



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 09:38 pm BST

PDB ID : 2NVX  
Title : RNA polymerase II elongation complex in 5 mM Mg+2 with 2'-dUTP  
Authors : Wang, D.; Bushnell, D.A.; Westover, K.D.; Kaplan, C.D.; Kornberg, R.D.  
Deposited on : 2006-11-13  
Resolution : 3.60 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

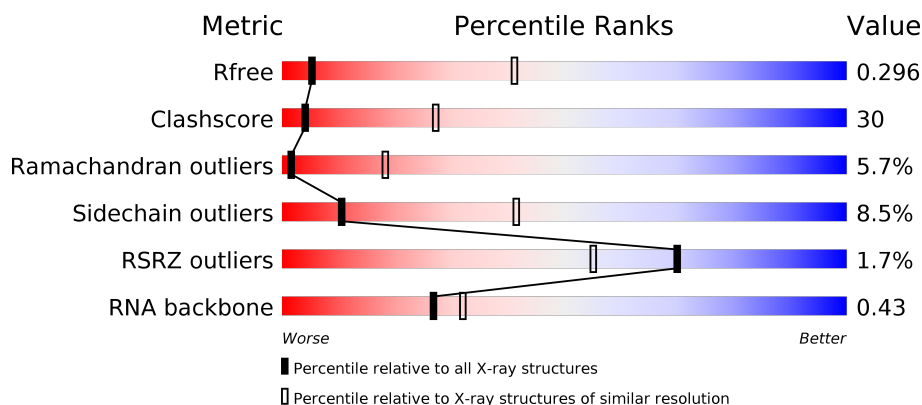
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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	 20% 70% 10%
2	N	14	 21% 93% 7%
3	T	28	 25% 46% 32% 21%
4	A	1733	 44% 29% 6% 19%

*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><div></div><div></div><div></div><div></div></div><div>48%35%7%9%</div></div>
6	C	318	<div><div><div></div><div></div><div></div><div></div></div><div>48%30%5%16%</div></div>
7	E	215	<div><div><div></div><div></div><div></div><div></div></div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>72%27%</div></div>
8	F	155	<div><div><div></div><div></div><div></div><div></div></div><div>38%15%43%</div></div>
9	H	146	<div><div><div></div><div></div><div></div><div></div></div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>55%31%6%8%</div></div>
10	I	122	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>71%24%</div></div>
11	J	70	<div><div><div></div><div></div><div></div><div></div></div><div>53%33%7%7%</div></div>
12	K	120	<div><div><div></div><div></div><div></div><div></div></div><div>67%27%5%</div></div>
13	L	70	<div><div><div></div><div></div><div></div><div></div></div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>40%21%34%</div></div>

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29436 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\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			216	98	45	64	9			

- Molecule 2 is a DNA chain called 5'-D(\*CP\*TP\*GP\*CP\*TP\*TP\*AP\*TP\*CP\*GP\*GP\*TP\*AP\*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

- Molecule 3 is a DNA chain called 28-MER DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1402	Total	C	N	O	S	0	0	0
			11028	6950	1934	2083	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
			8856	5605	1553	1644	54			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	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	88	Total	C	N	O	S	0	0	0
			712	455	120	134	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	134	Total	C	N	O	S	0	0	0
			1076	678	181	212	5			

- 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
			364	224	72	64	4			

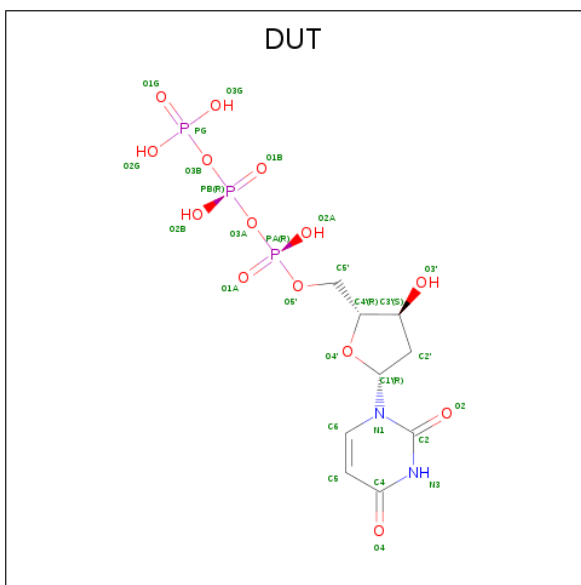
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		

- Molecule 16 is DEOXYURIDINE-5'-TRIPHOSPHATE (three-letter code: DUT) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>2</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	B	1	Total	C	N	O	P	0	1
			56	18	4	28	6		

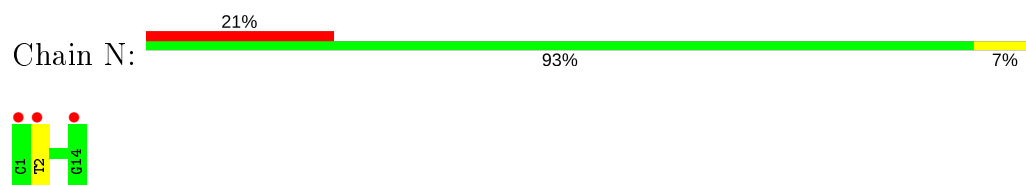
### 3 Residue-property plots

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

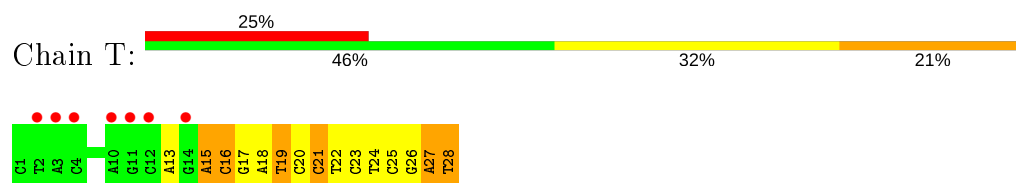
- Molecule 1: 5'-R(\*AP\*UP\*CP\*GP\*AP\*GP\*AP\*GP\*GP\*A)-3'



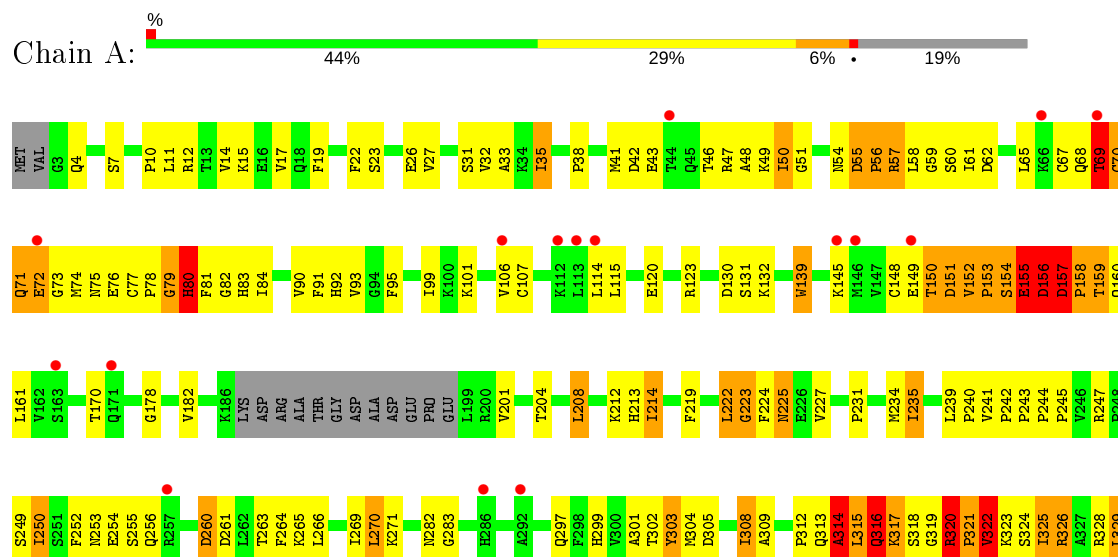
- Molecule 2: 5'-D(\*CP\*TP\*GP\*CP\*TP\*TP\*AP\*TP\*CP\*GP\*GP\*TP\*AP\*G)-3'



- Molecule 3: 28-MER DNA template strand



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

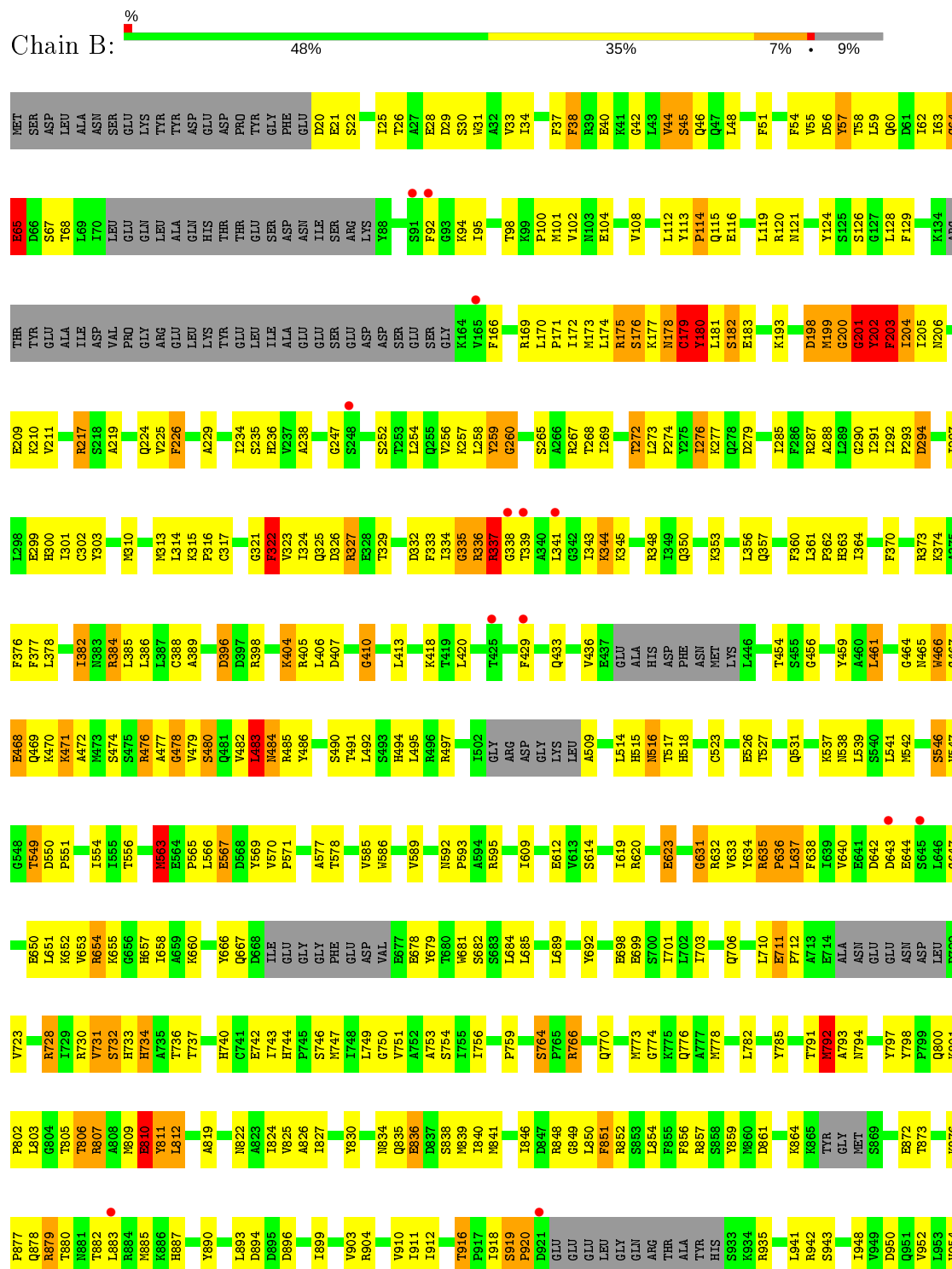


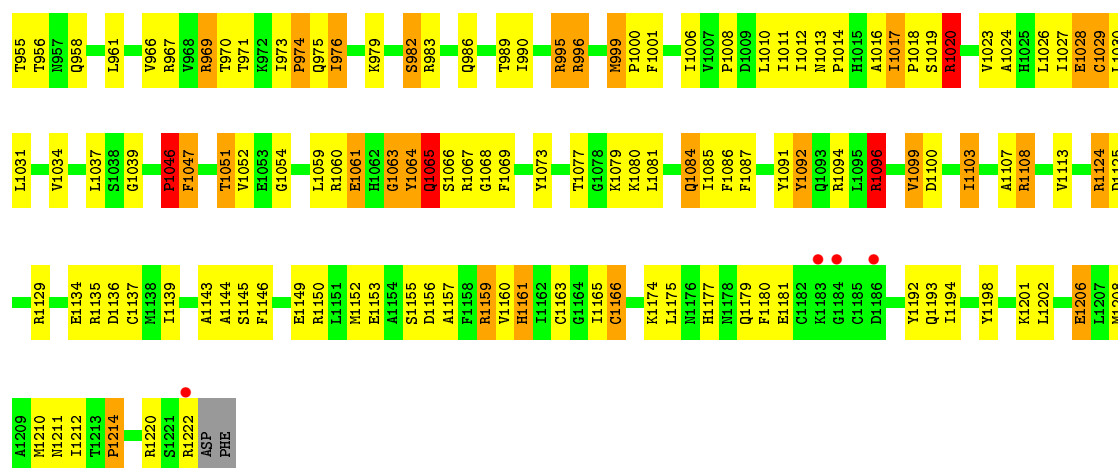




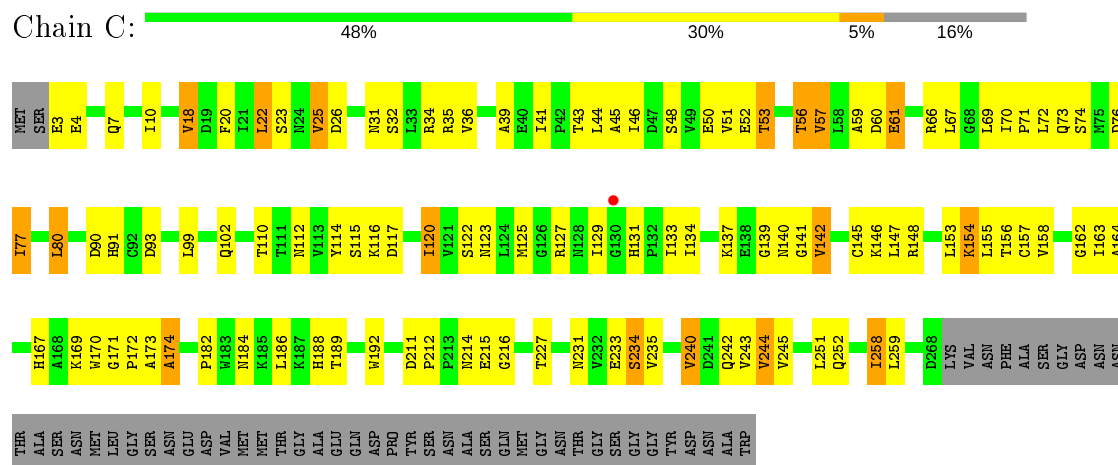
THR	THR
SER	SER
PRO	PRO
ALA	LYS
LEU	GLN
TYR	ASP
SER	ASP
PRO	GLU
THR	GLN
THR	GLN
THR	LYS
SER	HIS
PRO	ASN
ASN	ASN
GLY	GLU
THR	ASN
SER	GLU
PRO	ASP
THR	PRO
THR	THR
SER	THR
PRO	GLY
PRO	ASP
PRO	PHE
THR	ASP
SER	GLU
PRO	D20
THR	E21
SER	S22
PRO	LYS
PRO	Y88
THR	T26
THR	K27
SER	E28
PRO	D29
THR	S30
SER	W31
PRO	V165
SER	A32
PRO	V33
SER	T34
THR	T37
SER	F38
PRO	R39
THR	N103
SER	E104
PRO	E40
ASN	K41
TYR	G42
SER	L43
PRO	V44
THR	L112
THR	Y113
SER	S45
PRO	Q46
SER	Q47
PRO	L48
THR	F51
THR	L119
PRO	R120
THR	N121
SER	F54
PRO	D56
GLY	Y57
TYR	T58
SER	G201
PRO	S126
GLY	L127
PRO	O60
GLY	N61
SER	I62
PRO	I63
ALA	O64

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

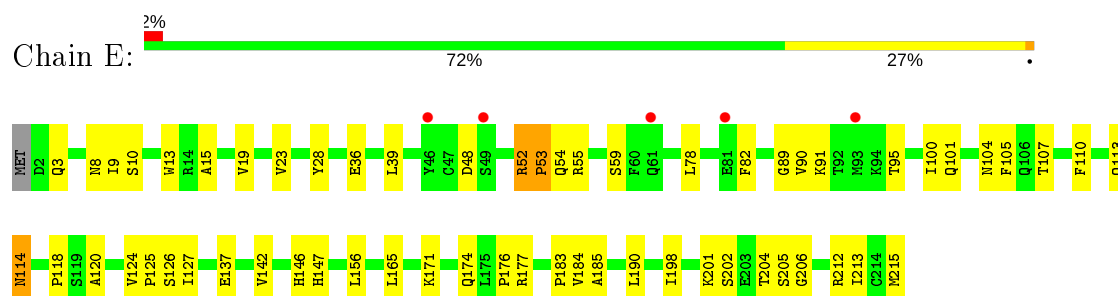




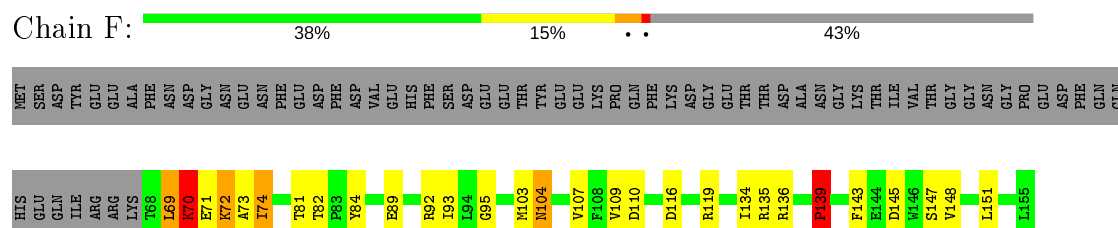
• Molecule 6: DNA-directed RNA polymerase II 45 kDa polypeptide



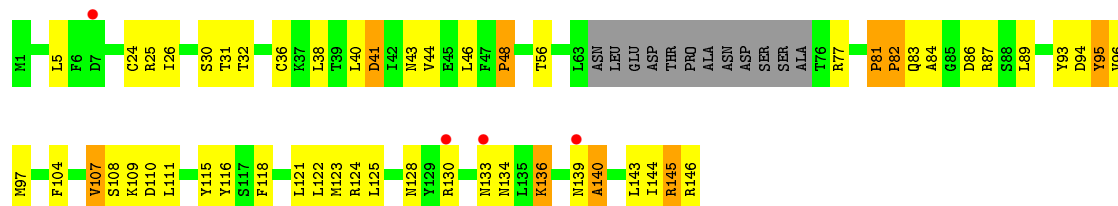
• Molecule 7: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide



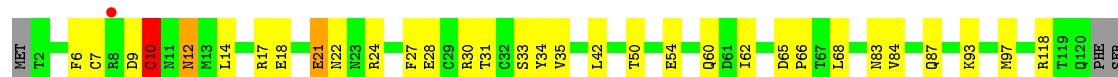
• Molecule 8: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



- Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



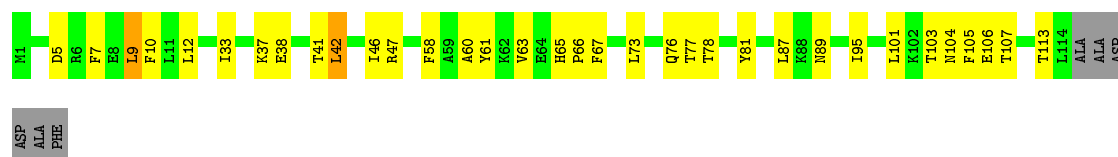
- Molecule 10: DNA-directed RNA polymerase II subunit 9



- Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10



- 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, $\alpha$ , $\beta$ , $\gamma$	168.72Å 222.41Å 193.07Å 90.00° 101.29° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 44.25 – 3.60	Depositor EDS
% Data completeness (in resolution range)	91.5 (50.00-3.60) 91.6 (44.25-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.285 , 0.304 0.282 , 0.296	Depositor DCC
$R_{free}$ test set	3721 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	104.2	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 59.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	29436	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, DUT, MG

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	1.16	1/243 (0.4%)	1.75	6/378 (1.6%)
2	N	0.74	0/317	1.27	0/488
3	T	1.18	4/634 (0.6%)	1.76	18/975 (1.8%)
4	A	0.68	8/11224 (0.1%)	0.67	2/15176 (0.0%)
5	B	0.82	11/9027 (0.1%)	0.73	3/12172 (0.0%)
6	C	0.71	0/2133	0.69	0/2891
7	E	0.58	1/1788 (0.1%)	0.61	0/2406
8	F	0.60	0/724	0.72	0/977
9	H	0.57	0/1094	0.65	0/1480
10	I	0.75	2/989 (0.2%)	0.68	0/1331
11	J	0.69	0/541	0.68	0/727
12	K	0.66	0/937	0.65	0/1265
13	L	0.70	0/366	0.78	0/485
All	All	0.74	27/30017 (0.1%)	0.76	29/40751 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	32
5	B	0	12
8	F	0	1
All	All	0	45

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	764	SER	CB-OG	13.86	1.60	1.42
5	B	490	SER	CB-OG	9.83	1.55	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	879	GLU	CD-OE1	7.99	1.34	1.25
3	T	19	DT	C5-C7	7.74	1.54	1.50
5	B	404	LYS	CE-NZ	7.54	1.67	1.49
3	T	23	DC	C1'-N1	7.16	1.58	1.49
5	B	1061	GLU	CD-OE1	6.57	1.32	1.25
5	B	1029	CYS	CB-SG	-6.50	1.71	1.82
5	B	114	PRO	N-CD	6.24	1.56	1.47
7	E	126	SER	CB-OG	6.17	1.50	1.42
5	B	546	SER	CB-OG	6.13	1.50	1.42
4	A	797	LYS	CD-CE	5.94	1.66	1.51
10	I	21	GLU	CD-OE1	5.88	1.32	1.25
3	T	24	DT	C5-C7	5.62	1.53	1.50
10	I	21	GLU	CD-OE2	5.51	1.31	1.25
5	B	836	GLU	CD-OE1	5.48	1.31	1.25
3	T	17	DG	C3'-O3'	-5.41	1.36	1.44
4	A	398	GLU	CD-OE1	5.36	1.31	1.25
4	A	951	GLU	CD-OE1	5.31	1.31	1.25
5	B	623	GLU	CD-OE2	5.31	1.31	1.25
5	B	1206	GLU	CD-OE2	5.29	1.31	1.25
4	A	271	LYS	CE-NZ	5.24	1.62	1.49
1	R	10	A	N9-C4	5.18	1.41	1.37
4	A	546	VAL	CB-CG1	5.17	1.63	1.52
4	A	879	GLU	CD-OE2	5.10	1.31	1.25
5	B	1100	ASP	CG-OD1	5.07	1.37	1.25
4	A	500	GLU	CD-OE1	5.06	1.31	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	19	DT	C4-C5-C7	10.26	125.16	119.00
3	T	19	DT	C6-C5-C7	-9.91	116.95	122.90
3	T	19	DT	N3-C2-O2	-9.91	116.36	122.30
3	T	16	DC	O4'-C1'-N1	9.72	114.80	108.00
3	T	28	DT	O4'-C1'-N1	8.42	113.89	108.00
1	R	10	A	O4'-C1'-N9	8.33	114.86	108.20
3	T	22	DT	O4'-C4'-C3'	-8.00	101.20	106.00
3	T	22	DT	C6-C5-C7	-7.56	118.36	122.90
1	R	9	G	O5'-P-OP1	7.45	119.64	110.70
1	R	10	A	C5-C6-N6	-7.03	118.08	123.70
3	T	27	DA	O4'-C4'-C3'	-6.77	101.79	104.50
3	T	15	DA	C1'-O4'-C4'	-6.57	103.53	110.10
1	R	10	A	N1-C6-N6	6.41	122.44	118.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	805	LEU	CA-CB-CG	6.36	129.92	115.30
5	B	996	ARG	NE-CZ-NH2	-6.34	117.13	120.30
3	T	15	DA	P-O3'-C3'	5.95	126.84	119.70
1	R	8	G	N1-C6-O6	5.74	123.35	119.90
5	B	766	ARG	NE-CZ-NH2	-5.63	117.48	120.30
3	T	22	DT	C5-C4-O4	-5.56	121.01	124.90
3	T	19	DT	C2-N3-C4	-5.47	123.92	127.20
3	T	25	DC	C6-N1-C2	5.46	122.49	120.30
1	R	8	G	C5-C6-O6	-5.46	125.32	128.60
3	T	21	DC	O5'-P-OP1	5.37	117.14	110.70
4	A	546	VAL	CG1-CB-CG2	-5.35	102.35	110.90
3	T	21	DC	OP1-P-OP2	-5.34	111.58	119.60
3	T	21	DC	C4'-C3'-C2'	-5.12	98.49	103.10
3	T	22	DT	N1-C2-N3	-5.10	111.54	114.60
3	T	22	DT	N3-C4-O4	5.08	122.95	119.90
5	B	782	LEU	CA-CB-CG	5.07	126.97	115.30

