



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 01:10 pm GMT

PDB ID : 5T0G
EMDB ID: : EMD-8334
Title : Structural basis for dynamic regulation of the human 26S proteasome
Authors : Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.;
Kirschner, M.W.; Mao, Y.
Deposited on : 2016-08-16
Resolution : 4.40 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

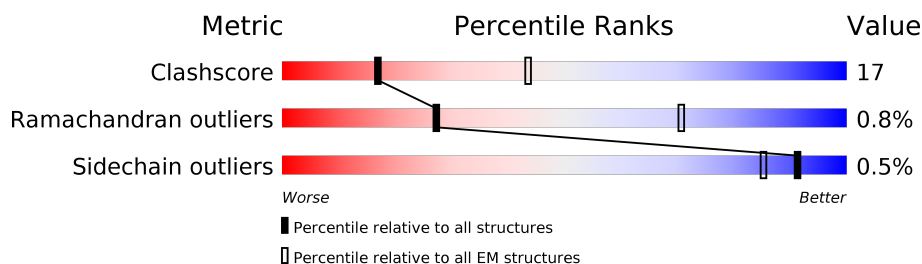
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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

Mol	Chain	Length	Quality of chain
1	G	245	
2	H	233	
3	I	260	
4	J	247	
5	K	240	
6	L	268	
7	M	254	
8	N	238	
9	O	276	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	P	204	
11	Q	201	
12	R	262	
13	S	240	
14	T	263	
15	A	433	
16	B	440	
17	D	418	
18	E	403	
19	F	439	
20	C	398	
21	U	953	
22	V	533	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	309	
30	d	349	
31	e	70	
32	f	749	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 77800 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	233	Total	C	N	O	S	0	0
			1713	1084	290	334	5		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 15 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A	361	Total	C	N	O	S	0	0
			2835	1788	501	528	18		

- Molecule 16 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	B	341	Total	C	N	O	S	0	0
			2662	1671	453	526	12		

- Molecule 17 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	E	353	Total	C	N	O	S	0	0
			2790	1755	494	525	16		

- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	F	366	Total	C	N	O	S	0	0
			2863	1802	496	549	16		

- Molecule 20 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	384	Total	C	N	O	S	0	0
			3015	1894	540	564	17		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	806	Total	C	N	O	S	0	0
			6287	3990	1075	1178	44		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

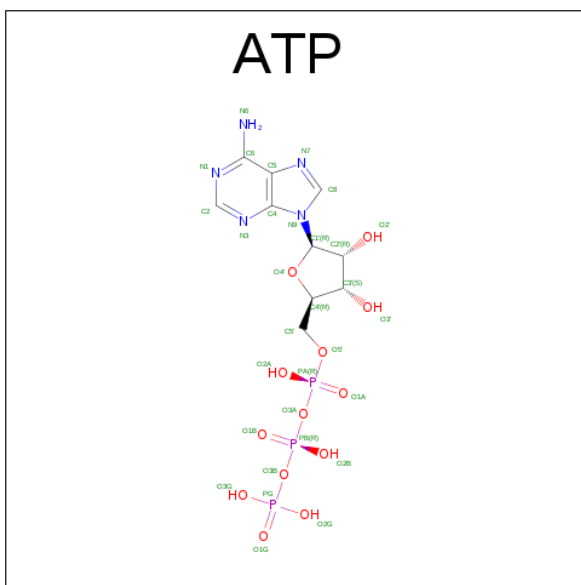
- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	694	Total	C	N	O	S	0	0
			5331	3364	899	1027	41		

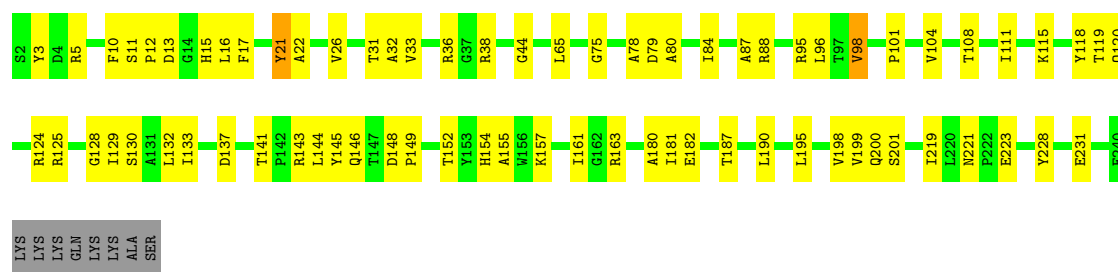
- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
34	c	1	Total Zn 1 1	0



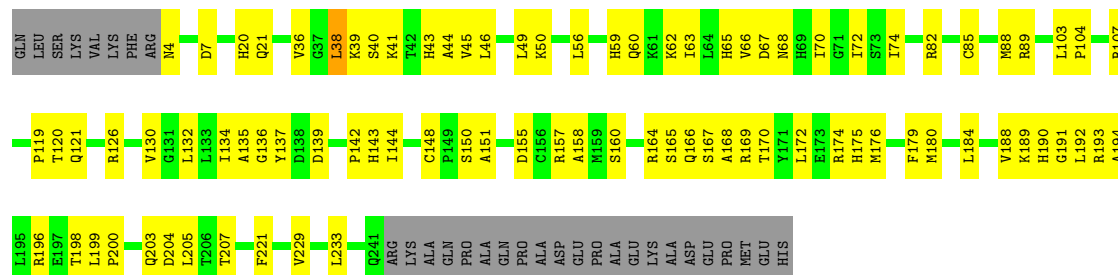
• Molecule 5: Proteasome subunit alpha type-5

Chain K: 64% 30% 5%



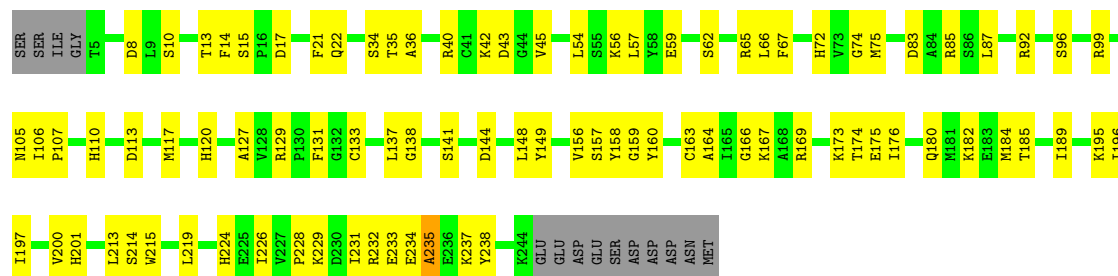
• Molecule 6: Proteasome subunit alpha type-1

Chain L: 56% 32% 11%



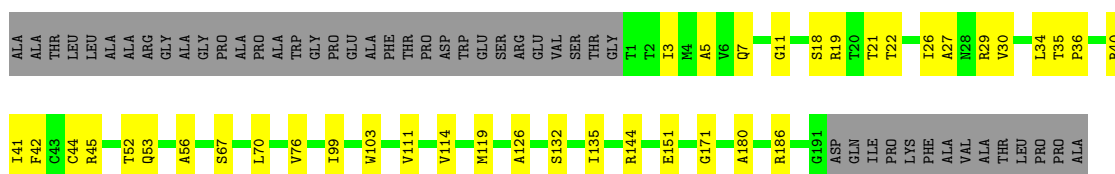
• Molecule 7: Proteasome subunit alpha type-3

Chain M: 60% 34% 6%

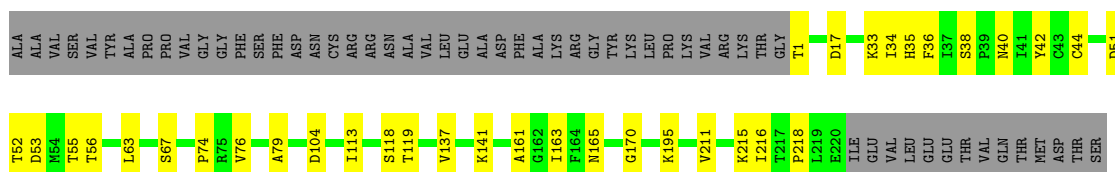


• Molecule 8: Proteasome subunit beta type-6

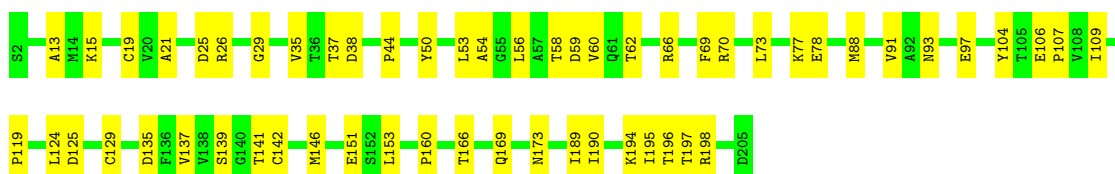
Chain N: 64% 16% 20%



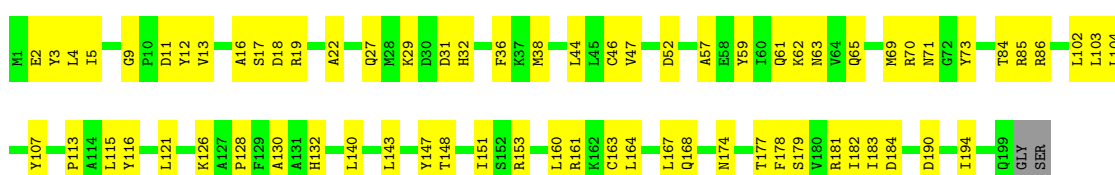
• Molecule 9: Proteasome subunit beta type-7



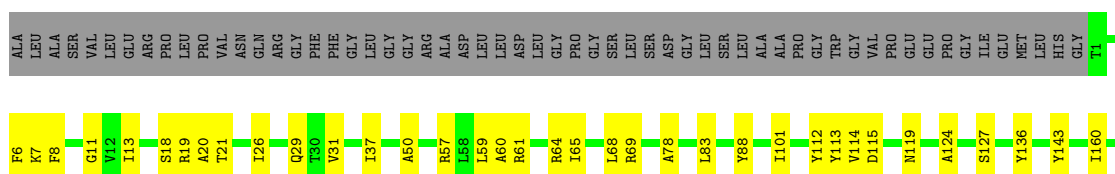
• Molecule 10: Proteasome subunit beta type-3



• Molecule 11: Proteasome subunit beta type-2

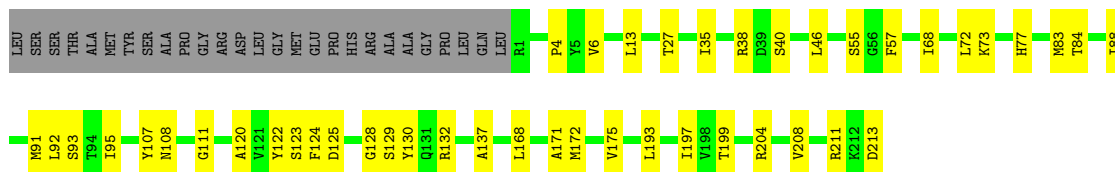


• Molecule 12: Proteasome subunit beta type-5



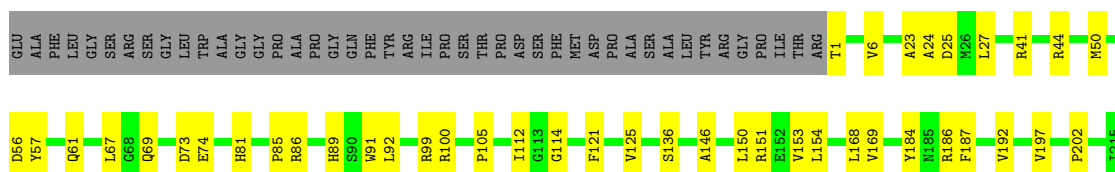
• Molecule 13: Proteasome subunit beta type-1

Chain S:



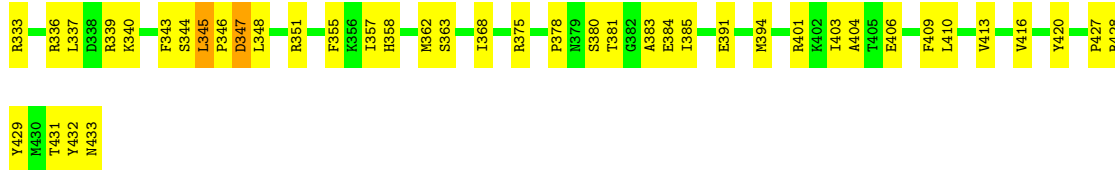
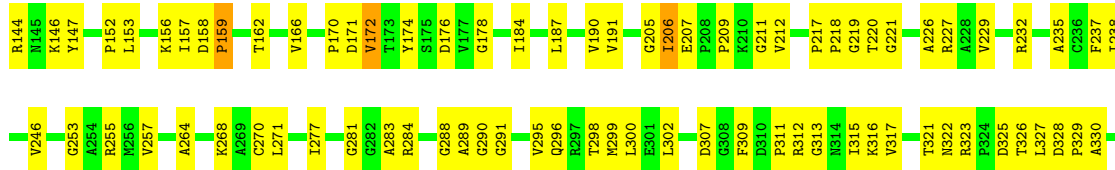
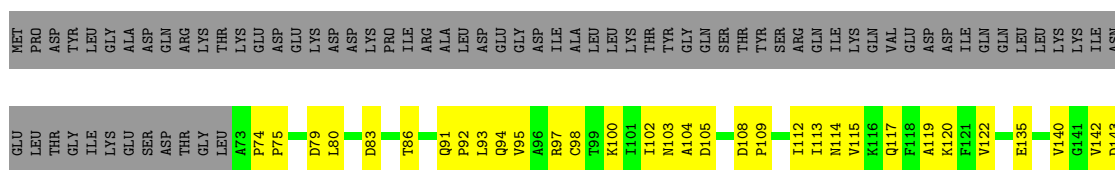
- Molecule 14: Proteasome subunit beta type-4

Chain T:



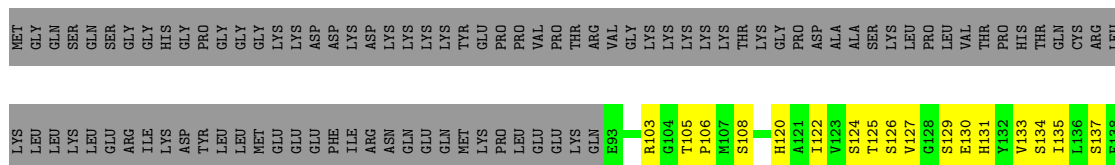
- Molecule 15: 26S protease regulatory subunit 7

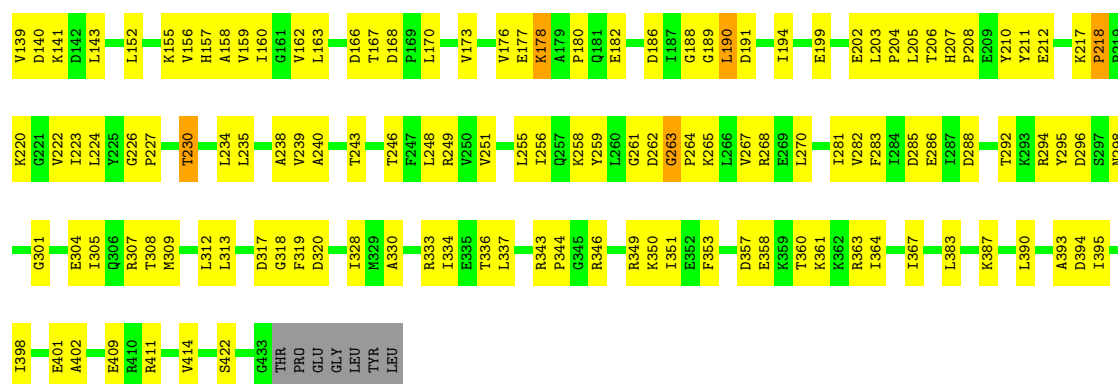
Chain A:



- Molecule 16: 26S protease regulatory subunit 4

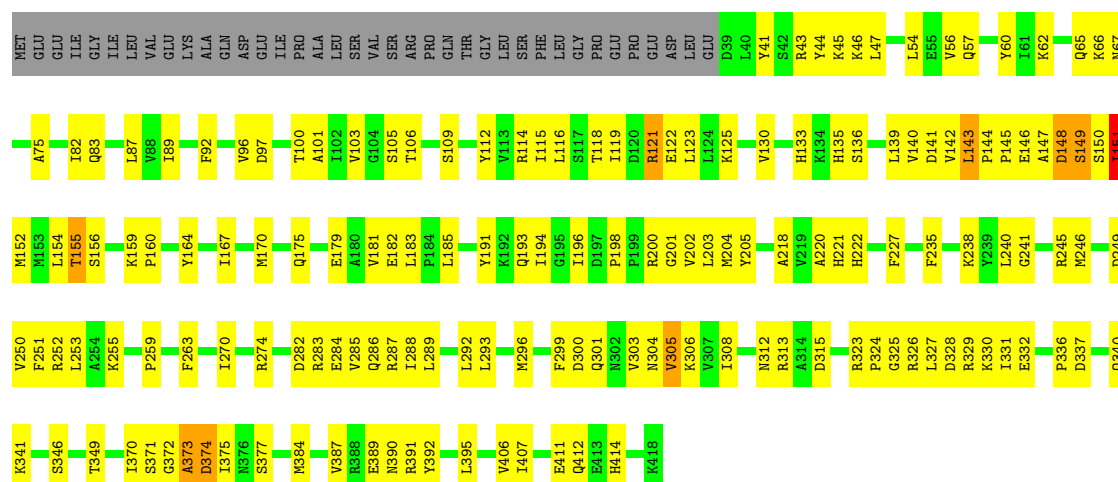
Chain B:





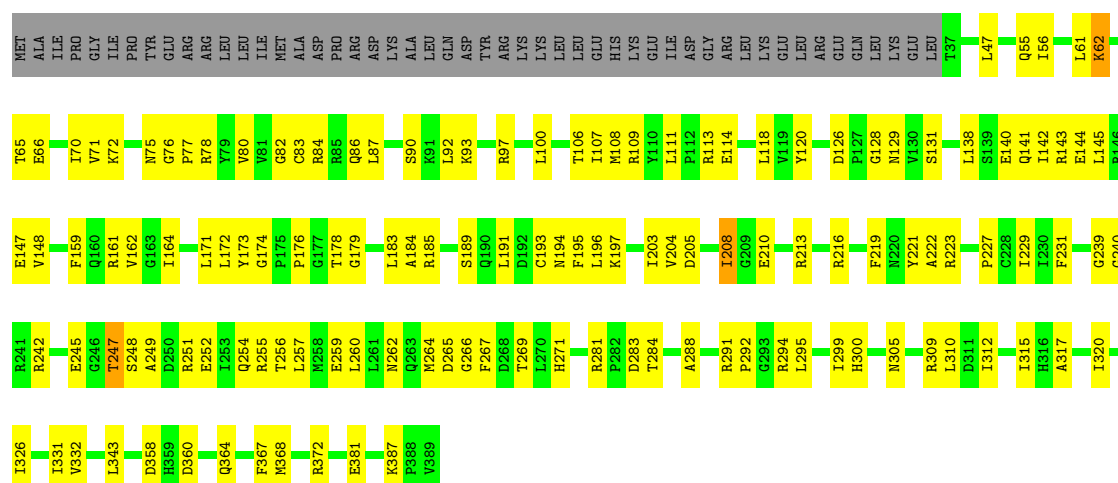
• Molecule 17: 26S protease regulatory subunit 6B

Chain D: 53% 36% 9%




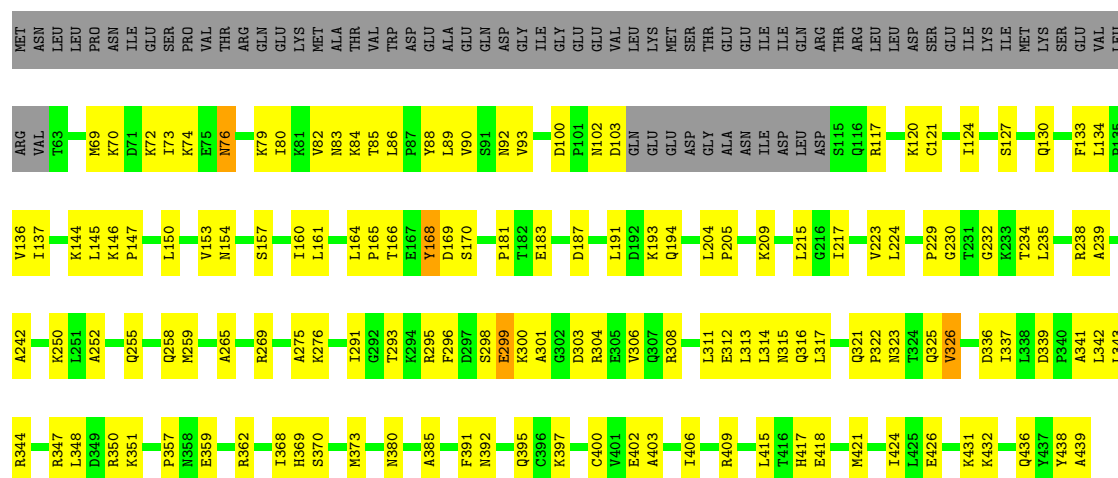
• Molecule 18: 26S protease regulatory subunit 10B

Chain E: 55% 32% 12%



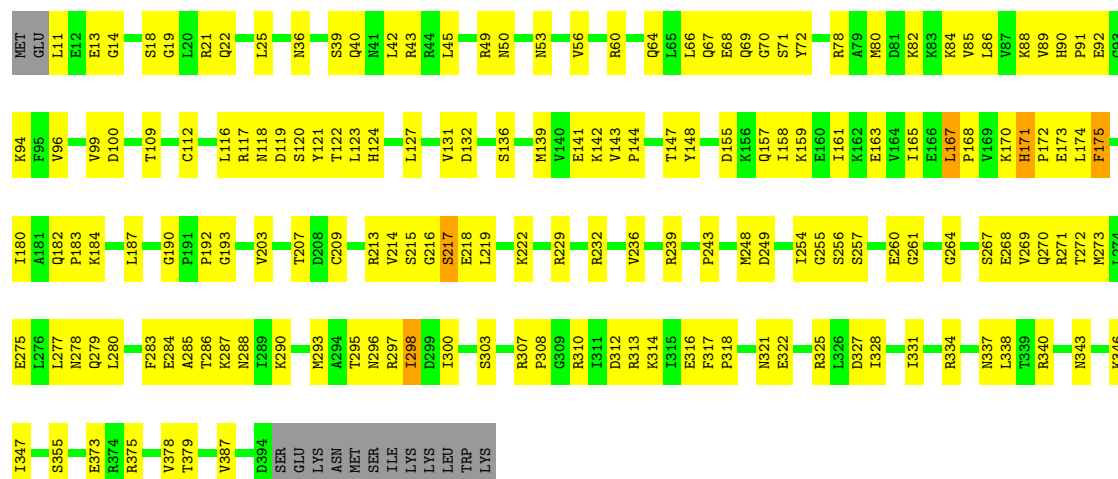
• Molecule 19: 26S protease regulatory subunit 6A

Chain F: 



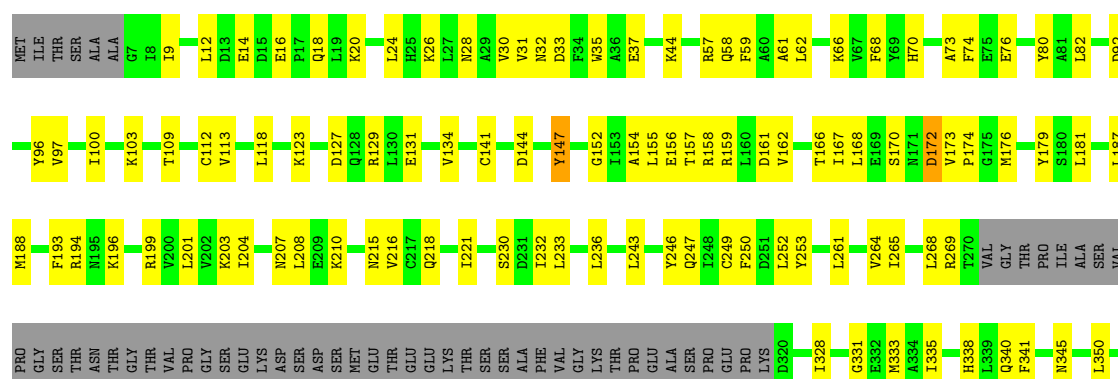
• Molecule 20: 26S protease regulatory subunit 8

Chain C: 

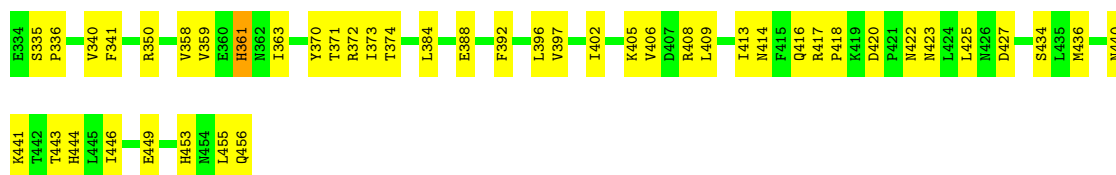


• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 

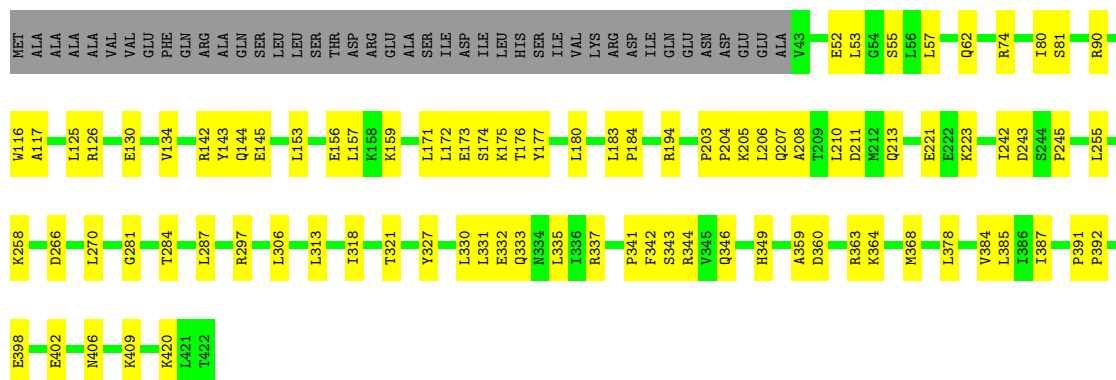






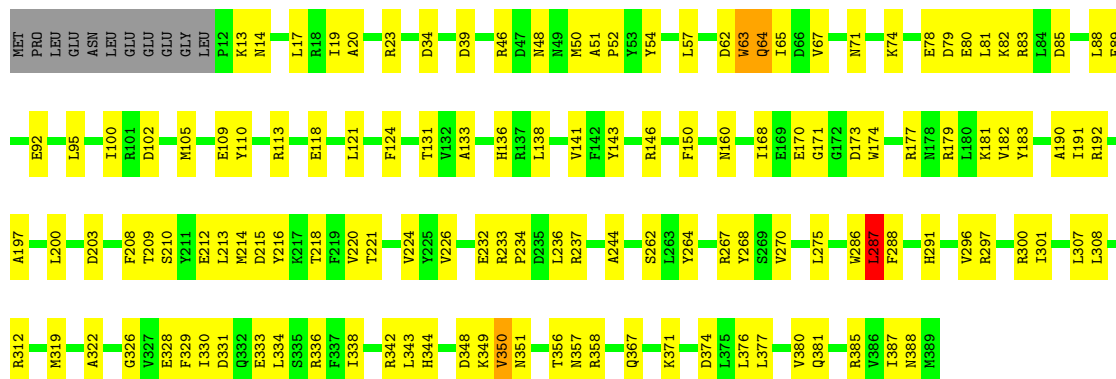
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 69% 21% 10%



- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 63% 33% 4%



- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

Chain Z: 55% 32% 12%



GLU
SER
LYS
LYS
ASP
ARG
LYS
GLU
ASP
LYS
GLU
LYS
ASP
LYS
ASP
LYS
GLU
LYS
SER
SER
ASP
VAL
LYS
LYS
GLU
GLU
LYS
LYS
GLU
LYS

- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

Chain a: 98% .

