



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 21, 2016 – 05:11 PM EST

PDB ID : 5T0H  
EMDB ID: : EMD-8335  
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 : 6.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : unknown  
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



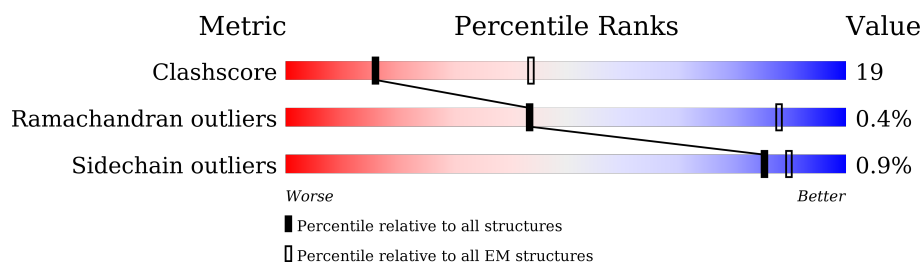
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.80 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









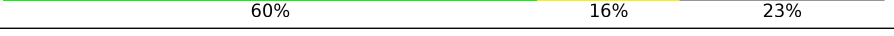

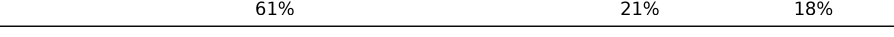
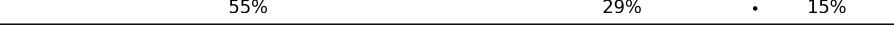

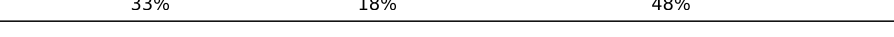



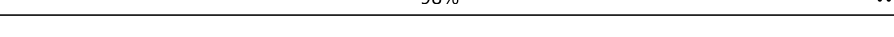
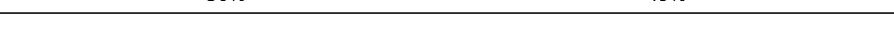



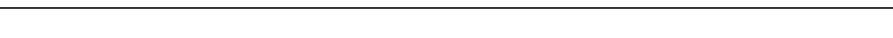
The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of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

Mol	Chain	Length	Quality of chain
1	A	433	34% 48% 17%
2	B	440	35% 41% 23%
3	C	398	41% 53% . .
4	D	418	38% 52% . 9%
5	E	403	43% 43% . 12%
6	F	439	37% 45% . 17%
7	G	245	64% 34% .
8	H	233	73% 26% .
9	I	260	72% 25% .

*Continued on next page...*



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Mol	Chain	Length	Quality of chain
10	J	247	
11	K	240	
12	L	268	
13	M	254	
14	N	238	
15	O	276	
16	P	204	
17	Q	201	
18	R	262	
19	S	240	
20	T	263	
21	U	953	
22	V	533	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	309	
30	d	349	
31	e	70	
32	f	749	



## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 73509 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
1	A	361	Total	C	N	O	S	0	0
			2835	1788	501	528	18		

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

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

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

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

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

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

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

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

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

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



- 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	232	Total	C	N	O	S	0	0
			1708	1081	289	333	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	236	Total	C	N	O	S	0	0
			1940	1237	331	361	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	81	Total	C	N	O	S	0	0
			647	414	107	124	2		

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

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

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

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

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

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

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



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

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

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

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

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

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

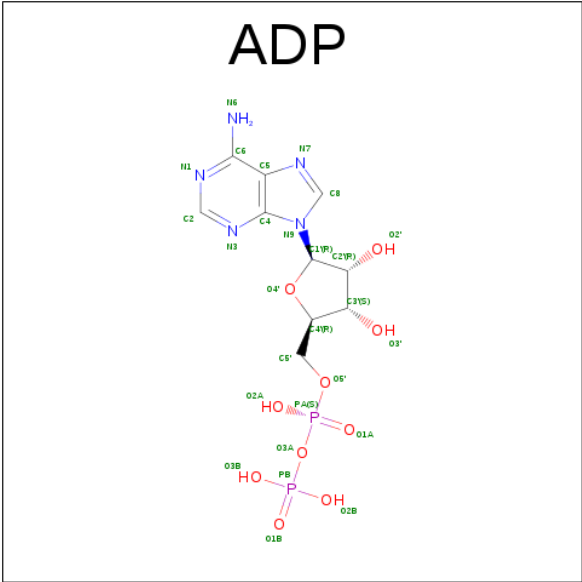
Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	24	Total	C	N	O	S	0	0
			197	121	34	40	2		

- 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'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).





Mol	Chain	Residues	Atoms					AltConf
33	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
33	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

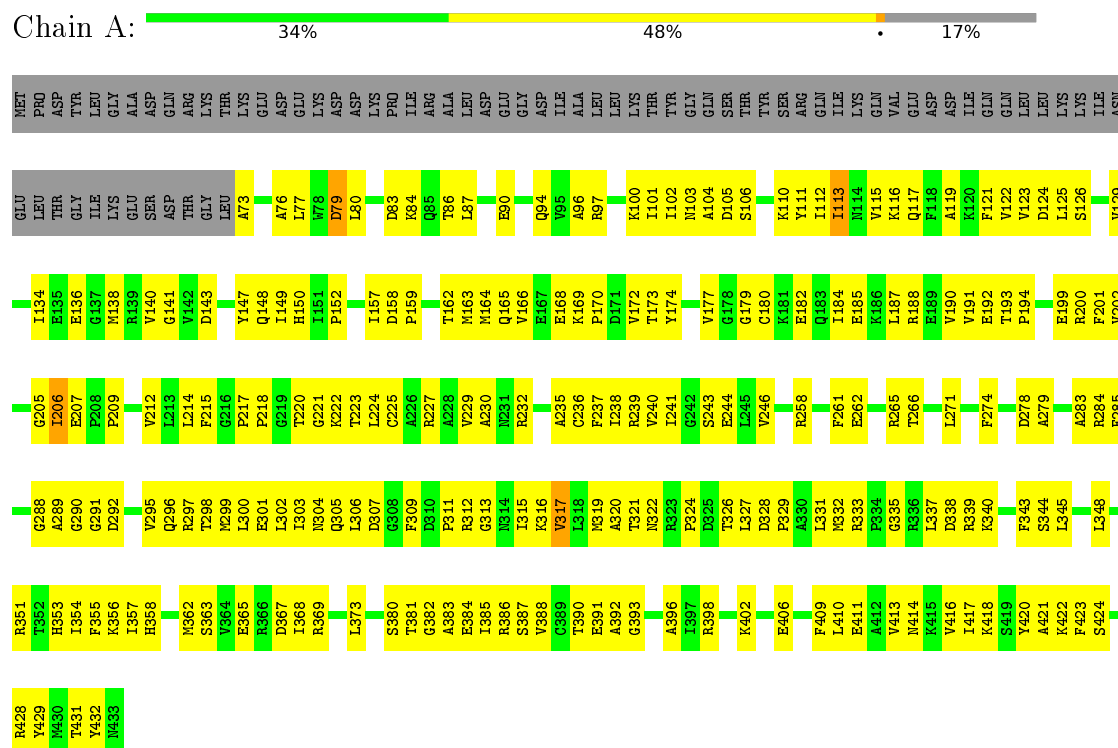
Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	Zn	0
			1	1	



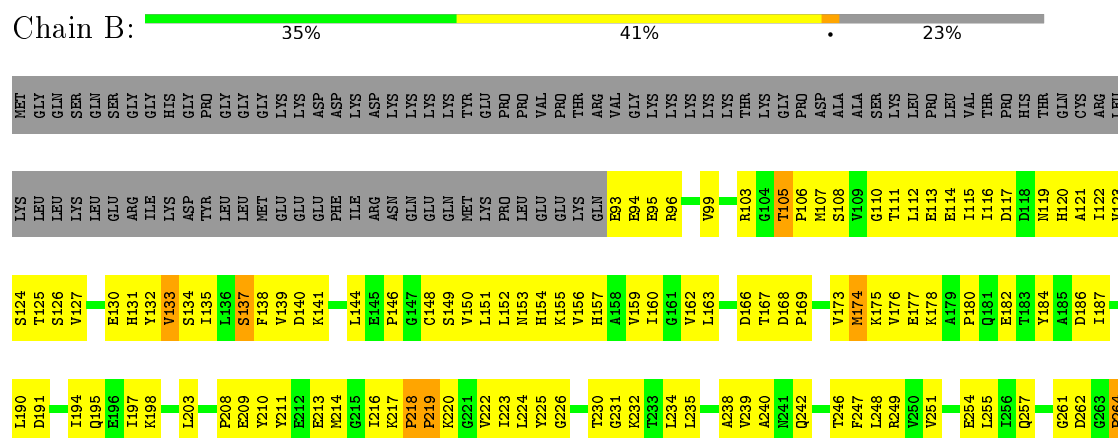
### 3 Residue-property plots

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.

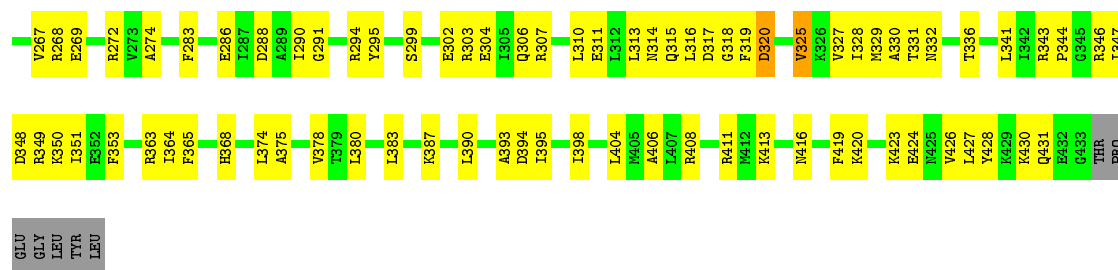
- Molecule 1: 26S protease regulatory subunit 7



