Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Nov 21, 2016 – 05:03 PM EST

PDB ID	:	5T0I
EMDB ID:	:	EMD-8336
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	:	8.00 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 (i) symbol.

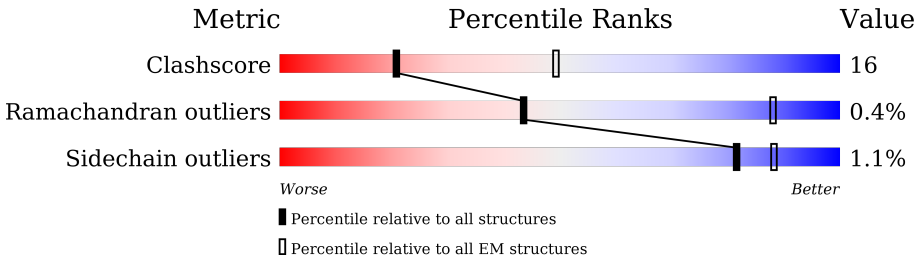
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis	:	NOT EXECUTED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	433	47% 35% • 17%
2	B	440	42% 36% • 21%
3	C	398	55% 39% • •
4	D	418	54% 37% 9%
5	E	403	51% 36% 12%
6	F	439	51% 31% • 17%
7	G	245	62% 35% • •
8	H	233	81% 19%
9	I	260	65% 31% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	J	247	71% 25%
11	K	240	61% 33% 5%
12	L	268	57% 31% 11%
13	M	254	66% 28% 6%
14	N	238	60% 20% 20%
15	O	276	66% 14% 20%
16	P	204	74% 25%
17	Q	201	71% 28%
18	R	262	62% 15% 23%
19	S	240	68% 21% 11%
20	T	263	64% 18% 18%
21	U	953	59% 25% 15%
22	V	533	50% 39% 10%
23	W	456	66% 33%
24	X	422	38% 18% 43%
25	Y	389	62% 34%
26	Z	324	60% 26% 12%
27	a	376	98%
28	b	377	50% 49%
29	c	309	87% 10%
30	d	349	72% 26%
31	e	70	56% 43%
32	f	749	90% 7%

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 76616 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 26S protease regulatory subunit 7.

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

- Molecule 2 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	348	2717	1708	460	537	12	0	0

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

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

- Molecule 4 is a protein called 26S protease regulatory subunit 6B.

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

- Molecule 5 is a protein called 26S protease regulatory subunit 10B.

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

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

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

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 14 is a protein called Proteasome subunit beta type-6.

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

- Molecule 15 is a protein called Proteasome subunit beta type-7.

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

- Molecule 16 is a protein called Proteasome subunit beta type-3.

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

- Molecule 17 is a protein called Proteasome subunit beta type-2.

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

- Molecule 18 is a protein called Proteasome subunit beta type-5.

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

- Molecule 19 is a protein called Proteasome subunit beta type-1.

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

- Molecule 20 is a protein called Proteasome subunit beta type-4.

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

- 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	241	Total	C	N	O	S	0	0
			1905	1212	320	365	8		

- 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	278	Total	C	N	O	S	0	0
			2187	1389	374	406	18		

- 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		

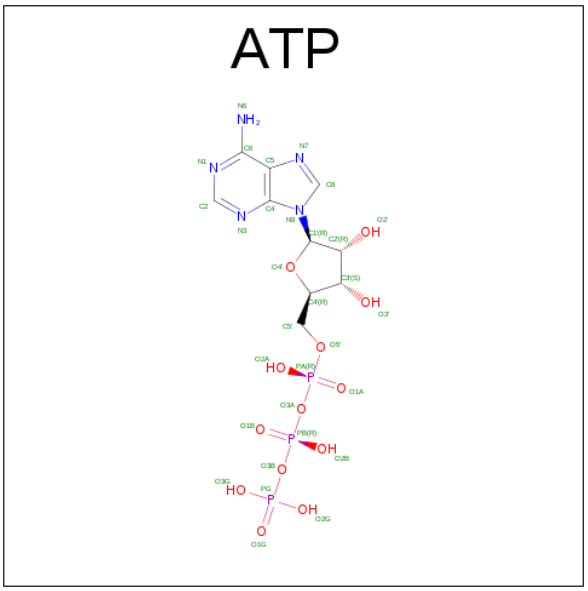
- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

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: $C_{10}H_{16}N_5O_{13}P_3$).



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

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

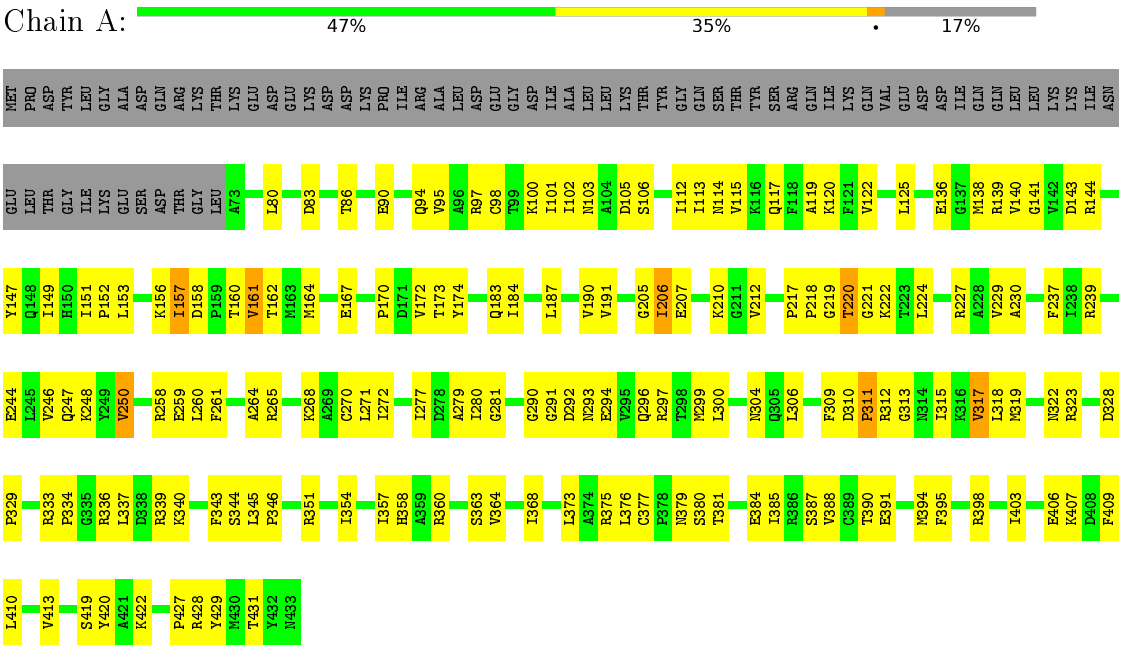
Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

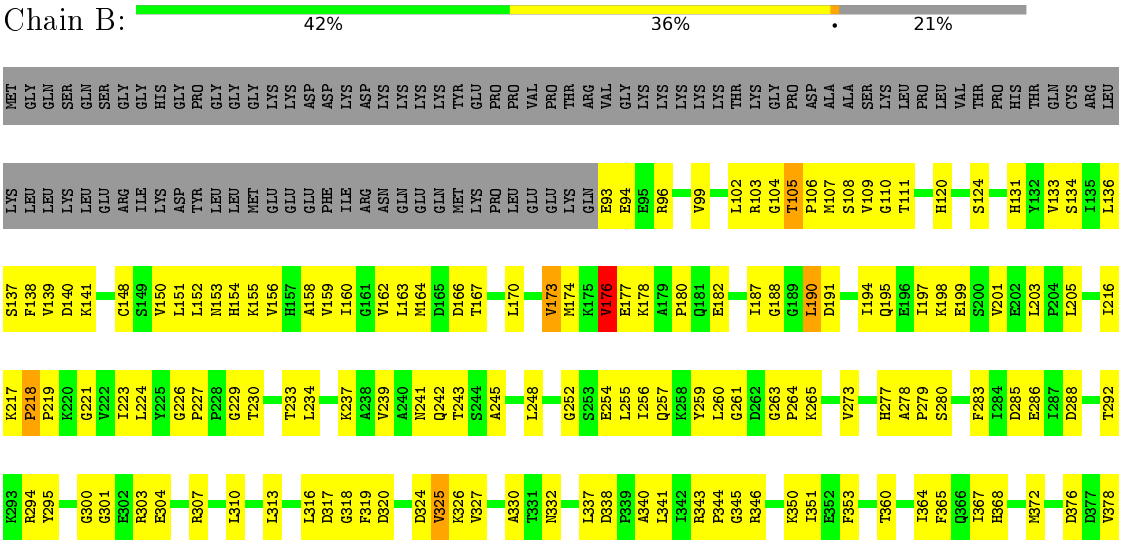
- Molecule 1: 26S protease regulatory subunit 7

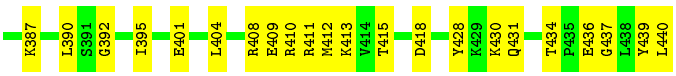
Chain A:



- Molecule 2: 26S protease regulatory subunit 4

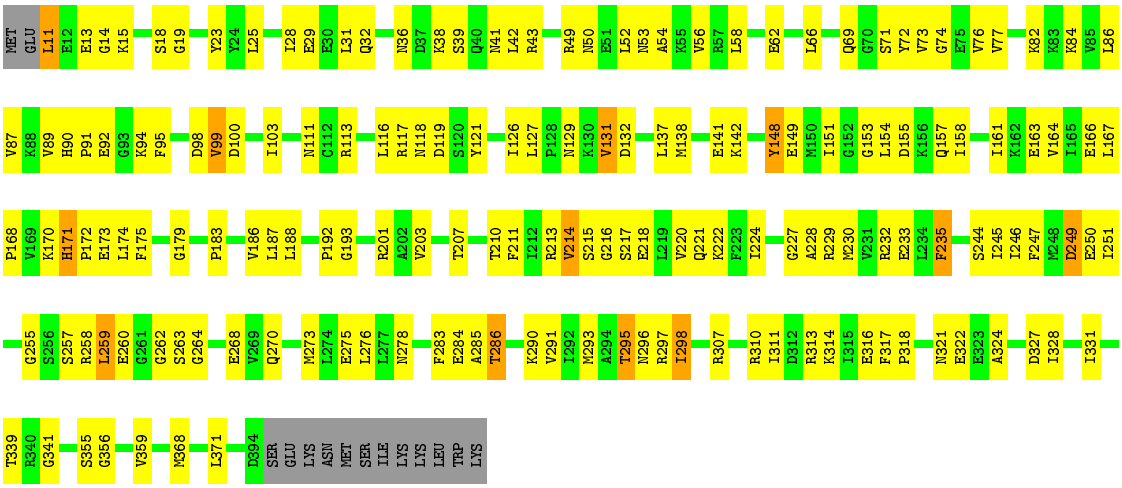
Chain B:





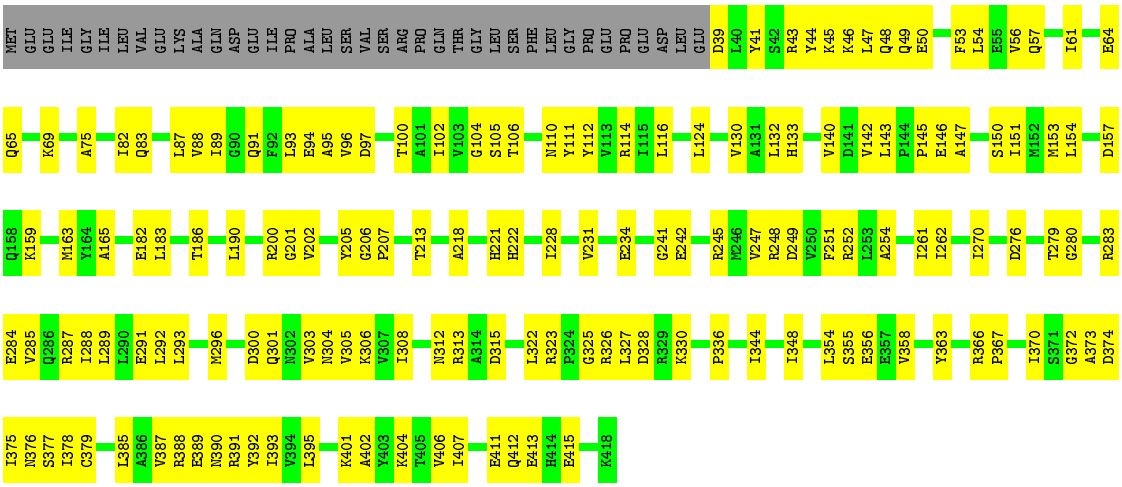
- Molecule 3: 26S protease regulatory subunit 8

Chain C:



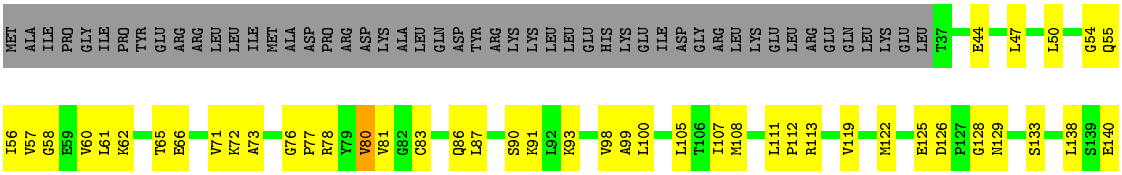
- Molecule 4: 26S protease regulatory subunit 6B

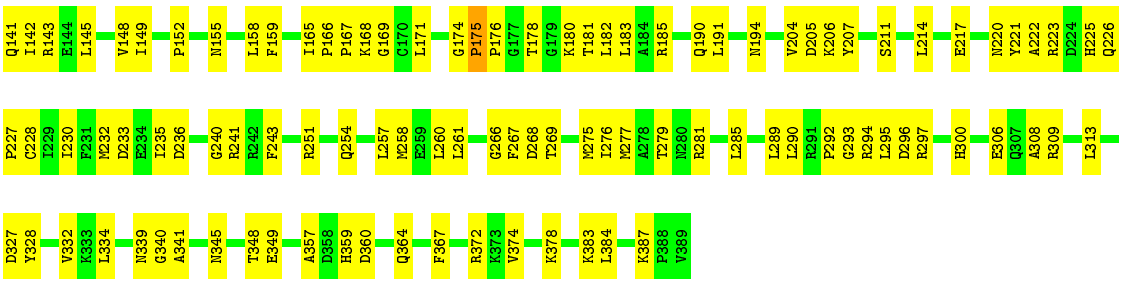
Chain D:



- Molecule 5: 26S protease regulatory subunit 10B

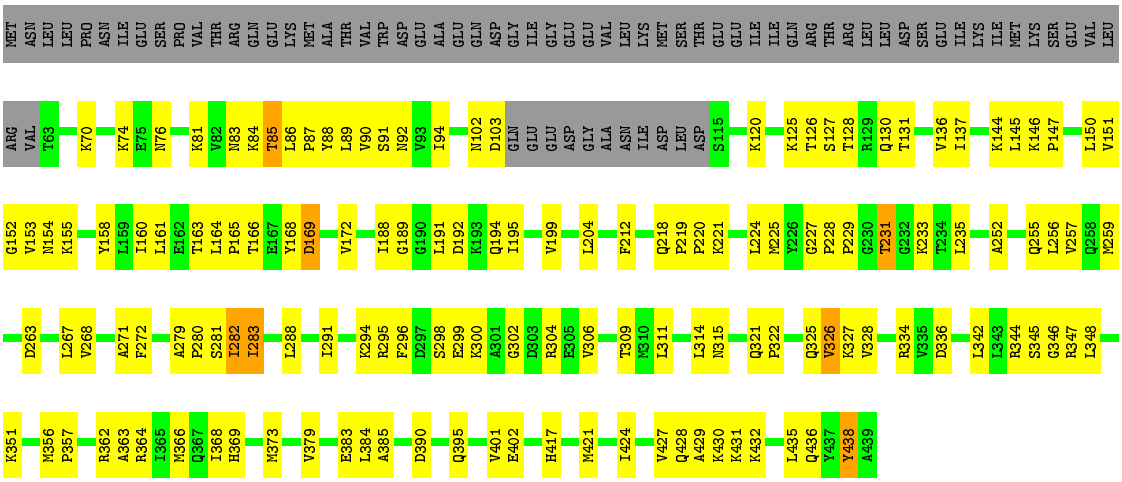
Chain E:





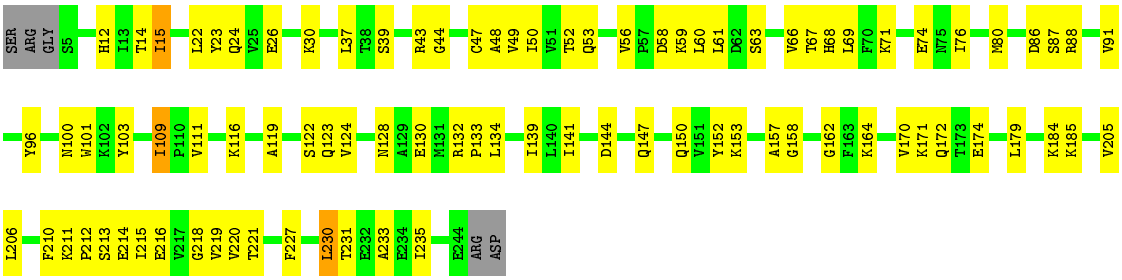
• Molecule 6: 26S protease regulatory subunit 6A

Chain F:



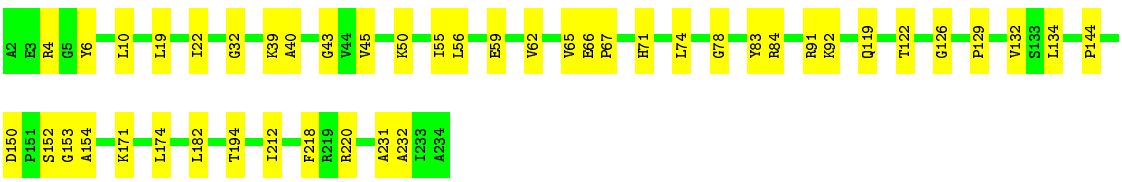
• Molecule 7: Proteasome subunit alpha type-6

Chain G:



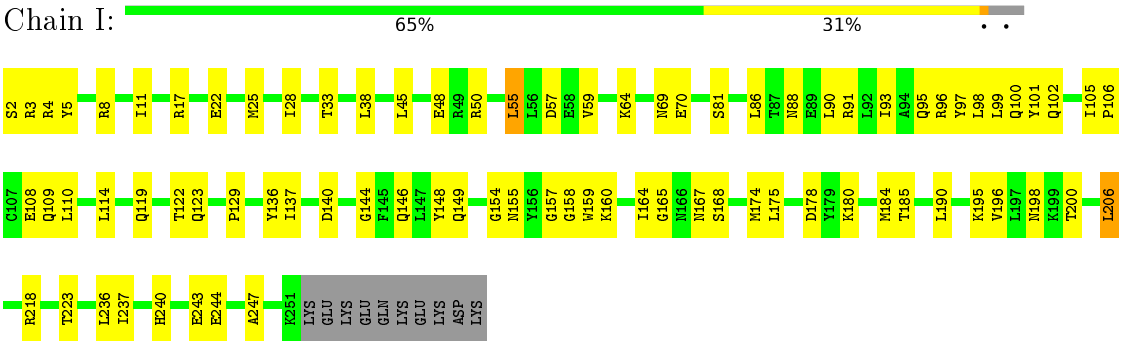
• Molecule 8: Proteasome subunit alpha type-2

Chain H:



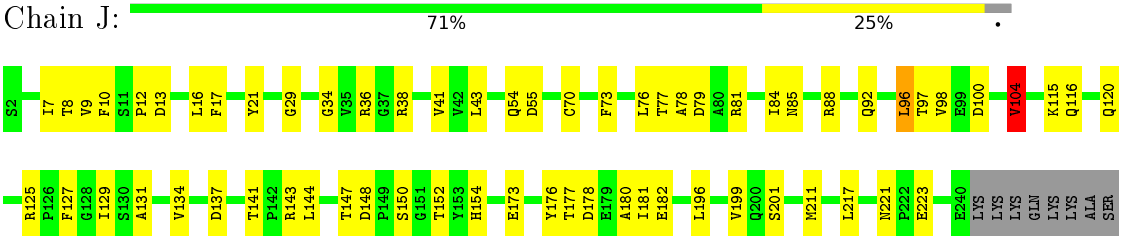
• Molecule 9: Proteasome subunit alpha type-4

Chain I:



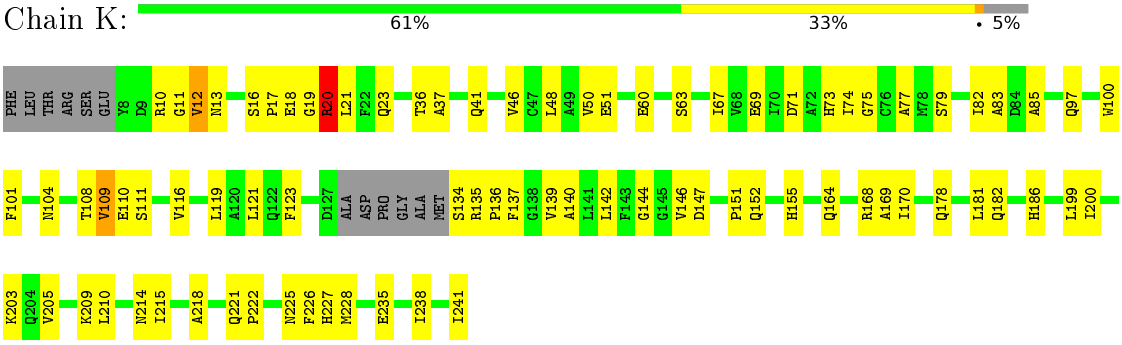
• Molecule 10: Proteasome subunit alpha type-7

Chain J:



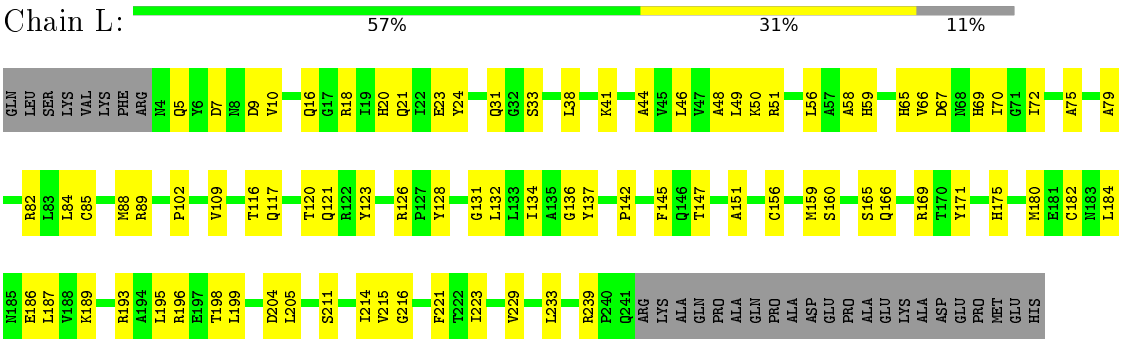
• Molecule 11: Proteasome subunit alpha type-5

Chain K:



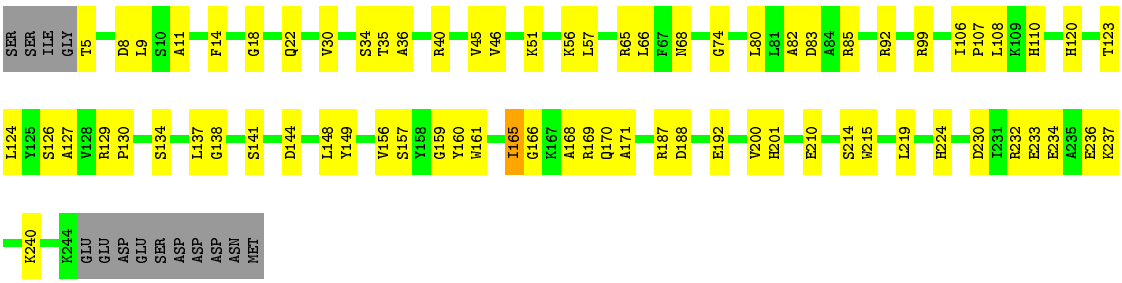
• Molecule 12: Proteasome subunit alpha type-1

Chain L:



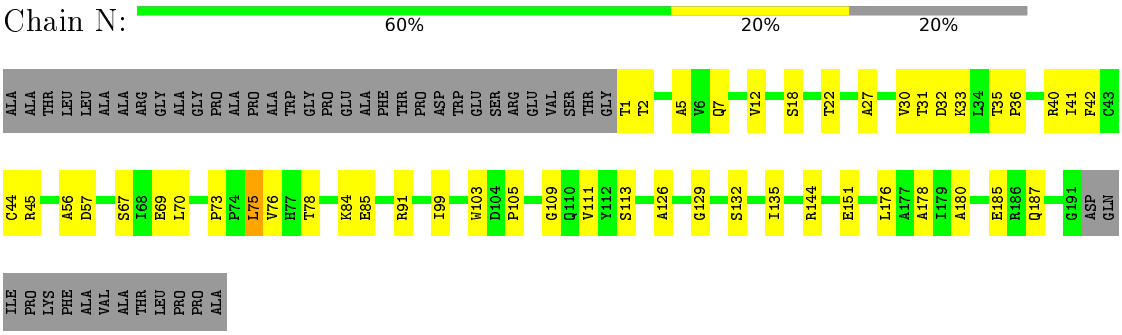
• Molecule 13: Proteasome subunit alpha type-3

Chain M:



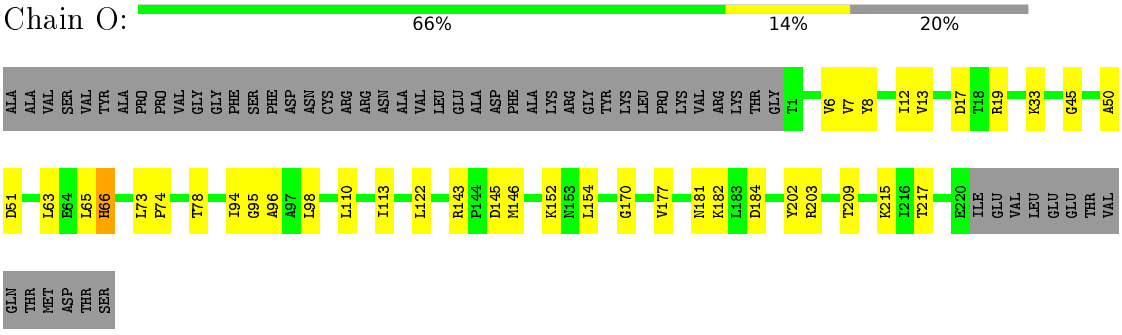
- Molecule 14: Proteasome subunit beta type-6

Chain N:



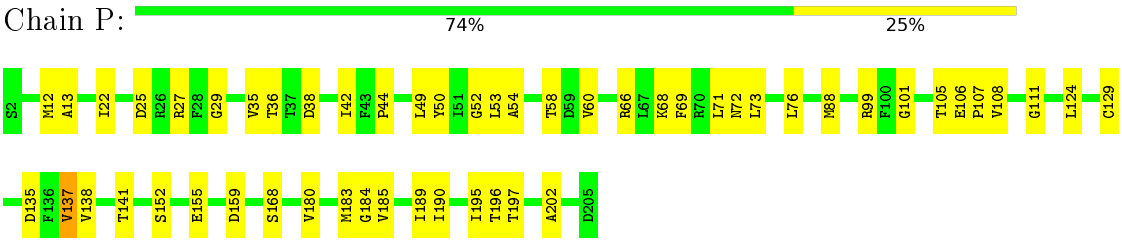
- Molecule 15: Proteasome subunit beta type-7

Chain O:



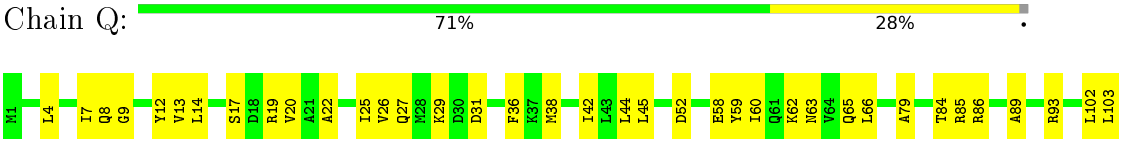
- Molecule 16: Proteasome subunit beta type-3

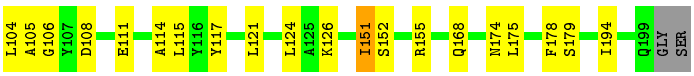
Chain P:



- Molecule 17: Proteasome subunit beta type-2

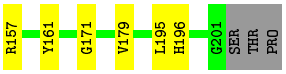
Chain Q:





- Molecule 18: Proteasome subunit beta type-5

Chain R:

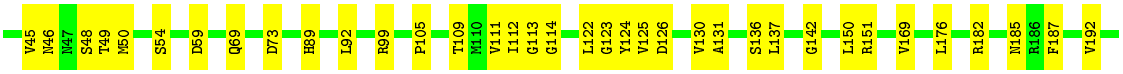


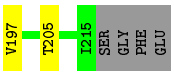
- Molecule 19: Proteasome subunit beta type-1

Chain S:

- Molecule 20: Proteasome subunit beta type-4

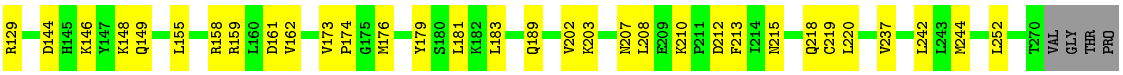
Chain T:

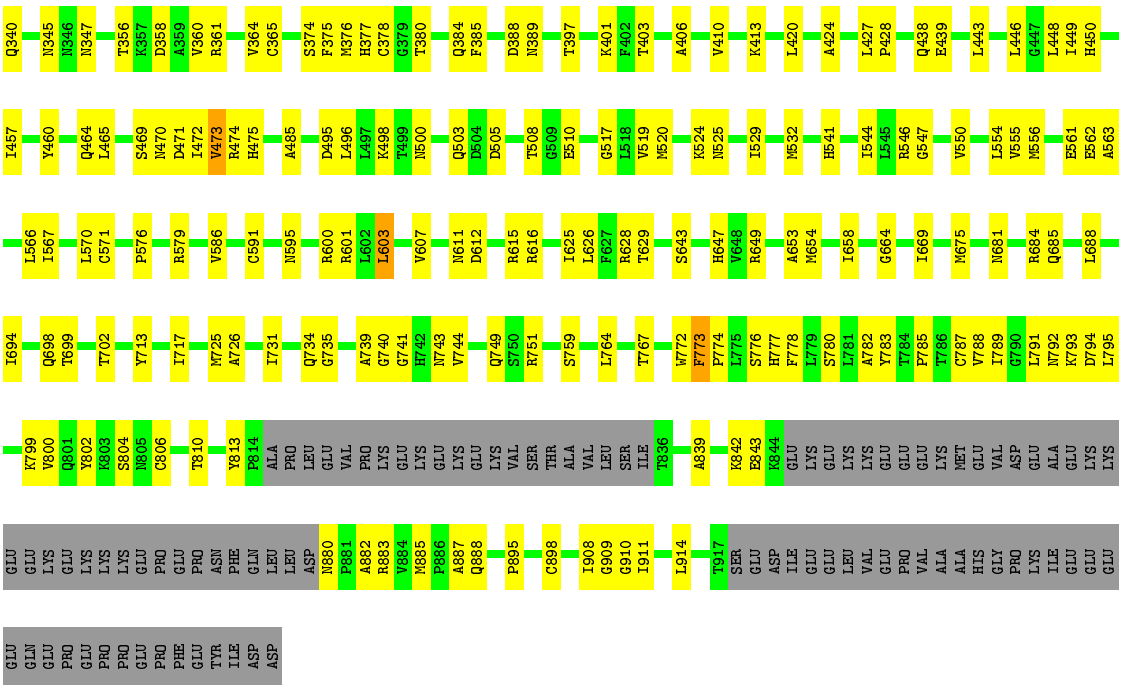




- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

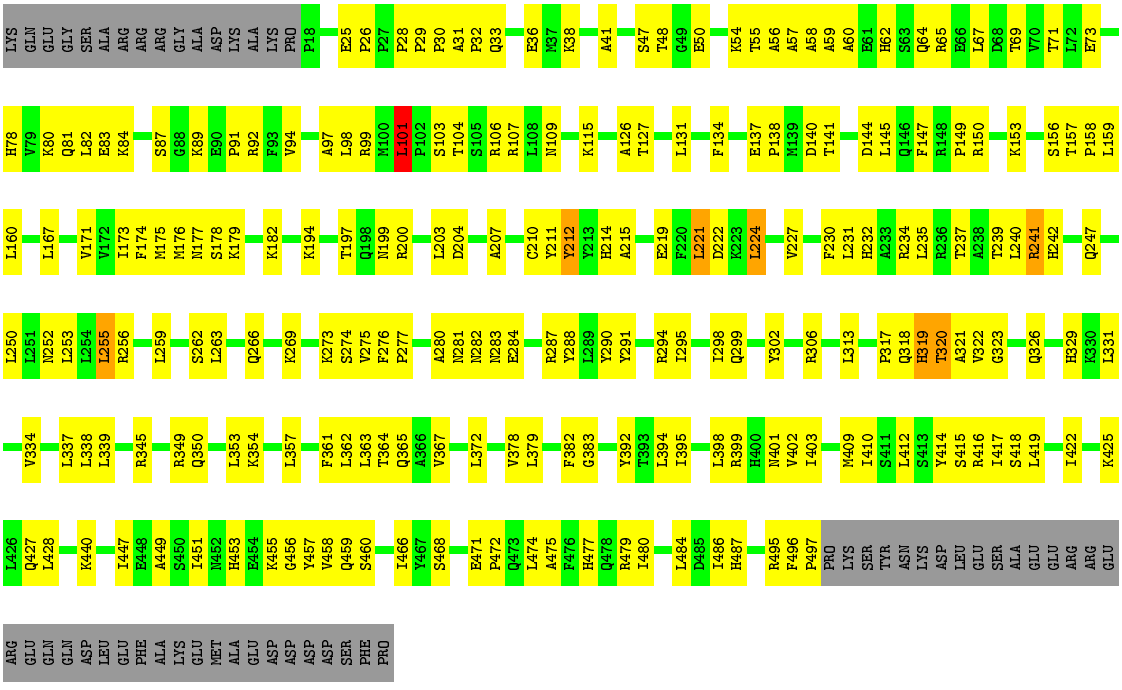
Chain U:





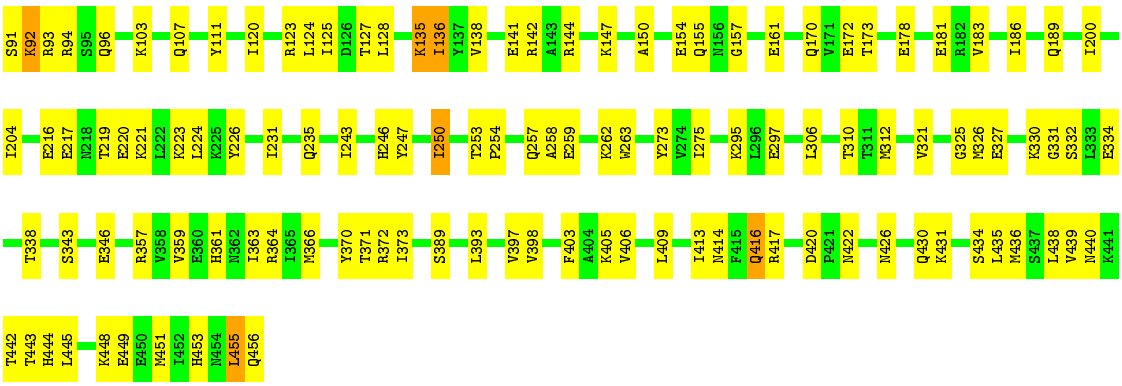
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



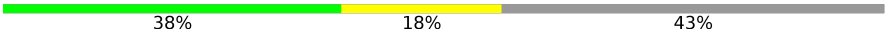
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

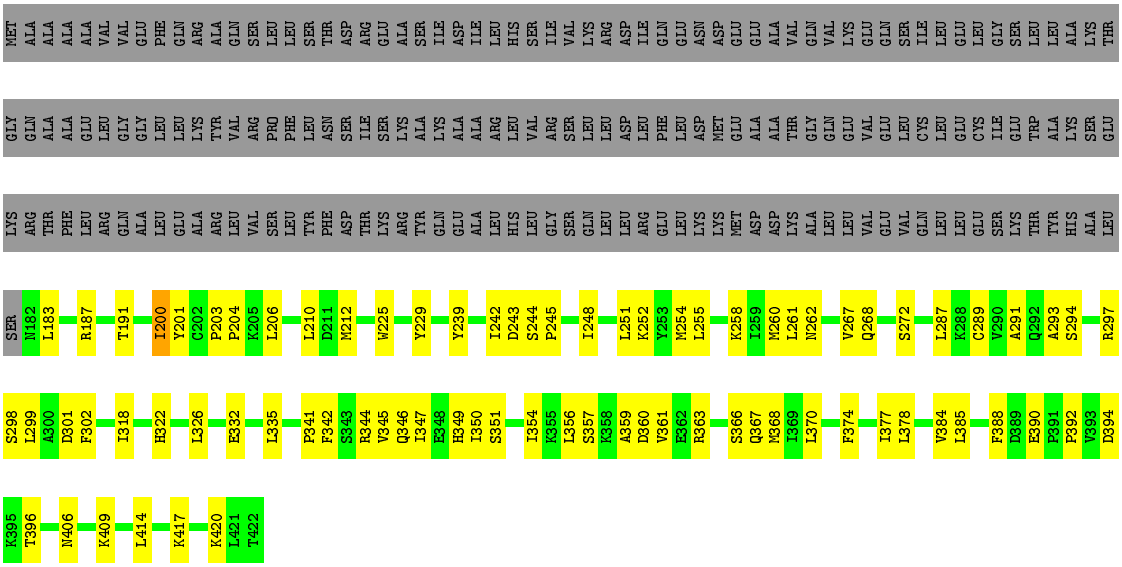
Chain W:



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

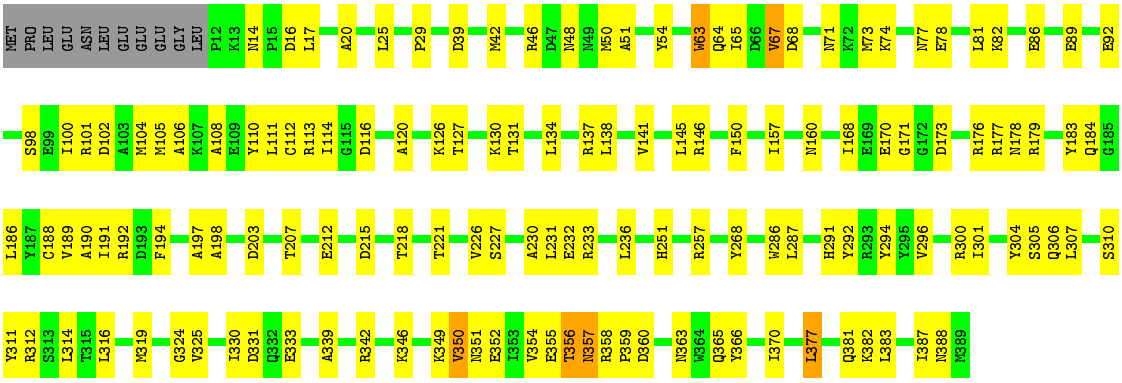
Chain X:





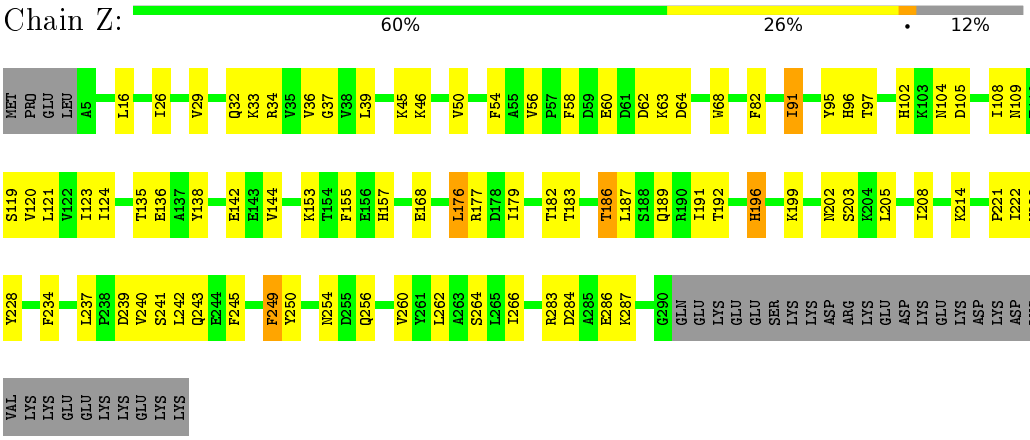
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:



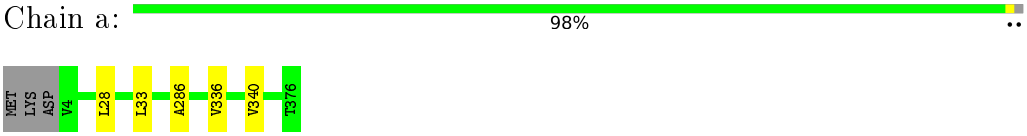
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

Chain Z:



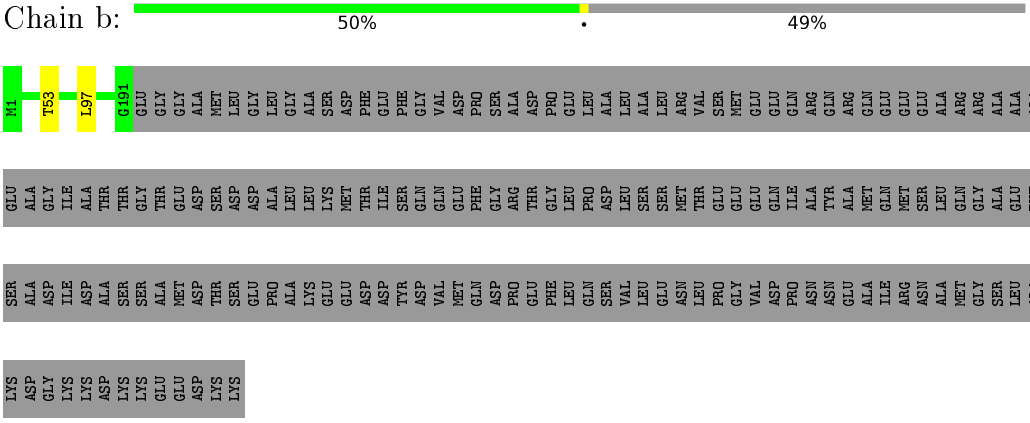
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

Chain a:



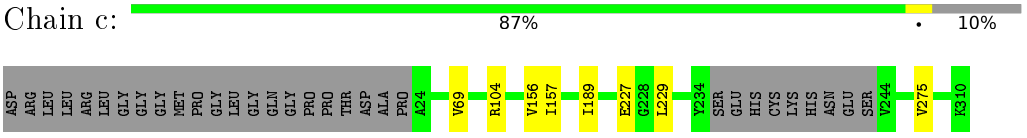
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain b:



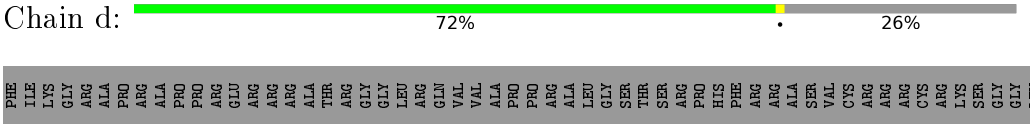
• Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

Chain c:



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

Chain d:

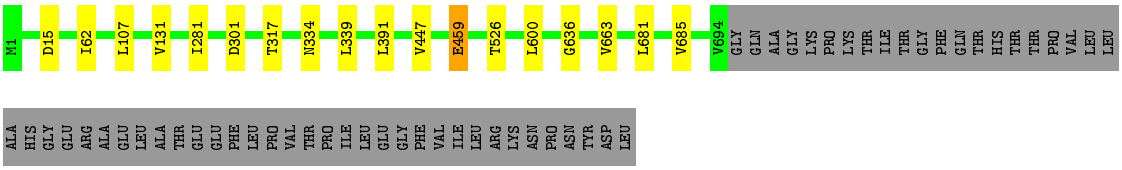


- Molecule 31: 26S proteasome complex subunit DSS1

Chain e:

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

Chain f:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	10622	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 ($e^-/Å^2$)	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	A	0.25	0/2886	0.48	0/3899
10	J	0.25	0/1728	0.45	0/2358
11	K	1.56	1/1747 (0.1%)	0.53	2/2364 (0.1%)
12	L	0.24	0/1885	0.44	0/2552
13	M	0.25	0/1891	0.44	0/2552
14	N	0.24	0/1454	0.41	0/1967
15	O	0.24	0/1669	0.46	0/2262
16	P	0.24	0/1613	0.41	0/2174
17	Q	0.24	0/1603	0.42	0/2174
18	R	0.23	0/1579	0.39	0/2134
19	S	0.24	0/1671	0.41	0/2253
2	B	0.26	0/2757	0.57	0/3724
20	T	0.23	0/1700	0.41	0/2305
21	U	0.23	0/6396	0.41	0/8646
22	V	1.26	6/3929 (0.2%)	0.51	0/5309
23	W	0.24	0/3751	0.48	3/5042 (0.1%)
24	X	0.23	0/1936	0.43	0/2614
25	Y	0.24	0/3173	0.49	1/4273 (0.0%)
26	Z	0.24	0/2324	0.49	0/3150
27	a	0.23	0/3053	0.43	0/4133
28	b	0.25	0/1478	0.44	0/2001
29	c	0.27	1/2226 (0.0%)	0.48	0/3007
3	C	0.26	0/3054	0.48	0/4107
30	d	0.25	0/2162	0.50	0/2919
31	e	3.67	1/338 (0.3%)	0.74	2/450 (0.4%)
32	f	0.35	1/5413 (0.0%)	0.52	2/7317 (0.0%)
4	D	0.24	0/3090	0.46	0/4168
5	E	0.24	0/2835	0.44	0/3821
6	F	1.42	6/2903 (0.2%)	0.49	0/3912
7	G	0.24	0/1859	0.44	0/2523
8	H	0.24	0/1747	0.44	0/2376
9	I	0.24	0/1942	0.45	0/2628

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
All	All	0.57	16/77792 (0.0%)	0.47	10/105114 (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
1	A	0	1
2	B	0	2
22	V	0	2
23	W	0	1
25	Y	0	1
27	a	0	1
3	C	0	2
30	d	0	1
32	f	0	1
All	All	0	12

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	e	4	LYS	CD-CE	67.35	3.19	1.51
11	K	20	ARG	CB-CG	64.16	3.25	1.52
22	V	212	TYR	CD2-CE2	40.36	1.99	1.39
22	V	212	TYR	CD1-CE1	40.15	1.99	1.39
6	F	438	TYR	CD2-CE2	39.43	1.98	1.39
6	F	438	TYR	CD1-CE1	38.54	1.97	1.39
22	V	212	TYR	CE1-CZ	29.35	1.76	1.38
6	F	438	TYR	CE2-CZ	28.75	1.75	1.38
6	F	438	TYR	CE1-CZ	28.65	1.75	1.38
22	V	212	TYR	CE2-CZ	28.64	1.75	1.38
22	V	212	TYR	CG-CD2	22.95	1.69	1.39
22	V	212	TYR	CG-CD1	22.77	1.68	1.39
6	F	438	TYR	CG-CD2	22.05	1.67	1.39
6	F	438	TYR	CG-CD1	21.68	1.67	1.39
32	f	681	LEU	C-N	18.07	1.68	1.34
29	c	104	ARG	C-N	6.56	1.46	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	20	ARG	CA-CB-CG	10.22	135.88	113.40
11	K	20	ARG	CB-CG-CD	8.29	133.16	111.60
31	e	4	LYS	CD-CE-NZ	8.20	130.57	111.70
31	e	4	LYS	CG-CD-CE	7.33	133.88	111.90
32	f	459	GLU	N-CA-C	6.21	127.77	111.00
25	Y	63	TRP	C-N-CA	5.57	135.62	121.70
32	f	636	GLY	N-CA-C	5.29	126.32	113.10
23	W	92	LYS	C-N-CA	5.25	134.84	121.70
23	W	135	LYS	C-N-CA	5.24	134.80	121.70
23	W	40	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	PRO	Peptide
2	B	176	VAL	Peptide
2	B	278	ALA	Peptide
3	C	171	HIS	Peptide
3	C	255	GLY	Peptide
22	V	101	LEU	Peptide
22	V	319	HIS	Peptide
23	W	416	GLN	Peptide
25	Y	357	ASN	Peptide
27	a	286	ALA	Peptide
30	d	3	GLU	Peptide
32	f	459	GLU	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	A	2835	0	2879	142	0
2	B	2717	0	2756	126	0
3	C	3015	0	3125	142	0
4	D	3040	0	3076	121	0
5	E	2790	0	2846	106	0
6	F	2863	0	2931	137	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1826	0	1796	67	0
8	H	1713	0	1598	28	0
9	I	1912	0	1851	66	0
10	J	1704	0	1517	59	0
11	K	1722	0	1673	101	0
12	L	1850	0	1822	63	0
13	M	1856	0	1814	63	0
14	N	1430	0	1398	29	0
15	O	1643	0	1643	32	0
16	P	1585	0	1597	39	0
17	Q	1570	0	1547	39	0
18	R	1548	0	1499	26	0
19	S	1641	0	1618	33	0
20	T	1667	0	1628	32	0
21	U	6287	0	6338	157	0
22	V	3852	0	3893	167	0
23	W	3703	0	3822	121	0
24	X	1905	0	1951	60	0
25	Y	3115	0	3120	126	0
26	Z	2281	0	2312	78	0
27	a	2995	0	3012	0	0
28	b	1458	0	1505	0	0
29	c	2187	0	2215	0	0
30	d	2116	0	2146	0	0
31	e	334	0	294	0	0
32	f	5331	0	5344	0	0
33	A	31	0	12	1	0
33	D	31	0	12	2	0
33	E	31	0	12	2	0
33	F	31	0	12	2	0
34	c	1	0	0	0	0
All	All	76616	0	76614	1913	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 16.