MET
LYS
ASP
V4
H69
L145
I166
D260
V336
V340
T376

- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain b:  50% 49%

[illegible]

GLY ILE THR THR GLY THR GLU ASP SER ASP ASP ALA LEU LEU LEU LYS MET THR ILE SER GLN GLN PHE GLY ARG THR GLY LEU LEU PRO ASP LEU LEU SER SER MET MET THR GLU GLU GLU GLN ILE ALA TYR ALA MET MET MET SER LEU LEU GLN GLY GLY PHE GLY ALA GLU ALA SER

ASP
ILE
ASP
SER
SER
ALA
MET
ASP
THR
SER
GLU
SER
PRO
ALA
LYS
GLU
GLU
ASP
TYR
ASP
ASP
VAL
MET
GLN
ASP
PRO
GLU
PHE
LEU
GLN
SER
VAL
GLU
LEU
ASN
PRO
GLY
VAL
ASP
PRO
ASN
ASN
GLU
ALA
ILE
ARG
ASN
ALA
MET
GLY
SER
LEU
ALA
SER
GLN
ALA
THR
LYS
ASP

GLY
LYS
LYS
ASP
LYS
LYS
GLU
GLU
ASP
LYS
LYS

- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

Chain c: 90% • 7%

ASP	ARG	LEU	ARG	LEU	GLY	GLY	MET	PRO	GLY	LEU	GLY	GLN	GLY	PRO	PRO	THR	ASP	ALA	PRO	A24	L38	P105	V151	V156	I157	I189	Y234	S243	V244	K310
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------

- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 72% . 26%

PHE	ILE	LYS	GLY	ARG	ALA	PRO	ARG	ALA	ALA	PRO	PRO	ARG	ARG	GLU	ARG	ARG	ALA	ALA	THR	ARG	GLY	LEU	GLY	ARG	GLN	VAL	VAL	ALA	ALA	PRO	PRO	PRO	ARG	ALA	ALA	LEU	GLY	THR	SER	SER	ARG	ALA	ALA	VAL	SER	CYS	ARG	ARG	ARG	CYS	LYS	ARG	GLY	GLY	LEU	LEU	ALA	ALA	SER
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ARG	LYS	MET	ALA	ALA	ALA	ALA	VAL	ASN	GLY	ALA	ALA	GLY	PHE	SER	SER	SER	GLY	PRO	ALA	ALA	THR	SER	GLY	VAL	LEU	GLN	ALA	ALA	THR	GLY	M1	Y2	E3		P37		R213	G214		V257
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----	--	-----	--	------	------	--	------

- Molecule 31: 26S proteasome complex subunit DSS1

Chain e:  56% . 43%

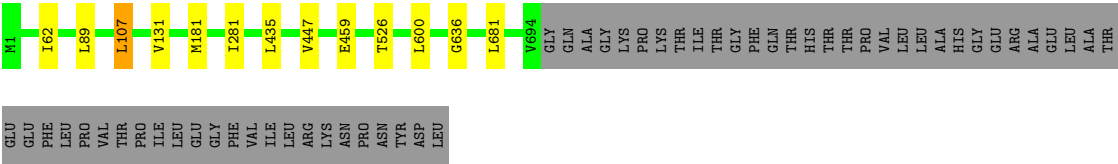
M1		K4		D9	LEU	GLY	LEU	LEU	GLU	GLU	ASP	ASP	GLU	PHE	GLU	GLU	PHE	PRO	ALA	GLU	ASP	TRP	ALA	GLY	LEU	ASP	GLU	ASP	GLU	ASP	ALA	HIS	VAL	TRP	E40	S70
----	--	----	--	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

Chain f:

91%

7%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	139236	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	G	0.30	0/1859	0.50	0/2523
10	P	0.28	0/1614	0.47	0/2177
11	Q	0.29	0/1603	0.49	0/2174
12	R	0.28	0/1579	0.45	0/2134
13	S	0.28	0/1671	0.47	0/2253
14	T	0.28	0/1700	0.46	0/2305
15	A	0.30	0/2886	0.53	0/3899
16	B	0.29	0/2700	0.51	0/3645
17	D	0.31	0/3090	0.59	2/4168 (0.0%)
18	E	0.30	0/2835	0.52	1/3821 (0.0%)
19	F	0.29	0/2903	0.51	1/3912 (0.0%)
2	H	0.30	0/1747	0.49	0/2376
20	C	0.29	0/3054	0.56	3/4107 (0.1%)
21	U	0.29	0/6396	0.49	0/8646
22	V	0.31	0/3929	0.57	0/5309
23	W	0.29	0/3751	0.54	3/5042 (0.1%)
24	X	0.27	0/3053	0.44	0/4115
25	Y	0.30	0/3173	0.53	2/4273 (0.0%)
26	Z	0.27	0/2324	0.55	0/3150
27	a	0.36	1/3053 (0.0%)	0.52	0/4133
28	b	0.27	0/1478	0.48	0/2001
29	c	0.33	0/2302	0.60	1/3110 (0.0%)
3	I	0.29	0/1942	0.51	0/2628
30	d	0.30	0/2162	0.57	0/2919
31	e	0.28	0/338	0.56	0/450
32	f	0.33	2/5413 (0.0%)	0.63	3/7317 (0.0%)
4	J	0.28	0/1728	0.48	0/2358
5	K	0.28	0/1747	0.48	0/2364
6	L	0.28	0/1885	0.48	0/2552
7	M	0.28	0/1891	0.46	0/2552
8	N	0.28	0/1454	0.48	0/1967
9	O	0.27	0/1670	0.49	0/2265

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
All	All	0.30	3/78930 (0.0%)	0.52	16/106645 (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
17	D	0	1
20	C	0	1
29	c	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	145	LEU	C-N	11.92	1.56	1.34
32	f	681	LEU	C-N	6.42	1.46	1.34
32	f	181	MET	C-N	-5.33	1.21	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	167	LEU	CB-CG-CD2	6.98	122.86	111.00
32	f	459	GLU	N-CA-C	6.02	127.25	111.00
20	C	217	SER	C-N-CA	5.95	136.58	121.70
17	D	151	ILE	C-N-CA	5.85	136.32	121.70
32	f	107	LEU	CA-CB-CG	5.62	128.22	115.30
25	Y	63	TRP	C-N-CA	5.52	135.51	121.70
23	W	40	LEU	CA-CB-CG	5.50	127.95	115.30
23	W	92	LYS	C-N-CA	5.44	135.31	121.70
32	f	636	GLY	N-CA-C	5.43	126.68	113.10
25	Y	287	LEU	CA-CB-CG	5.42	127.78	115.30
19	F	204	LEU	CA-CB-CG	5.37	127.64	115.30
23	W	135	LYS	C-N-CA	5.33	135.04	121.70
29	c	243	SER	C-N-CA	5.33	135.03	121.70
20	C	217	SER	CA-C-N	5.27	128.79	117.20
17	D	373	ALA	C-N-CA	5.04	134.31	121.70
18	E	62	LYS	CD-CE-NZ	5.04	123.28	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	C	171	HIS	Peptide
17	D	148	ASP	Peptide
29	c	243	SER	Peptide

