



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 12:30 PM EST

PDB ID : 1G65  
Title : Crystal structure of epoxomicin:20s proteasome reveals a molecular basis for selectivity of alpha,beta-epoxyketone proteasome inhibitors  
Authors : Groll, M.; Kim, K.B.; Kairies, N.; Huber, R.; Crews, C.  
Deposited on : 2000-11-03  
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

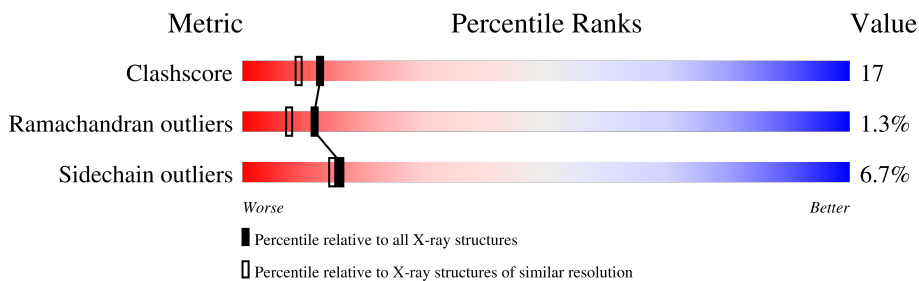
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)











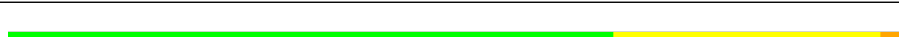


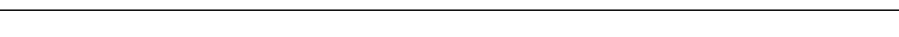
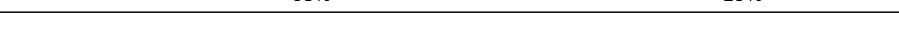
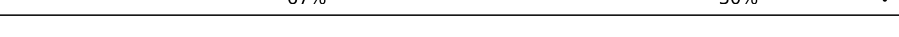






The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	250	71% 28% .
1	O	250	68% 30% .
2	B	244	60% 35% 5%
2	P	244	60% 35% 5%
3	C	241	63% 33% .
3	Q	241	56% 38% 6%
4	D	242	64% 34% .
4	R	242	69% 29% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	233	
5	S	233	
6	F	244	
6	T	244	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	
15	3	5	
15	4	5	

## 2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 52508 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			
2	P	244	Total	C	N	O	S	0	0	0
			1905	1201	321	380	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			
6	T	244	Total	C	N	O	S	0	0	0
			1897	1205	330	358	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is a protein called EPOXOMICIN (peptide inhibitor).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	3	5	Total	C	N	O	0	0	0
			39	28	4	7			
15	4	5	Total	C	N	O	0	0	0
			39	28	4	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	D	1	Total 1	Mg 1	0	0
16	F	2	Total 2	Mg 2	0	0
16	G	1	Total 1	Mg 1	0	0
16	H	1	Total 1	Mg 1	0	0
16	I	2	Total 2	Mg 2	0	0
16	K	1	Total 1	Mg 1	0	0
16	L	1	Total 1	Mg 1	0	0
16	N	1	Total 1	Mg 1	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	100	Total 100	O 100	0	0
17	B	72	Total 72	O 72	0	0
17	C	71	Total 71	O 71	0	0
17	D	86	Total 86	O 86	0	0
17	E	57	Total 57	O 57	0	0
17	F	98	Total 98	O 98	0	0
17	G	106	Total 106	O 106	0	0
17	H	129	Total 129	O 129	0	0
17	I	109	Total 109	O 109	0	0
17	J	114	Total 114	O 114	0	0
17	K	94	Total 94	O 94	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	L	147	Total 147	O 147	0	0
17	M	130	Total 130	O 130	0	0
17	N	115	Total 115	O 115	0	0
17	O	99	Total 99	O 99	0	0
17	P	72	Total 72	O 72	0	0
17	Q	68	Total 68	O 68	0	0
17	R	87	Total 87	O 87	0	0
17	S	56	Total 56	O 56	0	0
17	T	95	Total 95	O 95	0	0
17	U	111	Total 111	O 111	0	0
17	V	124	Total 124	O 124	0	0
17	W	111	Total 111	O 111	0	0
17	X	119	Total 119	O 119	0	0
17	Y	93	Total 93	O 93	0	0
17	Z	142	Total 142	O 142	0	0
17	1	142	Total 142	O 142	0	0
17	2	124	Total 124	O 124	0	0
17	3	1	Total 1	O 1	0	0



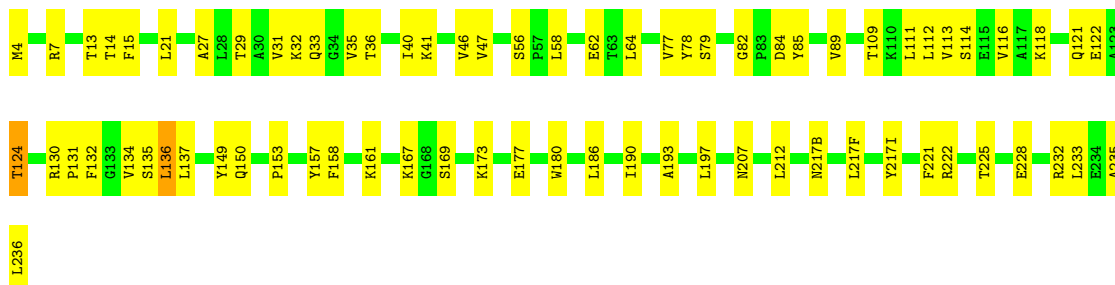
### 3 Residue-property plots [i](#)

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

Note EDS was not executed.

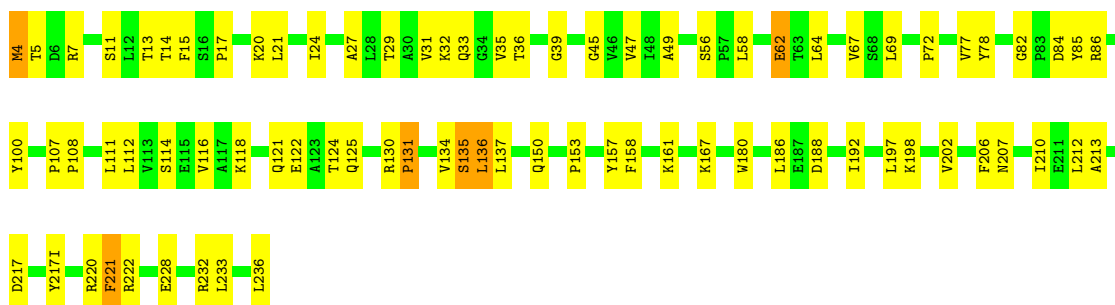
- Molecule 1: Proteasome component Y7

Chain A: 



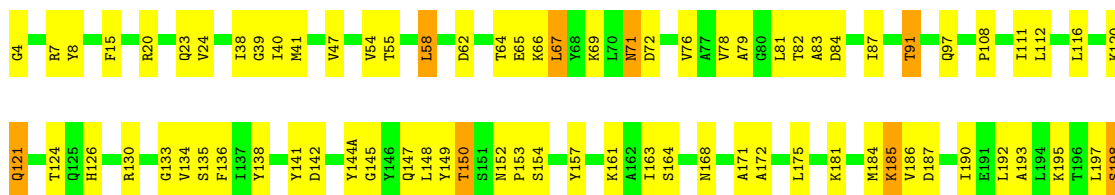
- Molecule 1: Proteasome component Y7

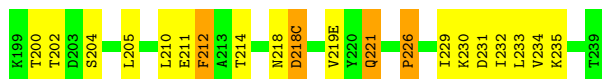
Chain O: 



- Molecule 2: Proteasome component Y13

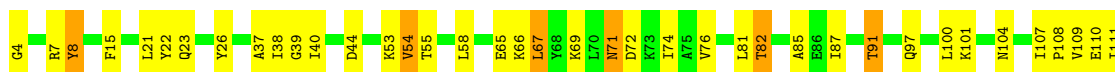
Chain B: 





- Molecule 2: Proteasome component Y13

Chain P: 60% 35% 5%



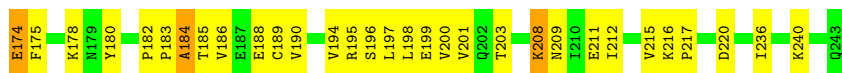
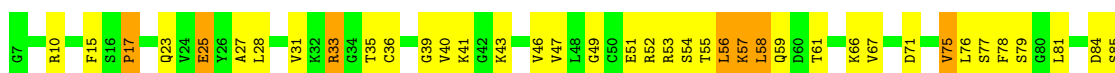
- Molecule 3: Proteasome component PRE6

Chain C: 63% 33%



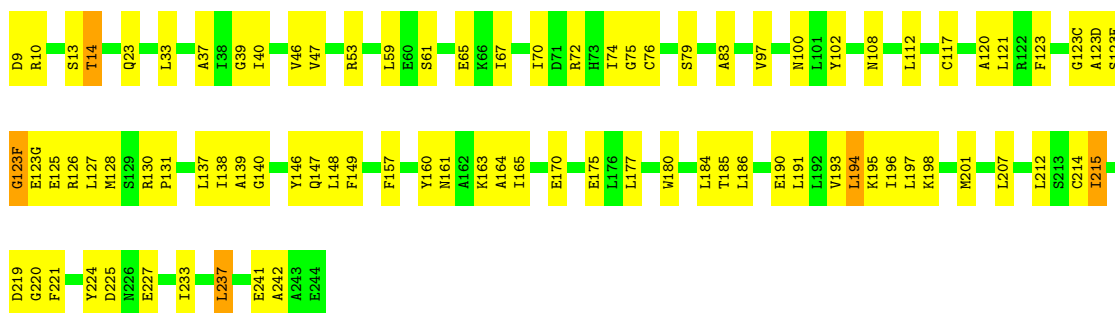
- Molecule 3: Proteasome component PRE6

Chain Q: 56% 38% 6%



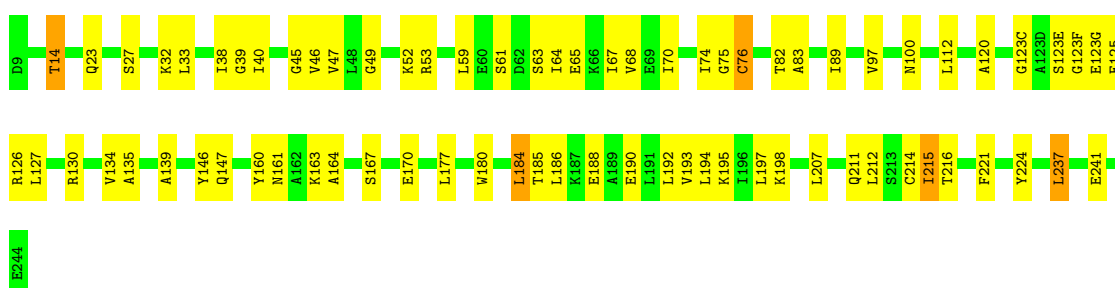
- Molecule 4: Proteasome component PUP2

Chain D: 64% 34%



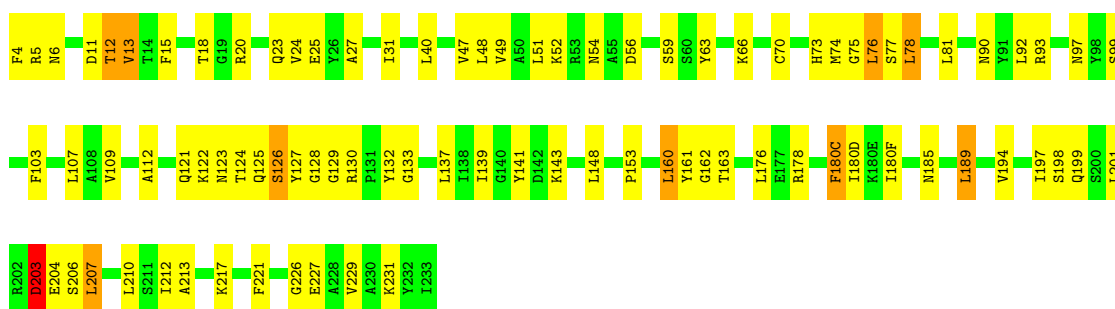
- Molecule 4: Proteasome component PUP2

Chain R: 69% 29%



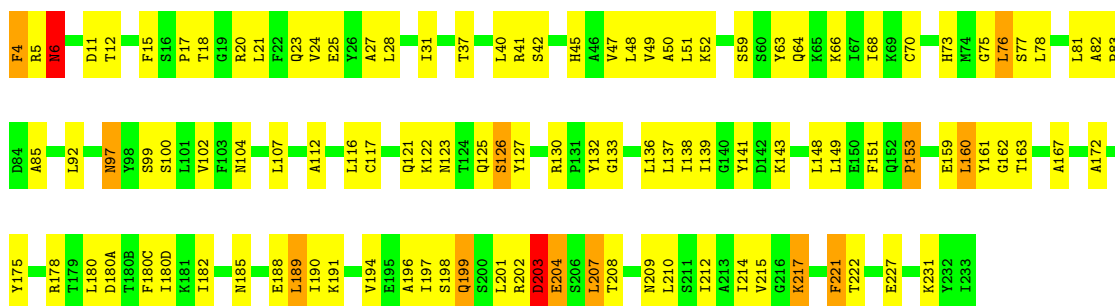
- Molecule 5: Proteasome component PRE5

Chain E: 62% 34%



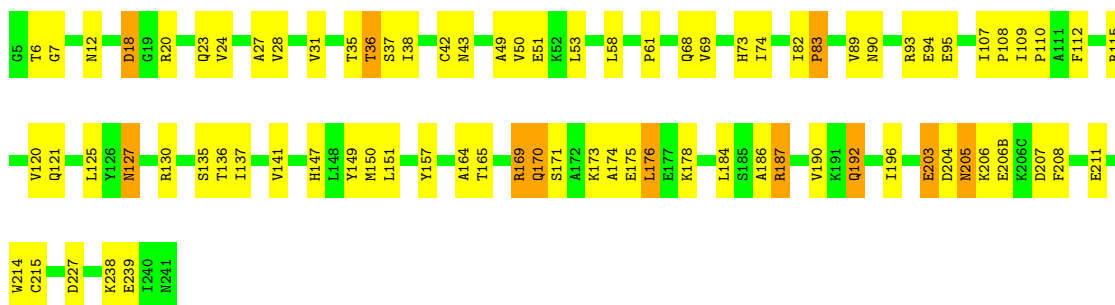
- Molecule 5: Proteasome component PRE5

Chain S: 52% 42% 5%



- Molecule 6: Proteasome component C1

Chain F:  66% 29% 5%



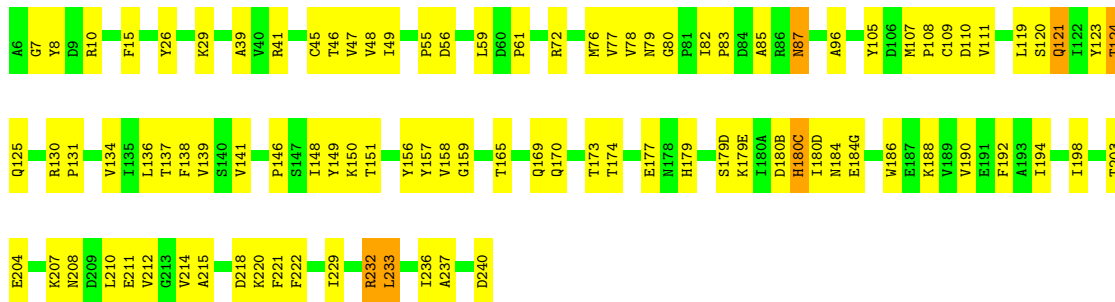
- Molecule 6: Proteasome component C1

Chain T:  58% 37% 5%



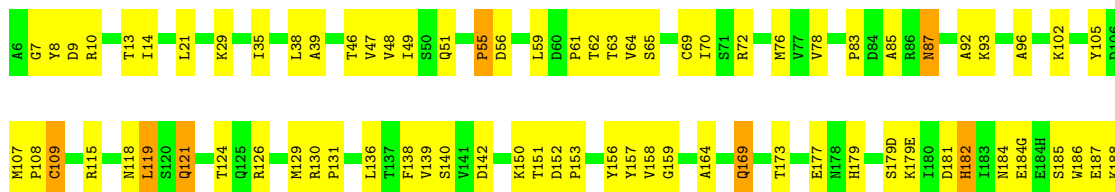
- Molecule 7: Proteasome component C7-alpha

Chain G:  60% 37% 3%



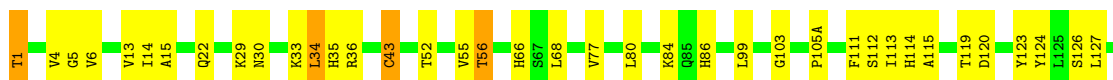
- Molecule 7: Proteasome component C7-alpha

Chain U:  59% 37% 4%

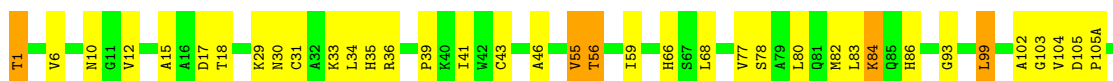




- Molecule 8: Proteasome component PUP1



- Molecule 8: Proteasome component PUP1



- Molecule 9: Proteasome component PUP3

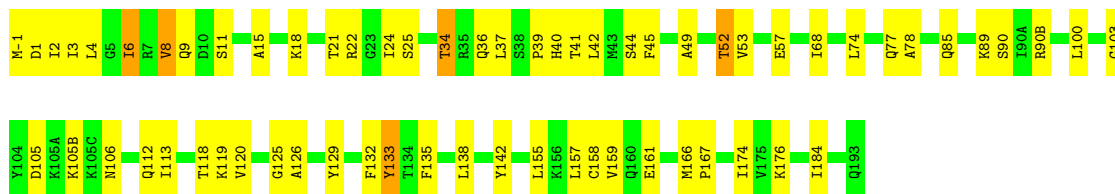


- Molecule 9: Proteasome component PUP3



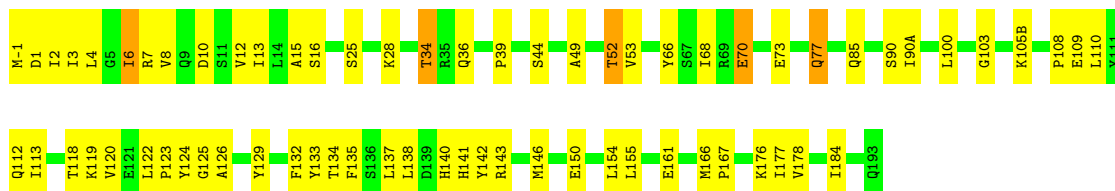
- Molecule 10: Proteasome component C11





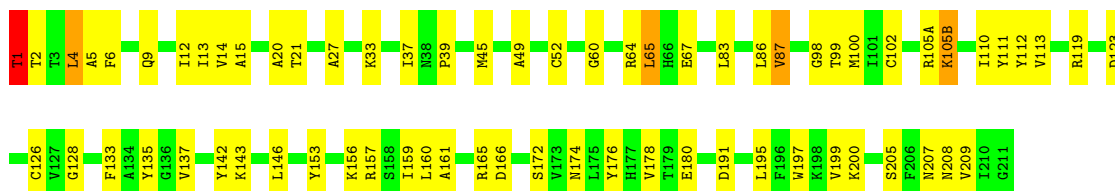
- Molecule 10: Proteasome component C11

Chain X: 66% 32%



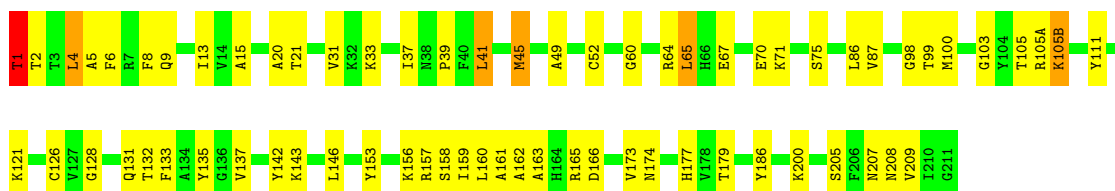
- Molecule 11: Proteasome component PRE2

Chain K: 68% 30%



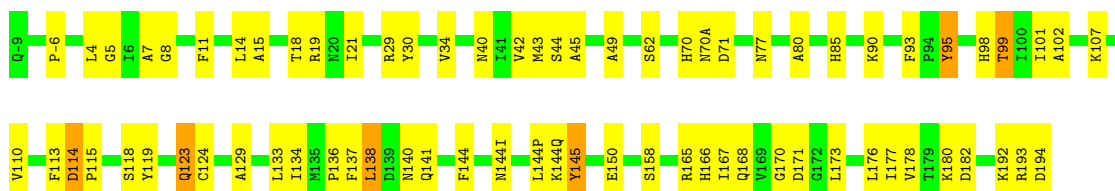
- Molecule 11: Proteasome component PRE2

Chain Y: 68% 29%



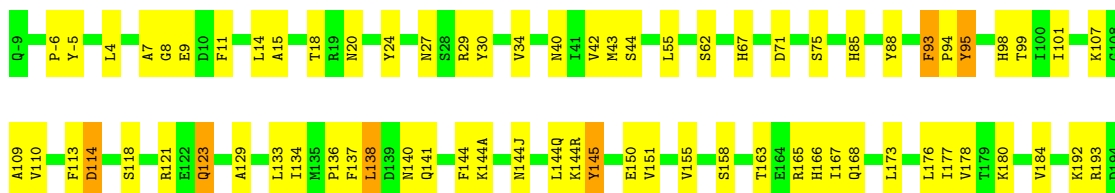
- Molecule 12: Proteasome component C5

Chain L: 67% 30%



- Molecule 12: Proteasome component C5

Chain Z:  68% 30%



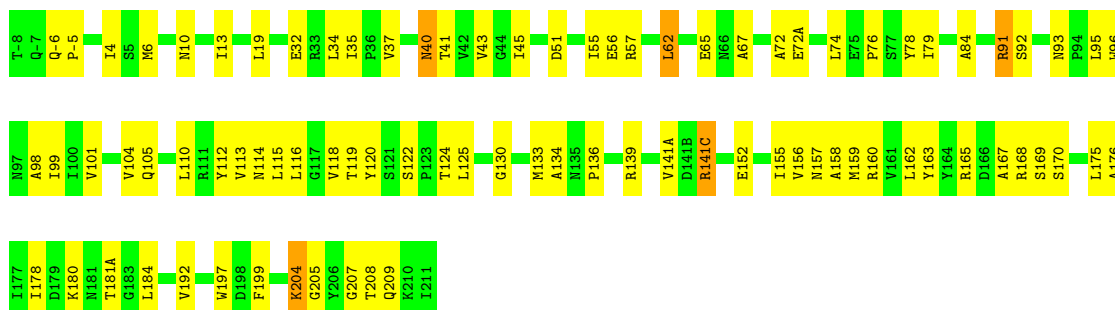
• Molecule 13: Proteasome component PRE4