All (1913) 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)
6:F:438:TYR:CZ	6:F:438:TYR:CE2	1.75	1.68
6:F:438:TYR:CZ	6:F:438:TYR:CE1	1.75	1.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:212:TYR:CZ	22:V:212:TYR:CE2	1.75	1.64
22:V:212:TYR:CE1	22:V:212:TYR:CZ	1.76	1.63
6:F:438:TYR:CE1	6:F:438:TYR:CD1	1.97	1.51
22:V:212:TYR:CD1	22:V:212:TYR:CE1	1.99	1.49
22:V:212:TYR:CD2	22:V:212:TYR:CE2	1.99	1.49
6:F:438:TYR:CE2	6:F:438:TYR:CD2	1.98	1.47
6:F:438:TYR:CZ	11:K:20:ARG:CG	2.34	1.11
6:F:438:TYR:CE1	11:K:20:ARG:CG	2.35	1.10
6:F:438:TYR:CD2	11:K:20:ARG:CB	2.38	1.06
6:F:438:TYR:CE2	11:K:20:ARG:CG	2.39	1.05
6:F:438:TYR:CD1	11:K:20:ARG:CB	2.43	1.02
6:F:438:TYR:CD1	11:K:20:ARG:CG	2.43	1.01
6:F:438:TYR:CE2	11:K:20:ARG:CB	2.42	1.01
6:F:438:TYR:CZ	11:K:20:ARG:HG2	1.94	1.00
6:F:438:TYR:CD2	11:K:20:ARG:HB3	1.97	1.00
6:F:438:TYR:CG	11:K:20:ARG:CB	2.45	0.99
6:F:438:TYR:CZ	11:K:20:ARG:CB	2.47	0.97
6:F:438:TYR:CE1	11:K:20:ARG:CB	2.46	0.97
6:F:438:TYR:CD2	11:K:20:ARG:CG	2.49	0.96
6:F:438:TYR:CG	11:K:20:ARG:CG	2.53	0.92
6:F:438:TYR:CD1	11:K:20:ARG:HB2	2.03	0.91
6:F:438:TYR:CD1	11:K:20:ARG:HG3	2.07	0.90
23:W:40:LEU:HB2	23:W:41:GLN:HA	1.56	0.87
8:H:231:ALA:HB3	8:H:232:ALA:HB3	1.55	0.85
4:D:389:GLU:HA	4:D:390:ASN:HB2	1.57	0.84
3:C:214:VAL:HG21	3:C:249:ASP:H	1.41	0.83
17:Q:8:GLN:HE21	17:Q:115:LEU:HB2	1.43	0.83
2:B:230:THR:HG23	2:B:353:PHE:HB3	1.60	0.82
23:W:416:GLN:HB3	23:W:417:ARG:HA	1.61	0.82
1:A:333:ARG:HH12	1:A:340:LYS:HD3	1.43	0.82
4:D:100:THR:HB	4:D:114:ARG:HD2	1.63	0.81
6:F:165:PRO:HB2	6:F:166:THR:HG22	1.63	0.80
4:D:354:LEU:HA	4:D:355:SER:HB3	1.62	0.80
2:B:265:LYS:HD3	3:C:227:GLY:HA3	1.63	0.80
11:K:225:ASN:HA	11:K:227:HIS:HB3	1.62	0.80
2:B:176:VAL:HG22	2:B:177:GLU:HA	1.63	0.79
21:U:361:ARG:HG3	21:U:365:CYS:HB2	1.64	0.79
9:I:33:THR:H	9:I:64:LYS:HZ3	1.28	0.79
4:D:104:GLY:HA2	4:D:110:ASN:HA	1.65	0.79
8:H:92:LYS:HG2	15:O:65:LEU:HD21	1.65	0.78
5:E:191:LEU:HD21	5:E:227:PRO:HG2	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:174:GLY:HA2	5:E:176:PRO:HD2	1.65	0.78
5:E:372:ARG:NH2	13:M:168:ALA:O	2.16	0.78
6:F:256:LEU:HB2	6:F:306:VAL:HG22	1.66	0.78
22:V:57:ALA:HB3	22:V:58:ALA:HB3	1.64	0.78
3:C:187:LEU:HA	3:C:293:MET:HB3	1.67	0.77
1:A:103:ASN:ND2	6:F:169:ASP:OD1	2.17	0.77
23:W:92:LYS:H	23:W:93:ARG:HB3	1.49	0.77
9:I:167:ASN:ND2	9:I:200:THR:O	2.17	0.76
6:F:92:ASN:HB3	6:F:125:LYS:HB2	1.66	0.76
6:F:299:GLU:HB3	6:F:300:LYS:HB2	1.68	0.76
22:V:99:ARG:HH22	22:V:147:PHE:H	1.34	0.76
4:D:293:LEU:O	4:D:326:ARG:NH1	2.20	0.75
5:E:113:ARG:HH11	5:E:220:ASN:HD21	1.34	0.75
24:X:370:LEU:HD13	25:Y:306:GLN:HB2	1.68	0.74
4:D:348:ILE:HG21	4:D:379:CYS:HB3	1.68	0.74
22:V:81:GLN:HB3	22:V:82:LEU:C	2.07	0.74
17:Q:4:LEU:HD22	17:Q:17:SER:HA	1.68	0.74
21:U:173:VAL:HG13	21:U:176:MET:HB2	1.70	0.74
8:H:39:LYS:HE2	8:H:144:PRO:HG2	1.69	0.74
25:Y:170:GLU:HG3	25:Y:171:GLY:HA3	1.70	0.74
6:F:137:ILE:HG21	6:F:160:ILE:HB	1.69	0.73
21:U:799:LYS:HA	21:U:843:GLU:HG3	1.69	0.73
1:A:170:PRO:HA	1:A:229:VAL:HG12	1.70	0.73
9:I:2:SER:N	12:L:123:TYR:HH	1.85	0.73
21:U:424:ALA:HA	21:U:427:LEU:HD13	1.69	0.73
22:V:255:LEU:HD22	22:V:291:TYR:HB3	1.70	0.73
1:A:312:ARG:HG3	1:A:336:ARG:HH11	1.53	0.73
21:U:337:LEU:HD13	21:U:789:ILE:HG12	1.70	0.73
14:N:75:LEU:HD13	14:N:78:THR:HB	1.71	0.73
12:L:67:ASP:HB3	12:L:70:ILE:HB	1.71	0.72
11:K:10:ARG:NH2	12:L:7:ASP:O	2.21	0.72
15:O:8:TYR:HA	15:O:145:ASP:HB2	1.70	0.72
9:I:100:GLN:HG3	17:Q:86:ARG:HG3	1.70	0.72
4:D:387:VAL:HG11	5:E:167:PRO:HD3	1.72	0.72
21:U:413:LYS:HA	21:U:449:ILE:HG12	1.71	0.72
24:X:366:SER:HB2	25:Y:310:SER:HB3	1.71	0.72
3:C:258:ARG:HD2	3:C:260:GLU:HB2	1.71	0.72
4:D:303:VAL:HG23	4:D:304:ASN:HB2	1.71	0.72
6:F:357:PRO:O	6:F:362:ARG:NH1	2.22	0.72
26:Z:102:HIS:HD2	26:Z:104:ASN:HB3	1.52	0.72
1:A:315:ILE:HD12	1:A:317:VAL:H	1.53	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:229:TYR:OH	24:X:258:LYS:NZ	2.23	0.72
25:Y:101:ARG:HB3	25:Y:130:LYS:HD3	1.72	0.72
25:Y:190:ALA:O	25:Y:291:HIS:NE2	2.23	0.71
3:C:229:ARG:HH11	3:C:232:ARG:HH11	1.35	0.71
9:I:154:GLY:O	10:J:81:ARG:NH1	2.24	0.71
23:W:417:ARG:NH1	23:W:420:ASP:OD1	2.23	0.71
4:D:270:ILE:HG22	5:E:251:ARG:HH21	1.55	0.71
13:M:34:SER:OG	13:M:65:ARG:NH1	2.24	0.71
26:Z:176:LEU:HD12	26:Z:177:ARG:H	1.54	0.71
23:W:44:ILE:HB	23:W:93:ARG:HD2	1.73	0.70
25:Y:101:ARG:HE	25:Y:127:THR:HA	1.56	0.70
22:V:447:ILE:HG13	22:V:449:ALA:H	1.56	0.70
24:X:225:TRP:HB3	24:X:261:LEU:HG	1.72	0.70
1:A:80:LEU:HD23	2:B:137:SER:HB3	1.73	0.70
23:W:257:GLN:HA	23:W:258:ALA:HB3	1.72	0.70
22:V:80:LYS:HA	22:V:81:GLN:HB2	1.73	0.70
23:W:436:MET:O	23:W:440:ASN:ND2	2.22	0.70
5:E:175:PRO:HD2	5:E:387:LYS:HE3	1.74	0.70
21:U:510:GLU:OE2	21:U:546:ARG:NH2	2.25	0.70
22:V:416:ARG:HG3	22:V:459:GLN:HA	1.73	0.70
6:F:153:VAL:HB	6:F:160:ILE:HG13	1.74	0.69
25:Y:357:ASN:HB2	25:Y:359:PRO:HD3	1.74	0.69
1:A:100:LYS:HZ3	1:A:140:VAL:HG23	1.57	0.69
3:C:168:PRO:HA	3:C:172:PRO:HG3	1.74	0.69
24:X:417:LYS:HD3	25:Y:383:LEU:HD23	1.74	0.69
4:D:105:SER:O	4:D:245:ARG:NH1	2.25	0.69
8:H:71:HIS:HA	8:H:218:PHE:H	1.56	0.69
23:W:91:SER:HB2	23:W:92:LYS:HD2	1.73	0.69
6:F:438:TYR:CE1	11:K:20:ARG:HG3	2.28	0.69
22:V:455:LYS:N	22:V:456:GLY:HA2	2.07	0.69
1:A:157:ILE:HG23	1:A:158:ASP:HB2	1.75	0.69
2:B:105:THR:HG23	2:B:106:PRO:HD3	1.74	0.69
8:H:40:ALA:HB1	8:H:182:LEU:H	1.57	0.69
22:V:283:ASN:HB2	22:V:317:PRO:HD2	1.75	0.69
17:Q:59:TYR:O	17:Q:63:ASN:ND2	2.22	0.69
7:G:63:SER:O	7:G:67:THR:OG1	2.11	0.68
25:Y:111:LEU:HA	25:Y:114:ILE:HD13	1.75	0.68
1:A:102:ILE:HA	1:A:113:ILE:HA	1.74	0.68
16:P:105:THR:HG23	16:P:107:PRO:HD3	1.75	0.68
25:Y:77:ASN:O	25:Y:81:LEU:N	2.27	0.68
6:F:84:LYS:HA	6:F:161:LEU:HD22	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:143:LEU:O	22:V:440:LYS:NZ	75.01	0.68
25:Y:358:ARG:HD2	25:Y:359:PRO:HD2	1.76	0.68
25:Y:64:GLN:HG2	25:Y:65:ILE:HG22	1.75	0.68
13:M:92:ARG:NH2	20:T:73:ASP:OD1	2.27	0.68
1:A:258:ARG:HD2	6:F:255:GLN:HE22	1.59	0.68
6:F:221:LYS:HD2	6:F:327:LYS:HG3	1.76	0.68
5:E:138:LEU:HD22	5:E:140:GLU:HG2	1.76	0.68
22:V:212:TYR:OH	22:V:287:ARG:NH2	2.26	0.68
21:U:842:LYS:HA	21:U:843:GLU:HB3	1.74	0.68
24:X:406:ASN:HA	24:X:409:LYS:HD3	1.75	0.68
2:B:372:MET:HB3	3:C:179:GLY:HA2	1.76	0.67
17:Q:168:GLN:NE2	17:Q:174:ASN:O	2.26	0.67
19:S:168:LEU:HD23	19:S:169:ASP:H	1.59	0.67
2:B:166:ASP:HB3	2:B:167:THR:HA	1.75	0.67
6:F:314:LEU:HD21	6:F:342:LEU:HD23	1.76	0.67
13:M:35:THR:HA	13:M:166:GLY:HA3	1.75	0.67
24:X:252:LYS:HD3	24:X:287:LEU:HD21	1.75	0.67
25:Y:145:LEU:HG	25:Y:160:ASN:HD21	1.59	0.67
18:R:19:ARG:HE	18:R:29:GLN:HE22	1.43	0.67
23:W:90:LEU:HA	23:W:94:ARG:HD2	1.75	0.67
9:I:198:ASN:HB2	9:I:206:LEU:HD12	1.75	0.67
6:F:188:ILE:HD11	6:F:195:ILE:HD12	1.76	0.67
2:B:217:LYS:HG3	2:B:219:PRO:HD3	1.76	0.67
12:L:38:LEU:HD11	12:L:187:LEU:HD11	1.77	0.67
19:S:55:SER:HB3	19:S:107:TYR:HB2	1.75	0.67
7:G:132:ARG:NH1	13:M:11:ALA:O	2.28	0.67
21:U:212:ASP:O	21:U:215:ASN:ND2	2.28	0.67
2:B:436:GLU:H	2:B:437:GLY:C	1.98	0.66
4:D:89:ILE:HD11	5:E:80:VAL:HG13	1.77	0.66
10:J:196:LEU:O	10:J:201:SER:OG	2.12	0.66
6:F:427:VAL:HA	6:F:431:LYS:HZ2	1.60	0.66
5:E:223:ARG:O	5:E:226:GLN:NE2	2.28	0.66
22:V:294:ARG:HH21	22:V:331:LEU:HD23	1.60	0.66
21:U:155:LEU:O	21:U:158:ARG:NH1	2.28	0.66
21:U:112:CYS:SG	21:U:159:ARG:NH1	2.68	0.66
7:G:30:LYS:HG3	13:M:18:GLY:HA3	1.76	0.66
11:K:85:ALA:HB2	11:K:139:VAL:HG21	1.76	0.66
13:M:46:VAL:HG22	13:M:215:TRP:HD1	1.61	0.66
23:W:331:GLY:HA2	23:W:332:SER:HB3	1.78	0.66
1:A:304:ASN:HD21	6:F:252:ALA:HB1	1.61	0.66
5:E:171:LEU:HB2	5:E:295:LEU:HD22	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:54:SER:HB2	20:T:109:THR:HB	1.78	0.66
23:W:397:VAL:HG13	24:X:341:PRO:HB2	1.78	0.65
2:B:197:ILE:HG21	2:B:234:LEU:HD13	1.77	0.65
5:E:81:VAL:HG11	5:E:105:LEU:HB2	1.78	0.65
5:E:266:GLY:HA2	5:E:267:PHE:HB2	1.77	0.65
26:Z:138:TYR:HB3	26:Z:155:PHE:HB3	1.77	0.65
3:C:153:GLY:HA3	3:C:324:ALA:HA	1.79	0.65
23:W:123:ARG:HH12	23:W:127:THR:HB	1.62	0.65
9:I:174:MET:SD	9:I:195:LYS:NZ	2.69	0.65
23:W:219:THR:HA	23:W:220:GLU:HB2	1.79	0.65
5:E:206:LYS:NZ	6:F:263:ASP:OD1	2.26	0.65
2:B:103:ARG:HD3	2:B:160:ILE:HG12	1.79	0.65
11:K:71:ASP:HB3	11:K:74:ILE:HB	1.78	0.65
22:V:266:GLN:HB3	22:V:299:GLN:HE22	1.61	0.65
25:Y:312:ARG:HA	25:Y:356:THR:HG22	1.78	0.65
12:L:10:VAL:HG13	12:L:21:GLN:HG3	1.79	0.65
21:U:338:HIS:CD2	21:U:785:PRO:HB2	2.32	0.65
2:B:221:GLY:O	2:B:346:ARG:NE	2.28	0.65
5:E:83:CYS:HB3	5:E:87:LEU:HD21	1.78	0.65
12:L:41:LYS:HG3	12:L:180:MET:HB3	1.78	0.65
4:D:411:GLU:OE1	4:D:412:GLN:NE2	2.30	0.65
3:C:42:LEU:HD13	26:Z:168:GLU:HA	40.55	0.65
1:A:306:LEU:O	1:A:336:ARG:NE	2.29	0.64
5:E:277:MET:HB2	5:E:295:LEU:HD21	1.78	0.64
9:I:17:ARG:HD2	9:I:22:GLU:HG3	1.79	0.64
25:Y:51:ALA:HA	25:Y:54:TYR:HB2	1.79	0.64
15:O:143:ARG:HH12	15:O:146:MET:HG2	1.62	0.64
19:S:193:LEU:HB3	19:S:208:VAL:HB	1.80	0.64
22:V:101:LEU:O	22:V:103:SER:N	2.31	0.64
1:A:100:LYS:NZ	1:A:141:GLY:O	2.30	0.64
1:A:246:VAL:HG23	2:B:260:LEU:HD23	1.79	0.64
12:L:137:TYR:HE2	12:L:215:VAL:HG13	1.63	0.64
24:X:242:ILE:HG22	24:X:243:ASP:H	1.63	0.64
4:D:374:ASP:HB3	4:D:378:ILE:HD12	1.79	0.64
22:V:99:ARG:NH1	22:V:144:ASP:O	2.31	0.64
1:A:293:ASN:HB2	6:F:295:ARG:HH11	1.61	0.64
9:I:119:GLN:HE22	10:J:79:ASP:HA	1.62	0.64
22:V:197:THR:HG21	22:V:200:ARG:HG3	1.78	0.64
4:D:91:GLN:O	4:D:104:GLY:N	2.31	0.64
3:C:164:VAL:O	3:C:290:LYS:NZ	2.28	0.63
10:J:38:ARG:HH22	10:J:182:GLU:HA	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:98:SER:HA	25:Y:130:LYS:HD2	1.79	0.63
3:C:69:GLN:HB2	3:C:118:ASN:HB2	1.80	0.63
5:E:91:LYS:HD2	5:E:107:ILE:HB	1.80	0.63
1:A:345:LEU:HG	1:A:346:PRO:HD2	1.79	0.63
3:C:213:ARG:HG3	3:C:214:VAL:HG12	1.80	0.63
14:N:41:ILE:HG12	14:N:76:VAL:HG22	1.80	0.63
26:Z:16:LEU:HD11	26:Z:135:THR:HG21	1.79	0.63
2:B:248:LEU:HD22	2:B:273:VAL:HG11	1.79	0.63
3:C:259:LEU:HD23	3:C:263:SER:HB3	1.79	0.63
13:M:99:ARG:HB3	20:T:69:GLN:HE22	1.64	0.63
11:K:164:GLN:HB3	12:L:58:ALA:HB3	1.81	0.63
22:V:252:ASN:ND2	22:V:284:GLU:OE2	2.31	0.63
26:Z:202:ASN:OD1	26:Z:203:SER:N	2.31	0.63
13:M:169:ARG:HD3	13:M:201:HIS:HB2	1.81	0.63
17:Q:60:ILE:HD12	17:Q:84:THR:HG22	1.78	0.63
22:V:211:TYR:HB3	22:V:253:LEU:HD11	1.81	0.63
25:Y:138:LEU:HD23	25:Y:176:ARG:HB2	1.80	0.63
1:A:346:PRO:HD3	1:A:381:THR:HA	1.79	0.63
2:B:218:PRO:HB2	2:B:346:ARG:HH12	1.64	0.63
4:D:50:GLU:HA	4:D:53:PHE:HB2	1.80	0.63
11:K:13:ASN:HD21	12:L:126:ARG:HH11	1.47	0.63
12:L:18:ARG:NH1	12:L:23:GLU:OE2	2.32	0.63
23:W:312:MET:SD	23:W:361:HIS:ND1	2.72	0.63
26:Z:245:PHE:O	26:Z:249:PHE:N	2.32	0.63
10:J:81:ARG:O	10:J:85:ASN:ND2	2.32	0.63
15:O:177:VAL:HB	15:O:184:ASP:HB2	1.81	0.63
22:V:275:VAL:H	22:V:276:PHE:HA	1.64	0.63
10:J:211:MET:HB2	10:J:217:LEU:HD23	1.81	0.62
11:K:74:ILE:HD11	11:K:109:VAL:H	1.64	0.62
26:Z:142:GLU:OE2	26:Z:153:LYS:NZ	2.32	0.62
22:V:80:LYS:HE2	22:V:87:SER:HA	1.81	0.62
2:B:411:ARG:HG2	2:B:412:MET:HG2	1.81	0.62
22:V:415:SER:O	22:V:460:SER:OG	2.16	0.62
4:D:373:ALA:HA	4:D:374:ASP:HB2	1.80	0.62
22:V:266:GLN:O	22:V:269:LYS:NZ	2.32	0.62
23:W:76:GLU:HA	23:W:79:GLU:HB2	1.81	0.62
2:B:252:GLY:O	2:B:257:GLN:NE2	2.33	0.62
11:K:104:ASN:ND2	19:S:130:TYR:OH	2.33	0.62
11:K:16:SER:O	11:K:19:GLY:HA3	2.00	0.62
22:V:353:LEU:HG	22:V:357:LEU:HD23	1.81	0.62
1:A:122:VAL:HG23	6:F:90:VAL:HG22	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:111:ASN:O	3:C:129:ASN:ND2	2.32	0.62
6:F:280:PRO:HB3	6:F:326:VAL:HA	1.82	0.62
6:F:83:ASN:O	6:F:154:ASN:ND2	2.32	0.62
7:G:43:ARG:HH11	7:G:150:GLN:HA	1.62	0.62
2:B:139:VAL:HA	2:B:140:ASP:HB3	1.81	0.62
2:B:408:ARG:O	2:B:410:ARG:NH1	2.33	0.62
6:F:224:LEU:HB3	6:F:351:LYS:HG2	1.80	0.62
17:Q:38:MET:O	17:Q:65:GLN:NE2	2.33	0.62
25:Y:190:ALA:HA	25:Y:287:LEU:HD13	1.82	0.62
1:A:112:ILE:HD12	6:F:150:LEU:HG	1.81	0.61
10:J:81:ARG:HA	10:J:84:ILE:HB	1.82	0.61
22:V:321:ALA:HB1	22:V:322:VAL:HB	1.81	0.61
23:W:78:LYS:HA	23:W:81:ASP:HB3	1.81	0.61
25:Y:138:LEU:HD12	25:Y:141:VAL:HB	1.82	0.61
3:C:214:VAL:HG22	3:C:215:SER:H	1.65	0.61
4:D:247:VAL:HG21	4:D:288:ILE:HG23	1.82	0.61
4:D:64:GLU:HB2	21:U:603:LEU:HD11	1.81	0.61
26:Z:199:LYS:HD3	26:Z:202:ASN:HD21	1.65	0.61
9:I:206:LEU:HD13	9:I:237:ILE:HG23	1.81	0.61
22:V:99:ARG:HB2	22:V:104:THR:HG22	1.82	0.61
22:V:337:LEU:O	22:V:401:ASN:ND2	2.33	0.61
23:W:55:ARG:NH1	23:W:75:TYR:O	2.33	0.61
1:A:141:GLY:N	1:A:151:ILE:O	2.29	0.61
2:B:440:LEU:HG	10:J:29:GLY:HA2	1.82	0.61
12:L:50:LYS:HB3	12:L:59:HIS:HB3	1.81	0.61
22:V:241:ARG:HG3	22:V:242:HIS:H	1.65	0.61
25:Y:349:LYS:HG3	25:Y:350:VAL:HG13	1.82	0.61
24:X:251:LEU:HA	24:X:254:MET:HG2	1.83	0.61
7:G:211:LYS:NZ	7:G:213:SER:OG	2.27	0.61
6:F:438:TYR:CG	11:K:20:ARG:HB2	2.32	0.61
3:C:246:ILE:HB	3:C:291:VAL:HG12	1.83	0.61
6:F:256:LEU:HD12	6:F:306:VAL:HG13	1.83	0.61
11:K:77:ALA:HB3	11:K:142:LEU:HB2	1.83	0.61
19:S:35:ILE:H	20:T:151:ARG:HH22	1.47	0.61
22:V:62:HIS:HA	22:V:65:ARG:HB3	1.81	0.61
14:N:5:ALA:HB3	14:N:126:ALA:HB3	1.81	0.61
3:C:214:VAL:HG11	3:C:249:ASP:HB3	1.83	0.60
2:B:313:LEU:O	2:B:317:ASP:N	2.34	0.60
6:F:438:TYR:CE1	11:K:20:ARG:HG2	2.32	0.60
22:V:54:LYS:N	22:V:55:THR:OG1	2.33	0.60
23:W:224:LEU:O	23:W:253:THR:OG1	2.19	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:71:ASN:HA	25:Y:74:LYS:HG2	1.81	0.60
22:V:416:ARG:HH12	22:V:418:SER:HB2	1.65	0.60
23:W:220:GLU:N	23:W:221:LYS:HA	2.15	0.60
1:A:264:ALA:O	1:A:268:LYS:N	2.34	0.60
21:U:12:LEU:HB2	21:U:44:LYS:HE3	1.83	0.60
23:W:397:VAL:HG21	24:X:342:PHE:HB3	1.83	0.60
24:X:262:ASN:HD21	24:X:326:LEU:HG	1.66	0.60
3:C:157:GLN:NE2	3:C:316:GLU:O	2.34	0.60
4:D:130:VAL:HB	4:D:142:VAL:HG12	1.82	0.60
10:J:116:GLN:NE2	10:J:150:SER:O	2.34	0.60
15:O:209:THR:HG21	16:P:168:SER:HB3	1.82	0.60
21:U:789:ILE:HG22	21:U:791:LEU:H	1.65	0.60
2:B:170:LEU:HD22	2:B:265:LYS:HE3	1.84	0.60
2:B:401:GLU:HA	2:B:404:LEU:HB3	1.83	0.60
8:H:32:GLY:HA3	8:H:78:GLY:HA2	1.83	0.60
10:J:154:HIS:HE1	11:K:60:GLU:H	1.49	0.60
19:S:145:LEU:HD21	19:S:178:VAL:HG21	1.84	0.60
5:E:334:LEU:HD23	5:E:372:ARG:HB2	1.83	0.60
7:G:144:ASP:HB3	7:G:147:GLN:HB2	1.84	0.60
23:W:135:LYS:HB3	23:W:136:ILE:HB	1.83	0.60
11:K:235:GLU:HA	11:K:238:ILE:HD12	1.84	0.60
23:W:430:GLN:O	23:W:434:SER:OG	2.14	0.60
24:X:332:GLU:HA	24:X:335:LEU:HB2	1.82	0.60
15:O:17:ASP:O	15:O:33:LYS:NZ	2.28	0.59
21:U:14:GLU:HG2	21:U:16:GLU:H	1.67	0.59
22:V:262:SER:HB2	22:V:263:LEU:HB2	1.82	0.59
3:C:11:LEU:N	21:U:144:ASP:OD2	2.35	0.59
4:D:370:ILE:HD13	4:D:404:LYS:HA	1.83	0.59
17:Q:85:ARG:HB2	17:Q:124:LEU:HD11	1.82	0.59
21:U:189:GLN:NE2	21:U:595:ASN:OD1	2.31	0.59
24:X:346:GLN:HE21	24:X:349:HIS:HB2	1.67	0.59
26:Z:97:THR:HA	26:Z:124:ILE:HG13	1.83	0.59
21:U:625:ILE:HG13	21:U:626:LEU:HG	1.85	0.59
23:W:125:ILE:HD12	23:W:128:LEU:HD12	1.84	0.59
23:W:431:LYS:O	23:W:435:LEU:HB2	2.02	0.59
26:Z:222:ILE:HG23	26:Z:224:HIS:HB2	1.85	0.59
26:Z:54:PHE:HB3	26:Z:82:PHE:HE2	1.67	0.59
1:A:339:ARG:NH2	6:F:402:GLU:OE1	2.35	0.59
8:H:231:ALA:H	8:H:232:ALA:C	2.05	0.59
23:W:92:LYS:N	23:W:93:ARG:HB3	2.15	0.59
2:B:436:GLU:HB3	2:B:437:GLY:HA3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:297:ARG:HG3	3:C:298:ILE:H	1.68	0.59
7:G:111:VAL:HG11	7:G:144:ASP:HB2	1.83	0.59
21:U:94:SER:OG	21:U:95:GLU:OE1	2.19	0.59
22:V:486:ILE:HD13	25:Y:377:LEU:HD22	1.84	0.59
4:D:391:ARG:HG2	4:D:395:LEU:HG	1.85	0.59
21:U:39:SER:HA	21:U:67:VAL:HG23	1.85	0.59
21:U:524:LYS:HE3	21:U:556:MET:HA	1.83	0.59
1:A:222:LYS:HD2	2:B:319:PHE:HB2	1.84	0.59
3:C:158:ILE:HA	3:C:161:ILE:HG22	1.84	0.59
6:F:87:PRO:HB2	6:F:152:GLY:HA3	1.84	0.59
23:W:235:GLN:NE2	23:W:247:TYR:OH	2.36	0.59
25:Y:101:ARG:NH2	25:Y:126:LYS:O	2.35	0.59
1:A:357:ILE:HG13	1:A:360:ARG:HH21	1.68	0.59
16:P:49:LEU:HG	16:P:111:GLY:HA3	1.84	0.59
22:V:349:ARG:HG3	22:V:357:LEU:HD21	1.84	0.59
7:G:14:THR:HG22	7:G:24:GLN:HG3	1.83	0.59
11:K:225:ASN:HB2	11:K:226:PHE:CG	2.38	0.59
24:X:203:PRO:HB3	24:X:206:LEU:HB2	1.85	0.59
1:A:281:GLY:HA2	1:A:299:MET:HB3	1.83	0.59
13:M:40:ARG:NH1	13:M:160:TYR:O	2.36	0.59
22:V:331:LEU:HD12	22:V:334:VAL:HG21	1.85	0.59
11:K:18:GLU:HB2	11:K:19:GLY:HA2	1.84	0.58
15:O:8:TYR:HE2	15:O:13:VAL:HG23	1.69	0.58
19:S:25:SER:HG	19:S:43:CYS:HG	1.48	0.58
1:A:381:THR:OG1	2:B:343:ARG:NH1	2.37	0.58
3:C:127:LEU:HD22	4:D:96:VAL:HG11	1.85	0.58
4:D:411:GLU:HB3	4:D:412:GLN:HB2	1.85	0.58
21:U:376:MET:HA	21:U:741:GLY:H	1.67	0.58
23:W:16:MET:HG2	23:W:27:ARG:HH22	1.67	0.58
24:X:255:LEU:HD12	24:X:287:LEU:HB3	1.85	0.58
25:Y:81:LEU:HD12	25:Y:111:LEU:HD13	1.85	0.58
26:Z:33:LYS:NZ	26:Z:34:ARG:O	2.33	0.58
26:Z:63:LYS:HB2	26:Z:64:ASP:HB2	1.84	0.58
2:B:223:ILE:HD12	2:B:346:ARG:H	1.68	0.58
13:M:36:ALA:HB2	13:M:65:ARG:HH21	1.67	0.58
14:N:31:THR:HB	14:N:33:LYS:HZ2	1.68	0.58
20:T:185:ASN:ND2	20:T:205:THR:OG1	2.34	0.58
3:C:270:GLN:O	3:C:307:ARG:NH1	2.36	0.58
6:F:231:THR:OG1	6:F:233:LYS:NZ	2.27	0.58
8:H:50:LYS:NZ	8:H:62:VAL:O	2.37	0.58
22:V:91:PRO:HG3	22:V:126:ALA:HB3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:422:ASN:O	23:W:426:ASN:ND2	2.35	0.58
23:W:445:LEU:HD12	23:W:448:LYS:HZ1	1.68	0.58
26:Z:102:HIS:CD2	26:Z:104:ASN:HB3	2.36	0.58
1:A:103:ASN:HB2	1:A:112:ILE:HG23	1.83	0.58
5:E:285:LEU:HB3	5:E:289:LEU:HB2	1.85	0.58
9:I:48:GLU:OE1	9:I:50:ARG:NH1	2.36	0.58
15:O:143:ARG:NH1	15:O:146:MET:HG2	2.18	0.58
21:U:759:SER:HA	21:U:782:ALA:HA	1.85	0.58
3:C:113:ARG:HG2	3:C:127:LEU:HD12	1.85	0.58
22:V:259:LEU:HD21	22:V:294:ARG:HD2	1.85	0.58
6:F:94:ILE:HA	6:F:147:PRO:HB3	1.84	0.58
10:J:176:TYR:HB3	10:J:180:ALA:HB3	1.84	0.58
12:L:66:VAL:HG13	12:L:89:ARG:HD3	1.86	0.58
24:X:262:ASN:O	24:X:297:ARG:NH2	2.33	0.58
25:Y:16:ASP:HB2	25:Y:113:ARG:HE	1.68	0.58
25:Y:357:ASN:HB2	25:Y:358:ARG:HA	1.86	0.58
2:B:229:GLY:O	2:B:233:THR:N	2.37	0.58
21:U:68:PHE:HB3	21:U:73:ALA:HB3	1.85	0.58
25:Y:178:ASN:HB3	25:Y:207:THR:HG22	1.85	0.58
26:Z:34:ARG:HH12	26:Z:102:HIS:HE1	1.51	0.58
2:B:316:LEU:HD11	2:B:327:VAL:HG11	1.86	0.58
3:C:230:MET:O	3:C:233:GLU:N	2.36	0.58
4:D:248:ARG:NH2	4:D:291:GLU:OE2	2.37	0.58
7:G:71:LYS:HE2	7:G:74:GLU:HA	1.85	0.58
9:I:123:GLN:NE2	10:J:79:ASP:OD1	2.37	0.58
12:L:215:VAL:HB	12:L:221:PHE:HD1	1.69	0.58
17:Q:38:MET:HG3	17:Q:44:LEU:HB2	1.86	0.58
23:W:52:LYS:HD3	23:W:55:ARG:HD3	1.86	0.58
2:B:133:VAL:HG11	2:B:159:VAL:HG12	1.85	0.58
2:B:190:LEU:HD12	2:B:194:ILE:HB	1.84	0.58
4:D:389:GLU:HB3	4:D:391:ARG:N	2.18	0.57
13:M:141:SER:HB3	13:M:144:ASP:HB2	1.86	0.57
21:U:213:PHE:HE2	21:U:244:MET:HB2	1.69	0.57
23:W:40:LEU:HB2	23:W:41:GLN:CA	2.31	0.57
1:A:310:ASP:N	1:A:312:ARG:HB2	2.19	0.57
2:B:280:SER:HB2	2:B:325:VAL:N	2.19	0.57
5:E:357:ALA:O	5:E:359:HIS:ND1	2.30	0.57
21:U:203:LYS:O	21:U:207:ASN:ND2	2.36	0.57
1:A:391:GLU:HA	1:A:394:MET:HB3	1.86	0.57
2:B:148:CYS:HB3	2:B:150:VAL:HG13	1.86	0.57
10:J:115:LYS:NZ	10:J:129:ILE:O	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:182:THR:H	26:Z:183:THR:HA	1.68	0.57
3:C:42:LEU:HD21	4:D:65:GLN:HE22	1.69	0.57
4:D:87:LEU:HB2	5:E:80:VAL:HG23	1.86	0.57
4:D:94:GLU:HG2	4:D:102:ILE:HD11	1.85	0.57
6:F:227:GLY:HA3	6:F:231:THR:HG21	1.87	0.57
19:S:35:ILE:O	20:T:151:ARG:NH2	2.37	0.57
21:U:740:GLY:HA3	21:U:744:VAL:HG22	1.86	0.57
22:V:383:GLY:O	22:V:392:TYR:OH	2.21	0.57
25:Y:330:ILE:HA	25:Y:333:GLU:HB3	1.85	0.57
22:V:479:ARG:HD2	25:Y:370:ILE:HG12	1.86	0.57
3:C:229:ARG:HE	3:C:232:ARG:HG3	1.68	0.57
3:C:245:ILE:HD12	3:C:290:LYS:HB2	1.87	0.57
11:K:101:PHE:HA	18:R:57:ARG:HE	1.69	0.57
22:V:28:PRO:HG2	22:V:84:LYS:HE2	1.87	0.57
1:A:380:SER:O	2:B:343:ARG:NH1	2.38	0.57
13:M:169:ARG:HD2	13:M:200:VAL:HG13	1.87	0.57
12:L:48:ALA:HB3	12:L:211:SER:HB2	1.85	0.57
12:L:5:GLN:HE21	13:M:5:THR:HA	1.70	0.57
15:O:94:ILE:HG22	15:O:95:GLY:H	1.69	0.57
23:W:223:LYS:HA	23:W:226:TYR:HB3	1.86	0.57
1:A:296:GLN:HB3	1:A:300:LEU:HD12	1.87	0.57
12:L:16:GLN:OE1	12:L:18:ARG:NH2	2.28	0.57
12:L:151:ALA:O	13:M:85:ARG:NH2	2.38	0.57
18:R:91:LYS:NZ	18:R:117:GLU:OE1	2.38	0.57
22:V:175:MET:O	22:V:178:SER:OG	2.21	0.57
26:Z:34:ARG:HB2	26:Z:97:THR:HG22	1.87	0.57
1:A:167:GLU:HB2	1:A:239:ARG:HG2	1.87	0.56
1:A:94:GLN:OE1	2:B:131:HIS:NE2	2.37	0.56
4:D:372:GLY:HA3	4:D:374:ASP:HB2	1.87	0.56
13:M:149:TYR:HA	13:M:159:GLY:HA3	1.87	0.56
1:A:138:MET:SD	1:A:156:LYS:NZ	2.69	0.56
9:I:122:THR:O	10:J:125:ARG:NH1	2.38	0.56
25:Y:388:ASN:ND2	26:Z:286:GLU:OE2	2.38	0.56
1:A:140:VAL:HA	1:A:152:PRO:HA	1.86	0.56
2:B:317:ASP:HB3	2:B:318:GLY:HA2	1.86	0.56
11:K:210:LEU:HG	11:K:238:ILE:HG23	1.87	0.56
15:O:96:ALA:HB1	15:O:98:LEU:HG	1.87	0.56
21:U:474:ARG:HH21	21:U:500:ASN:HB2	1.71	0.56
25:Y:314:LEU:HD21	25:Y:319:MET:HG2	1.87	0.56
11:K:23:GLN:HE22	11:K:135:ARG:HB2	1.71	0.56
16:P:36:THR:OG1	16:P:38:ASP:OD1	2.18	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:144:ARG:HA	23:W:147:LYS:HE2	1.86	0.56
24:X:318:ILE:O	24:X:322:HIS:ND1	2.38	0.56
25:Y:82:LYS:O	25:Y:86:GLU:N	2.36	0.56
33:E:401:ATP:O3'	6:F:344:ARG:NH2	2.37	0.56
10:J:10:PHE:CG	10:J:16:LEU:HD23	2.40	0.56
21:U:792:ASN:OD1	21:U:793:LYS:N	2.38	0.56
24:X:359:ALA:O	24:X:363:ARG:NE	2.37	0.56
1:A:364:VAL:HG13	1:A:368:ILE:HD12	1.86	0.56
2:B:198:LYS:HD3	2:B:237:LYS:HE2	1.86	0.56
21:U:541:HIS:HB2	21:U:544:ILE:HG22	1.86	0.56
23:W:334:GLU:OE1	23:W:338:THR:OG1	2.23	0.56
26:Z:224:HIS:CG	26:Z:225:GLN:HA	2.39	0.56
2:B:221:GLY:HA2	2:B:326:LYS:HE3	1.88	0.56
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.39	0.56
12:L:69:HIS:HE2	12:L:102:PRO:HB2	1.70	0.56
17:Q:45:LEU:HB3	17:Q:102:LEU:HD13	1.88	0.56
22:V:73:GLU:HB3	22:V:78:HIS:HA	1.87	0.56
25:Y:14:ASN:HA	25:Y:17:LEU:HB3	1.87	0.56
1:A:139:ARG:H	1:A:156:LYS:HE3	1.71	0.56
1:A:343:PHE:HA	1:A:344:SER:OG	2.06	0.56
3:C:157:GLN:HE22	3:C:318:PRO:HD3	1.71	0.56
12:L:121:GLN:HG3	13:M:129:ARG:HG2	1.86	0.56
13:M:8:ASP:O	13:M:22:GLN:NE2	2.39	0.56
2:B:205:LEU:HD21	2:B:245:ALA:HB2	1.87	0.56
6:F:89:LEU:HG	6:F:153:VAL:HG13	1.86	0.56
9:I:106:PRO:HD2	9:I:109:GLN:HE21	1.70	0.56
13:M:200:VAL:HG22	13:M:201:HIS:H	1.70	0.56
18:R:55:TRP:HB3	18:R:83:LEU:HD11	1.87	0.56
23:W:142:ARG:HH21	23:W:178:GLU:HB2	1.71	0.56
26:Z:225:GLN:HB2	26:Z:228:TYR:CE2	2.41	0.56
5:E:261:LEU:HD13	5:E:294:ARG:HE	1.69	0.56
5:E:327:ASP:O	5:E:364:GLN:NE2	2.38	0.56
22:V:200:ARG:O	22:V:204:ASP:N	2.36	0.56
22:V:302:TYR:HB3	22:V:339:LEU:HD23	1.87	0.56
23:W:440:ASN:O	23:W:443:THR:OG1	2.19	0.56
24:X:299:LEU:HA	24:X:302:PHE:HB3	1.88	0.56
2:B:188:GLY:HA3	2:B:367:ILE:HD12	1.87	0.56
10:J:73:PHE:HA	10:J:131:ALA:HA	1.88	0.56
22:V:410:ILE:HD13	22:V:425:LYS:HE3	1.88	0.56
2:B:170:LEU:HD13	3:C:228:ALA:HA	1.87	0.55
5:E:57:VAL:HA	5:E:99:ALA:HA	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:149:GLN:O	9:I:157:GLY:N	2.38	0.55
11:K:109:VAL:HG11	11:K:152:GLN:HB2	1.87	0.55
14:N:32:ASP:O	14:N:45:ARG:NH1	2.39	0.55
26:Z:62:ASP:OD2	26:Z:63:LYS:NZ	2.39	0.55
4:D:88:VAL:N	4:D:132:LEU:O	2.30	0.55
5:E:122:MET:SD	5:E:225:HIS:NE2	2.79	0.55
6:F:256:LEU:HD13	6:F:309:THR:HG21	1.88	0.55
11:K:100:TRP:O	18:R:57:ARG:NH2	2.39	0.55
11:K:178:GLN:HE22	11:K:181:LEU:HD22	1.71	0.55
22:V:319:HIS:HB2	22:V:320:THR:HA	1.88	0.55
25:Y:105:MET:HG3	25:Y:106:ALA:H	1.71	0.55
25:Y:179:ARG:NH2	25:Y:212:GLU:OE2	2.38	0.55
8:H:171:LYS:HE3	9:I:55:LEU:HD13	1.88	0.55
13:M:169:ARG:HG3	13:M:170:GLN:H	1.70	0.55
22:V:30:PRO:HA	22:V:33:GLN:HB2	1.88	0.55
23:W:259:GLU:HG2	23:W:262:LYS:HB3	1.88	0.55
2:B:257:GLN:N	2:B:257:GLN:OE1	2.37	0.55
3:C:32:GLN:O	3:C:36:ASN:N	2.36	0.55
6:F:438:TYR:CD2	11:K:20:ARG:CD	2.88	0.55
16:P:52:GLY:N	16:P:108:VAL:O	2.33	0.55
21:U:842:LYS:HG2	21:U:882:ALA:HB2	1.89	0.55
26:Z:33:LYS:HD3	26:Z:60:GLU:N	2.21	0.55
3:C:171:HIS:O	3:C:173:GLU:N	2.39	0.55
3:C:164:VAL:HG21	3:C:313:ARG:HB2	1.89	0.55
3:C:90:HIS:HB2	3:C:91:PRO:HD3	1.89	0.55
4:D:39:ASP:N	21:U:148:LYS:O	2.39	0.55
6:F:280:PRO:HA	6:F:281:SER:HB2	1.89	0.55
12:L:166:GLN:OE1	12:L:169:ARG:NH1	2.40	0.55
10:J:96:LEU:HG	17:Q:58:GLU:HB3	1.88	0.55
22:V:38:LYS:HA	22:V:41:ALA:HB3	1.88	0.55
22:V:67:LEU:O	22:V:71:THR:OG1	2.21	0.55
25:Y:232:GLU:O	25:Y:236:LEU:N	2.39	0.55
25:Y:301:ILE:HD12	25:Y:342:ARG:HB3	1.88	0.55
1:A:373:LEU:HD21	1:A:413:VAL:HG21	1.88	0.55
3:C:84:LYS:NZ	3:C:98:ASP:OD1	2.32	0.55
9:I:4:ARG:NH2	9:I:5:TYR:OH	2.40	0.55
21:U:685:GLN:HB2	21:U:726:ALA:HA	1.88	0.55
24:X:345:VAL:HG21	24:X:350:ILE:HD13	1.87	0.55
24:X:351:SER:OG	24:X:357:SER:OG	2.19	0.55
25:Y:194:PHE:HB3	25:Y:230:ALA:HB2	1.89	0.55
26:Z:241:SER:HB2	26:Z:242:LEU:HD12	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:7:GLN:HB3	14:N:111:VAL:HG23	1.89	0.55
20:T:92:LEU:HG	20:T:125:VAL:HG11	1.88	0.55
21:U:82:LEU:O	21:U:129:ARG:NE	2.40	0.55
21:U:520:MET:HE2	21:U:525:ASN:HB2	1.88	0.55
22:V:317:PRO:HD3	25:Y:382:LYS:HD2	1.89	0.55
24:X:414:LEU:HD23	24:X:417:LYS:HD2	1.87	0.55
3:C:87:VAL:O	3:C:95:PHE:N	2.26	0.55
5:E:293:GLY:N	5:E:296:ASP:OD1	2.40	0.55
22:V:173:ILE:O	22:V:177:ASN:ND2	2.40	0.55
6:F:306:VAL:HA	6:F:309:THR:HB	1.88	0.55
10:J:116:GLN:HE21	11:K:83:ALA:HB3	1.72	0.55
21:U:428:PRO:HB3	21:U:439:GLU:HB2	1.88	0.55
22:V:159:LEU:HD13	22:V:178:SER:HB3	1.88	0.55
23:W:435:LEU:HA	23:W:438:LEU:HG	1.88	0.55
24:X:183:LEU:HD22	25:Y:251:HIS:HD2	1.72	0.55
1:A:323:ARG:HE	1:A:431:THR:HB	1.72	0.54
4:D:287:ARG:O	4:D:291:GLU:N	2.40	0.54
4:D:354:LEU:HD23	4:D:356:GLU:HB3	1.88	0.54
7:G:124:VAL:O	7:G:128:ASN:ND2	2.40	0.54
9:I:25:MET:HA	9:I:28:ILE:HD13	1.88	0.54
15:O:13:VAL:HG21	15:O:152:LYS:HG2	1.89	0.54
26:Z:240:VAL:O	26:Z:243:GLN:N	2.39	0.54
11:K:37:ALA:HB2	11:K:50:VAL:HG23	1.88	0.54
22:V:484:LEU:HA	22:V:487:HIS:HD2	1.71	0.54
23:W:178:GLU:OE1	23:W:181:GLU:N	2.40	0.54
23:W:66:ILE:HA	23:W:67:LEU:HB2	1.89	0.54
25:Y:63:TRP:HB3	25:Y:64:GLN:HB3	1.88	0.54
1:A:143:ASP:O	1:A:147:TYR:N	2.33	0.54
2:B:256:ILE:HG12	3:C:268:GLU:HG3	1.88	0.54
3:C:371:LEU:HG	4:D:190:LEU:HD21	1.90	0.54
5:E:60:VAL:HG22	5:E:71:VAL:HG12	1.88	0.54
6:F:126:THR:OG1	6:F:130:GLN:O	2.25	0.54
19:S:13:LEU:HD23	19:S:175:VAL:HG22	1.89	0.54
22:V:451:ILE:HG13	22:V:458:VAL:HG13	1.89	0.54
2:B:390:LEU:HD13	2:B:430:LYS:HE2	1.89	0.54
3:C:321:ASN:OD1	3:C:322:GLU:N	2.40	0.54
6:F:369:HIS:NE2	33:F:501:ATP:N3	2.56	0.54
8:H:45:VAL:HG22	8:H:212:ILE:HG22	1.88	0.54
10:J:70:CYS:HB2	10:J:134:VAL:HB	1.89	0.54
21:U:208:LEU:HD23	21:U:210:LYS:H	1.72	0.54
21:U:356:THR:HG22	21:U:717:ILE:HG21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:SER:HB3	1:A:384:GLU:HB3	1.89	0.54
5:E:241:ARG:HG2	5:E:243:PHE:H	1.73	0.54
6:F:168:TYR:HB2	6:F:169:ASP:HB2	1.88	0.54
8:H:119:GLN:NE2	8:H:152:SER:O	2.40	0.54
16:P:190:ILE:HG22	16:P:195:ILE:HG23	1.90	0.54
20:T:7:THR:OG1	20:T:182:ARG:NH2	2.41	0.54
22:V:466:ILE:HD11	22:V:471:GLU:HB2	1.88	0.54
24:X:417:LYS:HZ2	26:Z:283:ARG:HH12	1.55	0.54
25:Y:67:VAL:O	25:Y:71:ASN:N	2.41	0.54
3:C:72:TYR:HB2	3:C:116:LEU:HD23	1.90	0.54
15:O:63:LEU:HA	15:O:66:HIS:HB2	1.89	0.54
17:Q:17:SER:OG	17:Q:179:SER:OG	2.25	0.54
21:U:220:LEU:HD11	21:U:252:LEU:HD13	1.90	0.54
22:V:372:LEU:HD21	22:V:399:ARG:HH22	1.73	0.54
1:A:344:SER:N	1:A:345:LEU:HB3	2.22	0.54
2:B:111:THR:OG1	2:B:124:SER:O	2.21	0.54
6:F:267:LEU:O	6:F:271:ALA:N	2.35	0.54
7:G:132:ARG:HG3	7:G:134:LEU:H	1.73	0.54
19:S:184:GLU:OE2	19:S:211:ARG:NH1	2.40	0.54
22:V:131:LEU:HD23	22:V:134:PHE:HD2	1.72	0.54
22:V:372:LEU:H	22:V:427:GLN:NE2	2.05	0.54
2:B:280:SER:HB2	2:B:325:VAL:H	1.73	0.54
9:I:69:ASN:OD1	9:I:70:GLU:N	2.41	0.54
13:M:46:VAL:HG22	13:M:215:TRP:CD1	2.41	0.54
3:C:155:ASP:HA	3:C:158:ILE:HG12	1.88	0.54
9:I:136:TYR:HB2	9:I:148:TYR:HB2	1.90	0.54
22:V:320:THR:HG23	22:V:321:ALA:HB2	1.90	0.54
3:C:19:GLY:O	3:C:23:TYR:N	2.37	0.54
3:C:153:GLY:N	3:C:327:ASP:OD2	2.41	0.54
10:J:77:THR:O	10:J:81:ARG:NH2	2.41	0.54
21:U:773:PHE:O	21:U:776:SER:OG	2.18	0.54
22:V:468:SER:O	22:V:472:PRO:HD2	2.07	0.54
25:Y:74:LYS:HA	25:Y:77:ASN:HB3	1.90	0.54
1:A:218:PRO:HD3	1:A:428:ARG:HH21	1.73	0.53
1:A:427:PRO:HB2	1:A:429:TYR:HD2	1.71	0.53
3:C:222:LYS:HE3	26:Z:179:ILE:HG12	58.79	0.53
12:L:184:LEU:H	12:L:184:LEU:HD12	1.74	0.53
22:V:379:LEU:HD13	22:V:395:ILE:HG12	1.89	0.53
3:C:49:ARG:HA	3:C:52:LEU:HB2	1.90	0.53
5:E:285:LEU:HB2	5:E:290:LEU:HG	1.90	0.53
7:G:88:ARG:NH2	13:M:157:SER:O	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:108:ASN:HB2	19:S:124:PHE:HD2	1.73	0.53
21:U:375:PHE:O	21:U:740:GLY:N	2.30	0.53
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.90	0.53
4:D:56:VAL:HG23	21:U:600:ARG:HE	1.74	0.53
23:W:247:TYR:HD2	23:W:273:TYR:HD2	1.56	0.53
23:W:65:ARG:HB2	23:W:66:ILE:HD13	1.88	0.53
24:X:394:ASP:OD1	24:X:394:ASP:N	2.41	0.53
6:F:257:VAL:HG23	6:F:306:VAL:HG23	1.89	0.53
6:F:88:TYR:CD2	6:F:155:LYS:HG3	2.43	0.53
20:T:112:ILE:O	20:T:123:GLY:N	2.37	0.53
23:W:59:ASP:O	23:W:63:THR:OG1	2.16	0.53
25:Y:68:ASP:HA	25:Y:71:ASN:HB2	1.91	0.53
3:C:28:ILE:HA	3:C:31:LEU:HB3	1.89	0.53
5:E:285:LEU:HD12	5:E:290:LEU:HD23	1.90	0.53
11:K:210:LEU:HD11	11:K:215:ILE:HG12	1.90	0.53
12:L:204:ASP:HA	12:L:205:LEU:HB3	1.89	0.53
22:V:345:ARG:HH12	22:V:357:LEU:HB2	1.72	0.53
26:Z:91:ILE:HD13	26:Z:115:TYR:HB3	1.89	0.53
26:Z:214:LYS:HE3	26:Z:221:PRO:HG2	1.89	0.53
1:A:428:ARG:HH22	2:B:340:ALA:HB2	1.72	0.53
4:D:201:GLY:HA3	4:D:327:LEU:HA	1.91	0.53
21:U:616:ARG:HH21	21:U:647:HIS:HA	1.73	0.53
1:A:205:GLY:HA2	1:A:206:ILE:HG22	1.89	0.53
3:C:142:LYS:HB2	3:C:213:ARG:HG2	1.90	0.53
4:D:182:GLU:HG3	4:D:183:LEU:HD12	1.90	0.53
4:D:280:GLY:O	4:D:284:GLU:N	2.41	0.53
4:D:354:LEU:HB3	4:D:356:GLU:H	1.73	0.53
8:H:122:THR:HG22	8:H:129:PRO:HB3	1.90	0.53
21:U:774:PRO:HA	21:U:777:HIS:CD2	2.44	0.53
21:U:802:TYR:HB3	21:U:895:PRO:HD3	1.89	0.53
22:V:234:ARG:HG3	22:V:250:LEU:HD11	1.91	0.53
25:Y:197:ALA:HB3	25:Y:226:VAL:HG21	1.89	0.53
3:C:119:ASP:OD1	3:C:119:ASP:N	2.41	0.53
11:K:48:LEU:HB3	11:K:218:ALA:HB3	1.91	0.53
3:C:28:ILE:O	3:C:32:GLN:N	2.26	0.53
4:D:91:GLN:HB2	4:D:245:ARG:HE	1.74	0.53
7:G:53:GLN:HA	7:G:215:ILE:HA	1.89	0.53
8:H:65:VAL:HB	8:H:220:ARG:HE	1.74	0.53
10:J:116:GLN:OE1	11:K:135:ARG:NH2	2.42	0.53
16:P:88:MET:HG3	16:P:124:LEU:HD11	1.90	0.53
16:P:58:THR:O	17:Q:85:ARG:NH2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:322:VAL:HG13	22:V:323:GLY:H	1.73	0.53
26:Z:68:TRP:CD2	26:Z:108:ILE:HG13	2.43	0.53
2:B:106:PRO:HB2	2:B:154:HIS:HD2	1.73	0.53
3:C:11:LEU:HD12	3:C:14:GLY:HA2	1.90	0.53
6:F:195:ILE:HG12	6:F:199:VAL:HG23	1.91	0.53
20:T:92:LEU:HD23	20:T:112:ILE:HD11	1.90	0.53
3:C:50:ASN:HD21	21:U:643:SER:HA	1.72	0.53
1:A:120:LYS:H	6:F:127:SER:HB2	1.73	0.53
2:B:304:GLU:HA	2:B:307:ARG:HG2	1.90	0.53
3:C:99:VAL:HA	3:C:100:ASP:HB3	1.91	0.53
3:C:82:LYS:HE2	3:C:84:LYS:HD3	1.90	0.53
4:D:242:GLU:OE2	5:E:78:ARG:NH2	2.42	0.53
14:N:18:SER:HB2	14:N:30:VAL:HA	1.90	0.53
25:Y:192:ARG:NH2	25:Y:294:TYR:HB3	2.24	0.53
3:C:11:LEU:HD23	21:U:146:LYS:HB3	1.91	0.52
4:D:293:LEU:O	4:D:296:MET:HG2	2.09	0.52
7:G:86:ASP:HA	13:M:120:HIS:CE1	2.44	0.52
12:L:75:ALA:HB3	12:L:131:GLY:HA3	1.90	0.52
26:Z:33:LYS:HG2	26:Z:34:ARG:HG2	1.90	0.52
1:A:384:GLU:H	2:B:343:ARG:HH11	1.57	0.52
3:C:214:VAL:HG13	3:C:215:SER:O	2.09	0.52
6:F:383:GLU:HB3	6:F:417:HIS:NE2	2.24	0.52
1:A:334:PRO:HB3	6:F:395:GLN:HE21	1.74	0.52
17:Q:52:ASP:OD1	18:R:88:TYR:OH	2.23	0.52
21:U:474:ARG:NH2	21:U:496:LEU:O	2.41	0.52
22:V:338:LEU:HD21	22:V:394:LEU:HB2	1.91	0.52
22:V:362:LEU:HD12	22:V:365:GLN:HB3	1.92	0.52
5:E:145:LEU:HA	5:E:148:VAL:HB	1.91	0.52
9:I:195:LYS:HB2	9:I:240:HIS:CD2	2.45	0.52
17:Q:84:THR:HG21	17:Q:104:LEU:HD11	1.91	0.52
21:U:643:SER:O	21:U:649:ARG:NH1	2.43	0.52
22:V:33:GLN:HB3	22:V:115:LYS:HD3	1.91	0.52
23:W:389:SER:O	23:W:393:LEU:N	2.41	0.52
25:Y:173:ASP:H	25:Y:177:ARG:HD3	1.74	0.52
1:A:102:ILE:HD11	1:A:136:GLU:HA	1.92	0.52
3:C:270:GLN:HA	3:C:273:MET:HE3	1.90	0.52
5:E:348:THR:HG21	6:F:218:GLN:HB2	1.92	0.52
22:V:59:ALA:N	22:V:60:ALA:HB3	2.25	0.52
23:W:55:ARG:NH1	23:W:79:GLU:HG3	2.24	0.52
4:D:153:MET:HG3	4:D:154:LEU:HD13	1.90	0.52
6:F:438:TYR:CZ	11:K:20:ARG:CA	2.93	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:184:GLY:H	16:P:202:ALA:HB3	1.75	0.52
21:U:237:VAL:HG13	21:U:321:GLN:HG3	1.91	0.52
22:V:480:ILE:HD11	26:Z:264:SER:HA	1.92	0.52
3:C:221:GLN:HB2	4:D:283:ARG:NH1	2.25	0.52
22:V:412:LEU:O	25:Y:346:LYS:NZ	2.31	0.52
23:W:361:HIS:CD2	23:W:364:ARG:HH11	2.27	0.52
24:X:203:PRO:HB2	24:X:204:PRO:C	2.30	0.52
3:C:229:ARG:HB3	3:C:232:ARG:HB2	1.92	0.52
3:C:193:GLY:H	3:C:355:SER:HB2	1.75	0.52
5:E:292:PRO:HA	5:E:295:LEU:O	2.10	0.52
9:I:95:GLN:HE21	16:P:69:PHE:HA	1.75	0.52
21:U:57:ARG:HA	21:U:60:ALA:HB3	1.91	0.52
21:U:628:ARG:NH1	21:U:749:GLN:OE1	2.38	0.52
23:W:5:GLY:HA3	23:W:47:LEU:HD13	1.91	0.52
25:Y:16:ASP:HB3	25:Y:146:ARG:HH21	1.75	0.52
1:A:427:PRO:HB3	10:J:13:ASP:HB3	1.91	0.52
7:G:74:GLU:O	7:G:227:PHE:N	2.42	0.52
10:J:131:ALA:N	10:J:147:THR:OG1	2.42	0.52
10:J:17:PHE:O	10:J:21:TYR:HB3	2.09	0.52
14:N:178:ALA:HB3	14:N:185:GLU:HB2	1.92	0.52
15:O:215:LYS:HB3	16:P:197:THR:HB	1.92	0.52
21:U:806:CYS:SG	21:U:888:GLN:HG2	2.50	0.52
1:A:220:THR:HB	33:A:501:ATP:C5	2.45	0.52
4:D:251:PHE:CE2	4:D:292:LEU:HB2	2.45	0.52
6:F:279:ALA:HA	6:F:325:GLN:HE21	1.73	0.52
8:H:150:ASP:OD1	8:H:154:ALA:N	2.43	0.52
11:K:146:VAL:HG11	11:K:222:PRO:HG3	1.92	0.52
13:M:187:ARG:O	13:M:232:ARG:NH1	2.41	0.52
21:U:764:LEU:HA	21:U:767:THR:HG23	1.92	0.52
2:B:338:ASP:H	2:B:341:LEU:HG	1.74	0.52
3:C:49:ARG:HH22	4:D:69:LYS:HG3	1.75	0.52
5:E:152:PRO:HG3	5:E:159:PHE:HE2	1.74	0.52
10:J:10:PHE:HB2	10:J:16:LEU:HA	1.91	0.52
14:N:35:THR:HG21	14:N:56:ALA:HB1	1.92	0.52
22:V:137:GLU:O	22:V:141:THR:N	2.40	0.52
26:Z:192:THR:O	26:Z:196:HIS:N	2.37	0.52
8:H:4:ARG:HD2	8:H:6:TYR:HB3	1.91	0.51
12:L:156:CYS:SG	12:L:159:MET:HG2	2.51	0.51
12:L:70:ILE:HG12	12:L:136:GLY:HA3	1.91	0.51
19:S:73:LYS:O	19:S:77:HIS:ND1	2.35	0.51
1:A:277:ILE:HG13	1:A:280:ILE:HD11	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:TYR:HA	4:D:44:TYR:HB3	1.92	0.51
5:E:56:ILE:HG23	5:E:100:LEU:HB2	1.90	0.51
16:P:13:ALA:HB3	16:P:137:VAL:HG23	1.92	0.51
25:Y:346:LYS:HB2	25:Y:355:GLU:HB3	1.93	0.51
4:D:336:PRO:HG2	4:D:375:ILE:HG21	1.91	0.51
8:H:74:LEU:HD21	8:H:134:LEU:HD22	1.91	0.51
20:T:11:VAL:HG13	20:T:24:ALA:HB2	1.91	0.51
21:U:774:PRO:O	21:U:778:PHE:N	2.43	0.51
22:V:474:LEU:HA	22:V:477:HIS:HD2	1.76	0.51
4:D:163:MET:HG3	4:D:165:ALA:H	1.75	0.51
6:F:435:LEU:HD13	12:L:31:GLN:HG3	1.90	0.51
7:G:172:GLN:OE1	7:G:172:GLN:N	2.42	0.51
9:I:2:SER:HA	9:I:5:TYR:HD2	1.74	0.51
10:J:137:ASP:N	10:J:141:THR:O	2.43	0.51
9:I:69:ASN:HA	16:P:76:LEU:HD22	1.90	0.51
22:V:69:THR:O	22:V:73:GLU:N	2.36	0.51
26:Z:37:GLY:HA2	26:Z:56:VAL:HG12	1.91	0.51
9:I:11:ILE:HG21	10:J:7:ILE:HD12	1.92	0.51
10:J:96:LEU:HD23	10:J:97:THR:HG23	1.93	0.51
12:L:184:LEU:HD23	12:L:214:ILE:HG21	1.92	0.51
13:M:30:VAL:HG11	13:M:134:SER:HB3	1.91	0.51
17:Q:19:ARG:NH2	17:Q:31:ASP:O	2.44	0.51
22:V:378:VAL:HG13	22:V:382:PHE:HD2	1.76	0.51
24:X:420:LYS:O	26:Z:287:LYS:NZ	2.28	0.51
25:Y:191:ILE:HG13	25:Y:192:ARG:H	1.74	0.51
3:C:137:LEU:O	3:C:141:GLU:HG3	2.11	0.51
3:C:246:ILE:HG22	3:C:247:PHE:H	1.76	0.51
3:C:89:VAL:HG12	3:C:91:PRO:HD2	1.92	0.51
6:F:334:ARG:HG2	6:F:336:ASP:H	1.75	0.51
6:F:70:LYS:HE2	6:F:74:LYS:HE3	1.93	0.51
10:J:36:ARG:HB3	10:J:144:LEU:HD23	1.93	0.51
11:K:182:GLN:HA	12:L:56:LEU:HD23	1.92	0.51
21:U:403:THR:HA	21:U:406:ALA:HB3	1.93	0.51
21:U:908:ILE:HG12	21:U:909:GLY:H	1.76	0.51
22:V:227:VAL:O	22:V:231:LEU:N	2.43	0.51
24:X:298:SER:O	24:X:301:ASP:N	2.43	0.51
1:A:260:LEU:HD13	1:A:272:ILE:HG13	1.92	0.51
1:A:95:VAL:HB	1:A:144:ARG:H	1.76	0.51
9:I:155:ASN:OD1	10:J:81:ARG:NH2	2.44	0.51
12:L:132:LEU:HB2	12:L:147:THR:HG21	1.93	0.51
16:P:12:MET:HG3	16:P:138:VAL:HG12	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:132:SER:O	18:R:135:ALA:N	2.34	0.51
22:V:227:VAL:HA	22:V:230:PHE:HB3	1.92	0.51
25:Y:20:ALA:HB2	25:Y:150:PHE:HD1	1.75	0.51
1:A:270:CYS:O	1:A:315:ILE:HG12	2.10	0.51
2:B:224:LEU:O	2:B:330:ALA:HA	2.11	0.51
2:B:337:LEU:HA	2:B:341:LEU:HD12	1.93	0.51
3:C:193:GLY:H	3:C:356:GLY:H	1.58	0.51
5:E:165:ILE:HD12	5:E:166:PRO:HD2	1.93	0.51
17:Q:22:ALA:HB2	17:Q:27:GLN:HG3	1.93	0.51
19:S:27:THR:HB	19:S:40:SER:H	1.74	0.51
20:T:20:VAL:HG11	20:T:122:LEU:HD13	1.92	0.51
1:A:191:VAL:HG21	1:A:271:LEU:HD21	1.93	0.51
4:D:202:VAL:HB	4:D:308:ILE:HA	1.92	0.51
7:G:130:GLU:OE1	13:M:126:SER:OG	2.29	0.51
11:K:108:THR:O	11:K:110:GLU:N	2.44	0.51
14:N:2:THR:HA	14:N:129:GLY:HA3	1.93	0.51
2:B:110:GLY:HA3	2:B:152:LEU:HD13	1.93	0.51
7:G:205:VAL:HG12	7:G:206:LEU:HG	1.92	0.51
12:L:84:LEU:O	12:L:88:MET:N	2.44	0.51
13:M:214:SER:OG	13:M:224:HIS:NE2	2.41	0.51
18:R:1:THR:O	18:R:130:SER:N	2.35	0.51
20:T:45:VAL:HB	20:T:49:THR:HG23	1.93	0.51
23:W:141:GLU:HB3	23:W:172:GLU:HG3	1.93	0.51
26:Z:256:GLN:HG3	26:Z:260:VAL:HG23	1.93	0.51
7:G:60:LEU:HD22	13:M:161:TRP:HB2	1.93	0.50
15:O:203:ARG:NH2	16:P:155:GLU:OE1	2.44	0.50
21:U:885:MET:HG2	21:U:887:ALA:H	1.75	0.50
3:C:201:ARG:HH11	3:C:211:PHE:HB3	1.76	0.50
6:F:325:GLN:HG2	6:F:326:VAL:HG23	1.93	0.50
9:I:105:ILE:HG12	9:I:110:LEU:HD13	1.93	0.50
15:O:98:LEU:HB2	15:O:113:ILE:HD12	1.92	0.50
18:R:50:ALA:HB2	19:S:129:SER:HB2	1.93	0.50
22:V:203:LEU:O	22:V:207:ALA:N	2.25	0.50
23:W:442:THR:HA	23:W:445:LEU:HB2	1.94	0.50
26:Z:199:LYS:HA	26:Z:202:ASN:ND2	2.25	0.50
1:A:333:ARG:O	1:A:337:LEU:N	2.45	0.50
23:W:5:GLY:HA2	23:W:34:LEU:HD13	1.92	0.50
2:B:254:GLU:HG3	2:B:292:THR:HG22	1.94	0.50
10:J:92:GLN:HE21	17:Q:66:LEU:HB2	1.75	0.50
21:U:20:LYS:HE2	21:U:48:LEU:HD21	1.94	0.50
23:W:216:GLU:CD	23:W:217:GLU:H	2.15	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:79:ALA:HA	12:L:82:ARG:HH21	1.77	0.50
13:M:234:GLU:HA	13:M:237:LYS:HB3	1.92	0.50
15:O:73:LEU:HD12	15:O:74:PRO:HD2	1.94	0.50
21:U:529:ILE:HD11	21:U:555:VAL:HG11	1.93	0.50
23:W:135:LYS:HB3	23:W:136:ILE:C	2.32	0.50
25:Y:73:MET:O	25:Y:77:ASN:N	2.28	0.50
3:C:13:GLU:N	3:C:14:GLY:HA3	2.27	0.50
4:D:231:VAL:HG11	5:E:258:MET:HB3	1.94	0.50
11:K:137:PHE:HB3	11:K:139:VAL:HG12	1.93	0.50
19:S:11:THR:HA	19:S:139:GLY:HA3	1.94	0.50
21:U:576:PRO:HB3	21:U:611:ASN:HD22	1.76	0.50
23:W:321:VAL:O	23:W:325:GLY:N	2.43	0.50
23:W:366:MET:HB3	23:W:370:TYR:CE2	2.47	0.50
26:Z:223:ASN:HB2	26:Z:227:ILE:HG12	1.93	0.50
1:A:205:GLY:HA2	1:A:206:ILE:CG2	2.41	0.50
1:A:333:ARG:HG3	1:A:334:PRO:HD3	1.92	0.50
5:E:206:LYS:HG3	5:E:207:TYR:H	1.77	0.50
7:G:12:HIS:CD2	13:M:9:LEU:HD12	2.46	0.50
16:P:13:ALA:HA	16:P:22:ILE:HA	1.92	0.50
19:S:49:LYS:HB3	19:S:113:LEU:HB2	1.94	0.50
7:G:171:LYS:HB3	7:G:205:VAL:HG11	1.94	0.50
13:M:123:THR:HG22	13:M:130:PRO:HB3	1.94	0.50
3:C:71:SER:HB2	4:D:112:TYR:O	2.12	0.50
15:O:217:THR:HB	16:P:195:ILE:HB	1.94	0.50
2:B:199:GLU:O	2:B:203:LEU:N	2.45	0.49
3:C:163:GLU:OE1	3:C:163:GLU:N	2.44	0.49
9:I:196:VAL:O	9:I:200:THR:OG1	2.22	0.49
10:J:104:VAL:HG23	10:J:143:ARG:HD3	1.94	0.49
12:L:72:ILE:HG22	12:L:134:ILE:HA	1.94	0.49
12:L:33:SER:HB2	12:L:49:LEU:HB3	1.94	0.49
23:W:438:LEU:HD22	26:Z:234:PHE:CD1	2.47	0.49
1:A:354:ILE:O	1:A:358:HIS:ND1	2.40	0.49
14:N:84:LYS:NZ	14:N:85:GLU:OE2	2.40	0.49
17:Q:151:ILE:HG13	17:Q:152:SER:HB2	1.94	0.49
24:X:258:LYS:HD3	24:X:267:VAL:HG22	1.93	0.49
25:Y:233:ARG:NH1	25:Y:306:GLN:OE1	2.45	0.49
1:A:218:PRO:O	1:A:221:GLY:N	2.45	0.49
1:A:373:LEU:HD13	1:A:410:LEU:HB2	1.93	0.49
5:E:141:GLN:NE2	5:E:300:HIS:O	2.41	0.49
22:V:26:PRO:O	22:V:29:PRO:HD2	2.12	0.49
23:W:170:GLN:HA	23:W:173:THR:HG23	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:455:LEU:HD12	23:W:456:GLN:H	1.78	0.49
25:Y:134:LEU:HD13	25:Y:168:ILE:HG23	1.94	0.49
26:Z:136:GLU:OE2	26:Z:157:HIS:ND1	2.34	0.49
9:I:108:GLU:OE2	9:I:146:GLN:NE2	2.35	0.49
14:N:22:THR:HG22	14:N:27:ALA:HB2	1.95	0.49
20:T:25:ASP:OD1	20:T:41:ARG:NH1	2.46	0.49
21:U:792:ASN:HA	21:U:914:LEU:HB3	1.93	0.49
1:A:86:THR:O	1:A:90:GLU:N	2.45	0.49
2:B:109:VAL:HG22	2:B:151:LEU:HD22	1.95	0.49
3:C:142:LYS:HA	4:D:323:ARG:HD2	1.95	0.49
3:C:188:LEU:HB3	3:C:317:PHE:HB2	1.93	0.49
7:G:220:VAL:HB	7:G:227:PHE:HD1	1.76	0.49
15:O:181:ASN:OD1	15:O:182:LYS:N	2.46	0.49
21:U:842:LYS:H	21:U:882:ALA:HB2	1.76	0.49
22:V:367:VAL:HG13	22:V:402:VAL:HG22	1.93	0.49
24:X:414:LEU:HA	24:X:417:LYS:HD2	1.94	0.49
9:I:48:GLU:O	9:I:64:LYS:NZ	2.40	0.49
21:U:27:LEU:O	21:U:31:VAL:N	2.45	0.49
1:A:217:PRO:HD2	1:A:343:PHE:HB2	1.94	0.49
2:B:364:ILE:O	2:B:368:HIS:ND1	2.32	0.49
4:D:89:ILE:O	4:D:106:THR:OG1	2.29	0.49
5:E:360:ASP:OD1	5:E:360:ASP:N	2.44	0.49
13:M:56:LYS:H	13:M:57:LEU:HA	1.77	0.49
20:T:46:ASN:OD1	20:T:48:SER:N	2.29	0.49
21:U:345:ASN:ND2	21:U:743:ASN:OD1	2.45	0.49
21:U:472:ILE:HG22	21:U:475:HIS:CE1	2.47	0.49
21:U:885:MET:HB3	21:U:888:GLN:HG3	1.94	0.49
22:V:326:GLN:HB3	22:V:353:LEU:HD22	1.93	0.49
23:W:372:ARG:HG2	23:W:414:ASN:HB3	1.93	0.49
26:Z:39:LEU:HD11	26:Z:50:VAL:HG11	1.94	0.49
1:A:151:ILE:HD12	1:A:152:PRO:HD2	1.94	0.49
1:A:297:ARG:NE	6:F:302:GLY:O	2.45	0.49
9:I:175:LEU:HA	9:I:178:ASP:HB2	1.94	0.49
9:I:190:LEU:HB3	9:I:236:LEU:HD21	1.95	0.49
16:P:72:ASN:O	16:P:76:LEU:HG	2.13	0.49
17:Q:7:ILE:HD13	17:Q:14:LEU:HD23	1.94	0.49
22:V:219:GLU:OE2	22:V:256:ARG:NH1	2.45	0.49
24:X:368:MET:HB3	24:X:374:PHE:HB3	1.95	0.49
25:Y:46:ARG:C	25:Y:48:ASN:H	2.16	0.49
1:A:120:LYS:HE2	6:F:90:VAL:HG11	1.95	0.49
3:C:131:VAL:HG13	3:C:132:ASP:H	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:328:ILE:HG23	3:C:359:VAL:HG11	1.95	0.49
4:D:285:VAL:HA	4:D:288:ILE:HB	1.94	0.49
5:E:133:SER:HA	5:E:142:ILE:HD13	1.95	0.49
17:Q:36:PHE:HB2	17:Q:44:LEU:HB3	1.95	0.49
21:U:118:LEU:HD21	21:U:123:LYS:HA	1.95	0.49
21:U:612:ASP:HA	21:U:615:ARG:HD3	1.95	0.49
22:V:81:GLN:HB3	22:V:83:GLU:N	2.27	0.49
23:W:2:ALA:HA	23:W:47:LEU:HD11	1.95	0.49
2:B:103:ARG:HG3	2:B:104:GLY:H	1.78	0.49
4:D:300:ASP:HA	4:D:301:GLN:HA	1.64	0.49
5:E:178:THR:HG21	5:E:340:GLY:H	1.77	0.49
18:R:115:ASP:HB2	18:R:119:ASN:HD22	1.78	0.49
24:X:260:MET:HE3	24:X:322:HIS:HA	1.95	0.49
26:Z:105:ASP:HA	26:Z:108:ILE:HD13	1.94	0.49
3:C:89:VAL:HB	3:C:92:GLU:HB2	1.95	0.48
4:D:116:LEU:HD12	4:D:140:VAL:HG22	1.94	0.48
6:F:438:TYR:CE2	11:K:20:ARG:HG2	2.40	0.48
11:K:46:VAL:HG23	11:K:151:PRO:HB2	1.95	0.48
11:K:210:LEU:HA	11:K:214:ASN:HD22	1.77	0.48
13:M:74:GLY:HA3	13:M:224:HIS:CE1	2.48	0.48
23:W:405:LYS:HG3	24:X:344:ARG:HG2	1.95	0.48
26:Z:189:GLN:O	26:Z:192:THR:OG1	2.27	0.48
24:X:420:LYS:NZ	26:Z:284:ASP:OD1	2.40	0.48
1:A:219:GLY:HA2	1:A:220:THR:HA	1.49	0.48
1:A:174:TYR:HD1	1:A:227:ARG:HD2	1.78	0.48
7:G:52:THR:HG22	7:G:53:GLN:H	1.77	0.48
7:G:76:ILE:HA	7:G:141:ILE:HD11	1.93	0.48
11:K:221:GLN:OE1	11:K:227:HIS:NE2	2.42	0.48
12:L:85:CYS:SG	12:L:89:ARG:NH1	2.86	0.48
21:U:384:GLN:HG2	21:U:385:PHE:H	1.78	0.48
21:U:401:LYS:HB3	21:U:438:GLN:NE2	2.29	0.48
21:U:338:HIS:HD2	21:U:785:PRO:HB2	1.77	0.48
21:U:800:VAL:HG21	21:U:914:LEU:HD21	1.94	0.48
25:Y:131:THR:O	25:Y:137:ARG:NH1	2.45	0.48
26:Z:32:GLN:HG3	26:Z:33:LYS:H	1.78	0.48
1:A:125:LEU:HB3	1:A:149:ILE:HD12	1.94	0.48
2:B:216:ILE:O	2:B:217:LYS:HG2	2.12	0.48
4:D:254:ALA:HB1	4:D:305:VAL:HG23	1.95	0.48
5:E:339:ASN:OD1	5:E:340:GLY:N	2.46	0.48
5:E:345:ASN:HD21	6:F:345:SER:HA	1.78	0.48
6:F:366:MET:HE1	6:F:384:LEU:HD22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:681:ASN:ND2	21:U:725:MET:SD	2.86	0.48
1:A:101:ILE:N	1:A:114:ASN:O	2.45	0.48
1:A:217:PRO:HA	1:A:428:ARG:NE	2.29	0.48
4:D:241:GLY:O	4:D:245:ARG:NH2	2.46	0.48
3:C:43:ARG:HG2	4:D:61:ILE:HD12	1.94	0.48
5:E:65:THR:HG22	5:E:66:GLU:H	1.79	0.48
7:G:39:SER:H	7:G:172:GLN:HE21	1.59	0.48
9:I:93:ILE:HA	9:I:96:ARG:HG2	1.94	0.48
12:L:205:LEU:HD22	12:L:239:ARG:HH22	1.78	0.48