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	G	1826	0	1796	69	0
2	H	1713	0	1598	58	0
3	I	1912	0	1851	60	0
4	J	1704	0	1517	59	0
5	K	1722	0	1673	64	0
6	L	1850	0	1822	72	0
7	M	1856	0	1814	66	0
8	N	1430	0	1398	24	0
9	O	1643	0	1644	23	0
10	P	1585	0	1598	40	0
11	Q	1570	0	1547	51	0
12	R	1548	0	1499	30	0
13	S	1641	0	1618	30	0
14	T	1667	0	1628	31	0
15	A	2835	0	2879	133	0
16	B	2662	0	2702	134	0
17	D	3040	0	3076	158	0
18	E	2790	0	2846	113	0
19	F	2863	0	2931	110	0
20	C	3015	0	3125	160	0
21	U	6287	0	6338	169	0
22	V	3852	0	3893	155	0
23	W	3703	0	3822	127	0
24	X	3009	0	3113	63	0
25	Y	3115	0	3120	99	0
26	Z	2281	0	2312	99	0
27	a	2995	0	3012	0	0
28	b	1458	0	1505	0	0
29	c	2260	0	2276	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	2116	0	2146	0	0
31	e	334	0	294	0	0
32	f	5331	0	5343	0	0
33	A	31	0	12	2	0
33	B	31	0	12	3	0
33	C	31	0	12	1	0
33	D	31	0	12	3	0
33	E	31	0	12	4	0
33	F	31	0	12	3	0
34	c	1	0	0	0	0
All	All	77800	0	77808	1973	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 (1973) 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)
26:Z:261:TYR:O	26:Z:265:LEU:HD13	1.20	1.35
26:Z:261:TYR:O	26:Z:265:LEU:CD1	1.86	1.24
20:C:217:SER:HB3	20:C:218:GLU:HB3	1.38	1.02
26:Z:261:TYR:C	26:Z:265:LEU:HD13	1.79	1.01
17:D:152:MET:CE	18:E:62:LYS:HG3	1.94	0.97
17:D:83:GLN:HE22	17:D:140:VAL:HG21	1.29	0.96
21:U:517:GLY:O	21:U:554:LEU:HD22	1.69	0.93
12:R:19:ARG:HE	12:R:29:GLN:HE22	1.18	0.90
26:Z:222:ILE:HG23	26:Z:223:ASN:HB3	1.54	0.89
25:Y:179:ARG:NH2	25:Y:212:GLU:OE2	2.07	0.88
17:D:201:GLY:HA3	17:D:327:LEU:HA	1.56	0.86
20:C:86:LEU:HD23	20:C:96:VAL:HB	1.58	0.86
7:M:36:ALA:HB2	7:M:65:ARG:HH21	1.41	0.85
20:C:229:ARG:HH12	20:C:232:ARG:HE	1.25	0.84
16:B:296:ASP:HB2	20:C:268:GLU:HG3	1.59	0.84
16:B:180:PRO:HG2	16:B:239:VAL:HG23	1.59	0.83
23:W:40:LEU:HB2	23:W:41:GLN:HA	1.60	0.83
4:J:88:ARG:HH22	11:Q:69:MET:HB2	1.42	0.83
22:V:57:ALA:HB3	22:V:58:ALA:HB3	1.60	0.83
6:L:67:ASP:HB3	6:L:70:ILE:HB	1.61	0.83
26:Z:224:HIS:HB3	26:Z:225:GLN:HA	1.60	0.83
6:L:151:ALA:O	7:M:85:ARG:NH2	2.12	0.83
20:C:22:GLN:HA	20:C:25:LEU:HD13	1.61	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:143:LEU:HD11	17:D:147:ALA:H	1.43	0.83
23:W:47:LEU:O	23:W:51:GLU:OE1	1.97	0.83
19:F:300:LYS:HD2	19:F:304:ARG:HE	1.43	0.82
22:V:153:LYS:O	22:V:157:THR:HG23	1.79	0.82
26:Z:33:LYS:NZ	26:Z:34:ARG:O	2.12	0.82
17:D:152:MET:HE1	18:E:62:LYS:HG3	1.60	0.82
22:V:321:ALA:HB1	22:V:322:VAL:HB	1.59	0.82
23:W:92:LYS:H	23:W:93:ARG:HB3	1.47	0.80
19:F:183:GLU:HG2	19:F:239:ALA:HB2	1.63	0.80
6:L:148:CYS:HG	6:L:150:SER:HG	1.28	0.80
1:G:22:LEU:HD13	1:G:25:VAL:HB	1.63	0.80
2:H:231:ALA:HB3	2:H:232:ALA:HB3	1.62	0.80
15:A:368:ILE:HG12	15:A:406:GLU:HB3	1.63	0.79
20:C:99:VAL:HA	20:C:100:ASP:HB2	1.64	0.79
19:F:191:LEU:HG	19:F:194:GLN:HE21	1.48	0.79
21:U:154:ALA:HB2	21:U:166:THR:HG21	1.64	0.79
21:U:799:LYS:HA	21:U:843:GLU:HG3	1.65	0.79
22:V:255:LEU:HD22	22:V:291:TYR:HB3	1.65	0.79
14:T:99:ARG:HG3	14:T:105:PRO:HA	1.63	0.79
2:H:123:GLN:HB2	3:I:128:ARG:HH21	1.49	0.78
23:W:268:LYS:HD3	23:W:299:ILE:HG21	1.64	0.78
4:J:104:VAL:HB	4:J:143:ARG:HD3	1.64	0.78
23:W:406:VAL:HG12	23:W:413:ILE:HB	1.65	0.78
11:Q:36:PHE:HB2	11:Q:44:LEU:HB3	1.66	0.78
23:W:257:GLN:HA	23:W:258:ALA:HB3	1.64	0.78
21:U:554:LEU:O	21:U:554:LEU:HD23	1.84	0.77
17:D:286:GLN:NE2	20:C:218:GLU:OE2	2.17	0.77
23:W:136:ILE:H	23:W:141:GLU:HG2	1.48	0.77
22:V:228:ARG:HH21	22:V:257:ASN:HB3	1.48	0.77
19:F:168:TYR:HB2	19:F:169:ASP:HB2	1.66	0.77
15:A:190:VAL:HG23	15:A:209:PRO:HG2	1.67	0.77
15:A:383:ALA:HB3	16:B:343:ARG:HH11	1.50	0.77
20:C:78:ARG:HB3	20:C:86:LEU:HD12	1.67	0.77
16:B:105:THR:HG23	16:B:106:PRO:HD3	1.67	0.77
19:F:83:ASN:O	19:F:154:ASN:ND2	2.18	0.76
22:V:67:LEU:HD21	22:V:205:LEU:HD23	1.67	0.76
23:W:257:GLN:HE22	23:W:262:LYS:HD2	1.51	0.76
15:A:413:VAL:HA	15:A:416:VAL:HG12	1.67	0.76
21:U:474:ARG:HH21	21:U:500:ASN:HB2	1.48	0.76
16:B:333:ARG:HD2	16:B:336:THR:HG23	1.66	0.76
26:Z:164:ALA:HB1	26:Z:168:GLU:HG3	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:261:TYR:O	26:Z:265:LEU:HD12	1.86	0.76
22:V:494:MET:HG3	26:Z:278:ASN:HD22	1.49	0.76
17:D:116:LEU:HD23	17:D:118:THR:H	1.51	0.76
15:A:211:GLY:HA3	15:A:317:VAL:HG23	1.67	0.76
3:I:8:ARG:HE	4:J:5:ARG:HH21	1.34	0.76
7:M:175:GLU:HG3	7:M:196:ILE:HG12	1.68	0.76
3:I:213:ILE:HB	3:I:228:LEU:HD11	1.66	0.76
17:D:115:ILE:HG22	17:D:139:LEU:HD12	1.66	0.75
4:J:11:SER:OG	4:J:15:HIS:O	2.02	0.75
23:W:44:ILE:HB	23:W:93:ARG:HD2	1.68	0.75
2:H:222:THR:OG1	2:H:225:GLU:OE1	2.04	0.75
23:W:416:GLN:HB3	23:W:417:ARG:HA	1.67	0.75
16:B:240:ALA:O	16:B:243:THR:OG1	2.05	0.74
15:A:232:ARG:NE	15:A:235:ALA:O	2.12	0.74
24:X:420:LYS:O	26:Z:283:ARG:NH2	2.19	0.74
21:U:607:VAL:O	21:U:615:ARG:NH1	2.20	0.74
8:N:5:ALA:HB3	8:N:126:ALA:HB3	1.69	0.74
5:K:107:MET:HG2	5:K:111:SER:OG	1.87	0.74
23:W:414:ASN:ND2	23:W:416:GLN:O	2.21	0.73
23:W:186:ILE:O	23:W:189:GLN:NE2	2.21	0.73
17:D:154:LEU:HD23	17:D:155:THR:H	1.51	0.73
2:H:39:LYS:HE2	2:H:144:PRO:HG2	1.69	0.73
23:W:340:VAL:HG13	23:W:350:ARG:HD2	1.70	0.73
15:A:218:PRO:HD3	15:A:428:ARG:HE	1.53	0.73
21:U:147:TYR:OH	21:U:170:SER:O	2.06	0.73
25:Y:89:GLU:HA	25:Y:92:GLU:HG2	1.70	0.73
26:Z:37:GLY:HA2	26:Z:56:VAL:HG12	1.70	0.73
23:W:90:LEU:HD11	23:W:135:LYS:HD3	1.71	0.73
15:A:217:PRO:HA	15:A:428:ARG:HG2	1.69	0.73
17:D:312:ASN:HD21	18:E:242:ARG:HH22	1.34	0.73
25:Y:268:TYR:HB2	25:Y:322:ALA:HB1	1.70	0.73
15:A:166:VAL:HA	15:A:238:ILE:HG13	1.71	0.73
23:W:173:THR:HG23	23:W:182:ARG:HH11	1.53	0.73
2:H:4:ARG:HD3	7:M:127:ALA:HB2	1.70	0.73
18:E:381:GLU:HG3	19:F:351:LYS:HD2	1.70	0.72
10:P:62:THR:OG1	11:Q:85:ARG:NH2	2.18	0.72
17:D:193:GLN:O	20:C:337:ASN:ND2	2.21	0.72
21:U:842:LYS:HA	21:U:843:GLU:HB3	1.71	0.72
16:B:176:VAL:HG22	16:B:177:GLU:HB2	1.70	0.72
20:C:18:SER:HA	20:C:21:ARG:HB2	1.69	0.72
18:E:128:GLY:O	18:E:189:SER:OG	2.07	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:266:GLY:HA2	18:E:267:PHE:HB2	1.71	0.72
15:A:174:TYR:HD1	15:A:227:ARG:HD2	1.56	0.71
20:C:187:LEU:HD11	20:C:314:LYS:HD2	1.72	0.71
5:K:85:ALA:HB2	5:K:139:VAL:HG21	1.72	0.71
6:L:160:SER:O	6:L:169:ARG:NH2	2.23	0.71
18:E:97:ARG:HD2	18:E:111:LEU:HD11	1.71	0.71
15:A:218:PRO:HB3	15:A:428:ARG:HH21	1.55	0.71
19:F:137:ILE:HG21	19:F:160:ILE:HB	1.71	0.71
26:Z:233:VAL:HA	26:Z:236:LEU:HD13	1.72	0.71
17:D:89:ILE:HD11	18:E:80:VAL:HG13	1.72	0.71
19:F:276:LYS:NZ	19:F:325:GLN:OE1	2.24	0.71
11:Q:38:MET:HA	11:Q:61:GLN:HE22	1.55	0.71
5:K:167:ALA:HB3	5:K:181:LEU:HD21	1.73	0.71
21:U:518:LEU:HD23	21:U:554:LEU:HD11	1.73	0.71
21:U:611:ASN:HB3	21:U:614:VAL:HG12	1.72	0.71
15:A:94:GLN:O	16:B:131:HIS:NE2	2.23	0.70
1:G:144:ASP:HB3	1:G:147:GLN:HB2	1.73	0.70
23:W:373:ILE:HG23	23:W:413:ILE:HG13	1.71	0.70
26:Z:7:GLN:OE1	26:Z:46:LYS:NZ	2.24	0.70
4:J:115:LYS:HE2	4:J:149:PRO:HA	1.72	0.70
4:J:120:GLN:OE1	5:K:134:SER:N	2.24	0.70
10:P:29:GLY:HA2	10:P:35:VAL:HG23	1.73	0.70
20:C:175:PHE:CE2	20:C:182:GLN:HG3	2.26	0.70
22:V:212:TYR:OH	22:V:287:ARG:NH2	2.24	0.70
25:Y:381:GLN:HB3	25:Y:385:ARG:HH12	1.55	0.70
19:F:238:ARG:HH11	19:F:250:LYS:HG2	1.57	0.70
15:A:191:VAL:HG23	15:A:316:LYS:HE2	1.72	0.70
16:B:177:GLU:H	16:B:178:LYS:HA	1.57	0.70
6:L:168:ALA:HB1	6:L:194:ALA:HB1	1.73	0.70
26:Z:222:ILE:HG23	26:Z:223:ASN:CB	2.21	0.70
21:U:356:THR:HG21	21:U:731:ILE:HD13	1.74	0.70
3:I:218:ARG:NH1	3:I:223:THR:OG1	2.25	0.70
21:U:522:GLY:O	21:U:559:ARG:NH2	2.25	0.70
16:B:103:ARG:HD3	16:B:160:ILE:HG12	1.71	0.69
6:L:174:ARG:HG3	6:L:175:HIS:ND1	2.07	0.69
6:L:66:VAL:HG13	6:L:89:ARG:HD3	1.73	0.69
15:A:92:PRO:HB2	15:A:93:LEU:HD12	1.71	0.69
23:W:123:ARG:HH12	23:W:127:THR:HB	1.56	0.69
24:X:194:ARG:HD2	24:X:210:LEU:HD21	1.74	0.69
19:F:392:ASN:HB2	19:F:395:GLN:HG3	1.74	0.69
19:F:298:SER:HB3	19:F:299:GLU:HG3	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:8:PHE:HE1	12:R:13:ILE:HG12	1.58	0.69
21:U:447:GLY:HA3	21:U:480:GLY:HA2	1.73	0.69
22:V:379:LEU:HD13	22:V:395:ILE:HG12	1.72	0.69
18:E:47:LEU:HD13	19:F:80:ILE:HG12	1.72	0.69
7:M:195:LYS:HG3	7:M:196:ILE:HD12	1.75	0.69
21:U:341:PHE:HB2	21:U:881:PRO:HD2	1.74	0.69
24:X:255:LEU:HD12	24:X:287:LEU:HD13	1.74	0.69
25:Y:344:HIS:HB3	25:Y:358:ARG:HG2	1.73	0.69
18:E:288:ALA:O	18:E:294:ARG:NH1	2.26	0.69
17:D:392:TYR:HB2	23:W:135:LYS:HA	1.75	0.68
23:W:409:LEU:HD21	24:X:344:ARG:HG2	1.74	0.68
21:U:155:LEU:O	21:U:158:ARG:NH1	2.25	0.68
15:A:170:PRO:HA	15:A:229:VAL:HG12	1.73	0.68
22:V:94:VAL:HG22	22:V:138:PRO:HD3	1.74	0.68
26:Z:105:ASP:HA	26:Z:108:ILE:HD13	1.74	0.68
15:A:333:ARG:HH12	15:A:340:LYS:HD3	1.58	0.68
17:D:82:ILE:HD11	20:C:60:ARG:HH21	1.58	0.68
21:U:406:ALA:HA	21:U:445:ALA:HB2	1.75	0.68
16:B:317:ASP:HB3	16:B:318:GLY:HA2	1.73	0.68
7:M:40:ARG:HH11	7:M:148:LEU:HB3	1.58	0.68
17:D:159:LYS:HB3	17:D:160:PRO:HA	1.75	0.68
12:R:7:LYS:O	12:R:143:TYR:OH	2.10	0.68
26:Z:142:GLU:OE2	26:Z:153:LYS:NZ	2.27	0.68
15:A:157:ILE:HG22	15:A:158:ASP:HB2	1.75	0.68
2:H:160:ALA:H	3:I:55:LEU:HD21	1.59	0.68
3:I:122:THR:O	4:J:125:ARG:NH1	2.27	0.68
9:O:38:SER:OG	9:O:40:ASN:OD1	2.12	0.68
13:S:55:SER:HB3	13:S:107:TYR:HB2	1.76	0.68
17:D:67:ASN:HD22	21:U:607:VAL:HG12	1.58	0.68
5:K:71:ASP:HB3	5:K:74:ILE:HB	1.75	0.68
1:G:206:LEU:HB3	1:G:208:ILE:HG12	1.75	0.67
22:V:479:ARG:NH2	25:Y:374:ASP:OD1	2.27	0.67
16:B:205:LEU:CD2	16:B:206:THR:HG23	2.24	0.67
6:L:7:ASP:O	6:L:21:GLN:NE2	2.26	0.67
22:V:466:ILE:HG23	22:V:467:TYR:H	1.58	0.67
8:N:40:ARG:NH1	8:N:180:ALA:O	2.27	0.67
8:N:67:SER:HA	8:N:70:LEU:HD12	1.76	0.67
21:U:885:MET:HB3	21:U:888:GLN:HG3	1.76	0.67
23:W:169:LEU:O	23:W:182:ARG:NH1	2.27	0.67
19:F:291:ILE:HB	19:F:306:VAL:HG11	1.77	0.67
21:U:109:THR:OG1	21:U:156:GLU:O	2.11	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:401:ARG:HH12	15:A:404:ALA:HA	1.60	0.67
22:V:455:LYS:N	22:V:456:GLY:HA2	2.10	0.67
26:Z:262:LEU:HD23	26:Z:265:LEU:HD22	1.76	0.67
15:A:218:PRO:HB3	15:A:428:ARG:NH2	2.08	0.67
22:V:282:ASN:O	22:V:315:LYS:NZ	2.28	0.67
22:V:337:LEU:O	22:V:401:ASN:ND2	2.28	0.67
1:G:159:TYR:HB3	2:H:81:PRO:HG3	1.75	0.66
6:L:67:ASP:OD1	6:L:68:ASN:N	2.28	0.66
23:W:331:GLY:HA2	23:W:332:SER:HB3	1.77	0.66
15:A:381:THR:OG1	16:B:343:ARG:NH1	2.29	0.66
10:P:88:MET:HG3	10:P:124:LEU:HD11	1.77	0.66
21:U:35:TRP:HB3	21:U:70:HIS:CG	2.30	0.66
23:W:55:ARG:HH12	23:W:79:GLU:HG3	1.60	0.66
25:Y:13:LYS:HG2	25:Y:146:ARG:HD2	1.77	0.66
21:U:247:GLN:HE22	21:U:912:ILE:HG22	1.60	0.66
23:W:384:LEU:HD13	23:W:388:GLU:HB3	1.76	0.66
22:V:265:ASP:O	22:V:269:LYS:NZ	2.28	0.66
22:V:336:GLU:HA	22:V:339:LEU:HD12	1.77	0.66
15:A:380:SER:HB3	15:A:384:GLU:HB3	1.77	0.66
15:A:255:ARG:NH2	19:F:259:MET:SD	2.69	0.66
26:Z:43:TRP:HB3	26:Z:90:ARG:HH21	1.60	0.66
16:B:182:GLU:HB2	16:B:239:VAL:HG21	1.76	0.66
1:G:110:PRO:O	1:G:111:VAL:HG12	1.96	0.66
17:D:373:ALA:HB3	17:D:375:ILE:HG12	1.78	0.66
3:I:178:ASP:HB3	3:I:192:LEU:HD11	1.76	0.66
17:D:287:ARG:HD3	20:C:222:LYS:HE2	1.76	0.66
11:Q:148:THR:HB	11:Q:151:ILE:HB	1.77	0.66
17:D:283:ARG:HG3	17:D:286:GLN:HE21	1.61	0.66
9:O:63:LEU:HD11	9:O:79:ALA:HB2	1.77	0.66
22:V:345:ARG:HD3	22:V:361:PHE:HD1	1.61	0.66
17:D:389:GLU:HB2	17:D:391:ARG:HB2	1.78	0.65
10:P:21:ALA:HB2	10:P:189:ILE:HD13	1.78	0.65
23:W:48:LEU:HD12	23:W:96:GLN:HE22	1.60	0.65
16:B:264:PRO:O	16:B:267:VAL:N	2.28	0.65
17:D:151:ILE:HB	17:D:152:MET:HA	1.78	0.65
19:F:275:ALA:HB1	19:F:326:VAL:HG11	1.77	0.65
22:V:322:VAL:HG13	22:V:323:GLY:H	1.62	0.65
22:V:79:VAL:HG13	22:V:80:LYS:H	1.60	0.65
15:A:420:TYR:CE1	16:B:350:LYS:HG2	2.32	0.65
18:E:193:CYS:SG	18:E:194:ASN:N	2.69	0.65
1:G:23:TYR:O	1:G:26:GLU:HG2	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:144:ARG:NH2	8:N:151:GLU:OE1	2.30	0.65
22:V:250:LEU:HA	22:V:253:LEU:HD12	1.77	0.65
21:U:338:HIS:CE1	21:U:785:PRO:HB3	2.31	0.65
24:X:171:LEU:O	24:X:213:GLN:NE2	2.28	0.65
15:A:316:LYS:NZ	15:A:317:VAL:O	2.28	0.65
18:E:174:GLY:HA2	18:E:176:PRO:HD2	1.79	0.65
6:L:46:LEU:HD13	6:L:63:ILE:HD13	1.78	0.65
21:U:742:HIS:O	21:U:883:ARG:NH2	2.29	0.65
20:C:171:HIS:O	20:C:173:GLU:N	2.30	0.65
19:F:103:ASP:OD2	26:Z:88:ARG:NH2	2.30	0.65
12:R:59:LEU:HD22	12:R:83:LEU:HD13	1.79	0.65
20:C:170:LYS:HB3	25:Y:95:LEU:HD23	1.79	0.65
22:V:80:LYS:HB3	22:V:81:GLN:C	2.17	0.65
22:V:333:ILE:HD11	22:V:360:TYR:HE2	1.60	0.65
22:V:447:ILE:HG13	22:V:449:ALA:H	1.61	0.65
16:B:205:LEU:HD23	16:B:206:THR:HG23	1.78	0.64
4:J:36:ARG:HE	4:J:157:LYS:HA	1.62	0.64
21:U:68:PHE:HB3	21:U:73:ALA:HB3	1.79	0.64
20:C:19:GLY:HA2	22:V:195:ILE:HD11	1.79	0.64
22:V:190:ASP:HA	22:V:200:ARG:HH21	1.63	0.64
26:Z:97:THR:HA	26:Z:124:ILE:HG13	1.80	0.64
18:E:173:TYR:CZ	18:E:300:HIS:HB3	2.33	0.64
11:Q:13:VAL:HB	11:Q:183:ILE:HB	1.79	0.64
21:U:199:ARG:O	21:U:203:LYS:NZ	2.27	0.64
4:J:22:ALA:HB1	4:J:128:GLY:HA2	1.80	0.64
19:F:373:MET:N	19:F:373:MET:SD	2.71	0.64
7:M:92:ARG:NH2	14:T:73:ASP:OD1	2.30	0.64
26:Z:54:PHE:HB3	26:Z:82:PHE:HE2	1.63	0.64
22:V:228:ARG:O	22:V:232:HIS:ND1	2.31	0.64
5:K:69:GLU:O	5:K:93:ARG:NH2	2.30	0.64
22:V:333:ILE:HD11	22:V:360:TYR:CE2	2.32	0.64
26:Z:225:GLN:HG2	26:Z:228:TYR:HE2	1.63	0.64
15:A:205:GLY:HA2	15:A:206:ILE:HG22	1.79	0.63
20:C:295:THR:HG22	20:C:296:ASN:H	1.63	0.63
10:P:169:GLN:O	10:P:173:ASN:ND2	2.24	0.63
17:D:241:GLY:O	17:D:245:ARG:NH2	2.31	0.63
1:G:52:THR:HG22	1:G:53:GLN:H	1.64	0.63
22:V:167:LEU:HD11	22:V:171:VAL:HB	1.79	0.63
24:X:90:ARG:HH21	24:X:125:LEU:HA	1.63	0.63
18:E:178:THR:OG1	33:E:401:ATP:O2A	2.15	0.63
23:W:340:VAL:HG22	23:W:350:ARG:HH11	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:205:LEU:HD23	16:B:206:THR:N	2.14	0.63
5:K:93:ARG:NH1	12:R:68:LEU:O	2.32	0.63
21:U:215:ASN:OD1	21:U:216:VAL:N	2.30	0.63
25:Y:356:THR:HA	25:Y:357:ASN:CG	2.19	0.63
5:K:108:THR:O	5:K:111:SER:OG	2.16	0.63
20:C:175:PHE:CZ	20:C:182:GLN:HA	2.34	0.63
1:G:126:THR:HG22	2:H:128:ARG:HH22	1.64	0.63
2:H:65:VAL:HG22	2:H:75:VAL:HG12	1.81	0.63
4:J:108:THR:HG22	4:J:133:ILE:HD13	1.80	0.63
4:J:96:LEU:HA	11:Q:62:LYS:HE2	1.81	0.63
5:K:209:LYS:O	5:K:214:ASN:ND2	2.32	0.63
25:Y:356:THR:OG1	25:Y:357:ASN:O	2.14	0.63
19:F:86:LEU:HB2	19:F:88:TYR:CE1	2.33	0.63
26:Z:250:TYR:O	26:Z:254:ASN:HB2	1.98	0.63
15:A:429:TYR:O	15:A:433:ASN:ND2	2.31	0.62
16:B:259:TYR:OH	17:D:274:ARG:NH2	2.32	0.62
20:C:66:LEU:HG	20:C:70:GLY:HA2	1.79	0.62
23:W:408:ARG:HD2	24:X:346:GLN:HE22	1.64	0.62
11:Q:38:MET:O	11:Q:65:GLN:NE2	2.32	0.62
21:U:789:ILE:HG23	21:U:844:LYS:HE2	1.79	0.62
22:V:224:LEU:HD12	22:V:228:ARG:HG3	1.80	0.62
17:D:167:ILE:O	17:D:167:ILE:HD12	1.97	0.62
17:D:45:LYS:NZ	21:U:156:GLU:OE2	2.32	0.62
22:V:318:GLN:O	22:V:319:HIS:ND1	2.33	0.62
20:C:260:GLU:HB3	24:X:409:LYS:HE2	70.11	0.62
25:Y:190:ALA:O	25:Y:291:HIS:NE2	2.26	0.62
6:L:121:GLN:HE22	7:M:131:PHE:HE1	1.47	0.62
25:Y:110:TYR:O	25:Y:113:ARG:HB3	2.00	0.62
26:Z:220:LEU:HB3	26:Z:221:PRO:HA	1.81	0.62
20:C:286:THR:HG23	20:C:287:LYS:H	1.64	0.62
1:G:163:PHE:HD1	2:H:58:ASP:H	1.47	0.62
24:X:346:GLN:HE21	24:X:349:HIS:HB2	1.64	0.62
13:S:4:PRO:HB2	14:T:100:ARG:HH21	1.65	0.62
22:V:157:THR:OG1	22:V:158:PRO:HD3	2.00	0.62
26:Z:91:ILE:HD12	26:Z:91:ILE:O	2.00	0.62
3:I:233:VAL:O	3:I:237:ILE:HG13	2.00	0.62
1:G:28:ALA:HB2	7:M:14:PHE:HE2	1.65	0.62
12:R:50:ALA:HB2	13:S:129:SER:HB2	1.81	0.62
25:Y:262:SER:HB3	25:Y:270:VAL:HG11	1.81	0.62
26:Z:144:VAL:HG12	26:Z:145:HIS:H	1.64	0.62
17:D:105:SER:O	17:D:245:ARG:NH1	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:62:SER:OG	3:I:65:ILE:O	2.15	0.62
9:O:17:ASP:O	9:O:33:LYS:NZ	2.31	0.62
11:Q:29:LYS:HD3	11:Q:32:HIS:HB2	1.80	0.62
25:Y:357:ASN:HB2	25:Y:358:ARG:HA	1.82	0.62
15:A:206:ILE:HG13	15:A:207:GLU:H	1.63	0.61
14:T:27:LEU:HD22	14:T:184:TYR:H	1.65	0.61
22:V:173:ILE:O	22:V:177:ASN:ND2	2.32	0.61
25:Y:17:LEU:HA	25:Y:150:PHE:HE1	1.64	0.61
5:K:50:VAL:HG21	5:K:66:LYS:HG2	1.82	0.61
20:C:347:ILE:HD11	20:C:387:VAL:HG21	1.82	0.61
21:U:203:LYS:O	21:U:207:ASN:ND2	2.31	0.61
23:W:219:THR:HG22	23:W:222:LEU:H	1.64	0.61
18:E:120:TYR:OH	19:F:147:PRO:O	2.17	0.61
7:M:180:GLN:HB2	7:M:184:MET:HG2	1.83	0.61
7:M:56:LYS:H	7:M:57:LEU:HA	1.65	0.61
7:M:8:ASP:O	7:M:22:GLN:NE2	2.29	0.61
10:P:190:ILE:HG22	10:P:195:ILE:HG23	1.80	0.61
1:G:17:SER:OG	1:G:21:ARG:N	2.33	0.61
2:H:71:HIS:HA	2:H:218:PHE:H	1.66	0.61
11:Q:168:GLN:NE2	11:Q:174:ASN:O	2.34	0.61
14:T:92:LEU:HG	14:T:125:VAL:HG11	1.82	0.61
1:G:111:VAL:HG11	1:G:142:GLY:HA3	1.83	0.61
25:Y:210:SER:HB3	25:Y:213:LEU:HB2	1.82	0.61
26:Z:63:LYS:HB2	26:Z:64:ASP:HB2	1.83	0.61
17:D:143:LEU:HD12	17:D:252:ARG:HH12	1.66	0.61
22:V:241:ARG:HG3	22:V:242:HIS:H	1.66	0.61
2:H:66:GLU:OE2	2:H:91:ARG:NH2	2.34	0.61
7:M:106:ILE:HD12	7:M:107:PRO:HD2	1.81	0.61
22:V:89:LYS:HD3	22:V:92:ARG:HH11	1.64	0.61
15:A:83:ASP:OD1	16:B:137:SER:OG	2.19	0.61
6:L:120:THR:O	7:M:129:ARG:NH1	2.34	0.61
7:M:141:SER:HB3	7:M:144:ASP:HB2	1.82	0.61
22:V:281:ASN:H	22:V:284:GLU:HB3	1.66	0.61
24:X:384:VAL:HB	25:Y:312:ARG:HH22	1.65	0.61
20:C:217:SER:HB3	20:C:218:GLU:CB	2.21	0.60
17:D:100:THR:HB	17:D:114:ARG:HD2	1.83	0.60
2:H:66:GLU:HG3	2:H:91:ARG:HH21	1.65	0.60
21:U:353:LEU:HD13	21:U:385:PHE:HZ	1.66	0.60
20:C:157:GLN:NE2	20:C:316:GLU:O	2.35	0.60
17:D:374:ASP:HA	18:E:291:ARG:NH1	2.16	0.60
23:W:241:LEU:HA	23:W:244:CYS:SG	2.41	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:12:TYR:HB3	11:Q:153:ARG:HH21	1.65	0.60
26:Z:210:SER:O	26:Z:214:LYS:HG2	2.01	0.60
1:G:39:SER:H	1:G:172:GLN:NE2	1.99	0.60
7:M:34:SER:OG	7:M:65:ARG:NH1	2.35	0.60
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.82	0.60
22:V:290:TYR:OH	22:V:294:ARG:NH2	2.35	0.60
16:B:223:ILE:HG13	16:B:346:ARG:HB2	1.84	0.60
16:B:390:LEU:HD23	16:B:394:ASP:HB3	1.84	0.60
18:E:86:GLN:OE1	19:F:117:ARG:NH2	2.34	0.60
1:G:138:MET:HB3	1:G:154:CYS:HB3	1.83	0.60
2:H:68:ILE:HG23	2:H:91:ARG:HD3	1.84	0.60
21:U:74:PHE:HB3	21:U:103:LYS:HE3	1.83	0.60
20:C:117:ARG:HG3	20:C:124:HIS:HB2	1.83	0.60
1:G:43:ARG:HH11	1:G:150:GLN:HA	1.66	0.60
9:O:35:HIS:NE2	9:O:53:ASP:OD1	2.34	0.60
25:Y:301:ILE:HD12	25:Y:342:ARG:HB3	1.82	0.60
20:C:158:ILE:HA	20:C:161:ILE:HG22	1.82	0.60
18:E:269:THR:OG1	18:E:271:HIS:ND1	2.34	0.60
16:B:255:LEU:HD12	16:B:256:ILE:HG12	1.84	0.60
17:D:238:LYS:HA	18:E:208:ILE:HG12	1.84	0.60
6:L:66:VAL:HG11	6:L:88:MET:HG3	1.82	0.60
11:Q:38:MET:HA	11:Q:61:GLN:NE2	2.16	0.60
23:W:72:LYS:HZ1	23:W:122:LEU:HB2	1.67	0.60
16:B:173:VAL:O	20:C:232:ARG:NH1	2.35	0.60
16:B:191:ASP:HA	16:B:194:ILE:HG22	1.83	0.60
2:H:231:ALA:H	2:H:232:ALA:C	2.05	0.60
11:Q:22:ALA:HB2	11:Q:27:GLN:HA	1.84	0.60
20:C:173:GLU:HB3	21:U:363:SER:HB3	84.80	0.60
16:B:248:LEU:HD21	16:B:270:LEU:HD22	1.84	0.59
17:D:263:PHE:HD1	17:D:308:ILE:HG13	1.67	0.59
19:F:312:GLU:O	19:F:316:GLN:HG3	2.01	0.59
5:K:104:ASN:OD1	12:R:57:ARG:NH2	2.31	0.59
21:U:615:ARG:HH21	21:U:645:ASN:HD21	1.49	0.59
18:E:65:THR:HG22	18:E:66:GLU:H	1.67	0.59
19:F:359:GLU:HB2	19:F:385:ALA:HB1	1.83	0.59
12:R:127:SER:HB3	12:R:136:TYR:CE2	2.37	0.59
21:U:252:LEU:HD21	21:U:264:VAL:HG11	1.84	0.59
2:H:19:LEU:HD13	2:H:22:ILE:HD12	1.83	0.59
26:Z:22:HIS:HA	26:Z:25:ARG:HG2	1.84	0.59
15:A:348:LEU:HA	15:A:351:ARG:HH21	1.66	0.59
17:D:285:VAL:HA	17:D:288:ILE:HB	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:86:LEU:O	19:F:88:TYR:N	2.34	0.59
6:L:65:HIS:HD2	6:L:221:PHE:HD2	1.50	0.59
6:L:85:CYS:SG	6:L:89:ARG:NH1	2.76	0.59
7:M:232:ARG:NH1	7:M:234:GLU:OE1	2.35	0.59
17:D:56:VAL:HG21	21:U:599:ILE:HG23	1.83	0.59
22:V:97:ALA:HB3	22:V:98:LEU:HA	1.85	0.59
15:A:218:PRO:O	15:A:221:GLY:N	2.29	0.59
15:A:237:PHE:HB2	15:A:271:LEU:HB2	1.84	0.59
19:F:92:ASN:OD1	19:F:93:VAL:N	2.36	0.59
22:V:275:VAL:H	22:V:276:PHE:HA	1.68	0.59
15:A:264:ALA:HB1	15:A:315:ILE:HG21	1.85	0.59
15:A:355:PHE:HE1	15:A:385:ILE:HB	1.68	0.59
20:C:229:ARG:HH12	20:C:232:ARG:NE	1.97	0.59
2:H:174:LEU:HD21	2:H:194:THR:HG21	1.84	0.59
26:Z:106:ILE:HD11	26:Z:153:LYS:HB3	1.85	0.59
26:Z:207:ASP:O	26:Z:210:SER:OG	2.11	0.59
15:A:212:VAL:HG12	15:A:339:ARG:HB3	1.85	0.59
16:B:108:SER:O	16:B:152:LEU:N	2.32	0.59
16:B:220:LYS:HB2	16:B:346:ARG:CZ	2.33	0.59
1:G:81:THR:OG1	1:G:137:CYS:HB3	2.03	0.59
21:U:788:VAL:HG13	21:U:884:VAL:HG11	1.84	0.59
25:Y:23:ARG:NH1	25:Y:52:PRO:O	2.35	0.59
17:D:392:TYR:HA	23:W:136:ILE:HG13	1.83	0.59
18:E:61:LEU:HD11	18:E:72:LYS:HB2	1.84	0.59
22:V:224:LEU:HB2	22:V:227:VAL:HB	1.84	0.59
17:D:44:TYR:HA	20:C:25:LEU:HD11	1.84	0.58
1:G:102:LYS:HD3	1:G:108:GLU:HA	1.85	0.58
1:G:56:VAL:HA	1:G:61:LEU:HD13	1.85	0.58
21:U:643:SER:O	21:U:649:ARG:NH1	2.37	0.58
22:V:326:GLN:HB3	22:V:353:LEU:HD13	1.85	0.58
23:W:48:LEU:HB2	23:W:96:GLN:OE1	2.03	0.58
17:D:255:LYS:HE2	17:D:299:PHE:HE1	1.68	0.58
18:E:239:GLY:HA2	18:E:257:LEU:HD11	1.84	0.58
2:H:40:ALA:HB1	2:H:182:LEU:H	1.67	0.58
21:U:14:GLU:O	21:U:20:LYS:NZ	2.36	0.58
21:U:842:LYS:HG2	21:U:882:ALA:HB2	1.84	0.58
23:W:236:HIS:ND1	23:W:237:GLU:OE1	2.36	0.58
26:Z:193:ASN:O	26:Z:196:HIS:ND1	2.19	0.58
15:A:345:LEU:HG	15:A:346:PRO:HD2	1.84	0.58
16:B:190:LEU:HD13	16:B:194:ILE:HB	1.85	0.58
22:V:416:ARG:HB3	25:Y:348:ASP:OD1	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:17:SER:OG	11:Q:179:SER:OG	2.21	0.58
15:A:119:ALA:HA	19:F:127:SER:HB3	1.85	0.58
16:B:304:GLU:O	16:B:307:ARG:HG2	2.03	0.58
19:F:357:PRO:O	19:F:362:ARG:NH1	2.35	0.58
8:N:7:GLN:HB3	8:N:111:VAL:HG23	1.85	0.58
21:U:96:TYR:O	21:U:100:ILE:HG12	2.03	0.58
25:Y:63:TRP:HB3	25:Y:64:GLN:HB3	1.85	0.58
20:C:236:VAL:HG22	20:C:239:ARG:HH12	1.68	0.58
19:F:165:PRO:HB2	19:F:166:THR:OG1	2.04	0.58
21:U:188:MET:HG2	21:U:194:ARG:HD3	1.86	0.58
20:C:72:TYR:HB2	20:C:116:LEU:HB3	1.84	0.58
18:E:86:GLN:NE2	18:E:108:MET:O	2.37	0.58
4:J:11:SER:OG	4:J:13:ASP:OD1	2.21	0.58
4:J:32:ALA:HB3	4:J:161:ILE:HD11	1.85	0.58
11:Q:52:ASP:OD1	12:R:88:TYR:OH	2.20	0.58
11:Q:84:THR:HG21	11:Q:104:LEU:HD11	1.85	0.58
19:F:89:LEU:HG	19:F:153:VAL:HG13	1.85	0.58
1:G:53:GLN:HA	1:G:215:ILE:HA	1.84	0.58
15:A:357:ILE:HG23	15:A:358:HIS:HD1	1.68	0.57
3:I:123:GLN:HG3	4:J:125:ARG:NH2	2.18	0.57
21:U:759:SER:HA	21:U:782:ALA:HA	1.86	0.57
15:A:277:ILE:HG22	15:A:321:THR:HB	1.85	0.57
7:M:8:ASP:HB3	7:M:21:PHE:HD2	1.68	0.57
11:Q:153:ARG:HH22	11:Q:184:ASP:HB3	1.70	0.57
15:A:237:PHE:HA	15:A:270:CYS:SG	2.45	0.57
20:C:136:SER:HA	20:C:139:MET:HB2	1.87	0.57
17:D:83:GLN:NE2	17:D:140:VAL:HG21	2.10	0.57
17:D:60:TYR:HD1	21:U:603:LEU:HD21	1.68	0.57
1:G:211:LYS:NZ	1:G:232:GLU:OE2	2.36	0.57
22:V:451:ILE:HG13	22:V:458:VAL:HG13	1.85	0.57
26:Z:186:THR:HG23	26:Z:187:LEU:H	1.70	0.57
1:G:180:GLU:HG2	2:H:56:LEU:HG	1.86	0.57
18:E:179:GLY:N	33:E:401:ATP:O2A	2.36	0.57
3:I:171:ALA:O	3:I:175:LEU:HG	2.03	0.57
3:I:83:ALA:O	3:I:86:LEU:N	2.38	0.57
23:W:45:GLU:HB2	23:W:93:ARG:HG3	1.85	0.57
17:D:148:ASP:HB3	17:D:149:SER:C	2.23	0.57
1:G:11:ARG:O	1:G:24:GLN:NE2	2.32	0.57
3:I:140:ASP:OD1	3:I:144:GLY:N	2.37	0.57
23:W:137:TYR:HB3	23:W:140:ILE:HD12	1.86	0.57
18:E:138:LEU:HD22	18:E:140:GLU:HG2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:92:GLU:HA	25:Y:100:ILE:HD13	1.86	0.57
15:A:281:GLY:O	15:A:326:THR:OG1	2.19	0.57
15:A:309:PHE:CZ	19:F:235:LEU:HG	2.38	0.57
1:G:203:SER:O	1:G:207:SER:N	2.38	0.57
11:Q:22:ALA:CB	11:Q:27:GLN:HA	2.35	0.57
12:R:11:GLY:HA3	12:R:179:VAL:O	2.05	0.57
16:B:211:TYR:OH	16:B:217:LYS:HA	2.05	0.57
20:C:303:SER:O	20:C:307:ARG:N	2.37	0.57
5:K:16:SER:O	5:K:19:GLY:HA3	2.05	0.57
21:U:112:CYS:SG	21:U:159:ARG:NH1	2.78	0.57
22:V:148:ARG:HG3	22:V:149:PRO:HD3	1.86	0.57
22:V:411:SER:HB2	22:V:447:ILE:HD13	1.86	0.57
17:D:389:GLU:HA	17:D:390:ASN:HB2	1.86	0.57
22:V:224:LEU:HD13	22:V:227:VAL:HB	1.87	0.57
22:V:79:VAL:O	22:V:80:LYS:NZ	2.27	0.57
23:W:416:GLN:HB3	23:W:417:ARG:CA	2.35	0.57
17:D:194:ILE:HD12	17:D:196:ILE:HD13	1.86	0.56
17:D:45:LYS:HG2	21:U:187:LEU:HD13	1.87	0.56
26:Z:195:VAL:HG13	26:Z:199:LYS:HD3	1.87	0.56
16:B:255:LEU:HB3	20:C:229:ARG:HG3	1.87	0.56
17:D:293:LEU:O	17:D:326:ARG:NH1	2.37	0.56
18:E:128:GLY:HA2	18:E:129:ASN:HB2	1.85	0.56
9:O:163:ILE:HG23	9:O:170:GLY:HA2	1.88	0.56
9:O:36:PHE:CD1	9:O:42:TYR:HE1	2.22	0.56
10:P:44:PRO:HA	10:P:50:TYR:HD1	1.70	0.56
15:A:157:ILE:HG22	15:A:158:ASP:CB	2.34	0.56
15:A:103:ASN:ND2	19:F:169:ASP:OD1	2.39	0.56
15:A:80:LEU:HD23	16:B:137:SER:HB3	1.87	0.56
18:E:84:ARG:HH11	18:E:108:MET:HG3	1.70	0.56
6:L:50:LYS:HB3	6:L:59:HIS:HB3	1.86	0.56
11:Q:140:LEU:HA	11:Q:143:LEU:HB3	1.88	0.56
5:K:212:ALA:HA	5:K:234:LEU:HD22	1.87	0.56
22:V:82:LEU:O	22:V:87:SER:OG	2.23	0.56
23:W:370:TYR:HA	23:W:371:THR:HB	1.87	0.56
16:B:139:VAL:HA	16:B:140:ASP:HB3	1.88	0.56
18:E:281:ARG:HD3	18:E:387:LYS:NZ	2.21	0.56
3:I:69:ASN:OD1	3:I:70:GLU:N	2.38	0.56
22:V:200:ARG:HH11	22:V:242:HIS:HB2	1.71	0.56
25:Y:79:ASP:HA	25:Y:82:LYS:HG2	1.87	0.56
20:C:90:HIS:HB2	20:C:91:PRO:HD3	1.86	0.56
17:D:303:VAL:HA	17:D:304:ASN:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:87:LEU:HB2	18:E:80:VAL:HG23	1.87	0.56
4:J:137:ASP:N	4:J:141:THR:O	2.39	0.56
23:W:405:LYS:HG3	24:X:342:PHE:HA	1.88	0.56
17:D:283:ARG:HA	17:D:286:GLN:HG2	1.87	0.56
1:G:163:PHE:HB2	1:G:166:THR:OG1	2.05	0.56
1:G:50:ILE:O	1:G:218:GLY:N	2.38	0.56
2:H:6:TYR:HE2	2:H:126:GLY:HA3	1.71	0.56
3:I:90:LEU:HD12	3:I:114:LEU:HB2	1.87	0.56
6:L:72:ILE:HG22	6:L:134:ILE:HA	1.86	0.56
21:U:705:LYS:HA	21:U:708:GLN:HG3	1.88	0.56
23:W:455:LEU:HD12	23:W:456:GLN:HG2	1.88	0.56
5:K:13:ASN:HD21	6:L:126:ARG:HH11	1.54	0.56
23:W:67:LEU:HD22	23:W:71:VAL:HB	1.88	0.56
17:D:160:PRO:HG2	17:D:221:HIS:CD2	2.41	0.56
3:I:105:ILE:HD12	3:I:106:PRO:HD2	1.88	0.56
16:B:188:GLY:O	33:B:501:ATP:N6	2.39	0.55
18:E:138:LEU:O	18:E:142:ILE:HG13	2.06	0.55
22:V:159:LEU:HD13	22:V:178:SER:HB2	1.88	0.55
20:C:229:ARG:NH1	20:C:279:GLN:OE1	2.40	0.55
2:H:15:PRO:HA	3:I:23:TYR:CD1	2.41	0.55
4:J:36:ARG:HB3	4:J:144:LEU:HD23	1.88	0.55
7:M:83:ASP:HB2	7:M:133:CYS:SG	2.47	0.55
23:W:65:ARG:HB2	23:W:66:ILE:HB	1.88	0.55
16:B:222:VAL:HG23	16:B:328:ILE:HG23	1.88	0.55
16:B:294:ARG:HB3	20:C:264:GLY:HA3	1.87	0.55
17:D:181:VAL:O	17:D:306:LYS:NZ	2.39	0.55
17:D:323:ARG:NH1	17:D:324:PRO:O	2.39	0.55
17:D:374:ASP:HA	18:E:291:ARG:HH12	1.70	0.55
1:G:173:THR:O	1:G:176:THR:OG1	2.24	0.55
2:H:45:VAL:HG22	2:H:212:ILE:HG22	1.89	0.55
21:U:181:LEU:HD11	21:U:201:LEU:HD12	1.89	0.55
21:U:571:CYS:HB2	21:U:601:ARG:HH21	1.71	0.55
24:X:359:ALA:O	24:X:363:ARG:HG3	2.06	0.55
20:C:171:HIS:HB3	20:C:174:LEU:HD21	1.88	0.55
17:D:75:ALA:HB1	20:C:56:VAL:HG21	1.88	0.55
18:E:142:ILE:HG12	18:E:183:LEU:HD11	1.89	0.55
6:L:204:ASP:HB3	6:L:205:LEU:C	2.26	0.55
23:W:371:THR:O	23:W:414:ASN:HB2	2.06	0.55
17:D:337:ASP:O	17:D:341:LYS:N	2.35	0.55
1:G:76:ILE:HG12	1:G:142:GLY:HA2	1.88	0.55
5:K:143:PHE:HB2	5:K:154:PHE:HB2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:174:THR:OG1	18:E:372:ARG:NH1	2.40	0.55
22:V:160:LEU:HB2	22:V:161:PRO:HD3	1.88	0.55
22:V:358:MET:HB2	22:V:359:PRO:HD3	1.87	0.55
15:A:295:VAL:O	15:A:298:THR:OG1	2.20	0.55
19:F:164:LEU:HD12	19:F:165:PRO:HD2	1.87	0.55
1:G:127:GLN:OE1	2:H:128:ARG:N	2.38	0.55
22:V:211:TYR:O	22:V:214:HIS:HB2	2.07	0.55
22:V:90:GLU:N	22:V:90:GLU:OE1	2.38	0.55
20:C:328:ILE:HG12	33:C:501:ATP:N1	2.22	0.55
3:I:148:TYR:HA	3:I:158:GLY:HA2	1.89	0.55
11:Q:116:TYR:CE1	11:Q:126:LYS:HD3	2.41	0.55
14:T:44:ARG:HA	14:T:50:MET:HG3	1.89	0.55
22:V:228:ARG:HH12	22:V:254:LEU:HA	1.71	0.55
22:V:342:ILE:HD12	22:V:343:PRO:HD2	1.87	0.55
23:W:274:VAL:O	23:W:283:GLN:NE2	2.39	0.55
23:W:84:ASN:O	23:W:87:ILE:HD12	2.07	0.55
23:W:408:ARG:NH1	24:X:349:HIS:HB3	2.22	0.55
17:D:96:VAL:HG11	20:C:127:LEU:HD13	1.89	0.55
15:A:120:LYS:HB2	19:F:90:VAL:HB	1.88	0.55
8:N:26:ILE:HG21	8:N:29:ARG:HD3	1.88	0.55
13:S:91:MET:O	13:S:95:ILE:HG13	2.06	0.55
22:V:290:TYR:CD1	22:V:328:VAL:HG23	2.41	0.55
17:D:390:ASN:O	23:W:135:LYS:HE2	2.07	0.55
6:L:104:PRO:HD2	6:L:107:ARG:HH11	1.71	0.55
26:Z:101:LEU:HD23	26:Z:123:ILE:HD11	1.89	0.55
15:A:363:SER:HB2	15:A:403:ILE:HG22	1.89	0.54
17:D:282:ASP:HA	17:D:285:VAL:HG22	1.88	0.54
18:E:252:GLU:O	18:E:255:ARG:HG2	2.07	0.54
18:E:364:GLN:HG2	18:E:367:PHE:HD2	1.72	0.54
19:F:224:LEU:HB3	19:F:351:LYS:HG2	1.88	0.54
11:Q:47:VAL:HB	11:Q:102:LEU:HG	1.87	0.54
13:S:108:ASN:HB2	13:S:124:PHE:HD2	1.72	0.54
25:Y:203:ASP:N	25:Y:203:ASP:OD1	2.36	0.54
15:A:323:ARG:HB2	15:A:325:ASP:OD1	2.06	0.54
18:E:56:ILE:HG23	18:E:100:LEU:HB2	1.89	0.54
21:U:428:PRO:HB3	21:U:439:GLU:HB2	1.88	0.54
23:W:5:GLY:HA3	23:W:47:LEU:HD22	1.88	0.54
15:A:75:PRO:O	15:A:79:ASP:HB2	2.08	0.54
20:C:168:PRO:HA	20:C:172:PRO:HG3	1.89	0.54
17:D:150:SER:OG	17:D:151:ILE:N	2.32	0.54
21:U:800:VAL:HG21	21:U:914:LEU:HD21	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:285:TRP:O	22:V:288:TYR:HB3	2.07	0.54
23:W:422:ASN:ND2	26:Z:247:LYS:O	2.41	0.54
24:X:172:LEU:HD12	24:X:175:LYS:HD3	1.89	0.54
25:Y:181:LYS:HA	25:Y:200:LEU:HD12	1.89	0.54
5:K:16:SER:HB3	5:K:20:ARG:H	1.71	0.54
8:N:22:THR:HG22	8:N:27:ALA:HB2	1.90	0.54
9:O:34:ILE:HG12	9:O:44:CYS:SG	2.47	0.54
23:W:328:LEU:HD11	23:W:341:PHE:HE2	1.72	0.54
24:X:174:SER:HA	24:X:177:TYR:HD2	1.73	0.54
16:B:224:LEU:HB3	16:B:234:LEU:HD13	1.89	0.54
3:I:119:GLN:NE2	4:J:78:ALA:O	2.39	0.54
7:M:228:PRO:HB2	7:M:231:ILE:HG12	1.89	0.54
18:E:171:LEU:HB2	18:E:295:LEU:HD22	1.90	0.54
6:L:207:THR:HG22	6:L:233:LEU:HD12	1.89	0.54
4:J:88:ARG:NH2	11:Q:69:MET:HB2	2.17	0.54
23:W:86:ASN:HB3	23:W:88:MET:HG3	1.90	0.54
15:A:346:PRO:HB2	15:A:351:ARG:HG2	1.89	0.54
20:C:275:GLU:O	20:C:279:GLN:HG3	2.08	0.54
19:F:70:LYS:O	19:F:73:ILE:HG13	2.08	0.54
10:P:107:PRO:HG2	10:P:124:LEU:HB2	1.89	0.54
21:U:233:LEU:HD13	21:U:268:LEU:HD21	1.89	0.54
22:V:475:ALA:O	22:V:479:ARG:HG2	2.08	0.54
22:V:97:ALA:N	22:V:98:LEU:HB2	2.23	0.54
23:W:62:SER:HB2	23:W:71:VAL:HG11	1.90	0.54
16:B:383:LEU:HB3	16:B:387:LYS:HZ1	1.73	0.54
18:E:90:SER:O	18:E:93:LYS:NZ	2.35	0.54
1:G:49:VAL:HG22	1:G:219:VAL:HG23	1.90	0.54
2:H:50:LYS:HZ1	2:H:62:VAL:HB	1.72	0.54
7:M:10:SER:O	7:M:13:THR:OG1	2.26	0.54
25:Y:349:LYS:O	25:Y:350:VAL:HG22	2.08	0.54
26:Z:102:HIS:CD2	26:Z:104:ASN:HB3	2.43	0.54
26:Z:56:VAL:HA	26:Z:74:TYR:HE2	1.73	0.54
16:B:298:ASN:ND2	18:E:245:GLU:OE1	2.42	0.53
19:F:150:LEU:HB3	19:F:164:LEU:O	2.08	0.53
1:G:86:ASP:HA	7:M:120:HIS:CE1	2.43	0.53
21:U:382:SER:O	21:U:384:GLN:NE2	2.41	0.53
23:W:416:GLN:HB3	23:W:418:PRO:HD3	1.89	0.53
16:B:402:ALA:HB1	16:B:414:VAL:HG11	1.90	0.53
20:C:42:LEU:O	20:C:45:LEU:HB2	2.08	0.53
17:D:200:ARG:NH2	17:D:300:ASP:OD1	2.40	0.53
17:D:54:LEU:HA	17:D:57:GLN:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:E:204:VAL:HG23	18:E:205:ASP:H	1.72	0.53
6:L:193:ARG:O	6:L:196:ARG:HG2	2.08	0.53
21:U:623:GLY:HA2	21:U:659:CYS:HB2	1.90	0.53
25:Y:349:LYS:HG3	25:Y:350:VAL:HG13	1.90	0.53
25:Y:71:ASN:HA	25:Y:74:LYS:HG2	1.89	0.53
18:E:141:GLN:NE2	18:E:300:HIS:O	2.41	0.53
18:E:55:GLN:O	19:F:133:PHE:N	2.35	0.53
2:H:184:LEU:O	2:H:188:ILE:HG13	2.08	0.53
5:K:109:VAL:HG23	5:K:147:ASP:HB3	1.91	0.53
25:Y:381:GLN:HB3	25:Y:385:ARG:NH1	2.23	0.53
19:F:370:SER:HA	19:F:373:MET:HG2	1.89	0.53
5:K:35:SER:HA	5:K:53:ARG:NH2	2.23	0.53
22:V:79:VAL:HG13	22:V:80:LYS:N	2.22	0.53
15:A:143:ASP:O	15:A:147:TYR:N	2.38	0.53
20:C:243:PRO:HB3	20:C:288:ASN:HB3	1.91	0.53
3:I:47:ALA:HB1	3:I:64:LYS:HD2	1.91	0.53
7:M:45:VAL:HG11	7:M:138:GLY:HA3	1.90	0.53
2:H:179:ASN:HD21	24:X:159:LYS:HE2	1.74	0.53
16:B:189:GLY:HA3	16:B:360:THR:HG23	1.91	0.53
17:D:326:ARG:HH21	20:C:141:GLU:HG2	1.74	0.53
17:D:89:ILE:O	17:D:106:THR:OG1	2.21	0.53
1:G:73:THR:HB	1:G:76:ILE:HB	1.91	0.53
2:H:71:HIS:CE1	2:H:104:PRO:HB3	2.44	0.53
6:L:148:CYS:SG	6:L:150:SER:OG	2.48	0.53
7:M:66:LEU:HD13	7:M:214:SER:HB2	1.91	0.53
24:X:130:GLU:HB3	24:X:153:LEU:HD21	1.90	0.53
24:X:143:TYR:HD2	24:X:144:GLN:HG2	1.72	0.53
25:Y:109:GLU:HG2	25:Y:124:PHE:CE1	2.44	0.53
16:B:301:GLY:O	16:B:305:ILE:HG13	2.09	0.53
20:C:155:ASP:OD1	20:C:155:ASP:N	2.42	0.53
19:F:230:GLY:H	19:F:392:ASN:HB3	1.73	0.53
1:G:61:LEU:HA	7:M:160:TYR:CD1	2.43	0.53
5:K:34:GLY:HA3	5:K:80:GLY:HA2	1.90	0.53
7:M:197:ILE:HA	7:M:200:VAL:HG12	1.90	0.53
15:A:355:PHE:CE1	15:A:385:ILE:HB	2.44	0.53
20:C:373:GLU:HG2	20:C:375:ARG:NH1	2.24	0.53
21:U:61:ALA:HB1	21:U:80:TYR:HB3	1.91	0.53
21:U:844:LYS:HD3	21:U:881:PRO:HD3	1.91	0.53
22:V:284:GLU:HG2	22:V:287:ARG:HE	1.74	0.53
23:W:405:LYS:HA	24:X:341:PRO:O	2.08	0.53
16:B:393:ALA:HB3	20:C:310:ARG:HD3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:313:LEU:O	19:F:317:LEU:HD12	2.09	0.53
10:P:66:ARG:O	10:P:69:PHE:HB3	2.09	0.53
13:S:197:ILE:HB	13:S:204:ARG:HB2	1.90	0.53
23:W:359:VAL:O	23:W:363:ILE:HG12	2.09	0.53
17:D:373:ALA:HB1	17:D:374:ASP:HB3	1.91	0.53
11:Q:103:LEU:HD23	11:Q:132:HIS:HE1	1.73	0.53
11:Q:4:LEU:HD22	11:Q:17:SER:HA	1.91	0.53
13:S:171:ALA:O	13:S:175:VAL:HG23	2.09	0.53
22:V:213:TYR:HD1	22:V:216:ARG:HD2	1.73	0.53
25:Y:170:GLU:N	25:Y:171:GLY:HA3	2.23	0.53
25:Y:326:GLY:HA2	25:Y:329:PHE:HD2	1.74	0.53
22:V:490:SER:HA	26:Z:275:LEU:HD21	1.89	0.53
15:A:140:VAL:HA	15:A:152:PRO:HA	1.91	0.52
15:A:219:GLY:HA3	15:A:381:THR:HB	1.91	0.52
16:B:258:LYS:HA	16:B:296:ASP:HB3	1.90	0.52
19:F:255:GLN:O	19:F:258:GLN:NE2	2.36	0.52
23:W:420:ASP:HB2	23:W:425:LEU:HD12	1.92	0.52
17:D:143:LEU:O	22:V:440:LYS:NZ	76.25	0.52
4:J:87:ALA:HB2	4:J:111:ILE:HD11	1.91	0.52
23:W:441:LYS:HA	23:W:444:HIS:CE1	2.43	0.52
24:X:330:LEU:HA	24:X:333:GLN:HB2	1.92	0.52
25:Y:34:ASP:OD1	25:Y:34:ASP:N	2.42	0.52
20:C:117:ARG:HD3	20:C:122:THR:OG1	2.10	0.52
20:C:297:ARG:HG3	20:C:298:ILE:H	1.73	0.52
17:D:143:LEU:HD13	17:D:144:PRO:HD2	1.91	0.52
2:H:123:GLN:HB2	3:I:128:ARG:NH2	2.22	0.52
2:H:123:GLN:HG3	3:I:128:ARG:HB3	1.90	0.52
22:V:269:LYS:HE2	22:V:295:ILE:HG13	1.92	0.52
23:W:135:LYS:HB3	23:W:136:ILE:HB	1.92	0.52
16:B:343:ARG:HB2	16:B:344:PRO:HD3	1.92	0.52
20:C:271:ARG:O	20:C:275:GLU:HG2	2.10	0.52
20:C:321:ASN:O	20:C:325:ARG:HG3	2.08	0.52
1:G:14:THR:HG22	1:G:24:GLN:HG3	1.91	0.52
3:I:100:GLN:HG3	11:Q:86:ARG:HG3	1.91	0.52
21:U:388:ASP:OD1	21:U:389:ASN:ND2	2.42	0.52
22:V:143:ALA:HB3	22:V:145:LEU:HB3	1.92	0.52
20:C:192:PRO:HD3	20:C:296:ASN:CG	2.30	0.52
20:C:338:LEU:O	25:Y:174:TRP:NE1	2.31	0.52
17:D:145:PRO:HB2	17:D:146:GLU:HB2	1.90	0.52
23:W:247:TYR:O	23:W:250:ILE:HG13	2.09	0.52
17:D:204:MET:HA	17:D:331:ILE:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:198:VAL:O	4:J:201:SER:OG	2.28	0.52
7:M:83:ASP:O	7:M:87:LEU:HG	2.10	0.52
21:U:424:ALA:HA	21:U:427:LEU:HD13	1.92	0.52
18:E:55:GLN:HB3	18:E:100:LEU:O	2.10	0.52
19:F:421:MET:HA	19:F:424:ILE:HD12	1.91	0.52
10:P:91:VAL:HG21	10:P:109:ILE:HD11	1.92	0.52
21:U:118:LEU:HD21	21:U:123:LYS:HA	1.92	0.52
25:Y:296:VAL:O	25:Y:300:ARG:HG3	2.10	0.52
17:D:251:PHE:CE2	17:D:292:LEU:HB2	2.45	0.52
1:G:61:LEU:HG	1:G:66:VAL:HG21	1.90	0.52
4:J:98:VAL:HG22	12:R:78:ALA:HB1	1.92	0.52
24:X:281:GLY:H	24:X:284:THR:HG22	1.74	0.52
26:Z:225:GLN:HG2	26:Z:228:TYR:CE2	2.43	0.52
15:A:172:VAL:HB	15:A:226:ALA:HB1	1.90	0.52
17:D:326:ARG:NH2	20:C:141:GLU:OE2	2.43	0.52
2:H:150:ASP:OD1	2:H:154:ALA:N	2.43	0.52
22:V:349:ARG:HD2	22:V:354:LYS:HD3	1.92	0.52
23:W:373:ILE:HG12	23:W:374:THR:O	2.09	0.52
26:Z:68:TRP:HH2	26:Z:111:LEU:HB2	1.75	0.52
15:A:100:LYS:HZ3	15:A:140:VAL:HG23	1.75	0.52
16:B:124:SER:HA	16:B:129:SER:O	2.10	0.52
16:B:170:LEU:O	16:B:173:VAL:HG22	2.10	0.52
20:C:217:SER:CB	20:C:218:GLU:HB3	2.28	0.52
20:C:88:LYS:HD2	20:C:94:LYS:HE3	1.90	0.52
17:D:337:ASP:O	17:D:341:LYS:HG2	2.10	0.52
19:F:252:ALA:HB3	19:F:255:GLN:HG2	1.92	0.52
7:M:43:ASP:OD1	7:M:43:ASP:N	2.42	0.52
21:U:377:HIS:O	21:U:380:THR:HG22	2.09	0.52
24:X:203:PRO:HB3	24:X:206:LEU:HG	1.92	0.52
5:K:205:VAL:O	15:A:375:ARG:NH2	2.42	0.51
16:B:305:ILE:O	16:B:308:THR:HG22	2.10	0.51
25:Y:307:LEU:HD21	25:Y:319:MET:HE3	1.92	0.51
16:B:203:LEU:HG	16:B:211:TYR:HD1	1.76	0.51
10:P:26:ARG:HH21	10:P:38:ASP:HA	1.75	0.51
11:Q:46:CYS:HA	11:Q:102:LEU:HB2	1.92	0.51
26:Z:9:VAL:HG12	26:Z:48:LEU:HB3	1.92	0.51
20:C:13:GLU:HG2	21:U:141:CYS:SG	2.50	0.51
21:U:246:TYR:HH	21:U:250:PHE:HE2	1.58	0.51
21:U:31:VAL:HG22	21:U:35:TRP:CD1	2.45	0.51
22:V:275:VAL:HB	22:V:277:PRO:HD3	1.91	0.51
15:A:205:GLY:HA2	15:A:206:ILE:CG2	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:167:THR:OG1	16:B:168:ASP:N	2.44	0.51
16:B:190:LEU:O	16:B:194:ILE:N	2.30	0.51
16:B:294:ARG:HG2	20:C:261:GLY:O	2.11	0.51
18:E:260:LEU:HB3	18:E:264:MET:HE2	1.92	0.51
4:J:26:VAL:HG22	4:J:129:ILE:HA	1.91	0.51
5:K:79:SER:O	5:K:139:VAL:HG23	2.10	0.51
10:P:189:ILE:HG23	10:P:196:THR:HB	1.91	0.51
6:L:107:ARG:NH2	14:T:74:GLU:HG3	2.26	0.51
21:U:742:HIS:HB2	21:U:883:ARG:HH12	1.75	0.51
22:V:179:LYS:O	22:V:183:GLU:HG3	2.11	0.51
15:A:104:ALA:H	15:A:112:ILE:HG23	1.75	0.51
16:B:224:LEU:O	16:B:330:ALA:HA	2.10	0.51
17:D:312:ASN:ND2	18:E:242:ARG:HH22	2.05	0.51
18:E:252:GLU:HA	18:E:255:ARG:HE	1.76	0.51
4:J:10:PHE:HA	4:J:16:LEU:HD23	1.91	0.51
4:J:195:LEU:O	4:J:201:SER:OG	2.29	0.51
6:L:121:GLN:HG3	7:M:129:ARG:HG2	1.93	0.51
7:M:229:LYS:HZ1	7:M:235:ALA:H	1.58	0.51
14:T:57:TYR:HE2	14:T:61:GLN:HE21	1.58	0.51
21:U:208:LEU:HD23	21:U:210:LYS:H	1.75	0.51
21:U:596:ASN:O	21:U:599:ILE:HG22	2.11	0.51
25:Y:131:THR:HG21	25:Y:136:HIS:HB2	1.92	0.51
20:C:269:VAL:O	20:C:272:THR:HB	2.11	0.51
17:D:250:VAL:O	17:D:253:LEU:HG	2.10	0.51
18:E:247:THR:OG1	18:E:248:SER:N	2.44	0.51
10:P:135:ASP:N	10:P:135:ASP:OD1	2.41	0.51
21:U:243:LEU:O	21:U:913:ILE:HG21	2.10	0.51
26:Z:225:GLN:HE22	26:Z:229:GLN:HB2	1.75	0.51
16:B:205:LEU:CD2	16:B:206:THR:H	2.24	0.51
17:D:121:ARG:HG3	17:D:122:GLU:OE1	2.10	0.51
19:F:403:ALA:HB1	19:F:415:LEU:HD11	1.92	0.51
3:I:149:GLN:O	3:I:157:GLY:N	2.40	0.51
21:U:16:GLU:OE1	21:U:18:GLN:NE2	2.44	0.51
23:W:312:MET:SD	23:W:361:HIS:ND1	2.73	0.51
25:Y:102:ASP:HA	25:Y:105:MET:HG2	1.92	0.51
15:A:187:LEU:O	15:A:190:VAL:HG12	2.10	0.51
20:C:119:ASP:OD1	20:C:119:ASP:N	2.44	0.51
33:D:501:ATP:PG	18:E:294:ARG:HH22	2.33	0.51
1:G:15:ILE:HD12	2:H:21:GLN:HE22	1.76	0.51
5:K:18:GLU:HB2	5:K:19:GLY:HA2	1.92	0.51
21:U:625:ILE:HG13	21:U:626:LEU:HG	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:99:VAL:HG13	20:C:100:ASP:C	2.31	0.51
17:D:133:HIS:CE1	17:D:135:HIS:H	2.29	0.51
17:D:255:LYS:HE2	17:D:299:PHE:CE1	2.45	0.51
17:D:167:ILE:HG22	33:D:501:ATP:N6	2.25	0.51
2:H:93:LEU:HD21	2:H:113:ARG:HB2	1.91	0.51
5:K:16:SER:N	5:K:20:ARG:O	2.44	0.51
6:L:189:LYS:O	6:L:193:ARG:HG3	2.11	0.51
21:U:692:ALA:HB1	21:U:736:ILE:HB	1.93	0.51
17:D:182:GLU:HG3	17:D:183:LEU:HD12	1.93	0.50
17:D:202:VAL:HB	17:D:308:ILE:HA	1.92	0.50
15:A:428:ARG:O	15:A:431:THR:OG1	2.22	0.50
18:E:210:GLU:O	18:E:213:ARG:HG2	2.11	0.50
15:A:339:ARG:NH1	19:F:402:GLU:OE2	2.43	0.50
1:G:185:LYS:HG3	1:G:187:PHE:H	1.76	0.50
4:J:228:TYR:HA	4:J:231:GLU:HG2	1.92	0.50
7:M:35:THR:HA	7:M:166:GLY:HA3	1.93	0.50
21:U:249:CYS:HB3	21:U:328:ILE:HG21	1.93	0.50
19:F:191:LEU:HG	19:F:194:GLN:NE2	2.22	0.50
19:F:303:ASP:O	19:F:306:VAL:N	2.44	0.50
4:J:146:GLN:HG2	4:J:154:HIS:O	2.11	0.50
5:K:227:HIS:HA	5:K:228:MET:C	2.30	0.50
8:N:114:VAL:HA	8:N:119:MET:O	2.12	0.50
12:R:83:LEU:HD22	12:R:101:ILE:HD11	1.93	0.50
15:A:316:LYS:HG2	15:A:317:VAL:H	1.76	0.50
16:B:251:VAL:HG22	16:B:285:ASP:H	1.76	0.50
18:E:71:VAL:HG11	18:E:107:ILE:HD11	1.93	0.50
17:D:270:ILE:HA	18:E:251:ARG:HH21	1.77	0.50
33:D:501:ATP:H1'	18:E:291:ARG:HH21	1.77	0.50
26:Z:45:LYS:HG3	26:Z:46:LYS:H	1.76	0.50
15:A:97:ARG:HB2	15:A:98:CYS:SG	2.52	0.50
5:K:37:ALA:HB2	5:K:50:VAL:HG23	1.93	0.50
21:U:692:ALA:HB2	21:U:733:ALA:HB1	1.93	0.50
21:U:808:PRO:HD3	21:U:836:THR:HB	1.93	0.50
22:V:255:LEU:CD2	22:V:291:TYR:HB3	2.39	0.50
16:B:395:ILE:HG13	16:B:398:ILE:HD11	1.94	0.50
20:C:214:VAL:HG12	20:C:249:ASP:H	1.76	0.50
20:C:39:SER:O	20:C:43:ARG:HG3	2.11	0.50
1:G:172:GLN:N	1:G:172:GLN:OE1	2.44	0.50
2:H:185:GLU:OE1	2:H:185:GLU:N	2.44	0.50
4:J:65:LEU:HD22	4:J:88:ARG:HG2	1.93	0.50
21:U:403:THR:HG23	21:U:777:HIS:HE2	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:89:LYS:HD2	22:V:93:PHE:CE2	2.46	0.50
23:W:257:GLN:HB3	23:W:259:GLU:N	2.26	0.50
23:W:61:VAL:O	23:W:64:SER:OG	2.27	0.50
24:X:364:LYS:O	24:X:368:MET:HG2	2.12	0.50
26:Z:214:LYS:HB3	26:Z:222:ILE:HG12	1.94	0.50
1:G:22:LEU:HD12	1:G:22:LEU:O	2.12	0.50
5:K:11:GLY:O	5:K:12:VAL:HG22	2.12	0.50
7:M:156:VAL:HG12	7:M:158:TYR:HD1	1.77	0.50
8:N:18:SER:HB2	8:N:30:VAL:HA	1.93	0.50
10:P:13:ALA:HB3	10:P:137:VAL:HG23	1.94	0.50
10:P:153:LEU:HB3	10:P:166:THR:HG23	1.94	0.50
14:T:25:ASP:HA	14:T:187:PHE:HA	1.93	0.50
14:T:6:VAL:O	14:T:56:ASP:HA	2.11	0.50
21:U:842:LYS:HA	21:U:843:GLU:CB	2.41	0.50
25:Y:191:ILE:HG13	25:Y:192:ARG:H	1.77	0.50
26:Z:237:LEU:HB2	26:Z:239:ASP:HB3	1.94	0.50
20:C:159:LYS:NZ	20:C:163:GLU:OE2	2.34	0.50
17:D:337:ASP:H	17:D:340:GLN:HB2	1.76	0.50
17:D:43:ARG:HA	17:D:46:LYS:HB2	1.94	0.50
18:E:174:GLY:CA	18:E:176:PRO:HD2	2.40	0.50
11:Q:178:PHE:HB2	11:Q:194:ILE:HB	1.92	0.50
12:R:113:TYR:OH	12:R:115:ASP:OD2	2.24	0.50
21:U:886:PRO:HA	21:U:889:LEU:HD12	1.93	0.50
23:W:183:VAL:O	23:W:186:ILE:HG22	2.12	0.50
23:W:75:TYR:HD1	23:W:78:LYS:HE2	1.76	0.50
17:D:115:ILE:HA	17:D:139:LEU:HB2	1.94	0.50
17:D:185:LEU:HD11	17:D:259:PRO:HB3	1.94	0.50
18:E:83:CYS:HB3	18:E:87:LEU:HD21	1.93	0.50
3:I:119:GLN:HE21	3:I:123:GLN:HE22	1.60	0.50
8:N:44:CYS:SG	8:N:99:ILE:HB	2.52	0.50
22:V:26:PRO:O	22:V:29:PRO:HD2	2.12	0.50
16:B:218:PRO:HB2	16:B:346:ARG:HH12	1.77	0.49
20:C:267:SER:HA	20:C:270:GLN:HB2	1.94	0.49
19:F:431:LYS:HB2	19:F:432:LYS:HB2	1.93	0.49
3:I:45:LEU:HD11	3:I:137:ILE:HG12	1.93	0.49
23:W:155:GLN:HG2	23:W:157:GLY:H	1.76	0.49
15:A:351:ARG:HH11	15:A:378:PRO:HA	1.76	0.49
2:H:22:ILE:HD13	2:H:152:SER:HA	1.94	0.49
5:K:191:LEU:O	5:K:195:ILE:HG13	2.12	0.49
21:U:436:ALA:HB1	21:U:472:ILE:HG12	1.93	0.49
22:V:235:LEU:HD12	22:V:247:GLN:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:105:ASP:N	15:A:105:ASP:OD1	2.44	0.49
15:A:97:ARG:HB3	16:B:131:HIS:HD2	1.77	0.49
20:C:184:LYS:HB3	20:C:277:LEU:HD22	1.93	0.49
20:C:89:VAL:HG12	20:C:91:PRO:HD2	1.94	0.49
18:E:118:LEU:HD11	18:E:196:LEU:HD11	1.93	0.49
19:F:232:GLY:HA2	33:F:501:ATP:PB	2.52	0.49
5:K:141:LEU:HB2	5:K:156:MET:HG2	1.95	0.49
14:T:114:GLY:HA2	14:T:192:VAL:HG21	1.93	0.49
14:T:89:HIS:HA	14:T:112:ILE:HD12	1.93	0.49
21:U:232:ILE:O	21:U:236:LEU:HG	2.12	0.49
21:U:478:SER:OG	21:U:511:ALA:HB1	2.12	0.49
22:V:144:ASP:OD1	22:V:150:ARG:NH2	2.31	0.49
22:V:194:LYS:O	22:V:242:HIS:NE2	2.33	0.49
23:W:142:ARG:HH21	23:W:178:GLU:HB2	1.77	0.49
23:W:392:PHE:O	23:W:396:LEU:HG	2.12	0.49
23:W:67:LEU:H	23:W:68:VAL:HA	1.77	0.49
18:E:216:ARG:NE	18:E:259:GLU:OE1	2.45	0.49
4:J:17:PHE:O	4:J:21:TYR:HB3	2.12	0.49
6:L:155:ASP:HB3	7:M:62:SER:HB2	1.93	0.49
8:N:132:SER:HA	8:N:135:ILE:HG12	1.93	0.49
9:O:51:ASP:O	9:O:55:THR:OG1	2.17	0.49
21:U:176:MET:HA	21:U:179:TYR:CD1	2.46	0.49
22:V:108:LEU:HA	22:V:111:TYR:HD2	1.77	0.49
22:V:408:ARG:O	22:V:411:SER:OG	2.23	0.49
23:W:92:LYS:N	23:W:93:ARG:HB3	2.24	0.49
26:Z:136:GLU:OE2	26:Z:157:HIS:ND1	2.46	0.49
16:B:395:ILE:HA	16:B:398:ILE:HG12	1.95	0.49
20:C:36:ASN:O	20:C:40:GLN:HG2	2.12	0.49
17:D:65:GLN:O	20:C:49:ARG:NH2	2.45	0.49
17:D:119:ILE:HG21	17:D:123:LEU:HG	1.93	0.49
18:E:251:ARG:HH12	18:E:255:ARG:CZ	2.26	0.49
19:F:84:LYS:HA	19:F:161:LEU:HD22	1.93	0.49
22:V:90:GLU:HG3	22:V:158:PRO:HB3	1.94	0.49
26:Z:222:ILE:CG2	26:Z:223:ASN:HB3	2.33	0.49
15:A:380:SER:O	16:B:343:ARG:NH1	2.45	0.49
16:B:249:ARG:HH11	20:C:283:PHE:HE1	1.60	0.49
17:D:154:LEU:C	17:D:156:SER:H	2.15	0.49
19:F:205:PRO:O	19:F:209:LYS:HG2	2.12	0.49
5:K:232:GLU:HA	5:K:235:GLU:HG3	1.94	0.49
5:K:70:ILE:HG23	5:K:93:ARG:HG2	1.93	0.49
6:L:160:SER:OG	6:L:165:SER:HB3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:34:LEU:HD21	8:N:186:ARG:CZ	2.42	0.49
21:U:374:SER:HB2	21:U:410:VAL:HB	1.93	0.49
24:X:205:LYS:HG3	24:X:208:ALA:HB3	1.94	0.49
26:Z:182:THR:N	26:Z:183:THR:HA	2.27	0.49
16:B:203:LEU:HG	16:B:211:TYR:CD1	2.47	0.49
17:D:141:ASP:OD1	17:D:142:VAL:N	2.46	0.49
19:F:150:LEU:HD22	19:F:164:LEU:HB3	1.95	0.49
19:F:223:VAL:HG23	19:F:350:ARG:HB2	1.94	0.49
4:J:11:SER:HB3	4:J:17:PHE:CZ	2.47	0.49
5:K:11:GLY:C	5:K:13:ASN:H	2.15	0.49
21:U:176:MET:HA	21:U:179:TYR:HD1	1.77	0.49
22:V:281:ASN:N	22:V:284:GLU:HB3	2.27	0.49
4:J:200:GLN:HB2	16:B:358:GLU:OE2	2.13	0.49
20:C:308:PRO:O	20:C:310:ARG:HG3	2.13	0.49
20:C:99:VAL:HA	20:C:100:ASP:CB	2.37	0.49
1:G:39:SER:H	1:G:172:GLN:HE21	1.59	0.49
5:K:91:LYS:O	5:K:95:GLU:HG3	2.13	0.49
8:N:45:ARG:HD2	8:N:52:THR:OG1	2.12	0.49
11:Q:36:PHE:O	11:Q:44:LEU:N	2.43	0.49
21:U:471:ASP:N	21:U:471:ASP:OD1	2.46	0.49
16:B:178:LYS:HG3	20:C:283:PHE:HA	1.94	0.49
16:B:294:ARG:NH1	16:B:295:TYR:O	2.45	0.49
1:G:71:LYS:O	1:G:95:ARG:NH2	2.46	0.49
2:H:49:GLU:HA	2:H:208:ILE:HG22	1.94	0.49
5:K:73:HIS:HA	5:K:226:PHE:CE2	2.48	0.49
13:S:38:ARG:HH12	14:T:151:ARG:HD3	1.78	0.49
21:U:113:VAL:HG22	21:U:158:ARG:HG3	1.94	0.49
21:U:167:ILE:HD12	21:U:204:ILE:HG21	1.94	0.49
21:U:525:ASN:OD1	21:U:526:ALA:N	2.46	0.49
21:U:541:HIS:HB2	21:U:544:ILE:HG22	1.93	0.49
22:V:234:ARG:O	22:V:237:THR:HG22	2.13	0.49
22:V:252:ASN:ND2	22:V:284:GLU:OE2	2.43	0.49
23:W:402:ILE:HG23	23:W:416:GLN:HE22	1.77	0.49
15:A:348:LEU:HA	15:A:351:ARG:NH2	2.28	0.49
16:B:248:LEU:HD23	16:B:282:VAL:HG22	1.95	0.49
17:D:149:SER:OG	18:E:78:ARG:NH2	2.46	0.49
6:L:167:SER:O	6:L:170:THR:OG1	2.25	0.49
7:M:15:SER:OG	7:M:17:ASP:OD1	2.17	0.49
22:V:47:SER:HA	22:V:50:GLU:HB2	1.94	0.49
25:Y:333:GLU:HA	25:Y:336:ARG:HH21	1.78	0.49
15:A:343:PHE:HA	15:A:344:SER:OG	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:102:ASN:HA	19:F:103:ASP:HA	1.59	0.48
1:G:184:LYS:HB2	1:G:185:LYS:O	2.13	0.48
21:U:73:ALA:HB1	21:U:76:GLU:HB3	1.95	0.48
23:W:72:LYS:NZ	23:W:119:PRO:O	2.42	0.48
18:E:161:ARG:HD2	23:W:175:GLY:HA2	1.95	0.48
24:X:406:ASN:HB2	25:Y:376:LEU:HD11	1.94	0.48
18:E:242:ARG:HD3	18:E:254:GLN:HG3	1.94	0.48