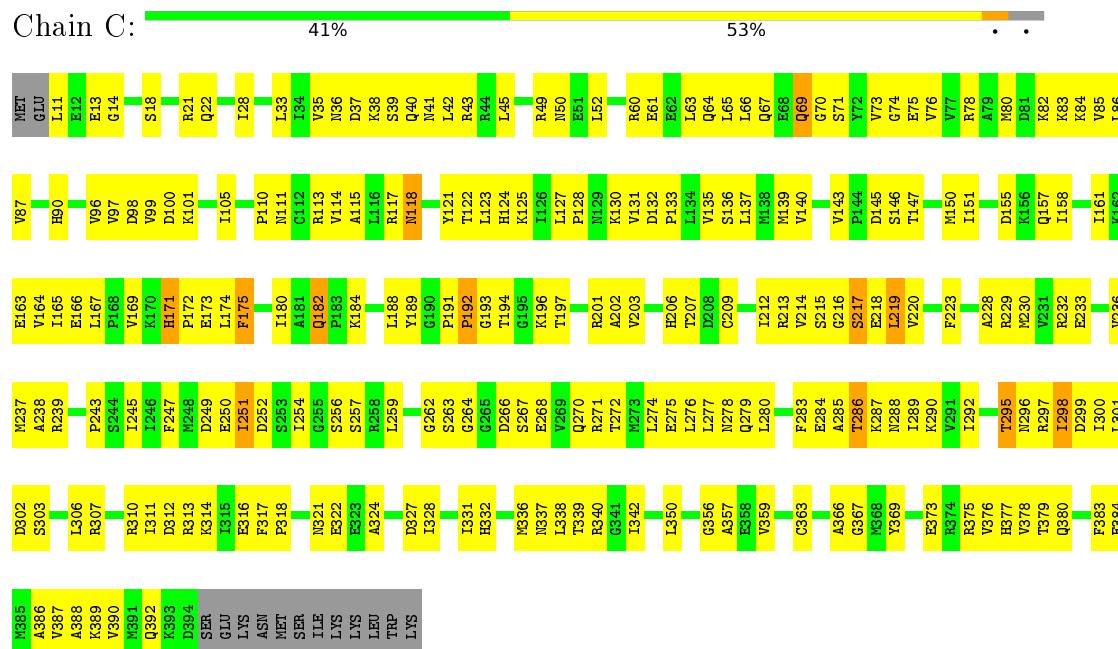
- Molecule 2: 26S protease regulatory subunit 4