Chain M:  70% 27%



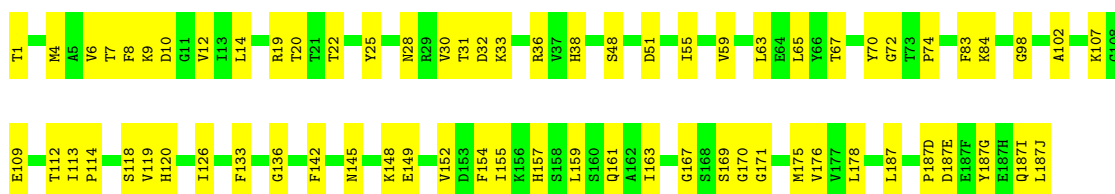
• Molecule 13: Proteasome component PRE4

Chain 1:  63% 35%



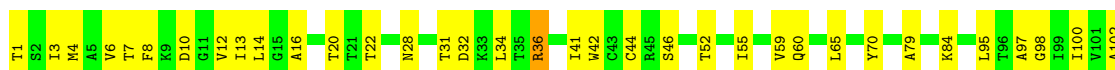
• Molecule 14: Proteasome component PRE3

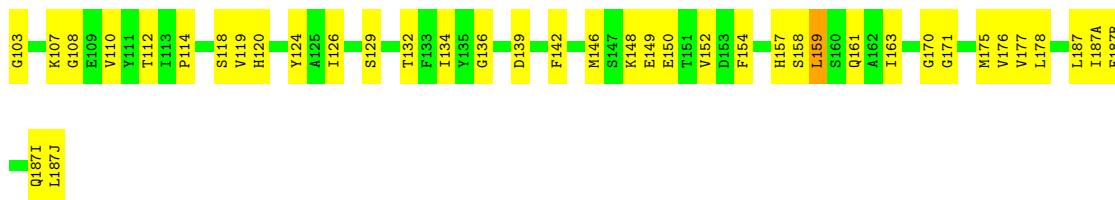
Chain N:  65% 35%



• Molecule 14: Proteasome component PRE3

Chain 2:  62% 37%





- Molecule 15: EPOXOMICIN (peptide inhibitor)



- Molecule 15: EPOXOMICIN (peptide inhibitor)





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.20Å 300.20Å 144.02Å 90.00° 112.98° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.25)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.283 , 0.336	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	52508	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, MG, 04D, IML

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.60	0/1952	0.80	0/2642
1	O	0.59	0/1952	0.79	0/2642
2	B	0.59	0/1935	0.76	0/2618
2	P	0.58	0/1935	0.77	0/2618
3	C	0.59	0/1920	0.78	1/2598 (0.0%)
3	Q	0.57	0/1920	0.78	1/2598 (0.0%)
4	D	0.59	0/1887	0.78	0/2541
4	R	0.58	0/1887	0.75	0/2541
5	E	0.53	0/1823	0.73	0/2463
5	S	0.55	0/1823	0.74	0/2463
6	F	0.54	0/1937	0.76	1/2614 (0.0%)
6	T	0.59	0/1937	0.79	1/2614 (0.0%)
7	G	0.61	0/1959	0.79	0/2652
7	U	0.65	1/1959 (0.1%)	0.80	0/2652
8	H	0.64	2/1716 (0.1%)	0.94	4/2326 (0.2%)
8	V	0.62	1/1716 (0.1%)	0.87	3/2326 (0.1%)
9	I	0.61	0/1611	0.81	0/2174
9	W	0.64	0/1611	0.83	1/2174 (0.0%)
10	J	0.62	0/1613	0.80	0/2173
10	X	0.63	0/1613	0.81	0/2173
11	K	0.64	1/1681 (0.1%)	0.83	4/2274 (0.2%)
11	Y	0.63	1/1681 (0.1%)	0.81	3/2274 (0.1%)
12	L	0.64	0/1795	0.78	2/2420 (0.1%)
12	Z	0.59	0/1795	0.78	1/2420 (0.0%)
13	1	0.64	0/1855	0.84	2/2514 (0.1%)
13	M	0.60	0/1855	0.79	2/2514 (0.1%)
14	2	0.64	0/1541	0.76	1/2087 (0.0%)
14	N	0.63	0/1541	0.80	2/2087 (0.1%)
15	3	1.51	0/14	1.53	0/18
15	4	1.25	0/14	1.38	0/18
All	All	0.61	6/50478 (0.0%)	0.80	29/68228 (0.0%)

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
2	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1	THR	C-N	-8.54	1.14	1.34
8	H	43	CYS	CB-SG	-5.80	1.72	1.81
11	K	1	THR	C-N	5.80	1.47	1.34
7	U	109	CYS	CB-SG	-5.53	1.72	1.81
8	V	31	CYS	CB-SG	-5.18	1.73	1.81
11	Y	1	THR	C-N	5.18	1.46	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	THR	O-C-N	-16.55	96.21	122.70
8	H	1	THR	C-N-CA	12.88	153.89	121.70
8	V	1	THR	O-C-N	-12.00	103.51	122.70
8	H	1	THR	CA-C-N	11.83	143.22	117.20
8	V	1	THR	C-N-CA	9.97	146.62	121.70
8	V	1	THR	CA-C-N	7.96	134.71	117.20
14	N	1	THR	C-N-CA	7.08	139.39	121.70
11	Y	1	THR	N-CA-CB	-6.46	98.03	110.30
11	K	1	THR	N-CA-CB	-6.21	98.50	110.30
14	N	98	GLY	N-CA-C	-5.80	98.60	113.10
11	K	1	THR	OG1-CB-CG2	-5.75	96.77	110.00
12	Z	95	TYR	N-CA-C	-5.74	95.49	111.00
6	F	125	LEU	CA-CB-CG	5.72	128.47	115.30
3	Q	56	LEU	CA-CB-CG	5.72	128.45	115.30
3	C	56	LEU	CA-CB-CG	5.59	128.15	115.30
12	L	93	PHE	N-CA-C	-5.58	95.93	111.00
12	L	95	TYR	N-CA-C	-5.49	96.18	111.00
9	W	95	TYR	N-CA-C	-5.47	96.22	111.00
11	Y	1	THR	OG1-CB-CG2	-5.41	97.55	110.00
11	K	1	THR	O-C-N	-5.38	114.08	122.70
11	K	98	GLY	N-CA-C	-5.38	99.64	113.10
14	2	98	GLY	N-CA-C	-5.35	99.72	113.10
13	1	95	LEU	N-CA-C	-5.24	96.85	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	98	GLY	N-CA-C	-5.23	100.03	113.10
6	T	93	ARG	NE-CZ-NH2	-5.18	117.71	120.30
13	1	98	ALA	N-CA-C	-5.13	97.16	111.00
13	M	27	ARG	N-CA-C	5.11	124.80	111.00
13	M	98	ALA	N-CA-C	-5.09	97.25	111.00
8	H	22	GLN	N-CA-C	-5.08	97.27	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	144(A)	TYR	Sidechain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	55	0
1	O	1915	0	1926	61	0
2	B	1905	0	1901	76	0
2	P	1905	0	1901	85	0
3	C	1891	0	1900	74	0
3	Q	1891	0	1900	102	0
4	D	1862	0	1836	70	0
4	R	1862	0	1836	61	0
5	E	1795	0	1797	70	0
5	S	1795	0	1797	92	0
6	F	1897	0	1886	57	0
6	T	1897	0	1886	79	0
7	G	1921	0	1910	79	0
7	U	1921	0	1910	79	0
8	H	1685	0	1687	46	0
8	V	1685	0	1687	63	0
9	I	1581	0	1573	38	0
9	W	1581	0	1574	50	0
10	J	1585	0	1590	52	0
10	X	1585	0	1590	55	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1644	0	1592	59	0
11	Y	1644	0	1593	60	0
12	L	1757	0	1711	70	0
12	Z	1757	0	1711	62	0
13	1	1824	0	1832	65	0
13	M	1824	0	1832	48	0
14	2	1512	0	1481	59	0
14	N	1512	0	1481	50	0
15	3	39	0	44	4	0
15	4	39	0	44	3	0
16	D	1	0	0	0	0
16	F	2	0	0	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0
16	I	2	0	0	0	0
16	K	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
17	1	142	0	0	1	0
17	2	124	0	0	0	0
17	3	1	0	0	0	0
17	A	100	0	0	2	0
17	B	72	0	0	1	0
17	C	71	0	0	0	0
17	D	86	0	0	5	0
17	E	57	0	0	1	0
17	F	98	0	0	2	0
17	G	106	0	0	4	0
17	H	129	0	0	2	0
17	I	109	0	0	1	0
17	J	114	0	0	3	0
17	K	94	0	0	5	0
17	L	147	0	0	4	0
17	M	130	0	0	0	0
17	N	115	0	0	1	0
17	O	99	0	0	1	0
17	P	72	0	0	2	0
17	Q	68	0	0	0	0
17	R	87	0	0	3	0
17	S	56	0	0	3	0
17	T	95	0	0	5	0
17	U	111	0	0	6	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	V	124	0	0	8	0
17	W	111	0	0	3	0
17	X	119	0	0	5	0
17	Y	93	0	0	9	0
17	Z	142	0	0	6	0
All	All	52508	0	49334	1644	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 17.

All (1644) 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)
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.09	1.09
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.13	1.05
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.44	1.00
7:G:96:ALA:HA	7:G:107:MET:HE2	1.40	0.99
12:L:18:THR:CG2	12:L:30:TYR:HA	1.95	0.97
14:N:136:GLY:HA2	14:2:161:GLN:NE2	1.81	0.94
11:K:4:LEU:HD11	11:K:15:ALA:HB3	1.50	0.94
6:T:37:SER:HB3	6:T:50:VAL:HG23	1.52	0.92
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.51	0.91
4:R:214:CYS:HG	4:R:224:TYR:HE2	1.15	0.88
12:Z:163:THR:O	17:Z:254:HOH:O	1.91	0.88
4:D:214:CYS:HG	4:D:224:TYR:HE2	1.16	0.86
3:C:35:THR:HB	3:C:51:GLU:HG3	1.56	0.86
12:Z:18:THR:CG2	12:Z:30:TYR:HA	2.05	0.86
1:O:7:ARG:HH22	4:R:123(C):GLY:HA3	1.41	0.85
11:Y:163:ALA:O	17:Y:334:HOH:O	1.94	0.85
7:U:121:GLN:O	7:U:124:THR:HB	1.76	0.84
8:H:1:THR:N	8:H:168:GLY:O	2.10	0.83
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.93	0.82
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.62	0.82
12:L:18:THR:HG22	12:L:29:ARG:O	1.78	0.82
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.20	0.82
12:L:18:THR:HG21	12:L:30:TYR:HD1	1.45	0.82
3:Q:47:VAL:HG23	3:Q:189:CYS:SG	2.20	0.81
7:U:96:ALA:HA	7:U:107:MET:HE2	1.60	0.81
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.60	0.81
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.63	0.81
6:F:35:THR:HG21	6:F:51:GLU:O	1.81	0.80

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:27:ALA:O	1:O:31:VAL:HG23	1.80	0.80
8:V:163:ILE:O	17:V:342:HOH:O	1.98	0.80
13:1:133:MET:O	13:1:136:PRO:HD2	1.82	0.80
3:Q:100:ARG:NH1	3:Q:106:PRO:HB3	1.97	0.80
13:1:6:MET:HG2	13:1:155:ILE:HD11	1.63	0.80
7:U:59:LEU:O	7:U:61:PRO:HD3	1.83	0.79
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.31	0.79
3:C:100:ARG:NH1	3:C:106:PRO:HB3	1.98	0.78
11:Y:208:ASN:HB3	17:Y:302:HOH:O	1.83	0.78
5:S:73:HIS:HE1	5:S:107:LEU:O	1.67	0.78
7:U:126:ARG:O	17:U:335:HOH:O	2.02	0.78
1:A:161:LYS:HD3	1:A:180:TRP:CH2	2.20	0.77
11:Y:33:LYS:HE2	15:4:5:04D:H23	1.66	0.77
3:Q:190:VAL:O	3:Q:194:VAL:HG23	1.84	0.77
9:W:163:ALA:O	17:W:234:HOH:O	2.01	0.77
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.19	0.77
8:H:1:THR:HG23	8:H:33:LYS:HD3	1.66	0.77
6:T:35:THR:HG21	6:T:51:GLU:O	1.84	0.77
14:N:8:PHE:CE1	14:N:10:ASP:HB2	2.20	0.76
3:C:163:GLN:HE21	3:C:164:THR:H	1.32	0.76
9:W:28:SER:HA	17:W:213:HOH:O	1.85	0.76
6:T:186:ALA:O	6:T:190:VAL:HG23	1.86	0.76
13:1:43:VAL:HG22	13:1:101:VAL:HG22	1.67	0.76
7:U:186:TRP:O	7:U:190:VAL:HG23	1.86	0.76
11:Y:45:MET:HB3	11:Y:52:CYS:HB3	1.68	0.76
7:G:96:ALA:HA	7:G:107:MET:CE	2.17	0.75
11:Y:105(B):LYS:H	11:Y:105(B):LYS:HD2	1.52	0.75
11:Y:105(A):ARG:HB3	11:Y:105(B):LYS:HE3	1.69	0.74
5:S:15:PHE:HB2	6:T:23:GLN:HE22	1.52	0.74
3:C:164:THR:HG21	3:C:172:VAL:HG13	1.68	0.74
11:K:208:ASN:HB3	17:K:461:HOH:O	1.85	0.74
10:X:44:SER:OG	10:X:100:LEU:HB2	1.86	0.74
5:E:47:VAL:HG23	5:E:189:LEU:HD13	1.70	0.74
8:H:1:THR:HA	8:H:33:LYS:NZ	2.03	0.74
11:K:1:THR:HA	17:K:445:HOH:O	1.88	0.74
4:D:215:ILE:HG22	4:D:221:PHE:HD2	1.53	0.73
2:P:76:VAL:HG12	2:P:138:TYR:CD2	2.22	0.73
11:K:4:LEU:CD1	11:K:15:ALA:HB3	2.17	0.73
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.51	0.73
5:E:15:PHE:HB2	6:F:23:GLN:HE22	1.54	0.73
6:T:141:VAL:HG23	6:T:215:CYS:SG	2.28	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:129:MET:O	17:U:335:HOH:O	2.08	0.72
10:X:6:ILE:HD11	10:X:142:TYR:CE1	2.24	0.72
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.70	0.72
6:T:176:LEU:HD22	6:T:196:ILE:HD13	1.72	0.72
14:2:157:HIS:HD2	14:2:187(J):LEU:HD13	1.54	0.72
13:1:41:THR:OG1	13:1:76:PRO:HG3	1.87	0.72
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.25	0.72
4:D:46:VAL:HG11	4:D:139:ALA:HB1	1.72	0.71
13:1:157:ASN:ND2	13:1:160:ARG:HH11	1.89	0.71
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.70	0.71
13:1:157:ASN:ND2	13:1:160:ARG:NH1	2.38	0.71
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.54	0.71
5:S:52:LYS:HB3	5:S:63:TYR:HB3	1.73	0.71
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.56	0.71
8:V:166:ASP:O	17:V:342:HOH:O	2.09	0.71
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.56	0.71
4:D:97:VAL:HG21	11:K:65:LEU:CD1	2.20	0.71
6:T:81:LEU:HD12	6:T:133:GLY:HA3	1.71	0.71
11:K:105(B):LYS:H	11:K:105(B):LYS:HD2	1.55	0.71
1:O:161:LYS:HD3	1:O:180:TRP:CH2	2.26	0.70
14:2:1:THR:HG21	14:2:46:SER:CB	2.21	0.70
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.27	0.70
2:P:130:ARG:HG3	2:P:130:ARG:HH11	1.55	0.70
3:Q:160:TRP:CE2	4:R:59:LEU:HD23	2.26	0.70
5:E:130:ARG:HG3	5:E:130:ARG:HH11	1.56	0.70
8:H:77:VAL:HB	13:1:208:THR:HG22	1.73	0.70
2:B:121:GLN:O	2:B:124:THR:HB	1.92	0.70
13:M:41:THR:OG1	13:M:76:PRO:HG3	1.91	0.70
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.56	0.70
4:R:75:GLY:HA3	4:R:221:PHE:CD2	2.27	0.70
12:Z:18:THR:HG23	12:Z:30:TYR:HA	1.73	0.69
11:K:142:TYR:O	11:K:143:LYS:HD2	1.91	0.69
14:2:8:PHE:CE1	14:2:10:ASP:HB2	2.28	0.69
8:H:103:GLY:HA2	8:H:178:MET:SD	2.32	0.69
4:R:46:VAL:HG11	4:R:139:ALA:HB1	1.73	0.69
2:P:185:LYS:HD3	2:P:187:ASP:H	1.56	0.69
9:I:28:SER:HA	17:I:388:HOH:O	1.93	0.69
11:K:105(A):ARG:HB3	11:K:105(B):LYS:HE3	1.74	0.69
14:N:157:HIS:HD2	14:N:187(J):LEU:HD13	1.56	0.69
10:X:-1:MET:HG2	10:X:1:ASP:H	1.57	0.69
10:X:2:ILE:HA	17:X:234:HOH:O	1.92	0.69