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1020	CYS	Peptide
4	A	1022	LEU	Peptide
4	A	1023	ARG	Peptide
4	A	1024	SER	Peptide
4	A	1219	THR	Peptide
4	A	1220	PHE	Peptide
4	A	1230	GLU	Peptide
4	A	1231	ASP	Peptide
4	A	1232	ASN	Peptide
4	A	1233	ASP	Peptide
4	A	1236	LEU	Peptide
4	A	1263	ILE	Peptide
4	A	1264	GLU	Peptide
4	A	153	PRO	Peptide
4	A	154	SER	Peptide
4	A	155	GLU	Peptide
4	A	156	ASP	Peptide
4	A	249	SER	Peptide
4	A	314	ALA	Peptide
4	A	315	LEU	Peptide
4	A	316	GLN	Peptide

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Group
4	A	320	ARG	Peptide
4	A	416	ARG	Peptide
4	A	451	HIS	Peptide
4	A	70	CYS	Peptide
4	A	71	GLN	Peptide
4	A	778	GLY	Peptide
4	A	79	GLY	Peptide
4	A	80	HIS	Peptide
4	A	850	VAL	Peptide
4	A	851	HIS	Peptide
4	A	852	TYR	Peptide
5	B	1063	GLY	Peptide
5	B	1065	GLN	Peptide
5	B	176	SER	Peptide
5	B	178	ASN	Peptide
5	B	179	CYS	Peptide
5	B	180	TYR	Peptide
5	B	201	GLY	Peptide
5	B	202	TYR	Peptide
5	B	203	PHE	Peptide
5	B	678	GLU	Peptide
5	B	810	GLU	Peptide
5	B	919	SER	Peptide
8	F	69	LEU	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	216	0	109	7	0
2	N	284	0	161	1	0
3	T	566	0	316	11	0
4	A	11028	0	11120	901	0
5	B	8856	0	8897	724	0
6	C	2095	0	2051	80	0
7	E	1752	0	1776	33	0
8	F	712	0	738	47	0
9	H	1076	0	1052	40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	971	0	930	21	0
11	J	532	0	542	41	0
12	K	919	0	929	20	0
13	L	364	0	387	20	0
14	A	2	0	0	1	0
14	B	1	0	0	1	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	B	56	0	22	1	0
All	All	29436	0	29030	1745	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (1745) 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)
5:B:404:LYS:NZ	5:B:404:LYS:CE	1.67	1.52
4:A:1287:TYR:CD2	4:A:1305:VAL:HB	1.59	1.36
4:A:1229:SER:HB2	4:A:1236:LEU:CD1	1.59	1.33
4:A:1229:SER:CB	4:A:1236:LEU:HD12	1.64	1.27
5:B:203:PHE:CA	5:B:204:ILE:HD12	1.63	1.27
4:A:810:PRO:HA	5:B:1047:PHE:CE2	1.69	1.26
4:A:1287:TYR:CE2	4:A:1305:VAL:HB	1.72	1.25
4:A:1174:PHE:HA	4:A:1175:SER:CB	1.65	1.25
5:B:728:ARG:HD2	5:B:730:ARG:NH2	1.52	1.24
4:A:315:LEU:CA	4:A:320:ARG:HH12	1.51	1.23
5:B:200:GLY:HA2	5:B:202:TYR:CE2	1.73	1.22
5:B:204:ILE:O	5:B:205:ILE:HD13	1.40	1.22
4:A:1215:ARG:O	4:A:1219:THR:HG23	1.35	1.22
5:B:302:CYS:CB	5:B:310:MET:HE3	1.70	1.21
5:B:175:ARG:HH11	5:B:182:SER:CA	1.56	1.19
5:B:302:CYS:SG	5:B:310:MET:CE	2.31	1.18
8:F:71:GLU:HA	8:F:72:LYS:HB2	1.25	1.17
4:A:157:ASP:HB2	4:A:158:PRO:CD	1.71	1.16
4:A:810:PRO:CA	5:B:1047:PHE:HE2	1.57	1.16
4:A:1025:ARG:HH11	4:A:1025:ARG:HG3	1.02	1.14
5:B:175:ARG:NH1	5:B:182:SER:HA	1.62	1.14

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1153:TYR:HE1	10:I:42:LEU:HD13	1.04	1.14
4:A:1231:ASP:HA	4:A:1233:ASP:OD1	1.45	1.14
5:B:302:CYS:HB2	5:B:310:MET:HE3	1.15	1.13
4:A:78:PRO:HB3	5:B:1201:LYS:HE2	1.27	1.13
4:A:58:LEU:HD23	4:A:59:GLY:H	1.09	1.13
4:A:857:ARG:NH2	8:F:139:PRO:HG2	1.61	1.13
4:A:1022:LEU:O	4:A:1023:ARG:HG3	1.48	1.13
4:A:857:ARG:HG2	4:A:863:VAL:HA	1.23	1.13
4:A:320:ARG:N	4:A:320:ARG:HD2	1.56	1.13
5:B:1065:GLN:NE2	5:B:1067:ARG:H	1.47	1.12
4:A:1170:ILE:HB	4:A:1171:GLN:HA	1.13	1.12
4:A:567:LYS:HB2	4:A:568:PRO:HD2	1.12	1.12
4:A:857:ARG:HH21	8:F:139:PRO:HG2	1.05	1.12
4:A:316:GLN:HE21	4:A:317:LYS:CG	1.63	1.11
4:A:153:PRO:HA	4:A:154:SER:OG	1.50	1.11
5:B:1159:ARG:HB3	5:B:1159:ARG:HH11	1.11	1.11
4:A:315:LEU:HB2	4:A:320:ARG:HH22	1.09	1.11
4:A:1153:TYR:CE1	10:I:42:LEU:HD13	1.86	1.11
4:A:1231:ASP:HA	4:A:1233:ASP:CG	1.70	1.10
5:B:1065:GLN:NE2	5:B:1068:GLY:H	1.50	1.10
4:A:316:GLN:HA	4:A:318:SER:H	1.17	1.10
5:B:224:GLN:HB3	5:B:226:PHE:HE1	1.12	1.10
5:B:969:ARG:NH2	6:C:59:ALA:HB1	1.65	1.10
4:A:1244:ARG:HH11	4:A:1244:ARG:CB	1.65	1.09
5:B:637:LEU:HD13	5:B:740:HIS:ND1	1.65	1.09
5:B:1124:ARG:HD2	5:B:1124:ARG:H	0.95	1.09
4:A:31:SER:HB2	4:A:82:GLY:HA2	1.29	1.09
7:E:53:PRO:CB	7:E:54:GLN:HA	1.83	1.08
4:A:1287:TYR:CD2	4:A:1305:VAL:CB	2.34	1.08
4:A:58:LEU:CD2	4:A:59:GLY:H	1.66	1.08
5:B:807:ARG:HG3	5:B:807:ARG:HH11	1.18	1.08
4:A:316:GLN:HG2	4:A:317:LYS:HA	1.22	1.08
4:A:316:GLN:HE21	4:A:317:LYS:HG3	1.16	1.08
4:A:316:GLN:HG2	4:A:317:LYS:CA	1.84	1.08
4:A:1244:ARG:NH1	4:A:1244:ARG:HB2	1.69	1.07
4:A:1030:ARG:HD3	4:A:1035:TYR:CE1	1.89	1.07
4:A:857:ARG:HH21	8:F:139:PRO:CG	1.67	1.07
4:A:1030:ARG:HG3	4:A:1030:ARG:HH11	1.11	1.07
4:A:302:THR:HG21	4:A:313:GLN:NE2	1.69	1.07
4:A:1025:ARG:CG	4:A:1025:ARG:HH11	1.67	1.07
7:E:53:PRO:HB2	7:E:54:GLN:CA	1.84	1.07

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1024:SER:HB3	4:A:1025:ARG:O	1.54	1.07
4:A:586:ILE:HD11	4:A:637:LYS:HD3	1.13	1.07
5:B:1124:ARG:HD2	5:B:1124:ARG:N	1.66	1.07
5:B:919:SER:HB3	5:B:920:PRO:HA	1.09	1.06
4:A:1265:ASN:HD21	5:B:265:SER:HB3	1.20	1.06
5:B:879:ARG:O	5:B:882:THR:HG22	1.55	1.06
4:A:1172:LEU:HB3	4:A:1173:HIS:HA	1.29	1.05
5:B:175:ARG:N	5:B:179:CYS:SG	2.30	1.05
5:B:969:ARG:HH21	6:C:59:ALA:HB1	0.97	1.05
5:B:1124:ARG:CD	5:B:1124:ARG:H	1.70	1.05
5:B:174:LEU:C	5:B:179:CYS:SG	2.35	1.04
4:A:1026:LEU:HD13	4:A:1026:LEU:N	1.69	1.04
4:A:315:LEU:HA	4:A:320:ARG:HH12	1.15	1.04
5:B:982:SER:HA	5:B:1092:TYR:CD2	1.92	1.04
5:B:1016:ALA:O	5:B:1017:ILE:HG13	1.55	1.04
5:B:48:LEU:HD22	5:B:175:ARG:O	1.58	1.04
4:A:157:ASP:HB2	4:A:158:PRO:HD3	1.07	1.04
4:A:151:ASP:CA	4:A:152:VAL:HB	1.86	1.03
4:A:810:PRO:HA	5:B:1047:PHE:HE2	0.91	1.03
4:A:451:HIS:HB3	4:A:453:MET:H	1.19	1.02
4:A:567:LYS:CB	4:A:568:PRO:HD2	1.86	1.02
4:A:1174:PHE:CA	4:A:1175:SER:HB2	1.89	1.02
5:B:1124:ARG:HG2	5:B:1124:ARG:HH11	1.19	1.02
5:B:982:SER:HB3	5:B:1092:TYR:CE2	1.95	1.02
4:A:1244:ARG:HH11	4:A:1244:ARG:HB2	0.86	1.02
5:B:302:CYS:SG	5:B:310:MET:HE2	2.00	1.02
4:A:151:ASP:HA	4:A:152:VAL:CB	1.85	1.01
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	1.41	1.01
4:A:67:CYS:O	4:A:68:GLN:HG3	1.61	1.01
4:A:1021:LEU:H	4:A:1024:SER:CB	1.73	1.01
5:B:203:PHE:CE1	5:B:461:LEU:HD21	1.96	1.01
5:B:176:SER:N	5:B:179:CYS:SG	2.33	1.00
7:E:52:ARG:HB2	7:E:53:PRO:HD3	1.37	1.00
4:A:779:PHE:CE2	4:A:785:PRO:HG3	1.96	1.00
4:A:1233:ASP:HB3	4:A:1235:LYS:O	1.61	1.00
5:B:203:PHE:HD1	5:B:204:ILE:N	1.59	1.00
4:A:830:LYS:NZ	4:A:1080:THR:HA	1.77	1.00
5:B:302:CYS:CB	5:B:310:MET:CE	2.38	1.00
4:A:417:TYR:O	4:A:418:SER:HB3	1.59	1.00
5:B:224:GLN:HB3	5:B:226:PHE:CE1	1.97	0.99
4:A:1174:PHE:CA	4:A:1175:SER:CB	2.40	0.99

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1167:GLU:O	4:A:1170:ILE:HG12	1.62	0.99
4:A:1174:PHE:HA	4:A:1175:SER:HB2	1.01	0.99
5:B:203:PHE:HA	5:B:204:ILE:HD12	1.01	0.98
5:B:299:GLU:HG2	5:B:571:PRO:HG2	1.46	0.98
4:A:666:ILE:CG2	5:B:1026:LEU:HB3	1.94	0.98
5:B:64:CYS:O	5:B:65:GLU:HG3	1.63	0.97
5:B:1065:GLN:HE22	5:B:1067:ARG:N	1.61	0.97
5:B:174:LEU:HA	5:B:179:CYS:SG	2.04	0.97
4:A:542:GLU:HG3	4:A:544:ASP:OD1	1.65	0.97
4:A:666:ILE:HD12	5:B:1052:VAL:HG13	1.44	0.97
4:A:852:TYR:CD2	4:A:1060:PRO:HB3	1.99	0.97
8:F:72:LYS:HB3	8:F:73:ALA:HA	1.46	0.97
4:A:1021:LEU:H	4:A:1024:SER:HB2	1.28	0.96
5:B:273:LEU:O	5:B:276:ILE:HG22	1.66	0.96
4:A:1265:ASN:ND2	5:B:265:SER:HB3	1.80	0.96
4:A:541:ILE:HD12	4:A:546:VAL:HG22	1.47	0.96
4:A:302:THR:HG21	4:A:313:GLN:HE22	1.22	0.95
5:B:177:LYS:HE2	5:B:178:ASN:ND2	1.81	0.95
5:B:175:ARG:HH11	5:B:182:SER:HA	0.81	0.95
4:A:253:ASN:HD22	4:A:256:GLN:H	1.05	0.95
5:B:174:LEU:CA	5:B:179:CYS:SG	2.55	0.95
5:B:200:GLY:HA2	5:B:202:TYR:CD2	2.01	0.95
4:A:1021:LEU:N	4:A:1024:SER:HB2	1.82	0.95
5:B:879:ARG:NH2	5:B:885:MET:SD	2.38	0.95
4:A:315:LEU:HA	4:A:320:ARG:NH1	1.81	0.95
4:A:779:PHE:HE2	4:A:785:PRO:CD	1.80	0.95
4:A:315:LEU:HB2	4:A:320:ARG:NH2	1.80	0.94
5:B:711:GLU:H	5:B:712:PRO:CD	1.80	0.94
4:A:151:ASP:HA	4:A:152:VAL:HB	0.96	0.94
4:A:586:ILE:CD1	4:A:637:LYS:HD3	1.97	0.94
4:A:1025:ARG:HD3	4:A:1030:ARG:NH2	1.83	0.94
4:A:1364:ASN:ND2	4:A:1366:ARG:HG2	1.81	0.94
4:A:535:THR:HG21	4:A:617:VAL:H	1.32	0.94
5:B:203:PHE:HA	5:B:204:ILE:CD1	1.95	0.94
4:A:779:PHE:HE2	4:A:785:PRO:HD3	1.31	0.94
4:A:779:PHE:HE1	5:B:517:THR:HG22	1.31	0.94
4:A:1287:TYR:CE2	4:A:1305:VAL:CB	2.51	0.93
4:A:779:PHE:CE2	4:A:785:PRO:HD3	2.02	0.93
4:A:451:HIS:HB3	4:A:453:MET:N	1.82	0.93
5:B:1159:ARG:NH1	5:B:1159:ARG:HB3	1.82	0.93
5:B:577:ALA:HB1	5:B:589:VAL:CG1	1.97	0.93

*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	1.10	0.93
4:A:1025:ARG:NH1	4:A:1025:ARG:HG3	1.70	0.93
9:H:81:PRO:CB	9:H:82:PRO:HD2	1.97	0.93
4:A:1172:LEU:CB	4:A:1173:HIS:HA	1.94	0.93
4:A:586:ILE:HD11	4:A:637:LYS:CD	1.98	0.93
4:A:1026:LEU:N	4:A:1026:LEU:CD1	2.31	0.93
5:B:825:VAL:HG23	5:B:1010:LEU:HB3	1.50	0.92
4:A:633:VAL:O	4:A:637:LYS:HG2	1.69	0.92
8:F:69:LEU:HB2	8:F:70:LYS:HB2	1.50	0.92
5:B:200:GLY:HA2	5:B:202:TYR:HE2	1.30	0.92
4:A:779:PHE:HE2	4:A:785:PRO:CG	1.82	0.92
5:B:211:VAL:O	5:B:480:SER:HA	1.68	0.92
4:A:1364:ASN:HD21	4:A:1366:ARG:HH11	1.10	0.91
5:B:955:THR:HG22	5:B:956:THR:H	1.31	0.91
5:B:919:SER:CB	5:B:920:PRO:HA	1.98	0.91
4:A:1016:THR:O	4:A:1020:CYS:SG	2.27	0.91
4:A:500:GLU:OE1	5:B:1145:SER:HB2	1.70	0.91
4:A:852:TYR:CE2	4:A:1060:PRO:HB2	2.05	0.91
4:A:1153:TYR:HE1	10:I:42:LEU:CD1	1.82	0.91
4:A:1209:MET:SD	4:A:1236:LEU:HD21	2.09	0.91
4:A:319:GLY:C	4:A:320:ARG:HD2	1.89	0.91
4:A:779:PHE:CE2	4:A:785:PRO:CG	2.54	0.91
4:A:1231:ASP:HA	4:A:1233:ASP:OD2	1.70	0.91
4:A:1287:TYR:HD2	4:A:1305:VAL:HB	1.25	0.90
4:A:636:GLU:HB3	4:A:637:LYS:HD2	1.52	0.90
4:A:250:ILE:HD11	4:A:254:GLU:OE2	1.71	0.90
4:A:666:ILE:HG22	5:B:1026:LEU:HB3	1.53	0.90
5:B:203:PHE:HE1	5:B:461:LEU:HD21	1.34	0.90
4:A:58:LEU:HD23	4:A:59:GLY:N	1.87	0.90
5:B:1065:GLN:HE22	5:B:1068:GLY:H	1.12	0.90
4:A:1170:ILE:CB	4:A:1171:GLN:HA	1.96	0.89
5:B:173:MET:O	5:B:179:CYS:SG	2.30	0.89
4:A:78:PRO:CB	5:B:1201:LYS:HE2	2.01	0.89
4:A:362:ASP:OD2	4:A:459:ARG:HD3	1.73	0.89
4:A:569:LYS:HD2	4:A:571:LEU:HD11	1.52	0.89
5:B:276:ILE:HG13	5:B:277:LYS:H	1.37	0.89
4:A:569:LYS:O	4:A:571:LEU:HD12	1.72	0.89
5:B:969:ARG:HH21	6:C:59:ALA:CB	1.85	0.89
4:A:852:TYR:CD2	4:A:1060:PRO:CB	2.56	0.89
5:B:1065:GLN:HE22	5:B:1067:ARG:H	0.91	0.89
11:J:45:CYS:SG	11:J:46:CYS:N	2.46	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:33:ALA:HB3	4:A:82:GLY:HA3	1.53	0.88
4:A:264:PHE:HE1	4:A:317:LYS:HG3	1.38	0.88
5:B:336:ARG:HD2	5:B:336:ARG:O	1.74	0.88
4:A:1345:ARG:HG3	4:A:1346:ALA:N	1.89	0.88
4:A:157:ASP:O	4:A:158:PRO:O	1.92	0.88
5:B:849:GLY:HA2	5:B:852:ARG:HD2	1.55	0.88
5:B:919:SER:HB3	5:B:920:PRO:CA	2.00	0.88
4:A:587:HIS:NE2	4:A:969:GLN:NE2	2.22	0.87
5:B:129:PHE:HE1	5:B:166:PHE:HD1	1.17	0.87
5:B:516:ASN:H	5:B:516:ASN:HD22	1.17	0.87
4:A:857:ARG:HH11	4:A:863:VAL:HG22	1.38	0.87
5:B:299:GLU:CG	5:B:571:PRO:HG2	2.05	0.87
4:A:1030:ARG:NH1	4:A:1030:ARG:HG3	1.87	0.87
4:A:777:PHE:CE1	4:A:782:ARG:HA	2.10	0.87
4:A:1030:ARG:HD3	4:A:1035:TYR:HE1	1.38	0.87
4:A:777:PHE:HB3	4:A:780:VAL:O	1.74	0.87
4:A:830:LYS:HZ3	4:A:1080:THR:HA	1.33	0.87
4:A:316:GLN:NE2	4:A:317:LYS:HG3	1.90	0.87
4:A:810:PRO:CA	5:B:1047:PHE:CE2	2.43	0.87
7:E:53:PRO:HB2	7:E:54:GLN:HA	0.92	0.86
4:A:416:ARG:NH2	4:A:417:TYR:CE2	2.43	0.86
4:A:541:ILE:HD11	4:A:577:ILE:HG12	1.57	0.86
5:B:48:LEU:CD2	5:B:175:ARG:O	2.24	0.86
5:B:173:MET:HA	5:B:203:PHE:HB3	1.56	0.86
4:A:315:LEU:CA	4:A:320:ARG:NH1	2.35	0.86
5:B:203:PHE:HE1	5:B:461:LEU:CD2	1.87	0.86
7:E:52:ARG:CB	7:E:53:PRO:HD3	2.05	0.86
4:A:1345:ARG:HG3	4:A:1346:ALA:H	1.40	0.86
4:A:149:GLU:HB3	4:A:152:VAL:HG21	1.58	0.86
4:A:754:SER:H	4:A:757:ASN:HD22	1.22	0.86
4:A:1026:LEU:O	4:A:1030:ARG:CB	2.24	0.85
4:A:809:THR:HB	4:A:810:PRO:HD2	1.55	0.85
5:B:64:CYS:C	5:B:65:GLU:HG3	1.92	0.85
5:B:565:PRO:HB2	5:B:567:GLU:OE1	1.76	0.85
4:A:320:ARG:CD	4:A:320:ARG:N	2.34	0.85
4:A:1234:GLU:C	4:A:1235:LYS:HD3	1.97	0.84
5:B:1016:ALA:O	5:B:1017:ILE:CG1	2.25	0.84
8:F:72:LYS:HB3	8:F:73:ALA:CA	2.06	0.84
4:A:1229:SER:HB2	4:A:1236:LEU:HD12	0.87	0.84
9:H:81:PRO:HB3	9:H:82:PRO:HD2	1.59	0.84
4:A:1030:ARG:CD	4:A:1035:TYR:HE1	1.91	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:129:PHE:CE1	5:B:166:PHE:HD1	1.96	0.83
5:B:638:PHE:O	5:B:740:HIS:HB2	1.78	0.83
5:B:203:PHE:HD1	5:B:204:ILE:H	1.24	0.83
4:A:1030:ARG:CD	4:A:1035:TYR:CE1	2.60	0.83
11:J:10:CYS:SG	11:J:43:ARG:HD2	2.18	0.83
8:F:71:GLU:HA	8:F:72:LYS:CB	2.02	0.83
4:A:567:LYS:HB2	4:A:568:PRO:CD	2.03	0.83
5:B:203:PHE:C	5:B:203:PHE:CD1	2.48	0.83
4:A:58:LEU:CG	4:A:80:HIS:O	2.26	0.83
4:A:353:ILE:HD13	4:A:487:MET:CE	2.09	0.83
4:A:783:THR:HG21	4:A:815:PHE:HE1	1.44	0.82
4:A:1118:VAL:HG23	4:A:1306:LEU:HB2	1.61	0.82
5:B:174:LEU:H	5:B:203:PHE:H	1.26	0.82
5:B:203:PHE:CE1	5:B:461:LEU:CD2	2.61	0.82
5:B:1084:GLN:NE2	6:C:192:TRP:H	1.77	0.82
13:L:60:ARG:HG3	13:L:61:THR:H	1.43	0.82
4:A:1441:PHE:CE2	8:F:89:GLU:HG3	2.14	0.82
4:A:1312:ASN:O	4:A:1316:VAL:HG23	1.79	0.82
4:A:153:PRO:CA	4:A:154:SER:OG	2.28	0.82
5:B:982:SER:CB	5:B:1092:TYR:CE2	2.63	0.82
5:B:982:SER:CA	5:B:1092:TYR:CE2	2.62	0.82
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.60	0.82
4:A:637:LYS:HZ3	4:A:637:LYS:HB3	1.45	0.82
4:A:316:GLN:HA	4:A:318:SER:N	1.94	0.81
4:A:873:MET:HG2	4:A:957:PRO:HG3	1.62	0.81
5:B:203:PHE:CD1	5:B:204:ILE:N	2.47	0.81
5:B:202:TYR:O	5:B:202:TYR:CG	2.33	0.81
4:A:316:GLN:CA	4:A:318:SER:H	1.92	0.81
4:A:450:LEU:O	4:A:451:HIS:CG	2.33	0.81
5:B:728:ARG:CD	5:B:730:ARG:NH2	2.39	0.81
5:B:986:GLN:HE22	5:B:1020:ARG:HD2	1.46	0.81
4:A:1153:TYR:CE1	10:I:42:LEU:CD1	2.62	0.81
4:A:65:LEU:HD22	4:A:72:GLU:C	2.01	0.80
5:B:1124:ARG:NH1	5:B:1124:ARG:HG2	1.93	0.80
4:A:482:PHE:HD2	5:B:836:GLU:O	1.63	0.80
4:A:1170:ILE:HB	4:A:1171:GLN:CA	2.06	0.80
4:A:1287:TYR:CD2	4:A:1305:VAL:CG2	2.65	0.80
4:A:153:PRO:HB2	4:A:154:SER:C	2.01	0.80
5:B:899:ILE:HD11	5:B:911:ILE:HG12	1.62	0.80
4:A:299:HIS:HA	4:A:302:THR:HG22	1.61	0.80
4:A:666:ILE:HG22	5:B:1026:LEU:CB	2.12	0.80