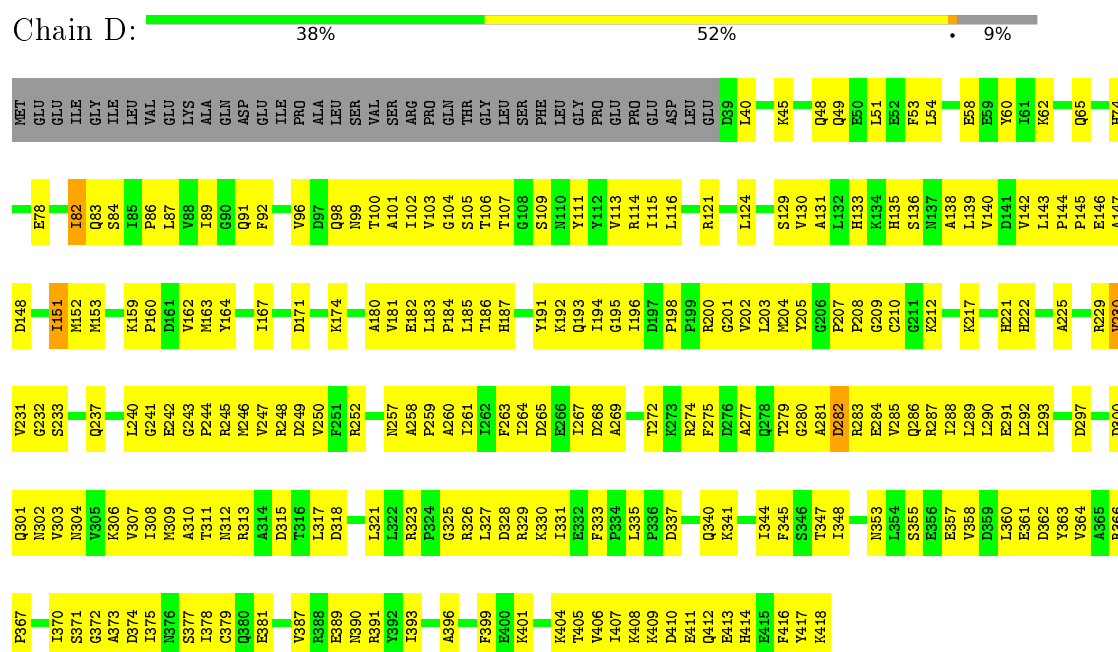




• Molecule 3: 26S protease regulatory subunit 8

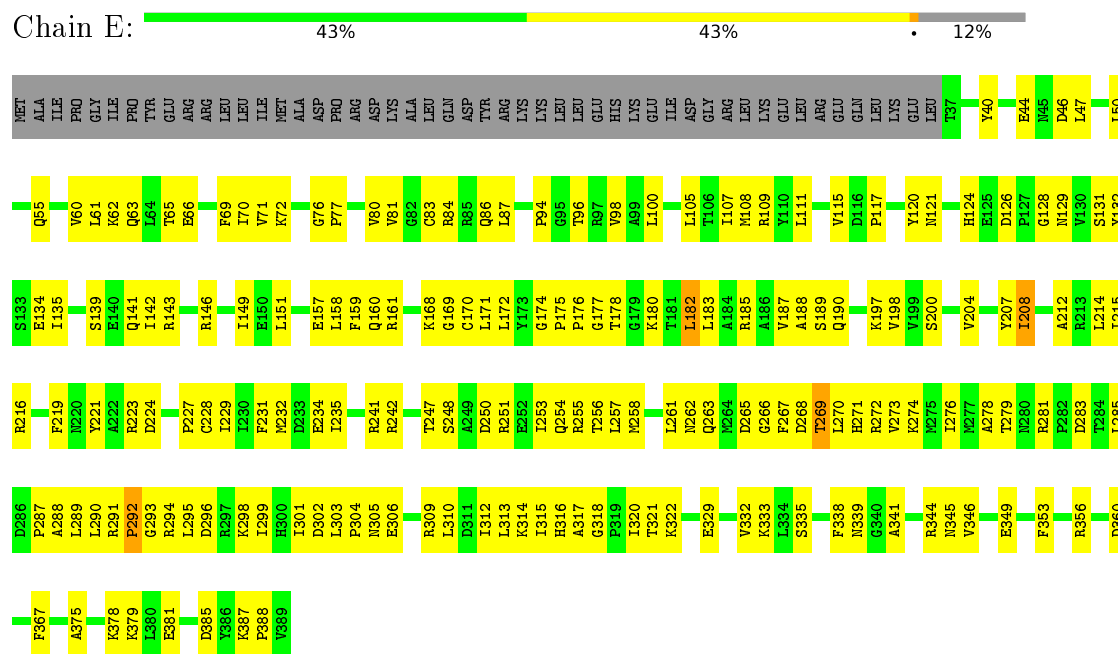


• Molecule 4: 26S protease regulatory subunit 6B

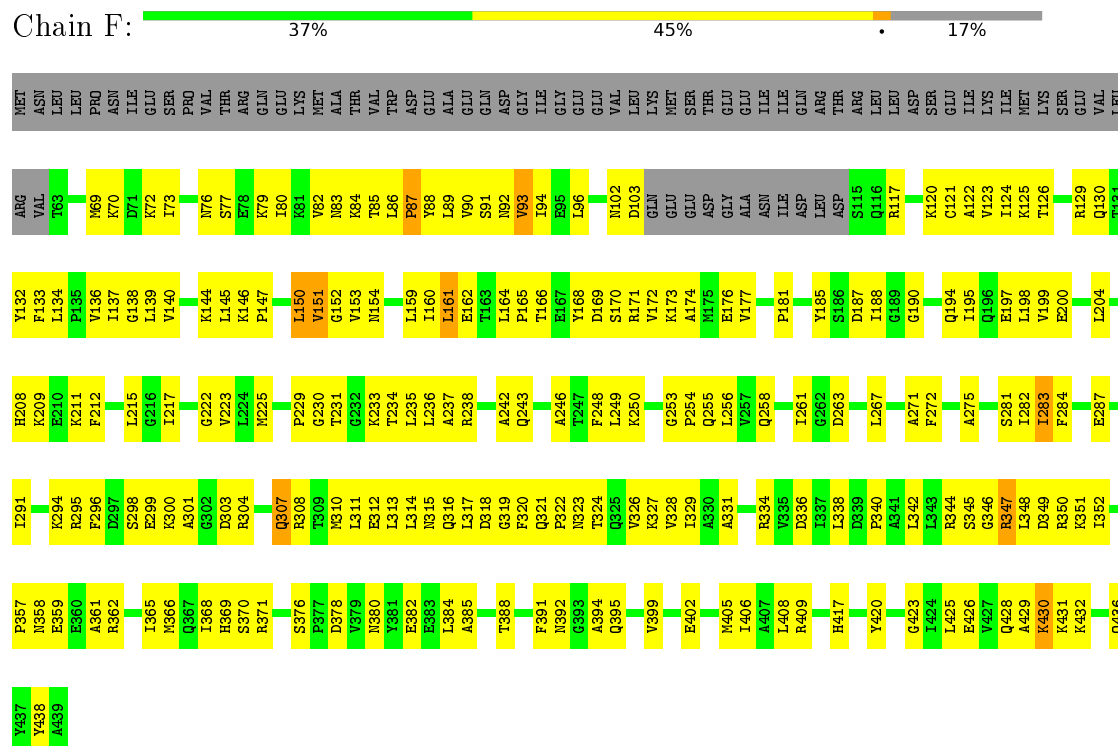




- Molecule 5: 26S protease regulatory subunit 10B



- Molecule 6: 26S protease regulatory subunit 6A



- Molecule 7: Proteasome subunit alpha type-6

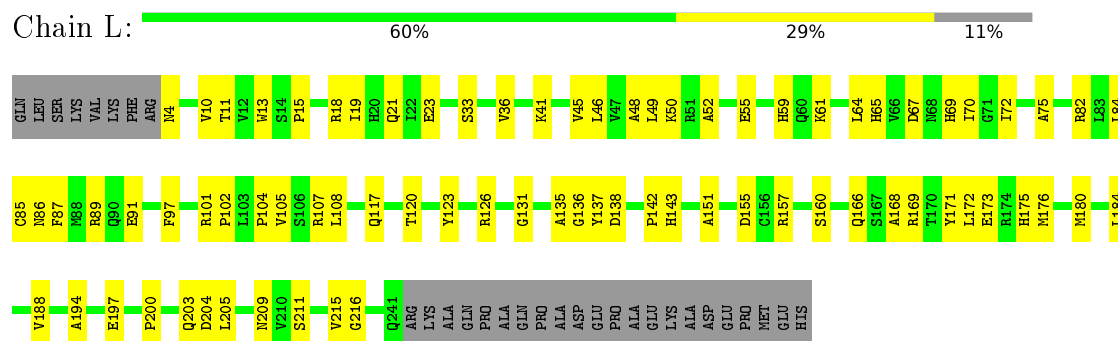




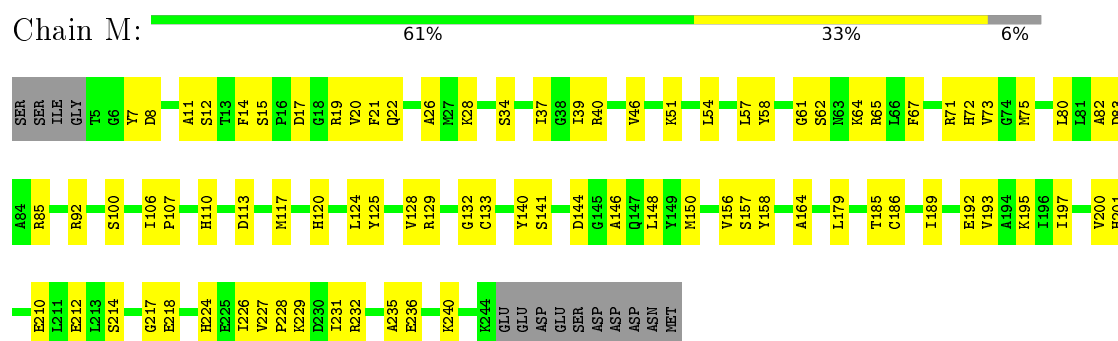




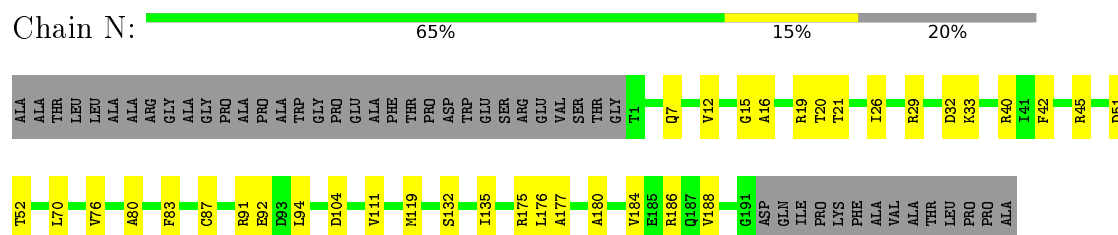
- Molecule 12: Proteasome subunit alpha type-1



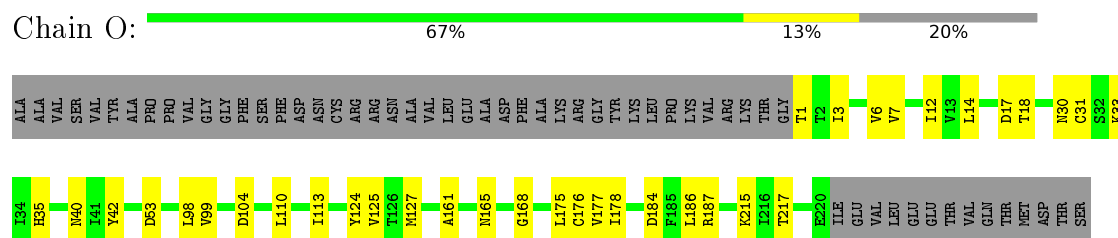
- Molecule 13: Proteasome subunit alpha type-3



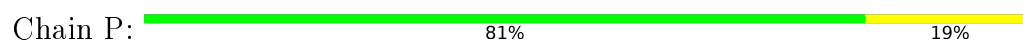
- Molecule 14: Proteasome subunit beta type-6



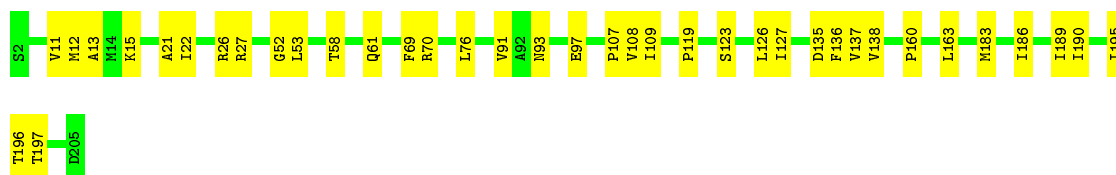
- Molecule 15: Proteasome subunit beta type-7



- Molecule 16: Proteasome subunit beta type-3

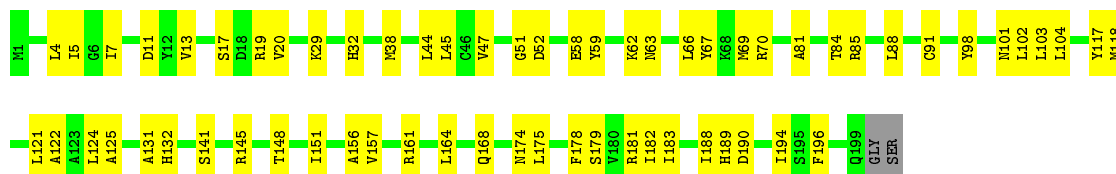






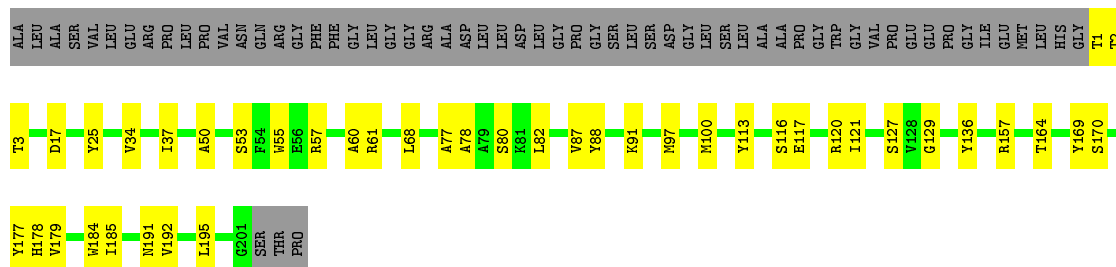
• Molecule 17: Proteasome subunit beta type-2

Chain Q: 68% 31%



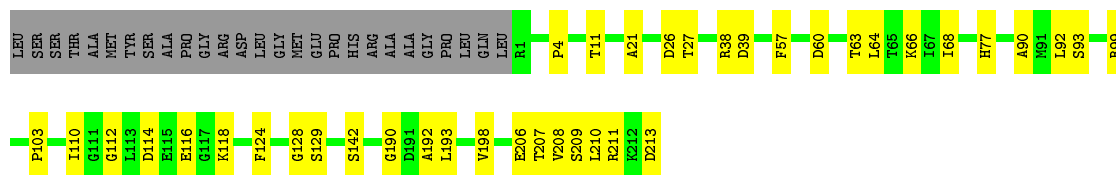
• Molecule 18: Proteasome subunit beta type-5

Chain R: 60% 16% 23%



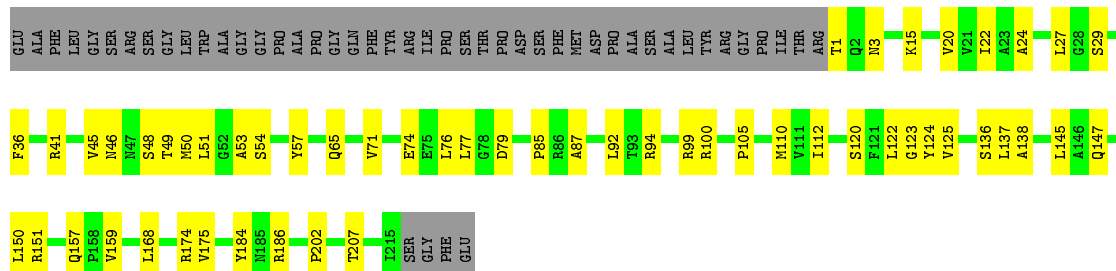
• Molecule 19: Proteasome subunit beta type-1

Chain S: 73% 16% 11%



• Molecule 20: Proteasome subunit beta type-4

Chain T: 61% 21% 18%



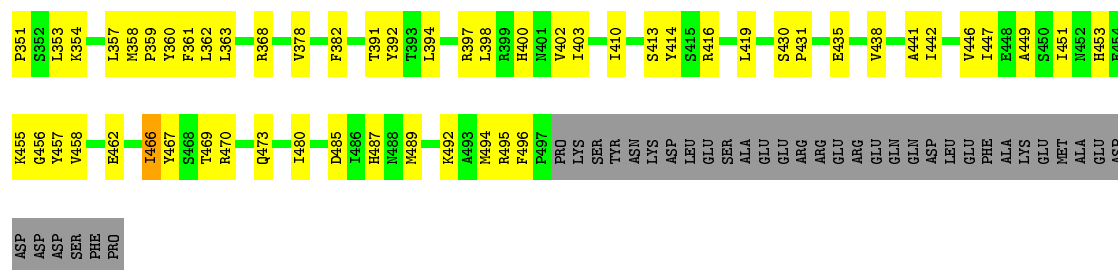


[illegible]

**Chain V:**

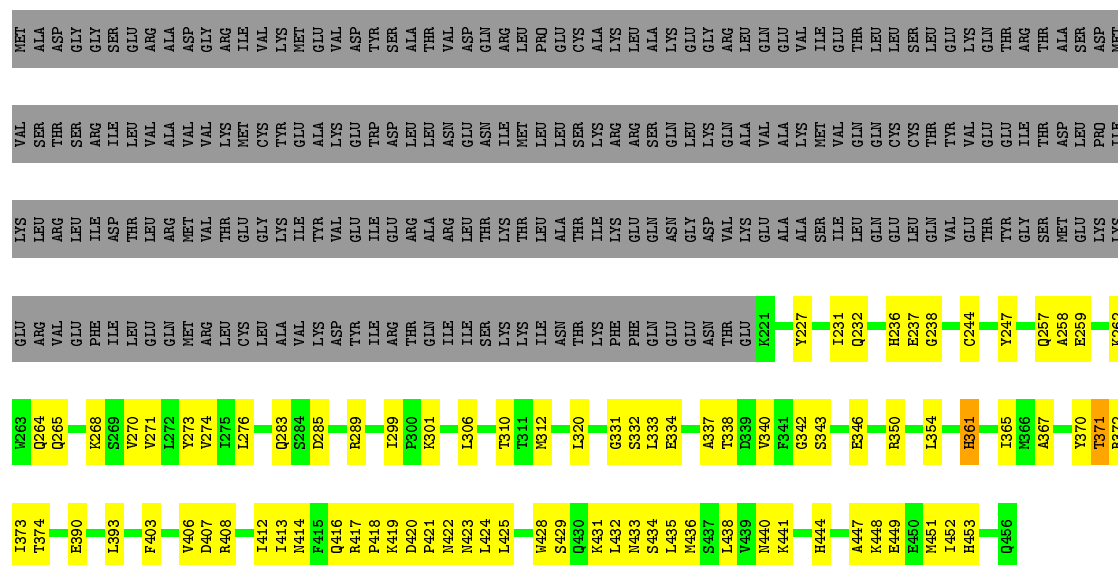
Category	Value (%)
LVS	51%
GLN	
GLY	
SER	
ALA	
ARG	
PHE	
ASP	
VAL	
PRO	
THR	
LEU	
ISL	
TYR	
ASN	
GLY	
ALA	
ASP	
VAL	
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ALA	