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.73	0.69
13:1:141(C):ARG:HG3	13:1:141(C):ARG:HH11	1.58	0.69
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.75	0.69
14:N:171:GLY:HA2	13:1:197:TRP:CH2	2.27	0.69
12:Z:18:THR:HG22	12:Z:29:ARG:O	1.92	0.68
12:L:90:LYS:HD3	12:L:95:TYR:CE1	2.28	0.68
12:Z:43:MET:HB2	12:Z:101:ILE:HG22	1.73	0.68
5:E:103:PHE:HE2	13:M:62:LEU:HD21	1.58	0.68
14:2:84:LYS:HE3	14:2:119:VAL:HG23	1.75	0.68
2:P:87:ILE:O	2:P:91:THR:HG23	1.92	0.68
13:M:80:PHE:CZ	13:M:111:ARG:HG2	2.28	0.68
1:O:121:GLN:O	1:O:124:THR:HB	1.94	0.68
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.07	0.68
7:U:96:ALA:HA	7:U:107:MET:CE	2.23	0.68
14:2:1:THR:HG21	14:2:46:SER:HB2	1.75	0.68
2:B:15:PHE:H	3:C:23:GLN:HE22	1.39	0.68
5:E:75:GLY:HA3	5:E:221:PHE:CZ	2.28	0.68
7:G:150:LYS:O	7:G:157:TYR:HA	1.93	0.68
4:R:75:GLY:HA3	4:R:221:PHE:CE2	2.29	0.68
9:I:48:LEU:HG	9:I:50:THR:HG22	1.76	0.68
3:C:57:LYS:HD2	3:C:58:LEU:N	2.09	0.67
11:Y:4:LEU:HD11	11:Y:15:ALA:HB3	1.76	0.67
11:K:157:ARG:O	11:K:160:LEU:HB3	1.94	0.67
11:Y:5:ALA:HA	11:Y:13:ILE:O	1.95	0.67
9:I:55:LEU:HD21	9:I:95:TYR:CD1	2.28	0.67
12:L:18:THR:HG21	12:L:30:TYR:CD1	2.30	0.67
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.77	0.67
3:Q:186:VAL:O	3:Q:190:VAL:HG23	1.95	0.67
5:S:161:TYR:OH	6:T:61:PRO:HD2	1.95	0.67
1:O:161:LYS:HD3	1:O:180:TRP:CZ3	2.30	0.67
1:A:121:GLN:O	1:A:124:THR:HB	1.95	0.67
3:C:15:PHE:H	4:D:23:GLN:HE22	1.43	0.67
10:J:-1:MET:HG2	10:J:1:ASP:H	1.60	0.67
2:P:121:GLN:O	2:P:124:THR:HB	1.94	0.67
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.77	0.66
5:E:73:HIS:HE1	5:E:107:LEU:O	1.78	0.66
8:H:29:LYS:HE2	12:Z:165:ARG:NH2	2.10	0.66
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.42	0.66
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.76	0.66
4:D:75:GLY:HA3	4:D:221:PHE:CD2	2.31	0.66
6:F:38:ILE:HG22	6:F:164:ALA:CB	2.25	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.23	0.66
1:O:130:ARG:HG3	1:O:130:ARG:HH11	1.60	0.66
12:Z:151:VAL:O	12:Z:155:VAL:HG23	1.96	0.66
3:C:57:LYS:O	3:C:58:LEU:HB2	1.95	0.66
3:C:160:TRP:CZ2	4:D:59:LEU:HD23	2.30	0.66
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.43	0.66
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.60	0.66
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.77	0.66
13:M:104:VAL:HG23	13:M:178:ILE:HG22	1.78	0.66
3:Q:130:ARG:HG3	3:Q:130:ARG:HH11	1.61	0.66
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.78	0.66
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.77	0.66
5:S:76:LEU:O	5:S:76:LEU:HD23	1.95	0.65
7:G:76:MET:SD	7:G:138:PHE:CE2	2.89	0.65
7:U:207:LYS:HG3	7:U:208:ASN:OD1	1.96	0.65
3:C:36:CYS:H	3:C:51:GLU:HG2	1.61	0.65
5:S:190:ILE:HG23	5:S:212:ILE:HD13	1.78	0.65
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.78	0.65
6:F:18:ASP:OD1	6:F:20:ARG:HD3	1.97	0.65
10:J:34:THR:HG23	10:J:42:LEU:HD11	1.78	0.65
2:P:4:GLY:HA3	5:S:127:TYR:CE1	2.32	0.65
3:Q:79:SER:OG	3:Q:165:ILE:HG13	1.97	0.65
4:R:215:ILE:HG22	4:R:221:PHE:HD2	1.61	0.65
3:C:163:GLN:NE2	3:C:164:THR:H	1.93	0.65
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.31	0.65
1:A:85:TYR:O	1:A:89:VAL:HG23	1.96	0.65
10:J:37:LEU:HB2	10:J:41:THR:HG22	1.79	0.65
12:L:194:ASP:OXT	17:V:342:HOH:O	2.15	0.65
7:G:130:ARG:HG3	7:G:131:PRO:O	1.96	0.64
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.95	0.64
6:T:120:VAL:HG21	6:T:151:LEU:HD21	1.78	0.64
4:D:125:GLU:HG2	4:D:127:LEU:HD13	1.79	0.64
5:E:194:VAL:O	5:E:197:ILE:HG22	1.97	0.64
3:C:160:TRP:CE2	4:D:59:LEU:HD23	2.32	0.64
12:L:18:THR:HG22	12:L:30:TYR:HA	1.77	0.64
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.79	0.64
4:D:14:THR:HG22	5:E:23:GLN:NE2	2.12	0.64
6:T:136:THR:O	6:T:150:MET:HA	1.97	0.64
10:X:6:ILE:HD11	10:X:142:TYR:HE1	1.61	0.64
14:2:103:GLY:HA2	14:2:178:LEU:HD23	1.78	0.64
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.78	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:134:ILE:HG23	12:Z:158:SER:HB3	1.79	0.64
1:A:217(B):ASN:HB3	1:A:217(F):LEU:HD12	1.78	0.64
8:H:167:LEU:HD22	12:Z:167:ILE:O	1.97	0.64
2:P:7:ARG:HB3	2:P:8:TYR:CE1	2.33	0.64
5:S:130:ARG:HG3	5:S:130:ARG:HH11	1.62	0.64
6:F:170:GLN:H	6:F:170:GLN:CD	2.00	0.64
12:Z:-6:PRO:HB2	13:1:91:ARG:NH1	2.13	0.64
7:G:229:ILE:O	7:G:232:ARG:HB2	1.97	0.64
10:J:44:SER:OG	10:J:100:LEU:HB2	1.96	0.64
13:M:141(C):ARG:HG3	13:M:141(C):ARG:HH11	1.62	0.64
3:Q:175:PHE:CZ	3:Q:195:ARG:HB3	2.32	0.64
2:P:141:TYR:CD1	2:P:219(A):VAL:HG21	2.32	0.63
3:C:130:ARG:HG3	3:C:130:ARG:HH11	1.63	0.63
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.29	0.63
2:B:163:ILE:HG13	2:B:164:SER:N	2.14	0.63
7:G:121:GLN:O	7:G:124:THR:HB	1.97	0.63
5:S:21:LEU:O	5:S:25:GLU:HG3	1.98	0.63
9:W:27:VAL:HG13	17:X:295:HOH:O	1.99	0.63
3:C:185:THR:HB	3:C:188:GLU:HG2	1.80	0.63
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.81	0.63
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.81	0.63
9:I:36:HIS:HB3	9:I:42:PHE:CD2	2.33	0.63
11:K:4:LEU:HD13	11:K:15:ALA:O	1.99	0.63
1:O:134:VAL:O	1:O:153:PRO:HG3	1.98	0.63
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.34	0.63
12:L:18:THR:HG23	12:L:30:TYR:HA	1.75	0.62
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.81	0.62
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.80	0.62
2:P:141:TYR:HA	2:P:145:GLY:O	2.00	0.62
2:B:163:ILE:HG13	2:B:164:SER:H	1.65	0.62
3:C:71:ASP:HA	10:J:68:ILE:CD1	2.29	0.62
11:K:21:THR:O	15:3:4:THR:HG22	1.99	0.62
12:L:133:LEU:O	12:L:136:PRO:HD2	2.00	0.62
3:Q:47:VAL:CG2	3:Q:189:CYS:SG	2.88	0.62
5:S:15:PHE:CE1	5:S:21:LEU:HD21	2.35	0.62
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.13	0.62
8:H:55:VAL:HG23	8:H:86:HIS:HD2	1.64	0.62
3:Q:160:TRP:CZ2	4:R:59:LEU:HD23	2.35	0.62
5:S:15:PHE:HB2	6:T:23:GLN:NE2	2.14	0.62
2:B:161:LYS:HE3	3:C:59:GLN:O	2.00	0.62
11:Y:4:LEU:HD12	11:Y:159:ILE:HD11	1.82	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:175:GLU:O	6:T:178:LYS:HB2	1.99	0.61
3:C:175:PHE:CZ	3:C:195:ARG:HB3	2.35	0.61
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.35	0.61
4:D:186:LEU:O	4:D:190:GLU:HG3	2.00	0.61
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.15	0.61
7:U:229:ILE:O	7:U:232:ARG:HB2	1.99	0.61
7:G:45:CYS:O	7:G:146:PRO:HB3	2.00	0.61
10:J:2:ILE:HA	17:J:301:HOH:O	2.00	0.61
12:Z:18:THR:HG21	12:Z:30:TYR:HD1	1.63	0.61
6:F:49:ALA:HA	6:F:211:GLU:O	2.00	0.61
7:U:158:VAL:HG22	7:U:159:GLY:N	2.15	0.61
10:X:53:VAL:HG21	17:Y:313:HOH:O	2.00	0.61
11:Y:157:ARG:O	11:Y:160:LEU:HB3	2.00	0.61
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.35	0.61
3:Q:106:PRO:HG2	3:Q:143:PRO:HG3	1.81	0.61
3:Q:168:ASN:CB	3:Q:200:VAL:HG11	2.31	0.61
12:Z:34:VAL:HG22	12:Z:44:SER:HB2	1.82	0.61
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.82	0.61
5:S:180(C):PHE:HA	5:S:182:ILE:HG13	1.81	0.61
9:W:19:ARG:HD3	9:W:168:LEU:O	2.01	0.61
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.83	0.61
1:A:14:THR:O	1:A:21:LEU:HD23	2.01	0.61
3:C:226:SER:HB2	3:C:227:GLU:OE1	2.01	0.61
6:F:42:CYS:HB2	6:F:184:LEU:O	2.00	0.61
2:P:8:TYR:CD1	2:P:8:TYR:N	2.69	0.61
6:T:130:ARG:HG3	6:T:130:ARG:HH11	1.66	0.61
3:Q:106:PRO:HG2	3:Q:143:PRO:CG	2.31	0.60
7:U:78:VAL:HG11	7:U:85:ALA:HB2	1.83	0.60
1:A:41:LYS:HG3	1:A:46:VAL:HG22	1.81	0.60
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.65	0.60
3:Q:40:VAL:HG12	3:Q:162:ALA:HB1	1.81	0.60
7:G:207:LYS:HG3	7:G:208:ASN:OD1	2.02	0.60
12:Z:-6:PRO:HB2	13:1:91:ARG:HH11	1.65	0.60
1:A:7:ARG:HH22	4:D:123(C):GLY:HA3	1.64	0.60
3:C:35:THR:HB	3:C:51:GLU:CG	2.31	0.60
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.01	0.60
6:T:170:GLN:CD	6:T:170:GLN:H	2.05	0.60
13:M:82:TYR:O	13:M:86:VAL:HG23	2.01	0.60
14:N:48:SER:HB3	14:N:51:ASP:HB2	1.84	0.60
1:O:207:ASN:HA	1:O:233:LEU:CD1	2.31	0.60
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.48	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.67	0.60
7:G:77:VAL:CG1	7:G:137:THR:HB	2.32	0.60
8:V:172:ASN:ND2	8:V:193:THR:HG22	2.16	0.60
9:W:55:LEU:HD21	9:W:95:TYR:CD1	2.36	0.60
11:K:137:VAL:HG21	11:K:161:ALA:HB2	1.82	0.60
5:S:81:LEU:HB2	5:S:133:GLY:O	2.02	0.60
6:T:38:ILE:HG22	6:T:164:ALA:CB	2.31	0.60
5:E:77:SER:OG	5:E:137:LEU:HB2	2.01	0.60
8:H:163:ILE:HG23	8:H:170:GLY:HA2	1.83	0.60
3:Q:164:THR:HG21	3:Q:172:VAL:HG13	1.82	0.60
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.02	0.60
2:B:41:MET:HB2	2:B:148:LEU:HD22	1.83	0.60
4:D:215:ILE:HG22	4:D:221:PHE:CD2	2.34	0.60
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.83	0.60
3:Q:185:THR:HB	3:Q:188:GLU:HG2	1.82	0.60
11:Y:99:THR:HA	17:Y:365:HOH:O	2.01	0.60
3:C:168:ASN:CB	3:C:200:VAL:HG11	2.31	0.59
6:F:192:GLN:O	6:F:196:ILE:HG13	2.02	0.59
9:W:101:VAL:O	9:W:110:ILE:HA	2.02	0.59
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.83	0.59
9:W:14:ILE:HG23	9:W:34:ILE:HD13	1.83	0.59
10:X:113:ILE:HA	10:X:118:THR:O	2.02	0.59
11:Y:1:THR:HA	17:Y:378:HOH:O	2.02	0.59
14:N:84:LYS:HB2	14:N:119:VAL:CG2	2.32	0.59
13:1:4:ILE:HD11	13:1:159:MET:SD	2.43	0.59
5:E:76:LEU:HD23	5:E:76:LEU:O	2.03	0.59
5:E:141:TYR:OH	5:E:217:LYS:HG3	2.02	0.59
7:G:80:GLY:HA3	7:G:134:VAL:HG12	1.84	0.59
5:S:24:VAL:O	5:S:28:LEU:HD13	2.03	0.59
9:W:6:MET:HB2	9:W:151:LEU:HD11	1.85	0.59
1:A:112:LEU:O	1:A:116:VAL:HG23	2.03	0.59
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.03	0.59
11:K:102:CYS:SG	11:K:110:ILE:HG23	2.43	0.59
3:Q:49:GLY:HA3	3:Q:212:ILE:HD13	1.85	0.59
5:S:175:TYR:HB2	5:S:199:GLN:HG2	1.84	0.59
6:F:176:LEU:HD22	6:F:196:ILE:HD13	1.83	0.59
7:G:76:MET:SD	7:G:138:PHE:HE2	2.25	0.59
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.84	0.59
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.84	0.59
10:J:21:THR:O	10:J:22:ARG:HD3	2.03	0.59
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.18	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:175:LEU:HB3	17:P:343:HOH:O	2.02	0.59
3:Q:57:LYS:O	3:Q:58:LEU:HB2	2.03	0.59
2:B:181:LYS:O	2:B:184:MET:HG3	2.03	0.59
13:M:57:ARG:HG2	13:M:57:ARG:HH11	1.67	0.59
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.16	0.58
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.38	0.58
7:U:83:PRO:HG2	17:U:355:HOH:O	2.02	0.58
7:U:158:VAL:HG22	7:U:159:GLY:H	1.68	0.58
2:P:112:LEU:C	2:P:112:LEU:HD23	2.23	0.58
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.83	0.58
9:I:16:CYS:SG	9:I:174:VAL:HG12	2.43	0.58
13:M:130:GLY:O	13:M:134:ALA:HB3	2.04	0.58
3:Q:52:ARG:HH21	3:Q:211:GLU:HB3	1.67	0.58
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.51	0.58
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.83	0.58
10:J:133:TYR:HD1	17:Y:337:HOH:O	1.85	0.58
13:M:157:ASN:ND2	13:M:160:ARG:HH11	2.02	0.58
7:U:76:MET:SD	7:U:138:PHE:CE2	2.96	0.58
7:G:173:THR:O	7:G:177:GLU:HG3	2.03	0.58
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.86	0.58
5:S:141:TYR:OH	5:S:217:LYS:HG3	2.03	0.58
6:T:69:VAL:HG12	17:T:362:HOH:O	2.04	0.58
8:V:78:SER:O	8:V:82:MET:HG3	2.02	0.58
12:Z:144(R):LYS:HG2	12:Z:145:TYR:N	2.18	0.58
12:Z:29:ARG:NH1	12:Z:193:ARG:HB3	2.19	0.58
2:B:76:VAL:HG12	2:B:138:TYR:CD2	2.38	0.58
11:K:14:VAL:HB	11:K:176:TYR:HB2	1.86	0.58
11:K:99:THR:HG22	11:K:113:VAL:O	2.04	0.58
8:V:18:THR:HG23	8:V:172:ASN:O	2.04	0.58
7:G:39:ALA:CB	7:G:48:VAL:HG12	2.33	0.58
14:N:4:MET:HB3	14:N:126:ILE:HG22	1.85	0.58
1:O:150:GLN:O	1:O:157:TYR:HA	2.03	0.58
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.68	0.58
11:Y:21:THR:O	15:4:4:THR:HG22	2.03	0.58
1:A:207:ASN:HA	1:A:233:LEU:CD1	2.34	0.58
2:B:141:TYR:CD1	2:B:219(E):VAL:HG21	2.39	0.58
2:P:202:THR:HG22	2:P:204:SER:H	1.69	0.58
8:V:172:ASN:HD22	8:V:193:THR:HG22	1.69	0.58
3:C:182:PRO:O	3:C:184:ALA:N	2.36	0.57
9:I:1:GLY:HA3	9:I:33:LYS:HE2	1.85	0.57
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.52	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:LYS:HA	5:E:78:LEU:HD21	1.86	0.57
13:M:35:ILE:CD1	13:M:56:GLU:HG2	2.33	0.57
5:S:148:LEU:HD23	5:S:162:GLY:HA2	1.85	0.57
3:C:168:ASN:HB2	3:C:200:VAL:HG11	1.86	0.57
3:Q:46:VAL:HG22	3:Q:146:PRO:HB2	1.86	0.57
3:Q:136:THR:O	3:Q:150:GLN:HA	2.04	0.57
11:Y:4:LEU:HD23	11:Y:6:PHE:HD2	1.69	0.57
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.86	0.57
3:Q:182:PRO:O	3:Q:184:ALA:N	2.38	0.57
6:T:221:HIS:HE1	6:T:223:PHE:CE1	2.22	0.57
8:V:132:LEU:HD12	8:V:132:LEU:N	2.19	0.57
3:Q:49:GLY:CA	3:Q:212:ILE:HD13	2.34	0.57
10:X:133:TYR:CE2	10:X:166:MET:SD	2.97	0.57
14:2:1:THR:CG2	14:2:46:SER:HB2	2.34	0.57
14:2:142:PHE:HB2	14:2:154:PHE:CZ	2.39	0.57
9:I:25:LEU:HD11	10:J:135:PHE:HD2	1.69	0.57
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.18	0.57
5:S:136:LEU:HD12	5:S:151:PHE:CD2	2.40	0.57
1:A:118:LYS:O	1:A:122:GLU:HG3	2.05	0.57
10:J:34:THR:CG2	10:J:42:LEU:HD11	2.35	0.57
1:O:45:GLY:HA3	1:O:186:LEU:HD13	1.86	0.57
7:U:39:ALA:CB	7:U:48:VAL:HG12	2.35	0.57
12:L:8:GLY:HA3	12:L:11:PHE:CZ	2.40	0.57
12:L:42:VAL:O	12:L:101:ILE:HA	2.04	0.57
7:U:105:TYR:OH	8:V:66:HIS:HE1	1.88	0.57
4:D:123(D):ALA:CB	5:E:129:GLY:HA2	2.35	0.57
2:B:87:ILE:O	2:B:91:THR:HG23	2.05	0.56
4:D:46:VAL:HG11	4:D:139:ALA:CB	2.34	0.56
6:F:74:ILE:HD13	6:F:112:PHE:CD2	2.40	0.56
7:G:130:ARG:HG3	7:G:130:ARG:HH11	1.70	0.56
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.87	0.56
9:I:171:TRP:HH2	11:Y:165:ARG:NH1	2.03	0.56
4:R:215:ILE:HG22	4:R:221:PHE:CD2	2.40	0.56
5:S:194:VAL:HG13	5:S:207:LEU:HD11	1.86	0.56
4:D:46:VAL:O	4:D:214:CYS:HA	2.05	0.56
6:F:171:SER:O	6:F:174:ALA:HB3	2.05	0.56
8:H:55:VAL:HG23	8:H:86:HIS:CD2	2.40	0.56
8:H:197:ARG:NH2	9:I:139:GLU:HG3	2.20	0.56
3:Q:71:ASP:HA	10:X:68:ILE:CD1	2.36	0.56
5:S:208:THR:H	5:S:209:ASN:HB3	1.70	0.56
6:T:121:GLN:HG3	7:U:83:PRO:O	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:20:THR:OG1	14:2:28:ASN:HB3	2.04	0.56
3:Q:174:GLU:O	3:Q:178:LYS:HG2	2.06	0.56
7:U:173:THR:O	7:U:177:GLU:HG3	2.05	0.56
9:W:8:GLY:HA3	9:W:11:CYS:SG	2.46	0.56
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.88	0.56
2:B:202:THR:HG22	2:B:204:SER:H	1.69	0.56
8:H:126:SER:O	8:H:127:LEU:HD23	2.05	0.56
13:M:208:THR:HG22	8:V:77:VAL:HB	1.86	0.56
1:A:130:ARG:HH21	7:G:124:THR:CG2	2.18	0.56
2:B:205:LEU:HG	2:B:210:LEU:HD11	1.87	0.56
3:C:163:GLN:HG3	3:C:164:THR:N	2.21	0.56
4:D:112:LEU:C	4:D:112:LEU:HD13	2.25	0.56
12:L:43:MET:HB2	12:L:101:ILE:HG22	1.86	0.56
2:P:111:ILE:HG12	10:X:70:GLU:OE2	2.05	0.56
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.39	0.56
8:V:55:VAL:HG23	8:V:86:HIS:HD2	1.71	0.56
11:Y:105(B):LYS:H	11:Y:105(B):LYS:CD	2.17	0.56
1:A:130:ARG:NH1	1:A:131:PRO:O	2.39	0.56
7:G:158:VAL:HG22	7:G:159:GLY:H	1.71	0.56
4:R:39:GLY:HA2	4:R:47:VAL:O	2.05	0.56
5:S:17:PRO:HG3	6:T:26:TYR:CE2	2.39	0.56
1:A:82:GLY:O	1:A:85:TYR:HB3	2.06	0.56
4:D:123:PHE:CE1	4:D:131:PRO:HG3	2.41	0.56
3:Q:39:GLY:HA2	3:Q:47:VAL:O	2.06	0.56
7:U:179(D):SER:O	7:U:179(E):LYS:HB2	2.05	0.56
4:D:79:SER:HB3	4:D:165:ILE:HD12	1.88	0.56
12:Z:42:VAL:O	12:Z:101:ILE:HA	2.06	0.56
12:Z:114:ASP:HB3	12:Z:118:SER:HB3	1.88	0.56
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.88	0.56
2:B:81:LEU:HD23	2:B:133:GLY:HA3	1.87	0.56
3:Q:33:ARG:HH11	3:Q:33:ARG:HB3	1.70	0.56
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.36	0.56
5:S:49:VAL:CG1	5:S:210:LEU:HD11	2.37	0.55
6:T:49:ALA:HA	6:T:211:GLU:O	2.06	0.55
12:Z:-6:PRO:HG2	12:Z:-5:TYR:CD1	2.41	0.55
9:I:41:VAL:HG22	9:I:76:PRO:HG3	1.86	0.55
11:Y:4:LEU:CD1	11:Y:15:ALA:HB3	2.36	0.55
17:A:387:HOH:O	2:B:83:ALA:HB3	2.07	0.55
6:F:169:ARG:HG3	6:F:173:LYS:HE3	1.88	0.55
10:J:45:PHE:CE1	10:J:52:THR:HG23	2.41	0.55
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.87	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:40:LEU:N	5:S:40:LEU:HD23	2.21	0.55
11:K:1:THR:HG23	11:K:33:LYS:HZ2	1.71	0.55
3:Q:27:ALA:O	3:Q:31:VAL:HG23	2.06	0.55
5:S:15:PHE:H	6:T:23:GLN:HE22	1.54	0.55
1:A:136:LEU:O	1:A:150:GLN:HA	2.07	0.55
5:E:15:PHE:H	6:F:23:GLN:HE22	1.52	0.55
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.88	0.55
13:M:132:HIS:O	13:M:136:PRO:HG2	2.07	0.55
13:M:157:ASN:ND2	13:M:160:ARG:NH1	2.54	0.55
2:P:71:ASN:ND2	2:P:72:ASP:N	2.54	0.55
10:X:-1:MET:HG2	10:X:1:ASP:N	2.21	0.55
13:1:160:ARG:HG3	13:1:192:VAL:CG1	2.37	0.55
14:2:44:CYS:HB2	14:2:100:ILE:HB	1.88	0.55
2:B:81:LEU:H	2:B:81:LEU:HD22	1.70	0.55
2:P:110:GLU:O	2:P:110:GLU:HG2	2.06	0.55
5:S:37:THR:OG1	5:S:50:ALA:HB2	2.06	0.55
8:V:84:LYS:HE2	8:V:119:THR:CG2	2.36	0.55
10:J:105(B):LYS:HB2	10:J:105(B):LYS:NZ	2.22	0.55
10:J:129:TYR:O	10:J:132:PHE:HB2	2.06	0.55
5:S:37:THR:HA	5:S:50:ALA:HA	1.89	0.55
17:V:302:HOH:O	14:2:31:THR:HG23	2.06	0.55
12:Z:15:ALA:HB1	12:Z:173:LEU:HD11	1.88	0.55
9:I:27:VAL:HG13	17:J:247:HOH:O	2.07	0.55
10:J:52:THR:HG22	10:J:53:VAL:N	2.22	0.55
2:P:163:ILE:HG13	2:P:164:SER:H	1.72	0.55
4:D:100:ASN:HB3	17:D:409:HOH:O	2.06	0.54
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.41	0.54
14:N:67:THR:HA	14:N:72:GLY:O	2.07	0.54
6:T:18:ASP:OD1	6:T:20:ARG:HD3	2.06	0.54
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.90	0.54
5:E:81:LEU:HB2	5:E:133:GLY:O	2.08	0.54
10:J:113:ILE:HA	10:J:118:THR:O	2.07	0.54
11:K:165:ARG:NH1	9:W:171:TRP:HH2	2.05	0.54
14:N:161:GLN:HE21	14:2:136:GLY:CA	2.04	0.54
5:S:77:SER:OG	5:S:137:LEU:HB2	2.06	0.54
3:Q:75:VAL:HG21	3:Q:215:VAL:HG11	1.89	0.54
2:B:81:LEU:HB2	2:B:84:ASP:HB2	1.90	0.54
3:C:53:ARG:HG2	3:C:54:SER:N	2.23	0.54
4:R:46:VAL:HG11	4:R:139:ALA:CB	2.37	0.54
5:S:194:VAL:O	5:S:197:ILE:HG22	2.07	0.54
7:U:49:ILE:HD13	7:U:193:ALA:HB1	1.88	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:1:THR:HG23	8:H:33:LYS:CD	2.36	0.54
3:Q:15:PHE:CE2	4:R:27:SER:HB3	2.42	0.54
1:O:130:ARG:HH21	7:U:124:THR:CG2	2.20	0.54
5:S:51:LEU:O	5:S:66:LYS:HE2	2.08	0.54
5:S:130:ARG:HG3	5:S:130:ARG:NH1	2.23	0.54
5:S:162:GLY:O	5:S:163:THR:HB	2.08	0.54
7:U:150:LYS:O	7:U:157:TYR:HA	2.07	0.54
8:V:200:LYS:HE3	9:W:140:SER:O	2.07	0.54
12:Z:133:LEU:O	12:Z:136:PRO:HD2	2.08	0.54
2:B:8:TYR:CD1	2:B:8:TYR:N	2.76	0.54
11:K:112:TYR:O	11:K:119:ARG:HA	2.07	0.54
4:R:186:LEU:O	4:R:190:GLU:HG3	2.07	0.54
