5:B:992:ILE:CA	2.17	0.71
4:A:1206:ASP:HB2	4:A:1274:ARG:HH22	1.55	0.71
4:A:84:ILE:HD11	4:A:270:LEU:HD12	1.70	0.71
8:F:155:LEU:HG	8:F:155:LEU:OXT	1.90	0.71
4:A:110:CYS:HB3	4:A:167:CYS:SG	2.30	0.71
4:A:182:VAL:HG12	4:A:183:GLY:H	1.55	0.71
5:B:1122:ARG:HH11	5:B:1122:ARG:HG3	1.50	0.71
4:A:218:ASP:N	4:A:219:PHE:HB3	2.05	0.71
5:B:1084:GLN:NE2	6:C:191:TYR:HA	2.06	0.71
4:A:308:ILE:HG22	4:A:309:ALA:H	1.56	0.70
5:B:1084:GLN:HE22	6:C:191:TYR:HA	1.54	0.70
4:A:353:ILE:HD13	4:A:487:MET:CE	2.20	0.70
4:A:993:LEU:HD23	4:A:1022:LEU:HD21	1.73	0.70
4:A:351:THR:HG23	5:B:1103:ILE:CD1	2.21	0.70
7:E:168:TYR:O	7:E:169:ARG:HG2	1.91	0.70
4:A:855:THR:CG2	4:A:857:ARG:HE	2.05	0.70
5:B:839:MET:HE1	5:B:841:MET:CE	2.21	0.70
4:A:343:LYS:NZ	5:B:1156:ASP:CG	2.45	0.70
4:A:351:THR:CG2	4:A:352:VAL:N	2.54	0.70
4:A:364:VAL:HG12	4:A:460:VAL:HA	1.72	0.70
4:A:709:THR:HB	4:A:712:GLU:H	1.57	0.70
6:C:186:LEU:HB2	6:C:188:HIS:HD2	1.56	0.70
10:I:10:CYS:SG	10:I:31:THR:HB	2.32	0.70
4:A:260:ASP:OD1	4:A:261:ASP:N	2.23	0.70
6:C:56:THR:HG22	6:C:57:VAL:N	2.07	0.70
7:E:130:ALA:HA	7:E:131:THR:CB	2.21	0.70
8:F:79:ARG:NH1	8:F:145:ASP:O	2.24	0.70
4:A:265:LYS:HE2	4:A:302:THR:HG23	1.74	0.70
4:A:596:THR:C	4:A:598:LEU:H	1.95	0.70
5:B:484:ASN:O	5:B:484:ASN:ND2	2.25	0.70
4:A:567:LYS:CB	9:H:96:VAL:H	1.98	0.70
4:A:117:GLU:H	4:A:118:HIS:CA	2.05	0.70
5:B:287:ARG:NH1	5:B:325:GLN:HA	2.06	0.70
5:B:451:LYS:HA	5:B:454:THR:HB	1.74	0.70
4:A:444:PHE:CE2	4:A:470:LEU:HD23	2.26	0.70
4:A:456:MET:HB2	4:A:478:TYR:OH	1.91	0.70
5:B:100:PRO:O	5:B:101:MET:HG3	1.91	0.70
4:A:344:ARG:NH2	5:B:1112:GLN:CD	2.44	0.70
4:A:1394:THR:HG22	4:A:1395:GLY:H	1.55	0.69
4:A:853:ASP:OD1	4:A:855:THR:CG2	2.39	0.69
4:A:882:SER:HB2	4:A:953:ASN:OD1	1.92	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1084:GLN:HE22	6:C:192:TRP:H	1.38	0.69
4:A:344:ARG:NH2	5:B:1112:GLN:NE2	2.41	0.69
5:B:955:THR:HG22	5:B:956:THR:H	1.56	0.69
2:T:10:DA:H61	3:N:5:DT:H3	1.40	0.69
4:A:302:THR:HA	4:A:305:ASP:O	1.93	0.69
5:B:815:ARG:HG2	5:B:816:GLU:OE1	1.92	0.69
5:B:879:ARG:O	5:B:882:THR:HB	1.93	0.69
5:B:1058:LEU:O	5:B:1062:HIS:HB2	1.92	0.69
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.25	0.69
4:A:855:THR:HG21	4:A:857:ARG:HE	1.57	0.68
5:B:361:LEU:CD2	5:B:377:PHE:HD2	2.06	0.68
5:B:955:THR:HG22	5:B:956:THR:N	2.08	0.68
4:A:364:VAL:CG1	4:A:460:VAL:HA	2.23	0.68
6:C:56:THR:HG22	6:C:57:VAL:H	1.56	0.68
5:B:313:MET:HE3	5:B:386:LEU:HD22	1.75	0.68
5:B:346:GLU:HG2	5:B:349:ILE:CD1	2.23	0.68
4:A:672:ASP:HB2	4:A:675:THR:OG1	1.93	0.68
4:A:535:THR:HG21	4:A:617:VAL:N	2.08	0.68
5:B:846:ILE:HG23	5:B:974:PRO:HD2	1.76	0.68
5:B:841:MET:HG2	5:B:842:ASN:H	1.59	0.68
5:B:957:ASN:HB3	5:B:961:LEU:HB2	1.76	0.68
6:C:31:ASN:ND2	6:C:35:ARG:HD2	2.09	0.68
4:A:444:PHE:HE2	4:A:470:LEU:HD23	1.58	0.68
4:A:48:ALA:HA	4:A:49:LYS:HB2	1.76	0.68
5:B:757:PRO:HG3	5:B:983:ARG:CZ	2.24	0.68
6:C:56:THR:HG21	6:C:145:CYS:SG	2.34	0.67
11:J:36:LEU:HD22	11:J:41:LEU:HD13	1.75	0.67
1:R:10:C:OP1	5:B:987:LYS:HD2	1.93	0.67
4:A:332:LYS:H	4:A:337:ARG:HB3	1.59	0.67
4:A:830:LYS:NZ	4:A:830:LYS:HB2	2.09	0.67
4:A:678:GLU:HA	4:A:681:GLU:HG2	1.76	0.67
5:B:1017:ILE:HD12	5:B:1026:LEU:HD21	1.76	0.67
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.75	0.67
5:B:487:THR:O	5:B:490:SER:N	2.27	0.67
5:B:486:TYR:HE2	5:B:1096:ARG:HG2	1.58	0.67
5:B:763:GLN:HG2	5:B:764:SER:N	2.08	0.67
5:B:313:MET:CE	5:B:390:LEU:HG	2.25	0.67
5:B:35:SER:HB3	5:B:39:ARG:HH21	1.60	0.67
10:I:117:LYS:HB3	10:I:118:ARG:CA	2.11	0.67
4:A:444:PHE:CE2	4:A:470:LEU:CD2	2.78	0.67
5:B:1175:LEU:HD23	5:B:1176:ASN:H	1.58	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:866:TYR:CD1	5:B:867:GLY:HA2	2.30	0.67
4:A:1418:LEU:HD22	5:B:1222:ARG:HH21	1.59	0.67
4:A:496:GLU:HB2	8:F:95:GLY:HA3	1.76	0.67
4:A:956:LEU:HD23	4:A:957:PRO:HD3	1.77	0.66
5:B:459:TYR:C	5:B:459:TYR:CD2	2.66	0.66
4:A:715:GLU:O	4:A:719:VAL:HG23	1.95	0.66
4:A:660:ASN:OD1	5:B:1082:MET:HB3	1.96	0.66
13:L:32:ALA:HB3	13:L:55:ILE:HB	1.77	0.66
4:A:423:ASP:OD2	4:A:424:ILE:N	2.29	0.66
4:A:336:ILE:CD1	4:A:1405:THR:CB	2.72	0.66
4:A:806:ARG:HH11	4:A:806:ARG:HG2	1.59	0.66
6:C:214:ASN:HD22	6:C:215:GLU:HB3	1.61	0.66
4:A:161:LEU:O	4:A:162:VAL:HG23	1.96	0.66
4:A:405:VAL:HG22	4:A:432:VAL:HG22	1.78	0.66
5:B:604:ARG:HD3	5:B:611:PRO:HA	1.76	0.66
5:B:744:HIS:CD2	5:B:746:SER:OG	2.48	0.66
4:A:1446:ASP:HB3	4:A:1448:GLU:N	2.09	0.66
5:B:1006:ILE:HG22	5:B:1007:VAL:N	2.10	0.66
4:A:526:ASP:OD2	5:B:829:CYS:HB3	1.95	0.66
6:C:18:VAL:O	6:C:231:ASN:HA	1.95	0.66
12:K:65:HIS:CD2	12:K:66:PRO:CD	2.78	0.66
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.60	0.66
5:B:619:ILE:HG13	10:I:65:ASP:HB2	1.77	0.66
9:H:38:LEU:HD13	9:H:125:LEU:HD13	1.77	0.66
4:A:148:CYS:O	4:A:149:GLU:HB2	1.94	0.66
5:B:190:TYR:CE1	11:J:62:ARG:HG2	2.31	0.66
5:B:841:MET:CE	5:B:990:ILE:CD1	2.73	0.65
4:A:340:LEU:HD21	5:B:1200:ALA:N	2.11	0.65
5:B:465:ASN:HA	5:B:476:ARG:HA	1.78	0.65
7:E:62:ALA:HB3	7:E:78:LEU:HB3	1.79	0.65
4:A:756:ILE:O	4:A:760:GLN:HG2	1.95	0.65
5:B:637:LEU:CD1	5:B:740:HIS:HB3	2.27	0.65
5:B:847:ASP:HB3	6:C:167:HIS:NE2	2.10	0.65
6:C:33:LEU:CD2	6:C:37:MET:CE	2.74	0.65
4:A:741:ASN:HD21	4:A:743:VAL:HG23	1.62	0.65
5:B:1175:LEU:HD23	5:B:1176:ASN:N	2.12	0.65
5:B:25:ILE:HD12	5:B:653:VAL:HB	1.77	0.65
6:C:123:ASN:HD22	6:C:125:MET:HG3	1.59	0.65
4:A:1111:MET:HG2	4:A:1114:PRO:HG3	1.78	0.65
4:A:340:LEU:HD23	5:B:1199:ALA:HB3	1.77	0.65
5:B:1106:ARG:NH2	5:B:1111:MET:HE3	2.12	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:175:LEU:O	7:E:177:ARG:HD2	1.97	0.65
5:B:839:MET:HE1	5:B:841:MET:HE3	1.78	0.65
5:B:850:LEU:CD2	5:B:1009:ASP:HB3	2.27	0.65
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.31	0.65
10:I:117:LYS:HD3	10:I:118:ARG:HH21	1.62	0.65
5:B:780:VAL:HB	5:B:817:LEU:HD22	1.77	0.65
5:B:870:ILE:O	5:B:870:ILE:HG22	1.96	0.65
5:B:1024:ALA:HA	5:B:1027:ILE:HD12	1.78	0.64
8:F:97:ARG:HG3	8:F:101:ILE:HD11	1.78	0.64
9:H:77:ARG:HB2	9:H:77:ARG:NH1	2.13	0.64
4:A:290:GLU:C	4:A:292:ALA:H	2.01	0.64
5:B:805:THR:N	5:B:1042:GLY:O	2.28	0.64
4:A:360:GLU:HB2	4:A:363:GLN:OE1	1.98	0.64
4:A:663:SER:OG	5:B:1085:ILE:HG23	1.98	0.64
5:B:879:ARG:HH12	5:B:882:THR:CG2	2.09	0.64
5:B:978:ASP:O	5:B:980:PHE:CD1	2.50	0.64
7:E:147:HIS:HB3	7:E:150:VAL:HG23	1.79	0.64
11:J:9:SER:OG	11:J:45:CYS:HB2	1.98	0.64
4:A:1364:ASN:HD21	4:A:1366:ARG:HG2	1.52	0.64
4:A:828:ALA:HB2	5:B:530:GLY:HA2	1.79	0.64
5:B:235:SER:OG	5:B:236:HIS:ND1	2.30	0.64
4:A:806:ARG:HG2	4:A:806:ARG:NH1	2.09	0.64
5:B:899:ILE:HG21	5:B:949:VAL:HG21	1.79	0.64
4:A:503:GLN:HE21	8:F:90:ARG:HH12	1.46	0.64
6:C:235:VAL:HG11	11:J:6:ARG:HH21	1.61	0.64
4:A:399:HIS:CD2	4:A:400:PRO:HG3	2.33	0.64
12:K:65:HIS:HD2	12:K:67:PHE:H	1.46	0.64
4:A:1101:LEU:HD13	4:A:1355:VAL:HG11	1.78	0.64
6:C:252:GLN:HG3	12:K:95:ILE:HG23	1.80	0.64
13:L:40:LEU:HD11	13:L:49:LYS:HE2	1.80	0.64
4:A:1446:ASP:HB3	4:A:1448:GLU:H	1.61	0.64
5:B:1033:LYS:O	5:B:1037:LEU:HG	1.97	0.64
4:A:265:LYS:HG2	4:A:303:TYR:HB2	1.79	0.64
4:A:913:LEU:HD12	4:A:914:GLU:N	2.12	0.64
5:B:999:MET:HG2	5:B:1008:PRO:CD	2.27	0.64
5:B:1107:ALA:O	5:B:1108:ARG:HG2	1.98	0.63
6:C:63:ILE:HA	6:C:66:ARG:HG3	1.80	0.63
5:B:448:ILE:CG2	5:B:449:ASN:N	2.60	0.63
6:C:71:PRO:O	6:C:133:ILE:HG12	1.98	0.63
6:C:78:GLU:HA	6:C:78:GLU:OE1	1.96	0.63
4:A:351:THR:CG2	4:A:352:VAL:H	2.08	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:465:TYR:CE1	12:K:67:PHE:CE2	2.86	0.63
6:C:67:LEU:HA	6:C:70:ILE:CD1	2.27	0.63
5:B:346:GLU:O	5:B:348:ARG:N	2.32	0.63
4:A:1151:GLU:HG2	10:I:45:ARG:HG3	1.80	0.63
4:A:508:PRO:O	4:A:510:GLN:N	2.28	0.63
5:B:839:MET:HE2	5:B:990:ILE:HG12	1.70	0.63
5:B:839:MET:SD	5:B:989:THR:O	2.56	0.63
5:B:886:LYS:HB3	5:B:887:HIS:CA	2.29	0.63
5:B:841:MET:HE3	5:B:990:ILE:CD1	2.29	0.63
4:A:53:LEU:HD12	4:A:54:ASN:H	1.62	0.63
4:A:760:GLN:HA	4:A:760:GLN:NE2	2.07	0.62
4:A:341:MET:SD	4:A:1428:VAL:HB	2.38	0.62
4:A:391:LEU:HD12	4:A:400:PRO:O	2.00	0.62
5:B:802:PRO:HA	5:B:822:ASN:HD21	1.65	0.62
7:E:16:PHE:CE2	7:E:20:LYS:HE2	2.33	0.62
7:E:9:ILE:HG12	7:E:53:PRO:HG3	1.80	0.62
4:A:1144:LYS:HB2	4:A:1268:LEU:O	1.99	0.62
4:A:364:VAL:CG1	4:A:364:VAL:O	2.47	0.62
6:C:33:LEU:CD2	6:C:37:MET:HE3	2.28	0.62
4:A:55:ASP:O	4:A:57:ARG:N	2.32	0.62
4:A:705:LYS:NZ	4:A:716:ASP:OD1	2.26	0.62
5:B:140:ILE:H	5:B:141:ASP:C	2.02	0.62
6:C:41:ILE:HG22	6:C:250:THR:OG1	1.99	0.62
6:C:211:ASP:HB3	6:C:212:PRO:HD2	1.81	0.62
7:E:55:ARG:O	7:E:57:MET:N	2.33	0.62
4:A:756:ILE:O	4:A:759:ALA:HB3	1.99	0.62
5:B:997:GLU:HG2	6:C:39:ALA:HB2	1.80	0.62
4:A:726:ARG:HD3	4:A:766:GLY:HA3	1.81	0.62
5:B:346:GLU:HG2	5:B:349:ILE:HD13	1.81	0.62
6:C:57:VAL:O	6:C:57:VAL:HG12	1.99	0.62
4:A:1161:THR:HG22	4:A:1163:ILE:H	1.64	0.62
4:A:1345:ARG:HD2	4:A:1373:ASP:OD1	1.99	0.62
4:A:1364:ASN:HD21	4:A:1366:ARG:HH11	1.45	0.62
5:B:448:ILE:HG23	5:B:449:ASN:N	2.14	0.62
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.35	0.62
10:I:63:GLY:HA3	10:I:104:LEU:HD11	1.82	0.62
4:A:353:ILE:HD11	4:A:480:ALA:HB1	1.81	0.62
5:B:1221:SER:C	5:B:1223:ASP:H	2.03	0.62
5:B:634:TYR:CE1	5:B:692:TYR:CD1	2.87	0.62
5:B:952:VAL:HG13	5:B:966:VAL:HG22	1.80	0.62
12:K:32:VAL:HG23	12:K:74:ARG:HG3	1.81	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:567:LYS:HB3	9:H:96:VAL:N	1.99	0.62
4:A:549:MET:SD	4:A:577:ILE:HD13	2.39	0.62
4:A:64:ASN:CB	4:A:66:LYS:HG2	2.30	0.62
5:B:803:LEU:O	5:B:1042:GLY:HA3	1.99	0.62
5:B:276:ILE:CD1	5:B:277:LYS:H	2.12	0.62
12:K:61:TYR:HA	12:K:72:LYS:O	2.00	0.62
4:A:1064:VAL:HG12	4:A:1064:VAL:O	1.99	0.61
4:A:1110:ASN:H	4:A:1110:ASN:HD22	1.48	0.61
4:A:635:ARG:HH11	4:A:635:ARG:HA	1.65	0.61
5:B:906:SER:HA	5:B:946:ASN:HB3	1.81	0.61
9:H:42:ILE:HG21	9:H:49:VAL:HG21	1.82	0.61
4:A:444:PHE:HE2	4:A:470:LEU:HD22	1.63	0.61
5:B:277:LYS:HE2	5:B:335:GLY:H	1.65	0.61
5:B:229:ALA:O	5:B:261:ARG:NH2	2.33	0.61
4:A:870:GLU:HG2	7:E:208:TYR:CG	2.36	0.61
7:E:64:PRO:HD3	7:E:76:GLY:HA2	1.80	0.61
4:A:830:LYS:HE2	4:A:1079:MET:O	1.99	0.61
4:A:341:MET:O	5:B:1132:GLU:HB3	2.00	0.61
5:B:990:ILE:HG22	5:B:991:GLY:N	2.14	0.61
2:T:21:DC:OP1	5:B:1129:ARG:HB3	2.01	0.61
4:A:313:GLN:HG3	4:A:314:ALA:H	1.64	0.61
6:C:11:ARG:HD3	6:C:21:ILE:HD11	1.81	0.61
13:L:48:CYS:SG	13:L:49:LYS:N	2.74	0.61
4:A:512:VAL:HA	4:A:519:PRO:HA	1.82	0.61
4:A:579:SER:HB3	4:A:611:GLN:HA	1.83	0.61
5:B:474:SER:HA	5:B:476:ARG:HG2	1.82	0.61
4:A:1384:VAL:HG23	4:A:1384:VAL:O	1.99	0.61
4:A:896:ARG:HD2	4:A:897:TYR:CE1	2.36	0.61
5:B:37:PHE:O	5:B:38:PHE:HB2	2.01	0.61
6:C:73:GLN:HE21	6:C:74:SER:H	1.49	0.61
5:B:185:THR:O	5:B:188:ASP:HB2	2.01	0.61
5:B:487:THR:O	5:B:490:SER:HB3	2.00	0.61
9:H:82:PRO:HB2	9:H:83:GLN:CA	2.15	0.61
5:B:711:GLU:H	5:B:712:PRO:HD3	1.65	0.60
5:B:826:ALA:HB3	5:B:1011:ILE:HA	1.83	0.60
5:B:863:GLU:CB	5:B:864:LYS:HA	2.30	0.60
4:A:276:LEU:HD11	4:A:292:ALA:CB	2.29	0.60
11:J:1:MET:N	11:J:56:LEU:H	2.00	0.60
12:K:37:LYS:O	12:K:38:GLU:HG2	2.01	0.60
5:B:869:SER:O	5:B:870:ILE:HG12	2.01	0.60