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1206:ASP:HB2	4:A:1274:ARG:HH12	1.46	0.80
5:B:982:SER:CA	5:B:1092:TYR:CD2	2.65	0.80
5:B:172:ILE:O	5:B:203:PHE:HB3	1.82	0.80
4:A:868:TYR:CE1	4:A:1064:VAL:HG11	2.16	0.80
6:C:102:GLN:HG2	6:C:154:LYS:HD2	1.64	0.80
5:B:567:GLU:CD	5:B:567:GLU:H	1.84	0.80
4:A:14:VAL:H	4:A:1432:GLN:HE22	1.30	0.79
8:F:71:GLU:CA	8:F:72:LYS:HB2	2.10	0.79
4:A:636:GLU:CB	4:A:637:LYS:HD2	2.12	0.79
4:A:453:MET:HE3	4:A:520:CYS:SG	2.22	0.79
4:A:1234:GLU:O	4:A:1235:LYS:HD3	1.81	0.79
4:A:541:ILE:CD1	4:A:577:ILE:HG12	2.11	0.79
4:A:1364:ASN:HD21	4:A:1366:ARG:NH1	1.80	0.79
5:B:202:TYR:O	5:B:204:ILE:HD11	1.82	0.79
4:A:67:CYS:O	4:A:68:GLN:CG	2.30	0.79
4:A:157:ASP:CB	4:A:158:PRO:HD3	2.02	0.79
5:B:1065:GLN:NE2	5:B:1068:GLY:N	2.30	0.79
4:A:1231:ASP:CA	4:A:1233:ASP:OD2	2.31	0.79
4:A:777:PHE:CB	4:A:780:VAL:O	2.31	0.79
4:A:779:PHE:CE1	5:B:517:THR:HG22	2.17	0.79
5:B:202:TYR:O	5:B:202:TYR:CD1	2.36	0.79
5:B:225:VAL:C	5:B:226:PHE:HD1	1.86	0.79
4:A:353:ILE:HD13	4:A:487:MET:HE3	1.64	0.78
5:B:652:LYS:O	5:B:654:ARG:HD3	1.83	0.78
9:H:26:ILE:HG22	9:H:40:LEU:O	1.83	0.78
4:A:1234:GLU:HB3	4:A:1235:LYS:HD3	1.65	0.78
4:A:316:GLN:HE21	4:A:317:LYS:HG2	1.45	0.78
5:B:879:ARG:HH12	5:B:885:MET:CE	1.96	0.78
4:A:777:PHE:CD1	4:A:782:ARG:CA	2.67	0.78
6:C:99:LEU:HD23	6:C:120:ILE:HA	1.67	0.78
4:A:1025:ARG:HD3	4:A:1030:ARG:CZ	2.15	0.77
5:B:104:GLU:OE2	13:L:54:ARG:CZ	2.32	0.77
4:A:500:GLU:OE2	5:B:1143:ALA:CA	2.31	0.77
5:B:1160:VAL:HG12	5:B:1161:HIS:H	1.47	0.77
4:A:1345:ARG:CG	4:A:1346:ALA:N	2.47	0.77
4:A:90:VAL:HG13	4:A:297:GLN:CD	2.04	0.77
4:A:500:GLU:OE2	5:B:1143:ALA:HA	1.85	0.77
5:B:299:GLU:HG2	5:B:571:PRO:CG	2.13	0.77
6:C:186:LEU:HB3	6:C:188:HIS:HD2	1.49	0.77
13:L:60:ARG:HG3	13:L:61:THR:N	1.98	0.77
4:A:1220:PHE:O	4:A:1221:LYS:HB2	1.84	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:325:ILE:HG21	5:B:1210:MET:SD	2.25	0.77
5:B:851:PHE:HB3	5:B:1094:ARG:HD2	1.65	0.77
4:A:1021:LEU:N	4:A:1024:SER:CB	2.43	0.77
4:A:607:ILE:HG12	4:A:612:ILE:HG22	1.67	0.77
4:A:315:LEU:N	4:A:320:ARG:HH12	1.82	0.77
4:A:381:THR:OG1	4:A:382:PRO:HD2	1.85	0.77
4:A:637:LYS:HB3	4:A:637:LYS:NZ	2.00	0.77
4:A:666:ILE:HD12	5:B:1052:VAL:CG1	2.14	0.77
5:B:807:ARG:HG3	5:B:807:ARG:NH1	1.98	0.76
4:A:645:LEU:HD11	4:A:649:ILE:HD11	1.68	0.76
4:A:154:SER:HA	4:A:155:GLU:O	1.85	0.76
5:B:1065:GLN:C	5:B:1065:GLN:NE2	2.38	0.76
4:A:329:LEU:HD13	4:A:336:ILE:HD11	1.65	0.76
4:A:544:ASP:CG	4:A:545:GLN:H	1.89	0.76
4:A:775:ILE:HG13	4:A:798:GLY:HA3	1.65	0.76
4:A:93:VAL:HG22	4:A:301:ALA:HA	1.68	0.76
4:A:91:PHE:HA	4:A:235:ILE:HG22	1.66	0.76
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.21	0.76
8:F:72:LYS:CB	8:F:73:ALA:HA	2.11	0.76
4:A:1026:LEU:O	4:A:1030:ARG:HB3	1.86	0.76
5:B:800:GLN:HB3	11:J:52:THR:CG2	2.15	0.76
4:A:1231:ASP:CA	4:A:1233:ASP:OD1	2.30	0.76
5:B:56:ASP:C	5:B:57:TYR:HD1	1.89	0.76
5:B:577:ALA:HB1	5:B:589:VAL:HG11	1.66	0.76
4:A:821:ARG:HH12	5:B:514:LEU:HD13	1.51	0.75
5:B:129:PHE:HE1	5:B:166:PHE:CD1	2.02	0.75
5:B:177:LYS:HD2	5:B:177:LYS:C	2.07	0.75
5:B:638:PHE:CE2	5:B:743:ILE:HD13	2.21	0.75
4:A:1234:GLU:HB3	4:A:1235:LYS:CD	2.16	0.75
4:A:777:PHE:HD1	4:A:782:ARG:C	1.89	0.75
5:B:172:ILE:O	5:B:203:PHE:CB	2.34	0.75
4:A:65:LEU:HD22	4:A:72:GLU:CA	2.16	0.75
4:A:79:GLY:O	4:A:243:PRO:HG3	1.87	0.75
5:B:637:LEU:CD1	5:B:740:HIS:ND1	2.48	0.75
4:A:1233:ASP:CB	4:A:1235:LYS:O	2.35	0.75
5:B:728:ARG:HD2	5:B:730:ARG:CZ	2.16	0.75
4:A:416:ARG:NH2	4:A:417:TYR:HE2	1.84	0.75
5:B:654:ARG:H	5:B:657:HIS:HD2	1.35	0.75
4:A:253:ASN:HD22	4:A:256:GLN:N	1.82	0.74
3:T:28:DT:H1'	4:A:317:LYS:O	1.87	0.74
4:A:1155:ASP:OD2	4:A:1161:THR:HG23	1.87	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:417:TYR:O	4:A:418:SER:CB	2.35	0.74
5:B:204:ILE:O	5:B:205:ILE:CD1	2.30	0.74
5:B:807:ARG:CG	5:B:807:ARG:HH11	1.98	0.74
4:A:1345:ARG:HD2	4:A:1346:ALA:HA	1.69	0.74
4:A:302:THR:CG2	4:A:313:GLN:HE22	2.00	0.74
4:A:347:PHE:HE1	4:A:375:THR:HG22	1.52	0.74
4:A:58:LEU:HG	4:A:80:HIS:O	1.87	0.74
4:A:157:ASP:CB	4:A:158:PRO:CD	2.57	0.74
5:B:177:LYS:HE2	5:B:178:ASN:HD21	1.53	0.74
5:B:577:ALA:HB1	5:B:589:VAL:HG13	1.70	0.74
4:A:1174:PHE:HB3	4:A:1175:SER:HB3	1.68	0.74
5:B:1047:PHE:CD1	5:B:1047:PHE:N	2.53	0.74
4:A:316:GLN:HG2	4:A:317:LYS:N	2.02	0.73
4:A:361:LEU:HD13	4:A:646:PHE:CD2	2.23	0.73
4:A:446:ARG:HH12	4:A:448:PRO:HD2	1.54	0.73
5:B:57:TYR:HD1	5:B:57:TYR:N	1.85	0.73
4:A:1024:SER:CB	4:A:1025:ARG:O	2.34	0.73
4:A:857:ARG:HD3	4:A:863:VAL:HG22	1.71	0.73
4:A:779:PHE:CE2	4:A:785:PRO:CD	2.62	0.73
4:A:869:GLY:O	7:E:204:THR:HG21	1.89	0.73
4:A:31:SER:HB2	4:A:82:GLY:CA	2.16	0.72
5:B:56:ASP:C	5:B:57:TYR:CD1	2.61	0.72
4:A:852:TYR:HD2	4:A:1060:PRO:HB3	1.53	0.72
4:A:316:GLN:CG	4:A:317:LYS:HA	2.11	0.72
5:B:40:GLU:OE2	5:B:681:TRP:HB3	1.88	0.72
4:A:1101:LEU:HD13	4:A:1355:VAL:HG11	1.71	0.72
4:A:51:GLY:HA2	4:A:56:PRO:HG3	1.71	0.72
5:B:1065:GLN:CD	5:B:1066:SER:N	2.42	0.72
5:B:176:SER:OG	5:B:177:LYS:HB3	1.89	0.72
13:L:32:ALA:HB3	13:L:55:ILE:HD12	1.71	0.72
4:A:1323:ASP:OD1	4:A:1325:THR:HG22	1.88	0.72
5:B:290:GLY:CA	5:B:327:ARG:NH1	2.52	0.72
4:A:1027:ALA:O	4:A:1030:ARG:N	2.22	0.72
4:A:596:THR:O	4:A:598:LEU:N	2.21	0.72
5:B:1065:GLN:C	5:B:1065:GLN:CD	2.47	0.72
5:B:1063:GLY:C	5:B:1064:TYR:HD1	1.93	0.72
5:B:1065:GLN:CD	5:B:1067:ARG:H	1.91	0.72
4:A:1209:MET:CG	4:A:1236:LEU:HD21	2.20	0.72
4:A:1287:TYR:HD2	4:A:1305:VAL:CB	1.87	0.72
5:B:344:LYS:HD3	5:B:348:ARG:HB3	1.71	0.72
4:A:1342:GLU:HG3	7:E:198:ILE:HD13	1.71	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.72	0.72
4:A:1407:GLU:H	4:A:1407:GLU:CD	1.92	0.72
5:B:179:CYS:O	5:B:181:LEU:HD12	1.90	0.72
4:A:222:LEU:O	4:A:224:PHE:CD2	2.42	0.71
4:A:69:THR:HG21	5:B:1174:LYS:HE3	1.72	0.71
5:B:701:ILE:HD12	5:B:740:HIS:NE2	2.05	0.71
5:B:60:GLN:HE22	5:B:94:LYS:HA	1.55	0.71
4:A:857:ARG:CG	4:A:863:VAL:HA	2.12	0.71
5:B:1166:CYS:SG	14:B:1307:ZN:ZN	1.78	0.71
5:B:57:TYR:CD1	5:B:57:TYR:N	2.56	0.71
4:A:58:LEU:HD21	4:A:80:HIS:O	1.89	0.71
4:A:35:ILE:CG2	4:A:84:ILE:HD13	2.21	0.71
5:B:203:PHE:CA	5:B:204:ILE:CD1	2.57	0.71
4:A:250:ILE:CD1	4:A:254:GLU:OE2	2.38	0.71
4:A:855:THR:HG23	4:A:856:THR:N	2.04	0.71
5:B:711:GLU:H	5:B:712:PRO:HD2	1.53	0.71
4:A:857:ARG:HH21	8:F:139:PRO:CB	2.04	0.71
4:A:335:ARG:HD2	5:B:1202:LEU:HD22	1.72	0.71
8:F:69:LEU:CB	8:F:70:LYS:HB2	2.21	0.71
4:A:19:PHE:HD2	4:A:1412:ALA:HB1	1.54	0.71
5:B:203:PHE:HD1	5:B:203:PHE:C	1.89	0.71
5:B:851:PHE:O	5:B:974:PRO:HD3	1.90	0.71
11:J:45:CYS:O	11:J:48:ARG:HG3	1.90	0.71
4:A:1173:HIS:O	4:A:1174:PHE:CG	2.44	0.71
4:A:463:ILE:HD13	4:A:469:ARG:HG3	1.72	0.71
5:B:336:ARG:HH11	5:B:336:ARG:H	1.36	0.71
5:B:770:GLN:OE1	5:B:983:ARG:HA	1.90	0.70
4:A:1364:ASN:ND2	4:A:1366:ARG:HH11	1.87	0.70
4:A:264:PHE:CE1	4:A:317:LYS:N	2.58	0.70
4:A:590:ARG:HH22	4:A:592:ASP:CG	1.94	0.70
4:A:636:GLU:HB3	4:A:637:LYS:CD	2.22	0.70
5:B:55:VAL:HG11	5:B:177:LYS:NZ	2.06	0.70
4:A:852:TYR:CE2	4:A:1060:PRO:CB	2.73	0.70
5:B:806:THR:H	5:B:809:MET:HE3	1.57	0.70
4:A:41:MET:C	4:A:50:ILE:HD11	2.12	0.70
6:C:56:THR:HG21	6:C:145:CYS:SG	2.30	0.70
4:A:83:HIS:CA	4:A:241:VAL:HG23	2.21	0.70
4:A:590:ARG:NH2	4:A:592:ASP:CG	2.45	0.70
4:A:637:LYS:HD2	4:A:637:LYS:N	2.06	0.70
4:A:857:ARG:HD3	4:A:863:VAL:CG2	2.22	0.70
4:A:1025:ARG:C	4:A:1026:LEU:HD13	2.11	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1231:ASP:CA	4:A:1233:ASP:CG	2.55	0.70
4:A:83:HIS:HA	4:A:241:VAL:HG23	1.71	0.70
5:B:104:GLU:OE1	5:B:120:ARG:NH2	2.20	0.70
6:C:186:LEU:HB3	6:C:188:HIS:CD2	2.26	0.70
4:A:1098:VAL:N	4:A:1099:PRO:HD2	2.06	0.70
4:A:1174:PHE:HA	4:A:1175:SER:HB3	1.70	0.70
4:A:55:ASP:O	4:A:58:LEU:N	2.25	0.70
4:A:795:GLU:OE2	5:B:731:VAL:HG11	1.91	0.70
5:B:225:VAL:C	5:B:226:PHE:CD1	2.65	0.70
5:B:703:ILE:HG12	5:B:740:HIS:CE1	2.26	0.70
4:A:795:GLU:OE2	5:B:731:VAL:CG1	2.40	0.70
11:J:8:PHE:H	11:J:49:MET:HE3	1.57	0.70
4:A:1364:ASN:HD22	4:A:1366:ARG:HG2	1.56	0.69
4:A:596:THR:C	4:A:598:LEU:H	1.96	0.69
5:B:653:VAL:HG22	5:B:689:LEU:HB3	1.74	0.69
4:A:1172:LEU:HA	4:A:1174:PHE:H	1.57	0.69
4:A:68:GLN:C	4:A:70:CYS:H	1.96	0.69
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.74	0.69
4:A:302:THR:CG2	4:A:313:GLN:NE2	2.53	0.69
4:A:567:LYS:CB	4:A:568:PRO:CD	2.65	0.69
4:A:90:VAL:HA	4:A:297:GLN:OE1	1.91	0.69
5:B:1068:GLY:HA3	5:B:1086:PHE:CD1	2.28	0.69
5:B:299:GLU:OE2	5:B:571:PRO:HD2	1.92	0.69
8:F:93:ILE:HD11	8:F:134:ILE:HD11	1.73	0.69
4:A:90:VAL:HG13	4:A:297:GLN:OE1	1.92	0.69
5:B:1084:GLN:HE22	6:C:192:TRP:N	1.87	0.69
6:C:67:LEU:HA	6:C:70:ILE:HD12	1.72	0.69
5:B:637:LEU:CD1	5:B:740:HIS:CE1	2.75	0.69
6:C:142:VAL:H	11:J:16:ASP:HB3	1.55	0.69
4:A:1287:TYR:HE2	4:A:1305:VAL:HB	1.51	0.69
4:A:156:ASP:CG	4:A:156:ASP:O	2.30	0.69
4:A:672:ASP:H	4:A:736:ASN:HD21	1.41	0.69
4:A:809:THR:HB	4:A:810:PRO:CD	2.22	0.69
4:A:1172:LEU:HB3	4:A:1173:HIS:CA	2.15	0.69
4:A:222:LEU:O	4:A:224:PHE:HD2	1.74	0.69
4:A:264:PHE:CE1	4:A:317:LYS:HG3	2.25	0.69
4:A:482:PHE:HE2	5:B:836:GLU:HB2	1.57	0.69
5:B:290:GLY:HA2	5:B:327:ARG:HH11	1.57	0.69
5:B:879:ARG:HH12	5:B:885:MET:HE1	1.56	0.69
4:A:777:PHE:CD1	4:A:782:ARG:HA	2.28	0.69
4:A:78:PRO:HB3	5:B:1201:LYS:CE	2.16	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:637:LEU:HD13	5:B:740:HIS:HD1	1.57	0.69
4:A:65:LEU:HD22	4:A:72:GLU:N	2.08	0.69
5:B:20:ASP:OD2	5:B:21:GLU:HG2	1.93	0.69
4:A:482:PHE:CE2	5:B:836:GLU:HB2	2.28	0.68
4:A:1026:LEU:O	4:A:1030:ARG:HB2	1.92	0.68
4:A:795:GLU:OE1	5:B:731:VAL:HG22	1.93	0.68
4:A:22:PHE:CD2	5:B:1211:ASN:HA	2.28	0.68
4:A:453:MET:CE	4:A:520:CYS:SG	2.81	0.68
8:F:69:LEU:HB2	8:F:70:LYS:CB	2.24	0.68
4:A:58:LEU:CD2	4:A:80:HIS:O	2.42	0.68
4:A:1199:ARG:NH2	4:A:1232:ASN:OD1	2.27	0.68
4:A:58:LEU:CD2	4:A:59:GLY:N	2.50	0.68
4:A:793:SER:HB2	4:A:794:PRO:HD2	1.76	0.68
4:A:852:TYR:HE2	4:A:1060:PRO:HB2	1.56	0.68
4:A:888:GLY:O	4:A:940:ARG:NH2	2.27	0.68
5:B:778:MET:HE3	5:B:794:ASN:HB3	1.74	0.68
4:A:67:CYS:HB3	4:A:70:CYS:HB3	1.76	0.68
4:A:765:VAL:HG22	4:A:800:VAL:HB	1.75	0.68
5:B:792:MET:HE1	5:B:857:ARG:CZ	2.24	0.68
9:H:81:PRO:CB	9:H:82:PRO:CD	2.71	0.67
5:B:40:GLU:OE2	5:B:682:SER:N	2.26	0.67
5:B:203:PHE:CZ	5:B:461:LEU:HD21	2.29	0.67
4:A:1287:TYR:HD2	4:A:1305:VAL:CG2	2.06	0.67
5:B:258:LEU:HD13	5:B:269:ILE:HG12	1.75	0.67
5:B:177:LYS:CE	5:B:178:ASN:ND2	2.55	0.67
4:A:909:ASP:OD1	4:A:910:PRO:HD2	1.93	0.67
5:B:302:CYS:HA	5:B:310:MET:HE1	1.77	0.67
5:B:483:LEU:HD11	5:B:491:THR:HG23	1.77	0.67
5:B:398:ARG:HD3	5:B:509:ALA:HB2	1.75	0.67
5:B:569:TYR:CE1	5:B:589:VAL:HG21	2.29	0.67
5:B:476:ARG:O	5:B:478:GLY:N	2.27	0.67
9:H:84:ALA:HB1	9:H:89:LEU:HD11	1.76	0.67
5:B:1047:PHE:N	5:B:1047:PHE:HD1	1.90	0.67
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.27	0.67
5:B:516:ASN:ND2	5:B:516:ASN:H	1.93	0.67
6:C:22:LEU:HD22	6:C:25:VAL:HG21	1.77	0.66
4:A:852:TYR:HD2	4:A:1060:PRO:CB	2.07	0.66
4:A:148:CYS:SG	14:A:1734:ZN:ZN	1.84	0.66
5:B:655:LYS:HA	5:B:658:ILE:HD12	1.75	0.66
5:B:64:CYS:C	5:B:65:GLU:CG	2.63	0.66
4:A:182:VAL:HG22	4:A:201:VAL:HG13	1.76	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:666:ILE:HG23	5:B:1026:LEU:HB3	1.74	0.66
5:B:1063:GLY:O	5:B:1064:TYR:CD1	2.49	0.66
5:B:711:GLU:H	5:B:712:PRO:HD3	1.61	0.66
5:B:793:ALA:HB3	5:B:856:PHE:HB2	1.77	0.66
5:B:982:SER:N	5:B:1092:TYR:CE2	2.64	0.66
5:B:40:GLU:CD	5:B:681:TRP:HB3	2.16	0.66
4:A:1199:ARG:CZ	4:A:1232:ASN:OD1	2.44	0.66
4:A:315:LEU:CB	4:A:320:ARG:HH12	2.07	0.66
4:A:535:THR:CG2	4:A:617:VAL:H	2.06	0.66
5:B:614:SER:H	5:B:632:ARG:HH12	1.42	0.66
4:A:1136:SER:O	4:A:1274:ARG:HD2	1.95	0.66
4:A:41:MET:C	4:A:50:ILE:CD1	2.64	0.66
5:B:1065:GLN:HE22	5:B:1068:GLY:N	1.89	0.66
5:B:637:LEU:HD13	5:B:740:HIS:CE1	2.31	0.66
5:B:879:ARG:HH11	5:B:879:ARG:HB3	1.59	0.66
4:A:567:LYS:HZ1	9:H:43:ASN:HB3	1.61	0.66
4:A:360:GLU:HB2	4:A:363:GLN:HG3	1.78	0.66
5:B:378:LEU:O	5:B:382:ILE:HG12	1.96	0.66
5:B:979:LYS:HA	5:B:989:THR:HG22	1.78	0.66
4:A:319:GLY:C	4:A:320:ARG:HH11	1.98	0.66
4:A:41:MET:CA	4:A:50:ILE:HD12	2.24	0.66
5:B:1016:ALA:O	5:B:1017:ILE:CB	2.42	0.66
5:B:236:HIS:HD2	5:B:389:ALA:HB2	1.59	0.66
5:B:728:ARG:HD2	5:B:730:ARG:HH22	1.55	0.66
6:C:7:GLN:HB2	6:C:23:SER:HB2	1.78	0.66
4:A:1400:CYS:SG	4:A:1409:LEU:HG	2.35	0.65
5:B:177:LYS:O	5:B:177:LYS:HD2	1.96	0.65
5:B:360:PHE:CE2	5:B:361:LEU:HD13	2.31	0.65
9:H:81:PRO:HB2	9:H:82:PRO:HD2	1.77	0.65
1:R:4:G:H2'	1:R:5:A:H8	1.61	0.65
4:A:1021:LEU:CA	4:A:1024:SER:HB2	2.26	0.65
4:A:1231:ASP:CG	4:A:1232:ASN:H	1.99	0.65
4:A:153:PRO:HB2	4:A:154:SER:O	1.96	0.65
5:B:952:VAL:HG22	5:B:966:VAL:HG13	1.78	0.65
4:A:1287:TYR:CE2	4:A:1305:VAL:CG1	2.79	0.65
4:A:648:ASN:O	4:A:652:VAL:HG23	1.97	0.65
4:A:850:VAL:HG12	4:A:851:HIS:N	2.10	0.65
4:A:981:LEU:HD13	4:A:986:ILE:HD11	1.78	0.65
5:B:322:PHE:C	5:B:322:PHE:CD2	2.70	0.65
4:A:47:ARG:NH1	5:B:920:PRO:HB2	2.12	0.65
4:A:1441:PHE:CE2	8:F:89:GLU:CG	2.80	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:35:ILE:HG22	4:A:84:ILE:HD13	1.79	0.65
4:A:1134:ILE:O	4:A:1138:ILE:HG12	1.97	0.65
4:A:153:PRO:HA	4:A:154:SER:CB	2.26	0.65
4:A:754:SER:N	4:A:757:ASN:HD22	1.92	0.65
4:A:1206:ASP:HB2	4:A:1274:ARG:NH1	2.11	0.65
4:A:457:ALA:O	4:A:507:VAL:HG23	1.97	0.65
4:A:779:PHE:CD2	4:A:785:PRO:HG3	2.32	0.65
11:J:48:ARG:HH21	11:J:49:MET:HE1	1.60	0.65
4:A:717:ASN:O	4:A:721:PHE:CD2	2.50	0.65
5:B:57:TYR:O	5:B:60:GLN:N	2.30	0.65
5:B:879:ARG:N	5:B:879:ARG:NE	2.45	0.65
4:A:68:GLN:O	4:A:70:CYS:N	2.30	0.64
5:B:30:SER:O	5:B:34:ILE:HD12	1.96	0.64
6:C:50:GLU:HB3	6:C:156:THR:HB	1.79	0.64
9:H:116:TYR:HB2	9:H:123:MET:HB3	1.78	0.64
11:J:48:ARG:HH21	11:J:49:MET:CE	2.10	0.64
4:A:337:ARG:HH21	4:A:839:ARG:HD2	1.63	0.64
4:A:717:ASN:O	4:A:721:PHE:HD2	1.80	0.64
5:B:969:ARG:NH2	6:C:59:ALA:CB	2.53	0.64
4:A:1236:LEU:C	4:A:1237:ILE:HG13	2.18	0.64
4:A:536:LEU:HB2	4:A:539:THR:HG22	1.79	0.64
5:B:1065:GLN:O	5:B:1065:GLN:NE2	2.30	0.64
5:B:982:SER:N	5:B:1092:TYR:HE2	1.96	0.64
5:B:376:PHE:HE2	5:B:569:TYR:HD2	1.45	0.64
5:B:176:SER:O	5:B:178:ASN:N	2.30	0.64
6:C:46:ILE:HD12	6:C:157:CYS:HB3	1.80	0.64
4:A:727:ASP:O	4:A:731:ARG:HG3	1.98	0.64
5:B:634:TYR:CD2	5:B:692:TYR:CD1	2.86	0.64
9:H:95:TYR:HE2	9:H:97:MET:CG	2.11	0.64
4:A:81:PHE:HE2	4:A:240:PRO:HB2	1.62	0.64
4:A:351:THR:HB	4:A:468:PHE:CD2	2.33	0.64
4:A:830:LYS:NZ	4:A:1080:THR:CA	2.57	0.64
4:A:664:THR:OG1	5:B:1014:PRO:HB3	1.97	0.64
5:B:175:ARG:NH1	5:B:181:LEU:O	2.31	0.64
5:B:1060:ARG:O	5:B:1063:GLY:N	2.29	0.64
4:A:1021:LEU:CA	4:A:1024:SER:CB	2.77	0.63
4:A:361:LEU:HD13	4:A:646:PHE:HD2	1.60	0.63
4:A:58:LEU:HD11	4:A:80:HIS:O	1.97	0.63
5:B:169:ARG:HB2	5:B:454:THR:HG23	1.79	0.63
4:A:324:SER:O	4:A:326:ARG:N	2.31	0.63
4:A:821:ARG:O	4:A:825:ILE:HG12	1.98	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1073:TYR:HE2	5:B:1080:LYS:HG3	1.63	0.63
5:B:203:PHE:N	5:B:204:ILE:HD12	2.13	0.63
5:B:986:GLN:HE22	5:B:1020:ARG:CD	2.10	0.63
4:A:830:LYS:HD3	4:A:1079:MET:O	1.98	0.63
4:A:68:GLN:O	4:A:68:GLN:CG	2.46	0.63
4:A:666:ILE:CD1	5:B:1052:VAL:HG13	2.24	0.63
4:A:779:PHE:HE1	5:B:517:THR:CG2	2.09	0.63
5:B:290:GLY:HA3	5:B:327:ARG:NH1	2.14	0.63
4:A:1021:LEU:N	4:A:1024:SER:OG	2.32	0.63
5:B:879:ARG:CZ	5:B:879:ARG:N	2.62	0.63
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.34	0.63
5:B:200:GLY:CA	5:B:202:TYR:HE2	2.09	0.63
5:B:903:VAL:HG12	5:B:904:ARG:H	1.64	0.63
6:C:56:THR:HG23	6:C:147:LEU:HD23	1.81	0.63
6:C:46:ILE:O	6:C:169:LYS:HE3	1.99	0.63
13:L:50:ASP:HA	13:L:51:CYS:C	2.19	0.63
4:A:830:LYS:HZ2	4:A:1080:THR:HA	1.60	0.63
5:B:1064:TYR:HD1	5:B:1064:TYR:N	1.96	0.63
5:B:1099:VAL:O	5:B:1103:ILE:HG12	1.98	0.63
5:B:202:TYR:HD1	5:B:209:GLU:HB3	1.63	0.63
5:B:336:ARG:CD	5:B:336:ARG:O	2.47	0.63
4:A:351:THR:HG22	4:A:352:VAL:N	2.14	0.63
4:A:41:MET:HA	4:A:50:ILE:HD12	1.81	0.63
4:A:541:ILE:CD1	4:A:546:VAL:HG22	2.27	0.63
4:A:947:PHE:CE1	4:A:954:TRP:CE2	2.86	0.63
5:B:40:GLU:OE2	5:B:681:TRP:N	2.32	0.63
4:A:11:LEU:HA	5:B:1193:GLN:O	1.99	0.62
5:B:982:SER:HA	5:B:1092:TYR:HD2	1.57	0.62
4:A:159:THR:CB	4:A:160:GLN:HA	2.30	0.62
4:A:853:ASP:O	4:A:855:THR:N	2.30	0.62
4:A:1209:MET:HE2	4:A:1236:LEU:HD11	1.81	0.62
4:A:155:GLU:HG3	4:A:156:ASP:N	2.12	0.62
6:C:112:ASN:ND2	6:C:146:LYS:HG2	2.14	0.62
5:B:181:LEU:C	5:B:183:GLU:H	2.03	0.62
4:A:101:LYS:HG2	4:A:139:TRP:CZ3	2.35	0.62
4:A:628:GLY:O	4:A:632:VAL:HG23	2.00	0.62
5:B:706:GLN:H	5:B:710:LEU:HD12	1.64	0.62
5:B:200:GLY:CA	5:B:202:TYR:CE2	2.68	0.62
4:A:1026:LEU:O	4:A:1027:ALA:HB3	1.98	0.62
4:A:963:ILE:HD13	4:A:1048:ASN:HB3	1.80	0.62
5:B:173:MET:HA	5:B:203:PHE:CD2	2.33	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:795:GLU:OE1	5:B:731:VAL:HG13	2.00	0.62
6:C:45:ALA:HA	6:C:72:LEU:HD12	1.82	0.62
11:J:41:LEU:HD22	11:J:46:CYS:O	2.00	0.62
4:A:1025:ARG:C	4:A:1026:LEU:CD1	2.67	0.62
4:A:523:ILE:O	4:A:528:LEU:HB2	1.99	0.62
4:A:636:GLU:CG	4:A:637:LYS:HD2	2.30	0.62
10:I:6:PHE:O	10:I:14:LEU:HD13	2.00	0.62
5:B:345:LYS:HG3	5:B:348:ARG:HH21	1.64	0.62
5:B:370:PHE:HD1	5:B:373:ARG:HG3	1.65	0.62
5:B:404:LYS:CD	5:B:404:LYS:NZ	2.61	0.62
5:B:515:HIS:H	5:B:518:HIS:HD2	1.48	0.62
6:C:35:ARG:HB2	12:K:41:THR:HG23	1.80	0.62
5:B:969:ARG:NH2	6:C:60:ASP:H	1.98	0.62
4:A:446:ARG:NH1	4:A:448:PRO:HD2	2.14	0.61
4:A:54:ASN:O	4:A:55:ASP:CB	2.48	0.61
4:A:590:ARG:HG3	4:A:605:MET:HB3	1.82	0.61
4:A:605:MET:SD	4:A:617:VAL:HG22	2.40	0.61
4:A:902:LEU:O	4:A:903:ASN:HB2	1.99	0.61
5:B:1017:ILE:HD13	5:B:1026:LEU:HD21	1.81	0.61
4:A:546:VAL:HG13	4:A:577:ILE:HG21	1.82	0.61
4:A:58:LEU:CD1	4:A:80:HIS:O	2.48	0.61
5:B:1017:ILE:HB	5:B:1018:PRO:CD	2.30	0.61
5:B:879:ARG:O	5:B:882:THR:CG2	2.40	0.61
8:F:136:ARG:O	8:F:143:PHE:HA	1.99	0.61
5:B:51:PHE:HD2	5:B:176:SER:HG	1.47	0.61
5:B:211:VAL:CG2	5:B:483:LEU:HD22	2.31	0.61
5:B:890:TYR:CD1	5:B:910:VAL:HG21	2.36	0.61
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	1.83	0.61
4:A:588:LEU:HD23	4:A:607:ILE:HD12	1.82	0.61
5:B:710:LEU:O	5:B:711:GLU:HB3	2.00	0.61
11:J:10:CYS:SG	11:J:43:ARG:CD	2.87	0.61
4:A:1172:LEU:CB	4:A:1173:HIS:CA	2.75	0.61
4:A:49:LYS:HZ1	4:A:61:ILE:H	1.48	0.61
4:A:777:PHE:HD1	4:A:782:ARG:CA	2.13	0.61
9:H:44:VAL:HG13	9:H:48:PRO:HA	1.82	0.61
5:B:848:ARG:HA	6:C:69:LEU:HD21	1.81	0.61
12:K:47:ARG:HD2	12:K:60:ALA:HA	1.81	0.61
4:A:1174:PHE:CB	4:A:1175:SER:HB3	2.30	0.61
4:A:93:VAL:CG2	4:A:301:ALA:HA	2.31	0.61
5:B:180:TYR:O	5:B:182:SER:N	2.33	0.61
5:B:805:THR:HG22	5:B:809:MET:SD	2.41	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:15:LYS:HE2	5:B:1220:ARG:HG2	1.83	0.60
4:A:668:ASP:HB3	4:A:743:VAL:HG23	1.82	0.60
4:A:669:THR:HG22	4:A:761:MET:HE3	1.82	0.60
5:B:302:CYS:SG	5:B:310:MET:HE1	2.34	0.60
1:R:3:C:H2'	1:R:4:G:C8	2.36	0.60
4:A:31:SER:OG	4:A:83:HIS:CD2	2.53	0.60
5:B:173:MET:CA	5:B:203:PHE:HD2	2.15	0.60
5:B:176:SER:O	5:B:179:CYS:N	2.30	0.60
4:A:332:LYS:HG3	4:A:333:GLU:HG2	1.83	0.60
5:B:57:TYR:O	5:B:59:LEU:N	2.33	0.60
5:B:706:GLN:O	5:B:710:LEU:HB2	2.01	0.60
4:A:1206:ASP:CB	4:A:1274:ARG:HH12	2.12	0.60
4:A:315:LEU:N	4:A:320:ARG:NH1	2.47	0.60
4:A:131:SER:HB3	4:A:223:GLY:HA2	1.83	0.60
5:B:1064:TYR:CD1	5:B:1064:TYR:N	2.67	0.60
5:B:541:LEU:HB2	5:B:747:MET:HE3	1.84	0.60
4:A:456:MET:HB2	4:A:478:TYR:OH	2.02	0.60
5:B:1073:TYR:CE2	5:B:1080:LYS:HG3	2.37	0.60
5:B:918:ILE:HD12	5:B:935:ARG:HD2	1.84	0.60
3:T:15:DA:H2''	3:T:16:DC:O5'	2.02	0.60
4:A:765:VAL:HG13	4:A:802:ASN:O	2.02	0.60
4:A:567:LYS:NZ	9:H:43:ASN:HB3	2.16	0.60
4:A:1170:ILE:HD12	4:A:1171:GLN:HG3	1.83	0.60
4:A:1345:ARG:HD2	4:A:1346:ALA:CA	2.31	0.60
4:A:811:GLN:HB3	4:A:815:PHE:HE2	1.67	0.60
4:A:1020:CYS:N	4:A:1021:LEU:O	2.35	0.60
4:A:1295:THR:HB	4:A:1297:GLU:OE1	2.02	0.60
4:A:666:ILE:CG2	5:B:1026:LEU:CB	2.74	0.60
5:B:592:ASN:HD21	5:B:595:ARG:HD2	1.65	0.59
4:A:857:ARG:HD2	4:A:861:GLY:C	2.22	0.59
4:A:35:ILE:HG13	4:A:241:VAL:HG21	1.84	0.59
4:A:313:GLN:O	4:A:321:PRO:HA	2.02	0.59
4:A:855:THR:HG23	4:A:856:THR:H	1.68	0.59
5:B:684:LEU:HD23	5:B:689:LEU:HD12	1.83	0.59
5:B:835:GLN:HA	5:B:1013:ASN:HD22	1.66	0.59
4:A:1022:LEU:HA	4:A:1026:LEU:CD1	2.32	0.59
4:A:676:MET:HA	4:A:679:ILE:HD12	1.84	0.59
13:L:30:ILE:O	13:L:56:LEU:HA	2.02	0.59
4:A:1390:ASN:O	4:A:1399:ARG:HD2	2.03	0.59
5:B:634:TYR:HD2	5:B:692:TYR:CD1	2.21	0.59
7:E:15:ALA:O	7:E:19:VAL:HG23	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1023:ARG:N	4:A:1025:ARG:O	2.35	0.59
4:A:1352:VAL:O	4:A:1355:VAL:HG12	2.03	0.59
4:A:1150:SER:HA	4:A:1195:LEU:HD23	1.85	0.59
4:A:1209:MET:CE	4:A:1236:LEU:HD11	2.32	0.59
4:A:115:LEU:HD21	4:A:145:LYS:HD2	1.84	0.59
5:B:1160:VAL:HG12	5:B:1161:HIS:N	2.18	0.59
5:B:202:TYR:OH	5:B:485:ARG:NH2	2.36	0.59
5:B:807:ARG:NH1	5:B:807:ARG:CG	2.62	0.59
4:A:598:LEU:HD13	9:H:25:ARG:HH22	1.68	0.59
4:A:508:PRO:O	4:A:511:ILE:HG13	2.03	0.59
4:A:814:PHE:CE1	5:B:514:LEU:HD21	2.38	0.59
5:B:857:ARG:NH2	5:B:942:ARG:NH1	2.50	0.59
4:A:1170:ILE:CD1	4:A:1171:GLN:HG3	2.32	0.59
4:A:1424:VAL:HG13	4:A:1436:ILE:HD11	1.85	0.59
5:B:800:GLN:HB3	11:J:52:THR:HG22	1.83	0.59
3:T:20:DC:H2'	3:T:21:DC:O4'	2.03	0.59
4:A:1174:PHE:CA	4:A:1175:SER:HB3	2.29	0.58
4:A:1231:ASP:CG	4:A:1232:ASN:N	2.55	0.58
4:A:465:TYR:HB3	5:B:976:ILE:HG21	1.85	0.58
5:B:179:CYS:O	5:B:181:LEU:CG	2.51	0.58
4:A:779:PHE:CE1	5:B:517:THR:HA	2.37	0.58
8:F:69:LEU:H	8:F:70:LYS:HB2	1.68	0.58
9:H:84:ALA:HA	9:H:87:ARG:HB2	1.83	0.58
4:A:69:THR:HA	4:A:71:GLN:HG3	1.84	0.58
4:A:1025:ARG:CD	4:A:1030:ARG:NH2	2.61	0.58
4:A:1244:ARG:HH11	4:A:1244:ARG:CG	2.16	0.58
4:A:314:ALA:HA	4:A:320:ARG:HB3	1.85	0.58
4:A:54:ASN:O	4:A:55:ASP:HB2	2.02	0.58
5:B:982:SER:HB3	5:B:1092:TYR:CZ	2.36	0.58
8:F:69:LEU:N	8:F:70:LYS:HB2	2.18	0.58
4:A:1018:PHE:O	4:A:1021:LEU:HB3	2.03	0.58
4:A:463:ILE:CD1	4:A:469:ARG:HG3	2.33	0.58
5:B:276:ILE:HG13	5:B:277:LYS:N	2.13	0.58
4:A:472:LEU:HD13	5:B:835:GLN:OE1	2.04	0.58
6:C:66:ARG:NH2	11:J:3:VAL:O	2.36	0.58
4:A:396:PRO:HB3	4:A:403:LYS:HB3	1.84	0.58
4:A:830:LYS:HZ2	4:A:1080:THR:CB	2.16	0.58
4:A:92:HIS:ND1	4:A:95:PHE:HD2	2.02	0.58
4:A:810:PRO:N	5:B:1047:PHE:HE2	1.99	0.58
5:B:1063:GLY:C	5:B:1064:TYR:CD1	2.77	0.58
5:B:37:PHE:O	5:B:38:PHE:HB2	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1392:SER:O	4:A:1394:THR:N	2.37	0.58
4:A:482:PHE:CD2	5:B:836:GLU:O	2.50	0.58
4:A:779:PHE:CD1	4:A:779:PHE:N	2.68	0.58
5:B:1084:GLN:OE1	5:B:1084:GLN:N	2.36	0.58
5:B:711:GLU:N	5:B:712:PRO:CD	2.56	0.58
5:B:406:LEU:HD12	5:B:633:VAL:CG2	2.33	0.58