12:Z:123:GLN:HG3	12:Z:145:TYR:OH	2.08	0.54
5:E:76:LEU:HD23	5:E:76:LEU:C	2.28	0.54
7:G:184(G):GLU:HG2	7:G:188:LYS:CB	2.38	0.54
12:Z:43:MET:CB	12:Z:101:ILE:HG22	2.38	0.54
12:Z:129:ALA:HB1	12:Z:166:HIS:CE1	2.43	0.54
5:E:49:VAL:HG13	5:E:212:ILE:HG12	1.89	0.54
8:H:15:ALA:HA	8:H:174:ASP:O	2.08	0.54
2:P:40:ILE:HD12	2:P:193:ALA:HB2	1.90	0.54
3:Q:43:LYS:O	3:Q:43:LYS:HG2	2.06	0.54
5:S:139:ILE:HG22	5:S:148:LEU:HD13	1.90	0.54
5:S:148:LEU:CD2	5:S:162:GLY:HA2	2.38	0.54
5:S:161:TYR:CE2	6:T:60:VAL:HA	2.43	0.54
8:V:34:LEU:HB2	17:V:376:HOH:O	2.08	0.54
8:H:123:TYR:HB3	8:H:142:TRP:CZ2	2.43	0.53
3:Q:159:SER:O	4:R:59:LEU:HD22	2.07	0.53
7:U:108:PRO:HB3	7:U:142:ASP:OD1	2.09	0.53
12:Z:109:ALA:HA	17:Z:306:HOH:O	2.07	0.53
7:G:79:ASN:OD1	7:G:165:THR:HB	2.08	0.53
7:G:184(G):GLU:HG2	7:G:188:LYS:HB3	1.89	0.53
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.41	0.53
1:O:108:PRO:HG2	1:O:111:LEU:HB2	1.91	0.53
5:S:66:LYS:HA	5:S:78:LEU:HD21	1.90	0.53
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.90	0.53
10:X:2:ILE:O	10:X:16:SER:HA	2.08	0.53
11:Y:100:MET:HA	11:Y:111:TYR:O	2.08	0.53
1:A:27:ALA:O	1:A:31:VAL:HG23	2.09	0.53
4:D:123(D):ALA:HA	5:E:129:GLY:HA2	1.90	0.53
7:G:158:VAL:HG22	7:G:159:GLY:N	2.24	0.53
10:J:6:ILE:HD11	10:J:142:TYR:CE1	2.42	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:136:PHE:O	2:P:150:THR:HA	2.09	0.53
7:U:55:PRO:HG2	7:U:56:ASP:H	1.74	0.53
3:C:93:ARG:O	3:C:96:ALA:HB3	2.09	0.53
4:D:237:LEU:HD22	4:D:241:GLU:HG3	1.90	0.53
4:D:39:GLY:HA2	4:D:47:VAL:O	2.09	0.53
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.39	0.53
3:Q:168:ASN:HB2	3:Q:200:VAL:HG11	1.91	0.53
1:A:130:ARG:HG3	1:A:130:ARG:NH1	2.23	0.53
2:B:39:GLY:HA2	2:B:47:VAL:O	2.09	0.53
2:P:185:LYS:HD3	2:P:187:ASP:N	2.23	0.53
11:Y:142:TYR:O	11:Y:143:LYS:HD2	2.07	0.53
13:1:112:TYR:O	13:1:119:THR:HA	2.09	0.53
2:B:40:ILE:HD12	2:B:193:ALA:HB2	1.90	0.53
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.91	0.53
3:C:49:GLY:HA3	3:C:212:ILE:HD13	1.90	0.53
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.90	0.53
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.91	0.53
1:O:14:THR:O	1:O:21:LEU:HD23	2.09	0.53
3:Q:28:LEU:O	3:Q:31:VAL:HB	2.09	0.53
4:D:130:ARG:HG3	4:D:130:ARG:HH11	1.73	0.53
13:M:7:LYS:HD2	13:M:141(G):ILE:HD13	1.89	0.53
1:O:125:GLN:HG3	2:P:130:ARG:HG2	1.91	0.53
5:S:68:ILE:HB	5:S:76:LEU:CD2	2.39	0.53
6:T:90:ASN:O	6:T:94:GLU:HG3	2.09	0.53
10:X:129:TYR:O	10:X:132:PHE:HB2	2.09	0.53
2:B:108:PRO:HB2	2:B:111:ILE:HG13	1.91	0.52
5:E:48:LEU:HD13	5:E:77:SER:HB3	1.90	0.52
8:V:114:HIS:HD2	17:V:410:HOH:O	1.92	0.52
10:X:15:ALA:HB2	10:X:155:LEU:HD13	1.90	0.52
14:2:31:THR:HG22	14:2:32:ASP:N	2.23	0.52
3:C:52:ARG:HD2	3:C:208:LYS:O	2.09	0.52
12:L:5:GLY:O	12:L:124:CYS:HA	2.09	0.52
12:L:29:ARG:NH1	12:L:193:ARG:HB3	2.24	0.52
8:V:123:TYR:HB3	8:V:142:TRP:CZ2	2.44	0.52
3:C:152:GLU:HG2	3:C:156:ILE:HG22	1.90	0.52
12:L:134:ILE:HG23	12:L:158:SER:HB3	1.90	0.52
1:O:221:PHE:C	1:O:221:PHE:CD2	2.82	0.52
5:S:31:ILE:HD11	5:S:153:PRO:HD2	1.90	0.52
5:S:160:LEU:HD13	5:S:163:THR:HB	1.91	0.52
7:U:69:CYS:O	7:U:93:LYS:HE2	2.08	0.52
13:1:37:VAL:HG11	13:1:79:ILE:HD13	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HG2	2:B:58:LEU:HD13	1.91	0.52
3:C:71:ASP:HA	10:J:68:ILE:HD11	1.92	0.52
3:C:195:ARG:HG3	3:C:236:ILE:HD13	1.91	0.52
5:E:130:ARG:HG3	5:E:130:ARG:NH1	2.20	0.52
5:E:226:GLY:O	5:E:229:VAL:HG22	2.09	0.52
2:P:76:VAL:CG1	2:P:138:TYR:CD2	2.92	0.52
2:P:130:ARG:HG3	2:P:130:ARG:NH1	2.23	0.52
7:U:109:CYS:HB3	17:U:402:HOH:O	2.09	0.52
10:X:28:LYS:HE3	11:Y:121:LYS:O	2.10	0.52
2:P:7:ARG:HB3	2:P:8:TYR:CD1	2.45	0.52
5:S:24:VAL:O	5:S:27:ALA:HB3	2.10	0.52
6:T:192:GLN:O	6:T:196:ILE:HG13	2.09	0.52
8:V:41:ILE:HA	8:V:103:GLY:HA3	1.90	0.52
11:Y:1:THR:CG2	11:Y:2:THR:N	2.73	0.52
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.74	0.52
4:R:65:GLU:HA	17:R:345:HOH:O	2.10	0.52
3:C:100:ARG:HH11	3:C:106:PRO:HB3	1.74	0.52
1:O:69:LEU:C	1:O:69:LEU:HD23	2.29	0.52
2:P:4:GLY:HA3	5:S:127:TYR:HE1	1.73	0.52
3:Q:52:ARG:NH2	3:Q:211:GLU:HB3	2.24	0.52
8:V:126:SER:O	8:V:127:LEU:HD23	2.09	0.52
3:C:106:PRO:HG2	3:C:143:PRO:HG3	1.91	0.52
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.92	0.52
7:G:180(B):ASP:O	7:G:180(C):HIS:HB3	2.09	0.52
14:N:14:LEU:O	14:N:175:MET:HA	2.09	0.52
2:P:67:LEU:HD22	2:P:211:GLU:HB3	1.91	0.52
2:P:100:LEU:O	2:P:104:ASN:N	2.40	0.52
6:T:24:VAL:O	6:T:27:ALA:HB3	2.10	0.52
8:V:1:THR:HA	8:V:33:LYS:HZ3	1.74	0.52
9:I:12:VAL:HG23	9:I:178:ILE:HB	1.90	0.52
9:W:156:SER:O	9:W:160:LEU:HB2	2.10	0.52
12:Z:8:GLY:HA3	12:Z:11:PHE:CE2	2.45	0.52
5:S:49:VAL:HG13	5:S:212:ILE:HG12	1.91	0.52
6:T:194:ALA:O	6:T:198:TYR:HD1	1.93	0.52
10:X:105(B):LYS:HB2	10:X:105(B):LYS:NZ	2.25	0.52
11:Y:41:LEU:HD23	11:Y:103:GLY:HA3	1.91	0.52
13:1:10:ASN:ND2	13:1:180:LYS:HE2	2.25	0.52
5:E:49:VAL:CG1	5:E:210:LEU:HD11	2.40	0.51
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.40	0.51
2:P:181:LYS:O	2:P:184:MET:HG3	2.10	0.51
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.39	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:1:GLY:HA3	9:W:33:LYS:HE2	1.91	0.51
14:2:84:LYS:CE	14:2:119:VAL:HG23	2.40	0.51
5:E:123:ASN:N	5:E:123:ASN:HD22	2.08	0.51
10:J:2:ILE:O	10:J:3:ILE:HD13	2.10	0.51
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.25	0.51
4:R:97:VAL:HG21	11:Y:65:LEU:CD1	2.40	0.51
13:1:163:TYR:HA	13:1:169:SER:OG	2.10	0.51
4:D:117:CYS:SG	4:D:157:PHE:HB3	2.50	0.51
5:E:103:PHE:CE2	13:M:62:LEU:HD21	2.42	0.51
12:L:43:MET:CB	12:L:101:ILE:HG22	2.41	0.51
12:L:90:LYS:HD3	12:L:95:TYR:CZ	2.44	0.51
13:M:35:ILE:HD13	13:M:56:GLU:HG2	1.90	0.51
4:R:194:LEU:HD22	4:R:212:LEU:HD11	1.91	0.51
14:2:163:ILE:HG23	14:2:170:GLY:HA2	1.92	0.51
1:A:15:PHE:HD2	2:B:23:GLN:NE2	2.09	0.51
3:C:70:ILE:HG21	3:C:112:LEU:HD21	1.90	0.51
4:D:215:ILE:CG2	4:D:221:PHE:HD2	2.21	0.51
5:E:162:GLY:O	5:E:163:THR:HB	2.10	0.51
4:R:194:LEU:HD12	4:R:207:LEU:HD11	1.91	0.51
6:T:28:VAL:O	6:T:31:VAL:HB	2.11	0.51
3:C:49:GLY:CA	3:C:212:ILE:HD13	2.40	0.51
8:H:4:VAL:HG22	8:H:159:ILE:HD11	1.91	0.51
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.93	0.51
11:K:5:ALA:HA	11:K:13:ILE:O	2.11	0.51
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.45	0.51
1:O:15:PHE:H	2:P:23:GLN:HE22	1.59	0.51
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.92	0.51
4:R:163:LYS:HG3	4:R:164:ALA:N	2.26	0.51
4:R:214:CYS:SG	4:R:224:TYR:HE2	2.25	0.51
9:W:45:ILE:HG22	9:W:52:VAL:HG22	1.92	0.51
11:Y:137:VAL:HG21	11:Y:161:ALA:HB2	1.93	0.51
10:J:52:THR:CG2	10:J:53:VAL:N	2.73	0.51
3:Q:33:ARG:HB3	3:Q:33:ARG:NH1	2.26	0.51
5:E:15:PHE:HB2	6:F:23:GLN:NE2	2.25	0.51
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.92	0.51
10:J:15:ALA:HB2	10:J:155:LEU:HD13	1.92	0.51
11:K:6:PHE:HA	11:K:123:ASP:O	2.10	0.51
5:S:180(C):PHE:CD1	5:S:180(D):ILE:N	2.79	0.51
7:U:218:ASP:O	7:U:220:LYS:HB2	2.11	0.51
9:W:160:LEU:HD12	9:W:191:MET:HE3	1.93	0.51
10:X:4:LEU:HD21	10:X:134:THR:HG21	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:ALA:O	2:B:175:LEU:HG	2.10	0.51
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.45	0.51
5:E:51:LEU:O	5:E:66:LYS:HE2	2.10	0.51
10:X:2:ILE:O	10:X:3:ILE:HD13	2.11	0.51
8:H:35:HIS:CB	8:H:56:THR:HG21	2.41	0.51
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.93	0.51
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.93	0.51
2:P:205:LEU:HG	2:P:210:LEU:HD11	1.93	0.51
3:Q:93:ARG:O	3:Q:96:ALA:HB3	2.11	0.51
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.93	0.51
17:E:304:HOH:O	6:F:12:ASN:HB2	2.10	0.51
7:G:151:THR:HA	7:G:156:TYR:O	2.11	0.51
10:J:155:LEU:O	10:J:159:VAL:HG23	2.11	0.51
14:N:114:PRO:HD2	14:N:118:SER:O	2.11	0.51
2:P:113:VAL:HG22	2:P:138:TYR:CD1	2.46	0.51
5:S:132:TYR:O	5:S:153:PRO:HB3	2.10	0.51
8:V:1:THR:HG21	8:V:46:ALA:CB	2.41	0.51
14:2:114:PRO:HD2	14:2:118:SER:O	2.11	0.51
2:B:7:ARG:HB3	2:B:8:TYR:CE1	2.45	0.50
2:B:71:ASN:ND2	2:B:72:ASP:N	2.58	0.50
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.91	0.50
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.93	0.50
11:Y:15:ALA:HA	11:Y:174:ASN:O	2.10	0.50
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.92	0.50
7:G:55:PRO:HG2	7:G:56:ASP:H	1.76	0.50
8:H:124:TYR:HD2	8:H:138:LEU:HD13	1.76	0.50
11:K:1:THR:HG23	11:K:33:LYS:NZ	2.26	0.50
5:S:47:VAL:HG23	5:S:189:LEU:HD13	1.92	0.50
13:1:45:ILE:HG23	13:1:99:ILE:HG12	1.93	0.50
13:1:157:ASN:HD22	13:1:160:ARG:NH1	2.07	0.50
3:C:47:VAL:O	3:C:48:LEU:HD23	2.12	0.50
5:E:47:VAL:HG12	5:E:48:LEU:N	2.26	0.50
12:L:11:PHE:HA	12:L:178:VAL:O	2.11	0.50
14:N:187(D):PRO:HA	14:N:187(G):TYR:CE2	2.47	0.50
1:O:100:TYR:CE1	1:O:107:PRO:HA	2.46	0.50
4:R:125:GLU:HG2	4:R:127:LEU:HD13	1.93	0.50
8:V:197:ARG:NH2	9:W:139:GLU:O	2.44	0.50
11:Y:128:GLY:O	11:Y:131:GLN:HG2	2.10	0.50
1:A:217(B):ASN:CB	1:A:217(F):LEU:HD12	2.41	0.50
2:B:81:LEU:H	2:B:81:LEU:CD2	2.25	0.50
10:J:36:GLN:HG3	10:J:184:ILE:CD1	2.41	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:85:GLN:O	10:J:89:LYS:HG3	2.10	0.50
6:T:54:ILE:HG13	6:T:208:PHE:HA	1.92	0.50
8:H:1:THR:HA	8:H:33:LYS:HZ3	1.74	0.50
9:I:51:ASP:OD1	10:J:90(B):ARG:NH2	2.45	0.50
4:R:14:THR:HG22	5:S:23:GLN:NE2	2.27	0.50
10:X:6:ILE:HD12	10:X:7:ARG:N	2.26	0.50
14:2:148:LYS:O	14:2:152:VAL:HG23	2.12	0.50
5:E:139:ILE:HG22	5:E:148:LEU:HD13	1.92	0.50
8:H:1:THR:HA	8:H:33:LYS:HZ2	1.75	0.50
9:I:20:LEU:HB3	9:I:28:SER:HB3	1.94	0.50
9:I:113:PHE:N	9:I:113:PHE:CD2	2.79	0.50
14:N:142:PHE:HB2	14:N:154:PHE:CZ	2.47	0.50
3:Q:152:GLU:HG2	3:Q:156:ILE:HG22	1.93	0.50
4:R:130:ARG:HG3	4:R:130:ARG:HH11	1.77	0.50
11:Y:159:ILE:CG2	11:Y:173:VAL:HG22	2.42	0.50
2:B:130:ARG:HG3	2:B:130:ARG:HH11	1.76	0.50
5:E:31:ILE:HD11	5:E:153:PRO:HD2	1.93	0.50
8:H:114:HIS:HD2	17:H:470:HOH:O	1.95	0.50
11:K:200:LYS:HG3	11:K:205:SER:O	2.12	0.50
1:O:136:LEU:O	1:O:150:GLN:HA	2.11	0.50
5:S:198:SER:HA	5:S:201:LEU:CD1	2.41	0.50
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.93	0.50
14:2:107:LYS:HG2	14:2:108:GLY:H	1.76	0.50
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.77	0.50
2:B:230:LYS:O	2:B:234:VAL:HG23	2.12	0.50
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.75	0.50
12:L:113:PHE:CD2	12:L:119:TYR:HB3	2.47	0.50
1:O:13:THR:O	2:P:130:ARG:HD3	2.11	0.50
2:B:172:ALA:HB2	2:B:200:THR:HG21	1.93	0.49
5:E:48:LEU:HD13	5:E:77:SER:CB	2.42	0.49
8:H:5:GLY:O	8:H:124:TYR:HA	2.12	0.49
1:O:17:PRO:HG3	2:P:26:TYR:CE2	2.47	0.49
2:P:163:ILE:HG13	2:P:164:SER:N	2.26	0.49
6:T:179:LEU:HD11	6:T:196:ILE:HD11	1.92	0.49
6:T:192:GLN:HE21	6:T:192:GLN:HA	1.77	0.49
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.12	0.49
4:D:70:ILE:HB	4:D:74:ILE:HG22	1.93	0.49
11:Y:8:PHE:CE2	11:Y:13:ILE:HG12	2.47	0.49
2:B:81:LEU:HD22	2:B:81:LEU:N	2.27	0.49
2:B:141:TYR:HA	2:B:145:GLY:O	2.12	0.49
2:B:185:LYS:HD3	2:B:187:ASP:H	1.75	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:ILE:O	4:D:149:PHE:N	2.45	0.49
5:E:148:LEU:CD2	5:E:162:GLY:HA2	2.41	0.49
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.93	0.49
9:I:36:HIS:HB3	9:I:42:PHE:CE2	2.47	0.49
12:L:144(Q):LYS:HG2	12:L:145:TYR:N	2.26	0.49
1:O:24:ILE:HD11	1:O:124:THR:HG23	1.93	0.49
2:B:168:ASN:ND2	2:B:200:THR:O	2.44	0.49
5:E:148:LEU:HD23	5:E:162:GLY:HA2	1.94	0.49
11:K:105(B):LYS:H	11:K:105(B):LYS:CD	2.21	0.49
11:K:137:VAL:HG21	11:K:161:ALA:CB	2.43	0.49
14:N:32:ASP:OD1	13:1:204:LYS:HA	2.12	0.49
1:O:118:LYS:O	1:O:122:GLU:HG3	2.12	0.49
6:T:139:GLY:HA3	6:T:147:HIS:O	2.12	0.49
12:Z:140:ASN:O	12:Z:144:PHE:HA	2.12	0.49
12:Z:178:VAL:HG22	12:Z:184:VAL:HG22	1.94	0.49
1:A:15:PHE:H	2:B:23:GLN:HE22	1.61	0.49
1:O:130:ARG:NH1	1:O:131:PRO:O	2.45	0.49
12:Z:177:ILE:HD12	12:Z:177:ILE:N	2.28	0.49
5:E:176:LEU:HD22	5:E:180(C):PHE:CE2	2.47	0.49
7:G:179:HIS:NE2	7:G:192:PHE:HE2	2.11	0.49
7:G:186:TRP:O	7:G:190:VAL:HG23	2.12	0.49
11:K:165:ARG:HH22	11:K:208:ASN:ND2	2.09	0.49
14:N:31:THR:HG22	14:N:32:ASP:N	2.28	0.49
1:O:112:LEU:O	1:O:116:VAL:HG23	2.13	0.49
3:Q:52:ARG:HD2	3:Q:208:LYS:O	2.11	0.49
9:W:48:LEU:HG	9:W:50:THR:HG22	1.95	0.49
1:A:228:GLU:O	1:A:232:ARG:NH1	2.46	0.49
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.43	0.49
12:L:180:LYS:HG3	12:L:182:ASP:OD1	2.13	0.49
6:T:160:TYR:HB3	6:T:162:GLY:O	2.12	0.49
8:V:93:GLY:HA2	8:V:115:ALA:O	2.13	0.49
9:W:12:VAL:CG2	9:W:178:ILE:HB	2.42	0.49
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.94	0.49
13:M:63:VAL:HG22	13:M:74:LEU:HD12	1.94	0.49
14:N:6:VAL:C	14:N:12:VAL:HG23	2.33	0.49
6:T:238:LYS:NZ	6:T:239:GLU:HG3	2.27	0.49
8:V:35:HIS:CB	8:V:56:THR:HG21	2.42	0.49
6:F:203:GLU:C	6:F:205:ASN:H	2.15	0.49
9:I:123:ASP:HB2	9:I:124:PHE:CD2	2.47	0.49
10:J:-1:MET:HG2	10:J:1:ASP:N	2.27	0.49
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.13	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:55:THR:O	3:Q:56:LEU:HD13	2.13	0.49
4:R:52:LYS:HG3	4:R:64:ILE:CG2	2.43	0.49
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.94	0.49
3:C:47:VAL:HG23	3:C:189:CYS:SG	2.53	0.49
7:G:180(D):ILE:N	7:G:180(D):ILE:HD13	2.27	0.49
12:Z:109:ALA:HB2	12:Z:121:ARG:NH2	2.28	0.49
6:F:141:VAL:HG23	6:F:215:CYS:SG	2.52	0.48
10:J:52:THR:HG22	10:J:53:VAL:H	1.78	0.48
14:N:84:LYS:HD3	17:N:375:HOH:O	2.13	0.48
3:Q:163:GLN:HE21	3:Q:164:THR:N	2.05	0.48
5:S:66:LYS:O	5:S:77:SER:HA	2.12	0.48
11:Y:1:THR:HG23	11:Y:33:LYS:NZ	2.28	0.48
2:B:15:PHE:H	3:C:23:GLN:NE2	2.09	0.48
3:C:101:LEU:HD11	10:J:57:GLU:HB3	1.96	0.48
11:K:4:LEU:HD23	11:K:6:PHE:HD2	1.77	0.48
9:W:152:PHE:HB2	9:W:177:ILE:HD11	1.94	0.48
12:L:123:GLN:HG3	12:L:145:TYR:OH	2.14	0.48
14:N:19:ARG:NH1	14:N:169:SER:O	2.46	0.48
13:1:4:ILE:CD1	13:1:159:MET:SD	3.01	0.48
14:2:1:THR:O	14:2:129:SER:N	2.47	0.48
14:2:4:MET:HG2	14:2:159:LEU:HD21	1.95	0.48
5:E:40:LEU:N	5:E:40:LEU:HD23	2.29	0.48
12:L:134:ILE:HG22	12:L:138:LEU:HD22	1.96	0.48
13:M:41:THR:HG21	13:M:79:ILE:HD12	1.95	0.48
6:T:159:GLY:HA3	7:U:63:THR:HG21	1.96	0.48
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	1.94	0.48
10:X:13:ILE:HG12	10:X:177:ILE:HG23	1.95	0.48
12:Z:18:THR:HG21	12:Z:30:TYR:CD1	2.46	0.48
12:Z:42:VAL:CG1	12:Z:176:LEU:HD23	2.44	0.48
13:1:57:ARG:HH11	13:1:57:ARG:HG2	1.77	0.48
13:1:158:ALA:O	13:1:162:LEU:HG	2.14	0.48
5:E:132:TYR:O	5:E:153:PRO:HB3	2.13	0.48
7:G:48:VAL:C	7:G:49:ILE:HD12	2.33	0.48
8:H:160:GLN:O	8:H:164:TRP:CD1	2.66	0.48
9:I:14:ILE:HG23	9:I:34:ILE:HD13	1.95	0.48
3:Q:100:ARG:HH11	3:Q:106:PRO:HB3	1.78	0.48
8:V:12:VAL:HG11	8:V:102:ALA:HB1	1.96	0.48
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.34	0.48
14:2:6:VAL:HG13	14:2:124:TYR:HB3	1.95	0.48
6:F:109:ILE:HB	6:F:110:PRO:HD3	1.94	0.48
7:G:136:LEU:O	7:G:150:LYS:HA	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:15:ALA:HB1	12:L:173:LEU:HD11	1.94	0.48
3:Q:109:VAL:HG21	3:Q:147:LYS:HB2	1.96	0.48
8:V:164:TRP:HA	8:V:164:TRP:CE3	2.49	0.48
5:E:48:LEU:O	5:E:212:ILE:HA	2.12	0.48
6:F:35:THR:CG2	6:F:36:THR:N	2.76	0.48
7:G:46:THR:OG1	7:G:146:PRO:HB3	2.14	0.48
11:K:45:MET:HB3	11:K:52:CYS:HB3	1.95	0.48
14:2:55:ILE:O	14:2:59:VAL:HG23	2.14	0.48
4:D:163:LYS:HG3	4:D:164:ALA:N	2.29	0.48
5:E:13:VAL:HG13	5:E:13:VAL:O	2.13	0.48
6:F:136:THR:O	6:F:150:MET:HA	2.14	0.48
13:M:139:ARG:HH11	8:V:165:ASN:ND2	2.12	0.48
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.13	0.48
10:X:10:ASP:HB3	17:X:283:HOH:O	2.13	0.48
6:F:147:HIS:HD2	17:F:449:HOH:O	1.97	0.48
14:N:9:LYS:HG3	14:N:145:ASN:HB3	1.96	0.48
3:Q:35:THR:HB	3:Q:51:GLU:CG	2.37	0.48
13:1:-5:PRO:HD3	13:1:96:TRP:CD2	2.49	0.48
14:2:6:VAL:C	14:2:12:VAL:HG23	2.34	0.48
1:A:186:LEU:O	1:A:190:ILE:HG13	2.13	0.48
4:D:215:ILE:HA	4:D:220:GLY:O	2.14	0.48
12:L:192:LYS:HE3	8:V:195:ASN:HB3	1.96	0.48
14:N:8:PHE:HE1	14:N:10:ASP:HB2	1.72	0.48
14:N:84:LYS:HB2	14:N:119:VAL:HG21	1.95	0.48
1:O:111:LEU:O	1:O:114:SER:HB3	2.13	0.48
8:V:55:VAL:HG23	8:V:86:HIS:CD2	2.49	0.48
10:X:112:GLN:NE2	10:X:126:ALA:H	2.11	0.48
14:2:146:MET:HE3	14:2:150:GLU:HB3	1.96	0.48
1:A:130:ARG:HG2	7:G:125:GLN:HG3	1.96	0.47
3:C:41:LYS:HG2	3:C:161:SER:O	2.15	0.47
14:N:4:MET:SD	14:N:159:LEU:CD2	3.02	0.47
1:O:20:LYS:HD2	17:O:348:HOH:O	2.13	0.47
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.78	0.47
2:P:125:GLN:HG3	3:Q:130:ARG:HG2	1.96	0.47
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.95	0.47
3:Q:186:VAL:HG21	3:Q:216:LYS:HE2	1.96	0.47
8:V:112:SER:OG	8:V:120:ASP:HB2	2.14	0.47
9:W:137:MET:CE	9:W:161:ASN:HB2	2.44	0.47
1:A:79:SER:HA	17:A:317:HOH:O	2.13	0.47
6:F:130:ARG:HG3	6:F:130:ARG:HH11	1.78	0.47
6:F:238:LYS:NZ	6:F:239:GLU:HG3	2.29	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:79:ASN:HA	17:G:433:HOH:O	2.14	0.47
3:Q:36:CYS:N	3:Q:51:GLU:HG2	2.29	0.47
3:Q:53:ARG:HG2	3:Q:54:SER:N	2.28	0.47
3:Q:152:GLU:CG	3:Q:156:ILE:HG22	2.43	0.47
5:S:41:ARG:NH1	5:S:42:SER:O	2.45	0.47
6:T:21:ASN:HB2	17:T:338:HOH:O	2.14	0.47
2:B:120:LYS:HZ1	2:B:136:PHE:HD1	1.60	0.47
6:F:192:GLN:HE21	6:F:192:GLN:HA	1.79	0.47
9:I:101:VAL:O	9:I:110:ILE:HA	2.14	0.47
12:L:19:ARG:HD2	12:L:168:GLN:O	2.14	0.47
13:M:40:ASN:H	13:M:40:ASN:ND2	2.12	0.47
4:R:32:LYS:O	4:R:167:SER:HA	2.14	0.47
8:V:103:GLY:HA2	8:V:178:MET:SD	2.54	0.47
13:1:104:VAL:HG23	13:1:178:ILE:HG22	1.97	0.47
2:B:112:LEU:HD23	2:B:112:LEU:C	2.35	0.47
3:C:169:SER:HA	3:C:172:VAL:HG12	1.96	0.47
4:D:160:TYR:CD2	5:E:59:SER:HB3	2.49	0.47
2:P:194:LEU:HG	2:P:212:PHE:CZ	2.49	0.47
7:U:179:HIS:NE2	7:U:192:PHE:HE2	2.12	0.47
10:X:140:HIS:HD2	10:X:141:HIS:CE1	2.32	0.47
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.50	0.47
9:I:93:GLY:N	9:I:94:PRO:CD	2.78	0.47
9:I:115:LEU:N	9:I:115:LEU:HD23	2.29	0.47
9:I:156:SER:O	9:I:160:LEU:HB2	2.15	0.47
11:K:33:LYS:HE2	15:3:5:04D:H23	1.96	0.47
12:L:136:PRO:HB2	9:W:137:MET:SD	2.54	0.47
13:M:165:ARG:HD3	8:V:139:GLU:OE1	2.14	0.47
9:W:12:VAL:HG23	9:W:178:ILE:HB	1.95	0.47
11:Y:208:ASN:OD1	11:Y:208:ASN:O	2.33	0.47
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	1.96	0.47
13:1:-6:GLN:O	13:1:-6:GLN:HG3	2.14	0.47
2:B:134:VAL:HG12	2:B:135:SER:N	2.29	0.47
4:D:123(D):ALA:HA	5:E:129:GLY:CA	2.45	0.47
6:F:175:GLU:O	6:F:178:LYS:HB2	2.14	0.47