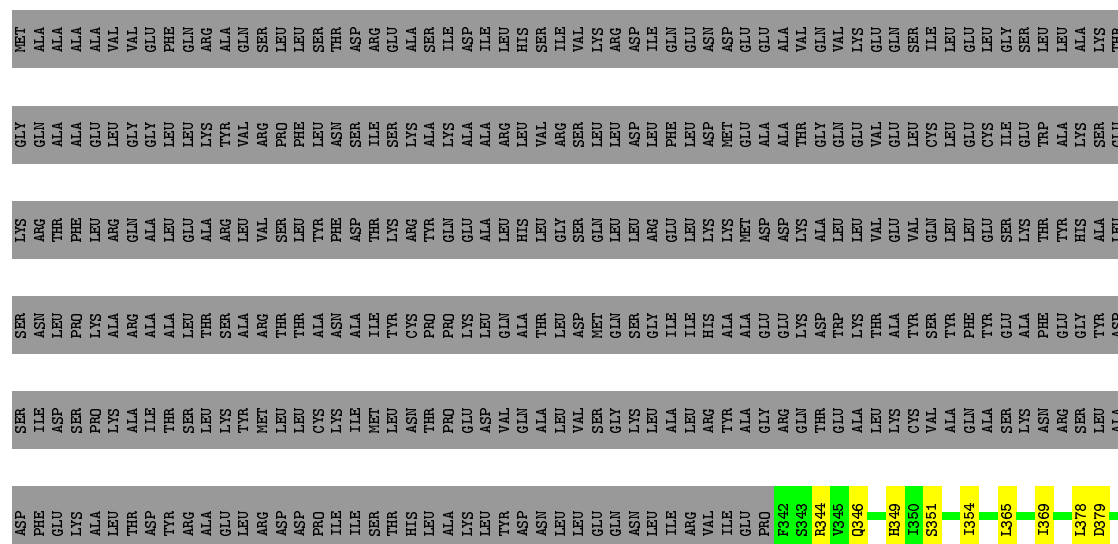
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 33% 18% 48%



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

Chain X: 14% 5% 81%

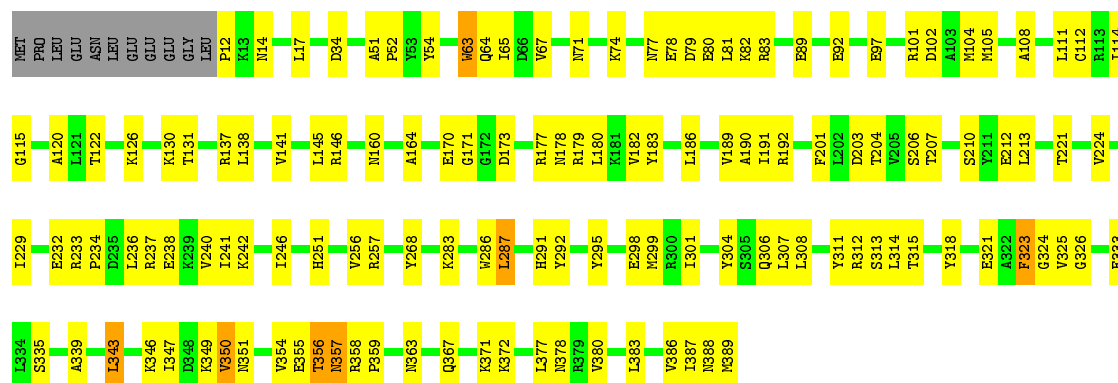






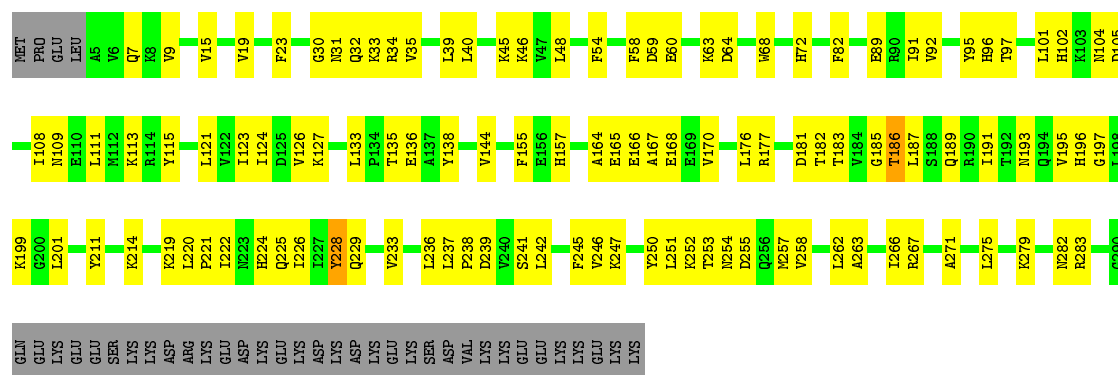
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:  63% 33% . .



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

Chain Z:  54% 34% 12%



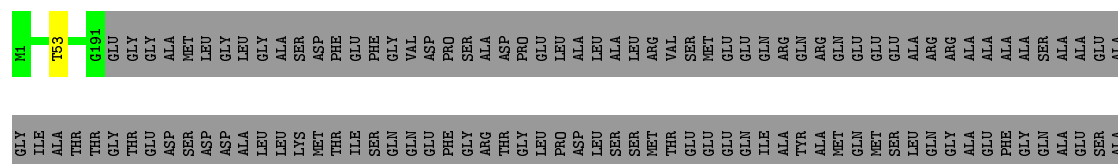
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

Chain a:  98% ..



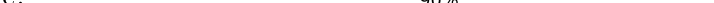
- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain b:  50% 49%





GLY  
LYS  
LYS  
ASP  
LYS  
LYS  
GLU  
GLU  
ASP  
LYS  
LYS

- Chain c:  90% • 7%

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

Chain d:  72% . 26%

ARG	LYS	MET	ALA	ALA	ALA	VAL	ASN	GLY	ALA	ALA	GLY	PHE	SER	SER	SER	GLY	PRO	ALA	ALA	THR	SER	GLY	ALA	VAL	LEU	GLN	ALA	ALA	THR	GLY	M1	Y2	E3	L107	H116	R121	R213	V257
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----	------	------	------	------	------

- Chain e:  34% 66%

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

Chain f:  90% • 7%

GLY	GLU	ARG	ALA	GLU	LEU	ALA	THR	GLU	GLU	PHE	LEU	PRO	VAL	THR	PRO	ILE	LEU	GLU	GLY	PHE	VAL	ILE	LEU	ARG	LYS	ASN	PRO	TYR	ASN	ASP	LEU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	18443	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.27	0/2886	0.54	0/3899
10	J	0.23	0/1728	0.44	0/2358
11	K	0.24	0/1747	0.44	0/2364
12	L	0.24	0/1885	0.44	0/2552
13	M	0.23	0/1891	0.42	0/2552
14	N	0.24	0/1454	0.42	0/1967
15	O	0.23	0/1670	0.43	0/2265
16	P	0.24	0/1614	0.41	0/2177
17	Q	0.23	0/1603	0.41	0/2174
18	R	0.23	0/1579	0.39	0/2134
19	S	0.24	0/1671	0.41	0/2253
2	B	0.27	0/2700	0.55	0/3645
20	T	0.25	0/1700	0.41	0/2305
21	U	0.23	0/6396	0.42	0/8646
22	V	0.25	0/3929	0.52	2/5309 (0.0%)
23	W	0.24	0/1975	0.46	0/2659
24	X	0.22	0/655	0.40	0/877
25	Y	0.24	0/3173	0.47	2/4273 (0.0%)
26	Z	1.86	6/2324 (0.3%)	0.53	0/3150
27	a	1.52	2/3052 (0.1%)	0.55	4/4130 (0.1%)
28	b	0.25	0/1478	0.43	0/2001
29	c	0.25	0/2302	0.53	2/3110 (0.1%)
3	C	0.25	0/3054	0.52	1/4107 (0.0%)
30	d	0.25	0/2162	0.51	0/2919
31	e	0.24	0/198	0.53	0/258
32	f	0.27	1/5413 (0.0%)	0.53	3/7317 (0.0%)
4	D	0.26	0/3090	0.53	0/4168
5	E	0.25	0/2835	0.48	0/3821
6	F	0.26	0/2903	0.54	0/3912
7	G	0.23	0/1859	0.45	0/2523
8	H	0.25	0/1743	0.46	0/2372
9	I	0.23	0/1942	0.45	0/2628



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
All	All	0.51	9/74611 (0.0%)	0.48	14/100825 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
21	U	0	3
22	V	0	2
25	Y	0	1
3	C	0	1
30	d	0	1
32	f	0	2
5	E	0	1
6	F	0	2
All	All	0	15