5:B:978:ASP:O	5:B:980:PHE:HD1	1.85	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:464:PRO:O	4:A:465:TYR:HB2	2.01	0.60
5:B:976:ILE:CG2	5:B:976:ILE:O	2.44	0.60
6:C:79:GLN:HG3	6:C:127:ARG:HD2	1.83	0.60
4:A:946:VAL:HG22	7:E:201:LYS:HB3	1.84	0.60
5:B:345:LYS:N	5:B:348:ARG:NE	2.50	0.60
5:B:973:ILE:H	5:B:973:ILE:HD12	1.67	0.60
10:I:77:LYS:HG2	10:I:108:HIS:ND1	2.17	0.60
5:B:1039:GLY:HA2	11:J:51:LEU:CD2	2.31	0.60
5:B:1037:LEU:HD12	5:B:1062:HIS:CD2	2.37	0.60
4:A:809:THR:CG2	4:A:810:PRO:HD2	2.30	0.60
5:B:1072:MET:HE2	5:B:1085:ILE:HB	1.83	0.60
5:B:515:HIS:CD2	5:B:517:THR:H	2.18	0.60
5:B:898:LEU:HB2	13:L:58:LYS:HE3	1.83	0.60
2:T:16:DT:H3'	2:T:17:DA:H8	1.67	0.60
4:A:116:ASP:CB	4:A:117:GLU:HB2	2.32	0.60
4:A:278:THR:O	4:A:282:ASN:HB3	2.02	0.60
5:B:1156:ASP:HB3	5:B:1198:TYR:H	1.66	0.60
4:A:808:LEU:HD13	5:B:760:ASP:O	2.02	0.60
10:I:106:CYS:SG	10:I:108:HIS:HB2	2.42	0.60
4:A:1319:VAL:HG13	4:A:1320:PRO:HD2	1.84	0.59
9:H:47:PHE:HB2	9:H:95:TYR:HD1	1.66	0.59
4:A:1140:HIS:HB2	4:A:1276:VAL:O	2.02	0.59
4:A:134:ARG:CD	4:A:221:SER:O	2.50	0.59
5:B:906:SER:HA	5:B:946:ASN:CB	2.32	0.59
5:B:872:GLU:HG2	5:B:916:THR:HB	1.84	0.59
6:C:41:ILE:HD11	6:C:243:VAL:HG13	1.84	0.59
4:A:1134:ILE:O	4:A:1138:ILE:HG13	2.02	0.59
4:A:1219:THR:HG21	4:A:1271:ILE:HD12	1.85	0.59
4:A:660:ASN:OD1	5:B:1082:MET:CB	2.50	0.59
7:E:147:HIS:HB3	7:E:150:VAL:CG2	2.32	0.59
7:E:36:GLU:O	7:E:38:PRO:HD3	2.02	0.59
12:K:91:CYS:O	12:K:95:ILE:HG13	2.03	0.59
4:A:244:PRO:O	4:A:246:VAL:N	2.36	0.59
4:A:90:VAL:HB	4:A:297:GLN:HE22	1.68	0.59
4:A:350:ARG:HG3	4:A:488:ASN:OD1	2.02	0.59
4:A:134:ARG:HD2	4:A:221:SER:O	2.03	0.59
4:A:1383:SER:O	4:A:1388:GLY:HA3	2.02	0.59
5:B:827:ILE:HG23	5:B:1012:ILE:HD12	1.84	0.59
5:B:863:GLU:O	5:B:872:GLU:HB2	2.02	0.59
5:B:889:THR:HG22	5:B:891:ASP:OD2	2.03	0.59
4:A:112:LYS:HG2	4:A:113:LEU:N	2.16	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:318:SER:O	4:A:320:ARG:NH2	2.36	0.59
4:A:63:ARG:HA	4:A:74:MET:HG3	1.84	0.59
10:I:98:VAL:HG11	10:I:113:ASP:HB2	1.85	0.59
5:B:664:THR:HG23	5:B:678:GLU:HB3	1.85	0.59
4:A:782:ARG:NH2	5:B:699:GLU:O	2.35	0.59
5:B:899:ILE:HG13	5:B:911:ILE:HG23	1.84	0.59
6:C:63:ILE:O	6:C:66:ARG:HB2	2.03	0.59
4:A:470:LEU:HD21	4:A:487:MET:HE3	1.84	0.59
4:A:549:MET:SD	4:A:577:ILE:CD1	2.91	0.59
4:A:830:LYS:HZ1	4:A:1082:ASN:HB3	1.67	0.59
4:A:875:ALA:HB2	4:A:1366:ARG:CD	2.26	0.59
5:B:778:MET:HE3	5:B:1094:ARG:HH11	1.67	0.59
5:B:209:GLU:OE2	5:B:485:ARG:HD3	2.03	0.59
5:B:744:HIS:HD2	5:B:746:SER:H	1.48	0.59
6:C:167:HIS:HE1	13:L:70:ARG:HA	1.68	0.59
6:C:36:VAL:HG13	6:C:40:GLU:HB2	1.85	0.59
4:A:106:VAL:HG12	4:A:107:CYS:H	1.67	0.58
5:B:899:ILE:HD11	5:B:911:ILE:HG12	1.85	0.58
6:C:244:VAL:HG21	12:K:105:PHE:CZ	2.37	0.58
7:E:130:ALA:HB1	7:E:131:THR:HB	1.85	0.58
4:A:1364:ASN:ND2	4:A:1366:ARG:H	2.01	0.58
4:A:583:PRO:O	4:A:610:GLY:HA3	2.03	0.58
4:A:979:SER:OG	4:A:981:LEU:HD12	2.02	0.58
5:B:276:ILE:HG23	5:B:277:LYS:N	2.18	0.58
5:B:363:HIS:O	5:B:364:ILE:HB	2.02	0.58
5:B:43:LEU:HD13	5:B:492:LEU:HD21	1.84	0.58
5:B:67:SER:HB2	5:B:92:PHE:HD1	1.68	0.58
4:A:567:LYS:HB2	9:H:95:TYR:HA	1.83	0.58
5:B:841:MET:HE1	5:B:990:ILE:CD1	2.34	0.58
5:B:863:GLU:HB2	5:B:864:LYS:HA	1.83	0.58
5:B:892:LYS:NZ	5:B:904:ARG:O	2.36	0.58
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.84	0.58
4:A:1037:LEU:HD12	4:A:1042:PHE:HA	1.85	0.58
4:A:336:ILE:HD13	4:A:1405:THR:HG21	0.58	0.58
4:A:382:PRO:HD3	4:A:428:TYR:CD2	2.37	0.58
4:A:839:ARG:HG2	4:A:839:ARG:NH1	2.16	0.58
5:B:244:LEU:HD11	5:B:366:GLN:HE22	1.68	0.58
6:C:46:ILE:HG12	6:C:157:CYS:HB3	1.85	0.58
1:R:9:G:H2'	1:R:10:C:H6	1.66	0.58
6:C:73:GLN:HA	6:C:133:ILE:HD11	1.86	0.58
4:A:744:LYS:O	4:A:748:MET:HG3	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.04	0.58
5:B:345:LYS:N	5:B:348:ARG:HE	2.00	0.58
4:A:296:LEU:O	4:A:296:LEU:HD23	2.03	0.58
4:A:323:LYS:HZ3	4:A:324:SER:N	1.98	0.58
4:A:370:ILE:HG12	5:B:1105:ALA:HB2	1.86	0.58
5:B:100:PRO:C	5:B:101:MET:HG3	2.24	0.58
5:B:446:LEU:CG	5:B:447:ALA:H	2.02	0.58
5:B:530:GLY:O	5:B:531:GLN:C	2.42	0.58
5:B:847:ASP:HB3	6:C:167:HIS:CD2	2.39	0.58
4:A:106:VAL:CG1	4:A:107:CYS:N	2.67	0.58
4:A:1206:ASP:O	4:A:1274:ARG:NH2	2.37	0.58
5:B:1002:THR:CG2	5:B:1006:ILE:HB	2.34	0.58
5:B:948:ILE:HD12	5:B:969:ARG:NH1	2.19	0.58
6:C:27:LEU:HA	6:C:228:PHE:CZ	2.38	0.58
5:B:850:LEU:HD12	11:J:8:PHE:CD1	2.39	0.58
4:A:645:LEU:O	4:A:649:ILE:HG13	2.04	0.58
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.22	0.58
4:A:179:LEU:HD13	4:A:297:GLN:HG3	1.84	0.58
4:A:352:VAL:HB	5:B:1099:VAL:HG12	1.85	0.58
4:A:92:HIS:O	4:A:92:HIS:CD2	2.57	0.58
6:C:31:ASN:HD22	6:C:35:ARG:HD2	1.69	0.58
4:A:336:ILE:HD11	4:A:1405:THR:CB	2.32	0.57
4:A:211:PHE:HD1	4:A:231:PRO:HB2	1.69	0.57
4:A:979:SER:OG	4:A:981:LEU:CD1	2.52	0.57
4:A:64:ASN:HB3	4:A:66:LYS:HG2	1.84	0.57
5:B:464:GLY:CA	5:B:478:GLY:HA2	2.34	0.57
5:B:25:ILE:HD11	5:B:653:VAL:HB	1.86	0.57
5:B:913:GLY:HA2	5:B:938:SER:HG	1.69	0.57
7:E:64:PRO:HG3	7:E:76:GLY:HA2	1.86	0.57
5:B:1039:GLY:HA2	11:J:51:LEU:HD21	1.86	0.57
4:A:377:PRO:CB	4:A:431:LYS:HE3	2.34	0.57
4:A:399:HIS:HB3	4:A:400:PRO:HD3	1.87	0.57
4:A:672:ASP:HB3	4:A:674:PRO:HG2	1.86	0.57
4:A:775:ILE:HG12	4:A:797:LYS:O	2.04	0.57
5:B:35:SER:HB3	5:B:39:ARG:NH2	2.18	0.57
5:B:680:THR:O	5:B:683:SER:N	2.34	0.57
5:B:634:TYR:HE1	5:B:692:TYR:CD1	2.22	0.57
12:K:49:GLU:HG3	12:K:94:ILE:HG13	1.86	0.57
4:A:401:GLY:C	4:A:435:HIS:HD1	2.08	0.57
4:A:37:PHE:HB2	4:A:52:GLY:CA	2.32	0.57
5:B:459:TYR:O	5:B:459:TYR:CD2	2.57	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:244:VAL:HG21	12:K:105:PHE:CE1	2.39	0.57
4:A:1213:GLY:HA3	4:A:1228:TRP:CZ3	2.39	0.57
5:B:827:ILE:HD11	5:B:1086:PHE:CD2	2.40	0.57
5:B:658:ILE:O	5:B:661:LEU:HB2	2.05	0.57
4:A:1100:ARG:HH21	4:A:1351:GLU:HG2	1.68	0.57
4:A:1345:ARG:HG3	4:A:1376:THR:HG21	1.86	0.57
4:A:367:PRO:HG2	4:A:370:ILE:HD12	1.86	0.57
4:A:455:MET:O	4:A:456:MET:HG3	2.05	0.57
4:A:449:SER:OG	5:B:1134:GLU:OE2	2.15	0.57
5:B:378:LEU:O	5:B:382:ILE:HG12	2.04	0.57
5:B:65:GLU:CD	5:B:66:ASP:HB3	2.24	0.57
6:C:214:ASN:HA	6:C:215:GLU:HB3	1.86	0.57
4:A:547:LEU:HD22	12:K:58:PHE:HD1	1.70	0.57
4:A:1110:ASN:HD22	4:A:1110:ASN:N	2.03	0.57
4:A:532:ARG:HG3	4:A:618:GLU:HB3	1.85	0.57
4:A:92:HIS:O	4:A:94:GLY:N	2.38	0.57
10:I:47:GLU:OE1	10:I:50:THR:HG23	2.04	0.57
11:J:18:TRP:CZ2	11:J:22:LEU:HD11	2.40	0.57
4:A:577:ILE:O	4:A:580:VAL:HG23	2.05	0.57
5:B:1065:GLN:HG2	5:B:1069:PHE:HB2	1.86	0.57
5:B:211:VAL:CG2	5:B:483:LEU:HD13	2.35	0.57
6:C:163:ILE:O	6:C:166:GLU:HB2	2.05	0.57
11:J:44:TYR:C	11:J:44:TYR:CD1	2.77	0.57
4:A:1312:ASN:O	4:A:1316:VAL:HG23	2.05	0.57
4:A:868:TYR:CE1	4:A:1064:VAL:CG1	2.69	0.57
4:A:1005:GLU:OE1	4:A:1005:GLU:N	2.37	0.56
4:A:447:GLN:HE22	4:A:488:ASN:ND2	2.03	0.56
4:A:48:ALA:CB	4:A:49:LYS:HZ3	2.18	0.56
5:B:1037:LEU:HD12	5:B:1062:HIS:HD2	1.69	0.56
5:B:406:LEU:HD12	5:B:633:VAL:CG2	2.35	0.56
5:B:765:PRO:O	5:B:766:ARG:C	2.43	0.56
4:A:116:ASP:CA	4:A:117:GLU:HB2	2.34	0.56
4:A:1198:ASP:O	4:A:1202:MET:HG2	2.04	0.56
1:R:10:C:O2'	4:A:446:ARG:NH2	2.37	0.56
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.86	0.56
6:C:46:ILE:O	6:C:169:LYS:NZ	2.38	0.56
9:H:123:MET:HE2	9:H:142:LEU:HD13	1.86	0.56
4:A:1080:THR:O	4:A:1081:LEU:C	2.43	0.56
4:A:731:ARG:HG3	4:A:755:PHE:CZ	2.41	0.56
11:J:6:ARG:HG2	11:J:11:GLY:O	2.04	0.56
9:H:41:ASP:HB3	9:H:121:LEU:HD13	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:52:GLU:HA	13:L:64:LEU:HD22	1.86	0.56
4:A:605:MET:HE3	4:A:614:PHE:O	2.06	0.56
4:A:662:PHE:HB3	5:B:829:CYS:SG	2.45	0.56
6:C:10:ILE:HG21	12:K:112:GLN:HG3	1.88	0.56
5:B:33:VAL:HG21	5:B:638:PHE:HZ	1.70	0.56
5:B:944:THR:HB	5:B:1122:ARG:NH2	2.20	0.56
6:C:54:ASN:O	6:C:56:THR:N	2.38	0.56
4:A:244:PRO:HB2	4:A:245:PRO:HD3	1.87	0.56
4:A:537:ARG:HD3	9:H:120:GLY:O	2.06	0.56
4:A:534:LEU:O	4:A:574:GLY:HA3	2.06	0.56
5:B:361:LEU:O	5:B:363:HIS:O	2.24	0.56
12:K:65:HIS:HD2	12:K:66:PRO:HD2	1.68	0.56
4:A:1155:ASP:OD1	4:A:1162:VAL:HG23	2.06	0.56
4:A:1295:THR:OG1	4:A:1297:GLU:OE1	2.24	0.56
4:A:55:ASP:H	4:A:56:PRO:CD	2.05	0.56
4:A:642:CYS:O	4:A:645:LEU:HB3	2.06	0.56
4:A:336:ILE:HD11	4:A:1405:THR:OG1	2.06	0.56
4:A:340:LEU:HD23	5:B:1199:ALA:CB	2.36	0.56
4:A:353:ILE:CD1	4:A:480:ALA:HB1	2.36	0.56
5:B:744:HIS:HD2	5:B:746:SER:OG	1.89	0.56
5:B:821:GLN:NE2	11:J:8:PHE:HE1	2.04	0.56
4:A:848:ILE:HD13	4:A:858:ASN:HB3	1.87	0.56
4:A:896:ARG:HH11	4:A:897:TYR:HE1	1.54	0.56
5:B:291:ILE:N	5:B:291:ILE:CD1	2.68	0.56
7:E:55:ARG:C	7:E:57:MET:H	2.10	0.56
4:A:739:ASP:OD2	9:H:19:ARG:HD3	2.06	0.56
5:B:1006:ILE:CG2	5:B:1007:VAL:N	2.69	0.56
5:B:1120:GLU:HG2	5:B:1121:GLY:N	2.21	0.56
5:B:448:ILE:CG2	5:B:449:ASN:H	2.17	0.56
5:B:710:LEU:O	5:B:711:GLU:CB	2.54	0.56
6:C:54:ASN:C	6:C:56:THR:H	2.09	0.56
4:A:447:GLN:CB	4:A:448:PRO:HA	2.21	0.55
5:B:60:GLN:HA	5:B:60:GLN:HE21	1.69	0.55
6:C:69:LEU:HD23	11:J:6:ARG:HB2	1.88	0.55
6:C:166:GLU:HG2	12:K:10:PHE:HZ	1.70	0.55
5:B:1016:ALA:O	5:B:1017:ILE:HG12	2.06	0.55
5:B:315:LYS:N	5:B:316:PRO:HD2	2.21	0.55
5:B:483:LEU:HD11	5:B:491:THR:HG23	1.87	0.55
6:C:67:LEU:HD13	6:C:157:CYS:SG	2.47	0.55
9:H:123:MET:CE	9:H:142:LEU:HD13	2.35	0.55
4:A:1392:SER:O	4:A:1399:ARG:HD3	2.07	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:679:ILE:O	4:A:682:THR:HB	2.07	0.55
5:B:364:ILE:HG22	5:B:365:THR:N	2.21	0.55
5:B:402:GLY:CA	5:B:695:ALA:HB3	2.36	0.55
5:B:705:MET:H	5:B:710:LEU:HD12	1.72	0.55
6:C:10:ILE:HD13	6:C:20:PHE:HB3	1.88	0.55
4:A:116:ASP:HA	4:A:117:GLU:CB	2.36	0.55
4:A:365:GLY:O	4:A:468:PHE:HA	2.06	0.55
4:A:91:PHE:HA	4:A:235:ILE:HG22	1.88	0.55
5:B:778:MET:HE3	5:B:1094:ARG:NH1	2.21	0.55
5:B:850:LEU:O	5:B:851:PHE:HB2	2.06	0.55
4:A:840:ARG:NH2	4:A:1106:ASN:OD1	2.39	0.55
4:A:567:LYS:CB	4:A:568:PRO:CD	2.84	0.55
5:B:1132:GLU:O	5:B:1135:ARG:HB3	2.05	0.55
5:B:597:MET:SD	5:B:624:LEU:HD11	2.47	0.55
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.88	0.55
4:A:1339:LEU:HD13	7:E:147:HIS:CD2	2.41	0.55
11:J:18:TRP:CE2	11:J:22:LEU:HD11	2.41	0.55
12:K:49:GLU:HG3	12:K:94:ILE:CG1	2.37	0.55
4:A:1116:LEU:H	4:A:1308:THR:HG22	1.71	0.55
4:A:475:THR:CG2	4:A:476:SER:N	2.70	0.55
5:B:581:PHE:HB2	5:B:625:LYS:HG3	1.89	0.55
2:T:24:DG:OP1	5:B:857:ARG:NH2	2.40	0.55
7:E:5:ASN:HD21	7:E:52:ARG:H	1.55	0.55
11:J:3:VAL:HG21	11:J:18:TRP:CD2	2.41	0.55
4:A:711:ARG:O	4:A:714:PHE:HB3	2.07	0.55
4:A:814:PHE:CE1	5:B:514:LEU:HD21	2.41	0.55
11:J:14:VAL:HG21	11:J:49:MET:HG3	1.89	0.55
11:J:44:TYR:CD1	11:J:45:CYS:N	2.75	0.55
4:A:225:ASN:HD22	4:A:227:VAL:H	1.55	0.55
9:H:10:PHE:HB3	9:H:28:ALA:HB1	1.88	0.55
11:J:24:LEU:CD2	11:J:30:LEU:HD12	2.37	0.55
4:A:447:GLN:HB3	4:A:448:PRO:CA	2.28	0.55
4:A:726:ARG:HG2	4:A:726:ARG:O	2.07	0.55
5:B:992:ILE:CD1	12:K:67:PHE:HE2	2.20	0.55
4:A:49:LYS:CD	4:A:55:ASP:OD2	2.48	0.54
4:A:609:ASP:O	4:A:611:GLN:N	2.40	0.54
5:B:1106:ARG:CD	5:B:1126:GLY:O	2.50	0.54
5:B:638:PHE:CE1	5:B:743:ILE:HD13	2.42	0.54
4:A:663:SER:HA	5:B:827:ILE:O	2.07	0.54
4:A:482:PHE:C	4:A:484:GLY:N	2.60	0.54