13:M:-6:GLN:HG3	13:M:-6:GLN:O	2.14	0.47
5:S:122:LYS:O	5:S:126:SER:HB2	2.15	0.47
6:T:191:LYS:HD3	6:T:235:PHE:CD1	2.48	0.47
9:W:49:ALA:HB3	10:X:118:THR:HG23	1.97	0.47
11:Y:2:THR:HG21	11:Y:162:ALA:HB3	1.97	0.47
11:Y:126:CYS:HB2	11:Y:135:TYR:CE1	2.50	0.47
13:1:112:TYR:CD2	13:1:120:TYR:CZ	3.03	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:ARG:NE	3:C:33:ARG:HH21	2.13	0.47
2:B:78:VAL:HG12	2:B:79:ALA:N	2.29	0.47
2:B:229:ILE:O	2:B:232:ILE:HG22	2.14	0.47
3:C:163:GLN:HE21	3:C:164:THR:N	2.04	0.47
4:D:195:LYS:HA	4:D:237:LEU:HD11	1.97	0.47
5:E:207:LEU:H	5:E:207:LEU:CD2	2.28	0.47
6:F:89:VAL:O	6:F:93:ARG:HG3	2.14	0.47
7:G:77:VAL:HG13	7:G:137:THR:HB	1.95	0.47
8:H:159:ILE:O	8:H:163:ILE:HG13	2.14	0.47
9:I:-2:ASN:HB3	9:I:20:LEU:HD22	1.95	0.47
9:I:55:LEU:HD21	9:I:95:TYR:CE1	2.49	0.47
9:I:115:LEU:HD23	9:I:115:LEU:H	1.79	0.47
10:J:4:LEU:HD23	10:J:126:ALA:HB2	1.96	0.47
11:K:195:LEU:O	11:K:199:VAL:HG23	2.15	0.47
3:Q:41:LYS:HG2	3:Q:161:SER:O	2.15	0.47
5:S:48:LEU:HG	5:S:139:ILE:HD13	1.96	0.47
5:S:143:LYS:HE3	13:1:78:TYR:OH	2.14	0.47
6:T:35:THR:CG2	6:T:36:THR:N	2.77	0.47
7:U:136:LEU:O	7:U:150:LYS:HA	2.14	0.47
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.45	0.47
8:V:162:GLY:O	8:V:166:ASP:HB3	2.15	0.47
13:1:130:GLY:O	13:1:134:ALA:HB3	2.14	0.47
3:C:185:THR:HG22	3:C:186:VAL:N	2.30	0.47
14:N:133:PHE:HA	14:2:132:THR:O	2.14	0.47
6:T:120:VAL:HG22	6:T:132:PHE:CD1	2.49	0.47
12:Z:55:LEU:HD13	12:Z:95:TYR:CD1	2.50	0.47
2:B:190:ILE:HG21	2:B:232:ILE:HG12	1.97	0.47
3:C:136:THR:O	3:C:150:GLN:HA	2.14	0.47
4:D:37:ALA:HB3	4:D:165:ILE:CG1	2.45	0.47
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.97	0.47
5:E:90:ASN:O	5:E:93:ARG:HB2	2.15	0.47
7:G:109:CYS:HB3	17:G:463:HOH:O	2.14	0.47
10:J:45:PHE:CD1	10:J:52:THR:HG23	2.50	0.47
11:Y:1:THR:HG23	11:Y:2:THR:H	1.80	0.47
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.48	0.47
12:Z:67:HIS:HD2	17:Z:329:HOH:O	1.97	0.47
13:1:141(C):ARG:HG3	13:1:141(C):ARG:NH1	2.26	0.47
14:2:52:THR:HG22	14:2:97:ALA:HB1	1.95	0.47
14:2:107:LYS:HG2	14:2:108:GLY:N	2.30	0.47
7:G:76:MET:HB2	7:G:138:PHE:CD2	2.50	0.47
10:J:36:GLN:HG3	10:J:184:ILE:HD12	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:195:LYS:O	2:P:198:SER:HB2	2.15	0.47
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.50	0.47
6:T:38:ILE:HG22	6:T:164:ALA:HB1	1.96	0.47
6:T:130:ARG:HG3	6:T:130:ARG:NH1	2.29	0.47
10:X:103:GLY:HA2	10:X:178:VAL:HG11	1.97	0.47
2:B:185:LYS:HD3	2:B:186:VAL:N	2.31	0.46
3:C:46:VAL:HG22	3:C:146:PRO:HB2	1.96	0.46
5:E:207:LEU:H	5:E:207:LEU:HD23	1.80	0.46
7:G:87:ASN:C	7:G:87:ASN:HD22	2.18	0.46
9:I:6:MET:HB2	9:I:151:LEU:HD11	1.98	0.46
13:M:18:ASN:HA	13:M:31:VAL:O	2.15	0.46
14:N:30:VAL:HG11	13:1:199:PHE:CE2	2.50	0.46
14:N:59:VAL:O	14:N:63:LEU:HG	2.16	0.46
2:P:108:PRO:HB2	2:P:111:ILE:HG13	1.96	0.46
2:P:190:ILE:HG21	2:P:232:ILE:HG12	1.97	0.46
5:S:82:ALA:O	5:S:85:ALA:HB3	2.15	0.46
9:W:14:ILE:HG12	9:W:34:ILE:CD1	2.44	0.46
9:W:59:PHE:CZ	9:W:83:VAL:HG22	2.50	0.46
11:Y:20:ALA:HB2	11:Y:31:VAL:HG21	1.96	0.46
2:B:205:LEU:O	2:B:233:LEU:HD21	2.15	0.46
6:F:24:VAL:O	6:F:27:ALA:HB3	2.15	0.46
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.97	0.46
13:M:6:MET:HG2	13:M:155:ILE:HD11	1.96	0.46
4:D:123:PHE:HA	4:D:128:MET:O	2.15	0.46
12:L:129:ALA:HB1	12:L:166:HIS:NE2	2.30	0.46
4:R:188:GLU:O	4:R:192:LEU:HD13	2.15	0.46
7:U:236:ILE:HD12	7:U:237:ALA:N	2.31	0.46
9:W:191:MET:HE3	9:W:191:MET:HB2	1.70	0.46
1:A:109:THR:O	1:A:113:VAL:HG23	2.15	0.46
7:G:139:VAL:HG12	7:G:148:ILE:HG12	1.98	0.46
8:H:135:MET:HE3	13:1:165:ARG:NH1	2.30	0.46
7:U:130:ARG:HG3	7:U:131:PRO:O	2.16	0.46
7:U:215:ALA:HB2	7:U:221:PHE:HD2	1.80	0.46
10:X:90(A):ILE:HD12	10:X:90(A):ILE:HA	1.83	0.46
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.97	0.46
14:2:14:LEU:HB3	14:2:34:LEU:HD22	1.96	0.46
5:E:143:LYS:HE3	13:M:78:TYR:OH	2.15	0.46
8:H:157:ASP:O	8:H:160:GLN:HB2	2.15	0.46
10:J:74:LEU:HD22	10:J:78:ALA:HB1	1.97	0.46
1:O:62:GLU:H	1:O:62:GLU:CD	2.18	0.46
3:Q:67:VAL:HG22	3:Q:77:SER:HB3	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:139:ALA:HA	4:R:147:GLN:O	2.16	0.46
5:S:47:VAL:HG12	5:S:48:LEU:N	2.30	0.46
6:T:167:LYS:O	6:T:170:GLN:NE2	2.48	0.46
12:Z:134:ILE:HA	17:Z:341:HOH:O	2.14	0.46
14:2:163:ILE:HD13	14:2:170:GLY:HA2	1.98	0.46
4:D:139:ALA:HB2	4:D:148:LEU:HD12	1.97	0.46
11:K:207:ASN:C	11:K:209:VAL:H	2.19	0.46
12:L:140:ASN:O	12:L:144:PHE:HA	2.16	0.46
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.97	0.46
3:Q:76:LEU:HD12	3:Q:138:ILE:HG12	1.98	0.46
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.97	0.46
5:S:48:LEU:O	5:S:212:ILE:HA	2.15	0.46
6:T:171:SER:O	6:T:174:ALA:HB3	2.16	0.46
7:U:115:ARG:O	7:U:119:LEU:HD22	2.16	0.46
9:W:13:ALA:HA	9:W:176:TYR:O	2.16	0.46
13:1:110:LEU:HD23	13:1:122:SER:O	2.15	0.46
2:B:47:VAL:HG22	2:B:214:THR:HG22	1.96	0.46
11:K:126:CYS:SG	11:K:135:TYR:CD2	3.03	0.46
3:Q:75:VAL:CG2	3:Q:215:VAL:HG11	2.45	0.46
3:Q:130:ARG:HH11	3:Q:130:ARG:CG	2.28	0.46
13:1:13:ILE:CG2	13:1:175:LEU:HD21	2.46	0.46
1:A:177:GLU:HG3	2:B:58:LEU:HD22	1.98	0.46
4:D:10:ARG:HE	4:D:10:ARG:HB2	1.55	0.46
4:D:195:LYS:O	4:D:198:LYS:HB3	2.16	0.46
5:E:198:SER:HA	5:E:201:LEU:CD1	2.45	0.46
7:G:56:ASP:HB3	7:G:59:LEU:HG	1.98	0.46
7:G:220:LYS:HG2	7:G:221:PHE:N	2.31	0.46
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.61	0.46
14:N:4:MET:SD	14:N:159:LEU:HD21	2.56	0.46
7:U:35:ILE:HG23	7:U:51:GLN:HB2	1.97	0.46
7:U:194:ILE:HG23	7:U:210:LEU:HD11	1.98	0.46
8:V:34:LEU:HD22	8:V:174:ASP:HB3	1.97	0.46
10:X:3:ILE:HG22	10:X:100:LEU:CD1	2.46	0.46
10:X:112:GLN:HE22	10:X:126:ALA:H	1.63	0.46
7:G:236:ILE:HD12	7:G:237:ALA:N	2.30	0.46
10:J:34:THR:CG2	10:J:176:LYS:HZ2	2.28	0.46
3:Q:161:SER:HB3	3:Q:180:TYR:CE1	2.51	0.46
3:Q:185:THR:HG22	3:Q:186:VAL:N	2.31	0.46
5:S:20:ARG:HB3	5:S:25:GLU:OE2	2.16	0.46
7:U:169:GLN:HG3	17:U:316:HOH:O	2.15	0.46
14:2:14:LEU:O	14:2:175:MET:HA	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:35:THR:HG22	6:F:36:THR:N	2.30	0.46
6:F:36:THR:HA	6:F:165:THR:O	2.16	0.46
8:H:6:VAL:HG11	8:H:154:LEU:HD23	1.97	0.46
10:J:133:TYR:CE2	10:J:166:MET:SD	3.09	0.46
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.98	0.46
12:L:42:VAL:CG2	12:L:102:ALA:HB3	2.46	0.46
6:T:116:LEU:HD23	6:T:116:LEU:HA	1.75	0.46
7:U:39:ALA:HB1	7:U:48:VAL:HG12	1.98	0.46
7:U:181:ASP:O	7:U:182:HIS:HB3	2.15	0.46
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.83	0.46
3:C:227:GLU:N	3:C:227:GLU:CD	2.70	0.45
5:E:12:THR:HG21	5:E:124:THR:HA	1.98	0.45
9:I:13:ALA:HA	9:I:176:TYR:O	2.15	0.45
2:P:185:LYS:HE2	2:P:187:ASP:OD1	2.15	0.45
2:P:231:ASP:O	2:P:235:LYS:HG2	2.16	0.45
3:Q:81:LEU:HB2	3:Q:84:ASP:HB2	1.98	0.45
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.98	0.45
4:R:100:ASN:HB3	17:R:353:HOH:O	2.15	0.45
14:2:13:ILE:HG23	14:2:176:VAL:O	2.16	0.45
1:A:137:LEU:HA	1:A:149:TYR:O	2.16	0.45
3:C:40:VAL:HG23	3:C:189:CYS:SG	2.56	0.45
7:G:214:VAL:HG12	7:G:215:ALA:N	2.31	0.45
11:K:153:TYR:O	11:K:156:LYS:HB3	2.17	0.45
2:P:215:ILE:HG12	2:P:221:GLN:HG2	1.98	0.45
3:Q:33:ARG:NH1	3:Q:33:ARG:CB	2.80	0.45
4:R:46:VAL:O	4:R:214:CYS:HA	2.16	0.45
7:U:48:VAL:CG1	7:U:139:VAL:HG11	2.46	0.45
10:X:52:THR:HG21	17:X:263:HOH:O	2.16	0.45
2:B:141:TYR:CD1	2:B:141:TYR:C	2.89	0.45
4:D:123(D):ALA:CA	5:E:129:GLY:HA2	2.45	0.45
5:E:125:GLN:HG3	6:F:130:ARG:HG2	1.98	0.45
10:J:6:ILE:HD11	10:J:142:TYR:HE1	1.82	0.45
11:K:1:THR:CG2	11:K:2:THR:N	2.79	0.45
12:L:21:ILE:C	12:L:21:ILE:HD12	2.36	0.45
14:N:167:GLY:O	13:1:167:ALA:HB1	2.17	0.45
4:R:195:LYS:O	4:R:198:LYS:HB3	2.15	0.45
5:S:15:PHE:CD1	5:S:21:LEU:HD21	2.51	0.45
7:U:8:TYR:C	7:U:10:ARG:H	2.20	0.45
7:U:130:ARG:HG3	7:U:130:ARG:HH11	1.82	0.45
10:X:36:GLN:HG3	10:X:184:ILE:CD1	2.47	0.45
3:C:125:GLN:HG3	3:C:125:GLN:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:-6:PRO:HB2	13:M:91:ARG:NH1	2.31	0.45
12:L:114:ASP:HB2	15:3:3:ILE:HD12	1.97	0.45
14:N:4:MET:CB	14:N:126:ILE:HG22	2.46	0.45
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.65	0.45
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.98	0.45
4:R:146:TYR:HE1	4:R:216:THR:HA	1.80	0.45
8:V:10:ASN:OD1	8:V:180:ILE:HD12	2.16	0.45
12:Z:88:TYR:CD1	12:Z:88:TYR:O	2.69	0.45
13:1:40:ASN:H	13:1:40:ASN:HD22	1.64	0.45
6:F:186:ALA:O	6:F:190:VAL:HG23	2.16	0.45
8:V:221:ILE:HG13	9:W:40:HIS:HA	1.99	0.45
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.51	0.45
12:L:70:HIS:HE1	17:L:355:HOH:O	2.00	0.45
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.65	0.45
2:P:218:ASN:O	2:P:218(B):ASP:HB2	2.17	0.45
4:R:160:TYR:CZ	4:R:163:LYS:HD3	2.52	0.45
5:S:64:GLN:HA	17:S:345:HOH:O	2.16	0.45
6:T:35:THR:HG22	6:T:36:THR:N	2.31	0.45
17:T:347:HOH:O	13:1:67:ALA:HB3	2.17	0.45
7:U:29:LYS:HA	7:U:29:LYS:HD2	1.58	0.45
8:V:1:THR:HA	8:V:33:LYS:NZ	2.30	0.45
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.99	0.45
9:W:55:LEU:HD21	9:W:95:TYR:CE1	2.52	0.45
10:X:77:GLN:NE2	10:X:77:GLN:C	2.70	0.45
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.99	0.45
8:H:1:THR:HG23	8:H:33:LYS:NZ	2.32	0.45
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.32	0.45
14:N:83:PHE:HB3	14:N:113:ILE:HD13	1.99	0.45
14:N:161:GLN:HE22	14:2:139:ASP:HB3	1.82	0.45
6:T:137:ILE:HA	6:T:149:TYR:O	2.16	0.45
6:T:195:LYS:O	6:T:198:TYR:N	2.49	0.45
10:X:7:ARG:O	10:X:7:ARG:HG2	2.16	0.45
11:Y:70:GLU:O	11:Y:71:LYS:HB2	2.16	0.45
12:Z:109:ALA:HB2	12:Z:121:ARG:HH21	1.82	0.45
1:A:40:ILE:HD11	1:A:193:ALA:HA	1.98	0.45
5:E:74:MET:HE1	5:E:109:VAL:HA	1.99	0.45
6:F:187:ARG:HG3	6:F:187:ARG:HH11	1.82	0.45
8:H:112:SER:OG	8:H:120:ASP:HB2	2.17	0.45
11:K:99:THR:HA	17:K:432:HOH:O	2.17	0.45
13:M:133:MET:C	13:M:136:PRO:HD2	2.37	0.45
3:Q:134:VAL:HG12	3:Q:135:SER:N	2.30	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:198:LEU:HD12	3:Q:236:ILE:HG21	1.99	0.45
4:R:112:LEU:HD13	4:R:112:LEU:C	2.37	0.45
11:Y:132:THR:HA	17:Y:337:HOH:O	2.17	0.45
12:Z:137:PHE:CE1	12:Z:141:GLN:CG	2.99	0.45
2:B:81:LEU:HD23	2:B:133:GLY:CA	2.47	0.45
10:J:24:ILE:HD11	10:X:129:TYR:HB3	1.98	0.45
1:O:130:ARG:HG3	1:O:130:ARG:NH1	2.27	0.45
5:S:66:LYS:HA	5:S:78:LEU:CD2	2.47	0.45
6:T:37:SER:HB3	6:T:50:VAL:CG2	2.34	0.45
7:U:214:VAL:HG12	7:U:215:ALA:N	2.31	0.45
14:2:175:MET:HE3	14:2:187(B):PHE:CE2	2.52	0.45
2:B:141:TYR:CD1	2:B:142:ASP:N	2.85	0.45
6:F:68:GLN:OE1	6:F:89:VAL:HG21	2.17	0.45
6:F:90:ASN:O	6:F:94:GLU:HG3	2.17	0.45
12:L:114:ASP:HB3	12:L:118:SER:HB3	1.99	0.45
12:L:166:HIS:HD2	12:L:168:GLN:H	1.64	0.45
1:O:197:LEU:HD23	1:O:210:ILE:HG23	1.99	0.45
4:R:215:ILE:CG2	4:R:221:PHE:HD2	2.27	0.45
17:S:327:HOH:O	6:T:12:ASN:HB2	2.15	0.45
12:Z:180:LYS:HG2	17:Z:265:HOH:O	2.16	0.45
13:1:160:ARG:HG3	13:1:192:VAL:HG11	1.99	0.45
2:B:24:VAL:HG11	2:B:154:SER:HB3	1.99	0.44
3:C:186:VAL:O	3:C:190:VAL:HG23	2.17	0.44
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.52	0.44
9:I:33:LYS:O	9:I:44:GLY:HA2	2.17	0.44
10:J:53:VAL:HG21	17:K:474:HOH:O	2.16	0.44
11:K:133:PHE:CE2	11:K:166:ASP:HB2	2.52	0.44
12:L:165:ARG:NH1	9:W:135:PHE:CE1	2.85	0.44
13:M:114:ASN:O	13:M:116:LEU:N	2.50	0.44
2:P:144:ARG:O	2:P:144:ARG:HG2	2.16	0.44
4:R:70:ILE:HB	4:R:74:ILE:HG22	2.00	0.44
1:A:134:VAL:O	1:A:153:PRO:HG3	2.17	0.44
1:A:221:PHE:C	1:A:221:PHE:CD2	2.89	0.44
4:D:214:CYS:SG	4:D:224:TYR:HE2	2.30	0.44
5:E:122:LYS:O	5:E:126:SER:HB2	2.17	0.44
13:M:40:ASN:H	13:M:40:ASN:HD22	1.66	0.44
2:P:161:LYS:HE3	3:Q:59:GLN:O	2.17	0.44
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.99	0.44
12:Z:144(R):LYS:CG	12:Z:145:TYR:N	2.81	0.44
13:1:32:GLU:OE1	13:1:34:LEU:HB2	2.18	0.44
14:2:157:HIS:CD2	14:2:187(J):LEU:HD13	2.44	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:111:PHE:CE1	13:1:207:GLY:HA2	2.51	0.44
1:O:188:ASP:O	1:O:192:ILE:HG13	2.18	0.44
3:Q:84:ASP:CG	3:Q:130:ARG:HH22	2.20	0.44
5:S:123:ASN:HD22	5:S:123:ASN:N	2.15	0.44
7:U:38:LEU:HA	7:U:164:ALA:HA	1.99	0.44
7:U:65:SER:HA	7:U:211:GLU:OE2	2.18	0.44
7:U:87:ASN:C	7:U:87:ASN:HD22	2.21	0.44
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.99	0.44
8:V:15:ALA:HA	8:V:174:ASP:O	2.18	0.44
9:W:160:LEU:HD12	9:W:191:MET:CE	2.48	0.44
11:Y:4:LEU:HD13	11:Y:15:ALA:O	2.18	0.44
13:1:133:MET:C	13:1:136:PRO:HD2	2.38	0.44
14:2:42:TRP:CD1	14:2:42:TRP:N	2.86	0.44
2:B:147:GLN:HB3	2:B:149:TYR:CE2	2.53	0.44
5:E:70:CYS:SG	5:E:92:LEU:HD23	2.57	0.44
8:H:34:LEU:HB2	17:H:434:HOH:O	2.17	0.44
12:L:107:LYS:HA	12:L:107:LYS:HD3	1.86	0.44
12:L:114:ASP:OD2	12:L:114:ASP:C	2.55	0.44
12:L:177:ILE:N	12:L:177:ILE:HD12	2.31	0.44
12:L:180:LYS:HG2	17:L:313:HOH:O	2.17	0.44
13:M:53:GLN:O	13:M:56:GLU:HB2	2.18	0.44
14:N:102:ALA:HA	14:N:109:GLU:O	2.17	0.44
2:P:15:PHE:H	3:Q:23:GLN:NE2	2.15	0.44
2:P:39:GLY:C	2:P:148:LEU:HD21	2.38	0.44
6:T:12:ASN:OD1	6:T:12:ASN:O	2.35	0.44
7:G:233:LEU:O	7:G:236:ILE:HG13	2.18	0.44
3:Q:194:VAL:HB	3:Q:236:ILE:CD1	2.47	0.44
5:S:82:ALA:HB3	5:S:83:PRO:HD3	1.99	0.44
6:T:221:HIS:CE1	6:T:223:PHE:CE1	3.05	0.44
7:U:46:THR:HG21	7:U:139:VAL:HB	1.98	0.44
8:V:175:VAL:HG12	8:V:176:CYS:N	2.32	0.44
2:B:138:TYR:O	2:B:148:LEU:HA	2.17	0.44
6:F:120:VAL:HG21	6:F:151:LEU:HD21	1.99	0.44
6:F:150:MET:O	6:F:157:TYR:HA	2.18	0.44
7:G:47:VAL:HG12	7:G:49:ILE:HD12	2.00	0.44
12:L:166:HIS:CD2	12:L:168:GLN:HB2	2.52	0.44
2:P:130:ARG:NH1	2:P:131:PRO:O	2.50	0.44
2:P:168:ASN:ND2	2:P:200:THR:O	2.51	0.44
4:R:134:VAL:HG22	4:R:135:ALA:N	2.33	0.44
7:U:198:ILE:HG23	7:U:203:THR:O	2.17	0.44
10:X:146:MET:CE	10:X:150:GLU:HB3	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:113:VAL:HA	13:1:118:VAL:O	2.18	0.44
3:C:41:LYS:HE2	3:C:161:SER:HA	1.98	0.44
8:H:29:LYS:HE2	12:Z:165:ARG:CZ	2.48	0.44
12:L:18:THR:CG2	12:L:18:THR:O	2.66	0.44
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.49	0.44
14:N:171:GLY:HA2	13:1:197:TRP:CZ3	2.52	0.44
1:O:217(I):TYR:CE1	8:V:36:ARG:HD2	2.52	0.44
6:T:50:VAL:HG22	6:T:51:GLU:O	2.18	0.44
10:X:39:PRO:HG2	10:X:73:GLU:OE1	2.18	0.44
13:1:175:LEU:HD23	13:1:176:ALA:N	2.33	0.44
14:2:134:ILE:HD12	14:2:158:SER:HB3	2.00	0.44
2:B:20:ARG:NE	3:C:33:ARG:NH2	2.66	0.44
2:B:116:LEU:HD23	2:B:116:LEU:HA	1.77	0.44
3:C:28:LEU:O	3:C:31:VAL:HB	2.17	0.44
7:G:26:TYR:CD1	7:G:26:TYR:N	2.84	0.44
9:I:12:VAL:CG2	9:I:178:ILE:HB	2.47	0.44
11:K:165:ARG:NH2	11:K:208:ASN:HD22	2.16	0.44
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.53	0.44
9:W:90:ARG:HA	9:W:90:ARG:HD3	1.87	0.44
10:X:12:VAL:HG21	10:X:109:GLU:O	2.18	0.44
11:Y:64:ARG:O	11:Y:67:GLU:HB2	2.18	0.44
4:D:123(D):ALA:HB1	5:E:129:GLY:HA2	1.99	0.44
7:G:39:ALA:HA	7:G:47:VAL:O	2.18	0.44
7:G:192:PHE:CD1	7:G:192:PHE:C	2.91	0.44
11:K:197:TRP:CD1	9:W:190:LYS:HE3	2.52	0.44
12:L:49:ALA:HA	17:L:350:HOH:O	2.17	0.44
1:O:77:VAL:HG12	1:O:137:LEU:HB2	1.99	0.44
2:P:107:ILE:HA	2:P:108:PRO:HD3	1.92	0.44
5:S:45:HIS:HD2	5:S:214:ILE:HD11	1.82	0.44
6:T:208:PHE:H	6:T:208:PHE:HD2	1.66	0.44
8:V:164:TRP:HA	8:V:164:TRP:HE3	1.82	0.44
9:W:113:PHE:HA	9:W:118:CYS:O	2.17	0.44
4:D:72:ARG:HG3	17:D:464:HOH:O	2.18	0.43
1:O:78:TYR:CE2	1:O:82:GLY:HA2	2.52	0.43
2:P:150:THR:O	2:P:157:TYR:HA	2.18	0.43
2:P:197:LEU:HD13	2:P:210:LEU:CD2	2.48	0.43
9:W:12:VAL:HG23	9:W:178:ILE:HD12	1.99	0.43
13:1:204:LYS:HD3	13:1:204:LYS:N	2.33	0.43
1:A:27:ALA:HB2	7:G:15:PHE:CE2	2.53	0.43
1:A:29:THR:O	1:A:33:GLN:HG2	2.17	0.43
3:C:84:ASP:CG	3:C:130:ARG:HH22	2.22	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:194:LEU:HD12	4:D:194:LEU:HA	1.82	0.43
4:D:197:LEU:O	4:D:201:MET:HG3	2.17	0.43
6:F:107:ILE:HA	6:F:108:PRO:HD3	1.79	0.43
7:G:211:GLU:HA	17:G:447:HOH:O	2.18	0.43
8:H:52:THR:O	8:H:56:THR:HB	2.18	0.43
9:I:-8:SER:O	9:I:-6:PRO:HD3	2.18	0.43
11:K:64:ARG:O	11:K:67:GLU:HB2	2.17	0.43
12:L:165:ARG:CZ	8:V:29:LYS:HE2	2.48	0.43
4:R:160:TYR:CD2	5:S:59:SER:HB3	2.53	0.43
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.33	0.43
13:1:114:ASN:O	13:1:116:LEU:N	2.51	0.43
1:A:13:THR:O	2:B:130:ARG:HD3	2.18	0.43
3:C:39:GLY:HA2	3:C:47:VAL:O	2.18	0.43
3:C:130:ARG:HG3	3:C:130:ARG:NH1	2.31	0.43
4:D:207:LEU:HD21	4:D:233:ILE:HG12	2.00	0.43
6:F:107:ILE:HG23	6:F:107:ILE:O	2.17	0.43
7:G:41:ARG:NH2	7:G:180(B):ASP:O	2.51	0.43
10:J:18:LYS:HG2	10:J:174:ILE:HG13	2.01	0.43
11:K:133:PHE:CD2	11:K:166:ASP:HB2	2.52	0.43
12:L:113:PHE:CD1	12:L:113:PHE:N	2.86	0.43
3:Q:78:PHE:CD1	3:Q:85:SER:HB3	2.53	0.43
3:Q:168:ASN:HB3	3:Q:200:VAL:HG11	2.00	0.43
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.00	0.43
13:1:35:ILE:CD1	13:1:56:GLU:HG2	2.48	0.43
1:A:217(I):TYR:CE1	8:H:36:ARG:HD2	2.53	0.43
7:G:120:SER:O	7:G:121:GLN:C	2.56	0.43
8:H:29:LYS:HE2	12:Z:165:ARG:HH21	1.80	0.43
10:J:138:LEU:HD21	10:J:158:CYS:SG	2.58	0.43
13:M:135:ASN:HB2	13:M:136:PRO:HD3	1.99	0.43
2:P:152:ASN:HB2	2:P:153:PRO:HD2	2.00	0.43
4:R:49:GLY:HA2	4:R:211:GLN:O	2.18	0.43
4:R:194:LEU:HD12	4:R:194:LEU:HA	1.81	0.43
7:U:14:ILE:O	7:U:21:LEU:HD23	2.19	0.43
9:W:99:PRO:HB2	9:W:113:PHE:CD2	2.53	0.43
14:2:1:THR:HG21	14:2:46:SER:HA	2.01	0.43
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.81	0.43
1:A:225:THR:OG1	1:A:228:GLU:HG3	2.19	0.43
3:C:229:ILE:O	3:C:232:TYR:N	2.51	0.43
6:F:38:ILE:HG22	6:F:164:ALA:HB1	1.98	0.43
12:L:43:MET:HG2	12:L:44:SER:N	2.34	0.43
3:Q:40:VAL:HA	3:Q:162:ALA:HA	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:156:ILE:HD11	4:R:82:THR:OG1	2.17	0.43
4:R:237:LEU:HD22	4:R:241:GLU:HG3	1.99	0.43
5:S:68:ILE:HB	5:S:76:LEU:HD21	2.00	0.43
5:S:125:GLN:HG3	6:T:130:ARG:HG2	1.99	0.43
5:S:207:LEU:HD23	5:S:207:LEU:H	1.84	0.43
6:T:37:SER:HA	6:T:50:VAL:HA	1.99	0.43
11:Y:200:LYS:HG3	11:Y:205:SER:O	2.18	0.43
13:1:62:LEU:HD13	13:1:74:LEU:CD1	2.48	0.43
2:B:4:GLY:CA	5:E:127:TYR:CE1	3.01	0.43
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.99	0.43
7:G:29:LYS:HA	7:G:29:LYS:HD2	1.81	0.43
7:G:194:ILE:HG23	7:G:210:LEU:HD11	1.99	0.43
8:H:157:ASP:O	8:H:160:GLN:N	2.51	0.43
10:J:40:HIS:O	10:J:103:GLY:HA2	2.18	0.43
14:N:148:LYS:O	14:N:152:VAL:HG23	2.17	0.43
2:P:74:ILE:HD11	2:P:109:VAL:HG22	2.01	0.43
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	2.01	0.43
3:Q:141:PHE:CE1	3:Q:217:PRO:HG3	2.53	0.43