5:B:578:THR:OG1	5:B:593:PRO:HG3	2.03	0.58
12:K:33:ILE:HD13	12:K:87:LEU:HD22	1.86	0.58
4:A:316:GLN:CG	4:A:317:LYS:N	2.67	0.57
4:A:519:PRO:HB2	4:A:630:ILE:HD12	1.85	0.57
5:B:1001:PHE:CE1	6:C:34:ARG:CZ	2.87	0.57
5:B:219:ALA:HB2	5:B:405:ARG:HG2	1.86	0.57
8:F:116:ASP:HB3	8:F:119:ARG:HB2	1.86	0.57
8:F:73:ALA:O	8:F:74:ILE:HB	2.04	0.57
4:A:1022:LEU:C	4:A:1023:ARG:HG3	2.22	0.57
4:A:690:VAL:HG21	4:A:718:VAL:HG13	1.86	0.57
4:A:80:HIS:ND1	4:A:80:HIS:N	2.51	0.57
4:A:851:HIS:N	4:A:851:HIS:CD2	2.72	0.57
6:C:67:LEU:HD11	6:C:155:LEU:HD13	1.85	0.57
8:F:147:SER:O	8:F:151:LEU:HD12	2.04	0.57
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.33	0.57
5:B:1039:GLY:HA2	11:J:51:LEU:HD22	1.86	0.57
4:A:545:GLN:HB3	4:A:549:MET:CE	2.35	0.57
4:A:588:LEU:HD13	4:A:632:VAL:HG21	1.85	0.57
5:B:173:MET:HA	5:B:203:PHE:HD2	1.69	0.57
4:A:159:THR:HB	4:A:160:GLN:HA	1.87	0.57
4:A:22:PHE:CD1	4:A:26:GLU:OE2	2.57	0.57
4:A:618:GLU:CD	4:A:619:LYS:N	2.58	0.57
5:B:203:PHE:C	5:B:204:ILE:HD12	2.23	0.57
5:B:314:LEU:HD23	5:B:317:CYS:SG	2.44	0.57
4:A:1101:LEU:HB2	4:A:1355:VAL:HG21	1.85	0.57
5:B:175:ARG:HH11	5:B:182:SER:N	2.03	0.57
5:B:178:ASN:C	5:B:180:TYR:N	2.58	0.57
4:A:1345:ARG:HD2	4:A:1346:ALA:N	2.19	0.57
4:A:500:GLU:OE2	5:B:1143:ALA:C	2.43	0.57
4:A:316:GLN:NE2	4:A:317:LYS:CG	2.48	0.57
5:B:292:ILE:H	5:B:293:PRO:HD2	1.70	0.57
5:B:731:VAL:HG12	5:B:732:SER:N	2.19	0.57
4:A:1161:THR:HG22	4:A:1162:VAL:N	2.20	0.57
5:B:1068:GLY:HA3	5:B:1086:PHE:CE1	2.39	0.57
5:B:202:TYR:C	5:B:203:PHE:O	2.42	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:7:CYS:SG	10:I:9:ASP:O	2.62	0.57
11:J:6:ARG:HA	11:J:12:LYS:O	2.04	0.57
5:B:685:LEU:HD11	5:B:692:TYR:CE2	2.39	0.57
5:B:698:GLU:HA	5:B:701:ILE:CD1	2.35	0.57
4:A:399:HIS:CE1	4:A:462:VAL:HG21	2.40	0.57
5:B:637:LEU:HD13	5:B:740:HIS:CG	2.37	0.57
5:B:995:ARG:HH22	12:K:9:LEU:HD11	1.69	0.57
5:B:800:GLN:HB3	11:J:52:THR:HG21	1.85	0.57
4:A:1234:GLU:C	4:A:1235:LYS:CD	2.72	0.56
4:A:1344:GLY:O	4:A:1345:ARG:O	2.22	0.56
5:B:824:ILE:HG12	11:J:48:ARG:HH12	1.70	0.56
4:A:49:LYS:O	4:A:50:ILE:HB	2.04	0.56
5:B:361:LEU:HD21	5:B:377:PHE:HD2	1.71	0.56
5:B:744:HIS:CD2	5:B:746:SER:H	2.23	0.56
8:F:69:LEU:CA	8:F:70:LYS:HB2	2.35	0.56
4:A:157:ASP:O	4:A:158:PRO:C	2.44	0.56
5:B:1019:SER:C	5:B:1020:ARG:HG2	2.26	0.56
5:B:983:ARG:HD2	5:B:1091:TYR:HB3	1.88	0.56
7:E:202:SER:OG	7:E:204:THR:HG22	2.04	0.56
4:A:1017:LEU:HB2	7:E:205:SER:HA	1.85	0.56
4:A:354:SER:HA	4:A:482:PHE:HD1	1.71	0.56
4:A:544:ASP:CG	4:A:545:GLN:N	2.56	0.56
4:A:90:VAL:CA	4:A:297:GLN:OE1	2.52	0.56
4:A:939:ASP:OD1	4:A:1023:ARG:NH1	2.39	0.56
4:A:10:PRO:O	5:B:1193:GLN:HB3	2.05	0.56
5:B:785:TYR:CE1	11:J:60:PHE:CE1	2.94	0.56
5:B:1066:SER:C	5:B:1067:ARG:HG2	2.26	0.56
5:B:301:ILE:O	5:B:303:TYR:CE2	2.59	0.56
6:C:173:ALA:O	6:C:233:GLU:O	2.23	0.56
4:A:225:ASN:HD22	4:A:227:VAL:H	1.54	0.56
4:A:476:SER:N	4:A:477:PRO:HD2	2.20	0.56
4:A:524:VAL:HG12	4:A:525:GLN:N	2.20	0.56
5:B:226:PHE:HD2	5:B:398:ARG:NH2	2.03	0.56
5:B:217:ARG:NH1	5:B:407:ASP:CG	2.58	0.56
11:J:64:ASN:HB3	11:J:65:PRO:HD3	1.87	0.56
4:A:353:ILE:HD13	4:A:487:MET:HE1	1.84	0.56
4:A:777:PHE:CD1	4:A:782:ARG:N	2.73	0.56
5:B:1065:GLN:NE2	5:B:1067:ARG:N	2.30	0.56
5:B:1124:ARG:NH1	5:B:1124:ARG:CG	2.65	0.56
4:A:11:LEU:HD12	5:B:1194:ILE:HA	1.87	0.56
5:B:124:TYR:OH	5:B:179:CYS:C	2.44	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:202:TYR:O	5:B:204:ILE:CD1	2.52	0.56
5:B:523:CYS:SG	5:B:750:GLY:N	2.78	0.56
7:E:52:ARG:CB	7:E:53:PRO:CD	2.80	0.56
4:A:883:LEU:HD22	4:A:1020:CYS:O	2.06	0.56
4:A:1187:GLN:N	4:A:1187:GLN:HE21	2.03	0.56
5:B:341:LEU:HB2	5:B:344:LYS:HE3	1.88	0.56
4:A:47:ARG:HH12	5:B:920:PRO:HB2	1.69	0.56
4:A:956:LEU:HD11	4:A:1017:LEU:HD22	1.87	0.56
5:B:173:MET:CA	5:B:203:PHE:HB3	2.32	0.56
5:B:969:ARG:NE	6:C:61:GLU:OE1	2.39	0.56
4:A:1024:SER:HB3	4:A:1025:ARG:C	2.25	0.56
5:B:797:TYR:HB3	5:B:798:TYR:CE1	2.39	0.56
4:A:351:THR:CG2	4:A:352:VAL:N	2.69	0.56
4:A:81:PHE:O	4:A:241:VAL:O	2.23	0.56
5:B:292:ILE:HD12	5:B:327:ARG:H	1.70	0.56
5:B:1160:VAL:O	5:B:1161:HIS:ND1	2.40	0.55
5:B:291:ILE:HG12	5:B:300:HIS:CE1	2.41	0.55
5:B:542:MET:HB3	5:B:636:PRO:HD3	1.87	0.55
5:B:851:PHE:CD1	5:B:1094:ARG:HB2	2.39	0.55
4:A:351:THR:HG21	4:A:466:SER:O	2.06	0.55
5:B:637:LEU:HD11	5:B:740:HIS:CE1	2.41	0.55
4:A:826:ASP:O	4:A:830:LYS:N	2.37	0.55
5:B:201:GLY:N	5:B:202:TYR:HD2	2.03	0.55
4:A:315:LEU:HG	4:A:316:GLN:HB2	1.89	0.55
5:B:179:CYS:O	5:B:181:LEU:CD1	2.54	0.55
9:H:82:PRO:O	9:H:83:GLN:HB2	2.06	0.55
4:A:1011:GLN:O	4:A:1015:VAL:HG23	2.05	0.55
4:A:1027:ALA:O	4:A:1028:THR:C	2.44	0.55
4:A:1161:THR:HG21	4:A:1239:ARG:HH22	1.70	0.55
5:B:301:ILE:HG21	5:B:314:LEU:HD11	1.87	0.55
5:B:955:THR:HG22	5:B:956:THR:N	2.12	0.55
7:E:124:VAL:HB	7:E:125:PRO:HD3	1.88	0.55
10:I:7:CYS:SG	10:I:10:CYS:O	2.65	0.55
4:A:1287:TYR:OH	4:A:1307:GLU:CD	2.45	0.55
4:A:1363:VAL:HB	4:A:1368:MET:CE	2.37	0.55
4:A:857:ARG:NH2	8:F:139:PRO:CG	2.42	0.55
5:B:234:ILE:HA	5:B:259:TYR:HA	1.89	0.55
5:B:879:ARG:NH1	5:B:879:ARG:HB3	2.21	0.55
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.42	0.55
5:B:104:GLU:OE2	13:L:54:ARG:NH1	2.39	0.55
4:A:810:PRO:N	5:B:1047:PHE:CE2	2.74	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1179:GLN:O	5:B:1180:PHE:CD1	2.60	0.55
5:B:172:ILE:O	5:B:203:PHE:HB2	2.04	0.55
5:B:996:ARG:NH2	6:C:174:ALA:O	2.40	0.55
4:A:1232:ASN:HA	4:A:1233:ASP:O	2.07	0.55
5:B:766:ARG:HH21	5:B:1020:ARG:HB3	1.72	0.55
5:B:824:ILE:HG12	11:J:48:ARG:NH1	2.22	0.55
9:H:95:TYR:HE2	9:H:97:MET:HG3	1.72	0.55
4:A:1234:GLU:O	4:A:1235:LYS:CD	2.54	0.55
5:B:173:MET:O	5:B:176:SER:HB3	2.07	0.55
5:B:879:ARG:H	5:B:879:ARG:NE	2.03	0.55
4:A:1027:ALA:HB3	4:A:1030:ARG:HB2	1.88	0.54
4:A:587:HIS:NE2	4:A:969:GLN:CD	2.60	0.54
4:A:91:PHE:N	4:A:297:GLN:OE1	2.40	0.54
5:B:290:GLY:HA2	5:B:327:ARG:NH1	2.18	0.54
5:B:290:GLY:CA	5:B:327:ARG:HH11	2.17	0.54
11:J:5:VAL:O	11:J:6:ARG:O	2.25	0.54
12:K:65:HIS:CD2	12:K:66:PRO:HD2	2.42	0.54
4:A:65:LEU:CD2	4:A:72:GLU:C	2.74	0.54
5:B:803:LEU:HD12	5:B:822:ASN:OD1	2.06	0.54
8:F:72:LYS:HB3	8:F:73:ALA:CB	2.36	0.54
4:A:253:ASN:ND2	4:A:256:GLN:H	1.89	0.54
4:A:590:ARG:O	4:A:591:PHE:HB2	2.07	0.54
5:B:33:VAL:HG21	5:B:638:PHE:CZ	2.43	0.54
5:B:890:TYR:CE1	5:B:910:VAL:HG21	2.42	0.54
6:C:99:LEU:HB2	6:C:157:CYS:HB2	1.89	0.54
6:C:99:LEU:CD2	6:C:120:ILE:HA	2.36	0.54
6:C:244:VAL:HG21	12:K:105:PHE:CZ	2.42	0.54
4:A:1171:GLN:N	4:A:1171:GLN:OE1	2.41	0.54
4:A:68:GLN:O	4:A:68:GLN:HG3	2.08	0.54
4:A:51:GLY:HA2	4:A:56:PRO:CG	2.37	0.54
5:B:1077:THR:HG23	5:B:1079:LYS:H	1.72	0.54
5:B:363:HIS:HD2	5:B:585:VAL:HG22	1.71	0.54
4:A:868:TYR:HE1	4:A:1064:VAL:HG11	1.71	0.54
4:A:841:LEU:HD23	4:A:1384:VAL:HG11	1.90	0.54
4:A:441:PRO:HD3	4:A:498:ARG:HH21	1.72	0.54
5:B:798:TYR:CD2	11:J:4:PRO:HG3	2.43	0.54
13:L:38:LEU:HD21	13:L:49:LYS:HG2	1.89	0.54
4:A:14:VAL:H	4:A:1432:GLN:NE2	2.03	0.54
4:A:315:LEU:HB2	4:A:320:ARG:CZ	2.37	0.54
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.88	0.54
5:B:302:CYS:CA	5:B:310:MET:CE	2.85	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:69:LEU:H	8:F:70:LYS:CB	2.20	0.54
9:H:104:PHE:CZ	9:H:136:LYS:HA	2.43	0.54
4:A:642:CYS:O	4:A:645:LEU:HB3	2.07	0.54
4:A:690:VAL:CG2	4:A:718:VAL:HG13	2.37	0.54
5:B:302:CYS:SG	5:B:310:MET:HE3	2.23	0.54
5:B:290:GLY:HA3	5:B:327:ARG:HH12	1.71	0.54
4:A:1291:VAL:HG13	4:A:1292:PRO:HD2	1.90	0.54
4:A:68:GLN:C	4:A:70:CYS:N	2.61	0.54
4:A:1019:CYS:C	4:A:1021:LEU:O	2.47	0.53
4:A:1340:GLY:HA3	7:E:184:VAL:HG23	1.90	0.53
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.08	0.53
5:B:55:VAL:HG11	5:B:177:LYS:HZ2	1.73	0.53
5:B:809:MET:HE1	5:B:983:ARG:NH2	2.23	0.53
7:E:177:ARG:HG2	7:E:215:MET:HG3	1.90	0.53
4:A:1196:GLU:HG2	4:A:1197:LEU:N	2.23	0.53
4:A:17:VAL:HB	4:A:1419:ASP:HB3	1.90	0.53
5:B:302:CYS:HA	5:B:310:MET:CE	2.38	0.53
5:B:698:GLU:HA	5:B:701:ILE:HD13	1.89	0.53
4:A:1363:VAL:HB	4:A:1368:MET:HE3	1.89	0.53
4:A:855:THR:OG1	4:A:865:GLN:O	2.24	0.53
4:A:635:ARG:HH21	4:A:877:HIS:HA	1.73	0.53
5:B:29:ASP:HB3	5:B:658:ILE:HD13	1.89	0.53
4:A:1364:ASN:HD22	4:A:1366:ARG:CG	2.22	0.53
5:B:175:ARG:NH1	5:B:182:SER:CA	2.40	0.53
6:C:214:ASN:O	6:C:216:GLY:N	2.41	0.53
7:E:171:LYS:HB2	7:E:174:GLN:HG3	1.90	0.53
5:B:181:LEU:O	5:B:183:GLU:N	2.42	0.53
5:B:710:LEU:O	5:B:711:GLU:CB	2.56	0.53
5:B:809:MET:HE1	5:B:983:ARG:HH22	1.73	0.53
4:A:22:PHE:HD2	5:B:1211:ASN:HA	1.74	0.53
5:B:181:LEU:C	5:B:183:GLU:N	2.62	0.53
5:B:912:ILE:HD11	5:B:966:VAL:HG23	1.90	0.53
6:C:242:GLN:HA	6:C:245:VAL:HB	1.90	0.53
5:B:1163:CYS:SG	5:B:1166:CYS:SG	2.99	0.53
5:B:101:MET:HG3	5:B:169:ARG:HH12	1.74	0.53
5:B:238:ALA:HB3	5:B:256:VAL:HB	1.90	0.53
4:A:23:SER:O	4:A:27:VAL:HG23	2.07	0.53
4:A:518:LYS:HB2	4:A:519:PRO:HD2	1.91	0.53
4:A:853:ASP:C	4:A:855:THR:H	2.12	0.53
5:B:33:VAL:HG21	5:B:638:PHE:CE1	2.44	0.53
5:B:640:VAL:HG23	5:B:740:HIS:HA	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1023:ARG:O	4:A:1024:SER:HB2	2.09	0.53
4:A:370:ILE:HG22	4:A:374:LEU:HD12	1.90	0.53
4:A:403:LYS:HA	4:A:415:LEU:HB2	1.91	0.53
4:A:354:SER:HA	4:A:482:PHE:CD1	2.45	0.53
4:A:497:THR:HG21	5:B:1146:PHE:HD1	1.74	0.53
5:B:516:ASN:N	5:B:516:ASN:HD22	1.97	0.53
5:B:567:GLU:OE1	5:B:567:GLU:N	2.42	0.53
5:B:67:SER:HB2	5:B:92:PHE:HB2	1.91	0.53
10:I:68:LEU:HB3	10:I:84:VAL:CG1	2.39	0.53
4:A:1021:LEU:HA	4:A:1024:SER:OG	2.10	0.52
4:A:1026:LEU:HD13	4:A:1026:LEU:H	1.65	0.52
4:A:4:GLN:OE1	5:B:1159:ARG:NH1	2.42	0.52
4:A:579:SER:HB3	4:A:611:GLN:HA	1.91	0.52
4:A:830:LYS:HZ3	4:A:1081:LEU:H	1.57	0.52
4:A:22:PHE:HE2	5:B:1212:ILE:H	1.56	0.52
5:B:315:LYS:N	5:B:316:PRO:HD2	2.23	0.52
5:B:51:PHE:HD2	5:B:176:SER:OG	1.92	0.52
5:B:986:GLN:NE2	5:B:1020:ARG:CD	2.72	0.52
4:A:1207:LEU:HG	4:A:1274:ARG:NH2	2.25	0.52
4:A:1317:MET:HA	4:A:1322:ILE:HD11	1.91	0.52
1:R:9:G:C2	3:T:21:DC:O2	2.63	0.52
4:A:777:PHE:HE1	4:A:782:ARG:HA	1.66	0.52
4:A:22:PHE:CE2	5:B:1212:ILE:N	2.78	0.52
5:B:40:GLU:OE2	5:B:681:TRP:CB	2.58	0.52
7:E:52:ARG:HB2	7:E:53:PRO:CD	2.26	0.52
5:B:986:GLN:NE2	5:B:1020:ARG:HD2	2.21	0.52
5:B:1065:GLN:NE2	5:B:1066:SER:N	2.57	0.52
5:B:619:ILE:HG13	10:I:65:ASP:HB2	1.92	0.52
9:H:93:TYR:HA	9:H:145:ARG:HB3	1.91	0.52
4:A:542:GLU:O	4:A:546:VAL:HG23	2.09	0.52
4:A:850:VAL:CG1	4:A:851:HIS:N	2.72	0.52
4:A:545:GLN:HB3	4:A:549:MET:HE1	1.92	0.52
5:B:1034:VAL:HG22	5:B:1059:LEU:HD13	1.91	0.52
5:B:1073:TYR:HE2	5:B:1080:LYS:CG	2.22	0.52
5:B:634:TYR:CE2	5:B:692:TYR:CD1	2.98	0.52
4:A:1234:GLU:HB3	4:A:1235:LYS:CE	2.39	0.52
4:A:153:PRO:CB	4:A:154:SER:O	2.58	0.52
5:B:202:TYR:HE1	5:B:209:GLU:CD	2.13	0.52
4:A:22:PHE:HE2	5:B:1212:ILE:N	2.08	0.52
4:A:58:LEU:HD22	4:A:59:GLY:H	1.68	0.52
11:J:36:LEU:HD11	11:J:51:LEU:HB2	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:939:ASP:CG	4:A:1023:ARG:HH11	2.12	0.52
4:A:472:LEU:O	4:A:475:THR:HB	2.10	0.52
4:A:779:PHE:O	4:A:780:VAL:C	2.48	0.52
4:A:666:ILE:HD11	5:B:1030:LEU:HD22	1.91	0.52
5:B:1047:PHE:H	5:B:1047:PHE:HD1	1.58	0.52
2:N:2:DT:H3	3:T:13:DA:H61	1.55	0.52
4:A:845:LEU:O	4:A:846:GLU:C	2.47	0.52
5:B:226:PHE:CD1	5:B:226:PHE:N	2.78	0.52
4:A:852:TYR:CE1	8:F:136:ARG:HG2	2.45	0.52
4:A:1035:TYR:CD2	4:A:1035:TYR:O	2.64	0.51
4:A:252:PHE:O	4:A:252:PHE:CD2	2.63	0.51
4:A:587:HIS:CD2	4:A:609:ASP:H	2.28	0.51
4:A:901:LEU:H	4:A:926:GLN:NE2	2.08	0.51
5:B:1001:PHE:CD1	6:C:34:ARG:NH2	2.78	0.51
5:B:642:ASP:O	5:B:644:GLU:N	2.42	0.51
5:B:803:LEU:HD12	5:B:822:ASN:CG	2.30	0.51
8:F:93:ILE:CD1	8:F:134:ILE:HD11	2.40	0.51
4:A:707:GLY:HA3	4:A:1281:ARG:HG3	1.91	0.51
4:A:447:GLN:HA	4:A:448:PRO:C	2.30	0.51
4:A:731:ARG:HG2	4:A:755:PHE:CZ	2.45	0.51
5:B:684:LEU:HD23	5:B:689:LEU:CD1	2.40	0.51
4:A:1266:THR:HG22	4:A:1266:THR:O	2.10	0.51
4:A:596:THR:C	4:A:598:LEU:N	2.64	0.51
4:A:496:GLU:HG2	8:F:95:GLY:O	2.11	0.51
4:A:1229:SER:OG	4:A:1236:LEU:HD12	2.06	0.51
4:A:544:ASP:OD2	4:A:545:GLN:HG3	2.10	0.51
6:C:114:TYR:CD2	6:C:140:ASN:HB3	2.45	0.51
4:A:1170:ILE:CB	4:A:1171:GLN:CA	2.77	0.51
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.92	0.51
4:A:316:GLN:CA	4:A:318:SER:N	2.64	0.51
5:B:361:LEU:HD21	5:B:377:PHE:CD2	2.46	0.51
4:A:1209:MET:HG3	4:A:1230:GLU:O	2.11	0.51
4:A:265:LYS:HD2	4:A:303:TYR:HA	1.92	0.51
4:A:795:GLU:OE1	5:B:731:VAL:CG2	2.58	0.51
5:B:839:MET:HE3	5:B:1010:LEU:HD11	1.91	0.51
4:A:845:LEU:HD12	4:A:1069:ALA:HB2	1.93	0.51
5:B:40:GLU:OE2	5:B:681:TRP:CA	2.58	0.51
6:C:77:ILE:HD13	6:C:77:ILE:O	2.10	0.51
4:A:1434:ALA:O	4:A:1436:ILE:N	2.43	0.51
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.93	0.51
4:A:569:LYS:HD2	4:A:571:LEU:CD1	2.32	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:587:HIS:CE1	4:A:969:GLN:CD	2.84	0.51
5:B:177:LYS:CD	5:B:177:LYS:C	2.75	0.51
5:B:202:TYR:CZ	5:B:485:ARG:NH2	2.78	0.51
5:B:203:PHE:C	5:B:204:ILE:CG1	2.79	0.51
4:A:1162:VAL:C	4:A:1163:ILE:HG13	2.32	0.51
4:A:151:ASP:CA	4:A:152:VAL:CB	2.65	0.51
4:A:313:GLN:OE1	4:A:322:VAL:HG11	2.10	0.51
4:A:365:GLY:HA3	4:A:469:ARG:HB2	1.92	0.51
5:B:55:VAL:HG11	5:B:177:LYS:HZ3	1.75	0.51
4:A:1287:TYR:CD2	4:A:1305:VAL:HG21	2.42	0.50
4:A:1345:ARG:CD	4:A:1346:ALA:N	2.74	0.50
4:A:1364:ASN:ND2	4:A:1366:ARG:CG	2.66	0.50
4:A:567:LYS:CG	4:A:568:PRO:HD2	2.40	0.50
4:A:337:ARG:NH2	4:A:839:ARG:HD2	2.25	0.50
6:C:167:HIS:CD2	13:L:70:ARG:HB3	2.45	0.50
4:A:852:TYR:CZ	8:F:136:ARG:HG2	2.46	0.50
4:A:821:ARG:NH1	5:B:514:LEU:HD13	2.23	0.50
4:A:1193:LEU:HG	4:A:1193:LEU:O	2.10	0.50
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.93	0.50
5:B:120:ARG:HG2	5:B:955:THR:HG21	1.92	0.50
4:A:325:ILE:CG2	5:B:1210:MET:SD	2.99	0.50
8:F:82:THR:HG22	8:F:84:TYR:H	1.77	0.50
9:H:95:TYR:CE2	9:H:97:MET:HG3	2.46	0.50
4:A:355:GLY:N	4:A:482:PHE:CE1	2.79	0.50
5:B:1017:ILE:HB	5:B:1018:PRO:HD2	1.94	0.50
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.93	0.50
6:C:31:ASN:O	6:C:35:ARG:HG3	2.12	0.50
5:B:200:GLY:CA	5:B:202:TYR:CD2	2.85	0.50
5:B:950:ASP:OD2	5:B:967:ARG:NH2	2.29	0.50
6:C:93:ASP:OD1	6:C:122:SER:HB2	2.11	0.50
10:I:33:SER:O	10:I:35:VAL:HG23	2.11	0.50
1:R:4:G:H2'	1:R:5:A:C8	2.45	0.50
4:A:468:PHE:CE1	4:A:489:LEU:HD13	2.47	0.50
4:A:631:HIS:CE1	4:A:879:GLU:HG2	2.47	0.50
5:B:226:PHE:HD1	5:B:226:PHE:N	2.08	0.50
5:B:785:TYR:CE1	11:J:60:PHE:HE1	2.30	0.50
5:B:63:ILE:HD11	5:B:95:ILE:HD12	1.92	0.50
7:E:113:GLN:HB3	7:E:137:GLU:OE1	2.12	0.50
4:A:899:VAL:HB	4:A:929:LEU:HD12	1.93	0.50
5:B:1017:ILE:CB	5:B:1018:PRO:CD	2.89	0.50
5:B:234:ILE:HD13	5:B:257:LYS:HD3	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:376:PHE:CE2	5:B:569:TYR:HD2	2.29	0.50
7:E:89:GLY:O	7:E:91:LYS:N	2.45	0.50
10:I:27:PHE:O	10:I:35:VAL:HG13	2.12	0.49
4:A:497:THR:CG2	5:B:1146:PHE:HD1	2.25	0.49
4:A:1339:LEU:HD13	7:E:147:HIS:CD2	2.47	0.49
4:A:106:VAL:HG11	4:A:214:ILE:HD11	1.93	0.49
4:A:336:ILE:HD12	4:A:336:ILE:H	1.77	0.49
4:A:612:ILE:HG13	4:A:612:ILE:O	2.11	0.49
4:A:1436:ILE:HD13	5:B:1139:ILE:HG23	1.93	0.49
5:B:515:HIS:H	5:B:518:HIS:CD2	2.29	0.49
9:H:38:LEU:HD11	9:H:123:MET:CE	2.43	0.49
5:B:334:ILE:O	5:B:336:ARG:HG3	2.13	0.49
5:B:797:TYR:HE1	5:B:854:LEU:HG	1.76	0.49
6:C:43:THR:OG1	6:C:44:LEU:N	2.45	0.49
7:E:89:GLY:HA2	7:E:120:ALA:HB2	1.95	0.49
4:A:381:THR:O	4:A:383:TYR:N	2.45	0.49
4:A:779:PHE:O	4:A:782:ARG:O	2.30	0.49
4:A:947:PHE:CD1	4:A:954:TRP:CE2	3.00	0.49
5:B:1155:SER:OG	5:B:1156:ASP:N	2.45	0.49
5:B:749:LEU:HD22	5:B:753:ALA:HB1	1.95	0.49
8:F:71:GLU:HB3	8:F:72:LYS:O	2.12	0.49
4:A:153:PRO:CB	4:A:154:SER:C	2.76	0.49
4:A:99:ILE:HG13	4:A:234:MET:SD	2.53	0.49
4:A:334:GLY:O	4:A:336:ILE:N	2.45	0.49
5:B:728:ARG:CD	5:B:730:ARG:HH22	2.17	0.49
4:A:830:LYS:HZ2	4:A:1080:THR:CA	2.21	0.49
5:B:179:CYS:O	5:B:181:LEU:HG	2.13	0.49
5:B:322:PHE:C	5:B:322:PHE:HD2	2.14	0.49
7:E:176:PRO:O	7:E:212:ARG:HA	2.13	0.49
4:A:830:LYS:HZ3	4:A:1080:THR:CA	2.14	0.49
4:A:22:PHE:HB2	5:B:1211:ASN:OD1	2.13	0.49
5:B:203:PHE:HE1	5:B:461:LEU:HD22	1.76	0.49
5:B:515:HIS:N	5:B:518:HIS:HD2	2.10	0.49
5:B:57:TYR:O	5:B:58:THR:C	2.51	0.49
5:B:976:ILE:O	5:B:990:ILE:O	2.31	0.49
7:E:19:VAL:O	7:E:23:VAL:HG23	2.12	0.49
4:A:1030:ARG:NH1	4:A:1030:ARG:CG	2.65	0.49
5:B:204:ILE:C	5:B:205:ILE:HD13	2.24	0.49
5:B:226:PHE:CD2	5:B:398:ARG:NH2	2.81	0.49
6:C:184:ASN:HD21	6:C:189:THR:H	1.61	0.49
13:L:31:CYS:HB2	13:L:48:CYS:SG	2.53	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:993:LEU:HD22	4:A:1046:LEU:HG	1.94	0.48
4:A:266:LEU:HA	4:A:269:ILE:HD12	1.94	0.48
4:A:795:GLU:CD	5:B:731:VAL:CG1	2.81	0.48
4:A:795:GLU:OE2	5:B:731:VAL:HG13	2.11	0.48
5:B:1064:TYR:O	5:B:1065:GLN:O	2.30	0.48
5:B:341:LEU:HD12	5:B:344:LYS:CE	2.42	0.48
5:B:824:ILE:HD12	11:J:44:TYR:HE1	1.78	0.48
6:C:3:GLU:HB3	12:K:104:ASN:OD1	2.12	0.48
4:A:1022:LEU:HA	4:A:1026:LEU:HD11	1.95	0.48
4:A:35:ILE:HG21	4:A:84:ILE:HD13	1.94	0.48
4:A:413:ILE:HD12	4:A:413:ILE:N	2.28	0.48
4:A:565:ILE:CG2	4:A:567:LYS:HG2	2.43	0.48
5:B:98:THR:OG1	5:B:126:SER:HB2	2.13	0.48
5:B:217:ARG:HH11	5:B:407:ASP:CG	2.16	0.48
5:B:756:ILE:HG12	5:B:770:GLN:HG2	1.95	0.48
6:C:91:HIS:CE1	6:C:158:VAL:HG21	2.47	0.48
4:A:1441:PHE:HE2	8:F:89:GLU:HG3	1.73	0.48
4:A:315:LEU:O	4:A:316:GLN:HB3	2.12	0.48
4:A:857:ARG:HG2	4:A:863:VAL:CA	2.16	0.48
4:A:90:VAL:HG13	4:A:297:GLN:NE2	2.28	0.48
5:B:1202:LEU:HD23	5:B:1202:LEU:C	2.34	0.48
5:B:25:ILE:HG22	5:B:26:THR:N	2.28	0.48
5:B:302:CYS:CA	5:B:310:MET:HE1	2.41	0.48
5:B:363:HIS:O	5:B:364:ILE:HB	2.13	0.48
5:B:732:SER:HB3	5:B:734:HIS:CD2	2.49	0.48
5:B:851:PHE:HD1	5:B:1094:ARG:HB2	1.78	0.48
5:B:322:PHE:HE1	10:I:30:ARG:HD2	1.78	0.48
4:A:1244:ARG:NH1	4:A:1244:ARG:CB	2.50	0.48
5:B:955:THR:HG23	13:L:54:ARG:O	2.13	0.48
4:A:795:GLU:OE1	5:B:731:VAL:CG1	2.62	0.48
5:B:1028:GLU:O	5:B:1031:LEU:N	2.46	0.48
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.14	0.48
5:B:252:SER:HB3	5:B:362:PRO:HG2	1.95	0.48
5:B:294:ASP:HA	5:B:297:ILE:CG1	2.43	0.48
5:B:569:TYR:CZ	5:B:589:VAL:HG21	2.48	0.48
4:A:567:LYS:HB3	9:H:96:VAL:H	1.79	0.48
4:A:1026:LEU:O	4:A:1027:ALA:CB	2.61	0.48
5:B:44:VAL:CG1	5:B:495:LEU:HD13	2.42	0.48
5:B:515:HIS:HD2	5:B:517:THR:OG1	1.97	0.48
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.94	0.48
4:A:795:GLU:CD	5:B:731:VAL:HG13	2.33	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:199:MET:N	5:B:199:MET:SD	2.83	0.48
5:B:357:GLN:HA	5:B:374:LYS:NZ	2.28	0.48
4:A:1116:LEU:CD2	4:A:1311:VAL:HA	2.44	0.48
4:A:308:ILE:CG1	4:A:309:ALA:H	2.27	0.48
4:A:633:VAL:HG13	4:A:637:LYS:HG3	1.96	0.48
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.14	0.48
5:B:199:MET:SD	5:B:200:GLY:N	2.86	0.48
6:C:148:ARG:NH1	11:J:64:ASN:HA	2.29	0.48
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.95	0.48
4:A:1151:GLU:O	4:A:1193:LEU:HD12	2.13	0.48
4:A:598:LEU:HB3	9:H:25:ARG:HH22	1.78	0.48
5:B:198:ASP:CG	5:B:202:TYR:HH	2.17	0.48
4:A:790:ASP:HB3	10:I:87:GLN:HG3	1.96	0.48
4:A:1271:ILE:HG22	4:A:1271:ILE:O	2.13	0.47
4:A:1384:VAL:C	4:A:1389:PHE:HE1	2.17	0.47
5:B:459:TYR:C	5:B:459:TYR:CD2	2.88	0.47
5:B:703:ILE:HA	5:B:740:HIS:O	2.14	0.47
6:C:71:PRO:HB2	6:C:133:ILE:HD13	1.96	0.47
4:A:326:ARG:HG2	4:A:1406:VAL:HG21	1.96	0.47
4:A:76:GLU:OE2	5:B:1159:ARG:NH1	2.45	0.47
5:B:175:ARG:NH1	5:B:181:LEU:C	2.67	0.47
5:B:259:TYR:OH	5:B:279:ASP:OD2	2.32	0.47
5:B:542:MET:HG2	5:B:747:MET:HB3	1.96	0.47
4:A:1144:LYS:HD2	4:A:1269:GLU:OE2	2.14	0.47
5:B:492:LEU:HB2	5:B:751:VAL:HG11	1.96	0.47
9:H:110:ASP:N	9:H:110:ASP:OD2	2.48	0.47
9:H:93:TYR:CD1	9:H:143:LEU:HD22	2.49	0.47
10:I:54:GLU:OE2	10:I:118:ARG:NH1	2.47	0.47
4:A:563:PRO:HB3	4:A:572:TRP:CE2	2.48	0.47
4:A:577:ILE:H	4:A:577:ILE:HG13	1.60	0.47
5:B:1159:ARG:HD3	5:B:1193:GLN:HG3	1.96	0.47
5:B:1202:LEU:HD21	5:B:1206:GLU:OE2	2.15	0.47
5:B:660:LYS:HE3	5:B:679:TYR:CD1	2.50	0.47
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.49	0.47
5:B:879:ARG:CZ	5:B:879:ARG:CA	2.92	0.47
4:A:474:VAL:HG12	4:A:478:TYR:CE2	2.48	0.47
4:A:41:MET:C	4:A:50:ILE:HD12	2.33	0.47
4:A:637:LYS:CD	4:A:637:LYS:N	2.72	0.47
4:A:856:THR:HB	4:A:865:GLN:HB2	1.96	0.47
5:B:1065:GLN:OE1	5:B:1067:ARG:N	2.47	0.47
5:B:999:MET:HG2	5:B:1008:PRO:HD2	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1428:VAL:HG21	5:B:1135:ARG:HD2	1.97	0.47
4:A:404:TYR:HA	4:A:413:ILE:O	2.14	0.47
4:A:777:PHE:CD1	4:A:782:ARG:C	2.77	0.47
5:B:483:LEU:O	5:B:484:ASN:CB	2.62	0.47
4:A:807:GLY:HA3	5:B:728:ARG:HH12	1.77	0.47
6:C:52:GLU:HB3	6:C:154:LYS:HB3	1.95	0.47
1:R:9:G:N2	3:T:21:DC:H1'	2.29	0.47
4:A:1244:ARG:NH1	4:A:1244:ARG:CG	2.76	0.47
4:A:569:LYS:O	4:A:571:LEU:CD1	2.54	0.47
5:B:1073:TYR:CE2	5:B:1080:LYS:CG	2.98	0.47
5:B:337:ARG:HA	5:B:337:ARG:HD3	1.55	0.47
5:B:350:GLN:HE22	5:B:353:LYS:HD3	1.79	0.47
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.96	0.47
4:A:588:LEU:HB3	4:A:607:ILE:HB	1.96	0.47
5:B:1024:ALA:HA	5:B:1027:ILE:HD12	1.97	0.47
5:B:292:ILE:N	5:B:293:PRO:HD2	2.29	0.47
5:B:364:ILE:HD13	5:B:585:VAL:HG13	1.96	0.47
4:A:1418:LEU:HD13	5:B:1222:ARG:HD2	1.97	0.47
4:A:675:THR:HG22	4:A:679:ILE:HD11	1.96	0.47
5:B:839:MET:HB3	5:B:1012:ILE:HG22	1.96	0.47
5:B:1063:GLY:O	5:B:1064:TYR:HD1	1.92	0.47
5:B:177:LYS:HE2	5:B:178:ASN:CG	2.34	0.47
4:A:526:ASP:HB2	5:B:835:GLN:NE2	2.30	0.47
7:E:114:ASN:HA	7:E:114:ASN:HD22	1.54	0.47
4:A:43:GLU:O	4:A:43:GLU:HG3	2.15	0.47
5:B:203:PHE:CE1	5:B:461:LEU:HD22	2.46	0.47
5:B:323:VAL:HG12	5:B:324:ILE:HG12	1.96	0.47
5:B:546:SER:OG	5:B:631:GLY:N	2.42	0.47
5:B:857:ARG:NH2	5:B:942:ARG:HH12	2.11	0.47
6:C:162:GLY:HA3	6:C:170:TRP:CD2	2.50	0.47
4:A:451:HIS:NE2	4:A:1074:GLU:HG3	2.29	0.47
4:A:1234:GLU:CB	4:A:1235:LYS:HD3	2.40	0.47
4:A:78:PRO:HA	5:B:1201:LYS:HE3	1.96	0.47
5:B:294:ASP:HA	5:B:297:ILE:HG13	1.97	0.47
4:A:476:SER:N	4:A:477:PRO:CD	2.77	0.46
4:A:490:HIS:HB3	5:B:1150:ARG:NH2	2.31	0.46
5:B:337:ARG:O	5:B:339:THR:N	2.48	0.46
5:B:470:LYS:C	5:B:472:ALA:H	2.18	0.46
4:A:857:ARG:NH2	8:F:139:PRO:CB	2.76	0.46
10:I:65:ASP:HA	10:I:66:PRO:HD3	1.67	0.46
4:A:1364:ASN:HD21	4:A:1366:ARG:HG2	1.74	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:321:GLY:O	5:B:323:VAL:N	2.48	0.46
5:B:236:HIS:CD2	5:B:389:ALA:HB2	2.44	0.46
4:A:483:ASP:OD1	4:A:485:ASP:OD1	2.33	0.46
4:A:810:PRO:HG3	5:B:1047:PHE:CD2	2.51	0.46
4:A:589:GLN:HB3	4:A:961:ARG:NH2	2.30	0.46
5:B:547:VAL:HG12	5:B:612:GLU:OE2	2.15	0.46
5:B:635:ARG:HB2	5:B:636:PRO:CD	2.45	0.46
6:C:73:GLN:O	6:C:129:ILE:HD12	2.15	0.46