4:A:723:ASN:O	4:A:724:GLU:C	2.46	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:848:ILE:HA	4:A:857:ARG:O	2.07	0.54
5:B:256:VAL:HG11	5:B:382:ILE:HD13	1.88	0.54
6:C:215:GLU:N	6:C:216:GLY:HA3	2.13	0.54
6:C:33:LEU:CD2	6:C:37:MET:HE1	2.36	0.54
6:C:67:LEU:HA	6:C:70:ILE:HG13	1.89	0.54
2:T:18:DC:H2'	2:T:19:DG:C8	2.42	0.54
4:A:806:ARG:HH11	4:A:806:ARG:CG	2.19	0.54
7:E:177:ARG:HG2	7:E:215:MET:SD	2.47	0.54
4:A:106:VAL:CG1	4:A:107:CYS:H	2.21	0.54
6:C:102:GLN:HG2	6:C:154:LYS:HG3	1.89	0.54
7:E:128:PRO:HB2	7:E:129:PRO:HD3	1.89	0.54
7:E:124:VAL:HA	7:E:132:ILE:HD11	1.90	0.54
4:A:347:PHE:CE2	5:B:1107:ALA:HB1	2.43	0.54
4:A:385:ILE:HG13	4:A:385:ILE:O	2.07	0.54
6:C:6:PRO:HB2	12:K:101:LEU:HD23	1.89	0.54
4:A:200:ARG:HH21	4:A:202:LEU:HA	1.71	0.54
4:A:475:THR:HG22	4:A:476:SER:N	2.23	0.54
4:A:839:ARG:HG3	4:A:839:ARG:HH11	1.71	0.54
5:B:521:LEU:HB3	5:B:633:VAL:HG11	1.88	0.54
7:E:130:ALA:CA	7:E:131:THR:CB	2.85	0.54
4:A:545:GLN:O	4:A:549:MET:HG3	2.07	0.54
5:B:277:LYS:CE	5:B:335:GLY:H	2.20	0.54
5:B:657:HIS:ND1	5:B:689:LEU:HD11	2.22	0.54
5:B:884:ARG:NH1	5:B:935:ARG:HE	2.06	0.54
4:A:353:ILE:HG21	4:A:487:MET:HG3	1.89	0.54
4:A:731:ARG:HG3	4:A:755:PHE:CE1	2.43	0.54
4:A:92:HIS:C	4:A:92:HIS:CD2	2.81	0.54
4:A:497:THR:CG2	5:B:1146:PHE:HD1	2.21	0.54
6:C:167:HIS:HD2	6:C:169:LYS:H	1.56	0.54
9:H:2:SER:CA	9:H:3:ASN:HB2	2.38	0.54
9:H:24:CYS:O	9:H:41:ASP:HA	2.07	0.54
9:H:78:SER:OG	9:H:79:TRP:N	2.41	0.54
4:A:1435:PRO:O	4:A:1436:ILE:HD12	2.06	0.54
4:A:494:SER:O	4:A:498:ARG:HG2	2.07	0.54
4:A:352:VAL:HB	5:B:1099:VAL:CG1	2.38	0.54
6:C:244:VAL:CG2	6:C:245:VAL:N	2.70	0.54
4:A:380:VAL:O	4:A:428:TYR:HA	2.07	0.54
5:B:918:ILE:HG13	5:B:935:ARG:HH12	1.73	0.54
7:E:64:PRO:CD	7:E:76:GLY:HA2	2.38	0.54
10:I:116:ASN:HD22	10:I:117:LYS:HG3	1.72	0.54
2:T:28:DT:H4'	4:A:318:SER:HA	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:14:VAL:N	4:A:1432:GLN:HE22	1.98	0.53
4:A:353:ILE:HG21	4:A:487:MET:HE3	1.90	0.53
4:A:665:GLY:O	4:A:668:ASP:HB2	2.09	0.53
4:A:758:ILE:HD13	4:A:758:ILE:N	2.22	0.53
5:B:459:TYR:C	5:B:459:TYR:HD2	2.11	0.53
5:B:522:VAL:HG12	5:B:523:CYS:N	2.23	0.53
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.90	0.53
5:B:763:GLN:HG2	5:B:765:PRO:CD	2.38	0.53
7:E:177:ARG:C	7:E:212:ARG:HD3	2.27	0.53
4:A:1123:GLY:CA	4:A:1124:HIS:HB2	2.38	0.53
4:A:152:VAL:HG22	4:A:163:SER:OG	2.08	0.53
4:A:215:SER:HB3	4:A:218:ASP:CB	2.37	0.53
4:A:387:ARG:O	4:A:391:LEU:HB2	2.07	0.53
4:A:879:GLU:O	4:A:881:GLN:N	2.41	0.53
5:B:1099:VAL:O	5:B:1102:LYS:HG2	2.08	0.53
5:B:202:TYR:N	5:B:202:TYR:CD2	2.76	0.53
5:B:648:HIS:CG	5:B:648:HIS:O	2.61	0.53
9:H:47:PHE:CB	9:H:95:TYR:HD1	2.20	0.53
5:B:1156:ASP:HB3	5:B:1198:TYR:N	2.23	0.53
5:B:955:THR:HG23	13:L:54:ARG:O	2.09	0.53
5:B:969:ARG:NH1	5:B:969:ARG:HB3	2.19	0.53
5:B:980:PHE:CZ	5:B:990:ILE:HD11	2.42	0.53
6:C:46:ILE:HA	6:C:159:ALA:HA	1.90	0.53
13:L:61:THR:HB	13:L:63:ARG:H	1.74	0.53
4:A:253:ASN:H	4:A:253:ASN:HD22	1.56	0.53
4:A:311:GLN:CB	4:A:312:PRO:CD	2.85	0.53
4:A:451:HIS:O	5:B:1137:CYS:HB3	2.07	0.53
5:B:424:LEU:O	5:B:428:ILE:HG12	2.09	0.53
5:B:757:PRO:HG3	5:B:983:ARG:NH2	2.23	0.53
5:B:839:MET:HE2	5:B:990:ILE:HG23	1.90	0.53
4:A:247:ARG:NH1	4:A:263:THR:HG23	2.22	0.53
6:C:244:VAL:HG23	6:C:245:VAL:N	2.23	0.53
4:A:596:THR:C	4:A:598:LEU:N	2.59	0.53
4:A:443:LEU:HD11	5:B:1138:MET:HE1	1.90	0.53
6:C:25:VAL:HG12	6:C:26:ASP:N	2.22	0.53
4:A:303:TYR:CD2	4:A:304:MET:HG3	2.44	0.53
4:A:531:ILE:HG13	4:A:653:VAL:HG21	1.91	0.53
5:B:592:ASN:OD1	5:B:594:ALA:HB3	2.09	0.53
5:B:656:GLY:O	5:B:657:HIS:C	2.47	0.53
5:B:796:LEU:O	5:B:799:PRO:HD3	2.08	0.53
4:A:323:LYS:HZ3	4:A:323:LYS:N	2.07	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1149:GLU:C	5:B:1151:LEU:H	2.12	0.53
7:E:89:GLY:O	7:E:120:ALA:HB2	2.09	0.53
10:I:53:GLY:HA3	10:I:90:GLN:HG3	1.90	0.53
4:A:1342:GLU:HG2	7:E:212:ARG:HH12	1.74	0.53
4:A:218:ASP:H	4:A:219:PHE:CB	2.14	0.53
4:A:465:TYR:CD1	12:K:67:PHE:CZ	2.96	0.53
5:B:635:ARG:NH1	5:B:742:GLU:OE2	2.42	0.53
5:B:760:ASP:OD1	5:B:760:ASP:N	2.41	0.53
4:A:1127:ASP:O	4:A:1130:GLN:HB3	2.09	0.53
4:A:826:ASP:HA	4:A:829:VAL:HB	1.91	0.53
4:A:946:VAL:HG12	4:A:947:PHE:N	2.23	0.53
4:A:981:LEU:HD23	4:A:1039:LYS:HA	1.90	0.53
5:B:850:LEU:HD21	5:B:1009:ASP:HB3	1.91	0.53
5:B:313:MET:HE2	5:B:390:LEU:HG	1.89	0.53
5:B:654:ARG:N	5:B:657:HIS:HD2	2.03	0.53
4:A:276:LEU:CD1	4:A:292:ALA:HB1	2.31	0.52
5:B:863:GLU:HG2	5:B:962:LYS:O	2.10	0.52
5:B:822:ASN:ND2	11:J:52:THR:HG21	2.16	0.52
5:B:848:ARG:NH1	11:J:8:PHE:O	2.42	0.52
4:A:1107:VAL:HG12	4:A:1107:VAL:O	2.08	0.52
5:B:1111:MET:HE2	5:B:1118:PRO:HA	1.90	0.52
5:B:211:VAL:O	5:B:480:SER:HA	2.10	0.52
5:B:952:VAL:HG22	5:B:966:VAL:HG13	1.92	0.52
6:C:167:HIS:CD2	6:C:169:LYS:H	2.28	0.52
5:B:1084:GLN:OE1	5:B:1084:GLN:N	2.42	0.52
5:B:1029:CYS:HB2	5:B:1090:THR:CG2	2.40	0.52
4:A:455:MET:HG2	5:B:1138:MET:CE	2.40	0.52
5:B:836:GLU:O	5:B:838:SER:N	2.40	0.52
6:C:88:CYS:SG	6:C:88:CYS:O	2.67	0.52
4:A:341:MET:CG	4:A:1429:ILE:HG13	2.38	0.52
4:A:508:PRO:C	4:A:510:GLN:H	2.12	0.52
5:B:100:PRO:HG3	5:B:172:ILE:HG13	1.91	0.52
5:B:317:CYS:HA	5:B:320:ASP:HB2	1.90	0.52
5:B:800:GLN:HB3	11:J:52:THR:HG22	1.91	0.52
1:R:8:G:N2	2:T:22:DT:C2	2.78	0.52
1:R:2:A:H2'	1:R:3:G:H8	1.74	0.52
4:A:741:ASN:HD22	4:A:741:ASN:C	2.12	0.52
5:B:1029:CYS:HG	5:B:1086:PHE:HE2	1.57	0.52
5:B:950:ASP:HB3	5:B:967:ARG:HG3	1.91	0.52
6:C:12:GLU:H	6:C:19:ASP:HB3	1.75	0.52
9:H:47:PHE:CB	9:H:95:TYR:CD1	2.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:52:ILE:HA	10:I:54:GLU:H	1.75	0.52
4:A:1166:ASP:O	4:A:1167:GLU:HB3	2.10	0.52
4:A:1313:LEU:C	4:A:1315:GLU:H	2.13	0.52
4:A:1364:ASN:HD21	4:A:1366:ARG:NH1	2.08	0.52
4:A:72:GLU:HB3	4:A:76:GLU:HG2	1.91	0.52
4:A:839:ARG:NH1	4:A:839:ARG:CG	2.61	0.52
5:B:264:SER:HA	5:B:265:SER:O	2.09	0.52
5:B:779:GLY:HA2	5:B:796:LEU:HB2	1.91	0.52
5:B:800:GLN:HB3	11:J:52:THR:CG2	2.39	0.52
4:A:618:GLU:O	4:A:622:VAL:HG12	2.09	0.52
4:A:869:GLY:O	7:E:204:THR:HG21	2.09	0.52
5:B:115:GLN:O	5:B:119:LEU:HD12	2.10	0.52
4:A:1364:ASN:ND2	4:A:1366:ARG:HH11	2.08	0.52
4:A:74:MET:CE	4:A:74:MET:HA	2.40	0.52
4:A:751:SER:HB2	5:B:1015:HIS:CE1	2.45	0.52
5:B:637:LEU:HD11	5:B:740:HIS:CD2	2.45	0.52
8:F:103:MET:O	8:F:104:ASN:CB	2.56	0.52
8:F:111:LEU:H	8:F:111:LEU:HD12	1.75	0.52
4:A:1080:THR:HG22	4:A:1081:LEU:H	1.75	0.52
5:B:102:VAL:HG21	5:B:112:LEU:HD13	1.92	0.52
5:B:756:ILE:HD11	5:B:770:GLN:HB3	1.92	0.52
4:A:356:ASP:OD1	5:B:833:TYR:CE2	2.62	0.52
5:B:978:ASP:HB2	5:B:980:PHE:HE1	1.75	0.52
6:C:142:VAL:HG12	6:C:144:ILE:HD13	1.91	0.52
4:A:148:CYS:HB3	4:A:168:GLY:HA2	1.92	0.51
4:A:364:VAL:HB	4:A:458:HIS:HB3	1.92	0.51
4:A:629:LEU:HD22	4:A:633:VAL:HG23	1.92	0.51
4:A:858:ASN:O	4:A:861:GLY:N	2.40	0.51
4:A:900:ASP:HA	4:A:926:GLN:NE2	2.25	0.51
5:B:638:PHE:CD2	5:B:653:VAL:HG21	2.45	0.51
7:E:157:SER:OG	7:E:160:GLU:HG3	2.10	0.51
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.91	0.51
12:K:42:LEU:CD2	12:K:46:ILE:HD12	2.41	0.51
12:K:38:GLU:O	12:K:69:ALA:O	2.27	0.51
4:A:1089:VAL:HB	4:A:1092:LYS:HB2	1.91	0.51
4:A:116:ASP:C	4:A:118:HIS:HB2	2.23	0.51
4:A:1323:ASP:OD1	4:A:1325:THR:HG22	2.10	0.51
5:B:1084:GLN:HE22	6:C:192:TRP:N	2.08	0.51
5:B:385:LEU:HD23	5:B:386:LEU:N	2.26	0.51
5:B:648:HIS:O	5:B:649:LYS:O	2.27	0.51
4:A:567:LYS:O	4:A:568:PRO:C	2.48	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:322:PHE:HZ	10:I:30:ARG:HB2	1.74	0.51
5:B:680:THR:O	5:B:681:TRP:C	2.48	0.51
5:B:841:MET:HE3	5:B:990:ILE:HG12	1.92	0.51
5:B:944:THR:CB	5:B:1122:ARG:HH21	2.23	0.51
5:B:994:TYR:N	5:B:994:TYR:CD2	2.77	0.51
6:C:167:HIS:HB3	6:C:169:LYS:HG2	1.92	0.51
6:C:168:ALA:C	6:C:170:TRP:H	2.13	0.51
11:J:1:MET:H1	11:J:56:LEU:H	1.59	0.51
12:K:42:LEU:HD23	12:K:46:ILE:HD12	1.93	0.51
2:T:18:DC:H2'	2:T:19:DG:H8	1.74	0.51
4:A:370:ILE:CG2	4:A:374:LEU:HD11	2.41	0.51
5:B:1056:SER:O	5:B:1059:LEU:N	2.44	0.51
5:B:1085:ILE:HG22	5:B:1086:PHE:O	2.10	0.51
6:C:180:TYR:O	6:C:181:ASP:HB3	2.09	0.51
6:C:66:ARG:NH2	11:J:4:PRO:HA	2.24	0.51
13:L:58:LYS:O	13:L:59:ALA:HB3	2.10	0.51
4:A:102:VAL:O	4:A:106:VAL:HG23	2.11	0.51
4:A:367:PRO:CG	4:A:370:ILE:HD12	2.41	0.51
5:B:1172:ILE:HD13	5:B:1183:LYS:HG2	1.93	0.51
5:B:461:LEU:HD23	5:B:466:TRP:CZ3	2.46	0.51
5:B:485:ARG:NH1	5:B:491:THR:HG21	2.24	0.51
5:B:498:THR:HB	5:B:537:LYS:O	2.10	0.51
5:B:988:GLY:C	5:B:989:THR:O	2.48	0.51
5:B:797:TYR:O	11:J:1:MET:HG2	2.11	0.51
4:A:109:HIS:H	4:A:210:ILE:HD12	1.76	0.51
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.91	0.51
5:B:850:LEU:CD1	11:J:8:PHE:CD1	2.93	0.51
4:A:108:MET:O	4:A:109:HIS:HB2	2.10	0.51
4:A:370:ILE:O	4:A:374:LEU:HD12	2.10	0.51
5:B:1002:THR:HG22	5:B:1006:ILE:HB	1.91	0.51
5:B:287:ARG:NH1	5:B:324:ILE:O	2.40	0.51
5:B:314:LEU:C	5:B:316:PRO:HD2	2.30	0.51
5:B:33:VAL:HG21	5:B:638:PHE:CZ	2.46	0.51
5:B:887:HIS:HB3	5:B:888:GLY:O	2.10	0.51
5:B:915:THR:HB	5:B:934:LYS:HB3	1.93	0.51
7:E:22:MET:HB2	7:E:187:TYR:CE1	2.45	0.51
4:A:1094:VAL:HA	4:A:1113:THR:HG21	1.93	0.51
4:A:588:LEU:HD12	4:A:632:VAL:HG21	1.92	0.51
5:B:879:ARG:NH1	5:B:882:THR:CG2	2.58	0.51
11:J:1:MET:HG3	11:J:1:MET:O	2.11	0.51
4:A:290:GLU:C	4:A:292:ALA:N	2.64	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:455:MET:HG2	5:B:1138:MET:HE3	1.92	0.51
5:B:956:THR:HB	13:L:46:VAL:CG2	2.40	0.51
9:H:104:PHE:CZ	9:H:136:LYS:HA	2.46	0.51
10:I:28:GLU:HB3	10:I:35:VAL:HG13	1.93	0.51
4:A:55:ASP:N	4:A:56:PRO:CD	2.70	0.50
5:B:653:VAL:HG13	5:B:689:LEU:HD13	1.93	0.50
6:C:101:LEU:HB3	6:C:155:LEU:CD1	2.41	0.50
7:E:99:HIS:CE1	7:E:103:LYS:HE2	2.47	0.50
4:A:14:VAL:O	4:A:15:LYS:HD3	2.11	0.50
4:A:86:LEU:HB2	4:A:237:THR:O	2.11	0.50
4:A:365:GLY:HA3	4:A:469:ARG:HG3	1.92	0.50
7:E:55:ARG:CZ	7:E:113:GLN:OE1	2.59	0.50
13:L:28:LYS:HB2	13:L:39:SER:HA	1.93	0.50
4:A:591:PHE:HD2	4:A:595:THR:HB	1.75	0.50
4:A:68:GLN:NE2	4:A:68:GLN:O	2.44	0.50
4:A:68:GLN:O	4:A:70:CYS:N	2.37	0.50
4:A:836:TYR:CZ	4:A:840:ARG:HD2	2.47	0.50
5:B:854:LEU:HD22	5:B:969:ARG:HD3	1.92	0.50
6:C:73:GLN:HB3	6:C:131:HIS:H	1.75	0.50
7:E:164:LEU:HD13	7:E:211:TYR:CE2	2.46	0.50
4:A:341:MET:SD	4:A:1429:ILE:N	2.84	0.50
4:A:1446:ASP:HA	4:A:1447:GLU:HB2	1.93	0.50
4:A:102:VAL:HG11	4:A:211:PHE:HE1	1.76	0.50
4:A:639:PRO:HD2	4:A:640:GLN:H	1.75	0.50
4:A:984:LYS:O	4:A:988:LEU:HB3	2.12	0.50
5:B:140:ILE:O	5:B:140:ILE:HG22	2.11	0.50
5:B:58:THR:O	5:B:62:ILE:HG12	2.11	0.50
5:B:866:TYR:CB	5:B:867:GLY:HA2	2.42	0.50
7:E:72:PHE:CD1	7:E:72:PHE:N	2.80	0.50
10:I:117:LYS:HD3	10:I:118:ARG:NH2	2.26	0.50
4:A:378:GLU:OE2	4:A:434:ARG:HD3	2.12	0.50
4:A:374:LEU:C	4:A:436:ILE:HD13	2.31	0.50
4:A:68:GLN:C	4:A:70:CYS:H	2.12	0.50
5:B:879:ARG:HH11	5:B:882:THR:HG22	1.64	0.50
5:B:980:PHE:CE1	5:B:990:ILE:HD12	2.45	0.50
11:J:45:CYS:O	11:J:48:ARG:HG3	2.11	0.50
4:A:12:ARG:O	5:B:1194:ILE:HG22	2.11	0.50
4:A:775:ILE:HG13	4:A:798:GLY:HA3	1.94	0.50
4:A:875:ALA:HA	4:A:878:ILE:HD12	1.94	0.50
5:B:976:ILE:HD13	5:B:991:GLY:O	2.03	0.50
4:A:465:TYR:HD1	12:K:67:PHE:CZ	2.30	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1197:LEU:HD12	4:A:1209:MET:SD	2.52	0.50