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	215	GLU	CG-CD	82.57	2.75	1.51
26	Z	228	TYR	CD2-CE2	46.09	2.08	1.39
26	Z	228	TYR	CD1-CE1	45.24	2.07	1.39
26	Z	228	TYR	CE1-CZ	34.72	1.83	1.38
26	Z	228	TYR	CE2-CZ	33.47	1.82	1.38
26	Z	228	TYR	CG-CD1	26.67	1.73	1.39
26	Z	228	TYR	CG-CD2	26.35	1.73	1.39
27	a	215	GLU	CB-CG	6.88	1.65	1.52
32	f	681	LEU	C-N	6.33	1.46	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	215	GLU	OE1-CD-OE2	-19.13	100.35	123.30
27	a	215	GLU	CG-CD-OE1	6.35	131.00	118.30
29	c	243	SER	C-N-CA	6.19	137.17	121.70
27	a	215	GLU	CB-CG-CD	6.17	130.86	114.20
32	f	459	GLU	N-CA-C	6.13	127.56	111.00
3	C	217	SER	C-N-CA	5.99	136.67	121.70
25	Y	63	TRP	C-N-CA	5.79	136.19	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	661	GLY	N-CA-C	5.68	127.29	113.10
25	Y	287	LEU	CA-CB-CG	5.54	128.04	115.30
22	V	195	ILE	C-N-CA	5.32	135.00	121.70
32	f	636	GLY	N-CA-C	5.27	126.28	113.10
27	a	215	GLU	CG-CD-OE2	5.17	128.65	118.30
29	c	243	SER	CA-C-N	5.09	128.40	117.20
22	V	81	GLN	C-N-CA	5.07	134.37	121.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	133	VAL	Peptide
2	B	264	PRO	Peptide
3	C	171	HIS	Peptide
5	E	292	PRO	Peptide
6	F	294	LYS	Peptide
6	F	87	PRO	Peptide
21	U	432	SER	Peptide
21	U	433	PRO	Peptide
21	U	435	SER	Peptide
22	V	193	GLN	Peptide
22	V	319	HIS	Peptide
25	Y	357	ASN	Peptide
30	d	3	GLU	Peptide
32	f	667	GLN	Peptide
32	f	681	LEU	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	226	0
2	B	2662	0	2702	193	0
3	C	3015	0	3125	201	0
4	D	3040	0	3076	224	0
5	E	2790	0	2846	182	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	2863	0	2931	202	0
7	G	1826	0	1796	74	0
8	H	1708	0	1594	45	0
9	I	1912	0	1851	46	0
10	J	1704	0	1517	49	0
11	K	1722	0	1673	68	0
12	L	1850	0	1822	63	0
13	M	1856	0	1814	67	0
14	N	1430	0	1398	23	0
15	O	1643	0	1644	21	0
16	P	1585	0	1598	26	0
17	Q	1570	0	1547	50	0
18	R	1548	0	1499	31	0
19	S	1641	0	1618	25	0
20	T	1667	0	1628	42	0
21	U	6287	0	6338	191	0
22	V	3852	0	3893	181	0
23	W	1940	0	1978	73	0
24	X	647	0	676	22	0
25	Y	3115	0	3120	100	0
26	Z	2281	0	2312	95	0
27	a	2995	0	3011	0	0
28	b	1458	0	1505	0	0
29	c	2260	0	2276	0	0
30	d	2116	0	2146	0	0
31	e	197	0	199	0	0
32	f	5331	0	5344	0	0
33	A	27	0	12	5	0
33	B	27	0	12	8	0
33	C	27	0	12	2	0
33	D	27	0	12	4	0
33	E	27	0	12	7	0
33	F	27	0	12	4	0
34	c	1	0	0	0	0
All	All	73509	0	73428	2249	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 19.