8:F:135:ARG:HG2	8:F:145:ASP:OD1	2.15	0.46
8:F:81:THR:HG21	8:F:136:ARG:HD3	1.98	0.46
12:K:12:LEU:HD12	12:K:12:LEU:H	1.80	0.46
4:A:1021:LEU:CA	4:A:1024:SER:OG	2.63	0.46
4:A:1344:GLY:O	4:A:1345:ARG:C	2.54	0.46
4:A:347:PHE:CE1	4:A:375:THR:HG22	2.43	0.46
4:A:523:ILE:HG23	4:A:527:THR:HB	1.97	0.46
4:A:68:GLN:O	4:A:68:GLN:CD	2.54	0.46
5:B:202:TYR:HA	5:B:203:PHE:O	2.15	0.46
5:B:376:PHE:HB3	5:B:586:TRP:CZ3	2.50	0.46
5:B:973:ILE:HG23	5:B:974:PRO:HD2	1.97	0.46
4:A:547:LEU:HD22	12:K:58:PHE:HD1	1.80	0.46
4:A:1284:MET:HG2	4:A:1306:LEU:CD2	2.46	0.46
4:A:575:LYS:HB3	4:A:612:ILE:HD11	1.98	0.46
4:A:519:PRO:HG3	4:A:630:ILE:HG13	1.97	0.46
4:A:73:GLY:O	4:A:76:GLU:N	2.48	0.46
5:B:1149:GLU:HG3	5:B:1153:GLU:OE1	2.14	0.46
5:B:224:GLN:HA	5:B:396:ASP:OD2	2.16	0.46
8:F:107:VAL:HG12	8:F:109:VAL:H	1.80	0.46
13:L:48:CYS:SG	13:L:51:CYS:SG	3.14	0.46
4:A:530:GLY:O	4:A:534:LEU:N	2.46	0.46
4:A:624:SER:HA	4:A:630:ILE:HD11	1.97	0.46
5:B:1175:LEU:C	5:B:1177:HIS:H	2.19	0.46
5:B:650:GLU:HG3	5:B:651:LEU:N	2.31	0.46
5:B:878:GLN:HA	5:B:879:ARG:HH21	1.79	0.46
4:A:67:CYS:CB	4:A:70:CYS:HB3	2.44	0.46
4:A:907:THR:HG22	4:A:908:LEU:N	2.30	0.46
5:B:1179:GLN:O	5:B:1180:PHE:HD1	1.98	0.46
5:B:325:GLN:HE22	10:I:12:ASN:HD21	1.64	0.46
5:B:526:GLU:HG2	5:B:538:ASN:ND2	2.31	0.46
5:B:518:HIS:CE1	5:B:537:LYS:HE2	2.50	0.46
12:K:37:LYS:O	12:K:38:GLU:HG2	2.15	0.46
1:R:3:C:H4'	4:A:323:LYS:NZ	2.30	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1173:HIS:O	4:A:1174:PHE:CD1	2.68	0.46
4:A:1345:ARG:O	4:A:1346:ALA:C	2.54	0.46
5:B:911:ILE:HG22	5:B:912:ILE:HG13	1.98	0.46
4:A:1209:MET:HE3	4:A:1228:TRP:HB2	1.97	0.46
4:A:1243:VAL:HG12	4:A:1244:ARG:H	1.81	0.46
4:A:1327:ILE:O	4:A:1327:ILE:HG23	2.16	0.46
4:A:495:GLU:O	4:A:498:ARG:HB2	2.16	0.46
4:A:649:ILE:O	4:A:653:VAL:HG23	2.16	0.46
4:A:587:HIS:CE1	4:A:969:GLN:NE2	2.82	0.46
5:B:1017:ILE:N	5:B:1018:PRO:HD2	2.30	0.46
5:B:1202:LEU:HD23	5:B:1202:LEU:O	2.16	0.46
5:B:37:PHE:O	5:B:38:PHE:CB	2.64	0.46
6:C:115:SER:OG	6:C:141:GLY:O	2.21	0.46
4:A:315:LEU:O	4:A:316:GLN:CB	2.64	0.46
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.97	0.46
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.98	0.46
9:H:82:PRO:C	9:H:84:ALA:H	2.18	0.46
13:L:48:CYS:SG	13:L:49:LYS:N	2.88	0.46
4:A:1116:LEU:HD22	4:A:1311:VAL:HA	1.97	0.45
4:A:1279:ILE:HA	4:A:1310:GLY:HA3	1.97	0.45
4:A:496:GLU:HG2	8:F:95:GLY:C	2.35	0.45
4:A:855:THR:CG2	4:A:856:THR:N	2.72	0.45
5:B:1016:ALA:O	5:B:1017:ILE:HB	2.16	0.45
5:B:102:VAL:HG12	5:B:102:VAL:O	2.16	0.45
5:B:785:TYR:HE1	11:J:60:PHE:CZ	2.34	0.45
6:C:134:ILE:HD13	6:C:139:GLY:O	2.16	0.45
4:A:545:GLN:HB3	4:A:549:MET:HE3	1.99	0.45
11:J:48:ARG:NH2	11:J:49:MET:HE1	2.30	0.45
4:A:1022:LEU:O	4:A:1022:LEU:HD23	2.16	0.45
4:A:939:ASP:CG	4:A:1023:ARG:NH1	2.70	0.45
4:A:830:LYS:NZ	4:A:1080:THR:HG23	2.32	0.45
4:A:851:HIS:O	4:A:853:ASP:OD1	2.34	0.45
5:B:1051:THR:O	5:B:1054:GLY:N	2.49	0.45
5:B:486:TYR:OH	5:B:1096:ARG:HB3	2.16	0.45
5:B:483:LEU:CD1	5:B:491:THR:HG23	2.46	0.45
9:H:5:LEU:HD22	9:H:133:ASN:O	2.17	0.45
10:I:33:SER:O	10:I:34:TYR:C	2.55	0.45
3:T:27:DA:N3	3:T:27:DA:H2'	2.32	0.45
4:A:156:ASP:C	4:A:157:ASP:CG	2.74	0.45
4:A:58:LEU:HG	4:A:80:HIS:C	2.36	0.45
5:B:1027:ILE:O	5:B:1028:GLU:C	2.54	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:113:TYR:HB3	5:B:114:PRO:HD2	1.97	0.45
5:B:177:LYS:HG3	5:B:178:ASN:N	2.31	0.45
5:B:329:THR:O	5:B:332:ASP:HB3	2.17	0.45
5:B:744:HIS:HD2	5:B:746:SER:CB	2.29	0.45
6:C:80:LEU:HD12	6:C:127:ARG:NH2	2.32	0.45
10:I:68:LEU:HB3	10:I:84:VAL:HG13	1.99	0.45
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.97	0.45
4:A:1345:ARG:O	4:A:1347:ALA:N	2.49	0.45
5:B:175:ARG:CA	5:B:179:CYS:SG	3.04	0.45
5:B:955:THR:CG2	5:B:956:THR:H	2.10	0.45
9:H:38:LEU:HD11	9:H:123:MET:HE2	1.99	0.45
4:A:1209:MET:SD	4:A:1236:LEU:CD2	2.94	0.45
4:A:1216:ILE:O	4:A:1219:THR:OG1	2.33	0.45
4:A:1236:LEU:O	4:A:1237:ILE:HG13	2.16	0.45
4:A:590:ARG:NH2	4:A:592:ASP:OD2	2.30	0.45
4:A:608:ILE:HG12	4:A:613:ILE:HG13	1.98	0.45
4:A:666:ILE:HG22	5:B:1026:LEU:HB2	1.96	0.45
4:A:775:ILE:O	4:A:797:LYS:HE2	2.16	0.45
4:A:784:LEU:HB3	4:A:786:HIS:HD2	1.82	0.45
5:B:1065:GLN:HG2	5:B:1069:PHE:HB2	1.98	0.45
5:B:1160:VAL:CG1	5:B:1161:HIS:H	2.22	0.45
5:B:405:ARG:CZ	5:B:632:ARG:HG2	2.47	0.45
5:B:903:VAL:HG12	5:B:904:ARG:N	2.29	0.45
6:C:51:VAL:HG22	6:C:155:LEU:CD2	2.47	0.45
4:A:1288:ASP:OD1	4:A:1300:LYS:NZ	2.49	0.45
4:A:208:LEU:HD22	4:A:212:LYS:HG3	1.99	0.45
4:A:447:GLN:H	4:A:447:GLN:HG2	1.67	0.45
4:A:857:ARG:HH11	4:A:863:VAL:CG2	2.19	0.45
5:B:1037:LEU:O	11:J:47:ARG:NH1	2.50	0.45
5:B:299:GLU:OE2	5:B:571:PRO:HG2	2.17	0.45
5:B:827:ILE:HG23	5:B:1012:ILE:HD12	1.98	0.45
5:B:956:THR:HA	5:B:961:LEU:O	2.17	0.45
9:H:139:ASN:O	9:H:140:ALA:HB2	2.17	0.45
13:L:32:ALA:HB3	13:L:55:ILE:CD1	2.44	0.45
4:A:308:ILE:HG13	4:A:309:ALA:H	1.81	0.45
4:A:646:PHE:O	4:A:647:GLY:C	2.55	0.45
5:B:1084:GLN:N	5:B:1084:GLN:CD	2.70	0.45
5:B:1107:ALA:O	5:B:1108:ARG:HB3	2.17	0.45
5:B:343:ILE:O	5:B:344:LYS:HG3	2.16	0.45
8:F:82:THR:HG22	8:F:84:TYR:HB2	1.99	0.45
4:A:1100:ARG:HH21	4:A:1351:GLU:HG2	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1169:ILE:O	4:A:1169:ILE:HG22	2.17	0.45
4:A:316:GLN:C	4:A:318:SER:N	2.70	0.45
4:A:453:MET:HE1	4:A:520:CYS:SG	2.57	0.45
4:A:49:LYS:HZ2	4:A:60:SER:HA	1.82	0.45
4:A:809:THR:H	4:A:812:GLU:HB2	1.82	0.45
6:C:18:VAL:CG2	6:C:240:VAL:HB	2.47	0.45
9:H:30:SER:HB2	9:H:36:CYS:SG	2.57	0.45
4:A:451:HIS:CE1	4:A:1074:GLU:HG3	2.52	0.45
4:A:19:PHE:CD2	4:A:1412:ALA:HB1	2.43	0.45
4:A:463:ILE:HD13	4:A:469:ARG:CG	2.46	0.45
4:A:598:LEU:O	4:A:599:SER:C	2.56	0.45
4:A:946:VAL:HG22	7:E:201:LYS:HB3	1.99	0.45
5:B:1068:GLY:HA3	5:B:1086:PHE:HD1	1.79	0.45
5:B:115:GLN:HE21	5:B:119:LEU:HD11	1.82	0.45
5:B:464:GLY:HA2	5:B:479:VAL:O	2.18	0.45
5:B:792:MET:CE	5:B:857:ARG:CZ	2.95	0.45
4:A:1031:VAL:HG13	4:A:1037:LEU:HD12	1.98	0.44
4:A:1231:ASP:C	4:A:1233:ASP:N	2.71	0.44
4:A:120:GLU:HG3	4:A:123:ARG:HD3	1.99	0.44
4:A:31:SER:CB	4:A:82:GLY:HA2	2.21	0.44
5:B:1028:GLU:O	5:B:1029:CYS:C	2.55	0.44
6:C:235:VAL:HG21	11:J:6:ARG:HH21	1.81	0.44
4:A:325:ILE:HG22	4:A:326:ARG:N	2.31	0.44
4:A:453:MET:HE1	4:A:520:CYS:HB3	2.00	0.44
5:B:1124:ARG:O	5:B:1125:ASP:C	2.54	0.44
5:B:494:HIS:HD2	5:B:497:ARG:NH1	2.15	0.44
5:B:1087:PHE:CE2	11:J:44:TYR:OH	2.70	0.44
4:A:1063:MET:CG	4:A:1436:ILE:HG23	2.46	0.44
4:A:325:ILE:O	4:A:328:ARG:N	2.33	0.44
4:A:586:ILE:HD11	4:A:637:LYS:CE	2.47	0.44
4:A:810:PRO:HD3	5:B:1047:PHE:HD2	1.82	0.44
5:B:31:TRP:HA	5:B:34:ILE:HD13	1.99	0.44
5:B:201:GLY:HA3	5:B:495:LEU:HD22	1.99	0.44
6:C:169:LYS:HZ2	13:L:70:ARG:HG3	1.82	0.44
4:A:38:PRO:HA	4:A:270:LEU:HD13	2.00	0.44
4:A:666:ILE:HA	5:B:1026:LEU:HD13	1.99	0.44
4:A:33:ALA:O	4:A:83:HIS:CD2	2.70	0.44
4:A:449:SER:OG	5:B:1134:GLU:OE2	2.21	0.44
5:B:202:TYR:CD1	5:B:209:GLU:HB3	2.48	0.44
12:K:65:HIS:CG	12:K:66:PRO:HD2	2.53	0.44
4:A:1206:ASP:C	4:A:1274:ARG:HH22	2.20	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1436:ILE:O	4:A:1437:GLY:C	2.54	0.44
4:A:260:ASP:OD1	4:A:261:ASP:N	2.50	0.44
4:A:304:MET:HE3	5:B:1210:MET:HG3	2.00	0.44
4:A:533:LYS:HE2	4:A:533:LYS:HB2	1.65	0.44
4:A:566:ILE:O	4:A:566:ILE:HG22	2.18	0.44
4:A:855:THR:OG1	4:A:866:PHE:HA	2.17	0.44
4:A:22:PHE:HZ	5:B:1208:MET:HG2	1.82	0.44
4:A:1154:TYR:CE1	10:I:18:GLU:HG3	2.52	0.44
4:A:1400:CYS:O	4:A:1402:PHE:N	2.42	0.44
4:A:452:LYS:NZ	4:A:1067:LEU:HD22	2.32	0.44
4:A:553:VAL:HG13	4:A:648:ASN:HB3	1.98	0.44
4:A:779:PHE:N	4:A:779:PHE:HD1	2.13	0.44
4:A:810:PRO:CD	5:B:1047:PHE:HD2	2.31	0.44
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.17	0.44
3:T:20:DC:H5"	5:B:1129:ARG:HD3	1.98	0.44
9:H:145:ARG:HD2	9:H:146:ARG:HD2	1.99	0.44
4:A:92:HIS:NE2	4:A:304:MET:CE	2.81	0.44
5:B:341:LEU:HD12	5:B:344:LYS:HE3	2.00	0.44
5:B:550:ASP:OD1	5:B:551:PRO:HD2	2.18	0.44
5:B:792:MET:HE3	5:B:857:ARG:NE	2.33	0.44
4:A:1424:VAL:HG11	5:B:1139:ILE:HD13	2.00	0.44
4:A:264:PHE:HE1	4:A:317:LYS:H	1.54	0.44
4:A:316:GLN:NE2	4:A:317:LYS:HG2	2.23	0.44
4:A:73:GLY:C	4:A:75:ASN:N	2.70	0.44
5:B:1060:ARG:HA	5:B:1060:ARG:HD2	1.71	0.44
4:A:455:MET:HG3	5:B:1137:CYS:CB	2.48	0.44
5:B:224:GLN:O	5:B:238:ALA:HA	2.18	0.44
5:B:34:ILE:HD11	5:B:743:ILE:HG22	1.98	0.44
5:B:258:LEU:HB2	5:B:385:LEU:HD21	1.99	0.44
5:B:468:GLU:HB3	5:B:469:GLN:H	1.53	0.44
5:B:810:GLU:O	5:B:811:TYR:C	2.56	0.44
6:C:73:GLN:HE21	6:C:74:SER:H	1.65	0.44
12:K:65:HIS:HD2	12:K:67:PHE:H	1.65	0.44
4:A:244:PRO:HD2	4:A:245:PRO:HD3	1.99	0.44
4:A:320:ARG:CD	4:A:320:ARG:H	2.23	0.44
4:A:588:LEU:CB	4:A:607:ILE:HB	2.48	0.44
4:A:618:GLU:O	4:A:622:VAL:HG12	2.17	0.44
4:A:857:ARG:CD	4:A:863:VAL:HG22	2.44	0.44
4:A:918:GLU:OE2	4:A:918:GLU:C	2.57	0.44
5:B:744:HIS:CD2	5:B:746:SER:HB3	2.52	0.44
6:C:184:ASN:ND2	6:C:189:THR:O	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:118:PHE:HB2	9:H:121:LEU:HB2	2.00	0.44
9:H:115:TYR:CE2	9:H:124:ARG:HG3	2.52	0.44
4:A:107:CYS:HB3	4:A:114:LEU:HD21	1.99	0.43
4:A:56:PRO:O	4:A:57:ARG:HB2	2.17	0.43
4:A:777:PHE:HB2	4:A:780:VAL:O	2.16	0.43
5:B:1013:ASN:OD1	5:B:1014:PRO:HD2	2.18	0.43
5:B:1156:ASP:OD2	5:B:1198:TYR:N	2.50	0.43
5:B:254:LEU:HD12	5:B:272:THR:O	2.18	0.43
5:B:754:SER:O	5:B:806:THR:OG1	2.26	0.43
5:B:872:GLU:HG2	5:B:916:THR:HB	2.00	0.43
7:E:100:ILE:HG23	7:E:105:PHE:HB2	2.00	0.43
10:I:87:GLN:HE22	10:I:97:MET:HG3	1.83	0.43
4:A:41:MET:HA	4:A:50:ILE:CD1	2.46	0.43
4:A:783:THR:HG21	4:A:815:PHE:CE1	2.36	0.43
4:A:837:ILE:HD13	4:A:840:ARG:HH12	1.83	0.43
5:B:1006:ILE:CD1	11:J:43:ARG:HB2	2.48	0.43
4:A:1153:TYR:HD2	4:A:1163:ILE:HD11	1.84	0.43
4:A:315:LEU:HB2	4:A:320:ARG:NH1	2.33	0.43
4:A:355:GLY:CA	4:A:482:PHE:CE1	3.02	0.43
4:A:807:GLY:HA3	5:B:728:ARG:NH1	2.33	0.43
4:A:93:VAL:HG21	4:A:304:MET:HB2	2.00	0.43
5:B:45:SER:OG	5:B:46:GLN:N	2.49	0.43
8:F:72:LYS:CE	8:F:72:LYS:HA	2.48	0.43
4:A:1021:LEU:HA	4:A:1024:SER:CB	2.46	0.43
4:A:159:THR:HB	4:A:160:GLN:HG3	2.00	0.43
4:A:41:MET:CA	4:A:50:ILE:CD1	2.93	0.43
5:B:350:GLN:NE2	5:B:353:LYS:HD3	2.34	0.43
5:B:766:ARG:HD3	5:B:766:ARG:HA	1.80	0.43
5:B:899:ILE:HD11	5:B:911:ILE:CG1	2.42	0.43
6:C:53:THR:O	6:C:153:LEU:HA	2.18	0.43
9:H:56:THR:O	9:H:144:ILE:HA	2.19	0.43
4:A:1017:LEU:HD23	4:A:1017:LEU:O	2.18	0.43
4:A:1230:GLU:HB3	4:A:1231:ASP:H	1.68	0.43
5:B:1081:LEU:HD13	5:B:1085:ILE:HD11	2.00	0.43
5:B:202:TYR:CA	5:B:203:PHE:O	2.66	0.43
5:B:429:PHE:O	5:B:433:GLN:HG3	2.19	0.43
5:B:48:LEU:HD22	5:B:175:ARG:C	2.35	0.43
5:B:890:TYR:HB3	5:B:893:LEU:HD12	2.01	0.43
6:C:60:ASP:HB3	13:L:67:PHE:CE1	2.54	0.43
7:E:9:ILE:O	7:E:13:TRP:N	2.43	0.43
11:J:8:PHE:CD1	11:J:49:MET:CE	3.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1161:THR:CG2	4:A:1162:VAL:N	2.82	0.43
4:A:709:THR:HG21	10:I:93:LYS:O	2.18	0.43
4:A:875:ALA:HA	4:A:878:ILE:HD12	1.99	0.43
5:B:1136:ASP:HA	5:B:1139:ILE:HD12	2.00	0.43
5:B:28:GLU:O	5:B:30:SER:N	2.51	0.43
5:B:800:GLN:CB	11:J:52:THR:HG22	2.48	0.43
4:A:1064:VAL:O	4:A:1065:GLY:C	2.56	0.43
4:A:1098:VAL:N	4:A:1099:PRO:CD	2.77	0.43
4:A:873:MET:HB3	4:A:878:ILE:HD11	2.00	0.43
4:A:7:SER:HB2	5:B:1193:GLN:OE1	2.19	0.43
5:B:285:ILE:O	5:B:288:ALA:HB3	2.18	0.43
5:B:335:GLY:HA3	5:B:336:ARG:HA	1.71	0.43
5:B:54:PHE:HA	5:B:58:THR:HB	1.99	0.43
5:B:801:LYS:O	11:J:52:THR:HG23	2.18	0.43
5:B:835:GLN:HA	5:B:1013:ASN:ND2	2.34	0.43
4:A:150:THR:O	4:A:151:ASP:CG	2.57	0.43
4:A:153:PRO:CB	4:A:154:SER:OG	2.67	0.43
4:A:779:PHE:HB2	4:A:782:ARG:O	2.18	0.43
4:A:873:MET:HG2	4:A:957:PRO:CG	2.39	0.43
4:A:915:SER:O	4:A:918:GLU:HG3	2.18	0.43
5:B:48:LEU:HD23	5:B:173:MET:SD	2.59	0.43
5:B:326:ASP:O	5:B:327:ARG:C	2.56	0.43
5:B:67:SER:HB2	5:B:92:PHE:HD2	1.84	0.43
5:B:876:LYS:HA	5:B:877:PRO:HD3	1.78	0.43
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.51	0.43
4:A:694:THR:HA	4:A:714:PHE:HE1	1.83	0.43
4:A:779:PHE:HA	5:B:699:GLU:OE1	2.18	0.43
5:B:1027:ILE:HG13	5:B:1027:ILE:H	1.71	0.43
4:A:12:ARG:NH1	5:B:1192:TYR:CE1	2.87	0.43
5:B:287:ARG:HA	5:B:291:ILE:O	2.19	0.43
9:H:38:LEU:HD13	9:H:125:LEU:HD13	2.01	0.43
5:B:954:VAL:O	13:L:55:ILE:O	2.37	0.43
4:A:264:PHE:CE1	4:A:317:LYS:CG	3.01	0.43
4:A:775:ILE:HG12	4:A:775:ILE:H	1.53	0.43
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.19	0.43
5:B:128:LEU:O	5:B:129:PHE:CD1	2.72	0.43
5:B:174:LEU:C	5:B:176:SER:H	2.23	0.43
5:B:203:PHE:C	5:B:204:ILE:HG13	2.38	0.43
7:E:205:SER:O	7:E:206:GLY:C	2.56	0.43
9:H:41:ASP:OD2	9:H:122:LEU:N	2.49	0.43
4:A:308:ILE:HG13	4:A:309:ALA:N	2.34	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:49:LYS:HZ1	4:A:61:ILE:N	2.14	0.42
4:A:618:GLU:OE1	4:A:619:LYS:N	2.52	0.42
12:K:61:TYR:HB3	12:K:73:LEU:HD12	2.01	0.42
4:A:1220:PHE:HA	4:A:1220:PHE:HD1	1.72	0.42
3:T:28:DT:C1'	4:A:317:LYS:O	2.62	0.42
4:A:319:GLY:CA	4:A:320:ARG:HD2	2.49	0.42
4:A:399:HIS:O	4:A:401:GLY:N	2.44	0.42
4:A:841:LEU:HD21	4:A:1105:LEU:HD22	2.00	0.42
4:A:983:ILE:HA	4:A:983:ILE:HD13	1.81	0.42
5:B:1010:LEU:HA	5:B:1010:LEU:HD12	1.81	0.42
5:B:112:LEU:HD12	5:B:116:GLU:HB3	2.00	0.42
5:B:40:GLU:CD	5:B:682:SER:H	2.19	0.42
9:H:125:LEU:HG	9:H:130:ARG:NH1	2.35	0.42
6:C:57:VAL:HG11	11:J:60:PHE:HB3	2.00	0.42
4:A:1279:ILE:HG13	4:A:1308:THR:HG21	2.00	0.42
4:A:635:ARG:HD3	4:A:635:ARG:HA	1.76	0.42
4:A:73:GLY:O	4:A:75:ASN:N	2.52	0.42
5:B:759:PRO:CG	5:B:1046:PRO:HG3	2.49	0.42
4:A:78:PRO:HA	5:B:1201:LYS:CE	2.49	0.42
5:B:301:ILE:HG22	5:B:302:CYS:N	2.33	0.42
5:B:44:VAL:O	5:B:45:SER:C	2.58	0.42
11:J:8:PHE:N	11:J:49:MET:HE3	2.30	0.42
4:A:155:GLU:HG3	4:A:156:ASP:HB3	2.02	0.42
4:A:65:LEU:HB3	4:A:72:GLU:H	1.85	0.42
5:B:1008:PRO:HG2	5:B:1011:ILE:HD11	2.00	0.42
5:B:1060:ARG:O	5:B:1061:GLU:C	2.57	0.42
5:B:1159:ARG:HH11	5:B:1159:ARG:CB	2.03	0.42
5:B:209:GLU:OE1	5:B:485:ARG:NE	2.45	0.42
6:C:41:ILE:HD11	6:C:243:VAL:HG13	2.01	0.42
6:C:36:VAL:HG21	6:C:251:LEU:HD13	2.01	0.42
4:A:1024:SER:HB3	4:A:1025:ARG:CA	2.50	0.42
4:A:376:TYR:HA	4:A:377:PRO:HD2	1.95	0.42
6:C:123:ASN:HD22	6:C:125:MET:HG2	1.84	0.42
6:C:252:GLN:HG3	12:K:95:ILE:HG23	2.02	0.42
4:A:335:ARG:HE	4:A:335:ARG:H	1.67	0.42
4:A:417:TYR:OH	5:B:887:HIS:NE2	2.31	0.42
4:A:741:ASN:ND2	4:A:741:ASN:C	2.73	0.42
5:B:260:GLY:O	5:B:267:ARG:HD3	2.20	0.42
5:B:830:TYR:CE2	5:B:1000:PRO:HD3	2.54	0.42
4:A:1022:LEU:HA	4:A:1026:LEU:HD13	2.01	0.42
4:A:567:LYS:HB2	9:H:95:TYR:HA	2.02	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:534:LEU:O	4:A:574:GLY:HA3	2.20	0.42
4:A:741:ASN:HD22	4:A:744:LYS:H	1.68	0.42
4:A:898:ARG:HB2	4:A:933:TYR:CE1	2.54	0.42
4:A:947:PHE:CD1	4:A:954:TRP:CZ2	3.07	0.42
5:B:179:CYS:O	5:B:181:LEU:HB2	2.19	0.42
5:B:198:ASP:OD1	5:B:485:ARG:NH2	2.52	0.42
5:B:62:ILE:HD12	5:B:418:LYS:HE2	2.01	0.42
5:B:841:MET:SD	5:B:990:ILE:HD11	2.59	0.42
6:C:18:VAL:HG22	6:C:240:VAL:HB	2.01	0.42
4:A:399:HIS:NE2	4:A:462:VAL:HG21	2.34	0.42
4:A:412:ARG:NH2	4:A:433:GLU:OE2	2.52	0.42
4:A:80:HIS:O	4:A:243:PRO:HB3	2.19	0.42
9:H:109:LYS:HD2	9:H:111:LEU:HD12	2.02	0.42
4:A:547:LEU:HB3	12:K:58:PHE:CE1	2.55	0.42
4:A:1187:GLN:N	4:A:1187:GLN:NE2	2.67	0.42
4:A:1274:ARG:HE	4:A:1274:ARG:HB2	1.69	0.42
4:A:242:PRO:O	4:A:247:ARG:NH2	2.52	0.42
4:A:541:ILE:HD13	4:A:577:ILE:HG12	1.99	0.42
4:A:618:GLU:CD	4:A:618:GLU:C	2.78	0.42
4:A:69:THR:CA	4:A:71:GLN:HG3	2.47	0.42
4:A:500:GLU:OE2	5:B:1144:ALA:N	2.53	0.42
5:B:203:PHE:C	5:B:204:ILE:CD1	2.87	0.42
5:B:710:LEU:HD23	5:B:733:HIS:HA	2.01	0.42
5:B:840:ILE:HB	5:B:1011:ILE:HB	2.00	0.42
3:T:18:DA:H2'	3:T:19:DT:C6	2.55	0.42
4:A:482:PHE:C	4:A:484:GLY:H	2.24	0.42
4:A:523:ILE:HG22	4:A:523:ILE:O	2.19	0.42
4:A:679:ILE:O	4:A:682:THR:HB	2.19	0.42
5:B:1037:LEU:CD2	11:J:44:TYR:HB3	2.49	0.42
13:L:55:ILE:O	13:L:56:LEU:HB2	2.19	0.42
4:A:1441:PHE:HE1	8:F:92:ARG:HD3	1.85	0.41
4:A:78:PRO:CA	5:B:1201:LYS:HE2	2.50	0.41
5:B:225:VAL:HG13	5:B:385:LEU:HD12	2.01	0.41
5:B:299:GLU:OE2	5:B:571:PRO:CD	2.64	0.41
6:C:10:ILE:HD13	6:C:20:PHE:HB3	2.02	0.41
7:E:28:TYR:HE1	7:E:78:LEU:HD13	1.84	0.41
8:F:72:LYS:HB3	8:F:73:ALA:HB2	2.02	0.41
4:A:529:CYS:O	4:A:533:LYS:HG2	2.20	0.41
5:B:812:LEU:HA	5:B:812:LEU:HD22	1.84	0.41
6:C:171:GLY:HA2	6:C:172:PRO:HD3	1.82	0.41
8:F:81:THR:HG22	8:F:82:THR:N	2.34	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1441:PHE:HZ	8:F:89:GLU:HA	1.79	0.41
5:B:896:ASP:OD2	13:L:58:LYS:HE2	2.19	0.41
4:A:1170:ILE:HG13	4:A:1171:GLN:HG3	2.02	0.41
4:A:452:LYS:O	4:A:455:MET:HB2	2.20	0.41
4:A:474:VAL:O	4:A:474:VAL:HG12	2.19	0.41
4:A:500:GLU:OE2	5:B:1143:ALA:CB	2.68	0.41
4:A:779:PHE:CE1	5:B:517:THR:CG2	2.95	0.41
4:A:69:THR:CG2	5:B:1174:LYS:HE3	2.47	0.41
5:B:345:LYS:CG	5:B:348:ARG:HH21	2.33	0.41
5:B:420:LEU:HD21	5:B:456:GLY:HA3	2.02	0.41
5:B:918:ILE:HG22	5:B:920:PRO:HD3	2.02	0.41
6:C:32:SER:O	6:C:36:VAL:HG23	2.20	0.41
1:R:6:G:H2'	1:R:7:A:H8	1.85	0.41
4:A:897:TYR:HE1	4:A:1024:SER:O	2.04	0.41
4:A:1209:MET:HE1	4:A:1236:LEU:HG	2.02	0.41
4:A:156:ASP:O	4:A:157:ASP:CG	2.58	0.41
4:A:451:HIS:CB	4:A:453:MET:N	2.70	0.41
4:A:525:GLN:HG3	5:B:836:GLU:HG2	2.02	0.41
5:B:287:ARG:HG2	5:B:292:ILE:HA	2.01	0.41
5:B:356:LEU:HA	5:B:360:PHE:HB3	2.03	0.41
5:B:63:ILE:O	5:B:67:SER:HB3	2.21	0.41
5:B:899:ILE:HD11	5:B:911:ILE:HA	2.02	0.41
5:B:955:THR:CG2	5:B:956:THR:N	2.78	0.41
5:B:983:ARG:HD2	5:B:1091:TYR:HD2	1.85	0.41
6:C:48:SER:HB3	6:C:158:VAL:HB	2.01	0.41
7:E:55:ARG:HB3	7:E:82:PHE:HB3	2.02	0.41
4:A:1173:HIS:O	4:A:1174:PHE:CB	2.67	0.41
4:A:474:VAL:CG1	4:A:478:TYR:HE2	2.34	0.41
4:A:567:LYS:O	4:A:569:LYS:N	2.53	0.41
4:A:77:CYS:HA	4:A:78:PRO:HD3	1.85	0.41
4:A:853:ASP:O	4:A:853:ASP:OD1	2.39	0.41
5:B:38:PHE:O	5:B:42:GLY:N	2.52	0.41
4:A:779:PHE:HE1	5:B:517:THR:HA	1.85	0.41
5:B:526:GLU:HG2	5:B:538:ASN:HD22	1.84	0.41
5:B:636:PRO:O	5:B:637:LEU:HG	2.21	0.41
5:B:711:GLU:N	5:B:712:PRO:HD2	2.28	0.41
5:B:785:TYR:CE1	11:J:60:PHE:CZ	3.08	0.41
5:B:841:MET:SD	5:B:846:ILE:HD11	2.61	0.41
9:H:130:ARG:HB3	9:H:134:ASN:HB2	2.03	0.41
4:A:1234:GLU:HB3	4:A:1235:LYS:HE2	2.03	0.41
4:A:1316:VAL:O	4:A:1322:ILE:HD11	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:132:LYS:NZ	4:A:1399:ARG:HH12	2.19	0.41
4:A:598:LEU:HA	9:H:122:LEU:HD13	2.03	0.41
4:A:715:GLU:OE2	4:A:774:ARG:HD3	2.21	0.41
4:A:840:ARG:HE	4:A:1385:THR:HG22	1.86	0.41
4:A:846:GLU:C	4:A:848:ILE:H	2.24	0.41
5:B:483:LEU:HB3	5:B:484:ASN:H	1.63	0.41
5:B:554:ILE:HD11	5:B:609:ILE:HG23	2.01	0.41
5:B:879:ARG:O	5:B:880:THR:OG1	2.34	0.41
7:E:23:VAL:HG12	7:E:28:TYR:HB2	2.02	0.41
4:A:1170:ILE:CG1	4:A:1171:GLN:HG3	2.51	0.41
4:A:1340:GLY:H	7:E:183:PRO:HG2	1.86	0.41
4:A:470:LEU:C	4:A:470:LEU:HD12	2.41	0.41
5:B:315:LYS:N	5:B:316:PRO:CD	2.83	0.41
5:B:549:THR:HG22	5:B:550:ASP:H	1.85	0.41
5:B:773:MET:O	5:B:776:GLN:N	2.47	0.41
6:C:114:TYR:CG	6:C:140:ASN:HB3	2.56	0.41
8:F:103:MET:O	8:F:104:ASN:C	2.59	0.41
8:F:70:LYS:HA	8:F:70:LYS:HD3	1.84	0.41
12:K:7:PHE:HA	12:K:10:PHE:CE2	2.56	0.41
3:T:26:DG:C2	3:T:27:DA:C8	3.09	0.41
4:A:1271:ILE:HG22	4:A:1273:LEU:HD12	2.03	0.41
4:A:1277:GLU:O	4:A:1278:ASN:HB2	2.21	0.41
4:A:1293:SER:HB2	4:A:1299:VAL:HG23	2.03	0.41
4:A:414:ASP:O	4:A:417:TYR:O	2.39	0.41
5:B:1161:HIS:CE1	5:B:1193:GLN:HB2	2.55	0.41
4:A:1410:PHE:HD2	5:B:1212:ILE:HD11	1.86	0.41
5:B:333:PHE:O	5:B:333:PHE:CG	2.73	0.41
6:C:73:GLN:HB3	6:C:131:HIS:H	1.86	0.41
13:L:48:CYS:CB	13:L:51:CYS:SG	3.08	0.41
4:A:1022:LEU:CA	4:A:1025:ARG:O	2.69	0.41
4:A:586:ILE:CD1	4:A:637:LYS:HE3	2.50	0.41
4:A:846:GLU:O	4:A:848:ILE:N	2.53	0.41
5:B:170:LEU:HA	5:B:171:PRO:HD2	1.84	0.41
5:B:310:MET:O	5:B:313:MET:HB2	2.20	0.41
5:B:324:ILE:O	5:B:324:ILE:HG22	2.20	0.41
5:B:879:ARG:CB	5:B:879:ARG:NH1	2.83	0.41
5:B:970:THR:HG22	5:B:971:THR:O	2.21	0.41
4:A:380:VAL:HG22	4:A:388:LEU:HD13	2.02	0.41
5:B:1019:SER:OG	16:B:1308[A]:DUT:H2'1	2.20	0.41
5:B:174:LEU:C	5:B:176:SER:N	2.73	0.41
5:B:292:ILE:N	5:B:293:PRO:CD	2.84	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1231:ASP:O	4:A:1233:ASP:N	2.53	0.40
4:A:315:LEU:HD12	4:A:316:GLN:HA	2.03	0.40
4:A:381:THR:C	4:A:383:TYR:N	2.75	0.40
4:A:909:ASP:C	4:A:911:SER:H	2.24	0.40
5:B:173:MET:HG2	5:B:174:LEU:O	2.21	0.40
5:B:410:GLY:O	5:B:413:LEU:N	2.54	0.40
5:B:479:VAL:O	5:B:480:SER:HB3	2.21	0.40
5:B:819:ALA:O	5:B:1091:TYR:OH	2.38	0.40
9:H:24:CYS:HB2	9:H:44:VAL:CG2	2.50	0.40
4:A:1345:ARG:O	4:A:1348:LEU:N	2.54	0.40
4:A:302:THR:HA	4:A:305:ASP:O	2.20	0.40
4:A:315:LEU:HB2	4:A:320:ARG:HH12	1.83	0.40
4:A:367:PRO:HB3	4:A:465:TYR:O	2.20	0.40
4:A:741:ASN:HD22	4:A:741:ASN:C	2.24	0.40
5:B:563:MET:HG3	5:B:563:MET:O	2.21	0.40
12:K:77:THR:HB	12:K:81:TYR:HB3	2.03	0.40
4:A:219:PHE:HE1	4:A:231:PRO:HD2	1.86	0.40
4:A:244:PRO:HB2	4:A:245:PRO:HD3	2.03	0.40
4:A:91:PHE:N	4:A:297:GLN:HE22	2.19	0.40
4:A:351:THR:HB	4:A:468:PHE:HD2	1.83	0.40
4:A:463:ILE:CD1	4:A:469:ARG:CG	2.99	0.40
4:A:365:GLY:N	4:A:469:ARG:O	2.47	0.40
6:C:234:SER:HB3	6:C:240:VAL:HG13	2.02	0.40
4:A:282:ASN:HB3	4:A:283:GLY:H	1.74	0.40
4:A:414:ASP:OD1	4:A:416:ARG:HD3	2.20	0.40
4:A:58:LEU:HD22	4:A:244:PRO:CD	2.50	0.40
4:A:685:GLU:O	4:A:689:LYS:HB2	2.21	0.40
4:A:737:LEU:HD11	4:A:758:ILE:CG2	2.50	0.40
4:A:344:ARG:HA	5:B:1129:ARG:HA	2.03	0.40
4:A:443:LEU:HD12	5:B:1146:PHE:CE2	2.56	0.40
5:B:37:PHE:HD1	5:B:681:TRP:CE2	2.40	0.40
5:B:384:ARG:NH2	5:B:623:GLU:OE1	2.53	0.40
5:B:635:ARG:HH22	5:B:742:GLU:CD	2.24	0.40
6:C:116:LYS:O	6:C:116:LYS:HG2	2.21	0.40
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.61	0.40
4:A:757:ASN:O	4:A:761:MET:HG3	2.21	0.40
4:A:79:GLY:O	4:A:243:PRO:CG	2.64	0.40
5:B:744:HIS:HD2	5:B:746:SER:H	1.64	0.40
5:B:826:ALA:HB3	5:B:1011:ILE:HG13	2.03	0.40
5:B:859:TYR:OH	5:B:941:LEU:HD22	2.22	0.40
6:C:211:ASP:HA	6:C:212:PRO:HD3	1.91	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:78:LEU:HD12	7:E:107:THR:HB	2.02	0.40
6:C:258:ILE:HD13	12:K:42:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	1392/1733 (80%)	1118 (80%)	182 (13%)	92 (7%)	1	16
5	B	1096/1224 (90%)	897 (82%)	124 (11%)	75 (7%)	1	15
6	C	264/318 (83%)	229 (87%)	28 (11%)	7 (3%)	5	35
7	E	212/215 (99%)	190 (90%)	15 (7%)	7 (3%)	4	31
8	F	86/155 (56%)	75 (87%)	6 (7%)	5 (6%)	1	18
9	H	130/146 (89%)	105 (81%)	18 (14%)	7 (5%)	2	19
10	I	117/122 (96%)	96 (82%)	18 (15%)	3 (3%)	5	35
11	J	63/70 (90%)	53 (84%)	8 (13%)	2 (3%)	4	31
12	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
13	L	44/70 (63%)	29 (66%)	13 (30%)	2 (4%)	2	23
All	All	3516/4173 (84%)	2899 (82%)	417 (12%)	200 (6%)	1	18