8:F:90:ARG:HD2	8:F:155:LEU:HD21	1.94	0.50
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.93	0.50
4:A:451:HIS:CE1	4:A:1074:GLU:HG3	2.46	0.50
4:A:672:ASP:HB2	4:A:675:THR:CB	2.41	0.50
4:A:828:ALA:CB	5:B:530:GLY:HA2	2.41	0.50
5:B:1002:THR:HG23	5:B:1006:ILE:H	1.75	0.50
5:B:464:GLY:O	5:B:466:TRP:N	2.45	0.50
5:B:744:HIS:CD2	5:B:746:SER:H	2.28	0.50
5:B:801:LYS:O	11:J:52:THR:HG22	2.11	0.50
6:C:180:TYR:CD1	6:C:180:TYR:O	2.65	0.50
7:E:164:LEU:HD23	7:E:165:LEU:N	2.26	0.50
12:K:56:VAL:HA	12:K:77:THR:HG22	1.92	0.50
1:R:9:G:O3'	5:B:979:LYS:NZ	2.45	0.50
11:J:48:ARG:NH1	11:J:48:ARG:HG2	2.24	0.50
4:A:1135:ARG:HG2	4:A:1282:VAL:HG12	1.94	0.49
4:A:1293:SER:HB2	4:A:1299:VAL:CG2	2.42	0.49
1:R:1:A:C2	4:A:252:PHE:HB3	2.47	0.49
12:K:47:ARG:HH11	12:K:47:ARG:HB3	1.76	0.49
4:A:117:GLU:C	4:A:118:HIS:O	2.48	0.49
4:A:303:TYR:HD2	4:A:304:MET:HG3	1.77	0.49
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.13	0.49
4:A:457:ALA:HB2	4:A:501:LEU:HD12	1.94	0.49
4:A:758:ILE:H	4:A:758:ILE:HD13	1.77	0.49
4:A:830:LYS:HZ2	4:A:830:LYS:HB2	1.78	0.49
4:A:848:ILE:O	4:A:1065:GLY:N	2.44	0.49
4:A:929:LEU:HD21	4:A:1028:THR:HG21	1.93	0.49
5:B:202:TYR:CD1	5:B:209:GLU:HB3	2.47	0.49
5:B:770:GLN:HG2	5:B:983:ARG:O	2.11	0.49
7:E:115:ASN:N	7:E:115:ASN:OD1	2.41	0.49
6:C:241:ASP:HB3	12:K:109:TRP:CZ2	2.46	0.49
2:T:13:DA:H2''	2:T:14:DC:C5	2.47	0.49
4:A:1042:PHE:CE2	4:A:1046:LEU:HD13	2.47	0.49
4:A:1434:ALA:HB1	4:A:1436:ILE:HD13	1.93	0.49
5:B:1106:ARG:NH2	5:B:1111:MET:CE	2.74	0.49
5:B:276:ILE:HD11	5:B:334:ILE:HG23	1.94	0.49
9:H:96:VAL:HG22	9:H:143:LEU:HG	1.94	0.49
4:A:1017:LEU:O	4:A:1020:CYS:HB2	2.13	0.49
4:A:1428:VAL:O	4:A:1431:GLY:N	2.44	0.49
4:A:376:TYR:CD2	4:A:376:TYR:C	2.86	0.49
4:A:464:PRO:HG2	12:K:67:PHE:CD1	2.47	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:707:PRO:O	5:B:711:GLU:HG2	2.12	0.49
6:C:57:VAL:HG11	11:J:60:PHE:HB2	1.85	0.49
4:A:1227:ILE:HG22	4:A:1228:TRP:N	2.27	0.49
4:A:1308:THR:HG23	4:A:1309:ASP:N	2.27	0.49
4:A:185:TRP:HB2	4:A:199:LEU:HG	1.93	0.49
4:A:370:ILE:HG23	4:A:374:LEU:HD11	1.95	0.49
4:A:440:ASP:O	4:A:460:VAL:HG23	2.11	0.49
4:A:340:LEU:HD22	5:B:1200:ALA:HB2	1.95	0.49
5:B:242:SER:HB2	5:B:362:PRO:HD2	1.95	0.49
5:B:759:PRO:CD	5:B:1046:PRO:HG3	2.43	0.49
5:B:769:TYR:O	5:B:770:GLN:C	2.51	0.49
5:B:769:TYR:O	5:B:771:SER:N	2.46	0.49
5:B:936:ASP:OD2	5:B:938:SER:HB2	2.12	0.49
7:E:93:MET:O	7:E:94:LYS:HG3	2.12	0.49
4:A:22:PHE:HB2	5:B:1211:ASN:CG	2.33	0.49
5:B:276:ILE:HD13	5:B:277:LYS:H	1.77	0.49
5:B:345:LYS:HB2	5:B:348:ARG:HE	1.78	0.49
5:B:313:MET:HE1	5:B:390:LEU:HG	1.95	0.49
5:B:821:GLN:HE22	11:J:8:PHE:HE1	1.61	0.49
10:I:52:ILE:HA	10:I:54:GLU:N	2.27	0.49
4:A:1363:VAL:HG12	4:A:1364:ASN:N	2.28	0.49
4:A:405:VAL:HG23	4:A:415:LEU:HD11	1.95	0.49
5:B:850:LEU:HD22	5:B:1009:ASP:HB3	1.94	0.49
5:B:979:LYS:O	5:B:980:PHE:CD1	2.66	0.49
6:C:29:MET:HA	12:K:45:LEU:HD13	1.95	0.49
4:A:464:PRO:HG2	12:K:67:PHE:CE1	2.48	0.49
4:A:519:PRO:O	4:A:624:SER:HB2	2.12	0.49
5:B:1120:GLU:HG2	5:B:1121:GLY:H	1.77	0.49
5:B:834:ASN:HA	5:B:838:SER:HB3	1.95	0.49
5:B:862:GLN:HG2	5:B:963:PHE:HB2	1.94	0.49
8:F:93:ILE:HG22	8:F:94:LEU:N	2.28	0.49
11:J:44:TYR:C	11:J:44:TYR:HD1	2.16	0.49
4:A:84:ILE:HD12	4:A:270:LEU:HD12	1.93	0.49
4:A:442:VAL:O	4:A:457:ALA:HA	2.12	0.49
4:A:760:GLN:HB3	4:A:804:TYR:HE1	1.78	0.49
4:A:899:VAL:HG12	4:A:929:LEU:HD13	1.95	0.49
5:B:546:SER:HA	5:B:612:GLU:OE2	2.12	0.49
9:H:137:GLN:HB3	9:H:139:ASN:H	1.78	0.49
1:R:10:C:OP1	5:B:987:LYS:CD	2.60	0.49
4:A:941:LYS:CG	4:A:942:PHE:N	2.76	0.49
5:B:763:GLN:CG	5:B:764:SER:N	2.76	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1084:GLN:NE2	6:C:192:TRP:H	2.07	0.49
4:A:548:ASN:OD1	12:K:60:ALA:HB1	2.12	0.49
4:A:368:LYS:HD2	4:A:399:HIS:HB2	1.96	0.48
4:A:662:PHE:O	5:B:828:ALA:HA	2.12	0.48
5:B:48:LEU:HD23	5:B:173:MET:SD	2.53	0.48
5:B:528:PRO:O	5:B:533:CYS:HB2	2.13	0.48
5:B:944:THR:HG23	5:B:945:GLU:HG3	1.95	0.48
6:C:147:LEU:HB3	6:C:151:GLN:HB2	1.95	0.48
4:A:496:GLU:CB	8:F:95:GLY:HA3	2.43	0.48
4:A:1148:ILE:HD11	4:A:1198:ASP:HB2	1.94	0.48
4:A:57:ARG:C	4:A:68:GLN:HG2	2.33	0.48
5:B:1006:ILE:CG2	5:B:1007:VAL:H	2.26	0.48
5:B:1016:ALA:HB1	5:B:1020:ARG:NH1	2.28	0.48
5:B:839:MET:CE	5:B:841:MET:CE	2.89	0.48
6:C:142:VAL:N	11:J:16:ASP:HB3	2.13	0.48
4:A:1242:VAL:HG12	4:A:1243:VAL:N	2.27	0.48
4:A:1402:PHE:CD2	4:A:1403:GLU:HB2	2.48	0.48
4:A:43:GLU:HB3	4:A:50:ILE:HG23	1.94	0.48
4:A:741:ASN:ND2	4:A:743:VAL:H	2.11	0.48
4:A:117:GLU:O	4:A:123:ARG:HG2	2.13	0.48
4:A:1374:VAL:C	4:A:1376:THR:H	2.17	0.48
4:A:93:VAL:HG13	4:A:301:ALA:HB1	1.95	0.48
4:A:75:ASN:O	4:A:76:GLU:HB2	2.13	0.48
5:B:278:GLN:CG	5:B:279:ASP:H	2.26	0.48
5:B:785:TYR:C	5:B:787:VAL:H	2.16	0.48
4:A:313:GLN:HB3	4:A:321:PRO:HA	1.95	0.48
4:A:340:LEU:CD2	5:B:1199:ALA:CB	2.92	0.48
4:A:774:ARG:NH2	4:A:792:TYR:O	2.45	0.48
5:B:1077:THR:HG22	6:C:27:LEU:HD21	1.95	0.48
5:B:523:CYS:SG	5:B:750:GLY:N	2.85	0.48
7:E:93:MET:HG3	7:E:120:ALA:HB1	1.94	0.48
4:A:540:PHE:CE1	9:H:43:ASN:ND2	2.81	0.48
4:A:1219:THR:HG21	4:A:1271:ILE:CD1	2.43	0.48
4:A:125:ALA:O	4:A:128:ILE:HG22	2.12	0.48
4:A:669:THR:HG22	4:A:762:SER:HB2	1.95	0.48
5:B:1037:LEU:HB3	5:B:1062:HIS:NE2	2.27	0.48
5:B:558:LEU:C	5:B:560:GLU:H	2.16	0.48
7:E:204:THR:CG2	7:E:205:SER:N	2.76	0.48
12:K:24:ASP:CG	12:K:74:ARG:HH11	2.17	0.48
4:A:775:ILE:CG1	4:A:797:LYS:O	2.62	0.48
5:B:1060:ARG:HB2	5:B:1066:SER:HB3	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:174:LEU:HD11	5:B:204:ILE:HG13	1.94	0.48
5:B:213:ILE:HG23	5:B:497:ARG:HB3	1.95	0.48
6:C:167:HIS:CD2	6:C:168:ALA:N	2.82	0.48
12:K:12:LEU:H	12:K:12:LEU:HD12	1.77	0.48
4:A:1059:HIS:ND1	8:F:87:LYS:HG2	2.29	0.48
4:A:381:THR:CG2	4:A:382:PRO:HD2	2.44	0.48
4:A:760:GLN:CA	4:A:760:GLN:NE2	2.68	0.48
4:A:896:ARG:HB3	4:A:897:TYR:CD1	2.49	0.48
5:B:1201:LYS:C	5:B:1201:LYS:HD3	2.34	0.48
5:B:990:ILE:CG2	5:B:991:GLY:H	2.22	0.48
11:J:57:ILE:HA	11:J:60:PHE:CD2	2.43	0.48
4:A:1388:GLY:O	4:A:1391:ARG:HG3	2.14	0.48
4:A:218:ASP:N	4:A:219:PHE:CB	2.74	0.48
4:A:360:GLU:OE1	4:A:360:GLU:HA	2.14	0.48
4:A:404:TYR:HA	4:A:413:ILE:O	2.13	0.48
4:A:541:ILE:HG22	4:A:545:GLN:NE2	2.28	0.48
5:B:129:PHE:CE2	5:B:166:PHE:HB2	2.49	0.48
5:B:246:LYS:NZ	5:B:246:LYS:HB3	2.29	0.48
7:E:163:GLU:O	7:E:166:LYS:N	2.46	0.48
4:A:494:SER:HB3	4:A:497:THR:OG1	2.13	0.48
4:A:550:LEU:HD13	4:A:556:TRP:CZ2	2.49	0.48
5:B:785:TYR:O	5:B:787:VAL:N	2.47	0.48
10:I:33:SER:O	10:I:35:VAL:HG23	2.14	0.48
12:K:32:VAL:CG2	12:K:74:ARG:HG3	2.42	0.48
4:A:553:VAL:HG23	4:A:652:VAL:HG22	1.96	0.47
4:A:718:VAL:HG12	4:A:719:VAL:N	2.28	0.47
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.45	0.47
5:B:901:PRO:HB3	5:B:950:ASP:O	2.14	0.47
8:F:116:ASP:HB3	8:F:119:ARG:HG3	1.95	0.47
9:H:137:GLN:HE21	9:H:139:ASN:HB2	1.78	0.47
4:A:619:LYS:O	4:A:623:GLY:HA3	2.14	0.47
5:B:827:ILE:HD11	5:B:1086:PHE:HD2	1.78	0.47
6:C:39:ALA:CA	6:C:164:ALA:HB3	2.36	0.47
6:C:195:GLN:N	6:C:200:GLU:OE2	2.29	0.47
4:A:577:ILE:HG13	4:A:578:LEU:N	2.29	0.47
4:A:11:LEU:HB2	5:B:1193:GLN:HG3	1.95	0.47
5:B:975:GLN:O	5:B:977:GLY:N	2.44	0.47
5:B:988:GLY:O	5:B:989:THR:O	2.33	0.47
9:H:22:LYS:O	9:H:44:VAL:N	2.47	0.47
4:A:1147:THR:HG22	4:A:1197:LEU:CD2	2.44	0.47
5:B:364:ILE:HG21	5:B:374:LYS:HG2	1.96	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:35:PHE:CD1	12:K:35:PHE:N	2.82	0.47
4:A:1363:VAL:CG1	4:A:1364:ASN:N	2.77	0.47
4:A:336:ILE:CG1	4:A:337:ARG:N	2.58	0.47
4:A:388:LEU:HD22	4:A:432:VAL:HG11	1.95	0.47
4:A:474:VAL:HG22	4:A:478:TYR:CE1	2.50	0.47
4:A:92:HIS:HD2	4:A:92:HIS:O	1.97	0.47
5:B:860:MET:SD	5:B:861:ASP:N	2.87	0.47
5:B:969:ARG:HE	6:C:59:ALA:HB1	1.78	0.47
12:K:63:VAL:HG23	12:K:63:VAL:O	2.14	0.47
4:A:1235:LYS:HB2	4:A:1237:ILE:CD1	2.45	0.47
4:A:338:GLY:O	4:A:339:ASN:OD1	2.32	0.47
4:A:590:ARG:HH11	4:A:590:ARG:HG3	1.80	0.47
4:A:612:ILE:HG13	4:A:612:ILE:O	2.14	0.47
5:B:126:SER:HB2	5:B:172:ILE:HD11	1.97	0.47
7:E:144:ILE:HG13	7:E:145:THR:N	2.30	0.47
7:E:164:LEU:HD13	7:E:211:TYR:CD2	2.50	0.47
5:B:424:LEU:O	5:B:427:ASP:HB2	2.13	0.47
6:C:69:LEU:HD23	11:J:6:ARG:HD3	1.97	0.47
4:A:1235:LYS:HB2	4:A:1237:ILE:HD12	1.96	0.47
4:A:208:LEU:O	4:A:212:LYS:HB2	2.14	0.47
4:A:401:GLY:C	4:A:435:HIS:ND1	2.67	0.47
5:B:277:LYS:HE3	5:B:277:LYS:HB2	1.44	0.47
6:C:136:ASP:OD1	6:C:139:GLY:N	2.47	0.47
8:F:71:GLU:HA	8:F:72:LYS:HA	1.61	0.47
4:A:134:ARG:HD3	4:A:221:SER:O	2.15	0.47
4:A:344:ARG:NH2	5:B:1112:GLN:OE1	2.48	0.47
4:A:353:ILE:HG21	4:A:487:MET:CE	2.44	0.47
5:B:1037:LEU:HD21	11:J:44:TYR:CD2	2.49	0.47
5:B:1072:MET:CE	5:B:1085:ILE:HB	2.45	0.47
4:A:814:PHE:HE1	5:B:514:LEU:HD21	1.78	0.47
5:B:95:ILE:O	5:B:95:ILE:HG23	2.15	0.47
6:C:242:GLN:HB3	6:C:246:ARG:HE	1.80	0.47
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.49	0.47
4:A:343:LYS:HZ1	5:B:1197:PRO:CB	2.17	0.47
5:B:801:LYS:O	11:J:52:THR:CG2	2.63	0.47
4:A:121:LEU:HA	4:A:124:GLN:HE22	1.79	0.47
4:A:816:HIS:O	4:A:817:ALA:C	2.54	0.47
4:A:488:ASN:OD1	5:B:1128:LEU:HD13	2.15	0.47
5:B:1171:VAL:HG21	5:B:1191:ILE:HG23	1.96	0.47
5:B:276:ILE:HD13	5:B:277:LYS:N	2.30	0.47
5:B:278:GLN:HG2	5:B:279:ASP:H	1.80	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:841:MET:HE3	5:B:990:ILE:HD13	1.96	0.47
6:C:226:ASP:O	6:C:227:THR:HB	2.14	0.47
12:K:7:PHE:C	12:K:9:LEU:H	2.18	0.47
4:A:382:PRO:HD3	4:A:428:TYR:HD2	1.79	0.46
4:A:582:ILE:HG22	4:A:610:GLY:HA2	1.97	0.46
4:A:696:GLU:C	4:A:698:GLN:H	2.19	0.46
5:B:663:ALA:O	5:B:667:GLN:HB2	2.15	0.46
6:C:167:HIS:CG	6:C:169:LYS:HG2	2.50	0.46
4:A:871:ASP:HB3	7:E:204:THR:HG23	1.95	0.46
7:E:89:GLY:HA2	7:E:117:THR:CG2	2.46	0.46
10:I:84:VAL:HG13	10:I:85:PHE:N	2.31	0.46
4:A:1342:GLU:HG2	7:E:212:ARG:NH1	2.30	0.46
4:A:1397:LEU:HD22	4:A:1429:ILE:HD13	1.96	0.46
4:A:491:VAL:HA	4:A:492:PRO:HD2	1.78	0.46
4:A:64:ASN:HB2	4:A:66:LYS:HG2	1.96	0.46
4:A:775:ILE:CG1	4:A:798:GLY:HA3	2.45	0.46
5:B:370:PHE:O	5:B:372:SER:N	2.48	0.46
5:B:649:LYS:O	5:B:650:GLU:HB2	2.15	0.46
5:B:804:GLY:HA2	5:B:1042:GLY:HA3	1.98	0.46
5:B:992:ILE:HD11	12:K:67:PHE:HE2	1.80	0.46
6:C:136:ASP:OD1	6:C:138:GLU:N	2.47	0.46
7:E:156:LEU:HD23	7:E:197:LYS:HB2	1.96	0.46
4:A:1083:THR:HB	4:A:1084:PHE:H	1.50	0.46
4:A:351:THR:HG21	4:A:467:THR:HA	1.98	0.46
4:A:951:GLU:OE1	4:A:951:GLU:HA	2.15	0.46
2:T:15:DT:H2''	2:T:16:DT:O5'	2.14	0.46
4:A:36:ARG:HB2	4:A:36:ARG:NH1	2.30	0.46
4:A:914:GLU:HB2	4:A:979:SER:O	2.15	0.46
5:B:278:GLN:HG2	5:B:279:ASP:N	2.31	0.46
5:B:577:ALA:HB1	5:B:589:VAL:HB	1.98	0.46
6:C:67:LEU:HA	6:C:70:ILE:CG1	2.46	0.46
6:C:75:MET:CE	6:C:239:PRO:HD3	2.45	0.46
7:E:167:ARG:HD3	7:E:167:ARG:HA	1.61	0.46
9:H:94:ASP:HB2	9:H:145:ARG:HA	1.98	0.46
5:B:190:TYR:CZ	11:J:62:ARG:HG2	2.50	0.46
4:A:64:ASN:HB3	4:A:66:LYS:HE2	1.97	0.46
5:B:269:ILE:O	5:B:282:ILE:HG23	2.15	0.46
5:B:308:TRP:HA	5:B:311:LEU:HB2	1.98	0.46
5:B:942:ARG:HB2	5:B:945:GLU:HG3	1.97	0.46
5:B:953:LEU:HD11	13:L:55:ILE:HG22	1.97	0.46
2:T:9:DA:OP2	2:T:9:DA:H2'	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:340:LEU:CD2	5:B:1200:ALA:N	2.78	0.46