19:F:406:ILE:HG22	19:F:409:ARG:HH11	1.78	0.48
21:U:265:ILE:HG12	21:U:269:ARG:HH11	1.78	0.48
22:V:322:VAL:HG13	22:V:323:GLY:N	2.27	0.48
26:Z:219:LYS:HG3	26:Z:220:LEU:HD23	1.94	0.48
20:C:331:ILE:HD13	20:C:334:ARG:HE	1.78	0.48
12:R:101:ILE:HB	12:R:112:TYR:HB2	1.96	0.48
13:S:92:LEU:HD23	13:S:124:PHE:CE2	2.48	0.48
23:W:98:LYS:HD3	23:W:138:VAL:HB	1.95	0.48
24:X:223:LYS:HE2	25:Y:244:ALA:HB2	1.95	0.48
26:Z:224:HIS:CB	26:Z:225:GLN:HA	2.35	0.48
16:B:120:HIS:ND1	16:B:134:SER:OG	2.44	0.48
16:B:230:THR:HG21	16:B:353:PHE:CE2	2.48	0.48
20:C:11:LEU:HD11	21:U:141:CYS:HA	1.95	0.48
17:D:112:TYR:HB3	20:C:71:SER:HB2	1.95	0.48
4:J:132:LEU:HG	4:J:146:GLN:HB2	1.95	0.48
5:K:191:LEU:HD21	5:K:221:GLN:HE21	1.77	0.48
12:R:7:LYS:HG2	12:R:124:ALA:HA	1.95	0.48
12:R:174:VAL:O	12:R:189:SER:HA	2.14	0.48
21:U:24:LEU:HD13	21:U:59:PHE:CD2	2.48	0.48
22:V:134:PHE:HA	22:V:137:GLU:OE1	2.14	0.48
22:V:273:LYS:HA	22:V:274:SER:HB2	1.95	0.48
23:W:51:GLU:OE1	23:W:51:GLU:N	2.46	0.48
25:Y:20:ALA:HB2	25:Y:150:PHE:HD1	1.77	0.48
25:Y:78:GLU:OE1	25:Y:81:LEU:HD22	2.13	0.48
16:B:166:ASP:HA	16:B:167:THR:OG1	2.14	0.48
20:C:69:GLN:HB2	20:C:118:ASN:HB2	1.94	0.48
17:D:370:ILE:HG23	17:D:371:SER:H	1.77	0.48
3:I:3:ARG:HH21	3:I:8:ARG:NH2	2.12	0.48
6:L:229:VAL:HG12	6:L:233:LEU:HG	1.96	0.48
12:R:20:ALA:HB3	12:R:31:VAL:HG21	1.95	0.48
21:U:506:ALA:HB2	21:U:541:HIS:HB3	1.96	0.48
23:W:139:GLU:HG2	23:W:142:ARG:HB2	1.95	0.48
24:X:406:ASN:HA	24:X:409:LYS:HD3	1.94	0.48
26:Z:228:TYR:O	26:Z:231:GLN:HB3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:333:ARG:O	15:A:337:LEU:N	2.31	0.48
20:C:255:GLY:N	20:C:256:SER:HB2	2.28	0.48
17:D:179:GLU:HA	17:D:183:LEU:HD13	1.94	0.48
18:E:184:ALA:HB1	18:E:231:PHE:CZ	2.49	0.48
19:F:85:THR:HA	19:F:86:LEU:HD23	1.94	0.48
1:G:152:TYR:HA	1:G:162:GLY:HA2	1.96	0.48
7:M:56:LYS:N	7:M:57:LEU:HA	2.26	0.48
9:O:113:ILE:HA	9:O:119:THR:HG22	1.95	0.48
9:O:215:LYS:HB3	10:P:197:THR:HB	1.95	0.48
23:W:135:LYS:HB3	23:W:136:ILE:C	2.33	0.48
23:W:235:GLN:OE1	23:W:243:ILE:HD13	2.13	0.48
25:Y:334:LEU:O	25:Y:338:ILE:HG13	2.14	0.48
16:B:133:VAL:HG13	16:B:158:ALA:HA	1.96	0.48
20:C:13:GLU:N	20:C:14:GLY:HA3	2.27	0.48
2:H:42:ASN:N	2:H:42:ASN:OD1	2.43	0.48
6:L:172:LEU:O	6:L:175:HIS:N	2.40	0.48
6:L:44:ALA:N	6:L:137:TYR:OH	2.46	0.48
21:U:159:ARG:HB3	21:U:162:VAL:HG12	1.95	0.48
21:U:32:ASN:OD1	21:U:33:ASP:N	2.43	0.48
21:U:493:VAL:HG21	21:U:519:VAL:HG11	1.96	0.48
23:W:441:LYS:NZ	26:Z:207:ASP:OD2	2.46	0.48
24:X:318:ILE:HG22	24:X:321:THR:H	1.79	0.48
26:Z:210:SER:HB2	26:Z:214:LYS:NZ	2.29	0.48
26:Z:43:TRP:HZ3	26:Z:48:LEU:HD12	1.78	0.48
16:B:261:GLY:HA3	16:B:263:GLY:H	1.79	0.48
17:D:112:TYR:O	20:C:71:SER:HB2	2.14	0.48
17:D:139:LEU:O	17:D:143:LEU:HD13	15.53	0.48
17:D:406:VAL:HG23	17:D:407:ILE:HB	1.96	0.48
18:E:173:TYR:OH	18:E:300:HIS:HB3	2.13	0.48
4:J:221:ASN:O	4:J:223:GLU:N	2.37	0.48
6:L:200:PRO:HD2	6:L:203:GLN:HE22	1.79	0.48
6:L:40:SER:OG	6:L:43:HIS:O	2.28	0.48
15:A:97:ARG:HA	15:A:98:CYS:HA	1.54	0.48
17:D:384:MET:HA	17:D:387:VAL:HG12	1.95	0.48
19:F:100:ASP:OD1	19:F:100:ASP:N	2.46	0.48
7:M:185:THR:O	7:M:189:ILE:HG12	2.14	0.48
7:M:200:VAL:HG22	7:M:201:HIS:H	1.79	0.48
7:M:40:ARG:NH1	7:M:160:TYR:O	2.47	0.48
10:P:106:GLU:HB3	10:P:139:SER:HB3	1.95	0.48
10:P:58:THR:OG1	11:Q:121:LEU:O	2.26	0.48
21:U:792:ASN:OD1	21:U:793:LYS:N	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:31:ALA:HB3	22:V:32:PRO:HD3	1.95	0.48
23:W:35:ALA:HB2	23:W:48:LEU:HD11	1.96	0.48
23:W:397:VAL:HG21	24:X:341:PRO:HA	1.95	0.48
26:Z:191:ILE:O	26:Z:195:VAL:HG23	2.13	0.48
20:C:60:ARG:O	20:C:64:GLN:HG2	2.14	0.48
17:D:92:PHE:HA	17:D:103:VAL:HG23	1.95	0.48
3:I:151:ASP:HB2	3:I:155:ASN:O	2.14	0.48
9:O:67:SER:HB3	9:O:74:PRO:HG3	1.95	0.48
10:P:56:LEU:HD21	10:P:58:THR:HB	1.95	0.48
20:C:248:MET:HG3	20:C:293:MET:SD	2.54	0.47
17:D:218:ALA:O	17:D:222:HIS:ND1	2.44	0.47
2:H:119:GLN:NE2	2:H:152:SER:O	2.47	0.47
6:L:137:TYR:CZ	6:L:142:PRO:HB3	2.50	0.47
11:Q:12:TYR:HB2	11:Q:182:ILE:HD11	1.95	0.47
23:W:100:ALA:O	23:W:104:MET:HG2	2.14	0.47
16:B:191:ASP:N	16:B:191:ASP:OD1	2.46	0.47
16:B:261:GLY:HA2	16:B:262:ASP:HB3	1.96	0.47
18:E:193:CYS:SG	18:E:227:PRO:HG2	2.54	0.47
19:F:369:HIS:ND1	19:F:397:LYS:HG2	2.29	0.47
4:J:118:TYR:HD1	4:J:124:ARG:HH21	1.61	0.47
21:U:567:ILE:HD13	21:U:570:LEU:HD12	1.96	0.47
23:W:446:ILE:HG21	26:Z:157:HIS:HB2	1.94	0.47
20:C:203:VAL:O	20:C:207:THR:OG1	2.21	0.47
17:D:251:PHE:HE2	17:D:292:LEU:HB2	1.79	0.47
2:H:50:LYS:NZ	2:H:62:VAL:O	2.48	0.47
24:X:134:VAL:HG13	24:X:172:LEU:HD23	1.97	0.47
18:E:61:LEU:HD12	18:E:70:ILE:HG22	1.97	0.47
19:F:314:LEU:HD21	19:F:342:LEU:HD23	1.95	0.47
19:F:76:ASN:O	19:F:80:ILE:HG13	2.13	0.47
6:L:103:LEU:HD22	6:L:107:ARG:HD2	1.96	0.47
14:T:153:VAL:HG21	14:T:168:LEU:HD11	1.96	0.47
21:U:474:ARG:NH2	21:U:500:ASN:HB2	2.25	0.47
22:V:80:LYS:CE	22:V:86:VAL:HB	2.44	0.47
23:W:423:ASN:N	23:W:423:ASN:OD1	2.46	0.47
19:F:90:VAL:HG13	19:F:150:LEU:HA	1.96	0.47
3:I:164:ILE:HA	3:I:165:GLY:HA2	1.69	0.47
3:I:31:ALA:O	3:I:50:ARG:NH2	2.47	0.47
21:U:35:TRP:HB3	21:U:70:HIS:CD2	2.49	0.47
22:V:207:ALA:HA	22:V:210:CYS:SG	2.54	0.47
22:V:54:LYS:N	22:V:55:THR:OG1	2.47	0.47
15:A:156:LYS:C	15:A:157:ILE:HD13	2.35	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:100:ASP:OD1	20:C:122:THR:HB	2.14	0.47
20:C:175:PHE:HD1	20:C:180:ILE:HG23	1.79	0.47
18:E:249:ALA:O	18:E:252:GLU:HG2	2.14	0.47
19:F:299:GLU:HA	19:F:300:LYS:HA	1.67	0.47
19:F:301:ALA:HB3	19:F:304:ARG:HB2	1.95	0.47
1:G:58:ASP:OD1	1:G:59:LYS:N	2.48	0.47
7:M:54:LEU:H	7:M:57:LEU:HD11	1.80	0.47
12:R:37:ILE:HG23	12:R:60:ALA:HB2	1.96	0.47
12:R:65:ILE:O	12:R:69:ARG:HG3	2.15	0.47
21:U:216:VAL:HG21	21:U:232:ILE:HD13	1.95	0.47
22:V:246:GLY:O	22:V:249:THR:OG1	2.28	0.47
24:X:242:ILE:HG13	24:X:243:ASP:H	1.79	0.47
25:Y:343:LEU:O	25:Y:343:LEU:HD23	2.14	0.47
25:Y:357:ASN:CB	25:Y:358:ARG:HA	2.45	0.47
25:Y:64:GLN:HG2	25:Y:65:ILE:HG22	1.96	0.47
16:B:180:PRO:CG	16:B:239:VAL:HG23	2.38	0.47
18:E:312:ILE:HG23	18:E:343:LEU:HD23	1.96	0.47
19:F:229:PRO:HA	19:F:230:GLY:HA2	1.56	0.47
4:J:180:ALA:HA	4:J:181:ILE:HA	1.44	0.47
13:S:84:THR:O	13:S:88:ILE:HG13	2.15	0.47
14:T:146:ALA:O	14:T:150:LEU:HG	2.15	0.47
13:S:35:ILE:O	14:T:151:ARG:NH2	2.47	0.47
23:W:446:ILE:HD13	26:Z:157:HIS:HB2	1.97	0.47
15:A:102:ILE:HD11	15:A:135:GLU:O	2.15	0.47
17:D:300:ASP:HA	17:D:301:GLN:HA	1.49	0.47
17:D:411:GLU:HA	17:D:412:GLN:HB2	1.96	0.47
18:E:145:LEU:HD21	18:E:299:ILE:HD13	1.97	0.47
1:G:13:ILE:HB	1:G:129:ALA:HB1	1.97	0.47
5:K:200:ILE:HA	5:K:203:LYS:NZ	2.29	0.47
13:S:93:SER:OG	13:S:128:GLY:O	2.21	0.47
24:X:80:ILE:HD12	24:X:81:SER:O	2.13	0.47
15:A:391:GLU:HA	15:A:394:MET:HB3	1.95	0.47
16:B:135:ILE:O	16:B:135:ILE:HD12	2.14	0.47
17:D:283:ARG:HG3	17:D:286:GLN:NE2	2.28	0.47
18:E:305:ASN:O	18:E:309:ARG:N	2.42	0.47
5:K:225:ASN:HA	5:K:227:HIS:HB3	1.97	0.47
7:M:169:ARG:O	7:M:173:LYS:HG2	2.15	0.47
13:S:6:VAL:HG12	13:S:57:PHE:CD1	2.50	0.47
21:U:566:LEU:O	21:U:570:LEU:HG	2.13	0.47
21:U:724:VAL:HA	21:U:727:LYS:HG2	1.96	0.47
18:E:310:LEU:HD13	18:E:332:VAL:HG21	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:200:ILE:O	5:K:204:GLN:HG3	2.15	0.47
9:O:36:PHE:HD1	9:O:42:TYR:HE1	1.60	0.47
22:V:153:LYS:O	22:V:157:THR:CG2	2.57	0.47
26:Z:239:ASP:OD1	26:Z:239:ASP:N	2.48	0.47
6:L:164:ARG:HD2	6:L:198:THR:O	2.15	0.47
9:O:211:VAL:HG21	10:P:198:ARG:HD3	1.96	0.47
11:Q:5:ILE:HG22	11:Q:16:ALA:HB3	1.97	0.47
21:U:168:LEU:HD13	21:U:204:ILE:HD11	1.97	0.47
21:U:427:LEU:HD23	21:U:429:LYS:NZ	2.29	0.47
24:X:176:THR:O	24:X:180:LEU:HG	2.14	0.47
16:B:133:VAL:HG11	16:B:159:VAL:HG12	1.97	0.46
20:C:100:ASP:CG	20:C:123:LEU:H	2.18	0.46
17:D:60:TYR:HE1	21:U:640:LEU:HD21	1.79	0.46
17:D:82:ILE:HA	17:D:83:GLN:HA	1.46	0.46
18:E:265:ASP:OD2	18:E:294:ARG:NH2	2.45	0.46
1:G:148:GLY:O	1:G:150:GLN:NE2	2.48	0.46
3:I:105:ILE:HD11	3:I:109:GLN:HG3	1.97	0.46
13:S:193:LEU:HD23	13:S:208:VAL:HB	1.97	0.46
14:T:186:ARG:HE	14:T:202:PRO:HB2	1.80	0.46
21:U:521:LEU:HB2	21:U:554:LEU:CD2	2.46	0.46
23:W:56:THR:HG21	23:W:103:LYS:HG2	1.97	0.46
24:X:258:LYS:HD3	24:X:266:ASP:HB2	1.95	0.46
15:A:406:GLU:HA	15:A:409:PHE:CE2	2.50	0.46
20:C:168:PRO:HG2	20:C:290:LYS:HE2	1.97	0.46
20:C:215:SER:HA	20:C:216:GLY:HA3	1.54	0.46
2:H:43:GLY:HA2	2:H:144:PRO:HG3	1.97	0.46
4:J:84:ILE:O	4:J:88:ARG:HG3	2.15	0.46
6:L:179:PHE:CE2	6:L:190:HIS:HB3	2.50	0.46
11:Q:44:LEU:HD21	11:Q:57:ALA:HA	1.96	0.46
14:T:27:LEU:HD13	14:T:184:TYR:HB3	1.96	0.46
21:U:766:PHE:HD1	21:U:776:SER:HA	1.80	0.46
23:W:32:ALA:O	23:W:36:LYS:HG3	2.15	0.46
23:W:440:ASN:O	23:W:443:THR:OG1	2.18	0.46
24:X:406:ASN:HA	24:X:409:LYS:HB2	1.96	0.46
15:A:103:ASN:HB2	15:A:112:ILE:HG23	1.96	0.46
15:A:100:LYS:HZ1	15:A:142:VAL:HB	1.80	0.46
15:A:176:ASP:HA	15:A:357:ILE:HD12	1.97	0.46
15:A:288:GLY:HA2	15:A:289:ALA:HA	1.69	0.46
20:C:255:GLY:CA	20:C:256:SER:HB2	2.45	0.46
18:E:162:VAL:HB	18:E:164:ILE:HG22	1.97	0.46
18:E:76:GLY:N	18:E:77:PRO:HD2	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:TYR:CE2	2:H:126:GLY:HA3	2.51	0.46
6:L:130:VAL:HG22	6:L:132:LEU:H	1.81	0.46
6:L:45:VAL:HG11	6:L:188:VAL:HA	1.98	0.46
7:M:213:LEU:O	7:M:226:ILE:HG13	2.15	0.46
11:Q:163:CYS:O	11:Q:167:LEU:HG	2.16	0.46
21:U:630:PRO:HA	21:U:659:CYS:SG	2.55	0.46
15:A:102:ILE:HG22	15:A:113:ILE:HG12	1.96	0.46
17:D:240:LEU:HB2	17:D:284:GLU:OE1	2.15	0.46
18:E:191:LEU:HD23	18:E:229:ILE:HD11	1.96	0.46
2:H:122:THR:HG22	2:H:129:PRO:HB3	1.98	0.46
3:I:3:ARG:HH11	5:K:11:GLY:N	2.13	0.46
7:M:229:LYS:NZ	7:M:235:ALA:H	2.14	0.46
20:C:214:VAL:HG22	20:C:215:SER:H	1.79	0.46
18:E:360:ASP:N	18:E:360:ASP:OD1	2.41	0.46
19:F:418:GLU:N	19:F:418:GLU:OE1	2.42	0.46
6:L:38:LEU:HD21	6:L:191:GLY:HA2	1.98	0.46
7:M:229:LYS:HD2	7:M:229:LYS:HA	1.48	0.46
21:U:350:LEU:HD12	21:U:353:LEU:HD12	1.96	0.46
22:V:62:HIS:HA	22:V:65:ARG:HB3	1.98	0.46
23:W:240:TYR:CD1	23:W:276:LEU:HB3	2.50	0.46
25:Y:208:PHE:HB3	25:Y:209:THR:H	1.55	0.46
15:A:158:ASP:OD1	15:A:159:PRO:HD2	2.16	0.46
15:A:171:ASP:OD1	15:A:171:ASP:N	2.48	0.46
17:D:130:VAL:HG21	17:D:139:LEU:HD22	1.96	0.46
18:E:70:ILE:HG12	18:E:80:VAL:HG12	1.98	0.46
19:F:181:PRO:HG3	19:F:238:ARG:HG2	1.97	0.46
19:F:265:ALA:O	19:F:269:ARG:HG3	2.16	0.46
1:G:60:LEU:HD11	7:M:176:ILE:HG21	1.98	0.46
4:J:10:PHE:HD1	5:K:23:GLN:HE21	1.64	0.46
6:L:184:LEU:H	6:L:184:LEU:HD12	1.80	0.46
6:L:204:ASP:HA	6:L:205:LEU:HB3	1.97	0.46
1:G:60:LEU:HB3	7:M:160:TYR:HB3	1.98	0.46
21:U:331:GLY:O	21:U:335:ILE:HG12	2.15	0.46
23:W:372:ARG:HG2	23:W:414:ASN:HB3	1.98	0.46
24:X:327:TYR:O	24:X:331:LEU:HD13	2.16	0.46
25:Y:183:TYR:OH	25:Y:212:GLU:HB2	2.15	0.46
25:Y:377:LEU:HA	25:Y:380:VAL:HG22	1.98	0.46
26:Z:12:HIS:ND1	26:Z:168:GLU:OE1	2.49	0.46
17:D:412:GLN:HG3	17:D:414:HIS:H	1.80	0.46
33:E:401:ATP:O1G	19:F:347:ARG:NH2	2.41	0.46
1:G:89:SER:HG	7:M:120:HIS:CE1	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:220:ASN:HA	3:I:221:GLY:HA2	1.46	0.46
6:L:36:VAL:HG22	6:L:160:SER:HB2	1.97	0.46
21:U:261:LEU:HA	21:U:264:VAL:HG12	1.97	0.46
22:V:133:PRO:O	22:V:137:GLU:HG3	2.15	0.46
25:Y:46:ARG:C	25:Y:48:ASN:H	2.19	0.46
16:B:249:ARG:HE	20:C:283:PHE:HE1	1.59	0.46
16:B:294:ARG:HB3	20:C:264:GLY:CA	2.45	0.46
18:E:174:GLY:C	18:E:176:PRO:HD2	2.36	0.46
1:G:116:LYS:HG2	1:G:160:TYR:CG	2.51	0.46
2:H:139:TRP:HA	2:H:144:PRO:HA	1.98	0.46
2:H:22:ILE:HG21	2:H:152:SER:HB3	1.96	0.46
13:S:197:ILE:HG22	13:S:199:THR:HG23	1.97	0.46
21:U:699:THR:HG21	21:U:812:ALA:O	2.16	0.46
21:U:243:LEU:HD21	21:U:913:ILE:HD13	1.98	0.46
20:C:11:LEU:HG	20:C:13:GLU:HB3	1.98	0.46
17:D:389:GLU:HB3	17:D:390:ASN:C	2.36	0.46
5:K:107:MET:HG2	5:K:111:SER:CB	2.45	0.46
22:V:482:PHE:O	22:V:486:ILE:HG13	2.15	0.46
25:Y:19:ILE:O	25:Y:23:ARG:HG2	2.15	0.46
25:Y:367:GLN:OE1	25:Y:371:LYS:HE2	2.16	0.46
15:A:347:ASP:O	15:A:351:ARG:HG3	2.16	0.46
16:B:202:GLU:OE1	16:B:206:THR:OG1	2.31	0.46
20:C:213:ARG:HH21	20:C:249:ASP:HB2	1.80	0.46
19:F:79:LYS:O	19:F:82:VAL:HG22	2.16	0.46
2:H:87:VAL:O	2:H:91:ARG:HG2	2.15	0.46
3:I:8:ARG:HD3	3:I:11:ILE:HD12	1.98	0.46
7:M:74:GLY:HA3	7:M:224:HIS:CE1	2.50	0.46
22:V:210:CYS:SG	22:V:211:TYR:N	2.89	0.46
25:Y:233:ARG:NH2	25:Y:264:TYR:O	2.41	0.46
15:A:206:ILE:HG13	15:A:207:GLU:N	2.30	0.45
20:C:248:MET:HE3	20:C:273:MET:HB3	1.97	0.45
4:J:219:ILE:H	4:J:219:ILE:HD12	1.80	0.45
6:L:89:ARG:HH21	13:S:77:HIS:HB3	1.80	0.45
10:P:70:ARG:NH2	10:P:97:GLU:OE2	2.40	0.45
21:U:173:VAL:N	21:U:174:PRO:HD3	2.32	0.45
21:U:380:THR:HG23	21:U:382:SER:H	1.82	0.45
22:V:144:ASP:N	22:V:145:LEU:HA	2.31	0.45
24:X:207:GLN:NE2	24:X:211:ASP:OD1	2.45	0.45
25:Y:138:LEU:HD22	25:Y:168:ILE:HD11	1.97	0.45
20:C:340:ARG:NH2	25:Y:179:ARG:HE	2.13	0.45
26:Z:205:LEU:HA	26:Z:208:ILE:HG22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:184:ILE:HD12	15:A:187:LEU:HD11	1.97	0.45
16:B:226:GLY:HA3	16:B:353:PHE:HB3	1.98	0.45
20:C:378:VAL:HG12	20:C:379:THR:H	1.82	0.45
17:D:143:LEU:HD22	17:D:144:PRO:HD2	1.98	0.45
18:E:281:ARG:HD3	18:E:387:LYS:HZ1	1.79	0.45
19:F:144:LYS:HA	19:F:145:LEU:HA	1.72	0.45
3:I:119:GLN:NE2	4:J:79:ASP:HA	2.31	0.45
7:M:72:HIS:CE1	7:M:105:ASN:HB3	2.50	0.45
21:U:510:GLU:OE2	21:U:546:ARG:NH2	2.50	0.45
22:V:259:LEU:HD11	22:V:294:ARG:HD2	1.97	0.45
22:V:350:GLN:HB3	22:V:353:LEU:HB3	1.98	0.45
23:W:148:THR:O	23:W:151:THR:OG1	2.28	0.45
25:Y:232:GLU:CD	25:Y:234:PRO:HD2	2.36	0.45
15:A:114:ASN:OD1	15:A:115:VAL:N	2.49	0.45
16:B:139:VAL:HA	16:B:140:ASP:CB	2.46	0.45
17:D:249:ASP:HA	17:D:252:ARG:HG2	1.98	0.45
18:E:144:GLU:O	18:E:148:VAL:HG23	2.16	0.45
18:E:109:ARG:NH2	19:F:121:CYS:SG	2.89	0.45
1:G:56:VAL:HG22	1:G:61:LEU:HD22	1.98	0.45
6:L:166:GLN:HA	6:L:169:ARG:HH11	1.81	0.45
10:P:26:ARG:HB3	10:P:37:THR:O	2.16	0.45
21:U:9:ILE:HD11	21:U:37:GLU:HG3	1.98	0.45
22:V:80:LYS:HE2	22:V:86:VAL:HB	1.98	0.45
23:W:124:LEU:O	23:W:128:LEU:HD23	2.17	0.45
15:A:146:LYS:HE2	15:A:146:LYS:HB2	1.80	0.45
15:A:290:GLY:HA2	15:A:291:GLY:HA3	1.66	0.45
16:B:152:LEU:HD23	16:B:157:HIS:HD1	1.81	0.45
20:C:255:GLY:H	20:C:256:SER:HB2	1.81	0.45
6:L:139:ASP:H	14:T:81:HIS:HE1	1.64	0.45
21:U:340:GLN:HG3	21:U:880:ASN:HB3	1.97	0.45
22:V:81:GLN:HB3	22:V:82:LEU:C	2.37	0.45
23:W:42:GLU:O	23:W:45:GLU:HB3	2.17	0.45
25:Y:118:GLU:O	25:Y:121:LEU:HG	2.17	0.45
25:Y:216:TYR:O	25:Y:220:VAL:HG23	2.16	0.45
26:Z:233:VAL:O	26:Z:236:LEU:HB2	2.17	0.45
16:B:108:SER:N	16:B:152:LEU:O	2.30	0.45
20:C:82:LYS:HG3	20:C:84:LYS:HB2	1.99	0.45
6:L:46:LEU:CD1	6:L:63:ILE:HD13	2.45	0.45
21:U:158:ARG:HD2	21:U:193:PHE:CE1	2.52	0.45
21:U:436:ALA:O	21:U:472:ILE:HD13	2.16	0.45
21:U:757:MET:HG3	21:U:758:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:455:LYS:H	22:V:456:GLY:HA2	1.81	0.45
23:W:33:LYS:O	23:W:37:GLU:HG3	2.17	0.45
25:Y:237:ARG:HD3	25:Y:264:TYR:CE1	2.52	0.45
25:Y:307:LEU:HD22	25:Y:308:LEU:HD22	1.98	0.45
23:W:440:ASN:HB3	26:Z:230:LEU:HD11	1.97	0.45
15:A:339:ARG:HA	15:A:339:ARG:HD3	2.34	0.45
15:A:357:ILE:HG23	15:A:358:HIS:ND1	2.30	0.45
20:C:184:LYS:NZ	20:C:280:LEU:HB3	2.32	0.45
12:R:7:LYS:HE2	12:R:124:ALA:HA	1.98	0.45
21:U:62:LEU:O	21:U:66:LYS:HG2	2.17	0.45
24:X:183:LEU:HB3	24:X:184:PRO:HD3	1.97	0.45
24:X:343:SER:HB2	24:X:387:ILE:HB	1.98	0.45
25:Y:39:ASP:N	25:Y:39:ASP:OD1	2.49	0.45
15:A:312:ARG:HA	15:A:313:GLY:HA2	1.55	0.45
20:C:131:VAL:HG13	20:C:132:ASP:H	1.80	0.45
17:D:304:ASN:O	17:D:305:VAL:HB	2.16	0.45
4:J:31:THR:HG22	4:J:163:ARG:N	2.32	0.45
10:P:125:ASP:HB2	10:P:129:CYS:HB3	1.98	0.45
21:U:460:TYR:HD2	21:U:461:LEU:HD12	1.82	0.45
22:V:80:LYS:HD2	22:V:82:LEU:O	2.17	0.45
23:W:441:LYS:HA	23:W:444:HIS:HE1	1.82	0.45
24:X:52:GLU:O	24:X:55:SER:OG	2.29	0.45
26:Z:164:ALA:HB3	26:Z:169:GLU:HG3	1.97	0.45
26:Z:176:LEU:HD12	26:Z:178:ASP:H	1.81	0.45
26:Z:208:ILE:HA	26:Z:211:TYR:CD2	2.51	0.45
15:A:108:ASP:HB2	15:A:109:PRO:HD3	1.97	0.45
15:A:420:TYR:HE1	16:B:350:LYS:HG2	1.79	0.45
20:C:327:ASP:O	20:C:331:ILE:HG12	2.17	0.45
17:D:203:LEU:HB3	17:D:330:LYS:HA	1.98	0.45
19:F:120:LYS:HG2	19:F:136:VAL:HG21	1.98	0.45
19:F:187:ASP:HA	19:F:368:ILE:HG21	1.97	0.45
19:F:181:PRO:HD2	19:F:242:ALA:HB2	1.98	0.45
19:F:311:LEU:O	19:F:315:ASN:HB2	2.16	0.45
19:F:436:GLN:C	19:F:438:TYR:H	2.20	0.45
1:G:144:ASP:OD2	1:G:147:GLN:HG3	2.16	0.45
2:H:66:GLU:HG2	2:H:87:VAL:HG11	1.99	0.45
4:J:33:VAL:O	4:J:44:GLY:N	2.49	0.45
11:Q:107:TYR:HA	11:Q:113:PRO:HA	1.98	0.45
21:U:632:GLN:O	21:U:636:VAL:HG22	2.16	0.45
22:V:197:THR:HG22	22:V:200:ARG:H	1.81	0.45
22:V:319:HIS:HB2	22:V:320:THR:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:349:LYS:C	25:Y:351:ASN:H	2.20	0.45
16:B:208:PRO:O	16:B:212:GLU:HG2	2.16	0.45
16:B:222:VAL:HA	16:B:346:ARG:HG2	1.97	0.45
16:B:288:ASP:O	16:B:292:THR:HG23	2.17	0.45
17:D:175:GLN:NE2	17:D:179:GLU:OE2	2.50	0.45
18:E:172:LEU:HD23	18:E:299:ILE:HB	1.99	0.45
19:F:293:THR:HG23	19:F:337:ILE:HG21	1.99	0.45
23:W:370:TYR:HA	23:W:371:THR:CB	2.46	0.45
24:X:297:ARG:HB2	24:X:337:ARG:NH1	2.31	0.45
25:Y:50:MET:SD	25:Y:74:LYS:HB3	2.57	0.45
15:A:100:LYS:NZ	15:A:142:VAL:HB	2.32	0.45
15:A:191:VAL:CG2	15:A:316:LYS:HE2	2.44	0.45
15:A:362:MET:HG2	15:A:363:SER:H	1.81	0.45
20:C:80:MET:HB2	20:C:84:LYS:O	2.17	0.45
20:C:89:VAL:HB	20:C:92:GLU:HB2	1.99	0.45
17:D:303:VAL:HG23	17:D:304:ASN:HB2	1.98	0.45
1:G:157:ALA:HB3	1:G:159:TYR:HD1	1.82	0.45
4:J:12:PRO:HG3	5:K:26:TYR:CZ	2.52	0.45
5:K:157:ASP:OD2	5:K:159:SER:OG	2.32	0.45
10:P:15:LYS:HD3	10:P:119:PRO:HG2	1.99	0.45
12:R:21:THR:HG22	12:R:26:ILE:HA	1.98	0.45
13:S:125:ASP:N	13:S:125:ASP:OD1	2.49	0.45
17:D:41:TYR:CD2	21:U:152:GLY:HA3	2.52	0.45
21:U:908:ILE:HG12	21:U:909:GLY:H	1.82	0.45
16:B:255:LEU:CD1	16:B:256:ILE:HG12	2.47	0.44
20:C:167:LEU:HD22	20:C:175:PHE:CE2	2.53	0.44
19:F:90:VAL:O	19:F:127:SER:OG	2.20	0.44
5:K:177:ALA:O	5:K:181:LEU:HB2	2.17	0.44
7:M:92:ARG:NH1	7:M:96:SER:OG	2.49	0.44
7:M:110:HIS:NE2	8:N:70:LEU:HA	2.32	0.44
11:Q:128:PRO:HB2	11:Q:147:TYR:OH	2.17	0.44
13:S:6:VAL:HG12	13:S:57:PHE:CE1	2.51	0.44
21:U:157:THR:OG1	21:U:159:ARG:NH2	2.50	0.44
21:U:193:PHE:HA	21:U:196:LYS:HD2	1.97	0.44
21:U:59:PHE:HA	21:U:62:LEU:HD13	1.99	0.44
22:V:100:MET:HG2	22:V:102:PRO:HD2	1.99	0.44
22:V:76:LYS:HA	22:V:77:GLU:HA	1.74	0.44
24:X:173:GLU:O	24:X:176:THR:HG22	2.17	0.44
26:Z:124:ILE:HA	26:Z:135:THR:HA	1.99	0.44
16:B:199:GLU:O	16:B:203:LEU:N	2.50	0.44
18:E:203:ILE:HG23	18:E:256:THR:HG21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:203:GLN:HG2	6:L:204:ASP:O	2.17	0.44
8:N:45:ARG:HB2	8:N:52:THR:HG21	2.00	0.44
21:U:28:ASN:HD22	21:U:59:PHE:HZ	1.65	0.44
22:V:137:GLU:HA	22:V:140:ASP:HB2	1.98	0.44
22:V:419:LEU:O	22:V:422:ILE:HG22	2.17	0.44
25:Y:387:ILE:HA	25:Y:388:ASN:HA	1.54	0.44
20:C:171:HIS:HE2	25:Y:95:LEU:H	1.64	0.44
26:Z:21:ASP:OD1	26:Z:22:HIS:N	2.50	0.44
26:Z:225:GLN:NE2	26:Z:229:GLN:HB2	2.33	0.44
20:C:285:ALA:HB1	20:C:286:THR:HB	2.00	0.44
18:E:195:PHE:CZ	18:E:197:LYS:HB2	2.53	0.44
18:E:210:GLU:O	18:E:213:ARG:N	2.50	0.44
18:E:219:PHE:O	18:E:223:ARG:HG3	2.18	0.44
18:E:240:GLY:HA2	18:E:284:THR:HB	1.99	0.44
19:F:313:LEU:O	19:F:316:GLN:HB2	2.17	0.44
5:K:79:SER:H	5:K:139:VAL:HG23	1.81	0.44
5:K:154:PHE:HB3	5:K:162:PHE:HE1	1.81	0.44
6:L:7:ASP:OD1	6:L:20:HIS:ND1	2.50	0.44
22:V:80:LYS:HD3	22:V:80:LYS:HA	1.61	0.44
23:W:333:LEU:O	23:W:333:LEU:HD12	2.17	0.44
24:X:258:LYS:HE3	24:X:270:LEU:HD11	1.98	0.44
25:Y:109:GLU:HG2	25:Y:124:PHE:HE1	1.82	0.44
16:B:224:LEU:HD13	16:B:234:LEU:HB3	1.98	0.44
16:B:283:PHE:CE2	16:B:285:ASP:HB2	2.52	0.44
17:D:374:ASP:OD1	17:D:377:SER:HB2	2.17	0.44
19:F:343:LEU:HD22	19:F:351:LYS:HZ3	1.82	0.44
19:F:70:LYS:HG3	19:F:74:LYS:HE3	1.98	0.44
2:H:50:LYS:NZ	2:H:62:VAL:HB	2.32	0.44
3:I:3:ARG:HH21	3:I:8:ARG:HH21	1.66	0.44
4:J:154:HIS:CE1	5:K:59:MET:HG3	2.52	0.44
11:Q:11:ASP:N	11:Q:11:ASP:OD1	2.48	0.44
14:T:23:ALA:HB3	14:T:169:VAL:HG11	1.99	0.44
21:U:26:LYS:O	21:U:30:VAL:HG22	2.17	0.44
22:V:161:PRO:O	22:V:164:GLU:HB2	2.17	0.44
23:W:144:ARG:HA	23:W:147:LYS:HE2	1.99	0.44
23:W:408:ARG:HD2	24:X:346:GLN:NE2	2.29	0.44
23:W:40:LEU:HB2	23:W:41:GLN:CA	2.41	0.44
15:A:311:PRO:HD2	15:A:313:GLY:HA2	1.99	0.44
16:B:173:VAL:HG12	20:C:232:ARG:HG2	2.00	0.44
16:B:235:LEU:O	16:B:238:ALA:N	2.48	0.44
20:C:187:LEU:HG	20:C:313:ARG:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:343:ASN:HB3	20:C:346:LYS:HG2	1.99	0.44
20:C:338:LEU:HD13	20:C:378:VAL:HB	1.98	0.44
17:D:312:ASN:HD21	18:E:242:ARG:NH2	2.08	0.44
18:E:82:GLY:O	18:E:106:THR:OG1	2.24	0.44
19:F:336:ASP:OD1	19:F:336:ASP:N	2.50	0.44
15:A:122:VAL:N	19:F:88:TYR:O	2.30	0.44
3:I:14:PRO:HA	4:J:21:TYR:CE1	2.52	0.44
4:J:88:ARG:NH2	11:Q:70:ARG:HG3	2.32	0.44
5:K:13:ASN:ND2	6:L:126:ARG:HH11	2.15	0.44
7:M:233:GLU:OE1	7:M:237:LYS:HG2	2.18	0.44
4:J:88:ARG:HH12	11:Q:69:MET:HB2	1.83	0.44
21:U:161:ASP:OD1	21:U:162:VAL:N	2.51	0.44
22:V:59:ALA:N	22:V:60:ALA:HB3	2.31	0.44
23:W:253:THR:HB	23:W:254:PRO:HD3	2.00	0.44
16:B:155:LYS:HA	16:B:156:VAL:HA	1.53	0.44
16:B:401:GLU:HG3	16:B:422:SER:HB2	1.98	0.44
1:G:171:LYS:HB3	1:G:205:VAL:HG11	1.99	0.44
10:P:59:ASP:OD2	10:P:104:TYR:N	2.45	0.44
11:Q:86:ARG:HA	11:Q:86:ARG:HD3	1.76	0.44
22:V:428:LEU:HD21	22:V:434:ALA:N	2.33	0.44
22:V:96:ARG:HA	22:V:98:LEU:HD12	1.99	0.44
25:Y:197:ALA:HB3	25:Y:226:VAL:HG21	1.98	0.44
26:Z:102:HIS:HD2	26:Z:104:ASN:HB3	1.81	0.44
15:A:119:ALA:HA	19:F:127:SER:CB	2.48	0.44
15:A:174:TYR:CD1	15:A:227:ARG:HD2	2.44	0.44
16:B:363:ARG:O	16:B:367:ILE:HG13	2.18	0.44
19:F:69:MET:HA	19:F:72:LYS:HG2	1.99	0.44
1:G:122:SER:HB2	1:G:158:GLY:HA2	1.99	0.44
4:J:120:GLN:OE1	5:K:135:ARG:N	2.49	0.44
8:N:19:ARG:HB3	8:N:171:GLY:C	2.38	0.44
10:P:142:CYS:O	10:P:146:MET:HG3	2.16	0.44
12:R:64:ARG:O	12:R:68:LEU:HG	2.18	0.44
25:Y:212:GLU:H	25:Y:212:GLU:HG2	1.57	0.44
26:Z:262:LEU:HA	26:Z:265:LEU:HD22	2.00	0.44
26:Z:52:ASN:OD1	26:Z:53:SER:N	2.40	0.44
18:E:326:ILE:HD12	18:E:326:ILE:O	2.17	0.44
18:E:75:ASN:HD21	19:F:130:GLN:HA	1.82	0.44
19:F:295:ARG:CZ	19:F:301:ALA:HA	2.48	0.44
3:I:139:TRP:HD1	3:I:145:PHE:CE1	2.35	0.44
9:O:195:LYS:NZ	10:P:151:GLU:OE1	2.51	0.44
22:V:55:THR:HB	22:V:198:GLN:CD	2.37	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:289:LEU:HA	22:V:292:THR:HG22	2.00	0.44
23:W:124:LEU:HA	23:W:127:THR:HG22	1.99	0.44
24:X:378:LEU:HA	24:X:385:LEU:HA	2.00	0.44
26:Z:190:ARG:HG3	26:Z:191:ILE:HD12	1.98	0.44
17:D:289:LEU:HD12	17:D:292:LEU:HD11	1.99	0.44
19:F:406:ILE:HG22	19:F:409:ARG:NH1	2.32	0.44
2:H:22:ILE:O	2:H:26:LEU:HG	2.18	0.44
8:N:41:ILE:HG12	8:N:76:VAL:HG22	2.00	0.44
13:S:27:THR:HB	13:S:40:SER:H	1.82	0.44
21:U:250:PHE:HA	21:U:253:TYR:HB3	2.00	0.44
24:X:306:LEU:HD11	24:X:313:LEU:HG	2.00	0.44
25:Y:141:VAL:HG13	25:Y:160:ASN:ND2	2.33	0.44
15:A:351:ARG:NH1	15:A:378:PRO:HA	2.32	0.43
20:C:337:ASN:OD1	25:Y:177:ARG:NH2	2.44	0.43
5:K:160:GLY:O	6:L:82:ARG:NH2	2.39	0.43
9:O:52:THR:O	9:O:56:THR:HG22	2.17	0.43
10:P:93:ASN:O	10:P:97:GLU:HG3	2.18	0.43
22:V:149:PRO:HG3	22:V:203:LEU:HG	2.00	0.43
22:V:279:GLN:NE2	22:V:285:TRP:CD1	2.85	0.43
26:Z:168:GLU:H	26:Z:168:GLU:HG2	1.60	0.43
20:C:190:GLY:HA3	20:C:317:PHE:HB3	2.00	0.43
17:D:152:MET:HE2	18:E:62:LYS:HG3	1.94	0.43
1:G:43:ARG:HA	1:G:48:ALA:HA	1.99	0.43
2:H:171:LYS:NZ	3:I:55:LEU:HD22	2.33	0.43
4:J:65:LEU:HD11	4:J:87:ALA:HB1	2.00	0.43
5:K:96:THR:HG22	5:K:107:MET:SD	2.58	0.43
6:L:193:ARG:HA	6:L:196:ARG:HD2	2.00	0.43
13:S:83:MET:HE2	13:S:88:ILE:HG12	2.00	0.43
14:T:86:ARG:HG2	14:T:121:PHE:CE1	2.53	0.43
14:T:136:SER:HB3	14:T:154:LEU:HD11	2.00	0.43
21:U:218:GLN:O	21:U:221:ILE:HG13	2.18	0.43
21:U:630:PRO:HG2	21:U:663:THR:HG21	2.00	0.43
26:Z:144:VAL:HG12	26:Z:145:HIS:N	2.30	0.43
26:Z:54:PHE:HB2	26:Z:78:MET:SD	2.58	0.43
16:B:203:LEU:HB3	16:B:204:PRO:HD3	2.01	0.43
16:B:309:MET:O	16:B:312:LEU:HB3	2.17	0.43
2:H:34:PRO:HA	2:H:163:MET:O	2.18	0.43
3:I:143:TYR:HB2	3:I:146:GLN:NE2	2.33	0.43
4:J:119:THR:OG1	5:K:135:ARG:NH2	2.49	0.43
6:L:175:HIS:HB3	6:L:179:PHE:CE2	2.53	0.43
8:N:21:THR:HA	8:N:27:ALA:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:9:GLY:HA3	11:Q:12:TYR:CZ	2.53	0.43
12:R:160:ILE:O	12:R:164:THR:HG23	2.19	0.43
13:S:111:GLY:HA2	13:S:120:ALA:O	2.17	0.43
13:S:46:LEU:HB3	13:S:72:LEU:HD11	2.00	0.43
21:U:707:ASN:O	21:U:711:GLN:HG2	2.17	0.43
22:V:27:PRO:O	22:V:30:PRO:HD2	2.18	0.43
22:V:30:PRO:HA	22:V:33:GLN:HB2	2.00	0.43
23:W:324:TYR:O	23:W:327:GLU:HG2	2.18	0.43
25:Y:377:LEU:O	25:Y:381:GLN:HG3	2.17	0.43
26:Z:118:ASN:N	26:Z:118:ASN:OD1	2.50	0.43
26:Z:182:THR:H	26:Z:183:THR:HA	1.84	0.43
16:B:162:VAL:O	16:B:163:LEU:HD12	2.18	0.43
20:C:295:THR:HB	20:C:300:ILE:HD11	2.01	0.43
20:C:328:ILE:HD12	20:C:328:ILE:HA	1.84	0.43
17:D:96:VAL:HG23	17:D:97:ASP:OD1	2.18	0.43
17:D:387:VAL:HG21	18:E:159:PHE:CE2	2.54	0.43
5:K:195:ILE:O	5:K:198:SER:OG	2.34	0.43
22:V:79:VAL:HG12	22:V:161:PRO:HB2	2.01	0.43
23:W:122:LEU:HA	23:W:125:ILE:HG22	2.01	0.43
23:W:328:LEU:HD11	23:W:341:PHE:CE2	2.53	0.43
23:W:87:ILE:O	23:W:88:MET:HB2	2.19	0.43
15:A:158:ASP:HB3	15:A:162:THR:HG23	2.00	0.43
20:C:321:ASN:OD1	20:C:322:GLU:N	2.52	0.43
20:C:82:LYS:HE2	20:C:84:LYS:HD3	2.00	0.43
20:C:85:VAL:C	20:C:96:VAL:HG23	2.38	0.43
18:E:126:ASP:HB2	18:E:185:ARG:HG2	2.00	0.43
18:E:331:ILE:HD11	18:E:368:MET:HG2	1.99	0.43
3:I:143:TYR:HB2	3:I:146:GLN:HE21	1.83	0.43
4:J:75:GLY:HA3	4:J:129:ILE:HG22	1.99	0.43
5:K:173:ALA:O	5:K:177:ALA:N	2.52	0.43
6:L:4:ASN:HB3	15:A:327:LEU:HD11	2.01	0.43
9:O:161:ALA:O	9:O:165:ASN:ND2	2.38	0.43
9:O:218:PRO:HA	10:P:194:LYS:HA	2.01	0.43
13:S:123:SER:O	13:S:130:TYR:HA	2.18	0.43
21:U:710:ARG:HA	21:U:713:TYR:HD2	1.83	0.43
22:V:487:HIS:NE2	26:Z:267:ARG:HD3	2.32	0.43
25:Y:14:ASN:HD21	25:Y:214:MET:HA	1.84	0.43
15:A:328:ASP:HB3	15:A:329:PRO:HD3	2.01	0.43
16:B:313:LEU:O	16:B:317:ASP:N	2.51	0.43
16:B:393:ALA:HB2	33:B:501:ATP:H4'	2.00	0.43
16:B:105:THR:HG21	20:C:120:SER:HA	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:175:PHE:CD2	20:C:182:GLN:HG3	2.53	0.43
20:C:229:ARG:NH2	20:C:232:ARG:HB2	2.33	0.43
3:I:237:ILE:O	3:I:241:GLU:HG3	2.18	0.43
11:Q:177:THR:HA	11:Q:194:ILE:O	2.19	0.43
13:S:122:TYR:HE1	13:S:132:ARG:HB2	1.83	0.43
22:V:363:LEU:HA	22:V:378:VAL:HG11	1.99	0.43
22:V:433:ASP:N	22:V:433:ASP:OD1	2.50	0.43
25:Y:57:LEU:HD11	25:Y:62:ASP:HA	2.00	0.43
15:A:226:ALA:HB2	16:B:319:PHE:HE1	1.83	0.43
20:C:209:CYS:HB3	20:C:243:PRO:HG2	1.99	0.43
20:C:297:ARG:CG	20:C:298:ILE:H	2.31	0.43
5:K:50:VAL:HG11	5:K:66:LYS:HB3	2.01	0.43
7:M:113:ASP:O	7:M:117:MET:HG2	2.18	0.43
21:U:250:PHE:HZ	21:U:333:MET:SD	2.42	0.43
22:V:286:ALA:HB2	22:V:315:LYS:HD3	2.00	0.43
23:W:55:ARG:NH1	23:W:75:TYR:O	2.52	0.43
23:W:90:LEU:HA	23:W:94:ARG:HD2	2.01	0.43
17:D:205:TYR:HD2	17:D:332:GLU:OE1	2.02	0.43
1:G:189:TRP:CE3	1:G:193:GLN:HG3	2.53	0.43
2:H:14:SER:OG	2:H:18:LYS:N	2.51	0.43
3:I:219:GLU:H	3:I:223:THR:HA	1.84	0.43
5:K:36:THR:HA	5:K:171:GLY:HA3	2.01	0.43
7:M:215:TRP:CZ3	7:M:219:LEU:HB3	2.53	0.43
10:P:54:ALA:HB3	10:P:106:GLU:HB2	1.99	0.43
10:P:141:THR:OG1	10:P:142:CYS:N	2.52	0.43
10:P:44:PRO:HA	10:P:50:TYR:CD1	2.50	0.43
11:Q:161:ARG:HH12	11:Q:194:ILE:HD12	1.83	0.43
21:U:92:ASP:HA	21:U:97:VAL:HG21	2.01	0.43
22:V:239:THR:HA	22:V:240:LEU:HA	1.73	0.43
22:V:80:LYS:HA	22:V:81:GLN:HB2	2.00	0.43
15:A:322:ASN:OD1	15:A:428:ARG:HD2	2.19	0.43
15:A:220:THR:HB	33:A:501:ATP:C8	2.53	0.43
16:B:178:LYS:HB2	20:C:283:PHE:HA	2.01	0.43
15:A:246:VAL:HG21	16:B:307:ARG:HH21	1.82	0.43
20:C:254:ILE:HA	20:C:257:SER:HB3	1.99	0.43
19:F:238:ARG:NH1	19:F:250:LYS:HG2	2.29	0.43
1:G:43:ARG:HD2	1:G:149:PRO:O	2.19	0.43
1:G:152:TYR:CD1	1:G:162:GLY:HA3	2.54	0.43
5:K:10:ARG:O	5:K:12:VAL:N	2.52	0.43
6:L:65:HIS:CD2	6:L:221:PHE:HD2	2.33	0.43
7:M:137:LEU:O	7:M:148:LEU:HD12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:53:GLN:OE1	9:O:118:SER:HA	2.18	0.43
20:C:11:LEU:HD13	21:U:144:ASP:HB3	2.00	0.43
21:U:356:THR:HG22	21:U:717:ILE:HG21	2.01	0.43
21:U:611:ASN:HB3	21:U:614:VAL:CG1	2.44	0.43
23:W:219:THR:HA	23:W:220:GLU:HB3	2.00	0.43
25:Y:143:TYR:HA	25:Y:146:ARG:HG2	2.01	0.43
25:Y:328:GLU:O	25:Y:331:ASP:HB3	2.18	0.43
20:C:183:PRO:HG2	20:C:290:LYS:HZ1	1.82	0.43
17:D:122:GLU:HG2	17:D:123:LEU:N	2.34	0.43
17:D:220:ALA:HA	17:D:227:PHE:CZ	2.54	0.43
17:D:235:PHE:HB2	17:D:246:MET:HE3	2.01	0.43
18:E:364:GLN:HA	18:E:367:PHE:HB2	2.01	0.43
19:F:215:LEU:HB2	19:F:217:ILE:HG12	2.01	0.43
3:I:148:TYR:HA	3:I:158:GLY:CA	2.48	0.43
3:I:196:VAL:HG12	3:I:197:LEU:HD12	2.00	0.43
3:I:68:LEU:HD22	3:I:90:LEU:HD22	2.00	0.43
9:O:163:ILE:HG12	9:O:170:GLY:HA2	2.00	0.43
12:R:8:PHE:CE1	12:R:13:ILE:HG12	2.47	0.43
14:T:192:VAL:HG12	14:T:197:VAL:HG22	2.01	0.43
21:U:172:ASP:HA	21:U:173:VAL:HB	2.00	0.43
15:A:299:MET:O	15:A:302:LEU:HB3	2.18	0.42
20:C:142:LYS:HA	20:C:142:LYS:HD2	1.90	0.42
1:G:18:PRO:HA	2:H:24:TYR:CE1	2.53	0.42
1:G:208:ILE:HB	1:G:210:PHE:HD1	1.84	0.42
11:Q:71:ASN:HB3	11:Q:73:TYR:CE2	2.54	0.42
12:R:164:THR:HG21	12:R:192:VAL:HG21	2.01	0.42
22:V:171:VAL:O	22:V:175:MET:HG3	2.19	0.42
24:X:142:ARG:HD3	24:X:145:GLU:HG3	1.99	0.42
24:X:360:ASP:HA	24:X:363:ARG:NE	2.33	0.42
25:Y:173:ASP:O	25:Y:177:ARG:NH2	2.42	0.42
26:Z:37:GLY:HA3	26:Z:95:TYR:CZ	2.54	0.42
26:Z:63:LYS:H	26:Z:64:ASP:HB2	1.83	0.42
15:A:74:PRO:HB2	15:A:75:PRO:HD3	2.00	0.42
17:D:109:SER:HA	20:C:91:PRO:HG2	2.00	0.42
19:F:234:THR:OG1	33:F:501:ATP:O1G	2.36	0.42
1:G:10:ASP:N	1:G:10:ASP:OD1	2.51	0.42
1:G:38:THR:HA	1:G:172:GLN:NE2	2.34	0.42
4:J:130:SER:OG	4:J:149:PRO:HD3	2.19	0.42
7:M:99:ARG:HB3	14:T:69:GLN:HE22	1.84	0.42
14:T:24:ALA:HB1	14:T:41:ARG:NH1	2.34	0.42
21:U:12:LEU:HB2	21:U:44:LYS:HE3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:398:GLU:O	24:X:402:GLU:HG3	2.19	0.42
24:X:420:LYS:HZ3	26:Z:279:LYS:HD2	1.84	0.42
26:Z:8:LYS:HG3	26:Z:47:VAL:HG23	2.00	0.42
16:B:246:THR:O	16:B:281:ILE:N	2.47	0.42
16:B:170:LEU:HD21	16:B:270:LEU:HG	2.01	0.42
16:B:334:ILE:HD12	16:B:337:LEU:HD12	2.00	0.42
20:C:171:HIS:HB3	20:C:174:LEU:CD2	2.50	0.42
17:D:83:GLN:HG3	17:D:133:HIS:CD2	2.54	0.42
17:D:325:GLY:N	17:D:328:ASP:OD1	2.47	0.42
17:D:62:LYS:O	17:D:66:LYS:HG3	2.20	0.42
6:L:200:PRO:HB2	6:L:203:GLN:OE1	2.19	0.42
12:R:196:HIS:O	12:R:200:SER:OG	2.27	0.42
21:U:127:ASP:O	21:U:131:GLU:HG2	2.19	0.42
23:W:449:GLU:O	23:W:453:HIS:ND1	2.44	0.42
23:W:70:VAL:O	23:W:73:MET:HG2	2.18	0.42
24:X:74:ARG:HH22	24:X:116:TRP:HB2	1.84	0.42
25:Y:210:SER:HB3	25:Y:213:LEU:CB	2.49	0.42
25:Y:232:GLU:O	25:Y:236:LEU:N	2.43	0.42
26:Z:120:VAL:HG23	26:Z:138:TYR:O	2.19	0.42
15:A:344:SER:N	15:A:345:LEU:HB3	2.34	0.42
15:A:98:CYS:HB3	16:B:130:GLU:HB2	2.02	0.42
17:D:259:PRO:HA	17:D:304:ASN:ND2	2.34	0.42
17:D:185:LEU:HB2	17:D:306:LYS:HZ1	1.84	0.42
18:E:143:ARG:O	18:E:147:GLU:HG3	2.19	0.42
18:E:317:ALA:O	18:E:320:ILE:HG22	2.18	0.42
19:F:224:LEU:HD22	19:F:348:LEU:HD13	2.00	0.42
19:F:85:THR:HA	19:F:86:LEU:HA	1.60	0.42
1:G:189:TRP:CH2	1:G:197:THR:HG21	2.54	0.42
3:I:135:LEU:HD11	3:I:162:THR:HG21	2.01	0.42
4:J:148:ASP:HB3	4:J:152:THR:H	1.84	0.42
4:J:187:THR:O	4:J:190:LEU:HB3	2.19	0.42
6:L:136:GLY:O	6:L:142:PRO:HA	2.19	0.42
11:Q:160:LEU:O	11:Q:164:LEU:HD13	2.18	0.42
8:N:119:MET:SD	14:T:6:VAL:HG21	2.59	0.42
21:U:82:LEU:O	21:U:129:ARG:NE	2.52	0.42
22:V:254:LEU:HG	22:V:258:TYR:HD2	1.84	0.42
26:Z:181:ASP:HA	26:Z:182:THR:HA	1.65	0.42
16:B:351:ILE:HD12	16:B:351:ILE:O	2.19	0.42
16:B:409:GLU:OE1	16:B:411:ARG:NE	2.44	0.42
20:C:109:THR:HG23	20:C:112:CYS:SG	2.59	0.42
20:C:193:GLY:HA3	20:C:317:PHE:HE2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:VAL:O	1:G:50:ILE:HD13	2.19	0.42
9:O:137:VAL:HG13	9:O:141:LYS:HD2	2.02	0.42
11:Q:3:TYR:OH	11:Q:130:ALA:O	2.29	0.42
23:W:192:LEU:O	23:W:196:VAL:HG23	2.20	0.42
25:Y:85:ASP:HA	25:Y:88:LEU:CD2	2.50	0.42
15:A:253:GLY:O	15:A:257:VAL:HG12	2.19	0.42
17:D:136:SER:HB3	20:C:67:GLN:HA	2.01	0.42
17:D:200:ARG:HD2	17:D:296:MET:HE3	2.02	0.42
18:E:113:ARG:HB3	18:E:221:TYR:OH	2.20	0.42
18:E:387:LYS:HA	18:E:387:LYS:HD2	1.88	0.42
2:H:124:SER:HA	3:I:127:LYS:NZ	2.34	0.42
3:I:180:LYS:HB2	3:I:183:GLU:OE1	2.18	0.42
3:I:245:ALA:O	3:I:249:ARG:HG2	2.20	0.42
6:L:189:LYS:HA	6:L:192:LEU:HG	2.00	0.42
11:Q:115:LEU:O	11:Q:126:LYS:HD2	2.19	0.42
22:V:392:TYR:O	22:V:395:ILE:HG22	2.19	0.42
22:V:89:LYS:HD2	22:V:93:PHE:HE2	1.83	0.42
23:W:127:THR:HA	23:W:130:MET:HG2	2.02	0.42
23:W:441:LYS:HD2	23:W:444:HIS:HE1	1.84	0.42
24:X:117:ALA:HB2	24:X:125:LEU:HD23	2.02	0.42
25:Y:267:ARG:HG3	25:Y:270:VAL:HG12	2.02	0.42
16:B:126:SER:HA	16:B:127:VAL:HA	1.50	0.42
15:A:226:ALA:HB2	16:B:319:PHE:CE1	2.54	0.42
16:B:357:ASP:O	16:B:361:LYS:HG3	2.19	0.42
17:D:130:VAL:HA	17:D:142:VAL:HA	2.02	0.42
17:D:336:PRO:HB2	17:D:341:LYS:NZ	2.34	0.42
3:I:136:TYR:HB2	3:I:148:TYR:HB2	2.02	0.42
5:K:94:VAL:O	5:K:98:ASN:ND2	2.52	0.42
6:L:41:LYS:HG3	6:L:180:MET:HB3	2.00	0.42
21:U:396:ALA:HB1	21:U:400:ALA:CB	2.50	0.42
21:U:772:TRP:HB3	21:U:775:LEU:HG	2.01	0.42
17:D:152:MET:HE1	18:E:62:LYS:CG	2.40	0.42
17:D:340:GLN:N	17:D:340:GLN:OE1	2.52	0.42
18:E:83:CYS:SG	18:E:107:ILE:HD13	2.60	0.42
2:H:106:PRO:HG2	10:P:78:GLU:OE2	2.20	0.42
2:H:15:PRO:HA	3:I:23:TYR:CE1	2.54	0.42
3:I:228:LEU:HD13	3:I:233:VAL:CG2	2.50	0.42
5:K:225:ASN:HB2	5:K:226:PHE:CG	2.55	0.42
6:L:39:LYS:HD3	6:L:144:ILE:HG12	2.02	0.42
6:L:157:ARG:HB3	7:M:59:GLU:OE2	2.19	0.42
13:S:73:LYS:O	13:S:77:HIS:ND1	2.41	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:182:LYS:HE3	22:V:182:LYS:HB3	1.83	0.42
23:W:237:GLU:HG2	23:W:238:GLY:H	1.83	0.42
23:W:317:TRP:CD1	23:W:358:VAL:HG21	2.54	0.42
24:X:243:ASP:OD1	24:X:245:PRO:HD2	2.20	0.42
25:Y:138:LEU:HD12	25:Y:141:VAL:HB	2.01	0.42
25:Y:191:ILE:HD12	25:Y:191:ILE:HA	1.93	0.42
25:Y:286:TRP:O	25:Y:287:LEU:HG	2.19	0.42
26:Z:22:HIS:HA	26:Z:25:ARG:CG	2.48	0.42
16:B:364:ILE:HG12	33:B:501:ATP:C6	2.55	0.42
17:D:283:ARG:NH2	20:C:218:GLU:OE1	2.53	0.42
6:L:119:PRO:HB2	6:L:126:ARG:O	2.20	0.42
7:M:42:LYS:HD3	7:M:182:LYS:O	2.20	0.42
10:P:19:CYS:SG	10:P:160:PRO:HG3	2.59	0.42
11:Q:181:ARG:HD3	11:Q:190:ASP:HA	2.02	0.42
21:U:913:ILE:HG13	21:U:913:ILE:H	1.71	0.42
23:W:434:SER:HA	26:Z:237:LEU:HD22	2.01	0.42
24:X:420:LYS:NZ	26:Z:279:LYS:HD2	2.35	0.42
15:A:83:ASP:HA	15:A:86:THR:HB	2.01	0.42
16:B:346:ARG:HG3	16:B:349:ARG:H	1.85	0.42
19:F:380:ASN:OD1	19:F:417:HIS:NE2	2.53	0.42
7:M:54:LEU:HD12	7:M:57:LEU:HD21	2.02	0.42
13:S:13:LEU:HD13	13:S:137:ALA:HB2	2.01	0.42
22:V:186:LYS:NZ	22:V:234:ARG:HD3	2.35	0.42
25:Y:215:ASP:OD2	25:Y:218:THR:HG23	2.20	0.42
15:A:329:PRO:O	15:A:333:ARG:HG2	2.21	0.41
15:A:410:LEU:HA	15:A:413:VAL:HB	2.02	0.41
16:B:205:LEU:CD2	16:B:206:THR:N	2.81	0.41
16:B:298:ASN:OD1	16:B:298:ASN:N	2.53	0.41
20:C:275:GLU:HA	20:C:278:ASN:HB2	2.01	0.41
17:D:116:LEU:HB2	17:D:139:LEU:O	2.19	0.41
1:G:116:LYS:HG2	1:G:160:TYR:CD1	2.55	0.41
7:M:149:TYR:HA	7:M:159:GLY:HA3	2.02	0.41
7:M:163:CYS:SG	7:M:164:ALA:N	2.93	0.41
21:U:383:ASP:OD2	21:U:387:ARG:NH2	2.53	0.41
21:U:612:ASP:HB3	21:U:647:HIS:CG	2.55	0.41
22:V:449:ALA:HB1	22:V:459:GLN:O	2.18	0.41
23:W:121:LYS:HG3	23:W:122:LEU:HD12	2.02	0.41
15:A:97:ARG:HB3	16:B:131:HIS:CD2	2.55	0.41
16:B:177:GLU:N	16:B:178:LYS:HA	2.30	0.41
16:B:283:PHE:CZ	16:B:285:ASP:HB2	2.54	0.41
20:C:312:ASP:OD1	20:C:313:ARG:N	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:D:285:VAL:HA	17:D:288:ILE:HD12	2.02	0.41
17:D:389:GLU:CA	17:D:390:ASN:HB2	2.50	0.41
18:E:111:LEU:HD11	18:E:114:GLU:HG2	2.00	0.41
18:E:172:LEU:CD2	18:E:299:ILE:HB	2.50	0.41
6:L:60:GLN:HG2	19:F:439:ALA:HB1	2.01	0.41
6:L:49:LEU:HD21	6:L:199:LEU:HD21	2.01	0.41
10:P:25:ASP:OD1	10:P:25:ASP:N	2.50	0.41
11:Q:59:TYR:O	11:Q:63:ASN:ND2	2.36	0.41
12:R:6:PHE:HA	12:R:124:ALA:O	2.20	0.41
14:T:1:THR:N	14:T:105:PRO:O	2.47	0.41
21:U:682:TYR:HB3	21:U:725:MET:SD	2.59	0.41
21:U:766:PHE:CD1	21:U:776:SER:HA	2.54	0.41
24:X:221:GLU:HB3	24:X:223:LYS:HG2	2.02	0.41
25:Y:182:VAL:HG11	25:Y:213:LEU:HD22	2.02	0.41
25:Y:286:TRP:C	25:Y:288:PHE:H	2.23	0.41
25:Y:51:ALA:HA	25:Y:54:TYR:HD2	1.84	0.41
26:Z:241:SER:HB3	26:Z:245:PHE:HB3	2.02	0.41
15:A:383:ALA:HB3	16:B:343:ARG:NH1	2.26	0.41
15:A:429:TYR:HA	15:A:432:TYR:CE2	2.55	0.41
16:B:122:ILE:HA	16:B:131:HIS:O	2.20	0.41
16:B:140:ASP:OD1	16:B:143:LEU:HB3	2.19	0.41
20:C:147:THR:OG1	20:C:148:TYR:N	2.54	0.41
20:C:193:GLY:H	20:C:355:SER:HB2	1.85	0.41
17:D:143:LEU:CD1	17:D:146:GLU:HA	2.51	0.41
17:D:191:TYR:CE2	17:D:198:PRO:HB3	2.55	0.41
17:D:252:ARG:HA	17:D:255:LYS:HE3	2.02	0.41
17:D:384:MET:O	17:D:387:VAL:HG12	2.21	0.41
17:D:313:ARG:HH22	18:E:242:ARG:HG3	1.85	0.41
18:E:204:VAL:HG11	19:F:308:ARG:HH22	1.85	0.41
2:H:4:ARG:HH21	7:M:127:ALA:HB2	1.85	0.41
6:L:158:ALA:HB3	6:L:176:MET:HE3	2.01	0.41
6:L:82:ARG:HA	6:L:85:CYS:HB3	2.03	0.41
12:R:18:SER:OG	12:R:173:ALA:N	2.37	0.41
21:U:388:ASP:OD1	21:U:389:ASN:N	2.48	0.41
25:Y:210:SER:HB3	25:Y:213:LEU:HG	2.02	0.41
15:A:112:ILE:H	15:A:112:ILE:HG13	4.42	0.41
16:B:261:GLY:HA3	16:B:263:GLY:N	2.35	0.41
18:E:281:ARG:HD3	18:E:387:LYS:CE	2.50	0.41
19:F:154:ASN:O	19:F:157:SER:OG	2.29	0.41
1:G:80:MET:SD	1:G:138:MET:HA	2.61	0.41
3:I:3:ARG:HH11	5:K:11:GLY:H	1.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:167:ALA:H	6:L:56:LEU:HD13	1.85	0.41
8:N:11:GLY:HA2	8:N:103:TRP:HD1	1.85	0.41
10:P:73:LEU:O	10:P:77:LYS:HG3	2.20	0.41
11:Q:2:GLU:HB2	11:Q:18:ASP:OD2	2.20	0.41
10:P:58:THR:O	11:Q:85:ARG:NH2	2.53	0.41
21:U:364:VAL:HG12	21:U:728:PHE:CD1	2.55	0.41
21:U:567:ILE:HD11	21:U:585:THR:HB	2.03	0.41
22:V:269:LYS:HB3	22:V:273:LYS:NZ	2.36	0.41
22:V:279:GLN:HB2	22:V:285:TRP:CG	2.55	0.41
22:V:98:LEU:HA	22:V:99:ARG:HA	1.68	0.41
23:W:436:MET:O	23:W:440:ASN:ND2	2.46	0.41
26:Z:210:SER:HB2	26:Z:214:LYS:HZ3	1.84	0.41
15:A:307:ASP:OD1	15:A:336:ARG:HD2	2.21	0.41
16:B:125:THR:HG22	16:B:129:SER:OG	2.20	0.41
16:B:139:VAL:HB	16:B:141:LYS:N	2.35	0.41
16:B:286:GLU:N	16:B:330:ALA:O	2.54	0.41
17:D:133:HIS:HB3	17:D:136:SER:OG	2.21	0.41
17:D:201:GLY:O	17:D:329:ARG:HB2	2.20	0.41
33:E:401:ATP:H4'	19:F:344:ARG:HE	1.85	0.41
5:K:104:ASN:ND2	13:S:130:TYR:OH	2.54	0.41
6:L:62:LYS:HD2	6:L:74:ILE:O	2.20	0.41
8:N:35:THR:HG21	8:N:56:ALA:HB1	2.02	0.41
14:T:136:SER:HB2	14:T:150:LEU:HD13	2.02	0.41
21:U:444:TYR:CE1	21:U:479:LEU:HD23	2.55	0.41
22:V:372:LEU:HD13	22:V:426:LEU:O	2.20	0.41
22:V:80:LYS:HG3	22:V:87:SER:HA	2.01	0.41
22:V:99:ARG:HG3	22:V:143:ALA:O	2.20	0.41
24:X:332:GLU:HA	24:X:335:LEU:HB2	2.02	0.41
25:Y:221:THR:O	25:Y:224:VAL:HG12	2.20	0.41
25:Y:330:ILE:HA	25:Y:333:GLU:HB3	2.02	0.41
16:B:265:LYS:HA	16:B:268:ARG:HB2	2.02	0.41
16:B:319:PHE:HA	16:B:320:ASP:HA	1.60	0.41
20:C:118:ASN:OD1	20:C:118:ASN:N	2.41	0.41
20:C:167:LEU:HB3	20:C:168:PRO:HD3	2.01	0.41
17:D:346:SER:O	17:D:349:THR:HG22	2.20	0.41
17:D:238:LYS:NZ	18:E:75:ASN:HA	2.36	0.41
19:F:295:ARG:HB3	19:F:296:PHE:H	1.55	0.41
4:J:95:ARG:HH22	4:J:101:PRO:HA	1.86	0.41
5:K:225:ASN:HA	5:K:226:PHE:HA	1.78	0.41
9:O:216:ILE:HG23	10:P:194:LYS:HD2	2.02	0.41
21:U:844:LYS:HE3	21:U:844:LYS:HB3	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:59:ALA:HA	22:V:60:ALA:C	2.40	0.41
23:W:254:PRO:HA	23:W:257:GLN:HB2	2.03	0.41
23:W:55:ARG:NH1	23:W:79:GLU:HG3	2.31	0.41
24:X:126:ARG:HH22	24:X:156:GLU:HG3	1.85	0.41
24:X:331:LEU:HD23	24:X:364:LYS:HG2	2.02	0.41
20:C:334:ARG:O	25:Y:174:TRP:N	2.54	0.41
15:A:115:VAL:HG13	15:A:117:GLN:H	1.86	0.41
15:A:427:PRO:HA	15:A:429:TYR:CZ	2.55	0.41
15:A:91:GLN:HB2	15:A:92:PRO:HD3	2.02	0.41
20:C:117:ARG:O	20:C:121:TYR:HA	2.20	0.41
20:C:147:THR:HG21	25:Y:133:ALA:HB2	2.03	0.41
18:E:109:ARG:NH1	19:F:133:PHE:HE2	2.18	0.41
4:J:143:ARG:HG3	4:J:143:ARG:O	2.21	0.41
21:U:500:ASN:HA	21:U:503:GLN:HG2	2.02	0.41
21:U:740:GLY:HA3	21:U:744:VAL:HG22	2.01	0.41
22:V:160:LEU:HD22	22:V:213:TYR:CD2	2.56	0.41
25:Y:221:THR:HA	25:Y:224:VAL:HG12	2.03	0.41
26:Z:77:ASN:O	26:Z:81:MET:HG3	2.20	0.41
17:D:326:ARG:HH21	20:C:141:GLU:CG	2.33	0.41
20:C:143:VAL:HG22	20:C:144:PRO:O	2.21	0.41
20:C:187:LEU:HA	20:C:293:MET:HB2	2.01	0.41
17:D:47:LEU:HD12	20:C:25:LEU:HB3	2.02	0.41
19:F:235:LEU:HD13	33:F:501:ATP:H3'	2.02	0.41
1:G:88:ARG:NH2	7:M:157:SER:O	2.53	0.41
5:K:225:ASN:OD1	5:K:225:ASN:N	2.54	0.41
6:L:40:SER:HA	6:L:180:MET:SD	2.60	0.41
9:O:1:THR:HG23	9:O:33:LYS:HE3	2.03	0.41
10:P:53:LEU:HD13	10:P:60:VAL:HA	2.03	0.41
14:T:99:ARG:CG	14:T:105:PRO:HA	2.42	0.41
21:U:208:LEU:HD23	21:U:210:LYS:N	2.36	0.41
22:V:100:MET:O	22:V:104:THR:HG23	2.20	0.41
22:V:194:LYS:O	22:V:195:ILE:HD13	2.21	0.41
22:V:31:ALA:O	22:V:35:VAL:HG22	2.21	0.41
22:V:360:TYR:O	22:V:363:LEU:HB3	2.20	0.41
25:Y:297:ARG:O	25:Y:301:ILE:HG22	2.20	0.41
15:A:330:ALA:HA	15:A:333:ARG:HE	1.86	0.41
15:A:409:PHE:O	15:A:413:VAL:HG23	2.19	0.41
20:C:165:ILE:O	20:C:168:PRO:HD2	2.20	0.41
20:C:171:HIS:N	20:C:172:PRO:HD3	2.35	0.41
19:F:339:ASP:OD2	19:F:341:ALA:HB3	2.20	0.41
3:I:149:GLN:HB3	3:I:157:GLY:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:65:LEU:CD2	4:J:88:ARG:HG2	2.50	0.41
7:M:34:SER:HA	7:M:167:LYS:NZ	2.36	0.41
8:N:3:ILE:HD12	8:N:44:CYS:SG	2.60	0.41
22:V:186:LYS:HZ3	22:V:234:ARG:HD3	1.85	0.41
22:V:276:PHE:HA	22:V:277:PRO:HD3	1.86	0.41
23:W:200:ILE:O	23:W:204:ILE:HG12	2.21	0.41
23:W:397:VAL:HG11	24:X:341:PRO:HB3	2.03	0.41
24:X:344:ARG:HA	24:X:385:LEU:O	2.21	0.41
26:Z:190:ARG:O	26:Z:193:ASN:HB2	2.20	0.41
15:A:178:GLY:HA3	33:A:501:ATP:N1	2.36	0.41
15:A:283:ALA:HA	15:A:284:ARG:HA	1.68	0.41
16:B:186:ASP:O	16:B:367:ILE:HG21	2.20	0.41
16:B:207:HIS:CE1	16:B:210:TYR:HD2	2.39	0.41
20:C:192:PRO:HA	20:C:193:GLY:HA3	1.82	0.41
20:C:157:GLN:NE2	20:C:318:PRO:HD3	2.35	0.41
17:D:143:LEU:HB3	17:D:252:ARG:HH22	1.86	0.41
17:D:371:SER:HA	17:D:372:GLY:HA3	1.72	0.41
19:F:295:ARG:NH2	19:F:300:LYS:O	2.54	0.41
19:F:391:PHE:HA	19:F:395:GLN:OE1	2.20	0.41
1:G:15:ILE:HD12	2:H:21:GLN:NE2	2.36	0.41
5:K:101:PHE:CE2	12:R:61:ARG:HB2	2.56	0.41
10:P:44:PRO:HB3	10:P:50:TYR:HE1	1.85	0.41
12:R:114:VAL:HA	12:R:119:ASN:O	2.21	0.41
25:Y:275:LEU:O	25:Y:275:LEU:HD23	2.21	0.41
20:C:42:LEU:HA	20:C:45:LEU:HD13	2.03	0.41
19:F:370:SER:HB3	19:F:400:CYS:SG	2.60	0.41
4:J:38:ARG:NH2	4:J:182:GLU:O	2.27	0.41
13:S:168:LEU:O	13:S:172:MET:HG2	2.21	0.41
14:T:85:PRO:HB2	14:T:121:PHE:CD2	2.56	0.41
22:V:156:SER:O	22:V:160:LEU:HG	2.21	0.41
24:X:203:PRO:HB2	24:X:204:PRO:C	2.41	0.41
20:C:283:PHE:CD2	20:C:284:GLU:HG2	2.56	0.40
18:E:219:PHE:HA	18:E:222:ALA:HB3	2.02	0.40
3:I:93:ILE:HA	3:I:96:ARG:HG2	2.01	0.40
21:U:230:SER:HA	21:U:268:LEU:HD11	2.04	0.40
21:U:712:LEU:O	21:U:716:VAL:HG22	2.21	0.40
23:W:335:SER:OG	23:W:336:PRO:HD3	2.21	0.40
23:W:86:ASN:CB	23:W:88:MET:HG3	2.51	0.40
26:Z:221:PRO:CD	26:Z:222:ILE:HA	2.51	0.40
26:Z:41:GLY:HA3	26:Z:92:VAL:HB	2.02	0.40
15:A:296:GLN:O	15:A:300:LEU:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:B:176:VAL:HA	16:B:177:GLU:HA	1.76	0.40
20:C:163:GLU:O	20:C:167:LEU:HB2	2.20	0.40
20:C:213:ARG:NH2	20:C:249:ASP:HB2	2.36	0.40
17:D:164:TYR:HB3	17:D:218:ALA:HB1	2.02	0.40
17:D:315:ASP:N	17:D:315:ASP:OD1	2.54	0.40
18:E:281:ARG:HG3	18:E:283:ASP:OD1	2.20	0.40
18:E:312:ILE:O	18:E:315:ILE:HG13	2.21	0.40
15:A:290:GLY:H	19:F:295:ARG:HD3	1.87	0.40
1:G:72:ILE:HG12	1:G:78:CYS:SG	2.60	0.40
7:M:40:ARG:NH1	7:M:148:LEU:HB3	2.31	0.40
9:O:76:VAL:HG23	9:O:104:ASP:OD1	2.21	0.40
13:S:211:ARG:HH21	13:S:213:ASP:CG	2.25	0.40
21:U:264:VAL:HG22	21:U:268:LEU:HD22	2.02	0.40
21:U:366:HIS:ND1	21:U:396:ALA:HA	2.36	0.40
22:V:275:VAL:N	22:V:276:PHE:HA	2.32	0.40
22:V:63:SER:O	22:V:66:GLU:HB3	2.21	0.40
23:W:268:LYS:HE2	23:W:301:LYS:HE2	2.03	0.40
25:Y:80:GLU:HA	25:Y:83:ARG:HG2	2.02	0.40
26:Z:68:TRP:CE3	26:Z:108:ILE:HG13	2.57	0.40
15:A:95:VAL:HG12	15:A:144:ARG:NH1	2.36	0.40
17:D:406:VAL:HA	17:D:407:ILE:HA	1.80	0.40
18:E:128:GLY:HA3	18:E:131:SER:OG	2.22	0.40
19:F:124:ILE:HA	19:F:124:ILE:HD12	1.96	0.40
19:F:146:LYS:HB2	19:F:147:PRO:HD2	2.04	0.40
19:F:193:LYS:HB2	19:F:193:LYS:HE3	1.80	0.40
19:F:321:GLN:HG3	19:F:322:PRO:HD3	2.02	0.40
2:H:46:LEU:HD13	2:H:75:VAL:HG22	2.03	0.40
3:I:107:CYS:HB2	3:I:146:GLN:OE1	2.20	0.40
4:J:80:ALA:O	4:J:84:ILE:HG13	2.20	0.40
6:L:166:GLN:NE2	6:L:169:ARG:HD2	2.36	0.40
11:Q:19:ARG:NH2	11:Q:31:ASP:O	2.54	0.40
14:T:67:LEU:HD21	14:T:91:TRP:CZ3	2.57	0.40
21:U:680:VAL:HB	21:U:683:VAL:HG12	2.04	0.40
23:W:268:LYS:HA	23:W:271:VAL:HG12	2.04	0.40
24:X:391:PRO:HG2	24:X:392:PRO:HD3	2.03	0.40
24:X:53:LEU:O	24:X:57:LEU:HG	2.21	0.40
26:Z:263:ALA:O	26:Z:267:ARG:HG2	2.22	0.40
17:D:96:VAL:HG22	17:D:101:ALA:HA	2.02	0.40
17:D:119:ILE:HG12	17:D:122:GLU:OE2	2.22	0.40
17:D:89:ILE:HB	18:E:78:ARG:HB2	2.03	0.40
18:E:92:LEU:HA	18:E:92:LEU:HD23	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:89:LEU:HD12	19:F:89:LEU:O	2.93	0.40
4:J:145:TYR:CE1	4:J:155:ALA:HB2	2.56	0.40
13:S:68:ILE:HD11	13:S:92:LEU:HD13	2.03	0.40
21:U:401:LYS:HE2	21:U:401:LYS:HB2	1.71	0.40
22:V:193:GLN:O	22:V:194:LYS:HB2	2.21	0.40
22:V:363:LEU:O	22:V:367:VAL:HG23	2.20	0.40
26:Z:96:HIS:CE1	26:Z:123:ILE:HG12	2.57	0.40
26:Z:266:ILE:O	26:Z:270:VAL:HG23	2.21	0.40
20:C:170:LYS:C	20:C:172:PRO:HD3	2.42	0.40
17:D:391:ARG:HH21	17:D:395:LEU:HG	1.87	0.40
2:H:42:ASN:O	2:H:144:PRO:HG3	2.21	0.40
3:I:125:GLY:HA2	4:J:3:TYR:CG	2.57	0.40
3:I:17:ARG:HD2	3:I:22:GLU:HG3	2.02	0.40
3:I:97:TYR:CG	3:I:105:ILE:HD13	2.57	0.40
6:L:135:ALA:HA	6:L:143:HIS:O	2.20	0.40
7:M:67:PHE:HB2	7:M:75:MET:HB2	2.03	0.40
8:N:36:PRO:HA	8:N:42:PHE:CE1	2.56	0.40
21:U:397:THR:OG1	21:U:398:ASN:N	2.54	0.40
21:U:57:ARG:HG3	21:U:58:GLN:N	2.35	0.40
22:V:275:VAL:HB	22:V:277:PRO:CD	2.52	0.40
22:V:494:MET:HG3	26:Z:278:ASN:ND2	2.27	0.40
23:W:243:ILE:HB	23:W:247:TYR:CD1	2.57	0.40
25:Y:233:ARG:HB3	25:Y:234:PRO:HD3	2.04	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 PDB entries followed by that with respect to all EM entries.