13:M:56:LYS:HB3	13:M:57:LEU:C	2.34	0.48
15:O:51:ASP:OD2	16:P:99:ARG:NH2	2.46	0.48
22:V:47:SER:HA	22:V:50:GLU:HB2	1.94	0.48
23:W:136:ILE:H	23:W:141:GLU:HG2	1.78	0.48
26:Z:58:PHE:CZ	26:Z:68:TRP:HB2	2.49	0.48
4:D:218:ALA:O	4:D:222:HIS:ND1	2.39	0.48
4:D:261:ILE:HG12	4:D:306:LYS:HB2	1.95	0.48
5:E:235:ILE:HG22	5:E:279:THR:HB	1.95	0.48
22:V:417:ILE:HG12	22:V:422:ILE:HD12	1.94	0.48
1:A:206:ILE:HG23	1:A:207:GLU:H	1.79	0.48
9:I:86:LEU:HB3	9:I:114:LEU:HD11	1.96	0.48
11:K:69:GLU:HA	11:K:75:GLY:HA2	1.96	0.48
25:Y:145:LEU:HA	25:Y:157:ILE:HG22	1.95	0.48
2:B:260:LEU:N	2:B:261:GLY:HA2	2.29	0.48
10:J:115:LYS:HE3	10:J:127:PHE:HB2	1.95	0.48
11:K:11:GLY:C	11:K:13:ASN:H	2.16	0.48
13:M:22:GLN:HB3	13:M:130:PRO:HG2	1.95	0.48
12:L:117:GLN:NE2	13:M:83:ASP:OD1	2.45	0.48
16:P:42:ILE:HG12	16:P:52:GLY:HA2	1.96	0.48
18:R:157:ARG:HD3	18:R:195:LEU:HD13	1.95	0.48
22:V:306:ARG:HB3	22:V:339:LEU:HD21	1.95	0.48
23:W:91:SER:HB2	23:W:92:LYS:HA	1.94	0.48
2:B:176:VAL:CG2	2:B:177:GLU:HA	2.38	0.48
20:T:142:GLY:HA2	20:T:176:LEU:HD21	1.96	0.48
24:X:360:ASP:OD1	24:X:361:VAL:N	2.45	0.48
25:Y:77:ASN:ND2	25:Y:114:ILE:HG21	2.29	0.48
1:A:164:MET:HG2	1:A:244:GLU:HG3	1.95	0.48
1:A:375:ARG:HG3	1:A:376:LEU:HD12	1.96	0.48
2:B:93:GLU:HG3	2:B:94:GLU:H	1.79	0.48
7:G:80:MET:HG3	7:G:87:SER:HB2	1.95	0.48
12:L:65:HIS:H	12:L:223:ILE:HD11	1.78	0.48
13:M:68:ASN:ND2	13:M:224:HIS:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:29:GLY:HA2	16:P:35:VAL:HG23	1.94	0.48
20:T:24:ALA:H	20:T:42:ILE:HD11	1.77	0.48
21:U:591:CYS:HA	21:U:625:ILE:HA	1.96	0.48
23:W:186:ILE:O	23:W:189:GLN:NE2	2.44	0.48
26:Z:222:ILE:N	26:Z:223:ASN:HA	2.28	0.48
1:A:80:LEU:HD21	2:B:138:PHE:HB2	1.96	0.48
2:B:151:LEU:HD11	2:B:163:LEU:HD13	1.96	0.48
3:C:103:ILE:HG13	3:C:126:ILE:HG22	1.95	0.48
4:D:91:GLN:N	4:D:104:GLY:O	2.33	0.48
8:H:19:LEU:HD13	8:H:22:ILE:HD12	1.96	0.48
20:T:23:ALA:HB3	20:T:169:VAL:HG11	1.94	0.48
22:V:471:GLU:HB3	22:V:472:PRO:HD3	1.96	0.48
24:X:347:ILE:HG22	24:X:385:LEU:HB2	1.96	0.48
1:A:312:ARG:HA	1:A:313:GLY:HA2	1.58	0.47
11:K:178:GLN:NE2	11:K:181:LEU:HD22	2.29	0.47
12:L:229:VAL:HG12	12:L:233:LEU:HG	1.96	0.47
18:R:83:LEU:HD21	18:R:97:MET:HE1	1.95	0.47
20:T:99:ARG:HG3	20:T:105:PRO:HA	1.95	0.47
23:W:231:ILE:HG21	23:W:250:ILE:HG22	1.96	0.47
3:C:295:THR:HG22	3:C:296:ASN:H	1.79	0.47
4:D:313:ARG:NH2	4:D:315:ASP:OD2	2.47	0.47
4:D:89:ILE:HD13	5:E:78:ARG:HB3	1.96	0.47
5:E:58:GLY:HA2	5:E:73:ALA:HA	1.96	0.47
12:L:123:TYR:N	13:M:127:ALA:O	2.47	0.47
14:N:176:LEU:HD12	14:N:187:GLN:HE21	1.78	0.47
17:Q:9:GLY:HA3	17:Q:12:TYR:CE2	2.49	0.47
3:C:38:LYS:HG2	22:V:495:ARG:HB3	1.95	0.47
24:X:417:LYS:HZ3	26:Z:283:ARG:HH22	1.60	0.47
1:A:247:GLN:HB2	1:A:248:LYS:O	2.13	0.47
11:K:108:THR:HB	11:K:147:ASP:HA	1.97	0.47
22:V:273:LYS:HA	22:V:274:SER:HB2	1.94	0.47
3:C:203:VAL:O	3:C:207:THR:OG1	2.22	0.47
3:C:56:VAL:HG21	4:D:75:ALA:HB1	1.96	0.47
4:D:366:ARG:HB3	4:D:367:PRO:HD3	1.96	0.47
13:M:66:LEU:HD13	13:M:214:SER:HB2	1.96	0.47
19:S:142:SER:HA	19:S:145:LEU:HB2	1.96	0.47
21:U:443:LEU:HD21	21:U:464:GLN:HB2	1.97	0.47
21:U:571:CYS:HB2	21:U:601:ARG:HH21	1.78	0.47
25:Y:51:ALA:CB	25:Y:116:ASP:H	2.27	0.47
1:A:429:TYR:CD2	10:J:12:PRO:HD2	2.49	0.47
7:G:69:LEU:HD11	7:G:216:GLU:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:49:VAL:HG22	7:G:219:VAL:HG23	1.96	0.47
11:K:121:LEU:HD13	11:K:123:PHE:HE2	1.79	0.47
11:K:16:SER:OG	11:K:17:PRO:HD2	2.14	0.47
13:M:106:ILE:HD12	13:M:107:PRO:HD2	1.97	0.47
19:S:23:VAL:O	19:S:196:CYS:N	2.41	0.47
25:Y:101:ARG:HD3	25:Y:130:LYS:HD3	1.95	0.47
25:Y:356:THR:OG1	25:Y:357:ASN:O	2.28	0.47
26:Z:45:LYS:HG3	26:Z:46:LYS:H	1.80	0.47
1:A:311:PRO:N	1:A:312:ARG:HA	2.30	0.47
2:B:99:VAL:O	2:B:103:ARG:HG2	2.14	0.47
2:B:106:PRO:HB3	3:C:121:TYR:HB2	1.95	0.47
2:B:261:GLY:C	2:B:263:GLY:H	2.17	0.47
5:E:257:LEU:HA	5:E:260:LEU:HD12	1.96	0.47
6:F:224:LEU:HB2	6:F:348:LEU:HD13	1.96	0.47
5:E:341:ALA:HB1	6:F:345:SER:H	1.78	0.47
11:K:69:GLU:HG2	11:K:71:ASP:O	2.15	0.47
22:V:179:LYS:HD3	22:V:214:HIS:HA	1.97	0.47
23:W:52:LYS:HA	23:W:55:ARG:HB3	1.95	0.47
25:Y:316:LEU:HG	25:Y:352:GLU:HG3	1.97	0.47
2:B:255:LEU:HD11	3:C:264:GLY:HA2	1.96	0.47
22:V:468:SER:HA	25:Y:363:ASN:HD21	1.79	0.47
24:X:377:ILE:HB	24:X:388:PHE:HE2	1.80	0.47
25:Y:138:LEU:HD22	25:Y:168:ILE:HD13	1.96	0.47
4:D:145:PRO:HB2	4:D:146:GLU:HB2	1.97	0.47
4:D:358:VAL:HG12	4:D:363:TYR:HE2	1.80	0.47
4:D:377:SER:CB	5:E:292:PRO:HB2	2.44	0.47
5:E:211:SER:HA	5:E:214:LEU:HB3	1.96	0.47
10:J:148:ASP:OD2	10:J:150:SER:OG	2.26	0.47
12:L:204:ASP:HB3	12:L:205:LEU:C	2.34	0.47
13:M:165:ILE:HG22	13:M:166:GLY:H	1.80	0.47
16:P:68:LYS:HD2	16:P:71:LEU:HD23	1.97	0.47
17:Q:85:ARG:O	17:Q:89:ALA:N	2.39	0.47
4:D:64:GLU:HG3	21:U:607:VAL:HG21	1.97	0.47
22:V:259:LEU:HD11	22:V:294:ARG:HD2	1.97	0.47
24:X:206:LEU:O	24:X:210:LEU:N	2.41	0.47
1:A:428:ARG:NH2	2:B:340:ALA:HB2	2.28	0.47
3:C:245:ILE:HG23	3:C:290:LYS:HB2	1.97	0.47
4:D:54:LEU:HA	4:D:57:GLN:HB2	1.97	0.47
5:E:119:VAL:HG21	6:F:147:PRO:HD2	1.97	0.47
9:I:122:THR:HG22	9:I:129:PRO:HB3	1.96	0.47
11:K:155:HIS:CG	11:K:168:ARG:HG2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:79:SER:HB2	11:K:140:ALA:H	1.80	0.47
15:O:66:HIS:HD2	15:O:78:THR:HG23	1.80	0.47
17:Q:29:LYS:HD2	18:R:122:SER:O	2.15	0.47
20:T:32:SER:HA	20:T:182:ARG:HG2	1.97	0.47
21:U:336:GLU:HA	21:U:339:LEU:HB3	1.96	0.47
22:V:363:LEU:HA	22:V:378:VAL:HG11	1.97	0.47
3:C:74:GLY:HA3	3:C:87:VAL:HG13	1.97	0.47
6:F:379:VAL:HG13	6:F:417:HIS:HD1	1.80	0.47
11:K:109:VAL:HB	11:K:147:ASP:HB3	1.97	0.47
14:N:103:TRP:HA	14:N:109:GLY:HA2	1.97	0.47
14:N:7:GLN:HA	14:N:12:VAL:HA	1.97	0.47
21:U:176:MET:HA	21:U:179:TYR:CE2	2.50	0.47
21:U:202:VAL:HG11	21:U:219:CYS:HB3	1.95	0.47
21:U:842:LYS:HB3	21:U:843:GLU:O	2.15	0.47
22:V:479:ARG:NH1	25:Y:370:ILE:HG21	2.29	0.47
3:C:86:LEU:HD21	3:C:94:LYS:HB3	1.97	0.47
4:D:95:ALA:HB2	4:D:124:LEU:HD21	1.97	0.47
9:I:99:LEU:HD11	16:P:66:ARG:HD3	1.96	0.47
21:U:510:GLU:HA	21:U:547:GLY:HA3	1.97	0.47
22:V:144:ASP:N	22:V:145:LEU:HA	2.29	0.47
22:V:56:ALA:O	22:V:59:ALA:HB3	2.15	0.47
25:Y:92:GLU:HA	25:Y:100:ILE:HD13	1.97	0.47
26:Z:109:ASN:ND2	26:Z:119:SER:O	2.43	0.47
26:Z:186:THR:HG23	26:Z:187:LEU:H	1.80	0.47
1:A:184:ILE:HD13	1:A:224:LEU:HD22	1.97	0.46
1:A:157:ILE:HG21	1:A:259:GLU:OE1	2.16	0.46
4:D:159:LYS:HD2	4:D:221:HIS:CE1	2.50	0.46
4:D:385:LEU:HD22	4:D:402:ALA:HB2	1.97	0.46
5:E:100:LEU:HD23	5:E:107:ILE:HG13	1.97	0.46
5:E:47:LEU:HA	5:E:50:LEU:HD12	1.96	0.46
6:F:438:TYR:CE2	11:K:20:ARG:HB3	2.43	0.46
15:O:7:VAL:HG22	15:O:12:ILE:HG12	1.97	0.46
16:P:99:ARG:NH1	16:P:99:ARG:O	2.42	0.46
18:R:59:LEU:HD22	18:R:83:LEU:HB2	1.96	0.46
21:U:653:ALA:HB2	21:U:675:MET:HE2	1.96	0.46
22:V:239:THR:HA	22:V:240:LEU:HA	1.68	0.46
23:W:16:MET:HG3	23:W:54:THR:HB	1.96	0.46
24:X:396:THR:HG23	25:Y:366:TYR:CD1	2.50	0.46
3:C:14:GLY:O	3:C:18:SER:N	2.25	0.46
4:D:377:SER:HB3	5:E:292:PRO:HB2	1.96	0.46
6:F:300:LYS:HE3	6:F:304:ARG:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:43:ARG:HG3	7:G:48:ALA:HB2	1.97	0.46
10:J:120:GLN:OE1	11:K:134:SER:N	2.48	0.46
12:L:49:LEU:HD21	12:L:199:LEU:HD21	1.97	0.46
7:G:88:ARG:HH12	13:M:156:VAL:HG13	1.81	0.46
15:O:177:VAL:N	15:O:184:ASP:O	2.48	0.46
16:P:27:ARG:HB2	16:P:183:MET:HB2	1.97	0.46
26:Z:96:HIS:HE1	26:Z:121:LEU:HD13	1.80	0.46
2:B:261:GLY:O	2:B:264:PRO:HD3	2.15	0.46
3:C:69:GLN:H	3:C:118:ASN:HD22	1.63	0.46
11:K:23:GLN:NE2	11:K:136:PRO:HD2	2.30	0.46
21:U:378:CYS:HB2	21:U:740:GLY:HA2	1.97	0.46
21:U:664:GLY:HA2	21:U:698:GLN:HE22	1.81	0.46
23:W:403:PHE:HB3	23:W:416:GLN:HG3	1.97	0.46
1:A:279:ALA:HB2	2:B:310:LEU:HD23	1.97	0.46
1:A:290:GLY:HA2	1:A:291:GLY:HA3	1.56	0.46
1:A:368:ILE:HG23	1:A:406:GLU:HB3	1.97	0.46
3:C:232:ARG:NE	3:C:275:GLU:OE1	2.42	0.46
5:E:232:MET:HB2	5:E:277:MET:HG2	1.97	0.46
7:G:119:ALA:HA	7:G:122:SER:HB2	1.97	0.46
7:G:96:TYR:O	7:G:100:ASN:ND2	2.46	0.46
9:I:105:ILE:HD12	9:I:106:PRO:HD2	1.98	0.46
12:L:109:VAL:HG21	12:L:145:PHE:HD2	1.80	0.46
16:P:135:ASP:N	16:P:135:ASP:OD1	2.48	0.46
18:R:9:ARG:NH2	18:R:146:ASP:OD2	2.47	0.46
21:U:378:CYS:SG	21:U:783:TYR:HD1	2.39	0.46
21:U:388:ASP:OD1	21:U:389:ASN:N	2.46	0.46
22:V:173:ILE:O	22:V:177:ASN:N	2.42	0.46
25:Y:356:THR:HA	25:Y:357:ASN:CG	2.35	0.46
1:A:160:THR:C	1:A:162:THR:H	2.19	0.46
2:B:239:VAL:HA	2:B:242:GLN:HG3	1.97	0.46
3:C:166:GLU:OE2	3:C:207:THR:OG1	2.33	0.46
4:D:322:LEU:HB3	4:D:330:LYS:HE2	1.97	0.46
4:D:376:ASN:HD21	33:D:501:ATP:H1'	1.80	0.46
7:G:116:LYS:HE3	8:H:84:ARG:HD2	1.97	0.46
9:I:164:ILE:HA	9:I:165:GLY:HA2	1.56	0.46
11:K:11:GLY:O	11:K:12:VAL:HG22	2.15	0.46
23:W:253:THR:HB	23:W:254:PRO:HD3	1.97	0.46
23:W:263:TRP:HH2	23:W:295:LYS:HG3	1.80	0.46
23:W:45:GLU:HA	23:W:96:GLN:HB3	1.98	0.46
25:Y:25:LEU:O	25:Y:29:PRO:HG2	2.16	0.46
25:Y:286:TRP:O	25:Y:287:LEU:HG	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:314:LEU:O	25:Y:354:VAL:N	2.48	0.46
25:Y:349:LYS:O	25:Y:350:VAL:HG22	2.16	0.46
25:Y:387:ILE:HA	25:Y:388:ASN:HA	1.54	0.46
4:D:153:MET:HB3	4:D:228:ILE:HD13	1.96	0.46
6:F:151:VAL:HG12	6:F:163:THR:HA	1.97	0.46
6:F:298:SER:HB2	6:F:299:GLU:HA	1.97	0.46
6:F:363:ALA:HB2	6:F:385:ALA:HB2	1.96	0.46
7:G:230:LEU:HD11	7:G:235:ILE:HG13	1.96	0.46
11:K:227:HIS:HA	11:K:228:MET:C	2.36	0.46
20:T:50:MET:N	20:T:113:GLY:O	2.49	0.46
21:U:735:GLY:O	21:U:739:ALA:N	2.48	0.46
2:B:155:LYS:HA	2:B:156:VAL:HA	1.62	0.46
2:B:182:GLU:HB2	2:B:239:VAL:HG21	1.96	0.46
3:C:251:ILE:HG23	3:C:262:GLY:HA2	1.97	0.46
4:D:49:GLN:O	4:D:53:PHE:N	2.40	0.46
11:K:79:SER:H	11:K:139:VAL:HG23	1.81	0.46
11:K:67:ILE:HG12	11:K:218:ALA:HB2	1.97	0.46
23:W:436:MET:HA	23:W:439:VAL:HG22	1.97	0.46
24:X:396:THR:HG21	25:Y:365:GLN:HB3	1.98	0.46
25:Y:89:GLU:HA	25:Y:92:GLU:HG2	1.97	0.46
26:Z:34:ARG:HH12	26:Z:102:HIS:CE1	2.34	0.46
1:A:387:SER:HA	1:A:390:THR:HB	1.97	0.46
2:B:428:TYR:HA	2:B:431:GLN:HB2	1.98	0.46
6:F:145:LEU:HG	6:F:146:LYS:H	1.81	0.46
6:F:221:LYS:HA	6:F:327:LYS:HG3	1.97	0.46
9:I:95:GLN:HE22	9:I:98:LEU:HD23	1.80	0.46
10:J:9:VAL:HG22	11:K:23:GLN:HE21	1.81	0.46
11:K:23:GLN:NE2	11:K:135:ARG:HB2	2.30	0.46
11:K:50:VAL:HG22	11:K:51:GLU:H	1.81	0.46
12:L:186:GLU:HA	12:L:189:LYS:HE3	1.97	0.46
23:W:135:LYS:CB	23:W:136:ILE:HB	2.46	0.46
26:Z:187:LEU:O	26:Z:191:ILE:HD12	2.16	0.46
2:B:409:GLU:OE1	2:B:413:LYS:HB3	2.16	0.46
6:F:436:GLN:C	6:F:438:TYR:H	2.19	0.46
7:G:139:ILE:HG13	7:G:153:LYS:HG3	1.97	0.46
9:I:167:ASN:O	9:I:168:SER:HB3	2.16	0.46
19:S:171:ALA:HA	19:S:174:LEU:HD12	1.98	0.46
21:U:328:ILE:HG13	21:U:329:LEU:N	2.31	0.46
21:U:586:VAL:HG11	21:U:601:ARG:HH12	1.81	0.46
21:U:764:LEU:O	21:U:767:THR:OG1	2.26	0.46
21:U:813:TYR:OH	21:U:883:ARG:NH1	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:326:MET:O	23:W:330:LYS:N	2.48	0.46
1:A:322:ASN:OD1	1:A:428:ARG:NH1	2.46	0.46
7:G:50:ILE:O	7:G:218:GLY:N	2.49	0.46
21:U:469:SER:OG	21:U:472:ILE:HG13	2.16	0.46
21:U:20:LYS:HD2	21:U:48:LEU:HD11	1.98	0.46
23:W:155:GLN:NE2	23:W:161:GLU:HG3	2.31	0.46
25:Y:203:ASP:N	25:Y:203:ASP:OD1	2.46	0.46
1:A:427:PRO:HB2	1:A:429:TYR:CD2	2.50	0.45
3:C:77:VAL:HG22	3:C:86:LEU:HD22	1.97	0.45
7:G:103:TYR:HE1	14:N:57:ASP:HB3	1.81	0.45
7:G:210:PHE:HE1	7:G:214:GLU:HB2	1.81	0.45
7:G:67:THR:HG22	7:G:69:LEU:H	1.81	0.45
10:J:76:LEU:HD13	10:J:78:ALA:HB3	1.98	0.45
18:R:143:TYR:HA	18:R:155:LEU:HD21	1.98	0.45
18:R:11:GLY:HA3	18:R:179:VAL:O	2.15	0.45
25:Y:170:GLU:CG	25:Y:171:GLY:HA3	2.44	0.45
22:V:282:ASN:OD1	25:Y:382:LYS:HG3	2.16	0.45
1:A:206:ILE:HG12	6:F:401:VAL:HA	1.99	0.45
1:A:398:ARG:NH2	2:B:195:GLN:HB2	2.31	0.45
2:B:194:ILE:O	2:B:237:LYS:NZ	2.35	0.45
6:F:128:THR:HG23	6:F:130:GLN:H	1.81	0.45
5:E:281:ARG:NH1	6:F:294:LYS:O	2.45	0.45
14:N:40:ARG:NH1	14:N:180:ALA:O	2.48	0.45
16:P:141:THR:HG21	16:P:180:VAL:HG11	1.98	0.45
20:T:187:PHE:CE2	20:T:205:THR:HG23	2.51	0.45
21:U:337:LEU:HD12	21:U:338:HIS:N	2.30	0.45
21:U:485:ALA:HB3	21:U:519:VAL:HG12	1.97	0.45
21:U:794:ASP:OD1	21:U:795:LEU:N	2.49	0.45
22:V:153:LYS:O	22:V:157:THR:OG1	2.28	0.45
23:W:275:ILE:O	23:W:357:ARG:NE	2.49	0.45
2:B:201:VAL:HB	2:B:241:ASN:HD21	1.82	0.45
2:B:300:GLY:HA3	2:B:301:GLY:HA2	1.70	0.45
1:A:420:TYR:CE1	2:B:350:LYS:HG2	2.51	0.45
2:B:415:THR:HB	2:B:418:ASP:HB3	1.98	0.45
4:D:276:ASP:O	4:D:280:GLY:N	2.49	0.45
13:M:171:ALA:HB3	13:M:200:VAL:HG21	1.99	0.45
9:I:101:TYR:HD1	17:Q:79:ALA:HB1	1.81	0.45
21:U:16:GLU:OE1	21:U:18:GLN:HG2	2.15	0.45
21:U:550:VAL:O	21:U:554:LEU:N	2.49	0.45
22:V:99:ARG:NH2	22:V:147:PHE:H	2.08	0.45
25:Y:48:ASN:O	25:Y:114:ILE:HG13	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:HD23	1:A:319:MET:N	2.31	0.45
1:A:409:PHE:O	1:A:413:VAL:HG23	2.16	0.45
2:B:254:GLU:HB2	2:B:288:ASP:HB2	1.99	0.45
2:B:324:ASP:HB2	2:B:326:LYS:HG2	1.98	0.45
4:D:401:LYS:HA	4:D:404:LYS:HE2	1.97	0.45
12:L:193:ARG:HA	12:L:196:ARG:HD2	1.99	0.45
22:V:290:TYR:OH	22:V:294:ARG:NH2	2.49	0.45
22:V:80:LYS:HB3	22:V:81:GLN:C	2.37	0.45
23:W:431:LYS:HA	23:W:435:LEU:HD13	1.97	0.45
1:A:160:THR:O	1:A:162:THR:N	2.49	0.45
1:A:292:ASP:OD1	2:B:303:ARG:NH1	2.49	0.45
4:D:279:THR:O	4:D:283:ARG:N	2.47	0.45
4:D:315:ASP:N	4:D:315:ASP:OD1	2.50	0.45
10:J:7:ILE:HG22	10:J:8:THR:HG23	1.98	0.45
11:K:73:HIS:CE1	11:K:108:THR:HG22	2.51	0.45
17:Q:42:ILE:HA	17:Q:106:GLY:HA2	1.97	0.45
21:U:106:ASP:HA	21:U:109:THR:HG22	1.98	0.45
21:U:173:VAL:N	21:U:174:PRO:HD3	2.32	0.45
23:W:142:ARG:NH2	23:W:178:GLU:HB2	2.30	0.45
23:W:259:GLU:HB3	23:W:263:TRP:HB2	1.99	0.45
1:A:310:ASP:HA	1:A:311:PRO:HA	1.58	0.45
2:B:96:ARG:HH22	3:C:84:LYS:HG3	1.82	0.45
5:E:230:ILE:HB	5:E:275:MET:HA	1.98	0.45
9:I:148:TYR:HA	9:I:158:GLY:HA2	1.98	0.45
14:N:132:SER:HA	14:N:135:ILE:HG12	1.99	0.45
21:U:14:GLU:O	21:U:20:LYS:NZ	2.37	0.45
21:U:804:SER:HB3	21:U:839:ALA:HB3	1.99	0.45
22:V:137:GLU:HA	22:V:140:ASP:HB2	1.97	0.45
22:V:318:GLN:O	22:V:319:HIS:ND1	2.50	0.45
23:W:13:ILE:HG22	23:W:54:THR:HG21	1.99	0.45
25:Y:110:TYR:O	25:Y:113:ARG:HB3	2.16	0.45
25:Y:78:GLU:HA	25:Y:81:LEU:HB3	1.99	0.45
5:E:236:ASP:N	5:E:236:ASP:OD1	2.50	0.45
13:M:110:HIS:NE2	14:N:70:LEU:HA	2.31	0.45
17:Q:25:ILE:HG13	17:Q:26:VAL:H	1.80	0.45
21:U:340:GLN:HG3	21:U:880:ASN:HB3	1.99	0.45
23:W:327:GLU:HA	23:W:330:LYS:HB3	1.98	0.45
9:I:3:ARG:HH11	11:K:11:GLY:H	1.65	0.45
13:M:110:HIS:HE1	14:N:69:GLU:HG2	1.82	0.45
16:P:54:ALA:HB3	16:P:106:GLU:HB2	1.98	0.45
20:T:111:VAL:HG13	20:T:137:LEU:HD12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:377:HIS:O	21:U:380:THR:HG22	2.17	0.45
21:U:500:ASN:HA	21:U:503:GLN:HG2	1.99	0.45
23:W:23:THR:HA	23:W:26:GLN:HB2	1.99	0.45
23:W:88:MET:SD	23:W:96:GLN:NE2	2.90	0.45
1:A:105:ASP:N	1:A:105:ASP:OD1	2.50	0.45
3:C:117:ARG:O	3:C:121:TYR:HA	2.17	0.45
6:F:228:PRO:O	6:F:231:THR:HG23	2.16	0.45
6:F:283:ILE:HG22	6:F:328:VAL:HG13	1.98	0.45
6:F:288:LEU:HD12	6:F:291:ILE:HD11	1.98	0.45
1:A:206:ILE:HA	6:F:373:MET:SD	2.57	0.45
7:G:43:ARG:HA	7:G:48:ALA:HA	1.99	0.45
8:H:153:GLY:O	9:I:81:SER:OG	2.30	0.45
9:I:45:LEU:HD11	9:I:137:ILE:HG12	1.98	0.45
13:M:40:ARG:HH11	13:M:148:LEU:HB3	1.82	0.45
21:U:54:PHE:CZ	21:U:56:SER:HB2	2.52	0.45
21:U:751:ARG:HG3	21:U:908:ILE:HG21	1.97	0.45
24:X:200:ILE:HG22	24:X:201:TYR:H	1.81	0.45
24:X:244:SER:O	24:X:248:ILE:N	2.45	0.45
25:Y:251:HIS:HA	25:Y:257:ARG:HD3	1.97	0.45
1:A:315:ILE:HG13	1:A:315:ILE:H	1.55	0.45
4:D:130:VAL:HA	4:D:142:VAL:HA	1.99	0.45
6:F:85:THR:HA	6:F:86:LEU:HA	1.59	0.45
12:L:160:SER:OG	12:L:165:SER:HB3	2.17	0.45
9:I:95:GLN:HG2	16:P:73:LEU:HG	1.98	0.45
18:R:8:PHE:HE2	18:R:13:ILE:HG12	1.82	0.45
19:S:57:PHE:HD2	19:S:60:ASP:H	1.65	0.45
11:K:111:SER:HB3	19:S:79:ASN:OD1	2.17	0.45
22:V:32:PRO:O	22:V:36:GLU:HB3	2.17	0.45
22:V:455:LYS:HD2	22:V:457:TYR:CE2	2.52	0.45
26:Z:68:TRP:HH2	26:Z:111:LEU:HD22	1.81	0.45
1:A:419:SER:HA	1:A:422:LYS:HE3	1.99	0.44
1:A:250:VAL:O	6:F:259:MET:N	2.50	0.44
7:G:47:CYS:HB3	7:G:221:THR:HG23	1.99	0.44
10:J:9:VAL:HG22	11:K:23:GLN:NE2	2.32	0.44
13:M:236:GLU:O	13:M:240:LYS:NZ	2.45	0.44
14:N:99:ILE:HG23	14:N:113:SER:HA	2.00	0.44
15:O:50:ALA:HB2	16:P:129:CYS:HB2	1.99	0.44
22:V:280:ALA:HB1	22:V:281:ASN:ND2	2.32	0.44
24:X:289:CYS:O	24:X:293:ALA:N	2.49	0.44
25:Y:215:ASP:O	25:Y:218:THR:OG1	2.27	0.44
24:X:417:LYS:HG2	26:Z:283:ARG:NH1	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:392:GLY:O	2:B:395:ILE:HG22	2.16	0.44
3:C:257:SER:O	3:C:258:ARG:HB2	2.17	0.44
3:C:41:ASN:HD21	22:V:495:ARG:HA	1.81	0.44
3:C:49:ARG:O	3:C:53:ASN:N	2.47	0.44
4:D:105:SER:HB3	4:D:111:TYR:CE2	2.53	0.44
4:D:406:VAL:HA	4:D:407:ILE:HA	1.51	0.44
6:F:430:LYS:O	6:F:431:LYS:HG3	2.17	0.44
11:K:199:LEU:HD13	11:K:241:ILE:HD12	1.99	0.44
18:R:41:LEU:HD23	18:R:103:GLY:HA3	1.98	0.44
23:W:55:ARG:NH1	23:W:78:LYS:HG3	2.32	0.44
24:X:258:LYS:HD2	24:X:294:SER:OG	2.18	0.44
3:C:235:PHE:HD1	3:C:276:LEU:HG	1.83	0.44
15:O:33:LYS:O	15:O:45:GLY:N	2.42	0.44
16:P:101:GLY:O	17:Q:93:ARG:NH1	2.50	0.44
18:R:97:MET:H	18:R:116:SER:HB3	1.81	0.44
19:S:211:ARG:NE	19:S:213:ASP:O	2.51	0.44
21:U:561:GLU:HG2	21:U:562:GLU:H	1.82	0.44
21:U:773:PHE:HD1	21:U:773:PHE:HA	1.69	0.44
22:V:156:SER:HB2	22:V:160:LEU:HD12	1.99	0.44
22:V:275:VAL:HB	22:V:277:PRO:HD3	1.98	0.44
23:W:120:ILE:O	23:W:124:LEU:N	2.45	0.44
24:X:187:ARG:O	24:X:191:THR:N	2.45	0.44
1:A:328:ASP:HB3	1:A:329:PRO:HD3	1.98	0.44
3:C:154:LEU:O	3:C:157:GLN:N	2.51	0.44
7:G:139:ILE:HG12	7:G:153:LYS:NZ	2.33	0.44
12:L:31:GLN:O	12:L:51:ARG:NH1	2.49	0.44
14:N:73:PRO:HB3	14:N:105:PRO:HG2	2.00	0.44
20:T:136:SER:HB2	20:T:150:LEU:HD13	1.99	0.44
20:T:89:HIS:CE1	20:T:131:ALA:HB1	2.52	0.44
1:A:395:PHE:HA	1:A:398:ARG:HB2	1.99	0.44
3:C:167:LEU:HD22	3:C:175:PHE:CZ	2.52	0.44
4:D:96:VAL:HG23	4:D:97:ASP:OD1	2.18	0.44
5:E:349:GLU:HG2	5:E:374:VAL:HG21	2.00	0.44
6:F:81:LYS:O	6:F:85:THR:HG22	2.18	0.44
7:G:184:LYS:NZ	8:H:55:ILE:O	2.38	0.44
11:K:41:GLN:NE2	11:K:152:GLN:HA	2.32	0.44
11:K:10:ARG:NH1	12:L:21:GLN:HE22	2.14	0.44
17:Q:114:ALA:HB1	17:Q:126:LYS:HE2	1.99	0.44
18:R:19:ARG:NE	18:R:29:GLN:HE22	2.11	0.44
1:A:261:PHE:O	1:A:265:ARG:HG3	2.18	0.44
1:A:375:ARG:HH12	11:K:205:VAL:HB	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:VAL:HG23	2:B:174:MET:H	1.83	0.44
4:D:412:GLN:NE2	4:D:415:GLU:H	2.16	0.44
6:F:125:LYS:HD2	6:F:131:THR:HG23	2.00	0.44
6:F:91:SER:OG	6:F:125:LYS:O	2.20	0.44
5:E:281:ARG:NH2	6:F:296:PHE:HA	2.32	0.44
7:G:141:ILE:HD13	7:G:220:VAL:HG11	1.99	0.44
10:J:96:LEU:HA	17:Q:62:LYS:HG2	1.99	0.44
21:U:446:LEU:O	21:U:450:HIS:ND1	2.34	0.44
21:U:470:ASN:OD1	21:U:471:ASP:HA	2.18	0.44
21:U:669:ILE:HG12	21:U:694:ILE:HG21	2.00	0.44
23:W:247:TYR:HA	23:W:250:ILE:HG23	1.99	0.44
25:Y:301:ILE:O	25:Y:305:SER:N	2.44	0.44
3:C:25:LEU:HD23	4:D:47:LEU:HB2	2.00	0.44
3:C:368:MET:HA	3:C:371:LEU:HB3	1.99	0.44
4:D:213:THR:OG1	33:D:501:ATP:O2A	2.26	0.44
5:E:129:ASN:H	5:E:190:GLN:HG2	1.82	0.44
5:E:76:GLY:N	5:E:77:PRO:HD2	2.32	0.44
6:F:268:VAL:HA	6:F:271:ALA:HB3	1.99	0.44
6:F:344:ARG:HB3	6:F:347:ARG:HB2	1.99	0.44
10:J:100:ASP:OD1	10:J:100:ASP:N	2.50	0.44
12:L:160:SER:O	12:L:169:ARG:NH2	2.51	0.44
21:U:242:LEU:HD13	21:U:324:LYS:HD2	1.99	0.44
23:W:403:PHE:HD2	23:W:416:GLN:HA	1.83	0.44
23:W:398:VAL:HA	24:X:341:PRO:HB3	1.98	0.44
2:B:182:GLU:HB2	2:B:239:VAL:HG11	2.00	0.44
2:B:364:ILE:HG23	2:B:368:HIS:CE1	2.52	0.44
4:D:207:PRO:HG2	4:D:312:ASN:HA	1.99	0.44
6:F:189:GLY:HA3	6:F:364:ARG:HB3	2.00	0.44
6:F:356:MET:HG2	6:F:390:ASP:HA	1.99	0.44
7:G:152:TYR:CD1	7:G:162:GLY:HA3	2.52	0.44
7:G:24:GLN:OE1	13:M:14:PHE:N	2.49	0.44
12:L:20:HIS:HB3	12:L:24:TYR:CZ	2.53	0.44
12:L:120:THR:O	13:M:129:ARG:NH1	2.51	0.44
17:Q:178:PHE:HB2	17:Q:194:ILE:HB	1.99	0.44
21:U:465:LEU:HA	21:U:473:VAL:HG11	1.99	0.44
21:U:563:ALA:O	21:U:567:ILE:HG12	2.18	0.44
1:A:363:SER:HB2	1:A:403:ILE:HG22	1.99	0.44
5:E:57:VAL:HG12	5:E:111:LEU:HD21	2.00	0.44
5:E:222:ALA:HB1	5:E:228:CYS:SG	2.58	0.44
5:E:374:VAL:O	5:E:378:LYS:HG2	2.18	0.44
12:L:196:ARG:HB2	12:L:239:ARG:HH21	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:108:ASP:OD2	17:Q:111:GLU:N	2.49	0.44
18:R:81:LYS:HD3	18:R:120:ARG:HD2	1.99	0.44
21:U:107:HIS:HA	21:U:110:LYS:HE3	2.00	0.44
21:U:428:PRO:HD2	21:U:464:GLN:NE2	2.32	0.44
22:V:323:GLY:HA2	22:V:326:GLN:HB2	1.99	0.44
23:W:343:SER:HB2	23:W:346:GLU:HB3	2.00	0.44
25:Y:311:TYR:HD2	25:Y:314:LEU:HD12	1.83	0.44
26:Z:205:LEU:HA	26:Z:208:ILE:HG22	1.99	0.44
3:C:285:ALA:HA	3:C:286:THR:HA	1.78	0.43
5:E:128:GLY:HA2	5:E:129:ASN:HB2	2.00	0.43
7:G:212:PRO:O	7:G:215:ILE:HG13	2.18	0.43
9:I:240:HIS:O	9:I:244:GLU:N	2.33	0.43
15:O:98:LEU:HB2	15:O:113:ILE:HB	2.00	0.43
21:U:161:ASP:OD1	21:U:162:VAL:N	2.47	0.43
21:U:26:LYS:O	21:U:30:VAL:HG22	2.18	0.43
21:U:327:LYS:HB2	21:U:333:MET:HE2	1.99	0.43
22:V:174:PHE:HA	22:V:177:ASN:HB2	2.00	0.43
22:V:419:LEU:HD23	22:V:458:VAL:HG23	1.99	0.43
22:V:486:ILE:HG12	25:Y:381:GLN:HE21	1.83	0.43
23:W:306:LEU:O	23:W:310:THR:HG22	2.17	0.43
23:W:409:LEU:HD23	24:X:384:VAL:HG21	2.00	0.43
25:Y:357:ASN:OD1	25:Y:358:ARG:N	2.51	0.43
25:Y:387:ILE:HD13	26:Z:283:ARG:HD3	2.00	0.43
26:Z:199:LYS:HA	26:Z:202:ASN:HD21	1.83	0.43
1:A:115:VAL:HG13	1:A:117:GLN:H	1.82	0.43
1:A:250:VAL:HG11	1:A:297:ARG:NH2	2.34	0.43
3:C:192:PRO:HA	3:C:193:GLY:HA3	1.68	0.43
5:E:149:ILE:O	5:E:152:PRO:HD2	2.17	0.43
17:Q:152:SER:HB3	17:Q:155:ARG:HB2	1.99	0.43
21:U:772:TRP:CD1	21:U:774:PRO:HD2	2.53	0.43
23:W:124:LEU:O	23:W:128:LEU:HG	2.19	0.43
26:Z:250:TYR:O	26:Z:254:ASN:HB2	2.18	0.43
2:B:319:PHE:HA	2:B:320:ASP:HA	1.49	0.43
2:B:313:LEU:HD13	2:B:341:LEU:HD22	2.01	0.43
4:D:147:ALA:O	5:E:62:LYS:HD2	2.18	0.43
4:D:388:ARG:HH12	5:E:143:ARG:HG2	1.83	0.43
4:D:83:GLN:HG3	4:D:133:HIS:CD2	2.54	0.43
5:E:112:PRO:O	5:E:113:ARG:HG3	2.18	0.43
11:K:116:VAL:HA	11:K:119:LEU:HG	2.00	0.43
16:P:53:LEU:HD13	16:P:60:VAL:HA	2.00	0.43
21:U:181:LEU:HB3	21:U:218:GLN:NE2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:374:SER:HB2	21:U:410:VAL:HG11	2.00	0.43
22:V:99:ARG:NH1	22:V:150:ARG:HH21	2.16	0.43
22:V:182:LYS:NZ	22:V:210:CYS:HB2	2.33	0.43
22:V:215:ALA:HB1	22:V:256:ARG:NH2	2.34	0.43
22:V:480:ILE:HG22	22:V:484:LEU:HD23	2.00	0.43
22:V:89:LYS:HD3	22:V:92:ARG:HH11	1.82	0.43
23:W:370:TYR:OH	23:W:373:ILE:HD12	2.18	0.43
23:W:444:HIS:HD2	23:W:448:LYS:NZ	2.16	0.43
24:X:354:ILE:HG21	24:X:361:VAL:HG11	2.00	0.43
1:A:139:ARG:HG3	1:A:156:LYS:HG3	2.01	0.43
3:C:215:SER:HB3	3:C:216:GLY:HA2	2.01	0.43
3:C:73:VAL:HB	4:D:110:ASN:HB2	1.99	0.43
3:C:76:VAL:O	3:C:111:ASN:N	2.44	0.43
4:D:82:ILE:HA	4:D:83:GLN:HA	1.64	0.43
5:E:171:LEU:N	5:E:297:ARG:O	2.49	0.43
6:F:421:MET:HA	6:F:424:ILE:HB	1.99	0.43
4:D:413:GLU:HG2	7:G:157:ALA:HB2	2.01	0.43
10:J:152:THR:HG22	11:K:82:ILE:HB	2.00	0.43
16:P:159:ASP:OD1	16:P:159:ASP:N	2.52	0.43
21:U:338:HIS:CE1	21:U:787:CYS:HB3	2.54	0.43
23:W:445:LEU:HA	23:W:448:LYS:HZ3	1.83	0.43
25:Y:301:ILE:HA	25:Y:304:TYR:HB2	1.99	0.43
25:Y:50:MET:SD	25:Y:74:LYS:HB3	2.58	0.43
1:A:183:GLN:HG2	1:A:344:SER:OG	2.19	0.43
2:B:107:MET:HB2	2:B:153:ASN:HA	1.99	0.43
3:C:72:TYR:N	3:C:116:LEU:O	2.50	0.43
5:E:155:ASN:HB3	5:E:158:LEU:HG	1.99	0.43
5:E:168:LYS:O	5:E:275:MET:HG2	2.17	0.43
6:F:188:ILE:HG22	33:F:501:ATP:H2	1.83	0.43
11:K:225:ASN:HB2	11:K:226:PHE:CD1	2.53	0.43
15:O:6:VAL:HG11	15:O:154:LEU:HD23	1.99	0.43
3:C:15:LYS:HZ1	21:U:149:GLN:HG2	1.83	0.43
22:V:414:TYR:OH	25:Y:331:ASP:O	2.37	0.43
1:A:100:LYS:HB3	1:A:115:VAL:HG23	2.01	0.43
1:A:97:ARG:HA	1:A:98:CYS:HA	1.52	0.43
2:B:139:VAL:HB	2:B:141:LYS:N	2.34	0.43
2:B:285:ASP:OD2	2:B:286:GLU:HG2	2.18	0.43
3:C:25:LEU:O	3:C:29:GLU:N	2.43	0.43
5:E:169:GLY:O	5:E:296:ASP:HB2	2.18	0.43
6:F:204:LEU:HB2	6:F:212:PHE:HZ	1.84	0.43
6:F:364:ARG:O	6:F:368:ILE:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:54:SER:N	20:T:109:THR:O	2.50	0.43
24:X:378:LEU:HG	24:X:385:LEU:HD13	2.01	0.43
25:Y:112:CYS:SG	25:Y:120:ALA:HB2	2.58	0.43
26:Z:26:ILE:HA	26:Z:29:VAL:HG12	1.99	0.43
1:A:206:ILE:HG13	1:A:207:GLU:H	1.84	0.43
3:C:161:ILE:HD13	3:C:186:VAL:HG21	2.00	0.43
4:D:218:ALA:HA	4:D:221:HIS:HD2	1.84	0.43
5:E:214:LEU:HA	5:E:217:GLU:HB3	2.00	0.43
5:E:383:LYS:HG3	5:E:384:LEU:HD12	2.00	0.43
5:E:58:GLY:N	5:E:98:VAL:O	2.41	0.43
7:G:123:GLN:HE21	7:G:158:GLY:HA3	1.82	0.43
9:I:4:ARG:NH2	13:M:9:LEU:HD13	2.33	0.43
10:J:173:GLU:HA	10:J:176:TYR:HD2	1.84	0.43
10:J:177:THR:OG1	10:J:178:ASP:N	2.52	0.43
11:K:74:ILE:HG23	11:K:144:GLY:O	2.19	0.43
13:M:40:ARG:HA	13:M:45:VAL:HA	1.99	0.43
20:T:124:TYR:CE2	20:T:126:ASP:HB2	2.54	0.43
21:U:413:LYS:NZ	21:U:448:LEU:O	2.51	0.43
22:V:221:LEU:HD12	22:V:222:ASP:H	1.82	0.43
23:W:221:LYS:HG3	23:W:224:LEU:HB2	2.01	0.43
23:W:3:ASP:OD1	23:W:4:GLY:N	2.52	0.43
1:A:271:LEU:HA	1:A:315:ILE:HD13	2.00	0.43
2:B:409:GLU:CD	2:B:413:LYS:HB3	2.39	0.43
5:E:182:LEU:HD11	33:E:401:ATP:H2'	1.99	0.43
6:F:120:LYS:HG2	6:F:136:VAL:HG21	2.00	0.43
9:I:98:LEU:HD12	9:I:102:GLN:HA	1.99	0.43
10:J:43:LEU:HD23	10:J:134:VAL:HG11	2.01	0.43
18:R:100:MET:HG2	18:R:113:TYR:HD1	1.84	0.43
22:V:167:LEU:HD11	22:V:171:VAL:HB	2.00	0.43
22:V:357:LEU:O	22:V:361:PHE:N	2.52	0.43
23:W:183:VAL:HA	23:W:186:ILE:HG22	2.00	0.43
23:W:55:ARG:O	23:W:58:SER:OG	2.31	0.43
25:Y:286:TRP:CD1	25:Y:287:LEU:HD23	2.53	0.43
3:C:154:LEU:O	3:C:158:ILE:HG23	2.19	0.43
5:E:55:GLN:HB3	5:E:100:LEU:O	2.19	0.43
5:E:306:GLU:C	5:E:308:ALA:H	2.22	0.43
9:I:8:ARG:HD3	10:J:7:ILE:HD11	2.01	0.43
10:J:180:ALA:HA	10:J:181:ILE:HA	1.68	0.43
10:J:34:GLY:HA2	10:J:43:LEU:HA	2.01	0.43
11:K:209:LYS:O	11:K:214:ASN:ND2	2.51	0.43
17:Q:103:LEU:HD23	17:Q:117:TYR:HD1	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:150:ASP:HB3	19:S:156:LYS:HD2	2.01	0.43
21:U:457:ILE:HG23	21:U:460:TYR:HB3	1.99	0.43
22:V:94:VAL:HG11	22:V:134:PHE:HB3	2.01	0.43
25:Y:104:MET:O	25:Y:108:ALA:HB3	2.19	0.43
25:Y:108:ALA:HA	25:Y:111:LEU:HG	2.00	0.43
1:A:237:PHE:HB2	1:A:271:LEU:HB2	2.01	0.43
3:C:170:LYS:C	3:C:172:PRO:HD3	2.40	0.43
3:C:215:SER:HB3	3:C:216:GLY:CA	2.49	0.43
3:C:285:ALA:HB1	3:C:286:THR:HB	2.00	0.43
4:D:53:PHE:O	4:D:57:GLN:HG2	2.19	0.43
5:E:240:GLY:HA2	6:F:299:GLU:HB2	2.01	0.43
24:X:245:PRO:HA	24:X:248:ILE:HG22	2.00	0.43
22:V:409:MET:HG3	25:Y:339:ALA:HB2	2.01	0.43
3:C:217:SER:N	3:C:218:GLU:HB3	2.34	0.42
4:D:325:GLY:N	4:D:328:ASP:OD1	2.52	0.42
5:E:205:ASP:OD2	5:E:211:SER:N	2.50	0.42
7:G:58:ASP:OD1	7:G:59:LYS:N	2.52	0.42
11:K:169:ALA:HB3	11:K:178:GLN:HG2	2.01	0.42
12:L:215:VAL:HB	12:L:221:PHE:CD1	2.52	0.42
13:M:120:HIS:NE2	13:M:124:LEU:HD21	2.34	0.42
15:O:45:GLY:HA2	15:O:98:LEU:HD22	2.00	0.42
21:U:699:THR:O	21:U:702:THR:OG1	2.30	0.42
23:W:49:SER:O	23:W:53:GLN:N	2.51	0.42
26:Z:121:LEU:HG	26:Z:138:TYR:HB2	2.01	0.42
26:Z:237:LEU:HB2	26:Z:239:ASP:OD1	2.19	0.42
26:Z:241:SER:HA	26:Z:242:LEU:HA	1.40	0.42
1:A:173:THR:HA	1:A:230:ALA:HB3	2.01	0.42
2:B:277:HIS:HB3	2:B:279:PRO:HD2	2.00	0.42
2:B:338:ASP:N	2:B:341:LEU:HG	2.34	0.42
4:D:392:TYR:CD2	4:D:393:ILE:HG13	2.53	0.42
5:E:141:GLN:HB3	5:E:183:LEU:HD11	2.02	0.42
5:E:254:GLN:O	5:E:258:MET:HG2	2.19	0.42
6:F:428:GLN:CG	6:F:429:ALA:HA	2.49	0.42
10:J:88:ARG:HB3	17:Q:66:LEU:HD11	2.01	0.42
13:M:230:ASP:N	13:M:230:ASP:OD1	2.52	0.42
21:U:470:ASN:HA	21:U:471:ASP:HA	1.84	0.42
23:W:86:ASN:HD22	23:W:88:MET:HG3	1.83	0.42
24:X:212:MET:SD	24:X:239:TYR:OH	2.75	0.42
26:Z:287:LYS:HE3	26:Z:287:LYS:HB2	1.79	0.42
2:B:120:HIS:ND1	2:B:134:SER:OG	2.52	0.42
5:E:126:ASP:OD2	5:E:185:ARG:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:78:ALA:HA	10:J:81:ARG:HH12	1.85	0.42
12:L:66:VAL:HG11	12:L:88:MET:HG3	2.01	0.42
14:N:44:CYS:SG	14:N:99:ILE:HB	2.59	0.42
15:O:8:TYR:CE2	15:O:13:VAL:HG23	2.51	0.42
22:V:350:GLN:O	22:V:354:LYS:N	2.53	0.42
22:V:394:LEU:O	22:V:398:LEU:N	2.50	0.42
25:Y:184:GLN:O	25:Y:188:CYS:N	2.45	0.42
25:Y:63:TRP:HB3	25:Y:64:GLN:C	2.40	0.42
1:A:291:GLY:O	1:A:294:GLU:HG2	2.19	0.42
2:B:320:ASP:N	2:B:320:ASP:OD1	2.52	0.42
2:B:360:THR:O	2:B:364:ILE:N	2.52	0.42
3:C:259:LEU:H	3:C:259:LEU:HD13	1.85	0.42
5:E:54:GLY:H	6:F:158:TYR:HD2	1.67	0.42
6:F:144:LYS:HA	6:F:145:LEU:HA	1.71	0.42
13:M:45:VAL:HG11	13:M:138:GLY:HA3	2.01	0.42
16:P:107:PRO:HG2	16:P:124:LEU:HB2	2.01	0.42
19:S:64:LEU:HD21	19:S:92:LEU:HD11	2.00	0.42
21:U:607:VAL:O	21:U:615:ARG:NH1	2.52	0.42
21:U:713:TYR:HB2	21:U:734:GLN:HE21	1.83	0.42
21:U:780:SER:HA	21:U:783:TYR:CD2	2.54	0.42
23:W:451:MET:HE1	26:Z:157:HIS:H	1.84	0.42
25:Y:105:MET:HB3	25:Y:127:THR:HG21	2.01	0.42
2:B:283:PHE:CE2	2:B:285:ASP:HB2	2.55	0.42
2:B:294:ARG:HG2	2:B:295:TYR:H	1.85	0.42
2:B:227:PRO:HD3	2:B:332:ASN:O	2.19	0.42
2:B:343:ARG:HB2	2:B:344:PRO:HD3	2.02	0.42
3:C:220:VAL:O	3:C:224:ILE:HB	2.19	0.42
5:E:113:ARG:HB3	5:E:221:TYR:OH	2.19	0.42
13:M:51:LYS:HB3	13:M:210:GLU:HB3	2.00	0.42
19:S:22:ILE:HG23	19:S:197:ILE:HG13	2.00	0.42
22:V:127:THR:HA	22:V:131:LEU:HG	2.01	0.42
1:A:375:ARG:HH22	11:K:205:VAL:C	2.22	0.42
1:A:385:ILE:HA	1:A:388:VAL:HG23	2.00	0.42
5:E:180:LYS:HG3	5:E:181:THR:N	2.34	0.42
5:E:313:LEU:HD21	5:E:328:TYR:CD2	2.54	0.42
8:H:83:TYR:HB2	8:H:132:VAL:HG21	2.01	0.42
8:H:66:GLU:HG3	8:H:91:ARG:NH2	2.33	0.42
11:K:17:PRO:HA	12:L:24:TYR:CZ	2.55	0.42
16:P:25:ASP:HA	16:P:185:VAL:HA	2.00	0.42
16:P:44:PRO:HA	16:P:50:TYR:HD1	1.85	0.42
17:Q:13:VAL:HG11	17:Q:105:ALA:HB1	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:529:ILE:HA	21:U:532:MET:HE3	2.02	0.42
22:V:232:HIS:HA	22:V:235:LEU:HB3	2.02	0.42
22:V:25:GLU:O	22:V:28:PRO:HD2	2.19	0.42
23:W:66:ILE:HG23	23:W:67:LEU:HB2	2.01	0.42
24:X:356:LEU:HD11	24:X:360:ASP:OD1	2.19	0.42
2:B:153:ASN:HD21	2:B:160:ILE:HB	1.85	0.42
2:B:387:LYS:HD2	2:B:430:LYS:HZ2	1.84	0.42
3:C:235:PHE:CD1	3:C:275:GLU:HG3	2.55	0.42
4:D:228:ILE:HB	4:D:262:ILE:HG12	2.01	0.42
8:H:10:LEU:HD23	8:H:126:GLY:H	1.84	0.42
16:P:189:ILE:HG23	16:P:196:THR:HB	2.02	0.42
21:U:358:ASP:O	21:U:360:VAL:HG23	2.20	0.42
22:V:157:THR:OG1	22:V:158:PRO:HD3	2.19	0.42
22:V:197:THR:HG22	22:V:199:ASN:H	1.83	0.42
22:V:345:ARG:HG2	22:V:364:THR:HG21	2.01	0.42
22:V:403:ILE:HD11	22:V:428:LEU:HD11	2.02	0.42
22:V:475:ALA:O	22:V:479:ARG:HG2	2.19	0.42
25:Y:324:GLY:N	25:Y:325:VAL:HA	2.35	0.42
26:Z:262:LEU:O	26:Z:266:ILE:HD12	2.20	0.42
3:C:171:HIS:HD2	3:C:174:LEU:HD21	1.85	0.42
3:C:214:VAL:HG21	3:C:249:ASP:N	2.22	0.42
3:C:327:ASP:O	3:C:331:ILE:HG12	2.20	0.42
2:B:108:SER:HA	3:C:95:PHE:HA	2.02	0.42
5:E:181:THR:O	5:E:185:ARG:HB2	2.20	0.42
6:F:172:VAL:HG22	6:F:267:LEU:HD11	2.01	0.42
6:F:188:ILE:O	6:F:188:ILE:HG13	2.20	0.42
7:G:43:ARG:NH2	7:G:164:LYS:HG2	2.35	0.42
7:G:44:GLY:N	7:G:47:CYS:O	2.44	0.42
9:I:218:ARG:NH1	9:I:223:THR:OG1	2.53	0.42
11:K:21:LEU:HD13	11:K:123:PHE:HZ	1.85	0.42
12:L:44:ALA:N	12:L:137:TYR:OH	2.53	0.42
21:U:181:LEU:HB3	21:U:218:GLN:HE22	1.84	0.42
21:U:684:ARG:O	21:U:688:LEU:HG	2.19	0.42
22:V:31:ALA:HB3	22:V:32:PRO:HD3	2.01	0.42
25:Y:111:LEU:HD23	25:Y:114:ILE:HD13	2.01	0.42
25:Y:218:THR:O	25:Y:221:THR:OG1	2.29	0.42
25:Y:349:LYS:C	25:Y:351:ASN:H	2.23	0.42
1:A:212:VAL:O	1:A:319:MET:HB2	2.20	0.42
1:A:90:GLU:O	1:A:94:GLN:HB2	2.19	0.42
3:C:54:ALA:O	3:C:58:LEU:N	2.53	0.42
4:D:205:TYR:CG	4:D:206:GLY:N	2.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:SER:O	5:E:93:LYS:NZ	2.40	0.42
7:G:87:SER:O	7:G:91:VAL:HG23	2.20	0.42
10:J:9:VAL:HB	10:J:10:PHE:HB3	2.01	0.42
10:J:120:GLN:O	11:K:134:SER:OG	2.37	0.42
13:M:108:LEU:HD11	13:M:137:LEU:HB3	2.02	0.42
18:R:19:ARG:CZ	18:R:171:GLY:HA3	2.50	0.42
21:U:517:GLY:HA3	21:U:554:LEU:HB3	2.01	0.42
21:U:810:THR:O	21:U:883:ARG:NH1	2.52	0.42
22:V:372:LEU:H	22:V:427:GLN:HE22	1.67	0.42
23:W:200:ILE:O	23:W:204:ILE:HG12	2.19	0.42
23:W:243:ILE:HA	23:W:246:HIS:HB3	2.02	0.42
2:B:191:ASP:N	2:B:191:ASP:OD1	2.52	0.42
2:B:226:GLY:HA2	2:B:227:PRO:HD3	1.90	0.42
4:D:385:LEU:O	4:D:388:ARG:HB3	2.20	0.42
19:S:20:PHE:HB2	19:S:198:VAL:O	2.20	0.42
21:U:654:MET:O	21:U:658:ILE:HG12	2.19	0.42
22:V:259:LEU:HD12	22:V:295:ILE:HG12	2.02	0.42
23:W:135:LYS:HB3	23:W:136:ILE:CA	2.48	0.42
23:W:136:ILE:N	23:W:141:GLU:OE2	2.53	0.42
25:Y:356:THR:HA	25:Y:357:ASN:OD1	2.18	0.42
22:V:497:PRO:HG3	26:Z:286:GLU:HG3	2.02	0.42
3:C:310:ARG:HA	3:C:311:ILE:HA	1.68	0.41
3:C:39:SER:O	3:C:43:ARG:N	2.48	0.41
4:D:93:LEU:HD23	4:D:102:ILE:HD12	2.02	0.41
5:E:194:ASN:ND2	5:E:227:PRO:O	2.53	0.41
6:F:191:LEU:HG	6:F:194:GLN:HE21	1.84	0.41
6:F:321:GLN:HG3	6:F:322:PRO:HD3	2.01	0.41
8:H:43:GLY:HA2	8:H:144:PRO:HG3	2.02	0.41
10:J:36:ARG:HA	10:J:41:VAL:HG12	2.02	0.41
11:K:36:THR:OG1	11:K:170:ILE:O	2.24	0.41
11:K:200:ILE:HA	11:K:203:LYS:NZ	2.34	0.41
12:L:137:TYR:CZ	12:L:216:GLY:HA2	2.55	0.41
14:N:1:THR:H1	14:N:33:LYS:HE2	1.85	0.41
15:O:19:ARG:CZ	15:O:170:GLY:HA3	2.50	0.41
20:T:192:VAL:HG12	20:T:197:VAL:HG22	2.01	0.41
21:U:789:ILE:HB	21:U:911:ILE:HB	2.02	0.41
22:V:48:THR:HG23	22:V:147:PHE:HE2	1.84	0.41
23:W:107:GLN:HB3	23:W:111:TYR:CZ	2.55	0.41
26:Z:182:THR:N	26:Z:183:THR:HA	2.30	0.41
3:C:141:GLU:OE2	4:D:326:ARG:NH2	2.52	0.41
3:C:149:GLU:O	3:C:331:ILE:HD12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:157:ASP:O	4:D:159:LYS:HG2	2.19	0.41
5:E:119:VAL:HG11	6:F:146:LYS:HD2	2.02	0.41
6:F:150:LEU:HB3	6:F:164:LEU:O	2.20	0.41
7:G:174:GLU:HB2	7:G:205:VAL:HG22	2.02	0.41
7:G:56:VAL:HA	7:G:61:LEU:HD13	2.02	0.41
9:I:33:THR:OG1	9:I:50:ARG:NH2	2.53	0.41
9:I:88:ASN:HA	9:I:91:ARG:HB3	2.02	0.41
10:J:154:HIS:CE1	11:K:60:GLU:H	2.32	0.41
22:V:313:LEU:HD22	22:V:329:HIS:CE1	2.54	0.41
23:W:90:LEU:HD22	23:W:135:LYS:HE2	2.02	0.41
23:W:150:ALA:O	23:W:154:GLU:HG3	2.20	0.41
25:Y:198:ALA:HB2	25:Y:226:VAL:HG13	2.03	0.41
26:Z:121:LEU:HD11	26:Z:138:TYR:HD2	1.85	0.41
1:A:106:SER:HB2	6:F:165:PRO:O	2.20	0.41
1:A:210:LYS:O	1:A:336:ARG:NH2	2.53	0.41
1:A:406:GLU:HG3	1:A:407:LYS:H	1.86	0.41
1:A:83:ASP:HB2	2:B:102:LEU:HD23	2.01	0.41
2:B:376:ASP:O	2:B:378:VAL:N	2.53	0.41
3:C:183:PRO:HA	3:C:311:ILE:HG13	2.02	0.41
4:D:289:LEU:HD12	4:D:292:LEU:HD11	2.02	0.41
7:G:231:THR:O	7:G:233:ALA:N	2.52	0.41
9:I:180:LYS:HE3	9:I:180:LYS:HB3	1.91	0.41
12:L:116:THR:HG22	12:L:128:TYR:HD2	1.84	0.41
12:L:195:LEU:O	12:L:198:THR:OG1	2.30	0.41
13:M:169:ARG:HG3	13:M:170:GLN:N	2.35	0.41
14:N:67:SER:HA	14:N:70:LEU:HD12	2.01	0.41
20:T:49:THR:HA	20:T:114:GLY:HA3	2.02	0.41
21:U:576:PRO:HA	21:U:579:ARG:HE	1.85	0.41
23:W:59:ASP:HA	23:W:63:THR:HG23	2.02	0.41
25:Y:307:LEU:HD11	25:Y:319:MET:SD	2.59	0.41
1:A:102:ILE:HG22	1:A:113:ILE:HG12	2.02	0.41
3:C:210:THR:HG23	3:C:244:SER:HB3	2.01	0.41
3:C:214:VAL:HG22	3:C:215:SER:N	2.33	0.41
3:C:283:PHE:HD1	3:C:284:GLU:HG2	1.85	0.41
4:D:358:VAL:HG12	4:D:363:TYR:CE2	2.55	0.41
4:D:375:ILE:HG23	4:D:376:ASN:H	1.84	0.41
5:E:232:MET:N	5:E:276:ILE:O	2.53	0.41
6:F:311:LEU:HD23	6:F:314:LEU:HD22	2.01	0.41
9:I:38:LEU:HD11	9:I:160:LYS:HB3	2.01	0.41
21:U:788:VAL:HG12	21:U:910:GLY:H	1.84	0.41
22:V:288:TYR:HA	22:V:291:TYR:HD2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:72:LYS:HD2	23:W:123:ARG:HD3	2.02	0.41
23:W:455:LEU:HD12	23:W:456:GLN:N	2.34	0.41
23:W:45:GLU:HB2	23:W:93:ARG:HA	2.02	0.41
24:X:268:GLN:O	24:X:272:SER:HB2	2.20	0.41
25:Y:292:TYR:O	25:Y:296:VAL:HG23	2.21	0.41
26:Z:109:ASN:OD1	26:Z:119:SER:HB2	2.20	0.41
2:B:313:LEU:HD22	2:B:341:LEU:HD22	2.03	0.41
2:B:431:GLN:HA	2:B:434:THR:OG1	2.21	0.41
5:E:268:ASP:OD1	5:E:269:THR:N	2.49	0.41
7:G:39:SER:H	7:G:172:GLN:NE2	2.18	0.41
7:G:61:LEU:HG	7:G:66:VAL:HG21	2.02	0.41
8:H:174:LEU:HD21	8:H:194:THR:HG21	2.02	0.41
8:H:59:GLU:N	8:H:59:GLU:OE1	2.52	0.41
8:H:67:PRO:O	8:H:91:ARG:NH2	2.54	0.41
14:N:144:ARG:NH2	14:N:151:GLU:OE1	2.54	0.41
18:R:161:TYR:CE1	18:R:196:HIS:HA	2.56	0.41
22:V:137:GLU:N	22:V:138:PRO:HD2	2.36	0.41
22:V:234:ARG:HA	22:V:237:THR:HG22	2.02	0.41
25:Y:145:LEU:HD23	25:Y:157:ILE:HB	2.02	0.41
25:Y:16:ASP:OD2	25:Y:113:ARG:HG3	2.21	0.41
3:C:186:VAL:HG23	3:C:313:ARG:HB3	2.03	0.41
3:C:339:THR:HG23	3:C:341:GLY:H	1.85	0.41
6:F:431:LYS:HG2	6:F:432:LYS:HD2	2.02	0.41
7:G:132:ARG:HD3	7:G:133:PRO:HD2	2.01	0.41
7:G:14:THR:O	7:G:15:ILE:HG23	2.21	0.41
11:K:178:GLN:HB3	11:K:182:GLN:NE2	2.36	0.41
14:N:36:PRO:HA	14:N:42:PHE:CE1	2.56	0.41
21:U:495:ASP:HA	21:U:498:LYS:NZ	2.36	0.41
1:A:212:VAL:HG12	1:A:339:ARG:HB3	2.02	0.41
2:B:436:GLU:HG2	2:B:439:TYR:CD1	2.56	0.41
3:C:163:GLU:O	3:C:167:LEU:HB2	2.21	0.41
7:G:101:TRP:CD1	7:G:109:ILE:HA	2.56	0.41
9:I:140:ASP:OD1	9:I:144:GLY:N	2.54	0.41
9:I:119:GLN:HB2	9:I:154:GLY:HA3	2.01	0.41
9:I:57:ASP:HB3	9:I:59:VAL:HG13	2.03	0.41
19:S:13:LEU:HD13	19:S:137:ALA:HB2	2.02	0.41
4:D:46:LYS:HZ3	21:U:183:LEU:HD22	1.85	0.41
22:V:496:PHE:HB2	22:V:497:PRO:HD3	2.03	0.41
23:W:406:VAL:HA	23:W:413:ILE:HG22	2.03	0.41
23:W:373:ILE:HG23	23:W:413:ILE:HG13	2.03	0.41
24:X:390:GLU:O	24:X:392:PRO:HD3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:LYS:HG2	3:C:98:ASP:HA	2.02	0.41
4:D:412:GLN:OE1	4:D:415:GLU:HB2	2.21	0.41
6:F:192:ASP:HA	6:F:195:ILE:HG22	2.03	0.41
6:F:221:LYS:HG3	6:F:346:GLY:HA2	2.02	0.41
9:I:184:MET:HA	9:I:185:THR:C	2.41	0.41
10:J:221:ASN:O	10:J:223:GLU:N	2.47	0.41
11:K:60:GLU:OE1	11:K:63:SER:N	2.54	0.41
13:M:110:HIS:CD2	14:N:70:LEU:HD23	2.55	0.41
21:U:566:LEU:O	21:U:570:LEU:HG	2.19	0.41
21:U:800:VAL:HG22	21:U:898:CYS:SG	2.60	0.41
22:V:104:THR:HA	22:V:107:ARG:HG2	2.02	0.41
22:V:235:LEU:HD12	22:V:247:GLN:HG3	2.02	0.41
22:V:349:ARG:HD2	22:V:354:LYS:HG3	2.03	0.41
22:V:417:ILE:HD11	22:V:422:ILE:HB	2.03	0.41
23:W:359:VAL:O	23:W:363:ILE:HG12	2.21	0.41
25:Y:227:SER:O	25:Y:231:LEU:HB3	2.21	0.41
25:Y:268:TYR:CZ	25:Y:307:LEU:HD12	2.56	0.41
26:Z:96:HIS:NE2	26:Z:123:ILE:HG12	2.36	0.41
2:B:180:PRO:HG3	2:B:243:THR:HG22	2.03	0.41
5:E:125:GLU:N	5:E:125:GLU:OE1	2.54	0.41
4:D:150:SER:HB3	5:E:61:LEU:HD22	2.03	0.41
5:E:72:LYS:HB2	5:E:78:ARG:HG2	2.02	0.41
6:F:88:TYR:HB2	6:F:154:ASN:HA	2.03	0.41
7:G:179:LEU:HB2	8:H:56:LEU:HD11	2.02	0.41
9:I:97:TYR:O	9:I:101:TYR:HB2	2.21	0.41
17:Q:8:GLN:HB2	17:Q:115:LEU:HD22	2.02	0.41
21:U:356:THR:HG21	21:U:731:ILE:HD13	2.02	0.41
22:V:295:ILE:O	22:V:298:ILE:HG22	2.21	0.41
22:V:455:LYS:H	22:V:456:GLY:HA2	1.83	0.41
23:W:56:THR:HG21	23:W:103:LYS:HE3	2.02	0.41
24:X:367:GLN:HA	24:X:370:LEU:HD12	2.02	0.41
25:Y:191:ILE:HD12	25:Y:191:ILE:HA	1.91	0.41
26:Z:120:VAL:HG23	26:Z:138:TYR:O	2.21	0.41
26:Z:33:LYS:HD3	26:Z:60:GLU:H	1.85	0.41
1:A:206:ILE:HG23	1:A:207:GLU:N	2.35	0.41
2:B:150:VAL:HG12	2:B:162:VAL:HG12	2.03	0.41
2:B:153:ASN:N	2:B:158:ALA:O	2.31	0.41
3:C:62:GLU:HG2	4:D:114:ARG:NH2	2.36	0.41
4:D:200:ARG:NH1	4:D:300:ASP:OD1	2.39	0.41
1:A:309:PHE:CZ	6:F:235:LEU:HD12	2.56	0.41
7:G:37:LEU:HD11	7:G:53:GLN:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:4:ARG:HH12	12:L:9:ASP:CG	2.21	0.41
12:L:171:TYR:O	12:L:175:HIS:ND1	2.48	0.41
21:U:427:LEU:HG	21:U:464:GLN:HE21	1.85	0.41
22:V:194:LYS:HG2	22:V:200:ARG:HH22	1.86	0.41
22:V:224:LEU:HB2	22:V:227:VAL:HB	2.01	0.41
22:V:392:TYR:O	22:V:395:ILE:HG22	2.21	0.41
24:X:377:ILE:HG12	25:Y:312:ARG:HB3	2.01	0.41
25:Y:48:ASN:ND2	25:Y:77:ASN:HB2	2.35	0.41
1:A:344:SER:CA	1:A:345:LEU:HB3	2.51	0.41
2:B:106:PRO:HB2	2:B:154:HIS:CD2	2.55	0.41
3:C:249:ASP:HA	3:C:250:GLU:HA	1.72	0.41
2:B:178:LYS:NZ	3:C:278:ASN:HB3	2.36	0.41
3:C:313:ARG:HH11	3:C:314:LYS:H	1.69	0.41
4:D:249:ASP:HA	4:D:252:ARG:HG2	2.03	0.41
6:F:225:MET:HG2	6:F:233:LYS:HD2	2.02	0.41
7:G:184:LYS:HB2	7:G:185:LYS:O	2.21	0.41
13:M:188:ASP:O	13:M:192:GLU:HG2	2.21	0.41
15:O:110:LEU:HB3	15:O:122:LEU:O	2.21	0.41
19:S:11:THR:HG21	19:S:141:ALA:HB3	2.01	0.41
21:U:347:ASN:HB3	21:U:813:TYR:HB2	2.01	0.41
22:V:283:ASN:ND2	22:V:317:PRO:O	2.54	0.41
22:V:455:LYS:HD2	22:V:457:TYR:HE2	1.86	0.41
22:V:64:GLN:OE1	22:V:64:GLN:N	2.54	0.41
25:Y:186:LEU:HA	25:Y:189:VAL:HG12	2.03	0.41
25:Y:39:ASP:HA	25:Y:42:MET:HB3	2.03	0.41
1:A:187:LEU:O	1:A:190:VAL:HG12	2.21	0.40
2:B:224:LEU:HD22	2:B:351:ILE:HG12	2.03	0.40
3:C:157:GLN:NE2	3:C:318:PRO:HD3	2.34	0.40
3:C:49:ARG:NH2	4:D:69:LYS:HG3	2.35	0.40
5:E:44:GLU:OE1	6:F:76:ASN:ND2	2.53	0.40
9:I:159:TRP:HB3	10:J:54:GLN:HB3	2.03	0.40
11:K:73:HIS:ND1	11:K:74:ILE:HG13	2.36	0.40
12:L:182:CYS:SG	12:L:187:LEU:HD13	2.61	0.40
13:M:215:TRP:HH2	13:M:219:LEU:H	1.69	0.40
13:M:80:LEU:HD23	13:M:82:ALA:H	1.86	0.40
13:M:8:ASP:N	13:M:8:ASP:OD1	2.54	0.40
15:O:202:TYR:HD2	16:P:152:SER:HB3	1.86	0.40
16:P:58:THR:OG1	17:Q:121:LEU:O	2.17	0.40
19:S:213:ASP:OD1	19:S:213:ASP:N	2.55	0.40
22:V:106:ARG:HA	22:V:109:ASN:HB2	2.02	0.40
22:V:176:MET:HA	22:V:179:LYS:HE2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:172:GLU:OE1	23:W:172:GLU:N	2.54	0.40
23:W:449:GLU:HG2	23:W:453:HIS:CE1	2.55	0.40
25:Y:300:ARG:O	25:Y:304:TYR:N	2.51	0.40
26:Z:36:VAL:HG22	26:Z:96:HIS:HB3	2.02	0.40
1:A:377:CYS:HB2	1:A:380:SER:OG	2.21	0.40
4:D:43:ARG:HA	4:D:46:LYS:HD2	2.02	0.40
5:E:309:ARG:HD3	5:E:332:VAL:HB	2.04	0.40
6:F:102:ASN:HA	6:F:103:ASP:HA	1.51	0.40
9:I:243:GLU:O	9:I:247:ALA:N	2.53	0.40
9:I:90:LEU:HD12	9:I:114:LEU:HB2	2.03	0.40
14:N:91:ARG:NH1	20:T:59:ASP:OD1	2.54	0.40
15:O:13:VAL:HG22	15:O:177:VAL:HA	2.03	0.40
21:U:93:ASN:OD1	21:U:94:SER:N	2.54	0.40
22:V:91:PRO:HA	22:V:94:VAL:HG12	2.02	0.40
22:V:97:ALA:N	22:V:98:LEU:HA	2.35	0.40
25:Y:101:ARG:HG3	25:Y:104:MET:SD	2.62	0.40
25:Y:63:TRP:HB3	25:Y:65:ILE:N	2.37	0.40
1:A:190:VAL:HG11	1:A:212:VAL:HG11	2.03	0.40
1:A:292:ASP:O	1:A:296:GLN:HG2	2.21	0.40
1:A:351:ARG:HH11	1:A:379:ASN:H	1.69	0.40
2:B:109:VAL:HB	3:C:94:LYS:HB2	2.03	0.40
2:B:345:GLY:HA2	2:B:346:ARG:HA	1.74	0.40
4:D:45:LYS:O	4:D:48:GLN:NE2	2.54	0.40
5:E:86:GLN:NE2	5:E:108:MET:HG3	2.36	0.40
5:E:233:ASP:OD2	6:F:315:ASN:ND2	2.54	0.40
6:F:228:PRO:HA	6:F:229:PRO:HD3	1.84	0.40
7:G:23:TYR:O	7:G:26:GLU:HG2	2.21	0.40
11:K:146:VAL:HG22	11:K:151:PRO:HA	2.03	0.40
17:Q:20:VAL:HG21	17:Q:175:LEU:HA	2.03	0.40
19:S:125:ASP:N	19:S:125:ASP:OD1	2.55	0.40
19:S:40:SER:O	19:S:42:LYS:HD2	2.21	0.40
21:U:420:LEU:HB2	21:U:457:ILE:HD11	2.03	0.40
25:Y:98:SER:O	25:Y:102:ASP:HB2	2.22	0.40
26:Z:62:ASP:OD1	26:Z:62:ASP:N	2.55	0.40
1:A:354:ILE:HB	1:A:385:ILE:HD11	2.04	0.40
1:A:95:VAL:HG12	1:A:144:ARG:HG2	2.03	0.40
2:B:365:PHE:HE2	2:B:378:VAL:HG11	1.87	0.40
2:B:187:ILE:O	2:B:367:ILE:HG21	2.22	0.40
3:C:148:TYR:HA	3:C:151:ILE:HG22	2.04	0.40
5:E:364:GLN:HA	5:E:367:PHE:HB2	2.02	0.40
6:F:219:PRO:HA	6:F:220:PRO:HD3	1.99	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:160:LYS:HG3	10:J:55:ASP:HB2	2.03	0.40
19:S:58:HIS:HB3	20:T:130:VAL:HG22	2.03	0.40
20:T:25:ASP:HA	20:T:187:PHE:HA	2.04	0.40
22:V:149:PRO:HG3	22:V:203:LEU:HG	2.03	0.40
22:V:416:ARG:HE	22:V:459:GLN:HB3	1.86	0.40
24:X:291:ALA:O	24:X:294:SER:OG	2.38	0.40
25:Y:183:TYR:OH	25:Y:212:GLU:OE1	2.39	0.40
25:Y:360:ASP:O	25:Y:365:GLN:HB2	2.21	0.40
26:Z:62:ASP:OD1	26:Z:63:LYS:HG2	2.22	0.40
1:A:115:VAL:HG12	1:A:119:ALA:O	2.21	0.40
7:G:68:HIS:HE2	7:G:80:MET:C	2.23	0.40
7:G:86:ASP:OD1	13:M:120:HIS:NE2	2.52	0.40
11:K:97:GLN:NE2	18:R:64:ARG:HG2	2.37	0.40
12:L:137:TYR:CZ	12:L:142:PRO:HB3	2.56	0.40
11:K:10:ARG:HH11	12:L:21:GLN:HE22	1.68	0.40
19:S:149:LEU:O	19:S:153:VAL:N	2.54	0.40
21:U:397:THR:HA	21:U:401:LYS:NZ	2.36	0.40
21:U:842:LYS:HA	21:U:843:GLU:CB	2.48	0.40
22:V:237:THR:OG1	22:V:241:ARG:NH2	2.54	0.40
23:W:155:GLN:HG2	23:W:157:GLY:H	1.86	0.40
23:W:62:SER:HB2	23:W:71:VAL:HG11	2.03	0.40
25:Y:110:TYR:CE1	25:Y:113:ARG:HD3	2.57	0.40
25:Y:145:LEU:HD13	25:Y:183:TYR:CD1	2.56	0.40
25:Y:357:ASN:CB	25:Y:358:ARG:HA	2.51	0.40
26:Z:39:LEU:HB2	26:Z:95:TYR:HD2	1.86	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	A	359/433 (83%)	311 (87%)	44 (12%)	4 (1%)	17 63