4:R:215:ILE:O	4:R:215:ILE:HG13	2.18	0.43
5:S:160:LEU:HD23	6:T:59:LEU:HD12	2.00	0.43
6:T:212:ILE:HG22	6:T:213:SER:N	2.32	0.43
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.33	0.43
5:E:161:TYR:OH	6:F:61:PRO:HD2	2.19	0.43
6:F:137:ILE:HA	6:F:149:TYR:O	2.18	0.43
7:G:77:VAL:HG12	7:G:137:THR:HB	2.01	0.43
9:I:171:TRP:HH2	11:Y:165:ARG:HH11	1.65	0.43
10:J:8:VAL:HG23	10:J:9:GLN:N	2.34	0.43
12:L:45:ALA:HA	12:L:99:THR:HB	2.00	0.43
1:O:217:ASP:HA	1:O:220:ARG:NH1	2.33	0.43
5:S:172:ALA:HB2	5:S:196:ALA:O	2.18	0.43
7:U:233:LEU:O	7:U:236:ILE:HG13	2.18	0.43
4:D:215:ILE:O	4:D:215:ILE:HG13	2.17	0.43
8:H:167:LEU:HG	12:Z:24:TYR:O	2.18	0.43
12:L:134:ILE:HA	17:L:388:HOH:O	2.18	0.43
2:P:121:GLN:NE2	2:P:121:GLN:C	2.72	0.43
6:T:212:ILE:HG22	6:T:213:SER:H	1.83	0.43
11:Y:65:LEU:HA	11:Y:65:LEU:HD12	1.75	0.43
11:Y:207:ASN:C	11:Y:209:VAL:H	2.21	0.43
13:1:19:LEU:HD23	13:1:168:ARG:O	2.19	0.43
2:B:130:ARG:HG3	2:B:130:ARG:NH1	2.33	0.43
2:P:82:THR:O	2:P:85:ALA:HB3	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:229:ILE:O	2:P:232:ILE:HG22	2.19	0.43
8:V:43:CYS:SG	8:V:99:LEU:HB3	2.58	0.43
9:W:8:GLY:HA2	17:W:221:HOH:O	2.19	0.43
10:X:137:LEU:C	10:X:137:LEU:HD23	2.39	0.43
11:Y:153:TYR:O	11:Y:156:LYS:HB3	2.19	0.43
12:Z:75:SER:OG	17:Z:253:HOH:O	2.22	0.43
2:B:218:ASN:O	2:B:218(C):ASP:HB2	2.18	0.43
7:G:49:ILE:CD1	7:G:212:VAL:HG13	2.49	0.43
7:G:121:GLN:C	7:G:121:GLN:NE2	2.73	0.43
10:J:112:GLN:NE2	10:J:125:GLY:HA3	2.34	0.43
14:N:25:TYR:CE1	13:1:165:ARG:HB3	2.54	0.43
14:N:51:ASP:O	14:N:55:ILE:HG13	2.19	0.43
1:O:15:PHE:HD2	2:P:23:GLN:NE2	2.17	0.43
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.48	0.43
1:O:72:PRO:HB3	17:V:304:HOH:O	2.18	0.43
4:R:68:VAL:HG21	4:R:89:ILE:HD12	2.01	0.43
5:S:138:ILE:O	5:S:148:LEU:HA	2.19	0.43
6:T:39:GLY:O	6:T:148:LEU:HD21	2.18	0.43
6:T:113:ALA:O	6:T:116:LEU:HB2	2.19	0.43
9:W:43:LEU:CD2	9:W:45:ILE:HD11	2.49	0.43
9:W:43:LEU:HD23	9:W:45:ILE:HD11	2.00	0.43
11:Y:33:LYS:O	11:Y:45:MET:HG3	2.18	0.43
2:B:190:ILE:HG23	2:B:212:PHE:CE2	2.54	0.42
3:C:112:LEU:HD22	3:C:112:LEU:HA	1.83	0.42
4:D:214:CYS:SG	4:D:224:TYR:CE2	3.09	0.42
7:G:198:ILE:HG23	7:G:203:THR:O	2.19	0.42
11:K:33:LYS:O	11:K:45:MET:HG3	2.19	0.42
2:P:7:ARG:HG2	7:U:8:TYR:CZ	2.54	0.42
3:Q:121:GLN:OE1	3:Q:125:GLN:NE2	2.52	0.42
3:Q:160:TRP:CZ3	4:R:59:LEU:HB2	2.54	0.42
4:R:53:ARG:O	4:R:53:ARG:HG2	2.18	0.42
6:T:160:TYR:CD2	6:T:163:ALA:HB2	2.53	0.42
10:X:110:LEU:N	17:X:258:HOH:O	2.48	0.42
7:G:59:LEU:O	7:G:61:PRO:HD3	2.19	0.42
11:K:157:ARG:HD2	11:K:160:LEU:HD23	2.00	0.42
12:L:18:THR:HG22	12:L:18:THR:O	2.19	0.42
14:N:112:THR:HG22	14:N:120:HIS:HB2	2.01	0.42
2:P:108:PRO:HD2	2:P:111:ILE:HD12	2.00	0.42
5:S:76:LEU:HD23	5:S:76:LEU:C	2.39	0.42
5:S:188:GLU:O	5:S:191:LYS:HB2	2.19	0.42
6:T:192:GLN:HA	6:T:192:GLN:NE2	2.35	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:70:ILE:HD12	7:U:92:ALA:HB3	2.01	0.42
8:V:84:LYS:HE2	8:V:119:THR:HG21	2.01	0.42
8:V:157:ASP:O	8:V:160:GLN:HB2	2.19	0.42
1:A:150:GLN:O	1:A:157:TYR:HA	2.20	0.42
6:F:112:PHE:O	6:F:115:ARG:HB2	2.19	0.42
6:F:135:SER:HA	6:F:151:LEU:O	2.19	0.42
8:H:195:ASN:HB3	12:Z:192:LYS:HE3	2.00	0.42
9:I:49:ALA:HB3	10:J:118:THR:HG23	2.02	0.42
10:J:119:LYS:HG2	10:J:120:VAL:N	2.34	0.42
12:L:167:ILE:O	8:V:167:LEU:HD22	2.19	0.42
14:N:7:THR:HA	14:N:12:VAL:HG23	2.01	0.42
4:R:52:LYS:HG3	4:R:64:ILE:HG21	2.01	0.42
6:T:79:SER:HA	17:T:361:HOH:O	2.19	0.42
9:W:33:LYS:O	9:W:44:GLY:HA2	2.19	0.42
1:O:29:THR:O	1:O:33:GLN:HG2	2.19	0.42
1:O:31:VAL:HG11	1:O:135:SER:HB2	2.01	0.42
1:O:35:VAL:HG12	1:O:36:THR:N	2.35	0.42
1:O:49:ALA:HB2	1:O:212:LEU:CG	2.49	0.42
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.17	0.42
2:P:101:LYS:NZ	10:X:85:GLN:NE2	2.67	0.42
6:T:68:GLN:OE1	6:T:89:VAL:HG21	2.20	0.42
7:U:152:ASP:OD2	7:U:156:TYR:HB3	2.20	0.42
8:V:77:VAL:HG13	17:V:422:HOH:O	2.19	0.42
1:A:161:LYS:HD3	1:A:180:TRP:CZ3	2.54	0.42
7:G:108:PRO:HB2	7:G:111:VAL:HG23	2.01	0.42
7:G:222:PHE:N	7:G:222:PHE:CD2	2.88	0.42
8:H:132:LEU:HD12	8:H:132:LEU:N	2.35	0.42
3:Q:156:ILE:HD12	4:R:83:ALA:HB2	2.02	0.42
14:2:7:THR:HA	14:2:12:VAL:HA	2.00	0.42
7:G:141:VAL:HA	7:G:146:PRO:HA	2.01	0.42
13:M:40:ASN:ND2	13:M:40:ASN:N	2.67	0.42
3:Q:112:LEU:O	3:Q:116:VAL:HG23	2.20	0.42
4:R:68:VAL:O	4:R:76:CYS:N	2.52	0.42
5:S:4:PHE:O	5:S:6:ASN:N	2.53	0.42
5:S:203:ASP:HB3	5:S:204:GLU:H	1.72	0.42
7:U:39:ALA:HA	7:U:47:VAL:O	2.18	0.42
9:W:113:PHE:CD2	9:W:113:PHE:N	2.88	0.42
2:B:195:LYS:O	2:B:198:SER:HB2	2.19	0.42
3:C:106:PRO:HG2	3:C:143:PRO:CG	2.49	0.42
7:G:47:VAL:HG12	7:G:49:ILE:CD1	2.50	0.42
10:J:52:THR:HG22	10:J:53:VAL:HG23	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:15:ALA:HA	11:K:174:ASN:O	2.19	0.42
11:K:86:LEU:C	11:K:86:LEU:HD13	2.40	0.42
14:N:9:LYS:O	14:N:107:LYS:HD3	2.20	0.42
5:S:92:LEU:HA	5:S:92:LEU:HD12	1.86	0.42
8:V:112:SER:HB3	8:V:125:LEU:CD1	2.47	0.42
10:X:3:ILE:HG22	10:X:100:LEU:HD12	2.00	0.42
10:X:166:MET:HA	10:X:167:PRO:HD3	1.75	0.42
12:Z:144(A):LYS:HD3	12:Z:144(A):LYS:HA	1.93	0.42
13:1:122:SER:HB3	13:1:124:THR:O	2.20	0.42
14:2:3:ILE:HG22	14:2:16:ALA:CB	2.50	0.42
14:2:41:ILE:HG21	14:2:79:ALA:CB	2.49	0.42
1:A:78:TYR:CE2	1:A:82:GLY:HA2	2.54	0.42
1:A:84:ASP:HB3	1:A:132:PHE:HD2	1.85	0.42
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.89	0.42
5:E:15:PHE:H	6:F:23:GLN:NE2	2.18	0.42
7:G:123:TYR:N	7:G:123:TYR:CD1	2.85	0.42
7:G:130:ARG:HB2	17:G:405:HOH:O	2.20	0.42
11:K:49:ALA:HA	15:3:5:04D:H25A	2.01	0.42
14:N:157:HIS:NE2	14:N:187(J):LEU:HD22	2.35	0.42
2:P:197:LEU:HD13	2:P:210:LEU:HD21	2.02	0.42
3:Q:41:LYS:HE2	3:Q:161:SER:HA	2.01	0.42
3:Q:158:SER:HB2	4:R:59:LEU:HD21	2.02	0.42
5:S:198:SER:HA	5:S:201:LEU:HG	2.02	0.42
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.00	0.42
12:Z:11:PHE:HA	12:Z:178:VAL:O	2.19	0.42
12:Z:93:PHE:N	12:Z:94:PRO:HD3	2.34	0.42
14:2:12:VAL:HG22	14:2:13:ILE:N	2.34	0.42
1:A:15:PHE:N	2:B:23:GLN:HE22	2.18	0.42
3:C:197:LEU:HD23	3:C:197:LEU:HA	1.93	0.42
7:G:47:VAL:HG12	7:G:48:VAL:N	2.34	0.42
8:H:165:ASN:ND2	13:1:139:ARG:HH11	2.18	0.42
10:J:119:LYS:HE2	17:J:201:HOH:O	2.20	0.42
12:L:18:THR:CG2	12:L:30:TYR:CD1	3.01	0.42
12:L:129:ALA:HB1	12:L:166:HIS:CE1	2.55	0.42
3:Q:130:ARG:HG3	3:Q:130:ARG:NH1	2.33	0.42
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.54	0.42
7:U:109:CYS:HB2	7:U:140:SER:OG	2.19	0.42
7:U:190:VAL:O	7:U:193:ALA:HB3	2.19	0.42
11:Y:137:VAL:HG21	11:Y:161:ALA:CB	2.50	0.42
12:Z:18:THR:CG2	12:Z:18:THR:O	2.68	0.42
1:A:35:VAL:HG12	1:A:36:THR:N	2.34	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:PRO:O	3:C:185:THR:N	2.53	0.42
4:D:108:ASN:HD22	4:D:108:ASN:HA	1.61	0.42
1:O:39:GLY:HA2	1:O:47:VAL:O	2.20	0.42
2:P:37:ALA:O	2:P:164:SER:HA	2.20	0.42
7:U:203:THR:HG22	7:U:204:GLU:N	2.35	0.42
11:Y:135:TYR:HB2	17:Y:337:HOH:O	2.19	0.42
13:1:51:ASP:O	13:1:55:ILE:HG13	2.20	0.42
13:1:170:SER:HA	17:1:312:HOH:O	2.18	0.42
1:A:58:LEU:HG	7:G:177:GLU:HG2	2.01	0.41
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.81	0.41
7:G:130:ARG:HH11	7:G:130:ARG:CG	2.33	0.41
1:O:11:SER:OG	2:P:129:LEU:HA	2.20	0.41
11:Y:4:LEU:HD12	11:Y:159:ILE:CD1	2.50	0.41
11:Y:75:SER:HA	11:Y:105:THR:HG21	2.01	0.41
12:Z:134:ILE:HG22	12:Z:138:LEU:CD2	2.50	0.41
1:A:169:SER:O	1:A:173:LYS:HG3	2.20	0.41
4:D:121:LEU:HD23	4:D:123:PHE:HE1	1.85	0.41
4:D:194:LEU:HD22	4:D:212:LEU:HD11	2.02	0.41
12:L:99:THR:HG23	12:L:113:PHE:HB2	2.01	0.41
13:M:-2:THR:O	13:M:20:GLY:HA2	2.21	0.41
14:N:38:HIS:NE2	14:N:74:PRO:HD2	2.35	0.41
4:R:146:TYR:C	4:R:147:GLN:HG3	2.41	0.41
5:S:102:VAL:O	5:S:102:VAL:HG12	2.20	0.41
10:X:112:GLN:NE2	10:X:125:GLY:HA3	2.35	0.41
12:Z:9:GLU:O	12:Z:107:LYS:HA	2.20	0.41
13:1:152:GLU:O	13:1:156:VAL:HG23	2.20	0.41
14:2:3:ILE:HG22	14:2:16:ALA:HB2	2.01	0.41
2:B:150:THR:O	2:B:157:TYR:HA	2.19	0.41
13:M:112:TYR:O	13:M:119:THR:HA	2.20	0.41
13:M:157:ASN:HD22	13:M:160:ARG:NH1	2.18	0.41
5:S:161:TYR:OH	6:T:61:PRO:CD	2.67	0.41
6:T:62:GLN:HA	6:T:209:GLU:OE2	2.20	0.41
6:T:223:PHE:CD1	6:T:223:PHE:N	2.87	0.41
7:U:185:SER:HB2	7:U:187:GLU:OE2	2.19	0.41
9:W:160:LEU:HD11	9:W:191:MET:HB3	2.02	0.41
10:X:36:GLN:HG3	10:X:184:ILE:HD12	2.01	0.41
11:Y:133:PHE:CD2	11:Y:166:ASP:HB2	2.56	0.41
12:Z:42:VAL:HG12	12:Z:176:LEU:HD23	2.02	0.41
13:1:62:LEU:HD13	13:1:74:LEU:HD13	2.02	0.41
13:1:155:ILE:O	13:1:159:MET:HG2	2.19	0.41
1:A:40:ILE:HD12	1:A:193:ALA:HB2	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HA	1:A:58:LEU:HD23	1.60	0.41
3:C:163:GLN:CG	3:C:164:THR:N	2.83	0.41
7:G:179(D):SER:O	7:G:179(E):LYS:HB2	2.20	0.41
13:M:204:LYS:N	13:M:204:LYS:HD3	2.35	0.41
5:S:207:LEU:H	5:S:207:LEU:CD2	2.33	0.41
7:U:76:MET:SD	7:U:138:PHE:HE2	2.40	0.41
9:W:93:GLY:N	9:W:94:PRO:CD	2.81	0.41
3:C:36:CYS:N	3:C:51:GLU:HG2	2.31	0.41
3:C:55:THR:O	3:C:56:LEU:HD13	2.21	0.41
4:D:123(D):ALA:O	4:D:123(F):GLY:N	2.53	0.41
4:D:130:ARG:HG3	4:D:130:ARG:NH1	2.34	0.41
7:G:82:ILE:CG2	7:G:83:PRO:HD3	2.49	0.41
11:K:165:ARG:HD3	11:K:165:ARG:HA	1.86	0.41
12:L:165:ARG:HH21	8:V:29:LYS:HE2	1.86	0.41
1:O:7:ARG:NH2	4:R:123(C):GLY:HA3	2.23	0.41
1:O:198:LYS:HA	1:O:206:PHE:CE1	2.56	0.41
4:R:184:LEU:HD23	4:R:188:GLU:OE1	2.21	0.41
5:S:149:LEU:HD12	5:S:159:GLU:HG3	2.02	0.41
5:S:167:ALA:HB3	17:S:355:HOH:O	2.21	0.41
7:U:131:PRO:HB3	17:U:345:HOH:O	2.21	0.41
1:A:77:VAL:HG12	1:A:137:LEU:HB2	2.01	0.41
1:A:212:LEU:C	1:A:212:LEU:HD23	2.40	0.41
3:C:194:VAL:O	3:C:198:LEU:HG	2.21	0.41
4:D:137:LEU:HD23	4:D:137:LEU:HA	1.86	0.41
5:E:180(C):PHE:HA	5:E:180(F):ILE:HG13	2.03	0.41
6:F:74:ILE:HG21	6:F:112:PHE:CE2	2.55	0.41
11:K:1:THR:CA	17:K:445:HOH:O	2.58	0.41
12:L:4:LEU:HD11	12:L:138:LEU:HD21	2.03	0.41
2:P:134:VAL:HG12	2:P:135:SER:N	2.35	0.41
3:Q:46:VAL:HB	3:Q:215:VAL:HG22	2.03	0.41
3:Q:85:SER:O	3:Q:89:ILE:HG13	2.21	0.41
17:R:366:HOH:O	12:Z:85:HIS:HD2	2.03	0.41
5:S:31:ILE:HD11	5:S:153:PRO:CD	2.50	0.41
6:T:198:TYR:CD1	6:T:236:ALA:HB1	2.56	0.41
8:V:1:THR:HG21	8:V:46:ALA:HA	2.01	0.41
9:W:22:SER:O	9:W:23:GLN:HB2	2.21	0.41
13:1:40:ASN:H	13:1:40:ASN:ND2	2.18	0.41
4:D:140:GLY:HA2	4:D:215:ILE:HG12	2.02	0.41
4:D:147:GLN:HA	17:D:450:HOH:O	2.20	0.41
5:E:20:ARG:HB3	5:E:25:GLU:OE2	2.20	0.41
6:F:6:THR:HB	6:F:7:GLY:H	1.77	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.51	0.41
11:K:208:ASN:OD1	11:K:208:ASN:O	2.39	0.41
13:M:99:ILE:HG22	13:M:100:ILE:N	2.36	0.41
2:P:71:ASN:HD22	2:P:72:ASP:N	2.19	0.41
3:Q:57:LYS:HB3	3:Q:57:LYS:HE3	1.90	0.41
5:S:76:LEU:HB2	5:S:137:LEU:O	2.20	0.41
6:T:95:GLU:CG	6:T:115:ARG:HH11	2.31	0.41
7:U:151:THR:HG22	7:U:157:TYR:HB2	2.02	0.41
7:U:158:VAL:CG2	7:U:159:GLY:N	2.82	0.41
8:V:17:ASP:HA	8:V:172:ASN:O	2.20	0.41
11:Y:174:ASN:ND2	11:Y:186:TYR:OH	2.54	0.41
4:D:53:ARG:O	4:D:53:ARG:HG2	2.20	0.41
10:J:105:ASP:O	10:J:106:ASN:N	2.53	0.41
10:J:166:MET:HA	10:J:167:PRO:HD3	1.86	0.41
11:K:1:THR:O	11:K:128:GLY:HA3	2.20	0.41
1:O:130:ARG:HD3	7:U:13:THR:O	2.21	0.41
2:P:15:PHE:HB2	3:Q:23:GLN:HE22	1.86	0.41
7:U:102:LYS:HB3	7:U:102:LYS:HE2	1.82	0.41
8:V:163:ILE:HG23	8:V:170:GLY:HA2	2.02	0.41
11:Y:1:THR:CA	17:Y:378:HOH:O	2.67	0.41
11:Y:49:ALA:HA	15:4:5:04D:H25A	2.03	0.41
14:2:6:VAL:HG13	14:2:124:TYR:CB	2.51	0.41
14:2:187(A):ILE:HG23	14:2:187(A):ILE:O	2.21	0.41
2:B:20:ARG:CZ	3:C:33:ARG:HH21	2.34	0.41
3:C:71:ASP:OD1	3:C:100:ARG:NH1	2.54	0.41
3:C:111:TYR:O	3:C:112:LEU:C	2.59	0.41
3:C:156:ILE:HD12	4:D:83:ALA:HB2	2.03	0.41
3:C:161:SER:HB3	3:C:180:TYR:CE1	2.56	0.41
4:D:146:TYR:C	4:D:147:GLN:HG3	2.42	0.41
4:D:175:GLU:HG2	4:D:196:ILE:HG12	2.03	0.41
17:D:422:HOH:O	12:L:85:HIS:HD2	2.03	0.41
5:E:48:LEU:HB2	5:E:213:ALA:HB3	2.02	0.41
7:G:8:TYR:C	7:G:10:ARG:H	2.23	0.41
7:G:218:ASP:O	7:G:220:LYS:HB2	2.21	0.41
8:H:172:ASN:HB3	8:H:192:LEU:O	2.21	0.41
9:I:115:LEU:H	9:I:115:LEU:CD2	2.33	0.41
11:K:100:MET:HA	11:K:111:TYR:O	2.21	0.41
11:K:172:SER:HB3	11:K:191:ASP:HA	2.03	0.41
12:L:114:ASP:OD2	12:L:115:PRO:N	2.54	0.41
12:L:166:HIS:HD2	12:L:168:GLN:HB2	1.85	0.41
12:L:170:GLY:O	12:L:171:ASP:HB2	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:42:VAL:HG23	13:M:178:ILE:HD11	2.02	0.41
13:M:114:ASN:OD1	13:M:114:ASN:C	2.58	0.41
14:N:19:ARG:O	14:N:33:LYS:NZ	2.52	0.41
1:O:4:MET:SD	1:O:5:THR:N	2.90	0.41
1:O:82:GLY:O	1:O:85:TYR:HB3	2.21	0.41
2:P:44:ASP:OD2	2:P:44:ASP:N	2.54	0.41
2:P:71:ASN:HD22	2:P:72:ASP:H	1.67	0.41
2:P:211:GLU:HA	17:P:335:HOH:O	2.20	0.41
6:T:122:ALA:HB2	17:T:358:HOH:O	2.21	0.41
6:T:169:ARG:HG3	6:T:173:LYS:HE3	2.03	0.41
7:U:39:ALA:HB2	7:U:48:VAL:HG12	2.01	0.41
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.50	0.41
8:V:59:ILE:HG12	8:V:83:LEU:HD23	2.03	0.41
9:W:25:LEU:HD11	10:X:135:PHE:HD2	1.86	0.41
10:X:34:THR:CG2	10:X:176:LYS:NZ	2.84	0.41
10:X:143:ARG:O	10:X:146:MET:HG3	2.20	0.41
12:Z:145:TYR:HD1	12:Z:145:TYR:HA	1.59	0.41
14:2:36:ARG:HH21	14:2:60:GLN:HE21	1.69	0.41
2:B:231:ASP:O	2:B:235:LYS:HG2	2.21	0.41
3:C:175:PHE:CD2	3:C:196:SER:HB3	2.56	0.41
4:D:65:GLU:HA	17:D:402:HOH:O	2.20	0.41
4:D:123:PHE:CD1	4:D:131:PRO:HG3	2.56	0.41
5:E:54:ASN:ND2	5:E:56:ASP:O	2.53	0.41
5:E:160:LEU:HD13	5:E:163:THR:HB	2.03	0.41
7:G:151:THR:HG22	7:G:157:TYR:CB	2.51	0.41
7:G:210:LEU:HA	7:G:210:LEU:HD23	1.83	0.41
8:H:13:VAL:CG2	8:H:14:ILE:N	2.84	0.41
9:I:19:ARG:HB2	9:I:171:TRP:HB2	2.03	0.41
10:J:34:THR:HG21	10:J:176:LYS:HZ2	1.86	0.41
13:M:113:VAL:HA	13:M:118:VAL:O	2.21	0.41
1:O:58:LEU:HD23	1:O:58:LEU:HA	1.77	0.41
2:P:38:ILE:HD12	2:P:197:LEU:HG	2.02	0.41
5:S:100:SER:O	5:S:104:ASN:HA	2.21	0.41
10:X:120:VAL:HG13	10:X:122:LEU:HG	2.02	0.41
4:D:227:GLU:H	4:D:227:GLU:CD	2.25	0.40
6:F:69:VAL:HG12	17:F:436:HOH:O	2.20	0.40
11:K:6:PHE:CE2	11:K:13:ILE:HB	2.56	0.40
11:K:12:ILE:HB	11:K:178:VAL:HB	2.04	0.40
11:K:83:LEU:O	11:K:87:VAL:HB	2.21	0.40
12:L:77:ASN:O	12:L:80:ALA:HB3	2.21	0.40
13:M:186:PHE:HE1	13:M:188:LYS:HG3	1.86	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:198:LEU:HA	3:Q:198:LEU:HD23	1.86	0.40
6:T:186:ALA:HB1	6:T:214:TRP:HE3	1.86	0.40
7:U:192:PHE:CD1	7:U:192:PHE:C	2.94	0.40
7:U:220:LYS:HG2	7:U:221:PHE:N	2.36	0.40
11:Y:1:THR:HG23	11:Y:2:THR:N	2.36	0.40
11:Y:45:MET:HB3	11:Y:52:CYS:CB	2.44	0.40
11:Y:177:HIS:CE1	11:Y:179:THR:CG2	3.03	0.40
14:2:175:MET:CE	14:2:187(B):PHE:CE2	3.04	0.40
1:A:233:LEU:C	1:A:235:ALA:H	2.23	0.40
4:D:97:VAL:HG11	11:K:65:LEU:HD13	2.03	0.40
5:E:203:ASP:HB3	5:E:204:GLU:H	1.71	0.40
6:F:53:LEU:HD23	6:F:53:LEU:HA	1.78	0.40
1:O:202:VAL:HG21	1:O:206:PHE:CE1	2.56	0.40
1:O:228:GLU:O	1:O:232:ARG:NH1	2.54	0.40
2:P:4:GLY:CA	5:S:127:TYR:CE1	3.01	0.40
2:P:7:ARG:HG3	2:P:7:ARG:HH11	1.86	0.40
2:P:81:LEU:HD23	2:P:133:GLY:HA3	2.04	0.40
3:Q:25:GLU:O	3:Q:28:LEU:HB2	2.22	0.40
3:Q:134:VAL:CG1	3:Q:135:SER:N	2.84	0.40
5:S:97:ASN:HD22	5:S:97:ASN:HA	1.61	0.40
6:T:67:ILE:HG13	6:T:211:GLU:OE1	2.21	0.40
6:T:203:GLU:C	6:T:205:ASN:H	2.23	0.40
11:Y:158:SER:O	11:Y:161:ALA:HB3	2.20	0.40
12:Z:20:ASN:O	12:Z:27:ASN:HB2	2.20	0.40
13:1:157:ASN:O	13:1:160:ARG:N	2.54	0.40
14:2:7:THR:CG2	14:2:110:VAL:HG23	2.51	0.40
10:J:8:VAL:HG22	10:J:11:SER:O	2.21	0.40
13:M:57:ARG:HG2	13:M:57:ARG:NH1	2.34	0.40
1:O:84:ASP:CG	1:O:130:ARG:HH22	2.24	0.40
1:O:108:PRO:CG	1:O:111:LEU:HD12	2.51	0.40
3:Q:15:PHE:H	4:R:23:GLN:NE2	2.13	0.40
5:S:116:LEU:HD23	5:S:116:LEU:HA	1.73	0.40
10:X:155:LEU:HD23	10:X:155:LEU:HA	1.85	0.40
2:B:64:THR:HG23	17:B:368:HOH:O	2.21	0.40
6:F:28:VAL:O	6:F:31:VAL:HB	2.21	0.40
6:F:127:ASN:HD22	6:F:127:ASN:C	2.24	0.40
6:F:170:GLN:CD	6:F:170:GLN:N	2.72	0.40
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.57	0.40
11:K:20:ALA:O	11:K:27:ALA:HB3	2.21	0.40
12:L:134:ILE:CG2	12:L:158:SER:HB3	2.50	0.40
14:N:6:VAL:HG23	14:N:155:ILE:HD11	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:53:LYS:O	2:P:54:VAL:HB	2.22	0.40
3:Q:130:ARG:CG	3:Q:130:ARG:NH1	2.83	0.40
6:T:173:LYS:O	6:T:177:GLU:HG3	2.21	0.40
7:U:78:VAL:HG21	7:U:85:ALA:HB1	2.04	0.40
8:V:6:VAL:HG11	8:V:154:LEU:HD23	2.02	0.40
9:W:84:SER:HB2	9:W:119:ILE:HD11	2.02	0.40
13:1:205:GLY:HA3	13:1:209:GLN:HB3	2.04	0.40
5:E:24:VAL:O	5:E:27:ALA:HB3	2.21	0.40
5:E:162:GLY:O	6:F:58:LEU:HD13	2.22	0.40
5:E:180(C):PHE:CD1	5:E:180(D):ILE:N	2.89	0.40
10:J:161:GLU:OE2	10:J:161:GLU:HA	2.21	0.40
3:Q:87:ILE:O	3:Q:91:LYS:HG3	2.22	0.40
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.86	0.40
10:X:123:PRO:HB2	10:X:124:TYR:CD1	2.57	0.40
10:X:124:TYR:CG	10:X:138:LEU:HD13	2.56	0.40
10:X:154:LEU:HD12	10:X:154:LEU:HA	1.81	0.40
13:1:91:ARG:HG3	13:1:92:SER:N	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	220 (89%)	26 (10%)	2 (1%)	19	17
1	O	248/250 (99%)	218 (88%)	28 (11%)	2 (1%)	19	17
2	B	242/244 (99%)	217 (90%)	21 (9%)	4 (2%)	9	4
2	P	242/244 (99%)	223 (92%)	15 (6%)	4 (2%)	9	4
3	C	239/241 (99%)	218 (91%)	16 (7%)	5 (2%)	7	3
3	Q	239/241 (99%)	214 (90%)	18 (8%)	7 (3%)	4	2
4	D	240/242 (99%)	215 (90%)	19 (8%)	6 (2%)	5	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	240/242 (99%)	213 (89%)	22 (9%)	5 (2%)	7	3
5	E	231/233 (99%)	207 (90%)	19 (8%)	5 (2%)	6	3
5	S	231/233 (99%)	207 (90%)	15 (6%)	9 (4%)	3	1
6	F	242/244 (99%)	220 (91%)	21 (9%)	1 (0%)	34	37
6	T	242/244 (99%)	220 (91%)	20 (8%)	2 (1%)	19	17
7	G	241/243 (99%)	224 (93%)	15 (6%)	2 (1%)	19	17
7	U	241/243 (99%)	222 (92%)	15 (6%)	4 (2%)	9	4
8	H	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	29	29
8	V	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	29	29
9	I	202/204 (99%)	189 (94%)	13 (6%)	0	100	100
9	W	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	29	29
10	J	196/198 (99%)	184 (94%)	9 (5%)	3 (2%)	10	6
10	X	196/198 (99%)	185 (94%)	9 (5%)	2 (1%)	15	13
11	K	210/212 (99%)	199 (95%)	10 (5%)	1 (0%)	29	29
11	Y	210/212 (99%)	201 (96%)	8 (4%)	1 (0%)	29	29
12	L	220/222 (99%)	205 (93%)	13 (6%)	2 (1%)	17	14
12	Z	220/222 (99%)	206 (94%)	13 (6%)	1 (0%)	29	29
13	1	231/233 (99%)	214 (93%)	14 (6%)	3 (1%)	12	8
13	M	231/233 (99%)	213 (92%)	13 (6%)	5 (2%)	6	3
14	2	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
14	N	194/196 (99%)	184 (95%)	10 (5%)	0	100	100
15	3	2/5 (40%)	2 (100%)	0	0	100	100
15	4	2/5 (40%)	2 (100%)	0	0	100	100
All	All	6316/6378 (99%)	5806 (92%)	431 (7%)	79 (1%)	12	8