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	G	238/245 (97%)	223 (94%)	13 (6%)	2 (1%)	22	67
2	H	230/233 (99%)	216 (94%)	14 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	248/260 (95%)	230 (93%)	17 (7%)	1 (0%)	38	77
4	J	237/247 (96%)	223 (94%)	12 (5%)	2 (1%)	22	67
5	K	224/240 (93%)	204 (91%)	16 (7%)	4 (2%)	10	50
6	L	236/268 (88%)	218 (92%)	18 (8%)	0	100	100
7	M	238/254 (94%)	219 (92%)	18 (8%)	1 (0%)	38	77
8	N	189/238 (79%)	182 (96%)	7 (4%)	0	100	100
9	O	218/276 (79%)	212 (97%)	6 (3%)	0	100	100
10	P	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
11	Q	197/201 (98%)	185 (94%)	12 (6%)	0	100	100
12	R	199/262 (76%)	191 (96%)	8 (4%)	0	100	100
13	S	211/240 (88%)	203 (96%)	8 (4%)	0	100	100
14	T	213/263 (81%)	207 (97%)	6 (3%)	0	100	100
15	A	359/433 (83%)	317 (88%)	37 (10%)	5 (1%)	13	54
16	B	339/440 (77%)	308 (91%)	27 (8%)	4 (1%)	15	58
17	D	378/418 (90%)	339 (90%)	32 (8%)	7 (2%)	9	49
18	E	351/403 (87%)	321 (92%)	27 (8%)	3 (1%)	20	63
19	F	362/439 (82%)	326 (90%)	33 (9%)	3 (1%)	22	67
20	C	382/398 (96%)	337 (88%)	42 (11%)	3 (1%)	22	67
21	U	798/953 (84%)	762 (96%)	34 (4%)	2 (0%)	44	81
22	V	478/533 (90%)	431 (90%)	39 (8%)	8 (2%)	11	52
23	W	454/456 (100%)	412 (91%)	38 (8%)	4 (1%)	20	63
24	X	378/422 (90%)	363 (96%)	15 (4%)	0	100	100
25	Y	376/389 (97%)	341 (91%)	31 (8%)	4 (1%)	17	60
26	Z	284/324 (88%)	257 (90%)	23 (8%)	4 (1%)	13	54
27	a	371/376 (99%)	343 (92%)	23 (6%)	5 (1%)	14	56
28	b	189/377 (50%)	180 (95%)	8 (4%)	1 (0%)	32	74
29	c	285/309 (92%)	253 (89%)	26 (9%)	6 (2%)	8	47
30	d	255/349 (73%)	227 (89%)	25 (10%)	3 (1%)	15	58
31	e	36/70 (51%)	32 (89%)	3 (8%)	1 (3%)	6	41
32	f	686/749 (92%)	571 (83%)	110 (16%)	5 (1%)	25	68
All	All	9841/11269 (87%)	9025 (92%)	738 (8%)	78 (1%)	27	67