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	346/440 (79%)	297 (86%)	46 (13%)	3 (1%)	21	67
3	C	382/398 (96%)	339 (89%)	41 (11%)	2 (0%)	34	77
4	D	378/418 (90%)	333 (88%)	44 (12%)	1 (0%)	46	83
5	E	351/403 (87%)	322 (92%)	28 (8%)	1 (0%)	46	83
6	F	362/439 (82%)	322 (89%)	38 (10%)	2 (1%)	30	74
7	G	238/245 (97%)	213 (90%)	23 (10%)	2 (1%)	24	69
8	H	229/233 (98%)	211 (92%)	18 (8%)	0	100	100
9	I	248/260 (95%)	220 (89%)	28 (11%)	0	100	100
10	J	237/247 (96%)	214 (90%)	20 (8%)	3 (1%)	15	60
11	K	224/240 (93%)	204 (91%)	18 (8%)	2 (1%)	21	67
12	L	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
13	M	238/254 (94%)	216 (91%)	22 (9%)	0	100	100
14	N	189/238 (79%)	180 (95%)	9 (5%)	0	100	100
15	O	216/276 (78%)	197 (91%)	19 (9%)	0	100	100
16	P	200/204 (98%)	185 (92%)	15 (8%)	0	100	100
17	Q	197/201 (98%)	180 (91%)	17 (9%)	0	100	100
18	R	199/262 (76%)	184 (92%)	15 (8%)	0	100	100
19	S	211/240 (88%)	200 (95%)	11 (5%)	0	100	100
20	T	213/263 (81%)	208 (98%)	5 (2%)	0	100	100
21	U	798/953 (84%)	735 (92%)	62 (8%)	1 (0%)	56	90
22	V	478/533 (90%)	413 (86%)	63 (13%)	2 (0%)	39	80
23	W	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	26	71
24	X	239/422 (57%)	213 (89%)	26 (11%)	0	100	100
25	Y	376/389 (97%)	335 (89%)	39 (10%)	2 (0%)	34	77
26	Z	284/324 (88%)	253 (89%)	30 (11%)	1 (0%)	39	80
27	a	371/376 (99%)	331 (89%)	38 (10%)	2 (0%)	34	77
28	b	189/377 (50%)	174 (92%)	15 (8%)	0	100	100
29	c	274/309 (89%)	242 (88%)	28 (10%)	4 (2%)	13	57
30	d	255/349 (73%)	227 (89%)	27 (11%)	1 (0%)	39	80
31	e	36/70 (51%)	31 (86%)	5 (14%)	0	100	100
32	f	686/749 (92%)	573 (84%)	109 (16%)	4 (1%)	30	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9693/11269 (86%)	8692 (90%)	961 (10%)	40 (0%)	43 80