All (200) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	55	ASP
4	A	56	PRO
4	A	74	MET
4	A	157	ASP
4	A	158	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	308	ILE
4	A	316	GLN
4	A	317	LYS
4	A	321	PRO
4	A	335	ARG
4	A	418	SER
4	A	544	ASP
4	A	597	LEU
4	A	1022	LEU
4	A	1023	ARG
4	A	1024	SER
4	A	1175	SER
4	A	1221	LYS
4	A	1232	ASN
4	A	1393	ASN
5	B	45	SER
5	B	64	CYS
5	B	179	CYS
5	B	202	TYR
5	B	203	PHE
5	B	274	PRO
5	B	338	GLY
5	B	477	ALA
5	B	484	ASN
5	B	531	GLN
5	B	636	PRO
5	B	643	ASP
5	B	711	GLU
5	B	728	ARG
5	B	810	GLU
5	B	811	TYR
5	B	883	LEU
5	B	1017	ILE
5	B	1065	GLN
6	C	215	GLU
7	E	52	ARG
7	E	59	SER
7	E	90	VAL
8	F	104	ASN
9	H	81	PRO
9	H	82	PRO
11	J	2	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	J	6	ARG
4	A	50	ILE
4	A	69	THR
4	A	80	HIS
4	A	178	GLY
4	A	223	GLY
4	A	255	SER
4	A	260	ASP
4	A	623	GLY
4	A	647	GLY
4	A	779	PHE
4	A	780	VAL
4	A	851	HIS
4	A	852	TYR
4	A	903	ASN
4	A	1027	ALA
4	A	1220	PHE
4	A	1233	ASP
4	A	1345	ARG
4	A	1388	GLY
4	A	1401	SER
4	A	1437	GLY
5	B	175	ARG
5	B	182	SER
5	B	229	ALA
5	B	260	GLY
5	B	294	ASP
5	B	322	PHE
5	B	327	ARG
5	B	410	GLY
5	B	471	LYS
5	B	563	MET
5	B	731	VAL
5	B	734	HIS
5	B	774	GLY
5	B	943	SER
5	B	958	GLN
5	B	982	SER
5	B	1181	GLU
6	C	90	ASP
6	C	142	VAL
7	E	3	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	F	70	LYS
9	H	108	SER
9	H	140	ALA
13	L	55	ILE
4	A	214	ILE
4	A	314	ALA
4	A	404	TYR
4	A	451	HIS
4	A	483	ASP
4	A	568	PRO
4	A	846	GLU
4	A	854	ASN
4	A	855	THR
4	A	922	ASP
4	A	958	VAL
4	A	1021	LEU
4	A	1170	ILE
4	A	1234	GLU
5	B	180	TYR
5	B	337	ARG
5	B	344	LYS
5	B	476	ARG
5	B	478	GLY
5	B	483	LEU
5	B	894	ASP
5	B	1020	ARG
6	C	110	THR
6	C	174	ALA
7	E	53	PRO
8	F	74	ILE
10	I	10	CYS
10	I	60	GLN
4	A	46	THR
4	A	48	ALA
4	A	57	ARG
4	A	62	ASP
4	A	150	THR
4	A	152	VAL
4	A	312	PRO
4	A	333	GLU
4	A	423	ASP
4	A	424	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
4	A	517	ASN
4	A	543	LEU
4	A	567	LYS
4	A	895	LYS
4	A	1025	ARG
4	A	1028	THR
4	A	1065	GLY
4	A	1229	SER
5	B	38	PHE
5	B	467	GLY
5	B	468	GLU
5	B	637	LEU
5	B	647	GLY
5	B	792	MET
5	B	864	LYS
5	B	1096	ARG
9	H	128	ASN
4	A	130	ASP
4	A	151	ASP
4	A	213	HIS
4	A	325	ILE
4	A	591	PHE
4	A	972	HIS
4	A	1243	VAL
4	A	1424	VAL
4	A	1433	MET
5	B	65	GLU
5	B	204	ILE
5	B	247	GLY
5	B	474	SER
5	B	480	SER
5	B	974	PRO
5	B	1028	GLU
5	B	1046	PRO
5	B	1108	ARG
7	E	36	GLU
8	F	148	VAL
9	H	77	ARG
10	I	12	ASN
13	L	50	ASP
4	A	35	ILE
4	A	72	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	250	ILE
4	A	1270	ASN
5	B	201	GLY
5	B	259	TYR
5	B	466	TRP
5	B	631	GLY
5	B	851	PHE
6	C	227	THR
4	A	910	PRO
5	B	802	PRO
5	B	920	PRO
5	B	1214	PRO
9	H	107	VAL
5	B	100	PRO
5	B	276	ILE
5	B	335	GLY
5	B	1165	ILE
4	A	1384	VAL
4	A	322	VAL
4	A	599	SER
4	A	837	ILE
4	A	1435	PRO
5	B	200	GLY
8	F	139	PRO
5	B	1103	ILE
6	C	182	PRO
7	E	118	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	1225/1520 (81%)	1128 (92%)	97 (8%)	12	44
5	B	967/1061 (91%)	886 (92%)	81 (8%)	11	42
6	C	234/274 (85%)	211 (90%)	23 (10%)	8	36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	196/197 (100%)	181 (92%)	15 (8%)	13	45
8	F	78/137 (57%)	74 (95%)	4 (5%)	24	58
9	H	118/128 (92%)	107 (91%)	11 (9%)	9	38
10	I	113/116 (97%)	103 (91%)	10 (9%)	10	40
11	J	60/65 (92%)	52 (87%)	8 (13%)	4	23
12	K	99/102 (97%)	87 (88%)	12 (12%)	5	26
13	L	40/57 (70%)	36 (90%)	4 (10%)	7	35
All	All	3130/3657 (86%)	2865 (92%)	265 (8%)	10	41