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	111	VAL
5	K	12	VAL
21	U	364	VAL
23	W	136	ILE
25	Y	350	VAL
29	c	157	ILE
29	c	244	VAL
32	f	62	ILE
32	f	447	VAL
4	J	199	VAL
15	A	159	PRO
15	A	206	ILE
16	B	218	PRO
16	B	263	GLY
17	D	149	SER
17	D	151	ILE
18	E	247	THR
22	V	82	LEU
27	a	340	VAL
32	f	131	VAL
1	G	185	LYS
3	I	108	GLU
17	D	305	VAL
20	C	219	LEU
20	C	298	ILE
22	V	59	ALA
22	V	96	ARG
25	Y	287	LEU
26	Z	144	VAL
27	a	336	VAL
32	f	281	ILE
16	B	230	THR
17	D	170	MET
17	D	374	ASP
19	F	168	TYR
23	W	40	LEU
23	W	138	VAL
25	Y	64	GLN
25	Y	67	VAL
26	Z	33	LYS
28	b	77	THR
29	c	156	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	d	213	ARG
32	f	435	LEU
5	K	179	SER
7	M	235	ALA
15	A	268	LYS
17	D	155	THR
18	E	208	ILE
19	F	426	GLU
23	W	427	ASP
27	a	69	HIS
27	a	260	ASP
30	d	214	GLY
31	e	4	LYS
18	E	292	PRO
20	C	68	GLU
22	V	54	LYS
22	V	319	HIS
4	J	98	VAL
15	A	345	LEU
29	c	105	PRO
16	B	227	PRO
17	D	125	LYS
19	F	326	VAL
22	V	464	ILE
26	Z	240	VAL
15	A	172	VAL
21	U	134	VAL
22	V	322	VAL
27	a	166	ILE
29	c	151	VAL
5	K	11	GLY
22	V	317	PRO
5	K	89	ILE
29	c	189	ILE
26	Z	221	PRO
30	d	37	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	193/209 (92%)	192 (100%)	1 (0%)	91	95
2	H	164/190 (86%)	164 (100%)	0	100	100
3	I	193/220 (88%)	193 (100%)	0	100	100
4	J	152/210 (72%)	151 (99%)	1 (1%)	87	93
5	K	186/202 (92%)	186 (100%)	0	100	100
6	L	198/229 (86%)	197 (100%)	1 (0%)	91	95
7	M	192/211 (91%)	191 (100%)	1 (0%)	91	95
8	N	148/180 (82%)	148 (100%)	0	100	100
9	O	177/227 (78%)	177 (100%)	0	100	100
10	P	172/173 (99%)	172 (100%)	0	100	100
11	Q	164/171 (96%)	164 (100%)	0	100	100
12	R	153/201 (76%)	153 (100%)	0	100	100
13	S	174/198 (88%)	174 (100%)	0	100	100
14	T	175/214 (82%)	175 (100%)	0	100	100
15	A	308/372 (83%)	306 (99%)	2 (1%)	89	94
16	B	298/385 (77%)	296 (99%)	2 (1%)	87	93
17	D	333/366 (91%)	331 (99%)	2 (1%)	89	94
18	E	308/353 (87%)	306 (99%)	2 (1%)	89	94
19	F	312/379 (82%)	307 (98%)	5 (2%)	68	85
20	C	332/346 (96%)	329 (99%)	3 (1%)	82	91
21	U	685/816 (84%)	681 (99%)	4 (1%)	89	94
22	V	414/459 (90%)	409 (99%)	5 (1%)	75	88
23	W	416/416 (100%)	413 (99%)	3 (1%)	87	93
24	X	327/362 (90%)	325 (99%)	2 (1%)	89	94
25	Y	334/344 (97%)	334 (100%)	0	100	100
26	Z	257/295 (87%)	256 (100%)	1 (0%)	93	95
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/267 (94%)	250 (99%)	2 (1%)	85	92
30	d	231/293 (79%)	230 (100%)	1 (0%)	93	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	e	38/63 (60%)	38 (100%)	0	100	100
32	f	582/628 (93%)	578 (99%)	4 (1%)	87	93
All	All	8368/9627 (87%)	8326 (100%)	42 (0%)	91	95