4:A:394:ASN:HB3	4:A:398:GLU:HB2	1.98	0.46
4:A:446:ARG:HD3	4:A:447:GLN:O	2.16	0.46
4:A:441:PRO:HG3	4:A:498:ARG:HB2	1.97	0.46
4:A:879:GLU:O	4:A:881:GLN:HG3	2.16	0.46
4:A:344:ARG:HA	5:B:1129:ARG:HA	1.97	0.46
5:B:172:ILE:HD12	5:B:178:ASN:HD22	1.80	0.46
6:C:39:ALA:HA	6:C:164:ALA:CB	2.36	0.46
4:A:354:SER:O	4:A:469:ARG:HA	2.16	0.46
4:A:531:ILE:O	4:A:535:THR:HB	2.16	0.46
4:A:567:LYS:HD3	9:H:95:TYR:CG	2.51	0.46
4:A:88:LYS:HA	4:A:89:PRO:HD2	1.64	0.46
5:B:410:GLY:O	5:B:413:LEU:N	2.49	0.46
5:B:485:ARG:HG3	5:B:485:ARG:HH11	1.81	0.46
7:E:51:GLY:HA2	7:E:52:ARG:C	2.36	0.46
7:E:55:ARG:C	7:E:57:MET:N	2.69	0.46
13:L:31:CYS:HA	13:L:56:LEU:HD23	1.98	0.46
5:B:1002:THR:CG2	5:B:1006:ILE:H	2.29	0.46
4:A:466:SER:CB	5:B:1100:ASP:OD1	2.64	0.46
5:B:216:GLU:HB3	5:B:500:THR:HG23	1.98	0.46
5:B:263:GLY:HA2	5:B:264:SER:C	2.36	0.46
5:B:914:LYS:O	5:B:937:ALA:HB3	2.16	0.46
6:C:186:LEU:CB	6:C:188:HIS:HD2	2.25	0.46
6:C:53:THR:O	6:C:153:LEU:HA	2.15	0.46
7:E:185:ALA:HA	7:E:190:LEU:HD12	1.98	0.46
8:F:93:ILE:HD11	8:F:134:ILE:HD11	1.96	0.46
10:I:101:PHE:HE1	10:I:112:SER:HB3	1.80	0.46
12:K:6:ARG:O	12:K:9:LEU:HD12	2.16	0.46
1:R:2:A:H61	2:T:27:DT:H3	1.63	0.46
4:A:1407:GLU:HA	4:A:1410:PHE:HB2	1.98	0.46
4:A:214:ILE:CG2	4:A:215:SER:H	2.12	0.46
4:A:34:LYS:HE2	4:A:57:ARG:NH2	2.31	0.46
4:A:483:ASP:N	5:B:837:ASP:HB2	2.31	0.46
4:A:92:HIS:HD2	4:A:94:GLY:H	1.64	0.46
5:B:350:GLN:O	5:B:353:LYS:N	2.49	0.46
5:B:520:GLY:HA3	5:B:635:ARG:HD2	1.98	0.46
5:B:778:MET:SD	5:B:794:ASN:HB3	2.56	0.46
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.51	0.46
5:B:890:TYR:CZ	5:B:910:VAL:HG21	2.51	0.46
5:B:843:GLN:HB3	5:B:995:ARG:HG3	1.97	0.46
6:C:115:SER:C	6:C:117:ASP:H	2.19	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:258:ILE:HG22	6:C:259:LEU:N	2.30	0.46
6:C:31:ASN:O	6:C:33:LEU:N	2.49	0.46
6:C:79:GLN:HG3	6:C:127:ARG:CD	2.45	0.46
7:E:64:PRO:CG	7:E:76:GLY:HA2	2.45	0.46
4:A:392:VAL:HG11	4:A:424:ILE:HG21	1.97	0.46
5:B:276:ILE:HG23	5:B:277:LYS:H	1.79	0.46
5:B:383:ASN:O	5:B:387:LEU:HB2	2.16	0.46
5:B:546:SER:N	5:B:634:TYR:HE2	2.14	0.46
5:B:681:TRP:O	5:B:684:LEU:N	2.49	0.46
9:H:98:TYR:C	9:H:118:PHE:HD2	2.19	0.46
10:I:115:LYS:HE2	10:I:115:LYS:HA	1.98	0.46
1:R:8:G:C2	2:T:22:DT:C2	3.04	0.46
4:A:17:VAL:HG23	4:A:1421:CYS:SG	2.56	0.45
5:B:1162:ILE:HA	5:B:1162:ILE:HD13	1.76	0.45
5:B:92:PHE:HD2	5:B:132:VAL:HG22	1.82	0.45
5:B:283:VAL:CG2	5:B:321:GLY:HA3	2.46	0.45
9:H:42:ILE:HG21	9:H:49:VAL:CG2	2.45	0.45
4:A:1428:VAL:HG13	5:B:1151:LEU:HD21	1.98	0.45
4:A:403:LYS:HA	4:A:415:LEU:HB2	1.98	0.45
4:A:49:LYS:HB2	4:A:49:LYS:NZ	2.31	0.45
5:B:840:ILE:CG2	5:B:1011:ILE:HD12	2.42	0.45
5:B:102:VAL:HG23	5:B:112:LEU:HD22	1.98	0.45
5:B:1094:ARG:HG3	5:B:1094:ARG:O	2.16	0.45
5:B:1171:VAL:HG11	5:B:1191:ILE:HG21	1.98	0.45
5:B:291:ILE:HD12	5:B:291:ILE:H	1.81	0.45
6:C:124:LEU:O	6:C:127:ARG:HG2	2.16	0.45
7:E:89:GLY:O	7:E:120:ALA:CB	2.64	0.45
11:J:1:MET:O	11:J:2:ILE:HB	2.16	0.45
4:A:1116:LEU:H	4:A:1308:THR:CG2	2.28	0.45
4:A:37:PHE:HA	4:A:38:PRO:HD3	1.81	0.45
5:B:782:LEU:HB3	5:B:784:ASN:OD1	2.17	0.45
7:E:130:ALA:CA	7:E:131:THR:HB	2.46	0.45
10:I:53:GLY:CA	10:I:90:GLN:HG3	2.46	0.45
11:J:2:ILE:HD12	11:J:3:VAL:H	1.81	0.45
13:L:34:CYS:HB3	13:L:51:CYS:SG	2.56	0.45
1:R:2:A:H2'	1:R:3:G:C8	2.52	0.45
4:A:116:ASP:HA	4:A:117:GLU:HB2	1.98	0.45
4:A:1187:GLN:NE2	4:A:1188:GLN:HG3	2.31	0.45
4:A:464:PRO:O	4:A:465:TYR:CB	2.63	0.45
4:A:527:THR:HG21	4:A:650:GLN:HG2	1.97	0.45
5:B:681:TRP:HA	5:B:684:LEU:HD12	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:841:MET:CE	5:B:990:ILE:HD11	2.33	0.45
5:B:620:ARG:NH2	10:I:68:LEU:HD21	2.32	0.45
4:A:1187:GLN:HE22	4:A:1188:GLN:HG3	1.82	0.45
4:A:693:VAL:HG21	4:A:721:PHE:HE1	1.81	0.45
5:B:1029:CYS:HB2	5:B:1090:THR:HG23	1.98	0.45
5:B:1027:ILE:O	5:B:1030:LEU:HB3	2.16	0.45
5:B:1090:THR:O	5:B:1091:TYR:C	2.54	0.45
4:A:344:ARG:HH21	5:B:1112:GLN:CD	2.20	0.45
5:B:57:TYR:CD1	5:B:57:TYR:N	2.84	0.45
5:B:871:THR:HG22	5:B:872:GLU:H	1.81	0.45
5:B:979:LYS:HE2	5:B:987:LYS:HG2	1.97	0.45
13:L:41:SER:O	13:L:43:THR:N	2.45	0.45
2:T:21:DC:H5''	5:B:1128:LEU:CD2	2.46	0.45
4:A:1174:PHE:CG	4:A:1174:PHE:O	2.70	0.45
4:A:1115:SER:HB3	4:A:1330:ASN:ND2	2.32	0.45
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	1.99	0.45
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.16	0.45
6:C:34:ARG:NH1	6:C:35:ARG:HG2	2.32	0.45
1:R:9:G:H2'	1:R:10:C:C5	2.51	0.45
4:A:1293:SER:HB2	4:A:1299:VAL:HG23	1.98	0.45
5:B:999:MET:HB3	5:B:1007:VAL:HG22	1.99	0.45
5:B:834:ASN:HB3	5:B:840:ILE:HG13	1.99	0.45
6:C:69:LEU:O	11:J:6:ARG:NH1	2.49	0.45
13:L:67:PHE:O	13:L:68:GLU:C	2.55	0.45
4:A:225:ASN:ND2	4:A:227:VAL:H	2.14	0.45
4:A:253:ASN:N	4:A:253:ASN:HD22	2.15	0.45
4:A:322:VAL:HG23	4:A:322:VAL:O	2.17	0.45
4:A:525:GLN:O	4:A:529:CYS:HB3	2.17	0.45
4:A:550:LEU:HD11	4:A:561:PRO:HD2	1.99	0.45
4:A:630:ILE:HD12	4:A:630:ILE:H	1.81	0.45
5:B:291:ILE:CD1	5:B:291:ILE:H	2.30	0.45
5:B:706:GLN:HB2	5:B:709:ASP:HB2	1.98	0.45
5:B:879:ARG:CA	5:B:879:ARG:NE	2.61	0.45
5:B:990:ILE:CG2	5:B:991:GLY:N	2.78	0.45
6:C:46:ILE:HG13	6:C:72:LEU:HD11	1.99	0.45
4:A:1134:ILE:H	4:A:1134:ILE:HD12	1.82	0.45
4:A:1449:SER:HA	4:A:1450:LEU:HA	1.58	0.45
4:A:90:VAL:HB	4:A:297:GLN:NE2	2.29	0.45
4:A:307:ASP:C	4:A:308:ILE:HG13	2.37	0.45
4:A:517:ASN:ND2	4:A:1364:ASN:OD1	2.50	0.45
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:845:LEU:O	4:A:848:ILE:HG12	2.16	0.45
4:A:965:GLN:O	4:A:969:GLN:HB2	2.17	0.45
5:B:1188:LYS:HB2	5:B:1189:ILE:HG13	1.99	0.45
5:B:548:GLY:HA3	5:B:630:ALA:HB2	1.99	0.45
5:B:792:MET:HG3	5:B:855:PHE:HE1	1.82	0.45
5:B:957:ASN:N	5:B:961:LEU:O	2.45	0.45
6:C:115:SER:C	6:C:117:ASP:N	2.70	0.45
6:C:226:ASP:O	6:C:227:THR:CB	2.65	0.45
6:C:4:GLU:HG3	6:C:5:GLY:N	2.32	0.45
9:H:77:ARG:HB2	9:H:77:ARG:HH11	1.82	0.45
4:A:154:SER:HB2	4:A:161:LEU:HD12	1.99	0.45
4:A:64:ASN:C	4:A:66:LYS:H	2.20	0.45
4:A:718:VAL:O	4:A:721:PHE:N	2.50	0.45
5:B:303:TYR:N	5:B:303:TYR:CD2	2.83	0.45
5:B:361:LEU:CD2	5:B:377:PHE:CD2	2.93	0.45
5:B:446:LEU:CG	5:B:447:ALA:N	2.73	0.45
5:B:841:MET:HE3	5:B:990:ILE:CG1	2.47	0.45
2:T:20:DC:H2'	2:T:21:DC:O4'	2.17	0.45
4:A:1344:GLY:O	4:A:1347:ALA:N	2.49	0.44
4:A:280:GLU:C	4:A:282:ASN:H	2.20	0.44
4:A:325:ILE:O	4:A:328:ARG:HB2	2.17	0.44
4:A:413:ILE:HG22	4:A:413:ILE:O	2.17	0.44
4:A:666:ILE:HD11	5:B:1023:VAL:HG12	1.99	0.44
4:A:741:ASN:HD22	4:A:743:VAL:H	1.65	0.44
5:B:762:ASN:HD22	5:B:762:ASN:HA	1.68	0.44
5:B:839:MET:CE	5:B:841:MET:HE3	2.47	0.44
9:H:83:GLN:N	9:H:87:ARG:HG3	2.32	0.44
1:R:9:G:C6	2:T:21:DC:N3	2.85	0.44
4:A:1155:ASP:HB3	4:A:1241:ARG:NH2	2.32	0.44
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.99	0.44
5:B:1032:SER:C	5:B:1089:PRO:HG2	2.37	0.44
5:B:1041:GLU:HA	5:B:1041:GLU:OE2	2.16	0.44
5:B:1099:VAL:HB	5:B:1103:ILE:HD11	2.00	0.44
5:B:944:THR:HB	5:B:1122:ARG:HH21	1.81	0.44
4:A:451:HIS:O	5:B:1137:CYS:CB	2.65	0.44
4:A:335:ARG:HH11	5:B:1202:LEU:HD12	1.82	0.44
5:B:221:ASN:OD1	5:B:242:SER:HA	2.17	0.44
5:B:1078:GLY:O	6:C:180:TYR:HE2	1.99	0.44
12:K:58:PHE:HE2	12:K:74:ARG:NE	2.06	0.44
4:A:1364:ASN:HD22	4:A:1366:ARG:H	1.65	0.44
4:A:977:LYS:HA	4:A:978:PRO:HD3	1.74	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1095:LEU:C	5:B:1096:ARG:O	2.54	0.44
8:F:79:ARG:HA	8:F:144:GLU:OE2	2.18	0.44
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.32	0.44
4:A:1308:THR:CG2	4:A:1309:ASP:N	2.80	0.44
5:B:619:ILE:HG21	10:I:62:ILE:HA	1.99	0.44
5:B:728:ARG:NH1	5:B:760:ASP:OD2	2.43	0.44
5:B:765:PRO:O	5:B:768:THR:N	2.50	0.44
5:B:845:SER:OG	5:B:846:ILE:N	2.50	0.44
5:B:866:TYR:CG	5:B:867:GLY:HA2	2.52	0.44
6:C:33:LEU:HD21	6:C:37:MET:HE1	1.99	0.44
7:E:122:LYS:HA	7:E:122:LYS:HE3	2.00	0.44
4:A:225:ASN:HD22	4:A:228:PHE:H	1.64	0.44
4:A:381:THR:HG22	4:A:382:PRO:HD2	2.00	0.44
4:A:474:VAL:O	4:A:478:TYR:HD1	2.00	0.44
4:A:673:GLY:N	4:A:674:PRO:HD2	2.32	0.44
5:B:1017:ILE:HD12	5:B:1026:LEU:CD2	2.47	0.44
5:B:578:THR:OG1	5:B:593:PRO:HG3	2.17	0.44
4:A:760:GLN:HB3	4:A:804:TYR:CE1	2.52	0.44
4:A:925:LEU:HD22	4:A:983:ILE:HB	2.00	0.44
4:A:779:PHE:CE2	5:B:517:THR:HG22	2.52	0.44
5:B:756:ILE:HA	5:B:757:PRO:HD3	1.46	0.44
5:B:782:LEU:C	5:B:784:ASN:H	2.20	0.44
8:F:97:ARG:HG3	8:F:101:ILE:CD1	2.45	0.44
11:J:7:CYS:CB	11:J:49:MET:HG2	2.30	0.44
4:A:1121:GLU:O	4:A:1125:ALA:HB2	2.18	0.44
4:A:116:ASP:CA	4:A:117:GLU:CB	2.94	0.44
4:A:102:VAL:HG11	4:A:211:PHE:CE1	2.53	0.44
4:A:768:GLN:HB3	4:A:775:ILE:HD11	2.00	0.44
5:B:1006:ILE:HG22	5:B:1007:VAL:H	1.81	0.44
5:B:1021:MET:HB2	5:B:1021:MET:HE2	1.83	0.44
5:B:1117:GLN:HA	5:B:1118:PRO:HD2	1.70	0.44
5:B:1111:MET:CE	5:B:1118:PRO:HD3	2.48	0.44
5:B:1150:ARG:CG	5:B:1150:ARG:O	2.53	0.44
5:B:102:VAL:HG21	5:B:122:LEU:HD13	1.98	0.44
5:B:256:VAL:HG12	5:B:385:LEU:HD13	1.99	0.44
5:B:555:ILE:HG12	5:B:555:ILE:H	1.53	0.44
4:A:503:GLN:NE2	8:F:90:ARG:HH12	2.14	0.44
2:T:16:DT:H3'	2:T:17:DA:C8	2.51	0.44
4:A:96:ILE:CG2	4:A:176:LYS:HE3	2.32	0.44
4:A:915:SER:OG	4:A:919:ILE:HD11	2.18	0.44
5:B:233:PRO:HG2	5:B:234:ILE:HD13	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:484:ASN:ND2	5:B:484:ASN:C	2.70	0.44
5:B:769:TYR:C	5:B:771:SER:N	2.69	0.44
6:C:120:ILE:HG22	6:C:121:VAL:H	1.83	0.44
6:C:186:LEU:N	6:C:186:LEU:CD1	2.81	0.44
7:E:130:ALA:CB	7:E:131:THR:HB	2.47	0.44
4:A:1198:ASP:OD2	4:A:1200:ALA:HB3	2.18	0.44
4:A:262:LEU:HD21	4:A:325:ILE:HD11	1.99	0.44
4:A:445:ASN:ND2	4:A:455:MET:SD	2.90	0.44
4:A:1410:PHE:HA	5:B:1212:ILE:HD11	1.98	0.44
10:I:18:GLU:HG2	10:I:20:LYS:H	1.83	0.44
12:K:60:ALA:O	12:K:73:LEU:HD12	2.18	0.44
1:R:3:G:N1	2:T:27:DT:O2	2.51	0.44
4:A:1206:ASP:HB2	4:A:1274:ARG:NH2	2.30	0.43
4:A:182:VAL:HG12	4:A:183:GLY:N	2.26	0.43
4:A:356:ASP:HA	4:A:357:PRO:HD2	1.66	0.43
4:A:401:GLY:O	4:A:435:HIS:ND1	2.46	0.43
5:B:1158:PHE:CE2	5:B:1160:VAL:HG13	2.53	0.43
5:B:782:LEU:O	5:B:784:ASN:N	2.50	0.43
6:C:41:ILE:HA	6:C:42:PRO:HD3	1.90	0.43
9:H:15:VAL:O	9:H:15:VAL:HG22	2.17	0.43
4:A:121:LEU:HA	4:A:124:GLN:NE2	2.34	0.43
4:A:16:GLU:HA	4:A:1419:ASP:O	2.18	0.43
4:A:265:LYS:HE2	4:A:302:THR:CG2	2.47	0.43
4:A:754:SER:N	4:A:757:ASN:HD22	2.07	0.43
5:B:766:ARG:HD3	5:B:766:ARG:HA	1.82	0.43
6:C:246:ARG:O	6:C:250:THR:OG1	2.34	0.43
7:E:61:GLN:HG3	7:E:105:PHE:CZ	2.52	0.43
9:H:10:PHE:HA	9:H:30:SER:HA	2.00	0.43
11:J:44:TYR:HD1	11:J:45:CYS:N	2.16	0.43
4:A:458:HIS:CE1	4:A:507:VAL:HG21	2.53	0.43
4:A:619:LYS:O	4:A:623:GLY:N	2.51	0.43
4:A:635:ARG:NH1	4:A:635:ARG:HA	2.31	0.43
12:K:40:HIS:H	12:K:40:HIS:CD2	2.35	0.43
4:A:49:LYS:C	4:A:50:ILE:HG13	2.37	0.43
4:A:567:LYS:HG3	4:A:568:PRO:HG2	2.00	0.43
4:A:920:LEU:HD23	4:A:921:GLY:H	1.82	0.43
5:B:1175:LEU:O	5:B:1176:ASN:HB3	2.18	0.43
4:A:340:LEU:CD2	5:B:1199:ALA:HB3	2.48	0.43
5:B:657:HIS:CE1	5:B:689:LEU:HD11	2.53	0.43
4:A:382:PRO:HA	4:A:385:ILE:HG22	2.01	0.43
4:A:397:ASN:HA	4:A:397:ASN:HD22	1.53	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:855:THR:O	4:A:855:THR:HG23	2.18	0.43
5:B:498:THR:CG2	5:B:499:ASN:N	2.80	0.43