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	VAL
10	J	104	VAL
11	K	12	VAL
11	K	109	VAL
21	U	364	VAL
23	W	68	VAL
23	W	136	ILE
25	Y	350	VAL
32	f	62	ILE
32	f	447	VAL
2	B	176	VAL
3	C	214	VAL
29	c	157	ILE
29	c	227	GLU
32	f	131	VAL
1	A	206	ILE
1	A	317	VAL
2	B	218	PRO
4	D	151	ILE
10	J	199	VAL
27	a	340	VAL
32	f	281	ILE
3	C	298	ILE
6	F	282	ILE
7	G	15	ILE
23	W	138	VAL
25	Y	67	VAL
29	c	156	VAL
22	V	241	ARG
26	Z	144	VAL
30	d	213	ARG
22	V	101	LEU
27	a	336	VAL
2	B	325	VAL
29	c	189	ILE
1	A	172	VAL
6	F	326	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	170	VAL
10	J	98	VAL
5	E	175	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	A	308/372 (83%)	303 (98%)	5 (2%)	70	88
2	B	304/385 (79%)	298 (98%)	6 (2%)	63	85
3	C	332/346 (96%)	321 (97%)	11 (3%)	45	76
4	D	333/366 (91%)	330 (99%)	3 (1%)	84	93
5	E	308/353 (87%)	306 (99%)	2 (1%)	90	95
6	F	312/379 (82%)	306 (98%)	6 (2%)	65	86
7	G	193/209 (92%)	190 (98%)	3 (2%)	70	88
8	H	164/190 (86%)	164 (100%)	0	100	100
9	I	193/220 (88%)	191 (99%)	2 (1%)	82	92
10	J	152/210 (72%)	150 (99%)	2 (1%)	76	89
11	K	186/202 (92%)	184 (99%)	2 (1%)	80	91
12	L	198/229 (86%)	197 (100%)	1 (0%)	92	96
13	M	192/211 (91%)	190 (99%)	2 (1%)	82	92
14	N	148/180 (82%)	147 (99%)	1 (1%)	88	94
15	O	177/227 (78%)	176 (99%)	1 (1%)	90	95
16	P	172/173 (99%)	171 (99%)	1 (1%)	90	95
17	Q	164/171 (96%)	163 (99%)	1 (1%)	90	95
18	R	153/201 (76%)	153 (100%)	0	100	100
19	S	174/198 (88%)	173 (99%)	1 (1%)	90	95
20	T	175/214 (82%)	175 (100%)	0	100	100
21	U	685/816 (84%)	681 (99%)	4 (1%)	90	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	V	414/459 (90%)	409 (99%)	5 (1%)	78 90
23	W	416/416 (100%)	412 (99%)	4 (1%)	82 92
24	X	208/362 (58%)	207 (100%)	1 (0%)	92 96
25	Y	334/344 (97%)	332 (99%)	2 (1%)	90 95
26	Z	257/295 (87%)	252 (98%)	5 (2%)	65 86
27	a	333/336 (99%)	331 (99%)	2 (1%)	90 95
28	b	167/312 (54%)	165 (99%)	2 (1%)	78 90
29	c	243/267 (91%)	240 (99%)	3 (1%)	78 90
30	d	231/293 (79%)	229 (99%)	2 (1%)	84 93
31	e	38/63 (60%)	38 (100%)	0	100 100
32	f	582/628 (93%)	571 (98%)	11 (2%)	65 86
All	All	8246/9627 (86%)	8155 (99%)	91 (1%)	81 91