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
2	B	218(C)	ASP
3	C	58	LEU
3	C	184	ALA
4	D	123(E)	SER
5	E	5	ARG

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	203	ASP
12	L	71	ASP
13	M	71	GLU
2	P	218(B)	ASP
3	Q	58	LEU
3	Q	184	ALA
4	R	123(E)	SER
5	S	5	ARG
5	S	203	ASP
3	C	183	PRO
3	C	203	THR
6	F	206	LYS
10	J	49	ALA
1	O	167	LYS
3	Q	183	PRO
3	Q	203	THR
4	R	123(G)	GLU
6	T	206	LYS
7	U	7	GLY
7	U	182	HIS
13	1	72(A)	GLU
3	C	240	LYS
4	D	61	SER
4	D	120	ALA
4	D	123(G)	GLU
5	E	6	ASN
5	E	227	GLU
7	G	180(C)	HIS
10	J	39	PRO
11	K	39	PRO
13	M	115	LEU
3	Q	240	LYS
4	R	120	ALA
7	U	9	ASP
13	1	115	LEU
4	D	242	ALA
8	H	115	ALA
13	M	70(E)	ALA
13	M	96	TRP
3	Q	17	PRO
4	R	123(F)	GLY
5	S	202	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
5	S	221	PHE
5	S	227	GLU
6	T	143	LYS
7	U	55	PRO
13	1	72	ALA
2	B	62	ASP
12	L	70(A)	ASN
2	P	22	TYR
2	P	54	VAL
2	P	182	ASP
3	Q	199	GLU
4	R	61	SER
5	S	6	ASN
5	S	180	LEU
5	S	217	LYS
10	X	49	ALA
12	Z	71	ASP
1	A	56	SER
2	B	54	VAL
5	E	128	GLY
5	S	180(A)	ASP
8	V	115	ALA
7	G	7	GLY
10	J	8	VAL
13	M	-4	ILE
1	O	56	SER
10	X	8	VAL
11	Y	39	PRO
4	D	123(F)	GLY
9	W	93	GLY
2	B	226	PRO