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	32	VAL
4	A	42	ASP
4	A	69	THR
4	A	80	HIS
4	A	139	TRP
4	A	155	GLU
4	A	156	ASP
4	A	157	ASP
4	A	159	THR
4	A	161	LEU
4	A	170	THR
4	A	204	THR
4	A	208	LEU
4	A	222	LEU
4	A	225	ASN
4	A	235	ILE
4	A	263	THR
4	A	270	LEU
4	A	303	TYR
4	A	320	ARG
4	A	322	VAL
4	A	326	ARG
4	A	329	LEU
4	A	335	ARG
4	A	388	LEU
4	A	391	LEU
4	A	409	SER
4	A	416	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	443	LEU
4	A	447	GLN
4	A	485	ASP
4	A	504	LEU
4	A	535	THR
4	A	539	THR
4	A	569	LYS
4	A	590	ARG
4	A	592	ASP
4	A	596	THR
4	A	602	ASP
4	A	618	GLU
4	A	637	LYS
4	A	703	THR
4	A	709	THR
4	A	740	LEU
4	A	741	ASN
4	A	743	VAL
4	A	765	VAL
4	A	775	ILE
4	A	821	ARG
4	A	851	HIS
4	A	852	TYR
4	A	854	ASN
4	A	859	SER
4	A	871	ASP
4	A	889	SER
4	A	890	ASP
4	A	896	ARG
4	A	902	LEU
4	A	913	LEU
4	A	915	SER
4	A	918	GLU
4	A	920	LEU
4	A	953	ASN
4	A	961	ARG
4	A	982	THR
4	A	1017	LEU
4	A	1025	ARG
4	A	1026	LEU
4	A	1029	ARG
4	A	1030	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	1048	ASN
4	A	1054	LEU
4	A	1058	VAL
4	A	1064	VAL
4	A	1094	VAL
4	A	1116	LEU
4	A	1118	VAL
4	A	1128	GLN
4	A	1174	PHE
4	A	1187	GLN
4	A	1220	PHE
4	A	1227	ILE
4	A	1231	ASP
4	A	1232	ASN
4	A	1233	ASP
4	A	1234	GLU
4	A	1235	LYS
4	A	1244	ARG
4	A	1258	HIS
4	A	1265	ASN
4	A	1308	THR
4	A	1309	ASP
4	A	1314	SER
4	A	1345	ARG
4	A	1366	ARG
4	A	1391	ARG
4	A	1394	THR
5	B	22	SER
5	B	44	VAL
5	B	57	TYR
5	B	65	GLU
5	B	68	THR
5	B	108	VAL
5	B	121	ASN
5	B	198	ASP
5	B	199	MET
5	B	203	PHE
5	B	206	ASN
5	B	210	LYS
5	B	217	ARG
5	B	226	PHE
5	B	235	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	B	268	THR
5	B	272	THR
5	B	322	PHE
5	B	336	ARG
5	B	337	ARG
5	B	382	ILE
5	B	384	ARG
5	B	388	CYS
5	B	396	ASP
5	B	436	VAL
5	B	461	LEU
5	B	465	ASN
5	B	466	TRP
5	B	471	LYS
5	B	482	VAL
5	B	483	LEU
5	B	516	ASN
5	B	527	THR
5	B	539	LEU
5	B	549	THR
5	B	556	THR
5	B	563	MET
5	B	567	GLU
5	B	570	VAL
5	B	620	ARG
5	B	635	ARG
5	B	654	ARG
5	B	666	TYR
5	B	667	GLN
5	B	723	VAL
5	B	732	SER
5	B	736	THR
5	B	737	THR
5	B	764	SER
5	B	791	THR
5	B	792	MET
5	B	806	THR
5	B	807	ARG
5	B	812	LEU
5	B	838	SER
5	B	850	LEU
5	B	861	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	B	873	THR
5	B	879	ARG
5	B	916	THR
5	B	948	ILE
5	B	969	ARG
5	B	975	GLN
5	B	976	ILE
5	B	995	ARG
5	B	999	MET
5	B	1020	ARG
5	B	1046	PRO
5	B	1047	PHE
5	B	1051	THR
5	B	1064	TYR
5	B	1065	GLN
5	B	1084	GLN
5	B	1092	TYR
5	B	1096	ARG
5	B	1099	VAL
5	B	1113	VAL
5	B	1124	ARG
5	B	1159	ARG
5	B	1161	HIS
5	B	1166	CYS
6	C	4	GLU
6	C	18	VAL
6	C	22	LEU
6	C	25	VAL
6	C	26	ASP
6	C	53	THR
6	C	56	THR
6	C	57	VAL
6	C	61	GLU
6	C	76	ASP
6	C	77	ILE
6	C	80	LEU
6	C	117	ASP
6	C	120	ILE
6	C	137	LYS
6	C	154	LYS
6	C	163	ILE
6	C	231	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	C	234	SER
6	C	240	VAL
6	C	244	VAL
6	C	258	ILE
6	C	259	LEU
7	E	8	ASN
7	E	10	SER
7	E	39	LEU
7	E	48	ASP
7	E	95	THR
7	E	101	GLN
7	E	104	ASN
7	E	110	PHE
7	E	114	ASN
7	E	127	ILE
7	E	142	VAL
7	E	146	HIS
7	E	156	LEU
7	E	165	LEU
7	E	213	ILE
8	F	70	LYS
8	F	72	LYS
8	F	110	ASP
8	F	139	PRO
9	H	31	THR
9	H	32	THR
9	H	41	ASP
9	H	46	LEU
9	H	48	PRO
9	H	86	ASP
9	H	94	ASP
9	H	95	TYR
9	H	107	VAL
9	H	136	LYS
9	H	145	ARG
10	I	10	CYS
10	I	17	ARG
10	I	21	GLU
10	I	22	ASN
10	I	24	ARG
10	I	28	GLU
10	I	31	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
10	I	50	THR
10	I	62	ILE
10	I	83	ASN
11	J	2	ILE
11	J	5	VAL
11	J	7	CYS
11	J	13	VAL
11	J	14	VAL
11	J	20	SER
11	J	45	CYS
11	J	48	ARG
12	K	5	ASP
12	K	9	LEU
12	K	42	LEU
12	K	46	ILE
12	K	63	VAL
12	K	78	THR
12	K	89	ASN
12	K	101	LEU
12	K	103	THR
12	K	106	GLU
12	K	107	THR
12	K	113	THR
13	L	27	LEU
13	L	55	ILE
13	L	61	THR
13	L	65	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	80	HIS
4	A	83	HIS
4	A	225	ASN
4	A	253	ASN
4	A	306	ASN
4	A	316	GLN
4	A	339	ASN
4	A	435	HIS
4	A	503	GLN
4	A	631	HIS
4	A	736	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	A	741	ASN
4	A	742	ASN
4	A	757	ASN
4	A	768	GLN
4	A	851	HIS
4	A	926	GLN
4	A	969	GLN
4	A	1106	ASN
4	A	1218	GLN
4	A	1265	ASN
4	A	1364	ASN
4	A	1427	ASN
4	A	1432	GLN
5	B	121	ASN
5	B	178	ASN
5	B	215	GLN
5	B	300	HIS
5	B	325	GLN
5	B	350	GLN
5	B	363	HIS
5	B	366	GLN
5	B	415	GLN
5	B	484	ASN
5	B	494	HIS
5	B	515	HIS
5	B	516	ASN
5	B	518	HIS
5	B	592	ASN
5	B	657	HIS
5	B	686	ASN
5	B	734	HIS
5	B	744	HIS
5	B	822	ASN
5	B	984	HIS
5	B	986	GLN
5	B	1015	HIS
5	B	1062	HIS
5	B	1065	GLN
5	B	1084	GLN
5	B	1195	HIS
6	C	73	GLN
6	C	91	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	C	112	ASN
6	C	123	ASN
6	C	188	HIS
7	E	61	GLN
7	E	101	GLN
7	E	104	ASN
7	E	114	ASN
9	H	33	GLN
9	H	83	GLN
9	H	137	GLN
10	I	46	HIS
10	I	83	ASN
10	I	90	GLN
10	I	116	ASN
12	K	65	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	8/10 (80%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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, 9 are monoatomic - leaving 2 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
16	DUT	B	1308[A]	-	22,29,29	0.71	1 (4%)	27,45,45	1.06	1 (3%)
16	DUT	B	1308[B]	15	22,29,29	0.67	0	27,45,45	1.31	2 (7%)