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	161	CYS
4	J	21	TYR
6	L	38	LEU
7	M	238	TYR
15	A	153	LEU
15	A	347	ASP
16	B	178	LYS
16	B	190	LEU
17	D	121	ARG
17	D	143	LEU
18	E	262	ASN
18	E	358	ASP
19	F	76	ASN
19	F	134	LEU
19	F	170	SER
19	F	299	GLU
19	F	323	ASN
20	C	50	ASN
20	C	53	ASN
20	C	175	PHE
21	U	147	TYR
21	U	172	ASP
21	U	345	ASN
21	U	384	GLN
22	V	36	GLU
22	V	240	LEU
22	V	258	TYR
22	V	281	ASN
22	V	324	PHE
23	W	214	PHE
23	W	273	TYR
23	W	361	HIS
24	X	62	GLN
24	X	157	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	Z	196	HIS
29	c	38	LEU
29	c	234	TYR
30	d	3	GLU
32	f	89	LEU
32	f	107	LEU
32	f	526	THR
32	f	600	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
3	I	119	GLN
4	J	68	ASN
5	K	23	GLN
11	Q	24	ASN
12	R	29	GLN
15	A	94	GLN
15	A	197	HIS
16	B	368	HIS
17	D	83	GLN
17	D	286	GLN
17	D	414	HIS
18	E	75	ASN
19	F	194	GLN
20	C	296	ASN
21	U	18	GLN
21	U	338	HIS
22	V	33	GLN
23	W	257	GLN
23	W	414	ASN
27	a	244	ASN
29	c	172	HIS
29	c	298	GLN
31	e	6	GLN
32	f	39	HIS
32	f	40	ASN
32	f	212	ASN
32	f	228	GLN
32	f	237	ASN
32	f	269	GLN
32	f	293	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	f	316	ASN
32	f	372	ASN
32	f	406	ASN
32	f	491	GLN
32	f	565	ASN
32	f	578	ASN
32	f	588	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	ATP	A	501	-	27,33,33	0.90	1 (3%)	25,52,52	1.74	3 (12%)
33	ATP	B	501	-	27,33,33	0.92	1 (3%)	25,52,52	1.67	2 (8%)
33	ATP	C	501	-	27,33,33	0.93	1 (3%)	25,52,52	1.65	3 (12%)
33	ATP	D	501	-	27,33,33	0.93	1 (3%)	25,52,52	1.68	2 (8%)
33	ATP	E	401	-	27,33,33	0.95	1 (3%)	25,52,52	1.76	3 (12%)
33	ATP	F	501	-	27,33,33	0.92	1 (3%)	25,52,52	1.64	2 (8%)