5:B:578:THR:HG23	5:B:623:GLU:N	2.34	0.43
7:E:156:LEU:HD23	7:E:197:LYS:CB	2.48	0.43
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.49	0.43
5:B:850:LEU:CD1	11:J:8:PHE:HD1	2.31	0.43
4:A:746:MET:HG2	5:B:1015:HIS:CE1	2.54	0.43
5:B:1111:MET:HE1	5:B:1118:PRO:HD3	2.00	0.43
5:B:836:GLU:C	5:B:838:SER:H	2.18	0.43
5:B:842:ASN:O	5:B:845:SER:N	2.49	0.43
6:C:227:THR:C	6:C:228:PHE:CD1	2.92	0.43
7:E:161:LYS:O	7:E:162:ARG:C	2.57	0.43
7:E:167:ARG:C	7:E:169:ARG:H	2.22	0.43
9:H:83:GLN:O	9:H:85:GLY:N	2.52	0.43
10:I:101:PHE:CE1	10:I:112:SER:HB3	2.54	0.43
4:A:1394:THR:HG22	4:A:1395:GLY:N	2.29	0.43
4:A:1424:VAL:HG22	4:A:1436:ILE:HD11	1.99	0.43
4:A:315:LEU:HB3	4:A:316:GLN:H	1.30	0.43
4:A:673:GLY:O	4:A:677:ARG:HB2	2.19	0.43
5:B:26:THR:O	5:B:27:ALA:C	2.56	0.43
5:B:581:PHE:HA	5:B:585:VAL:O	2.18	0.43
5:B:858:SER:HA	5:B:967:ARG:HA	2.00	0.43
5:B:916:THR:HA	5:B:917:PRO:HD2	1.91	0.43
5:B:956:THR:HG22	13:L:54:ARG:HD3	2.01	0.43
5:B:762:ASN:OD1	5:B:984:HIS:CD2	2.72	0.43
6:C:168:ALA:C	6:C:170:TRP:N	2.72	0.43
7:E:156:LEU:CD2	7:E:197:LYS:HB2	2.49	0.43
8:F:99:LEU:HD13	8:F:99:LEU:O	2.17	0.43
4:A:1105:LEU:HD22	4:A:1384:VAL:HG21	2.01	0.43
4:A:1434:ALA:HB3	4:A:1436:ILE:HB	2.00	0.43
4:A:332:LYS:O	4:A:334:GLY:N	2.43	0.43
5:B:1033:LYS:HG2	5:B:1059:LEU:HD11	2.00	0.43
7:E:196:VAL:HG12	7:E:212:ARG:HB2	2.00	0.43
4:A:1396:ALA:HA	4:A:1399:ARG:NH2	2.34	0.43
4:A:71:GLN:O	4:A:73:GLY:N	2.52	0.43
5:B:1106:ARG:HG3	5:B:1108:ARG:O	2.19	0.43
5:B:549:THR:HG22	5:B:550:ASP:H	1.84	0.43
5:B:57:TYR:O	5:B:60:GLN:N	2.51	0.43
4:A:806:ARG:HG3	5:B:728:ARG:HA	2.01	0.43
5:B:976:ILE:CG1	5:B:991:GLY:C	2.81	0.43
6:C:186:LEU:HB2	6:C:188:HIS:CD2	2.45	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:19:ASP:O	10:I:21:GLU:N	2.44	0.43
5:B:190:TYR:CD1	11:J:62:ARG:HG2	2.53	0.43
11:J:64:ASN:N	11:J:65:PRO:HD2	2.34	0.43
13:L:32:ALA:CB	13:L:55:ILE:HB	2.46	0.43
4:A:206:GLU:O	4:A:210:ILE:HG12	2.19	0.43
4:A:535:THR:HG23	4:A:616:VAL:HA	2.00	0.43
4:A:543:LEU:HG	4:A:547:LEU:CD1	2.44	0.43
5:B:1002:THR:HG21	5:B:1006:ILE:HD12	2.00	0.43
5:B:1136:ASP:HA	5:B:1139:ILE:HD12	2.00	0.43
5:B:514:LEU:HD12	5:B:518:HIS:CD2	2.54	0.43
5:B:65:GLU:OE2	5:B:66:ASP:HB3	2.19	0.43
5:B:994:TYR:CB	5:B:999:MET:HE3	2.38	0.43
9:H:4:THR:HG22	9:H:5:LEU:N	2.33	0.43
4:A:11:LEU:HA	5:B:1193:GLN:O	2.18	0.42
4:A:325:ILE:HG12	4:A:325:ILE:H	1.55	0.42
4:A:49:LYS:CB	4:A:49:LYS:NZ	2.81	0.42
4:A:541:ILE:HG13	4:A:546:VAL:HG22	2.01	0.42
5:B:367:LEU:HB3	5:B:368:GLU:H	1.69	0.42
5:B:680:THR:O	5:B:682:SER:N	2.51	0.42
6:C:34:ARG:O	6:C:38:ILE:HG12	2.19	0.42
6:C:84:ARG:HD2	12:K:11:LEU:HD21	2.01	0.42
9:H:81:PRO:O	9:H:82:PRO:C	2.57	0.42
6:C:254:LYS:HD3	12:K:42:LEU:HD12	2.01	0.42
4:A:1029:ARG:O	4:A:1033:GLN:HB2	2.19	0.42
4:A:849:MET:HB3	4:A:1063:MET:SD	2.59	0.42
4:A:417:TYR:O	4:A:418:SER:CB	2.67	0.42
5:B:557:PHE:O	5:B:560:GLU:HB2	2.19	0.42
5:B:769:TYR:H	5:B:769:TYR:HD2	1.66	0.42
6:C:215:GLU:H	6:C:216:GLY:CA	2.25	0.42
11:J:59:LYS:O	11:J:62:ARG:HB3	2.18	0.42
4:A:1436:ILE:O	4:A:1437:GLY:C	2.56	0.42
4:A:553:VAL:HA	4:A:554:PRO:HD3	1.91	0.42
4:A:648:ASN:O	4:A:652:VAL:HG23	2.19	0.42
5:B:471:LYS:O	5:B:476:ARG:HD3	2.19	0.42
5:B:475:SER:C	5:B:477:ALA:N	2.72	0.42
7:E:61:GLN:HG3	7:E:105:PHE:CE2	2.55	0.42
9:H:30:SER:HG	9:H:36:CYS:HB3	1.85	0.42
4:A:464:PRO:CG	12:K:67:PHE:CD1	3.03	0.42
4:A:1015:VAL:CG1	4:A:1019:CYS:SG	2.94	0.42
4:A:1072:ILE:HD13	4:A:1371:LEU:HD22	2.00	0.42
4:A:146:MET:CE	4:A:146:MET:H	2.32	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:639:PRO:HD2	4:A:640:GLN:HG2	2.00	0.42
4:A:784:LEU:C	4:A:786:HIS:H	2.22	0.42
5:B:658:ILE:HA	5:B:661:LEU:HD12	2.02	0.42
5:B:942:ARG:HD2	5:B:945:GLU:CD	2.39	0.42
5:B:955:THR:CG2	5:B:956:THR:N	2.77	0.42
6:C:25:VAL:HG12	6:C:26:ASP:H	1.83	0.42
13:L:47:ARG:HG3	13:L:48:CYS:H	1.84	0.42
2:T:9:DA:H2"	2:T:10:DA:OP2	2.19	0.42
4:A:1011:GLN:NE2	4:A:1015:VAL:HG21	2.34	0.42
5:B:1009:ASP:OD2	11:J:48:ARG:NH2	2.52	0.42
5:B:346:GLU:C	5:B:348:ARG:H	2.23	0.42
5:B:594:ALA:HA	5:B:617:ARG:NH1	2.34	0.42
5:B:781:PHE:HE2	5:B:795:ILE:HD11	1.84	0.42
5:B:832:GLY:O	5:B:835:GLN:HG3	2.18	0.42
12:K:62:LYS:HG3	12:K:62:LYS:O	2.20	0.42
4:A:152:VAL:HG22	4:A:163:SER:HG	1.83	0.42
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.85	0.42
4:A:900:ASP:HA	4:A:926:GLN:HE22	1.85	0.42
5:B:601:ARG:HA	5:B:615:MET:HE1	2.02	0.42
10:I:96:SER:HB2	10:I:98:VAL:HG23	2.00	0.42
11:J:56:LEU:O	11:J:57:ILE:C	2.57	0.42
12:K:65:HIS:CD2	12:K:67:PHE:H	2.30	0.42
13:L:61:THR:HG21	13:L:63:ARG:HG3	2.01	0.42
4:A:826:ASP:HB2	4:A:1082:ASN:HD21	1.84	0.42
4:A:1335:ILE:HG23	4:A:1339:LEU:HD12	2.02	0.42
5:B:1084:GLN:NE2	6:C:191:TYR:HD2	2.17	0.42
5:B:1099:VAL:O	5:B:1103:ILE:HG12	2.19	0.42
5:B:778:MET:HE2	5:B:1094:ARG:HG3	2.02	0.42
6:C:145:CYS:SG	6:C:146:LYS:N	2.93	0.42
8:F:93:ILE:HD11	8:F:134:ILE:CD1	2.49	0.42
9:H:139:ASN:HB3	9:H:140:ALA:H	1.53	0.42
4:A:366:VAL:HA	4:A:367:PRO:HD2	1.72	0.42
4:A:589:GLN:HG3	4:A:606:LEU:HD13	2.01	0.42
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.19	0.42
5:B:1221:SER:C	5:B:1223:ASP:N	2.72	0.42
5:B:240:ILE:HG23	5:B:240:ILE:O	2.19	0.42
5:B:596:LEU:O	5:B:596:LEU:HD12	2.20	0.42
5:B:60:GLN:CA	5:B:60:GLN:HE21	2.32	0.42
5:B:805:THR:HA	5:B:809:MET:CE	2.49	0.42
5:B:970:THR:HG22	5:B:971:THR:N	2.35	0.42
6:C:186:LEU:CB	6:C:188:HIS:CD2	3.03	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:81:THR:HG23	8:F:144:GLU:OE1	2.20	0.42
10:I:89:GLN:O	10:I:91:ARG:N	2.53	0.42
2:T:26:DC:H2''	2:T:27:DT:C5'	2.50	0.42
4:A:361:LEU:HD22	4:A:646:PHE:CD1	2.55	0.42
4:A:403:LYS:C	4:A:404:TYR:CD1	2.93	0.42
5:B:1155:SER:HB3	5:B:1156:ASP:H	1.46	0.42
5:B:54:PHE:HA	5:B:58:THR:HB	2.01	0.42
5:B:653:VAL:HG23	5:B:653:VAL:H	1.58	0.42
5:B:656:GLY:O	5:B:658:ILE:N	2.52	0.42
5:B:637:LEU:HD11	5:B:740:HIS:HD2	1.82	0.42
6:C:11:ARG:NH1	6:C:209:TYR:CE1	2.88	0.42
6:C:167:HIS:HD2	6:C:168:ALA:N	2.18	0.42
6:C:254:LYS:CD	12:K:42:LEU:HD12	2.50	0.42
4:A:1072:ILE:O	4:A:1075:PRO:HD2	2.19	0.42
4:A:1220:PHE:CD1	4:A:1220:PHE:N	2.88	0.42
4:A:1337:GLU:O	7:E:183:PRO:HG3	2.20	0.42
4:A:1344:GLY:O	4:A:1345:ARG:C	2.59	0.42
4:A:211:PHE:O	4:A:214:ILE:HG12	2.19	0.42
4:A:211:PHE:CD1	4:A:231:PRO:HB2	2.51	0.42
4:A:99:ILE:CD1	4:A:234:MET:HB3	2.50	0.42
4:A:353:ILE:HD12	4:A:482:PHE:CE2	2.55	0.42
4:A:482:PHE:HD1	5:B:836:GLU:O	2.03	0.42
4:A:697:ALA:HA	4:A:702:LEU:HB2	2.01	0.42
5:B:261:ARG:HB3	5:B:262:GLU:H	1.67	0.42
5:B:34:ILE:HG21	5:B:747:MET:HE1	2.02	0.42
5:B:448:ILE:HD13	5:B:448:ILE:HA	1.63	0.42
5:B:901:PRO:HG3	5:B:952:VAL:HG23	2.02	0.42
5:B:973:ILE:N	5:B:973:ILE:HD12	2.32	0.42
7:E:180:ARG:HB2	7:E:215:MET:OXT	2.20	0.42
9:H:77:ARG:HB2	9:H:77:ARG:CZ	2.49	0.42
12:K:58:PHE:CE2	12:K:74:ARG:NE	2.74	0.42
4:A:1021:LEU:HD11	4:A:1025:ARG:NH1	2.35	0.41
4:A:79:GLY:C	4:A:243:PRO:HG3	2.36	0.41
4:A:541:ILE:H	4:A:541:ILE:HG12	1.81	0.41
4:A:921:GLY:O	4:A:922:ASP:HB3	2.20	0.41
5:B:280:ILE:HB	5:B:285:ILE:HD11	2.01	0.41
5:B:641:GLU:HG3	5:B:642:ASP:H	1.85	0.41
5:B:778:MET:O	5:B:819:ALA:CB	2.58	0.41
6:C:171:GLY:HA2	6:C:172:PRO:HD3	1.80	0.41
6:C:57:VAL:CG1	6:C:57:VAL:O	2.68	0.41
4:A:465:TYR:CE1	12:K:67:PHE:CZ	3.08	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:260:ASP:OD1	4:A:262:LEU:N	2.51	0.41
4:A:48:ALA:HB2	4:A:49:LYS:HZ3	1.83	0.41
4:A:877:HIS:CD2	4:A:877:HIS:N	2.88	0.41
4:A:344:ARG:NE	5:B:1118:PRO:O	2.37	0.41
5:B:383:ASN:C	5:B:383:ASN:ND2	2.72	0.41
5:B:757:PRO:HG3	5:B:983:ARG:NH1	2.35	0.41
6:C:31:ASN:O	6:C:35:ARG:HG3	2.20	0.41
6:C:54:ASN:CG	6:C:54:ASN:O	2.59	0.41
9:H:47:PHE:HA	9:H:48:PRO:HD2	1.94	0.41
4:A:356:ASP:OD2	12:K:65:HIS:HE1	2.03	0.41
4:A:658:LEU:HD23	4:A:659:HIS:NE2	2.34	0.41
4:A:837:ILE:HA	4:A:837:ILE:HD13	1.88	0.41
4:A:836:TYR:CE2	4:A:840:ARG:HD2	2.55	0.41
4:A:886:ILE:HD11	4:A:943:LEU:HB2	1.99	0.41
5:B:1059:LEU:HA	5:B:1059:LEU:HD12	1.81	0.41
5:B:1111:MET:HE2	5:B:1118:PRO:CA	2.50	0.41
5:B:1170:THR:O	5:B:1171:VAL:C	2.58	0.41
5:B:1188:LYS:HE3	5:B:1189:ILE:HD11	2.02	0.41
5:B:1200:ALA:HA	5:B:1203:LEU:HB3	2.01	0.41
4:A:1376:THR:HG23	7:E:212:ARG:NH2	2.35	0.41
4:A:613:ILE:HG21	9:H:102:TYR:CG	2.55	0.41
9:H:23:VAL:CG1	9:H:24:CYS:N	2.83	0.41
12:K:73:LEU:HA	12:K:73:LEU:HD12	1.83	0.41
2:T:13:DA:N3	3:N:3:DA:N1	2.69	0.41
4:A:1064:VAL:O	4:A:1064:VAL:CG1	2.65	0.41
4:A:1266:THR:O	4:A:1270:ASN:HB2	2.20	0.41
4:A:1313:LEU:O	4:A:1315:GLU:N	2.53	0.41
5:B:1074:ASN:OD1	5:B:1076:HIS:N	2.52	0.41
5:B:1072:MET:HE2	5:B:1085:ILE:HD13	2.02	0.41
5:B:984:HIS:ND1	5:B:1025:HIS:HB2	2.36	0.41
7:E:204:THR:HG23	7:E:205:SER:HB3	2.02	0.41
1:R:3:G:C4	1:R:4:A:C8	3.08	0.41
4:A:852:TYR:CD2	4:A:1060:PRO:HB2	2.56	0.41
4:A:1389:PHE:O	4:A:1392:SER:HB3	2.21	0.41
4:A:344:ARG:O	5:B:1118:PRO:HG2	2.20	0.41
4:A:614:PHE:C	4:A:614:PHE:CD1	2.94	0.41
4:A:949:ASP:N	4:A:949:ASP:OD1	2.48	0.41
5:B:1109:GLY:HA3	5:B:1110:PRO:HD2	1.91	0.41
5:B:1178:ASN:HD22	5:B:1178:ASN:HA	1.66	0.41
5:B:416:LEU:HD22	5:B:420:LEU:CD1	2.50	0.41
5:B:905:VAL:O	5:B:946:ASN:HB2	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:241:ASP:HB3	12:K:109:TRP:CE2	2.56	0.41
7:E:168:TYR:C	7:E:169:ARG:HG2	2.40	0.41
10:I:98:VAL:CG1	10:I:113:ASP:HB2	2.50	0.41
1:R:6:C:H2'	1:R:7:A:H8	1.85	0.41
4:A:1193:LEU:C	4:A:1193:LEU:HD12	2.41	0.41
4:A:16:GLU:CD	4:A:1418:LEU:HD11	2.41	0.41
4:A:399:HIS:CB	4:A:400:PRO:HD3	2.50	0.41
4:A:741:ASN:ND2	4:A:741:ASN:C	2.73	0.41
5:B:404:LYS:O	5:B:405:ARG:HD3	2.20	0.41
5:B:978:ASP:O	5:B:980:PHE:CE1	2.72	0.41
6:C:101:LEU:HB3	6:C:155:LEU:HD12	2.01	0.41
4:A:1175:SER:HA	4:A:1176:LEU:HA	1.81	0.41
4:A:243:PRO:HB2	4:A:244:PRO:CD	2.51	0.41
4:A:845:LEU:O	4:A:847:ASP:N	2.54	0.41
11:J:7:CYS:HA	11:J:49:MET:CG	2.51	0.41
12:K:65:HIS:HD2	12:K:66:PRO:CD	2.26	0.41
4:A:1030:ARG:HG2	4:A:1034:GLU:OE2	2.21	0.41
4:A:1205:LYS:HB3	4:A:1274:ARG:NH1	2.35	0.41
4:A:1141:THR:CG2	4:A:1205:LYS:HD3	2.51	0.41
4:A:455:MET:HB3	5:B:1141:HIS:HE1	1.86	0.41
4:A:811:GLN:HB2	4:A:811:GLN:HE21	1.42	0.41
5:B:817:LEU:HA	5:B:817:LEU:HD23	1.86	0.41
5:B:978:ASP:CB	5:B:980:PHE:HE1	2.34	0.41
5:B:992:ILE:HD11	12:K:67:PHE:CE2	2.55	0.41
6:C:241:ASP:CB	12:K:109:TRP:CE2	3.04	0.41
9:H:10:PHE:HE2	9:H:36:CYS:SG	2.43	0.41
5:B:956:THR:CB	13:L:46:VAL:HG21	2.43	0.41
4:A:1242:VAL:CG1	4:A:1243:VAL:N	2.84	0.41
4:A:434:ARG:NH2	4:A:440:ASP:OD1	2.46	0.41
4:A:608:ILE:O	4:A:609:ASP:O	2.38	0.41
4:A:639:PRO:CD	4:A:640:GLN:H	2.34	0.41
4:A:896:ARG:HB3	4:A:897:TYR:HD1	1.86	0.41
4:A:896:ARG:NH1	4:A:897:TYR:HE1	2.18	0.41
4:A:497:THR:HG23	5:B:1146:PHE:HA	2.02	0.41
5:B:264:SER:HA	5:B:265:SER:HB2	2.03	0.41
5:B:778:MET:HG2	5:B:794:ASN:HB3	2.02	0.41
5:B:830:TYR:HB3	5:B:831:SER:H	1.56	0.41
7:E:88:VAL:HB	7:E:116:ILE:HD13	2.02	0.41
8:F:89:GLU:HG2	8:F:134:ILE:HD12	2.03	0.41
8:F:90:ARG:O	8:F:91:ALA:C	2.57	0.41
5:B:164:LYS:O	5:B:165:VAL:HB	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:31:TRP:CZ3	5:B:747:MET:HE1	2.56	0.41
5:B:244:LEU:CD1	5:B:366:GLN:HE22	2.34	0.41
10:I:61:ASP:OD2	10:I:61:ASP:N	2.54	0.41
12:K:7:PHE:CD1	12:K:7:PHE:C	2.94	0.41