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	LEU
1	A	157	ILE
1	A	161	VAL
1	A	220	THR
1	A	250	VAL
2	B	105	THR
2	B	136	LEU
2	B	164	MET
2	B	173	VAL
2	B	190	LEU
2	B	259	TYR
3	C	11	LEU
3	C	66	LEU
3	C	99	VAL
3	C	131	VAL
3	C	138	MET
3	C	148	TYR
3	C	235	PHE
3	C	249	ASP
3	C	259	LEU
3	C	286	THR
3	C	295	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	186	THR
4	D	234	GLU
4	D	344	ILE
5	E	80	VAL
5	E	204	VAL
6	F	85	THR
6	F	169	ASP
6	F	231	THR
6	F	272	PHE
6	F	282	ILE
6	F	283	ILE
7	G	22	LEU
7	G	109	ILE
7	G	230	LEU
9	I	55	LEU
9	I	206	LEU
10	J	96	LEU
10	J	104	VAL
11	K	20	ARG
11	K	186	HIS
12	L	46	LEU
13	M	165	ILE
13	M	233	GLU
14	N	75	LEU
15	O	66	HIS
16	P	137	VAL
17	Q	151	ILE
19	S	168	LEU
21	U	473	VAL
21	U	603	LEU
21	U	629	THR
21	U	773	PHE
22	V	221	LEU
22	V	224	LEU
22	V	255	LEU
22	V	320	THR
22	V	453	HIS
23	W	250	ILE
23	W	297	GLU
23	W	371	THR
23	W	455	LEU
24	X	200	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	Y	356	THR
25	Y	377	LEU
26	Z	91	ILE
26	Z	176	LEU
26	Z	186	THR
26	Z	196	HIS
26	Z	249	PHE
27	a	28	LEU
27	a	33	LEU
28	b	53	THR
28	b	97	LEU
29	c	69	VAL
29	c	229	LEU
29	c	275	VAL
30	d	122	LEU
30	d	158	ILE
32	f	15	ASP
32	f	107	LEU
32	f	301	ASP
32	f	317	THR
32	f	334	ASN
32	f	339	LEU
32	f	391	LEU
32	f	526	THR
32	f	600	LEU
32	f	663	VAL
32	f	685	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	305	GLN
1	A	314	ASN
2	B	154	HIS
2	B	241	ASN
3	C	50	ASN
3	C	205	HIS
3	C	241	HIS
4	D	187	HIS
4	D	302	ASN
4	D	376	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	412	GLN
5	E	190	GLN
5	E	220	ASN
5	E	316	HIS
5	E	364	GLN
6	F	255	GLN
6	F	323	ASN
6	F	325	GLN
6	F	395	GLN
7	G	128	ASN
8	H	119	GLN
9	I	95	GLN
9	I	119	GLN
10	J	92	GLN
10	J	146	GLN
11	K	13	ASN
11	K	23	GLN
11	K	97	GLN
11	K	178	GLN
11	K	214	ASN
12	L	20	HIS
12	L	21	GLN
14	N	187	GLN
15	O	66	HIS
16	P	169	GLN
17	Q	8	GLN
17	Q	71	ASN
17	Q	99	HIS
18	R	29	GLN
18	R	119	ASN
18	R	162	GLN
20	T	65	GLN
21	U	70	HIS
21	U	107	HIS
21	U	145	HIS
21	U	258	GLN
21	U	345	ASN
21	U	389	ASN
21	U	438	GLN
21	U	453	HIS
21	U	475	HIS
21	U	698	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	U	734	GLN
21	U	777	HIS
22	V	177	ASN
22	V	279	GLN
22	V	281	ASN
22	V	427	GLN
22	V	459	GLN
22	V	477	HIS
22	V	487	HIS
23	W	235	GLN
23	W	246	HIS
23	W	426	ASN
23	W	444	HIS
24	X	207	GLN
24	X	262	ASN
24	X	406	ASN
25	Y	302	HIS
25	Y	363	ASN
25	Y	365	GLN
25	Y	378	ASN
26	Z	102	HIS
26	Z	194	GLN
26	Z	224	HIS
27	a	23	HIS
27	a	249	GLN
27	a	290	GLN
27	a	337	GLN
28	b	76	HIS
28	b	142	ASN
29	c	30	GLN
29	c	115	HIS
29	c	199	HIS
29	c	219	ASN
29	c	283	HIS
30	d	102	ASN
30	d	109	GLN
31	e	6	GLN
32	f	228	GLN
32	f	246	HIS
32	f	269	GLN
32	f	293	ASN
32	f	406	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	f	611	HIS