All (2249) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:228:TYR:CZ	26:Z:228:TYR:CE1	1.83	1.63
26:Z:228:TYR:CZ	26:Z:228:TYR:CE2	1.82	1.60
26:Z:228:TYR:CD2	26:Z:228:TYR:CE2	2.08	1.42
26:Z:228:TYR:CD1	26:Z:228:TYR:CE1	2.07	1.40
1:A:362:MET:HB2	2:B:216:ILE:HD11	1.47	0.97
3:C:217:SER:HB3	3:C:218:GLU:HB3	1.45	0.96
26:Z:63:LYS:HB2	26:Z:64:ASP:HB2	1.52	0.91
5:E:50:LEU:HD13	6:F:138:GLY:HA2	1.50	0.91
3:C:70:GLY:O	3:C:118:ASN:ND2	2.05	0.89
26:Z:224:HIS:HB3	26:Z:225:GLN:HA	1.56	0.88
4:D:151:ILE:HB	4:D:152:MET:HA	1.54	0.88
1:A:205:GLY:HA2	1:A:206:ILE:HG22	1.58	0.83
4:D:83:GLN:HE22	4:D:140:VAL:HG21	1.44	0.83
3:C:84:LYS:HA	3:C:98:ASP:HA	1.61	0.82
23:W:416:GLN:HB3	23:W:417:ARG:HA	1.60	0.82
3:C:299:ASP:HA	3:C:302:ASP:HB3	1.61	0.82
6:F:299:GLU:HG3	6:F:300:LYS:HB3	1.61	0.82
1:A:271:LEU:HA	1:A:315:ILE:HB	1.61	0.81
1:A:385:ILE:HA	1:A:388:VAL:HB	1.62	0.80
22:V:57:ALA:HB3	22:V:58:ALA:HB3	1.64	0.80
4:D:89:ILE:HA	4:D:131:ALA:HA	1.64	0.80
4:D:389:GLU:HB2	4:D:391:ARG:HB2	1.64	0.80
4:D:113:VAL:HG11	4:D:138:ALA:HA	1.64	0.79
4:D:184:PRO:HB2	4:D:306:LYS:HE2	1.63	0.79
11:K:225:ASN:HA	11:K:227:HIS:HB3	1.65	0.79
3:C:99:VAL:HA	3:C:100:ASP:HB2	1.63	0.79
6:F:316:GLN:HA	6:F:320:PHE:HB2	1.64	0.79
22:V:193:GLN:HB3	22:V:194:LYS:HA	1.64	0.79
4:D:243:GLY:HA3	4:D:288:ILE:HD13	1.65	0.79
5:E:126:ASP:HB2	5:E:185:ARG:HG2	1.62	0.79
26:Z:233:VAL:HA	26:Z:236:LEU:HD13	1.64	0.79
1:A:344:SER:N	1:A:345:LEU:HB2	1.98	0.78
5:E:250:ASP:HB2	6:F:300:LYS:HD3	1.66	0.78
22:V:148:ARG:HG3	22:V:149:PRO:HD3	1.67	0.77
3:C:157:GLN:NE2	3:C:316:GLU:O	2.18	0.77
2:B:387:LYS:HB3	2:B:390:LEU:HD11	1.65	0.77
5:E:262:ASN:HA	5:E:265:ASP:HB2	1.67	0.77
6:F:120:LYS:HD2	6:F:136:VAL:HG21	1.68	0.76
2:B:232:LYS:N	33:B:501:ADP:O1A	2.19	0.76
6:F:84:LYS:N	6:F:85:THR:HA	1.98	0.76
3:C:41:ASN:HD21	22:V:492:LYS:HD3	1.48	0.76
5:E:320:ILE:HD13	6:F:217:ILE:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:279:THR:O	4:D:283:ARG:N	2.17	0.75
2:B:261:GLY:HA2	2:B:262:ASP:HB3	1.69	0.74
5:E:60:VAL:HG23	5:E:98:VAL:HG21	1.70	0.74
6:F:94:ILE:HB	6:F:123:VAL:HB	1.70	0.74
22:V:192:MET:HA	22:V:193:GLN:HB2	1.68	0.74
1:A:90:GLU:O	1:A:94:GLN:HB2	1.87	0.74
2:B:105:THR:HG23	2:B:106:PRO:HD3	1.68	0.73
5:E:109:ARG:HH12	6:F:121:CYS:HB2	1.53	0.73
1:A:157:ILE:HG22	1:A:158:ASP:HA	1.69	0.73
5:E:290:LEU:HA	5:E:295:LEU:HD12	1.70	0.73
2:B:131:HIS:NE2	2:B:156:VAL:O	2.22	0.73
23:W:257:GLN:HA	23:W:258:ALA:HB3	1.71	0.73
7:G:219:VAL:HG12	7:G:230:LEU:HD11	1.70	0.73
24:X:417:LYS:HD2	25:Y:383:LEU:HD23	1.70	0.73
3:C:118:ASN:OD1	3:C:118:ASN:N	2.21	0.72
3:C:65:LEU:O	3:C:69:GLN:NE2	2.22	0.72
26:Z:97:THR:HA	26:Z:124:ILE:HG13	1.70	0.72
8:H:71:HIS:HA	8:H:218:PHE:H	1.52	0.72
12:L:105:VAL:HG21	12:L:136:GLY:HA3	1.71	0.72
22:V:435:GLU:HG2	22:V:453:HIS:CE1	2.24	0.72
22:V:195:ILE:H	22:V:196:SER:HB3	1.53	0.72
4:D:133:HIS:HB3	4:D:138:ALA:H	1.53	0.72
6:F:233:LYS:N	33:F:501:ADP:O1A	2.23	0.72
23:W:418:PRO:HA	23:W:419:LYS:HB2	1.72	0.72
3:C:263:SER:O	3:C:267:SER:N	2.20	0.71
4:D:83:GLN:HG3	4:D:133:HIS:CD2	2.25	0.71
6:F:168:TYR:HB2	6:F:169:ASP:HB2	1.72	0.71
3:C:137:LEU:HA	3:C:140:VAL:HG12	1.71	0.71
2:B:264:PRO:HG3	2:B:311:GLU:HG2	1.72	0.71
6:F:86:LEU:HD12	6:F:87:PRO:HD2	1.72	0.71
1:A:90:GLU:HG3	1:A:94:GLN:HE21	1.53	0.71
6:F:267:LEU:O	6:F:271:ALA:N	2.22	0.71
22:V:326:GLN:HB3	22:V:353:LEU:HD13	1.73	0.71
3:C:42:LEU:HB2	26:Z:167:ALA:HB1	41.20	0.71
2:B:307:ARG:HA	2:B:310:LEU:HB3	1.73	0.71
10:J:115:LYS:HE3	10:J:127:PHE:HB2	1.70	0.71
4:D:185:LEU:HD11	4:D:259:PRO:HB3	1.71	0.71
21:U:799:LYS:HA	21:U:843:GLU:HG3	1.72	0.71
6:F:85:THR:H	6:F:159:LEU:HD11	1.56	0.70
21:U:740:GLY:HA3	21:U:744:VAL:HG22	1.74	0.70
1:A:284:ARG:O	1:A:296:GLN:NE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:266:GLY:HA2	5:E:267:PHE:HB2	1.71	0.70
9:I:29:GLY:O	9:I:166:ASN:ND2	2.25	0.70
26:Z:33:LYS:NZ	26:Z:34:ARG:O	2.25	0.70
4:D:167:ILE:HG21	33:D:501:ADP:HN62	1.55	0.70
4:D:285:VAL:HA	4:D:288:ILE:HB	1.74	0.70
16:P:61:GLN:HE22	17:Q:124:LEU:HB2	1.57	0.70
2:B:111:THR:OG1	2:B:124:SER:O	2.10	0.69
4:D:401:LYS:HG3	4:D:404:LYS:HE2	1.74	0.69
21:U:191:LYS:HG3	21:U:194:ARG:HE	1.57	0.69
7:G:16:PHE:HB2	8:H:128:ARG:HH22	1.56	0.69
21:U:842:LYS:HA	21:U:843:GLU:HB3	1.72	0.69
1:A:380:SER:HB3	1:A:385:ILE:HG21	1.74	0.69
2:B:378:VAL:HG22	2:B:416:ASN:HB2	1.73	0.69
4:D:246:MET:O	4:D:250:VAL:N	2.25	0.69
17:Q:117:TYR:HB3	17:Q:125:ALA:HB3	1.75	0.69
3:C:328:ILE:HG23	3:C:359:VAL:HG11	1.75	0.69
4:D:230:VAL:HG23	4:D:264:ILE:HA	1.73	0.69
1:A:232:ARG:HH12	1:A:271:LEU:HD13	1.56	0.69
1:A:384:GLU:H	2:B:343:ARG:HH11	1.40	0.69
3:C:113:ARG:NH1	3:C:128:PRO:O	2.25	0.69
8:H:25:ALA:HB2	8:H:128:ARG:HE	1.58	0.69
12:L:75:ALA:HB3	12:L:131:GLY:HA3	1.74	0.69
21:U:112:CYS:SG	21:U:159:ARG:NH1	2.66	0.69
23:W:432:LEU:HD23	23:W:435:LEU:HD22	1.74	0.69
3:C:145:ASP:HB3	3:C:201:ARG:HG2	1.75	0.69
4:D:248:ARG:NH2	4:D:291:GLU:OE2	2.26	0.69
21:U:356:THR:HG21	21:U:731:ILE:HD13	1.72	0.69
23:W:407:ASP:H	23:W:413:ILE:HG22	1.58	0.69
1:A:240:VAL:HB	1:A:274:PHE:HA	1.74	0.68
4:D:194:ILE:HG13	4:D:196:ILE:H	1.58	0.68
5:E:207:TYR:HD1	5:E:208:ILE:HD12	1.58	0.68
7:G:183:VAL:HG12	7:G:184:LYS:HG2	1.72	0.68
22:V:275:VAL:HB	22:V:277:PRO:HD3	1.73	0.68
1:A:409:PHE:O	1:A:413:VAL:N	2.25	0.68
22:V:413:SER:OG	25:Y:335:SER:OG	2.09	0.68
1:A:112:ILE:HA	1:A:122:VAL:HA	1.75	0.68
8:H:231:ALA:HB3	8:H:232:ALA:HB3	1.74	0.68
11:K:209:LYS:O	11:K:214:ASN:ND2	2.25	0.68
25:Y:138:LEU:HD11	25:Y:180:LEU:HD11	1.75	0.68
1:A:413:VAL:HA	1:A:416:VAL:HG12	1.74	0.68
2:B:103:ARG:HG2	2:B:160:ILE:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:64:GLN:HG2	25:Y:65:ILE:HG22	1.74	0.68
24:X:395:LYS:HD3	26:Z:258:VAL:HG13	1.75	0.68
11:K:16:SER:HB3	11:K:20:ARG:H	1.59	0.68
21:U:155:LEU:O	21:U:158:ARG:NH1	2.26	0.68
21:U:446:LEU:O	21:U:450:HIS:ND1	2.26	0.68
22:V:259:LEU:HD11	22:V:294:ARG:HD2	1.76	0.68
6:F:308:ARG:HA	6:F:311:LEU:HB2	1.76	0.68
1:A:410:LEU:O	1:A:414:ASN:ND2	2.27	0.68
1:A:182:GLU:HA	1:A:185:GLU:HB3	1.73	0.68
2:B:175:LYS:O	3:C:232:ARG:NH1	2.27	0.68
1:A:80:LEU:HD22	2:B:99:VAL:HG11	1.75	0.68
21:U:418:GLU:HG3	21:U:421:GLN:HE21	1.59	0.68
22:V:262:SER:HB2	22:V:263:LEU:HB2	1.74	0.68
21:U:108:TYR:OH	21:U:159:ARG:NH2	2.27	0.67
23:W:441:LYS:HE3	26:Z:233:VAL:HG12	1.75	0.67
1:A:398:ARG:NH1	2:B:195:GLN:O	2.21	0.67
2:B:294:ARG:NH1	2:B:295:TYR:O	2.26	0.67
23:W:373:ILE:HG12	23:W:374:THR:H	1.59	0.67
1:A:123:VAL:HG21	1:A:147:TYR:HB2	1.74	0.67
4:D:260:ALA:H	4:D:304:ASN:HD22	1.40	0.67
3:C:218:GLU:OE2	4:D:286:GLN:NE2	2.25	0.67
2:B:175:LYS:HB3	2:B:176:VAL:HB	1.76	0.67
6:F:249:LEU:HB2	6:F:283:ILE:HG13	1.76	0.67
21:U:808:PRO:HD3	21:U:836:THR:HB	1.76	0.67
9:I:76:VAL:HG23	9:I:134:LEU:HB3	1.76	0.67
17:Q:183:ILE:HG12	17:Q:188:ILE:HG13	1.75	0.67
22:V:255:LEU:HD22	22:V:291:TYR:HB3	1.76	0.67
23:W:420:ASP:HB3	23:W:422:ASN:HB3	1.76	0.67
1:A:292:ASP:O	1:A:296:GLN:N	2.25	0.67
1:A:258:ARG:NH2	6:F:255:GLN:OE1	2.28	0.67
15:O:30:ASN:OD1	15:O:187:ARG:NH2	2.27	0.67
22:V:321:ALA:HB1	22:V:322:VAL:HB	1.75	0.67
2:B:174:MET:HA	2:B:248:LEU:HD13	1.76	0.66
4:D:249:ASP:HA	4:D:252:ARG:HG2	1.77	0.66