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
33	ATP	A	501	-	-	0/18/38/38	0/3/3/3
33	ATP	B	501	-	-	0/18/38/38	0/3/3/3
33	ATP	C	501	-	-	0/18/38/38	0/3/3/3
33	ATP	D	501	-	-	0/18/38/38	0/3/3/3
33	ATP	E	401	-	-	0/18/38/38	0/3/3/3
33	ATP	F	501	-	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	501	ATP	C5-C4	2.97	1.47	1.40
33	B	501	ATP	C5-C4	2.98	1.47	1.40
33	F	501	ATP	C5-C4	2.99	1.47	1.40
33	D	501	ATP	C5-C4	3.00	1.47	1.40
33	C	501	ATP	C5-C4	3.05	1.47	1.40
33	E	401	ATP	C5-C4	3.13	1.47	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	A	501	ATP	N3-C2-N1	-6.47	123.22	128.86
33	E	401	ATP	N3-C2-N1	-6.24	123.42	128.86
33	B	501	ATP	N3-C2-N1	-6.18	123.48	128.86
33	C	501	ATP	N3-C2-N1	-6.03	123.61	128.86
33	D	501	ATP	N3-C2-N1	-6.03	123.61	128.86
33	F	501	ATP	N3-C2-N1	-5.98	123.65	128.86
33	D	501	ATP	C4-C5-N7	-2.88	106.63	109.41
33	A	501	ATP	C4-C5-N7	-2.73	106.77	109.41
33	B	501	ATP	C4-C5-N7	-2.70	106.81	109.41
33	C	501	ATP	C4-C5-N7	-2.64	106.86	109.41
33	E	401	ATP	C4-C5-N7	-2.62	106.88	109.41
33	F	501	ATP	C4-C5-N7	-2.56	106.94	109.41
33	E	401	ATP	C2-N1-C6	2.02	122.30	118.77
33	C	501	ATP	C2-N1-C6	2.04	122.34	118.77
33	A	501	ATP	C2-N1-C6	2.08	122.42	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	501	ATP	2	0
33	B	501	ATP	3	0
33	C	501	ATP	1	0
33	D	501	ATP	3	0
33	E	401	ATP	4	0
33	F	501	ATP	3	0

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
32	f	3
2	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	f	110:ALA	C	111:LEU	N	9.72
1	f	79:ASN	C	80:TYR	N	7.23
1	f	348:ASP	C	349:SER	N	5.88
1	H	2:ALA	C	3:GLU	N	5.52