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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	-	26,33,33	0.96	1 (3%)	26,52,52	1.72	1 (3%)
33	ATP	D	501	-	26,33,33	0.97	1 (3%)	26,52,52	1.79	3 (11%)
33	ATP	E	401	-	26,33,33	0.96	1 (3%)	26,52,52	1.67	1 (3%)
33	ATP	F	501	-	26,33,33	0.96	1 (3%)	26,52,52	1.58	1 (3%)

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	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	A	501	ATP	C5-C4	3.08	1.47	1.40
33	D	501	ATP	C5-C4	3.11	1.47	1.40
33	E	401	ATP	C5-C4	3.12	1.47	1.40
33	F	501	ATP	C5-C4	3.12	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	A	501	ATP	N3-C2-N1	-6.85	123.49	128.87
33	E	401	ATP	N3-C2-N1	-6.66	123.64	128.87
33	D	501	ATP	N3-C2-N1	-6.39	123.85	128.87
33	F	501	ATP	N3-C2-N1	-6.32	123.91	128.87
33	D	501	ATP	C4'-O4'-C1'	-2.78	106.69	109.64
33	D	501	ATP	O4'-C1'-N9	3.49	114.69	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	501	ATP	1	0
33	D	501	ATP	2	0
33	E	401	ATP	2	0
33	F	501	ATP	2	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	4
16	P	1
15	O	1
8	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	9.37
1	f	79:ASN	C	80:TYR	N	8.13
1	f	348:ASP	C	349:SER	N	6.07
1	P	81:GLN	C	82:ILE	N	4.19
1	O	74:PRO	C	75:ARG	N	3.14
1	H	79:MET	C	80:GLY	N	3.08
1	f	681:LEU	C	682:PRO	N	1.68