4:D:345:PHE:HB3	4:D:360:LEU:HD13	1.76	0.66
9:I:12:PHE:HB2	10:J:18:GLN:HB3	1.78	0.66
16:P:58:THR:OG1	17:Q:121:LEU:O	2.12	0.66
7:G:43:ARG:HB3	7:G:164:LYS:HA	1.76	0.66
12:L:151:ALA:O	13:M:85:ARG:NH2	2.27	0.66
1:A:140:VAL:HA	1:A:152:PRO:HA	1.77	0.66
6:F:263:ASP:O	6:F:267:LEU:N	2.22	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:474:ARG:NH1	21:U:500:ASN:O	2.24	0.66
1:A:304:ASN:HD22	6:F:254:PRO:HG2	1.59	0.66
22:V:349:ARG:HH12	22:V:361:PHE:HB2	1.59	0.66
26:Z:220:LEU:HB3	26:Z:221:PRO:HA	1.78	0.66
1:A:410:LEU:HA	1:A:413:VAL:HB	1.77	0.66
5:E:178:THR:HG23	33:E:401:ADP:C8	2.31	0.66
3:C:38:LYS:HA	22:V:492:LYS:HB3	1.77	0.66
1:A:362:MET:HG2	1:A:363:SER:H	1.61	0.66
4:D:355:SER:HB2	4:D:393:ILE:HG21	1.78	0.65
6:F:209:LYS:NZ	6:F:217:ILE:O	2.28	0.65
15:O:42:TYR:HB2	15:O:178:ILE:HD11	1.79	0.65
3:C:182:GLN:NE2	3:C:286:THR:O	2.30	0.65
3:C:268:GLU:HA	3:C:271:ARG:HB3	1.79	0.65
4:D:287:ARG:O	4:D:291:GLU:N	2.27	0.65
2:B:191:ASP:HA	2:B:194:ILE:HG22	1.77	0.65
2:B:416:ASN:HA	2:B:419:PHE:HB3	1.77	0.65
4:D:89:ILE:O	4:D:106:THR:OG1	2.15	0.65
21:U:14:GLU:O	21:U:20:LYS:NZ	2.26	0.65
21:U:341:PHE:HB2	21:U:881:PRO:HD2	1.77	0.65
3:C:188:LEU:HB3	3:C:317:PHE:HB2	1.78	0.65
4:D:335:LEU:HD11	4:D:372:GLY:HA2	1.78	0.65
1:A:122:VAL:HG21	6:F:150:LEU:HD21	1.79	0.65
1:A:348:LEU:HD21	11:K:32:LYS:HE3	1.79	0.65
4:D:373:ALA:HB1	4:D:374:ASP:HB3	1.77	0.65
5:E:47:LEU:HA	5:E:50:LEU:HD12	1.78	0.65
7:G:109:ILE:HD11	7:G:114:LEU:HB2	1.79	0.65
25:Y:79:ASP:HA	25:Y:82:LYS:HG2	1.78	0.65
3:C:169:VAL:HG21	3:C:207:THR:HG21	1.78	0.65
5:E:281:ARG:HD3	5:E:387:LYS:HE3	1.78	0.65
6:F:417:HIS:HA	6:F:420:TYR:HB2	1.78	0.65
9:I:26:GLU:O	9:I:30:HIS:ND1	2.27	0.65
1:A:303:ILE:HD12	1:A:332:MET:HG2	1.77	0.65
4:D:129:SER:HB2	4:D:252:ARG:HH12	1.62	0.65
2:B:291:GLY:HA2	2:B:336:THR:HG21	1.79	0.64
3:C:182:GLN:HE21	3:C:287:LYS:HG2	1.61	0.64
8:H:135:LEU:HD23	8:H:148:GLN:HB2	1.78	0.64
1:A:290:GLY:O	6:F:295:ARG:NH1	2.30	0.64
4:D:406:VAL:HG23	4:D:407:ILE:HB	1.79	0.64
5:E:309:ARG:NH2	5:E:338:PHE:O	2.30	0.64
21:U:208:LEU:HD23	21:U:210:LYS:H	1.62	0.64
25:Y:251:HIS:HA	25:Y:257:ARG:HD3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:63:TRP:HB3	25:Y:64:GLN:HB3	1.79	0.64
26:Z:241:SER:HB3	26:Z:245:PHE:HB3	1.79	0.64
4:D:100:THR:HB	4:D:114:ARG:HD2	1.78	0.64
4:D:229:ARG:NH2	5:E:267:PHE:O	2.29	0.64
6:F:138:GLY:O	6:F:160:ILE:N	2.31	0.64
6:F:150:LEU:HD22	6:F:164:LEU:HB3	1.78	0.64
21:U:376:MET:O	21:U:741:GLY:N	2.31	0.64
22:V:362:LEU:HB3	22:V:382:PHE:HE2	1.63	0.64
23:W:432:LEU:HA	23:W:435:LEU:HB2	1.80	0.64
2:B:112:LEU:HB2	2:B:150:VAL:HG13	1.80	0.64
20:T:51:LEU:HD11	20:T:110:MET:HB3	1.80	0.64
22:V:281:ASN:ND2	25:Y:389:MET:SD	2.71	0.64
22:V:344:ASP:HB2	22:V:368:ARG:HH11	1.62	0.64
22:V:97:ALA:HB3	22:V:98:LEU:HA	1.79	0.64
3:C:14:GLY:O	3:C:18:SER:N	2.31	0.64
5:E:310:LEU:O	5:E:314:LYS:NZ	2.27	0.64
11:K:93:ARG:NH1	18:R:68:LEU:O	2.31	0.64
21:U:249:CYS:HB3	21:U:328:ILE:HD12	1.78	0.64
20:T:99:ARG:HG3	20:T:105:PRO:HA	1.80	0.64
5:E:86:GLN:OE1	6:F:117:ARG:NH2	2.31	0.63
1:A:339:ARG:NH2	6:F:402:GLU:OE1	2.32	0.63
21:U:444:TYR:HB2	21:U:476:GLY:HA3	1.81	0.63
6:F:298:SER:HB3	6:F:299:GLU:HB2	1.80	0.63
23:W:331:GLY:HA2	23:W:332:SER:HB3	1.79	0.63
4:D:284:GLU:O	4:D:288:ILE:N	2.31	0.63
9:I:45:LEU:HD11	9:I:137:ILE:HG12	1.80	0.63
16:P:11:VAL:HG11	16:P:52:GLY:HA3	1.81	0.63
1:A:103:ASN:HB2	1:A:112:ILE:HG23	1.78	0.63
1:A:205:GLY:HA2	1:A:206:ILE:CG2	2.29	0.63
20:T:174:ARG:HG3	20:T:207:THR:HG22	1.79	0.63
2:B:317:ASP:HB3	2:B:318:GLY:HA2	1.79	0.63
3:C:22:GLN:HB3	22:V:195:ILE:HD13	1.81	0.63
1:A:168:GLU:HA	1:A:236:CYS:HB2	1.79	0.63
6:F:79:LYS:HA	6:F:82:VAL:HG22	1.80	0.63
7:G:211:LYS:NZ	7:G:213:SER:OG	2.31	0.63
2:B:133:VAL:HG21	2:B:159:VAL:HG12	1.81	0.63
16:P:27:ARG:HB2	16:P:183:MET:HB2	1.79	0.63
1:A:333:ARG:HB2	1:A:337:LEU:HB2	1.81	0.63
5:E:171:LEU:HD22	5:E:295:LEU:HD13	1.81	0.63
7:G:86:ASP:OD2	7:G:132:ARG:NH2	2.32	0.63
17:Q:178:PHE:HB2	17:Q:194:ILE:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:TYR:CE2	2:B:350:LYS:HE3	2.34	0.62
2:B:398:ILE:HG22	2:B:426:VAL:HG11	1.80	0.62
5:E:288:ALA:O	5:E:294:ARG:NH1	2.32	0.62
5:E:177:GLY:H	5:E:303:LEU:HD12	1.63	0.62
11:K:203:LYS:HD3	11:K:241:ILE:HD11	1.81	0.62
4:D:286:GLN:HA	4:D:289:LEU:HB3	1.80	0.62
5:E:131:SER:HA	5:E:134:GLU:HB2	1.79	0.62
21:U:685:GLN:HB2	21:U:726:ALA:HA	1.80	0.62
13:M:236:GLU:O	13:M:240:LYS:NZ	2.27	0.62
1:A:122:VAL:O	6:F:88:TYR:HA	1.99	0.62
1:A:353:HIS:HA	1:A:356:LYS:HB2	1.82	0.62
3:C:171:HIS:O	3:C:173:GLU:N	2.32	0.62
3:C:63:LEU:HD11	4:D:133:HIS:CD2	2.34	0.62
7:G:22:LEU:HD13	7:G:25:VAL:HB	1.81	0.62
3:C:313:ARG:NH1	3:C:314:LYS:O	2.32	0.62
4:D:269:ALA:HB2	5:E:258:MET:HG3	1.80	0.62
11:K:10:ARG:NH2	12:L:4:ASN:O	2.31	0.62
21:U:247:GLN:HE22	21:U:912:ILE:HG22	1.64	0.62
1:A:115:VAL:HG13	1:A:117:GLN:H	1.65	0.62
1:A:206:ILE:HG23	1:A:207:GLU:H	1.64	0.62
6:F:392:ASN:HB2	6:F:395:GLN:HG3	1.80	0.62
21:U:842:LYS:HG2	21:U:882:ALA:HB2	1.81	0.62
7:G:49:VAL:HG22	7:G:219:VAL:HG23	1.81	0.62
10:J:23:GLN:HG2	10:J:149:PRO:HG2	1.81	0.62
15:O:215:LYS:HB3	16:P:197:THR:HB	1.81	0.62
21:U:800:VAL:HG21	21:U:914:LEU:HD21	1.81	0.62
25:Y:232:GLU:HG2	25:Y:234:PRO:HD2	1.81	0.62
26:Z:33:LYS:HE2	26:Z:59:ASP:HA	1.81	0.62
3:C:386:ALA:HA	3:C:389:LYS:HB2	1.80	0.62
4:D:414:HIS:NE2	7:G:21:ARG:HB2	2.15	0.62
5:E:292:PRO:HA	5:E:295:LEU:O	2.00	0.62
6:F:137:ILE:HG21	6:F:160:ILE:HB	1.80	0.62
24:X:420:LYS:HD2	26:Z:283:ARG:HD2	1.81	0.62
1:A:184:ILE:HD13	1:A:224:LEU:HD22	1.82	0.62
5:E:329:GLU:HA	5:E:332:VAL:HB	1.82	0.62
6:F:121:CYS:SG	6:F:122:ALA:N	2.73	0.62
8:H:93:LEU:HD21	8:H:113:ARG:HE	1.64	0.62
21:U:374:SER:HA	21:U:411:ILE:HG12	1.81	0.62
3:C:83:LYS:HA	3:C:105:ILE:HD11	1.81	0.62
25:Y:173:ASP:HB2	25:Y:177:ARG:HG3	1.82	0.62
25:Y:312:ARG:HG3	25:Y:313:SER:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:MET:HG3	3:C:96:VAL:HG13	1.82	0.61
5:E:178:THR:HG22	5:E:339:ASN:HB3	1.82	0.61
6:F:303:ASP:O	6:F:307:GLN:N	2.33	0.61
1:A:111:TYR:HE2	1:A:125:LEU:HD23	1.64	0.61
4:D:151:ILE:CB	4:D:152:MET:HA	2.29	0.61
17:Q:45:LEU:HB3	17:Q:102:LEU:HD13	1.83	0.61
17:Q:13:VAL:HB	17:Q:183:ILE:HB	1.81	0.61
10:J:88:ARG:HH22	17:Q:69:MET:HB2	1.66	0.61
21:U:792:ASN:HA	21:U:914:LEU:HB3	1.81	0.61
25:Y:112:CYS:SG	25:Y:120:ALA:N	2.73	0.61
6:F:229:PRO:HB3	33:F:501:ADP:H5'1	1.82	0.61
19:S:57:PHE:HD2	19:S:60:ASP:H	1.49	0.61
4:D:121:ARG:HA	22:V:262:SER:HB3	73.02	0.61
1:A:191:VAL:HG13	1:A:192:GLU:H	1.66	0.61
21:U:429:LYS:HA	21:U:430:ASP:HB3	1.82	0.61
25:Y:323:PHE:HD2	25:Y:326:GLY:HA3	1.66	0.61
26:Z:7:GLN:OE1	26:Z:46:LYS:NZ	2.32	0.61
4:D:247:VAL:HA	4:D:250:VAL:HB	1.82	0.61
8:H:75:VAL:HG23	8:H:135:LEU:HB2	1.82	0.61
21:U:12:LEU:HD22	21:U:20:LYS:HG3	1.80	0.61
22:V:224:LEU:O	22:V:227:VAL:N	2.29	0.61
3:C:192:PRO:HG3	3:C:296:ASN:HD21	1.64	0.61
3:C:236:VAL:HG22	3:C:239:ARG:HH12	1.64	0.61
3:C:271:ARG:HD3	3:C:274:LEU:HB2	1.81	0.61
6:F:233:LYS:O	6:F:237:ALA:N	2.29	0.61
21:U:388:ASP:OD1	21:U:389:ASN:ND2	2.34	0.61
25:Y:357:ASN:HB2	25:Y:358:ARG:HA	1.82	0.61
26:Z:124:ILE:HA	26:Z:135:THR:HA	1.83	0.61
4:D:212:LYS:HE3	4:D:310:ALA:HB1	1.83	0.61