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
16	DUT	B	1308[A]	-	-	6/19/34/34	0/2/2/2
16	DUT	B	1308[B]	15	-	4/19/34/34	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1308[A]	DUT	C4-N3	2.22	1.36	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1308[B]	DUT	PB-O3B-PG	-2.88	122.94	132.83
16	B	1308[B]	DUT	C2'-C1'-N1	-2.39	108.75	114.27
16	B	1308[A]	DUT	O3G-PG-O2G	2.14	115.81	107.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	1308[B]	DUT	C5'-O5'-PA-O1A
16	B	1308[B]	DUT	C5'-O5'-PA-O2A
16	B	1308[A]	DUT	PB-O3B-PG-O1G
16	B	1308[A]	DUT	C4'-C5'-O5'-PA
16	B	1308[A]	DUT	PB-O3B-PG-O2G
16	B	1308[A]	DUT	PB-O3B-PG-O3G
16	B	1308[A]	DUT	C5'-O5'-PA-O3A

*Continued on next page...*

*Continued from previous page...*

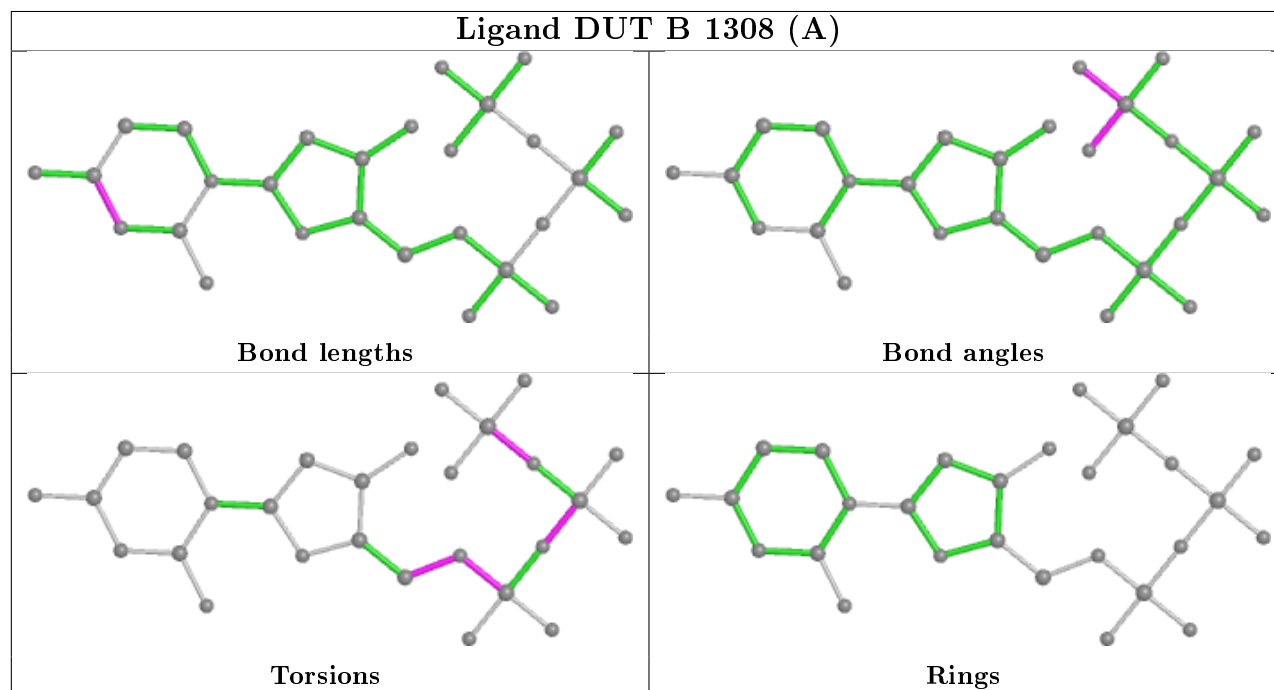
Mol	Chain	Res	Type	Atoms
16	B	1308[B]	DUT	C5'-O5'-PA-O3A
16	B	1308[A]	DUT	PA-O3A-PB-O2B
16	B	1308[B]	DUT	PB-O3A-PA-O2A

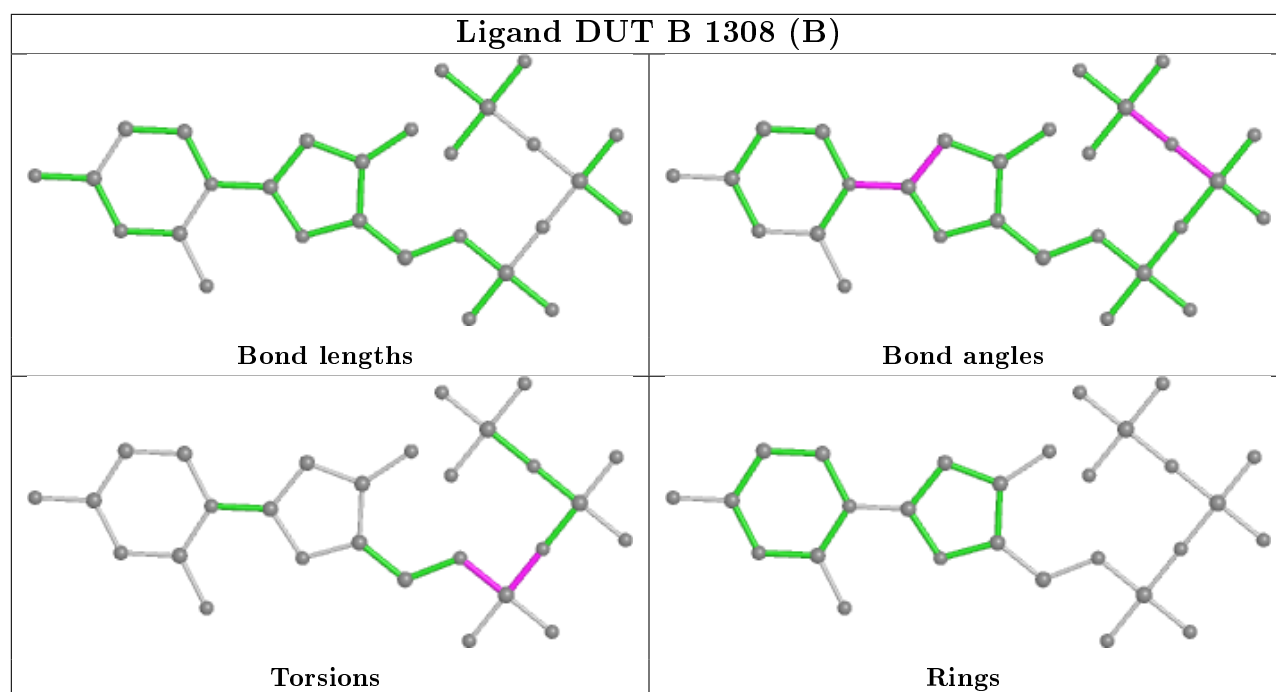
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1308[A]	DUT	1	0

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%)	-0.58	0 100 100	85, 109, 154, 170	0
2	N	14/14 (100%)	1.46	3 (21%) 0 0	178, 182, 198, 202	0
3	T	28/28 (100%)	0.74	7 (25%) 0 0	93, 173, 189, 192	0
4	A	1402/1733 (80%)	-0.04	21 (1%) 73 60	75, 103, 150, 163	0
5	B	1114/1224 (91%)	-0.05	17 (1%) 73 60	26, 102, 133, 143	0
6	C	266/318 (83%)	-0.23	1 (0%) 92 86	81, 100, 128, 144	0
7	E	214/215 (99%)	0.07	5 (2%) 60 44	91, 131, 165, 167	0
8	F	88/155 (56%)	-0.12	0 100 100	84, 104, 130, 137	0
9	H	134/146 (91%)	0.12	4 (2%) 50 34	100, 119, 152, 155	0
10	I	119/122 (97%)	-0.08	1 (0%) 86 75	87, 104, 122, 138	0
11	J	65/70 (92%)	-0.28	0 100 100	92, 102, 122, 125	0
12	K	114/120 (95%)	-0.28	0 100 100	82, 105, 119, 121	0
13	L	46/70 (65%)	0.31	2 (4%) 35 22	108, 145, 156, 157	0
All	All	3614/4225 (85%)	-0.04	61 (1%) 70 55	26, 104, 150, 202	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	69	THR	5.0
4	A	72	GLU	4.8
5	B	338	GLY	4.0
7	E	46	TYR	4.0
4	A	44	THR	3.9
5	B	339	THR	3.9
4	A	146	MET	3.8
13	L	38	LEU	3.4
2	N	2	DT	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	A	286	HIS	3.4
5	B	429	PHE	3.4
3	T	11	DG	3.4
7	E	93	MET	3.3
5	B	1183	LYS	3.2
5	B	1222	ARG	3.2
2	N	14	DG	3.1
2	N	1	DC	3.1
4	A	171	GLN	3.0
4	A	1166	ASP	3.0
3	T	4	DC	2.9
4	A	1169	ILE	2.8
3	T	10	DA	2.7
5	B	1186	ASP	2.7
7	E	81	GLU	2.7
5	B	248	SER	2.6
4	A	113	LEU	2.6
5	B	92	PHE	2.6
4	A	66	LYS	2.5
5	B	645	SER	2.5
5	B	425	THR	2.5
3	T	14	DG	2.5
5	B	883	LEU	2.4
4	A	163	SER	2.4
7	E	49	SER	2.4
5	B	341	LEU	2.4
4	A	292	ALA	2.4
3	T	12	DC	2.3
4	A	885	THR	2.3
5	B	921	ASP	2.3
9	H	139	ASN	2.3
4	A	257	ARG	2.3
4	A	114	LEU	2.3
13	L	26	THR	2.3
4	A	112	LYS	2.3
4	A	426	LEU	2.2
5	B	165	VAL	2.2
5	B	1184	GLY	2.2
4	A	1176	LEU	2.2
3	T	2	DT	2.2
6	C	130	GLY	2.2
4	A	106	VAL	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	T	3	DA	2.1
9	H	130	ARG	2.1
4	A	145	LYS	2.1
7	E	61	GLN	2.1
9	H	133	ASN	2.1
4	A	149	GLU	2.1
5	B	91	SER	2.0
5	B	643	ASP	2.0
10	I	8	ARG	2.0
9	H	7	ASP	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.

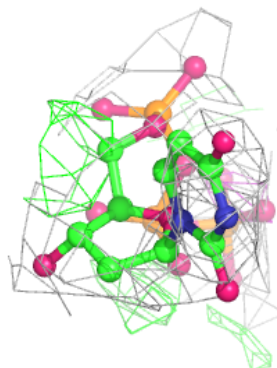
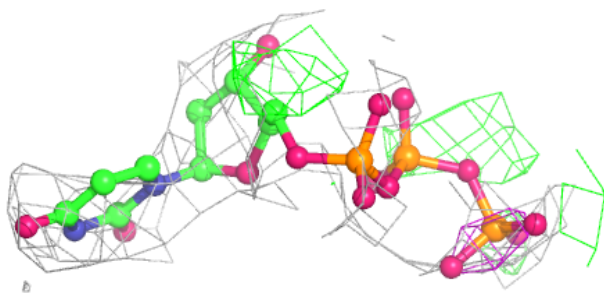
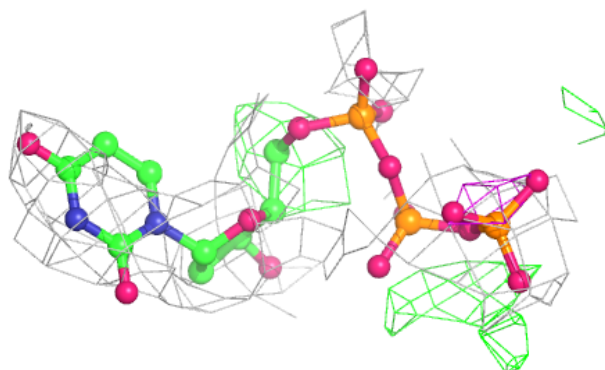
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
16	DUT	B	1308[A]	28/28	0.79	0.35	131,133,149,150	28
16	DUT	B	1308[B]	28/28	0.79	0.35	57,59,61,62	28
14	ZN	A	1734	1/1	0.89	0.05	159,159,159,159	0
14	ZN	I	203	1/1	0.93	0.07	97,97,97,97	0
14	ZN	B	1307	1/1	0.96	0.10	126,126,126,126	0
15	MG	A	2000	1/1	0.97	0.22	74,74,74,74	0
14	ZN	L	105	1/1	0.97	0.06	181,181,181,181	0
14	ZN	I	204	1/1	0.97	0.09	107,107,107,107	0
14	ZN	J	101	1/1	0.98	0.12	149,149,149,149	0
14	ZN	A	1735	1/1	0.98	0.09	142,142,142,142	0
14	ZN	C	319	1/1	0.99	0.06	104,104,104,104	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.

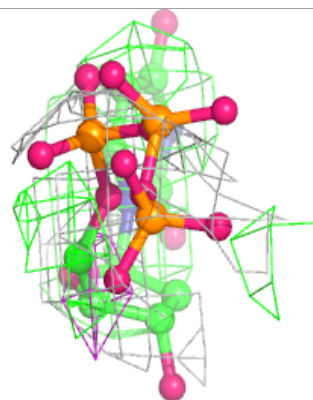
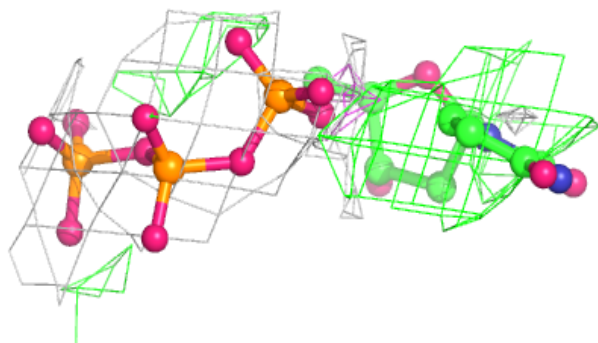
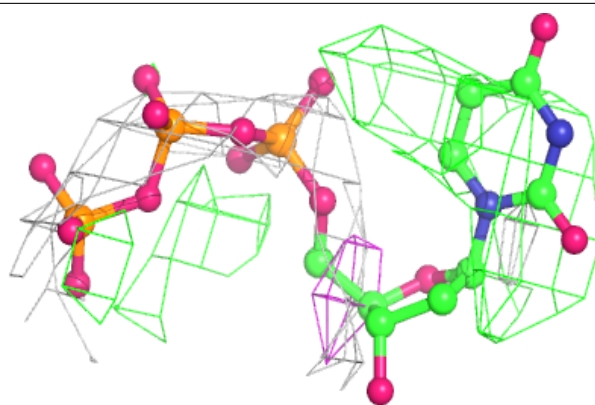
**Electron density around DUT B 1308 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around DUT B 1308 (B):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.