4:A:1339:LEU:CD1	7:E:147:HIS:CD2	3.03	0.41
4:A:323:LYS:HZ3	4:A:323:LYS:CA	2.34	0.41
4:A:705:LYS:HD2	4:A:713:SER:HB2	2.03	0.41
5:B:244:LEU:HD21	5:B:366:GLN:NE2	2.36	0.41
5:B:617:ARG:CG	5:B:618:ASP:N	2.83	0.41
5:B:951:GLN:O	5:B:952:VAL:CG2	2.69	0.41
5:B:848:ARG:HH22	5:B:996:ARG:NH1	2.18	0.41
6:C:134:ILE:HG23	6:C:141:GLY:H	1.85	0.41
8:F:85:MET:O	8:F:155:LEU:HD22	2.21	0.41
8:F:93:ILE:O	8:F:94:LEU:C	2.59	0.41
4:A:465:TYR:N	12:K:2:ASN:O	2.29	0.41
4:A:482:PHE:N	4:A:482:PHE:CD1	2.88	0.40
5:B:1013:ASN:HA	5:B:1014:PRO:HD2	1.70	0.40
5:B:1090:THR:O	5:B:1092:TYR:HD1	2.04	0.40
5:B:275:TYR:HB3	5:B:355:ILE:HD11	2.03	0.40
5:B:299:GLU:OE2	5:B:572:HIS:HB3	2.21	0.40
5:B:557:PHE:CZ	5:B:561:TRP:CD1	3.09	0.40
7:E:89:GLY:HA2	7:E:117:THR:HG23	2.03	0.40
9:H:45:GLU:HG2	9:H:45:GLU:O	2.20	0.40
9:H:4:THR:HG22	9:H:5:LEU:H	1.84	0.40
11:J:3:VAL:HA	11:J:4:PRO:HD2	1.94	0.40
13:L:34:CYS:O	13:L:35:SER:HB2	2.20	0.40
4:A:1004:ASN:ND2	7:E:167:ARG:HD2	2.36	0.40
4:A:315:LEU:HD23	4:A:320:ARG:NH2	2.36	0.40
4:A:376:TYR:HA	4:A:377:PRO:HD3	1.81	0.40
4:A:549:MET:O	4:A:550:LEU:C	2.56	0.40
4:A:709:THR:HG22	4:A:710:LEU:N	2.36	0.40
4:A:821:ARG:O	4:A:825:ILE:HG12	2.21	0.40
5:B:370:PHE:HD2	5:B:373:ARG:HD2	1.87	0.40
5:B:57:TYR:O	5:B:59:LEU:N	2.54	0.40
5:B:37:PHE:HD1	5:B:681:TRP:CZ2	2.39	0.40
5:B:526:GLU:OE1	5:B:752:ALA:HB3	2.21	0.40
6:C:148:ARG:H	6:C:151:GLN:HG3	1.87	0.40
9:H:139:ASN:HA	9:H:139:ASN:HD22	1.70	0.40
10:I:86:PHE:CD2	10:I:86:PHE:N	2.88	0.40
11:J:19:GLU:CA	11:J:19:GLU:OE1	2.54	0.40
13:L:46:VAL:HG12	13:L:47:ARG:N	2.35	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:4:A:C4	1:R:5:C:C5	3.10	0.40
4:A:756:ILE:HD13	4:A:756:ILE:N	2.36	0.40
5:B:1057:LYS:O	5:B:1061:GLU:HG2	2.21	0.40
5:B:46:GLN:H	5:B:46:GLN:HG3	1.63	0.40
9:H:47:PHE:HB2	9:H:95:TYR:CD1	2.50	0.40
4:A:1152:ILE:HB	10:I:44:TYR:HB3	2.03	0.40
4:A:1038:THR:O	4:A:1039:LYS:C	2.59	0.40
4:A:108:MET:O	4:A:109:HIS:CB	2.69	0.40
4:A:299:HIS:O	4:A:301:ALA:N	2.54	0.40
4:A:471:ASN:O	4:A:474:VAL:HG12	2.22	0.40
5:B:1207:LEU:HA	5:B:1207:LEU:HD23	1.79	0.40
5:B:658:ILE:HA	5:B:658:ILE:HD12	1.93	0.40
5:B:911:ILE:HD11	5:B:941:LEU:CD1	2.45	0.40
6:C:148:ARG:HB3	6:C:151:GLN:HG3	2.03	0.40
7:E:16:PHE:CZ	7:E:20:LYS:HE2	2.56	0.40
4:A:1075:PRO:O	4:A:1078:GLN:N	2.47	0.40
4:A:1407:GLU:O	4:A:1411:GLU:HG2	2.21	0.40
4:A:219:PHE:HZ	4:A:230:ARG:HD3	1.87	0.40
5:B:745:PRO:HB2	5:B:1047:PHE:CD1	2.57	0.40
5:B:825:VAL:N	5:B:1088:GLY:O	2.48	0.40
5:B:287:ARG:HA	5:B:291:ILE:O	2.22	0.40
5:B:638:PHE:HD2	5:B:653:VAL:HG21	1.86	0.40
5:B:402:GLY:HA3	5:B:695:ALA:HB3	2.04	0.40
5:B:745:PRO:O	5:B:748:ILE:HG12	2.21	0.40
9:H:118:PHE:HB2	9:H:121:LEU:HB2	2.03	0.40
12:K:47:ARG:HD2	12:K:60:ALA:HA	2.03	0.40
12:K:7:PHE:C	12:K:9:LEU:N	2.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:418:SER:OG	6:C:87:PHE:O[2_555]	1.88	0.32

## 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	
4	A	1401/1733 (81%)	1073 (77%)	223 (16%)	105 (8%)	1	7
5	B	1096/1224 (90%)	823 (75%)	190 (17%)	83 (8%)	1	7
6	C	265/318 (83%)	211 (80%)	38 (14%)	16 (6%)	1	11
7	E	212/215 (99%)	178 (84%)	25 (12%)	9 (4%)	3	19
8	F	83/155 (54%)	65 (78%)	14 (17%)	4 (5%)	2	16
9	H	129/146 (88%)	90 (70%)	25 (19%)	14 (11%)	0	3
10	I	117/122 (96%)	86 (74%)	24 (20%)	7 (6%)	1	11
11	J	63/70 (90%)	53 (84%)	6 (10%)	4 (6%)	1	10
12	K	112/120 (93%)	94 (84%)	16 (14%)	2 (2%)	8	35
13	L	44/70 (63%)	26 (59%)	12 (27%)	6 (14%)	0	1
All	All	3522/4173 (84%)	2699 (77%)	573 (16%)	250 (7%)	1	8

All (250) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	50	ILE
4	A	56	PRO
4	A	68	GLN
4	A	69	THR
4	A	72	GLU
4	A	76	GLU
4	A	89	PRO
4	A	93	VAL
4	A	109	HIS
4	A	118	HIS
4	A	130	ASP
4	A	182	VAL
4	A	255	SER
4	A	282	ASN
4	A	312	PRO
4	A	315	LEU
4	A	423	ASP
4	A	426	LEU
4	A	485	ASP
4	A	567	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	610	GLY
4	A	760	GLN
4	A	793	SER
4	A	801	GLU
4	A	880	LYS
4	A	916	GLY
4	A	1221	LYS
5	B	25	ILE
5	B	27	ALA
5	B	66	ASP
5	B	67	SER
5	B	264	SER
5	B	266	ALA
5	B	347	LYS
5	B	469	GLN
5	B	476	ARG
5	B	648	HIS
5	B	649	LYS
5	B	681	TRP
5	B	711	GLU
5	B	731	VAL
5	B	766	ARG
5	B	783	THR
5	B	837	ASP
5	B	863	GLU
5	B	870	ILE
5	B	881	ASN
5	B	989	THR
5	B	1055	ILE
5	B	1096	ARG
5	B	1157	ALA
5	B	1171	VAL
5	B	1181	GLU
6	C	55	THR
6	C	142	VAL
7	E	131	THR
7	E	163	GLU
9	H	77	ARG
9	H	109	LYS
9	H	136	LYS
10	I	51	ASN
10	I	54	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
10	I	69	PRO
12	K	70	ARG
13	L	42	ARG
13	L	64	LEU
4	A	40	THR
4	A	46	THR
4	A	49	LYS
4	A	65	LEU
4	A	74	MET
4	A	149	GLU
4	A	168	GLY
4	A	219	PHE
4	A	250	ILE
4	A	254	GLU
4	A	283	GLY
4	A	291	GLU
4	A	364	VAL
4	A	404	TYR
4	A	410	GLY
4	A	419	LYS
4	A	466	SER
4	A	536	LEU
4	A	609	ASP
4	A	759	ALA
4	A	846	GLU
4	A	1081	LEU
4	A	1083	THR
4	A	1234	GLU
4	A	1314	SER
4	A	1375	MET
4	A	1394	THR
4	A	1416	ALA
4	A	1447	GLU
5	B	38	PHE
5	B	58	THR
5	B	68	THR
5	B	137	TYR
5	B	165	VAL
5	B	364	ILE
5	B	369	GLY
5	B	371	GLU
5	B	411	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	B	465	ASN
5	B	480	SER
5	B	516	ASN
5	B	765	PRO
5	B	880	THR
5	B	1046	PRO
5	B	1054	GLY
5	B	1150	ARG
5	B	1221	SER
6	C	32	SER
6	C	196	ASP
6	C	225	ALA
7	E	56	LYS
7	E	162	ARG
7	E	168	TYR
8	F	110	ASP
9	H	18	GLY
9	H	34	ASP
9	H	61	SER
9	H	62	SER
9	H	82	PRO
9	H	84	ALA
9	H	111	LEU
9	H	131	ASN
10	I	47	GLU
11	J	2	ILE
11	J	6	ARG
12	K	10	PHE
13	L	46	VAL
13	L	55	ILE
4	A	55	ASP
4	A	117	GLU
4	A	119	ASN
4	A	245	PRO
4	A	285	PRO
4	A	297	GLN
4	A	316	GLN
4	A	483	ASP
4	A	486	GLU
4	A	509	LEU
4	A	1166	ASP
4	A	1438	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	B	111	ALA
5	B	139	ALA
5	B	261	ARG
5	B	650	GLU
5	B	733	HIS
5	B	786	ASN
5	B	865	LYS
5	B	879	ARG
5	B	977	GLY
5	B	978	ASP
5	B	1017	ILE
5	B	1118	PRO
5	B	1155	SER
5	B	1211	ASN
6	C	214	ASN
6	C	227	THR
7	E	76	GLY
8	F	73	ALA
8	F	104	ASN
8	F	154	ASP
9	H	3	ASN
9	H	132	LEU
10	I	90	GLN
10	I	91	ARG
11	J	58	GLU
13	L	45	ALA
13	L	59	ALA
4	A	44	THR
4	A	54	ASN
4	A	318	SER
4	A	332	LYS
4	A	335	ARG
4	A	336	ILE
4	A	597	LEU
5	B	231	PRO
5	B	278	GLN
5	B	467	GLY
5	B	531	GLN
5	B	559	SER
5	B	792	MET
5	B	976	ILE
5	B	1086	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	B	1102	LYS
6	C	90	ASP
6	C	121	VAL
6	C	181	ASP
7	E	3	GLN
10	I	3	THR
4	A	35	ILE
4	A	120	GLU
4	A	214	ILE
4	A	248	PRO
4	A	418	SER
4	A	424	ILE
4	A	592	ASP
4	A	634	THR
4	A	677	ARG
4	A	1218	GLN
5	B	276	ILE
5	B	288	ALA
5	B	563	MET
5	B	646	LEU
6	C	206	ASN
6	C	213	PRO
6	C	231	ASN
9	H	19	ARG
11	J	19	GLU
4	A	325	ILE
4	A	395	GLY
4	A	465	TYR
4	A	568	PRO
4	A	569	LYS
4	A	599	SER
4	A	724	GLU
5	B	292	ILE
5	B	471	LYS
5	B	484	ASN
6	C	60	ASP
6	C	129	ILE
7	E	93	MET
4	A	183	GLY
4	A	785	PRO
4	A	848	ILE
4	A	986	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	B	725	PRO
5	B	1172	ILE
5	B	1184	GLY
7	E	183	PRO
4	A	399	HIS
4	A	632	VAL
4	A	958	VAL
4	A	1437	GLY
5	B	260	GLY
5	B	263	GLY
5	B	750	GLY
5	B	991	GLY
4	A	583	PRO
4	A	1107	VAL
5	B	410	GLY
4	A	27	VAL
4	A	308	ILE
4	A	639	PRO
5	B	290	GLY
6	C	202	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1231/1520 (81%)	1008 (82%)	223 (18%)	1	7
5	B	967/1061 (91%)	774 (80%)	193 (20%)	1	4
6	C	235/274 (86%)	205 (87%)	30 (13%)	4	18
7	E	196/197 (100%)	164 (84%)	32 (16%)	2	10
8	F	75/137 (55%)	70 (93%)	5 (7%)	16	47
9	H	117/128 (91%)	93 (80%)	24 (20%)	1	4
10	I	113/116 (97%)	97 (86%)	16 (14%)	3	14
11	J	60/65 (92%)	46 (77%)	14 (23%)	1	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	99/102 (97%)	88 (89%)	11 (11%)	6	24
13	L	40/57 (70%)	30 (75%)	10 (25%)	0	2
All	All	3133/3657 (86%)	2575 (82%)	558 (18%)	2	7

All (558) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	11	LEU
4	A	28	ARG
4	A	30	ILE
4	A	32	VAL
4	A	41	MET
4	A	43	GLU
4	A	49	LYS
4	A	50	ILE
4	A	54	ASN
4	A	58	LEU
4	A	61	ILE
4	A	68	GLN
4	A	69	THR
4	A	70	CYS
4	A	74	MET
4	A	86	LEU
4	A	93	VAL
4	A	99	ILE
4	A	119	ASN
4	A	121	LEU
4	A	124	GLN
4	A	126	LEU
4	A	133	LYS
4	A	140	THR
4	A	143	LYS
4	A	146	MET
4	A	173	THR
4	A	179	LEU
4	A	201	VAL
4	A	208	LEU
4	A	209	ASN
4	A	218	ASP
4	A	222	LEU
4	A	227	VAL

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
4	A	249	SER
4	A	252	PHE
4	A	253	ASN
4	A	265	LYS
4	A	266	LEU
4	A	271	LYS
4	A	274	ILE
4	A	278	THR
4	A	282	ASN
4	A	298	PHE
4	A	302	THR
4	A	315	LEU
4	A	318	SER
4	A	320	ARG
4	A	323	LYS
4	A	330	LYS
4	A	335	ARG
4	A	350	ARG
4	A	374	LEU
4	A	375	THR
4	A	383	TYR
4	A	385	ILE
4	A	386	ASP
4	A	403	LYS
4	A	404	TYR
4	A	409	SER
4	A	416	ARG
4	A	424	ILE
4	A	427	GLN
4	A	428	TYR
4	A	434	ARG
4	A	438	ASP
4	A	440	ASP
4	A	443	LEU
4	A	450	LEU
4	A	451	HIS
4	A	452	LYS
4	A	455	MET
4	A	466	SER
4	A	467	THR
4	A	469	ARG
4	A	472	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	475	THR
4	A	482	PHE
4	A	485	ASP
4	A	496	GLU
4	A	501	LEU
4	A	505	CYS
4	A	513	SER
4	A	518	LYS
4	A	529	CYS
4	A	532	ARG
4	A	535	THR
4	A	541	ILE
4	A	544	ASP
4	A	567	LYS
4	A	597	LEU
4	A	598	LEU
4	A	612	ILE
4	A	618	GLU
4	A	629	LEU
4	A	635	ARG
4	A	637	LYS
4	A	663	SER
4	A	666	ILE
4	A	669	THR
4	A	679	ILE
4	A	688	LYS
4	A	695	LYS
4	A	702	LEU
4	A	708	MET
4	A	710	LEU
4	A	716	ASP
4	A	720	ARG
4	A	722	LEU
4	A	740	LEU
4	A	741	ASN
4	A	760	GLN
4	A	764	CYS
4	A	770	VAL
4	A	771	GLU
4	A	774	ARG
4	A	777	PHE
4	A	797	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	801	GLU
4	A	805	LEU
4	A	806	ARG
4	A	809	THR
4	A	811	GLN
4	A	821	ARG
4	A	826	ASP
4	A	830	LYS
4	A	834	THR
4	A	838	GLN
4	A	839	ARG
4	A	859	SER
4	A	878	ILE
4	A	880	LYS
4	A	882	SER
4	A	895	LYS
4	A	896	ARG
4	A	920	LEU
4	A	927	VAL
4	A	935	GLN
4	A	938	LYS
4	A	941	LYS
4	A	948	VAL
4	A	960	ILE
4	A	961	ARG
4	A	969	GLN
4	A	974	ASP
4	A	976	THR
4	A	981	LEU
4	A	982	THR
4	A	984	LYS
4	A	985	ASP
4	A	990	VAL
4	A	1000	LEU
4	A	1022	LEU
4	A	1029	ARG
4	A	1035	TYR
4	A	1037	LEU
4	A	1047	SER
4	A	1067	LEU
4	A	1080	THR
4	A	1083	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	1084	PHE
4	A	1094	VAL
4	A	1095	THR
4	A	1109	LYS
4	A	1110	ASN
4	A	1111	MET
4	A	1113	THR
4	A	1121	GLU
4	A	1129	GLU
4	A	1135	ARG
4	A	1141	THR
4	A	1146	VAL
4	A	1159	ARG
4	A	1161	THR
4	A	1163	ILE
4	A	1168	GLU
4	A	1170	ILE
4	A	1172	LEU
4	A	1174	PHE
4	A	1193	LEU
4	A	1199	ARG
4	A	1215	ARG
4	A	1219	THR
4	A	1220	PHE
4	A	1221	LYS
4	A	1237	ILE
4	A	1240	CYS
4	A	1243	VAL
4	A	1255	GLU
4	A	1256	GLU
4	A	1259	MET
4	A	1264	GLU
4	A	1266	THR
4	A	1270	ASN
4	A	1274	ARG
4	A	1277	GLU
4	A	1280	GLU
4	A	1297	GLU
4	A	1308	THR
4	A	1322	ILE
4	A	1325	THR
4	A	1333	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	1334	ASP
4	A	1354	ASN
4	A	1355	VAL
4	A	1359	ASP
4	A	1361	SER
4	A	1366	ARG
4	A	1372	VAL
4	A	1376	THR
4	A	1382	THR
4	A	1385	THR
4	A	1386	ARG
4	A	1391	ARG
4	A	1392	SER
4	A	1393	ASN
4	A	1398	MET
4	A	1400	CYS
4	A	1406	VAL
4	A	1426	GLU
4	A	1444	MET
4	A	1447	GLU
4	A	1449	SER
5	B	22	SER
5	B	43	LEU
5	B	46	GLN
5	B	60	GLN
5	B	66	ASP
5	B	89	GLU
5	B	98	THR
5	B	108	VAL
5	B	109	THR
5	B	112	LEU
5	B	138	GLU
5	B	164	LYS
5	B	175	ARG
5	B	183	GLU
5	B	191	LYS
5	B	199	MET
5	B	202	TYR
5	B	217	ARG