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

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

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	197 (94%)	12 (6%)	20	20
1	O	209/209 (100%)	198 (95%)	11 (5%)	22	23
2	B	203/203 (100%)	189 (93%)	14 (7%)	15	14
2	P	203/203 (100%)	187 (92%)	16 (8%)	12	10
3	C	213/213 (100%)	193 (91%)	20 (9%)	8	6
3	Q	213/213 (100%)	198 (93%)	15 (7%)	15	13
4	D	198/198 (100%)	181 (91%)	17 (9%)	10	9
4	R	198/198 (100%)	187 (94%)	11 (6%)	21	21
5	E	192/192 (100%)	171 (89%)	21 (11%)	6	4
5	S	192/192 (100%)	170 (88%)	22 (12%)	5	3
6	F	201/201 (100%)	181 (90%)	20 (10%)	7	5
6	T	201/201 (100%)	180 (90%)	21 (10%)	7	5
7	G	207/207 (100%)	196 (95%)	11 (5%)	22	23
7	U	207/207 (100%)	196 (95%)	11 (5%)	22	23
8	H	181/181 (100%)	168 (93%)	13 (7%)	14	12
8	V	181/181 (100%)	167 (92%)	14 (8%)	13	11
9	I	172/172 (100%)	164 (95%)	8 (5%)	26	29
9	W	172/172 (100%)	166 (96%)	6 (4%)	36	43
10	J	175/175 (100%)	167 (95%)	8 (5%)	27	30
10	X	175/175 (100%)	167 (95%)	8 (5%)	27	30
11	K	169/169 (100%)	161 (95%)	8 (5%)	26	29
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	23
12	L	185/185 (100%)	173 (94%)	12 (6%)	17	16
12	Z	185/185 (100%)	172 (93%)	13 (7%)	15	13
13	1	199/199 (100%)	189 (95%)	10 (5%)	24	26
13	M	199/199 (100%)	188 (94%)	11 (6%)	21	21
14	2	162/162 (100%)	155 (96%)	7 (4%)	29	33
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	33
15	3	2/2 (100%)	2 (100%)	0	100	100
15	4	2/2 (100%)	2 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	5336/5336 (100%)	4980 (93%)	356 (7%)	16	15

All (356) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	32	LYS
1	A	47	VAL
1	A	62	GLU
1	A	64	LEU
1	A	114	SER
1	A	124	THR
1	A	135	SER
1	A	136	LEU
1	A	158	PHE
1	A	222	ARG
1	A	236	LEU
2	B	55	THR
2	B	58	LEU
2	B	67	LEU
2	B	71	ASN
2	B	82	THR
2	B	91	THR
2	B	121	GLN
2	B	150	THR
2	B	185	LYS
2	B	192	LEU
2	B	198	SER
2	B	212	PHE
2	B	221	GLN
2	B	226	PRO
3	C	10	ARG
3	C	25	GLU
3	C	33	ARG
3	C	57	LYS
3	C	61	THR
3	C	66	LYS
3	C	75	VAL
3	C	82	ASN
3	C	121	GLN
3	C	131	PRO
3	C	135	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	150	GLN
3	C	156	ILE
3	C	163	GLN
3	C	174	GLU
3	C	208	LYS
3	C	209	ASN
3	C	215	VAL
3	C	237	GLU
3	C	239	GLU
4	D	9	ASP
4	D	13	SER
4	D	14	THR
4	D	33	LEU
4	D	76	CYS
4	D	102	TYR
4	D	126	ARG
4	D	170	GLU
4	D	177	LEU
4	D	184	LEU
4	D	185	THR
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	219	ASP
4	D	225	ASP
4	D	237	LEU
5	E	4	PHE
5	E	11	ASP
5	E	12	THR
5	E	13	VAL
5	E	18	THR
5	E	76	LEU
5	E	78	LEU
5	E	97	ASN
5	E	99	SER
5	E	121	GLN
5	E	126	SER
5	E	160	LEU
5	E	178	ARG
5	E	180(C)	PHE
5	E	185	ASN
5	E	189	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	199	GLN
5	E	203	ASP
5	E	206	SER
5	E	207	LEU
5	E	231	LYS
6	F	18	ASP
6	F	36	THR
6	F	43	ASN
6	F	73	HIS
6	F	83	PRO
6	F	121	GLN
6	F	127	ASN
6	F	169	ARG
6	F	170	GLN
6	F	176	LEU
6	F	187	ARG
6	F	192	GLN
6	F	203	GLU
6	F	204	ASP
6	F	205	ASN
6	F	206(B)	GLU
6	F	207	ASP
6	F	208	PHE
6	F	214	TRP
6	F	227	ASP
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	184	ASN
7	G	204	GLU
7	G	232	ARG
7	G	233	LEU
7	G	240	ASP
8	H	30	ASN
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	84	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	H	99	LEU
8	H	105(A)	PRO
8	H	135	MET
8	H	172	ASN
8	H	197	ARG
8	H	217	SER
8	H	221	ILE
9	I	-5	SER
9	I	58	MET
9	I	113	PHE
9	I	118	CYS
9	I	122(A)	LYS
9	I	123	ASP
9	I	135	PHE
9	I	160	LEU
10	J	6	ILE
10	J	25	SER
10	J	34	THR
10	J	52	THR
10	J	77	GLN
10	J	90	SER
10	J	133	TYR
10	J	157	LEU
11	K	1	THR
11	K	4	LEU
11	K	9	GLN
11	K	65	LEU
11	K	87	VAL
11	K	105(B)	LYS
11	K	146	LEU
11	K	180	GLU
12	L	14	LEU
12	L	40	ASN
12	L	62	SER
12	L	98	HIS
12	L	99	THR
12	L	114	ASP
12	L	123	GLN
12	L	138	LEU
12	L	144(I)	ASN
12	L	144(P)	LEU
12	L	145	TYR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	L	150	GLU
13	M	-8	THR
13	M	40	ASN
13	M	62	LEU
13	M	65	GLU
13	M	91	ARG
13	M	93	ASN
13	M	141(A)	VAL
13	M	141(C)	ARG
13	M	181(A)	THR
13	M	184	LEU
13	M	204	LYS
14	N	22	THR
14	N	36	ARG
14	N	65	LEU
14	N	70	TYR
14	N	149	GLU
14	N	187(E)	ASP
14	N	187(I)	GLN
1	O	4	MET
1	O	32	LYS
1	O	62	GLU
1	O	64	LEU
1	O	131	PRO
1	O	135	SER
1	O	136	LEU
1	O	158	PHE
1	O	221	PHE
1	O	222	ARG
1	O	236	LEU
2	P	8	TYR
2	P	55	THR
2	P	58	LEU
2	P	67	LEU
2	P	71	ASN
2	P	82	THR
2	P	91	THR
2	P	121	GLN
2	P	142	ASP
2	P	150	THR
2	P	153	PRO
2	P	185	LYS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	P	192	LEU
2	P	206	THR
2	P	212	PHE
2	P	226	PRO
3	Q	10	ARG
3	Q	17	PRO
3	Q	25	GLU
3	Q	33	ARG
3	Q	57	LYS
3	Q	61	THR
3	Q	66	LYS
3	Q	75	VAL
3	Q	121	GLN
3	Q	135	SER
3	Q	150	GLN
3	Q	163	GLN
3	Q	174	GLU
3	Q	208	LYS
3	Q	209	ASN
4	R	14	THR
4	R	33	LEU
4	R	63	SER
4	R	76	CYS
4	R	126	ARG
4	R	170	GLU
4	R	177	LEU
4	R	184	LEU
4	R	185	THR
4	R	215	ILE
4	R	237	LEU
5	S	4	PHE
5	S	6	ASN
5	S	11	ASP
5	S	12	THR
5	S	18	THR
5	S	76	LEU
5	S	97	ASN
5	S	99	SER
5	S	117	CYS
5	S	121	GLN
5	S	126	SER
5	S	153	PRO

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	S	160	LEU
5	S	178	ARG
5	S	185	ASN
5	S	189	LEU
5	S	199	GLN
5	S	203	ASP
5	S	204	GLU
5	S	207	LEU
5	S	222	THR
5	S	231	LYS
6	T	18	ASP
6	T	36	THR
6	T	43	ASN
6	T	59	LEU
6	T	73	HIS
6	T	83	PRO
6	T	121	GLN
6	T	127	ASN
6	T	135	SER
6	T	169	ARG
6	T	170	GLN
6	T	171	SER
6	T	187	ARG
6	T	192	GLN
6	T	203	GLU
6	T	204	ASP
6	T	205	ASN
6	T	206(A)	GLU
6	T	208	PHE
6	T	214	TRP
6	T	227	ASP
7	U	62	THR
7	U	72	ARG
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	169	GLN
7	U	184	ASN
7	U	204	GLU
7	U	232	ARG
7	U	233	LEU
7	U	240	ASP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	V	30	ASN
8	V	39	PRO
8	V	55	VAL
8	V	56	THR
8	V	68	LEU
8	V	84	LYS
8	V	99	LEU
8	V	104	VAL
8	V	120	ASP
8	V	121	VAL
8	V	135	MET
8	V	172	ASN
8	V	197	ARG
8	V	221	ILE
9	W	-5	SER
9	W	55	LEU
9	W	113	PHE
9	W	122(A)	LYS
9	W	135	PHE
9	W	160	LEU
10	X	6	ILE
10	X	25	SER
10	X	34	THR
10	X	52	THR
10	X	66	TYR
10	X	70	GLU
10	X	77	GLN
10	X	90	SER
11	Y	1	THR
11	Y	4	LEU
11	Y	9	GLN
11	Y	41	LEU
11	Y	45	MET
11	Y	65	LEU
11	Y	87	VAL
11	Y	105(B)	LYS
11	Y	146	LEU
12	Z	14	LEU
12	Z	40	ASN
12	Z	62	SER
12	Z	93	PHE
12	Z	98	HIS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	Z	99	THR
12	Z	114	ASP
12	Z	123	GLN
12	Z	138	LEU
12	Z	144(J)	ASN
12	Z	144(Q)	LEU
12	Z	145	TYR
12	Z	150	GLU
13	1	40	ASN
13	1	62	LEU
13	1	65	GLU
13	1	91	ARG
13	1	93	ASN
13	1	141(A)	VAL
13	1	141(C)	ARG
13	1	181(A)	THR
13	1	184	LEU
13	1	204	LYS
14	2	22	THR
14	2	36	ARG
14	2	65	LEU
14	2	70	TYR
14	2	149	GLU
14	2	159	LEU
14	2	187(I)	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	33	GLN
1	A	191	HIS
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
3	C	23	GLN
3	C	82	ASN
3	C	97	GLN
3	C	121	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
4	D	23	GLN
4	D	108	ASN
4	D	114	GLN
4	D	199	GLN
4	D	211	GLN
4	D	218	GLN
4	D	226	ASN
5	E	73	HIS
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	123	ASN
5	E	125	GLN
5	E	185	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	123	HIS
6	F	147	HIS
6	F	192	GLN
6	F	241	ASN
7	G	33	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	180(C)	HIS
7	G	184	ASN
7	G	196	HIS
8	H	30	ASN
8	H	66	HIS
8	H	109	HIS
8	H	190	ASN
9	I	81	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	I	145	ASN
9	I	193	GLN
10	J	9	GLN
10	J	54	GLN
10	J	64	GLN
10	J	77	GLN
10	J	112	GLN
10	J	140	HIS
10	J	141	HIS
10	J	186	GLN
11	K	85	ASN
11	K	174	ASN
11	K	189	ASN
11	K	208	ASN
12	L	61	ASN
12	L	70	HIS
12	L	82	ASN
12	L	144(B)	ASN
12	L	144(C)	GLN
12	L	144(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	191	GLN
14	N	28	ASN
14	N	69	GLN
14	N	161	GLN
1	O	191	HIS
2	P	23	GLN
2	P	71	ASN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	168	ASN
2	P	177	GLN
3	Q	23	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	Q	82	ASN
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	114	GLN
4	R	150	HIS
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	125	GLN
5	S	185	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	147	HIS
6	T	192	GLN
6	T	221	HIS
6	T	241	ASN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	178	ASN
7	U	184	ASN
7	U	239	GLN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	91	GLN
8	V	109	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	V	160	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	29	ASN
9	W	81	GLN
9	W	145	ASN
10	X	9	GLN
10	X	54	GLN
10	X	64	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	140	HIS
10	X	141	HIS
10	X	186	GLN
11	Y	85	ASN
11	Y	174	ASN
11	Y	189	ASN
11	Y	208	ASN
12	Z	144(B)	ASN
12	Z	144(C)	GLN
12	Z	144(J)	ASN
12	Z	166	HIS
13	1	10	ASN
13	1	18	ASN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	28	ASN
14	2	157	HIS
14	2	161	GLN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	IML	4	2	15	7,8,9	2.22	1 (14%)	8,9,11	1.46	2 (25%)
15	IML	3	2	15	7,8,9	2.36	2 (28%)	8,9,11	1.46	2 (25%)

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
15	IML	4	2	15	-	0/10/10/12	-
15	IML	3	2	15	-	0/10/10/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	4	2	IML	OXT-C	-5.18	1.20	1.42
15	3	2	IML	OXT-C	-4.96	1.21	1.42
15	3	2	IML	CB-CA	2.31	1.59	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	4	2	IML	OXT-C-CA	3.13	118.69	111.09
15	3	2	IML	C-CA-CB	2.74	122.88	114.25
15	3	2	IML	OXT-C-CA	2.65	117.53	111.09
15	4	2	IML	C-CA-CB	2.31	121.52	114.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1:THR	C	2:THR	N	1.14

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.