5	B	223	VAL
5	B	232	SER
5	B	234	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	B	244	LEU
5	B	248	SER
5	B	249	ARG
5	B	261	ARG
5	B	268	THR
5	B	275	TYR
5	B	276	ILE
5	B	291	ILE
5	B	296	GLU
5	B	300	HIS
5	B	305	VAL
5	B	311	LEU
5	B	333	PHE
5	B	345	LYS
5	B	346	GLU
5	B	355	ILE
5	B	366	GLN
5	B	372	SER
5	B	383	ASN
5	B	384	ARG
5	B	391	ASP
5	B	398	ARG
5	B	408	LEU
5	B	416	LEU
5	B	429	PHE
5	B	430	ARG
5	B	437	GLU
5	B	448	ILE
5	B	449	ASN
5	B	451	LYS
5	B	459	TYR
5	B	463	THR
5	B	468	GLU
5	B	469	GLN
5	B	471	LYS
5	B	474	SER
5	B	480	SER
5	B	484	ASN
5	B	485	ARG
5	B	489	SER
5	B	498	THR
5	B	500	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	B	527	THR
5	B	533	CYS
5	B	547	VAL
5	B	549	THR
5	B	555	ILE
5	B	563	MET
5	B	568	ASP
5	B	579	ARG
5	B	581	PHE
5	B	591	ARG
5	B	602	THR
5	B	604	ARG
5	B	612	GLU
5	B	613	VAL
5	B	620	ARG
5	B	623	GLU
5	B	625	LYS
5	B	626	ILE
5	B	628	THR
5	B	635	ARG
5	B	642	ASP
5	B	646	LEU
5	B	649	LYS
5	B	651	LEU
5	B	655	LYS
5	B	667	GLN
5	B	668	ASP
5	B	706	GLN
5	B	708	GLU
5	B	730	ARG
5	B	731	VAL
5	B	732	SER
5	B	751	VAL
5	B	762	ASN
5	B	769	TYR
5	B	782	LEU
5	B	783	THR
5	B	786	ASN
5	B	790	ASP
5	B	791	THR
5	B	792	MET
5	B	801	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	B	807	ARG
5	B	812	LEU
5	B	815	ARG
5	B	827	ILE
5	B	829	CYS
5	B	831	SER
5	B	838	SER
5	B	843	GLN
5	B	844	SER
5	B	871	THR
5	B	878	GLN
5	B	879	ARG
5	B	880	THR
5	B	881	ASN
5	B	882	THR
5	B	885	MET
5	B	886	LYS
5	B	889	THR
5	B	894	ASP
5	B	904	ARG
5	B	905	VAL
5	B	909	ASP
5	B	916	THR
5	B	918	ILE
5	B	938	SER
5	B	941	LEU
5	B	944	THR
5	B	956	THR
5	B	959	ASP
5	B	963	PHE
5	B	964	VAL
5	B	967	ARG
5	B	969	ARG
5	B	972	LYS
5	B	973	ILE
5	B	989	THR
5	B	995	ARG
5	B	996	ARG
5	B	997	GLU
5	B	999	MET
5	B	1007	VAL
5	B	1010	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	B	1022	THR
5	B	1029	CYS
5	B	1034	VAL
5	B	1037	LEU
5	B	1050	ILE
5	B	1052	VAL
5	B	1057	LYS
5	B	1060	ARG
5	B	1065	GLN
5	B	1090	THR
5	B	1091	TYR
5	B	1094	ARG
5	B	1095	LEU
5	B	1096	ARG
5	B	1099	VAL
5	B	1101	ASP
5	B	1102	LYS
5	B	1111	MET
5	B	1113	VAL
5	B	1122	ARG
5	B	1125	ASP
5	B	1134	GLU
5	B	1137	CYS
5	B	1138	MET
5	B	1147	LEU
5	B	1148	LYS
5	B	1150	ARG
5	B	1155	SER
5	B	1159	ARG
5	B	1160	VAL
5	B	1162	ILE
5	B	1176	ASN
5	B	1178	ASN
5	B	1185	CYS
5	B	1186	ASP
5	B	1188	LYS
5	B	1189	ILE
5	B	1191	ILE
5	B	1194	ILE
5	B	1196	ILE
5	B	1202	LEU
5	B	1203	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	B	1220	ARG
5	B	1221	SER
5	B	1222	ARG
5	B	1223	ASP
6	C	15	LYS
6	C	16	ASP
6	C	18	VAL
6	C	33	LEU
6	C	66	ARG
6	C	77	ILE
6	C	78	GLU
6	C	79	GLN
6	C	86	CYS
6	C	93	ASP
6	C	106	GLU
6	C	109	SER
6	C	137	LYS
6	C	140	ASN
6	C	143	LEU
6	C	145	CYS
6	C	163	ILE
6	C	166	GLU
6	C	170	TRP
6	C	186	LEU
6	C	193	TYR
6	C	199	LYS
6	C	221	TYR
6	C	231	ASN
6	C	240	VAL
6	C	241	ASP
6	C	250	THR
6	C	251	LEU
6	C	254	LYS
6	C	258	ILE
7	E	3	GLN
7	E	20	LYS
7	E	31	THR
7	E	45	LYS
7	E	48	ASP
7	E	54	GLN
7	E	72	PHE
7	E	83	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	E	87	SER
7	E	92	THR
7	E	95	THR
7	E	98	ILE
7	E	100	ILE
7	E	101	GLN
7	E	104	ASN
7	E	106	GLN
7	E	107	THR
7	E	119	SER
7	E	122	LYS
7	E	127	ILE
7	E	146	HIS
7	E	150	VAL
7	E	162	ARG
7	E	164	LEU
7	E	165	LEU
7	E	166	LYS
7	E	169	ARG
7	E	171	LYS
7	E	177	ARG
7	E	192	ARG
7	E	204	THR
7	E	210	SER
8	F	74	ILE
8	F	87	LYS
8	F	111	LEU
8	F	153	VAL
8	F	155	LEU
9	H	2	SER
9	H	3	ASN
9	H	11	GLN
9	H	15	VAL
9	H	24	CYS
9	H	31	THR
9	H	35	GLN
9	H	52	GLN
9	H	76	THR
9	H	77	ARG
9	H	83	GLN
9	H	86	ASP
9	H	91	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	H	92	ASP
9	H	95	TYR
9	H	109	LYS
9	H	110	ASP
9	H	114	VAL
9	H	121	LEU
9	H	130	ARG
9	H	132	LEU
9	H	136	LYS
9	H	138	GLU
9	H	139	ASN
10	I	3	THR
10	I	20	LYS
10	I	29	CYS
10	I	31	THR
10	I	55	THR
10	I	60	GLN
10	I	70	ARG
10	I	71	SER
10	I	75	CYS
10	I	78	CYS
10	I	84	VAL
10	I	90	GLN
10	I	95	THR
10	I	115	LYS
10	I	118	ARG
10	I	119	THR
11	J	2	ILE
11	J	5	VAL
11	J	7	CYS
11	J	9	SER
11	J	13	VAL
11	J	14	VAL
11	J	19	GLU
11	J	24	LEU
11	J	41	LEU
11	J	43	ARG
11	J	44	TYR
11	J	48	ARG
11	J	49	MET
11	J	52	THR
12	K	5	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	K	6	ARG
12	K	12	LEU
12	K	18	LYS
12	K	20	LYS
12	K	47	ARG
12	K	78	THR
12	K	91	CYS
12	K	103	THR
12	K	107	THR
12	K	114	LEU
13	L	27	LEU
13	L	33	GLU
13	L	34	CYS
13	L	42	ARG
13	L	43	THR
13	L	47	ARG
13	L	50	ASP
13	L	51	CYS
13	L	55	ILE
13	L	61	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	54	ASN
4	A	68	GLN
4	A	92	HIS
4	A	119	ASN
4	A	225	ASN
4	A	253	ASN
4	A	282	ASN
4	A	306	ASN
4	A	397	ASN
4	A	399	HIS
4	A	445	ASN
4	A	447	GLN
4	A	503	GLN
4	A	515	GLN
4	A	517	ASN
4	A	545	GLN
4	A	631	HIS
4	A	741	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	757	ASN
4	A	760	GLN
4	A	767	GLN
4	A	811	GLN
4	A	877	HIS
4	A	926	GLN
4	A	935	GLN
4	A	965	GLN
4	A	969	GLN
4	A	1078	GLN
4	A	1082	ASN
4	A	1085	HIS
4	A	1110	ASN
4	A	1187	GLN
4	A	1278	ASN
4	A	1330	ASN
4	A	1364	ASN
4	A	1432	GLN
5	B	60	GLN
5	B	115	GLN
5	B	178	ASN
5	B	215	GLN
5	B	255	GLN
5	B	366	GLN
5	B	383	ASN
5	B	449	ASN
5	B	484	ASN
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	657	HIS
5	B	744	HIS
5	B	822	ASN
5	B	842	ASN
5	B	881	ASN
5	B	1015	HIS
5	B	1040	ASN
5	B	1062	HIS
5	B	1084	GLN
5	B	1161	HIS
5	B	1178	ASN
6	C	31	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	C	65	HIS
6	C	73	GLN
6	C	112	ASN
6	C	123	ASN
6	C	167	HIS
6	C	188	HIS
6	C	214	ASN
6	C	231	ASN
6	C	242	GLN
7	E	5	ASN
7	E	8	ASN
7	E	61	GLN
7	E	99	HIS
7	E	104	ASN
7	E	147	HIS
9	H	33	GLN
9	H	43	ASN
9	H	52	GLN
9	H	131	ASN
9	H	137	GLN
9	H	139	ASN
10	I	83	ASN
10	I	90	GLN
10	I	114	GLN
10	I	116	ASN
10	I	120	GLN
12	K	65	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/10 (100%)	3 (30%)	1 (10%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	A
1	R	3	G
1	R	8	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	A

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	G2P	T	3000	-	26,34,34	2.60	8 (30%)	30,54,54	1.56	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
14	G2P	T	3000	-	-	3/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	3000	G2P	C5-C6	-8.02	1.39	1.52
14	T	3000	G2P	C4-N9	-6.71	1.38	1.47
14	T	3000	G2P	PB-O3B	4.10	1.62	1.58
14	T	3000	G2P	PA-O5'	3.03	1.61	1.57

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	3000	G2P	C8-N9	-2.43	1.37	1.45
14	T	3000	G2P	C6-N1	2.31	1.37	1.33
14	T	3000	G2P	PA-O1A	-2.31	1.51	1.56
14	T	3000	G2P	C5-C4	-2.28	1.39	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	3000	G2P	C4-C5-N7	4.27	108.12	102.46
14	T	3000	G2P	PG-O3B-PB	-3.48	120.37	132.62
14	T	3000	G2P	O4'-C4'-C5'	3.12	119.65	109.37
14	T	3000	G2P	O5'-C5'-C4'	2.42	117.32	108.99
14	T	3000	G2P	O6-C6-N1	-2.41	119.45	122.69

There are no chirality outliers.

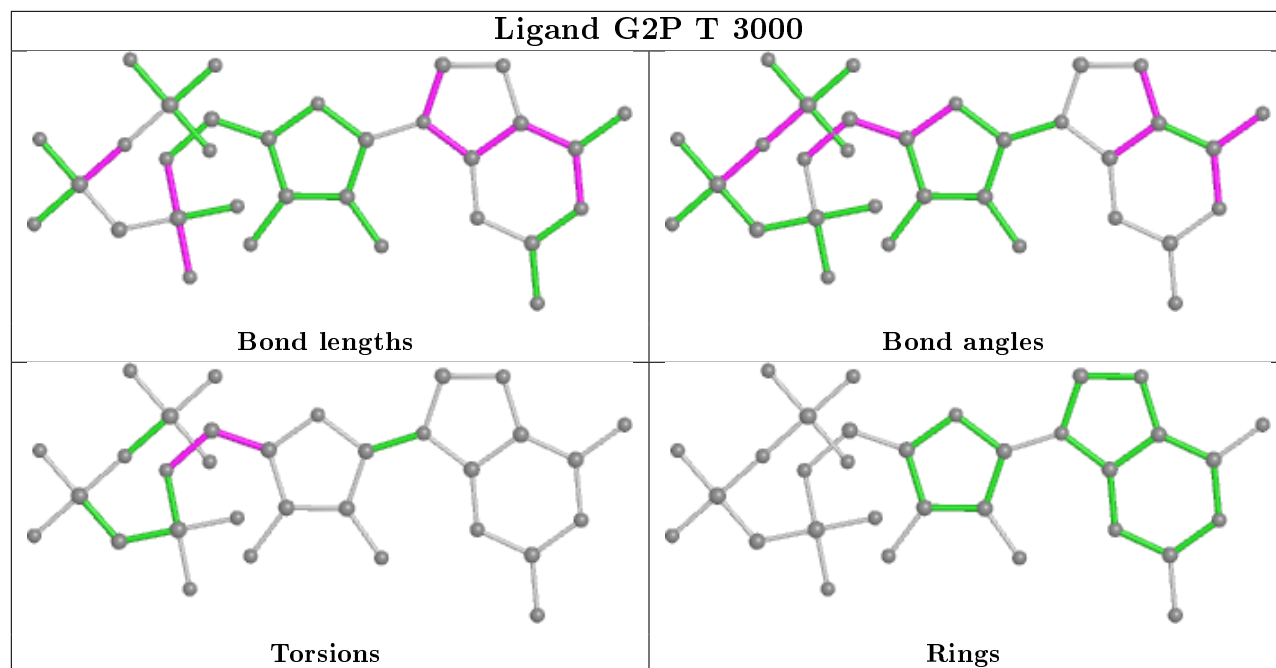
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	T	3000	G2P	O4'-C4'-C5'-O5'
14	T	3000	G2P	C3'-C4'-C5'-O5'
14	T	3000	G2P	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	R	10/10 (100%)	-0.60	0 <span>100</span> <span>100</span>	76, 118, 173, 179	0
2	T	21/21 (100%)	0.38	3 (14%) <span>2</span> <span>3</span>	100, 128, 234, 236	0
3	N	7/7 (100%)	1.52	2 (28%) <span>0</span> <span>0</span>	225, 230, 244, 248	0
4	A	1411/1733 (81%)	0.06	49 (3%) <span>44</span> <span>46</span>	83, 119, 142, 195	0
5	B	1114/1224 (91%)	0.18	30 (2%) <span>54</span> <span>57</span>	76, 121, 146, 177	0
6	C	267/318 (83%)	-0.08	3 (1%) <span>80</span> <span>84</span>	104, 119, 141, 159	0
7	E	214/215 (99%)	0.15	11 (5%) <span>28</span> <span>30</span>	100, 124, 146, 151	0
8	F	85/155 (54%)	-0.16	0 <span>100</span> <span>100</span>	107, 126, 146, 152	0
9	H	133/146 (91%)	0.14	4 (3%) <span>50</span> <span>53</span>	115, 134, 153, 156	0
10	I	119/122 (97%)	-0.01	0 <span>100</span> <span>100</span>	101, 122, 146, 158	0
11	J	65/70 (92%)	-0.03	0 <span>100</span> <span>100</span>	94, 118, 138, 145	0
12	K	114/120 (95%)	-0.09	0 <span>100</span> <span>100</span>	114, 123, 134, 140	0
13	L	46/70 (65%)	0.52	5 (10%) <span>5</span> <span>6</span>	131, 170, 177, 179	0
All	All	3606/4211 (85%)	0.09	107 (2%) <span>50</span> <span>53</span>	76, 121, 147, 248	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	1	DG	6.0
5	B	474	SER	5.5
4	A	1085	HIS	5.4
4	A	1089	VAL	5.2
4	A	175	ARG	5.1
4	A	69	THR	5.0
4	A	1088	GLY	5.0
7	E	2	ASP	4.8
5	B	883	LEU	4.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	B	1224	PHE	4.6
13	L	45	ALA	4.6
4	A	1090	ALA	4.3
4	A	151	ASP	4.0
4	A	154	SER	4.0
4	A	1176	LEU	3.9
4	A	250	ILE	3.9
4	A	141	LEU	3.8
6	C	213	PRO	3.6
2	T	10	DA	3.6
5	B	645	SER	3.4
13	L	38	LEU	3.4
4	A	341	MET	3.3
5	B	136	THR	3.3
5	B	1221	SER	3.3
5	B	709	ASP	3.2
7	E	121	MET	3.2
7	E	118	PRO	3.2
4	A	150	THR	3.2
4	A	153	PRO	3.2
13	L	27	LEU	3.1
4	A	286	HIS	3.0
4	A	257	ARG	3.0
4	A	146	MET	3.0
4	A	147	VAL	3.0
4	A	278	THR	3.0
5	B	1223	ASP	3.0
4	A	176	LYS	3.0
4	A	1083	THR	2.9
7	E	122	LYS	2.9
4	A	152	VAL	2.8
7	E	49	SER	2.8
4	A	162	VAL	2.8
4	A	1091	SER	2.8
5	B	134	LYS	2.7
9	H	132	LEU	2.7
4	A	1082	ASN	2.7
4	A	149	GLU	2.7
3	N	2	DT	2.6
5	B	869	SER	2.6
2	T	12	DT	2.6
4	A	256	GLN	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
5	B	666	TYR	2.5
2	T	9	DA	2.5
5	B	246	LYS	2.5
5	B	249	ARG	2.5
7	E	50	MET	2.5
5	B	868	MET	2.5
7	E	93	MET	2.5
4	A	1175	SER	2.5
5	B	714	GLU	2.4
4	A	1449	SER	2.4
4	A	163	SER	2.4
4	A	45	GLN	2.4
4	A	144	THR	2.4
5	B	141	ASP	2.4
5	B	429	PHE	2.4
13	L	26	THR	2.4
5	B	998	ASP	2.4
5	B	1190	ASP	2.4
4	A	285	PRO	2.4
13	L	25	ALA	2.4
4	A	426	LEU	2.4
9	H	85	GLY	2.3
7	E	110	PHE	2.3
9	H	86	ASP	2.3
4	A	44	THR	2.3
5	B	132	VAL	2.3
6	C	214	ASN	2.3
4	A	142	CYS	2.3
4	A	1087	ALA	2.3
5	B	842	ASN	2.3
4	A	1084	PHE	2.3
5	B	844	SER	2.3
9	H	112	ILE	2.2
6	C	4	GLU	2.2
5	B	1191	ILE	2.2
4	A	660	ASN	2.2
5	B	472	ALA	2.2
4	A	105	CYS	2.2
7	E	123	LEU	2.2
7	E	94	LYS	2.2
7	E	86	PRO	2.2
4	A	284	ALA	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	A	1234	GLU	2.1
5	B	1078	GLY	2.1
5	B	647	GLY	2.1
5	B	92	PHE	2.1
4	A	1108	ALA	2.1
4	A	173	THR	2.1
4	A	145	LYS	2.1
4	A	318	SER	2.1
5	B	509	ALA	2.0
5	B	1180	PHE	2.0
5	B	1189	ILE	2.0
4	A	1451	VAL	2.0
4	A	57	ARG	2.0
4	A	280	GLU	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

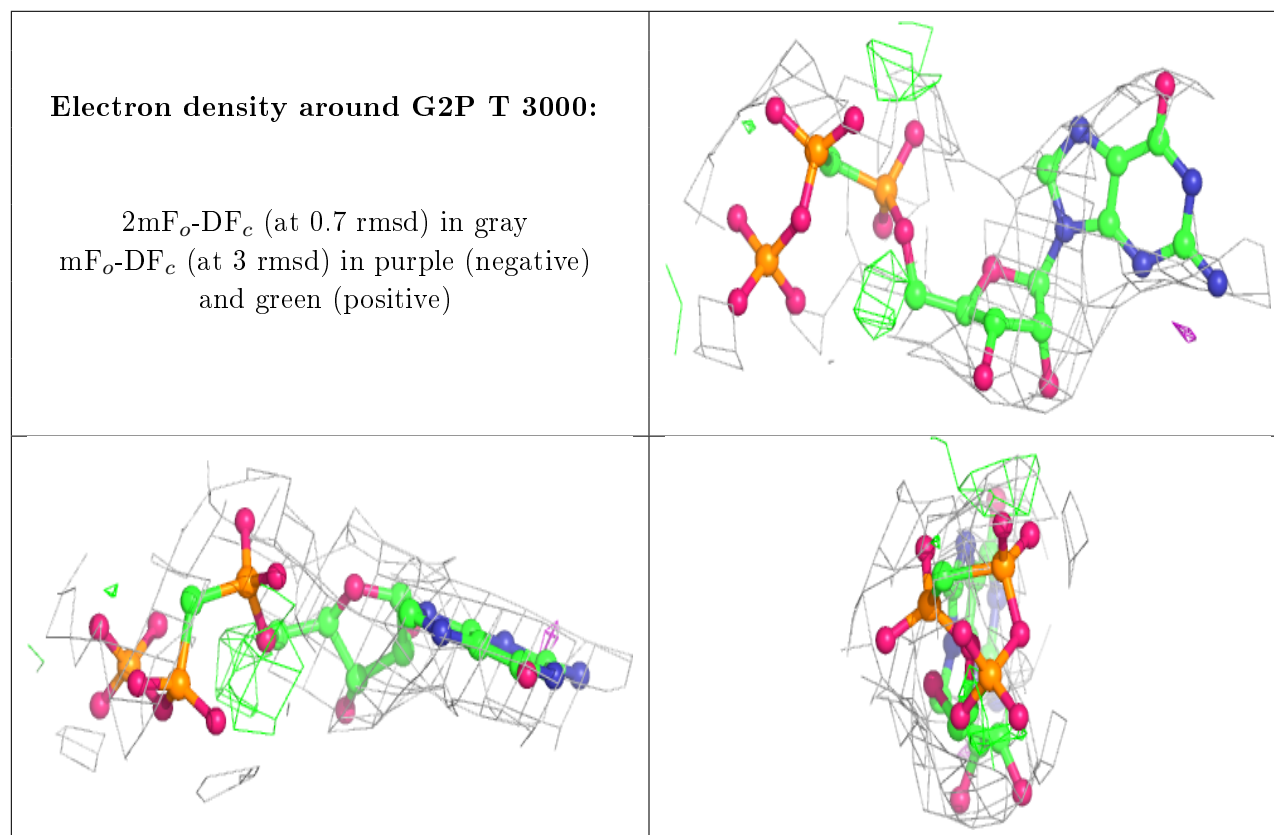
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	G2P	T	3000	32/32	0.85	0.27	120,126,149,149	0
15	ZN	A	1734	1/1	0.86	0.07	141,141,141,141	0
16	MG	A	2002	1/1	0.93	0.61	79,79,79,79	0
15	ZN	A	1735	1/1	0.94	0.09	141,141,141,141	0
15	ZN	B	1307	1/1	0.94	0.07	134,134,134,134	0
15	ZN	L	105	1/1	0.94	0.04	170,170,170,170	0
15	ZN	I	204	1/1	0.96	0.04	128,128,128,128	0
15	ZN	I	203	1/1	0.97	0.11	114,114,114,114	0
16	MG	A	2003	1/1	0.98	0.15	50,50,50,50	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	ZN	J	101	1/1	0.99	0.18	107,107,107,107	0
15	ZN	C	319	1/1	0.99	0.07	120,120,120,120	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.