6:F:366:MET:O	6:F:370:SER:N	2.29	0.61
21:U:789:ILE:HB	21:U:911:ILE:HA	1.83	0.61
2:B:346:ARG:NH1	2:B:348:ASP:OD2	2.33	0.61
3:C:67:GLN:HB2	4:D:135:HIS:HB3	1.82	0.61
4:D:207:PRO:HB3	4:D:210:CYS:HA	1.83	0.61
5:E:178:THR:OG1	33:E:401:ADP:O5'	2.18	0.61
6:F:284:PHE:HD1	6:F:329:ILE:HB	1.64	0.61
13:M:141:SER:HB3	13:M:144:ASP:HB2	1.83	0.61
23:W:416:GLN:HB3	23:W:417:ARG:CA	2.29	0.61
1:A:305:GLN:O	1:A:312:ARG:NE	2.33	0.61
1:A:386:ARG:NH2	33:A:501:ADP:O2'	2.34	0.61
11:K:225:ASN:HB2	11:K:226:PHE:CG	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:60:VAL:HA	5:E:71:VAL:HG12	1.82	0.60
4:D:87:LEU:HD11	4:D:133:HIS:HA	1.82	0.60
11:K:199:LEU:HD13	11:K:241:ILE:HD12	1.83	0.60
1:A:232:ARG:HE	1:A:235:ALA:H	1.47	0.60
6:F:388:THR:HG22	6:F:391:PHE:HD2	1.65	0.60
11:K:94:VAL:O	11:K:98:ASN:ND2	2.32	0.60
21:U:252:LEU:HD21	21:U:264:VAL:HG11	1.82	0.60
5:E:229:ILE:HG23	5:E:274:LYS:HB3	1.82	0.60
5:E:241:ARG:O	5:E:242:ARG:HG2	2.02	0.60
20:T:1:THR:HG22	20:T:3:ASN:H	1.67	0.60
21:U:757:MET:HG3	21:U:758:PRO:HD3	1.84	0.60
23:W:390:GLU:HG3	23:W:408:ARG:HH21	1.66	0.60
4:D:203:LEU:O	4:D:331:ILE:HB	2.02	0.60
12:L:160:SER:O	12:L:169:ARG:NH2	2.35	0.60
3:C:85:VAL:N	3:C:97:VAL:O	2.33	0.60
4:D:202:VAL:HB	4:D:308:ILE:HA	1.83	0.60
4:D:261:ILE:HG23	4:D:306:LYS:HB2	1.83	0.60
17:Q:19:ARG:HD2	17:Q:179:SER:HB3	1.83	0.60
21:U:188:MET:HG2	21:U:194:ARG:HD3	1.83	0.60
22:V:81:GLN:HB3	22:V:82:LEU:C	2.22	0.60
3:C:76:VAL:O	3:C:111:ASN:N	2.30	0.60
4:D:130:VAL:HA	4:D:142:VAL:HA	1.84	0.60
22:V:195:ILE:N	22:V:196:SER:HB3	2.17	0.60
2:B:173:VAL:HA	3:C:232:ARG:HG2	1.83	0.60
6:F:230:GLY:H	6:F:392:ASN:HB3	1.65	0.60
21:U:221:ILE:HB	21:U:754:HIS:HB2	1.83	0.60
21:U:233:LEU:HD22	21:U:268:LEU:HD21	1.83	0.60
22:V:143:ALA:HB3	22:V:145:LEU:HB3	1.83	0.60
22:V:252:ASN:ND2	22:V:284:GLU:OE2	2.35	0.60
4:D:348:ILE:HG21	4:D:379:CYS:HB3	1.83	0.60
4:D:91:GLN:NE2	4:D:244:PRO:HB2	2.16	0.60
5:E:172:LEU:HB2	5:E:278:ALA:HB2	1.84	0.60
9:I:239:LYS:NZ	9:I:243:GLU:OE2	2.35	0.60
25:Y:308:LEU:HB3	25:Y:356:THR:HG21	1.84	0.60
11:K:16:SER:OG	11:K:18:GLU:OE1	2.19	0.59
1:A:365:GLU:HB3	1:A:368:ILE:HG13	1.84	0.59
4:D:181:VAL:O	4:D:306:LYS:NZ	2.32	0.59
5:E:50:LEU:CD1	6:F:138:GLY:HA2	2.30	0.59
7:G:38:THR:HB	7:G:53:GLN:HE22	1.67	0.59
13:M:100:SER:O	20:T:65:GLN:NE2	2.35	0.59
20:T:51:LEU:HD13	20:T:112:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:122:THR:O	22:V:125:ASN:ND2	2.35	0.59
1:A:303:ILE:HA	1:A:306:LEU:HB2	1.85	0.59
3:C:171:HIS:HB3	3:C:174:LEU:HG	1.84	0.59
1:A:327:LEU:O	1:A:331:LEU:N	2.32	0.59
1:A:381:THR:OG1	2:B:343:ARG:NH1	2.35	0.59
2:B:217:LYS:C	2:B:219:PRO:HD3	2.23	0.59
4:D:408:LYS:HB3	4:D:409:LYS:HB2	1.83	0.59
6:F:314:LEU:O	6:F:318:ASP:N	2.35	0.59
10:J:120:GLN:OE1	11:K:134:SER:N	2.34	0.59
18:R:91:LYS:NZ	18:R:117:GLU:OE1	2.35	0.59
2:B:224:LEU:HB2	2:B:330:ALA:HB2	1.85	0.59
25:Y:12:PRO:O	25:Y:146:ARG:NH1	2.35	0.59
3:C:69:GLN:HB2	3:C:118:ASN:HB2	1.84	0.59
4:D:121:ARG:HD3	22:V:263:LEU:HD13	71.05	0.59
4:D:337:ASP:H	4:D:340:GLN:HB2	1.67	0.59
6:F:181:PRO:HG2	6:F:242:ALA:HB2	1.84	0.59
9:I:49:ARG:NH1	9:I:211:VAL:O	2.36	0.59
20:T:1:THR:N	20:T:105:PRO:O	2.26	0.59
23:W:237:GLU:HG2	23:W:238:GLY:H	1.67	0.59
3:C:307:ARG:HE	3:C:312:ASP:HB2	1.66	0.59
5:E:128:GLY:HA2	5:E:129:ASN:HB2	1.85	0.59
17:Q:88:LEU:HD23	17:Q:122:ALA:HA	1.84	0.59
25:Y:170:GLU:N	25:Y:171:GLY:HA3	2.17	0.59
21:U:194:ARG:HH22	21:U:222:PHE:HB3	1.68	0.59
21:U:361:ARG:HG3	21:U:365:CYS:HB2	1.84	0.59
1:A:311:PRO:HD2	1:A:313:GLY:HA2	1.83	0.59
3:C:60:ARG:O	3:C:64:GLN:N	2.33	0.59
4:D:171:ASP:HA	4:D:174:LYS:HE2	1.84	0.59
4:D:318:ASP:HB2	4:D:321:LEU:HG	1.85	0.59
4:D:237:GLN:HG3	4:D:242:GLU:HB3	1.85	0.58
4:D:410:ASP:HA	4:D:411:GLU:HB2	1.84	0.58
5:E:335:SER:HB3	5:E:338:PHE:CE2	2.37	0.58
6:F:406:ILE:HA	6:F:409:ARG:HG2	1.84	0.58
23:W:373:ILE:HG12	23:W:374:THR:N	2.16	0.58
24:X:379:ASP:N	24:X:384:VAL:O	2.32	0.58
3:C:165:ILE:HA	3:C:290:LYS:HE3	1.85	0.58
4:D:153:MET:SD	4:D:257:ASN:ND2	2.76	0.58
5:E:223:ARG:NE	5:E:268:ASP:OD2	2.36	0.58
22:V:275:VAL:H	22:V:276:PHE:HA	1.67	0.58
12:L:120:THR:O	13:M:129:ARG:NH1	2.26	0.58
14:N:20:THR:OG1	14:N:33:LYS:NZ	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:89:ILE:HG21	4:D:143:LEU:HD11	1.86	0.58
16:P:123:SER:HB3	16:P:137:VAL:HB	1.86	0.58
23:W:423:ASN:HA	26:Z:251:LEU:HD21	1.85	0.58
3:C:202:ALA:O	3:C:206:HIS:N	2.30	0.58
4:D:284:GLU:HA	4:D:287:ARG:HB2	1.85	0.58
6:F:195:ILE:HG13	6:F:198:LEU:HD23	1.86	0.58
6:F:320:PHE:HB3	6:F:322:PRO:HD2	1.84	0.58
8:H:67:PRO:O	8:H:91:ARG:NH2	2.36	0.58
21:U:599:ILE:O	21:U:603:LEU:HB3	2.03	0.58
23:W:436:MET:O	23:W:440:ASN:ND2	2.26	0.58
2:B:220:LYS:HB2	2:B:346:ARG:HH21	1.69	0.58
2:B:404:LEU:O	2:B:408:ARG:N	2.32	0.58
3:C:338:LEU:HD13	3:C:383:PHE:HE2	1.68	0.58
3:C:67:GLN:HA	4:D:136:SER:HA	1.85	0.58
9:I:180:LYS:HB2	9:I:183:GLU:HG2	1.85	0.58
18:R:97:MET:H	18:R:116:SER:HB3	1.69	0.58
2:B:120:HIS:HB3	2:B:132:TYR:HB3	1.84	0.58
9:I:159:TRP:HB3	10:J:54:GLN:HG3	1.85	0.58
21:U:792:ASN:OD1	21:U:793:LYS:N	2.36	0.58
25:Y:108:ALA:O	25:Y:112:CYS:N	2.35	0.58
5:E:200:SER:O	6:F:308:ARG:NH1	2.36	0.58
5:E:316:HIS:CE1	5:E:344:ARG:HB2	2.39	0.58
7:G:147:GLN:HB2	7:G:150:GLN:HE21	1.67	0.58
24:X:420:LYS:HD3	25:Y:387:ILE:HG21	1.86	0.58
3:C:214:VAL:HG12	3:C:249:ASP:H	1.68	0.58
3:C:270:GLN:HB3	3:C:306:LEU:HD21	1.86	0.58
5:E:197:LYS:NZ	5:E:198:VAL:O	2.37	0.58
1:A:102:ILE:HA	1:A:113:ILE:HA	1.86	0.57
1:A:119:ALA:HB1	1:A:121:PHE:HE2	1.70	0.57
1:A:303:ILE:O	1:A:307:ASP:N	2.34	0.57
1:A:390:THR:HA	2:B:216:ILE:HG21	1.86	0.57
4:D:183:LEU:HA	4:D:186:THR:HG22	1.85	0.57
9:I:181:GLU:C	9:I:183:GLU:HB2	2.25	0.57
13:M:192:GLU:HA	13:M:195:LYS:HE3	1.86	0.57
17:Q:7:ILE:HD13	17:Q:156:ALA:HB1	1.85	0.57
2:B:349:ARG:HE	2:B:351:ILE:HG22	1.68	0.57
4:D:83:GLN:HG2	4:D:84:SER:N	2.19	0.57
7:G:14:THR:HG22	7:G:24:GLN:HB2	1.85	0.57
15:O:1:THR:N	15:O:168:GLY:O	2.36	0.57
21:U:493:VAL:O	21:U:497:LEU:HB2	2.05	0.57
22:V:174:PHE:HA	22:V:177:ASN:HD22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ILE:HG13	2:B:346:ARG:HB3	1.86	0.57
4:D:201:GLY:HA3	4:D:328:ASP:H	1.69	0.57
17:Q:52:ASP:OD1	18:R:88:TYR:OH	2.21	0.57
21:U:576:PRO:HA	21:U:579:ARG:HE	1.68	0.57
1:A:333:ARG:HH22	1:A:340:LYS:HD3	1.69	0.57
1:A:406:GLU:HA	1:A:409:PHE:CE2	2.40	0.57
2:B:294:ARG:HB3	3:C:264:GLY:H	1.70	0.57
5:E:149:ILE:HG23	5:E:274:LYS:HG2	1.87	0.57
8:H:128:ARG:HB2	8:H:129:PRO:HD2	1.85	0.57
12:L:117:GLN:NE2	13:M:83:ASP:OD1	2.37	0.57
22:V:480:ILE:HG23	26:Z:271:ALA:HB2	1.84	0.57
3:C:299:ASP:O	3:C:303:SER:N	2.36	0.57
3:C:67:GLN:CB	4:D:135:HIS:HB3	2.35	0.57
6:F:185:TYR:HE2	6:F:243:GLN:HG3	1.68	0.57
26:Z:101:LEU:HD23	26:Z:123:ILE:HD11	1.86	0.57
1:A:223:THR:O	1:A:227:ARG:N	2.30	0.57
4:D:115:ILE:HA	4:D:139:LEU:HB2	1.85	0.57
4:D:283:ARG:HA	4:D:286:GLN:HG2	1.87	0.57
9:I:136:TYR:HB2	9:I:148:TYR:HB2	1.87	0.57
11:K:90:ASP:HA	11:K:93:ARG:HD2	1.85	0.57
21:U:17:PRO:HA	21:U:20:LYS:HD3	1.86	0.57
1:A:313:GLY:C	1:A:315:ILE:H	2.08	0.57
1:A:383:ALA:HB3	2:B:343:ARG:HE	1.68	0.57
22:V:331:LEU:HD12	22:V:334:VAL:HG21	1.85	0.57
23:W:268:LYS:HE2	23:W:301:LYS:HE2	1.87	0.57
1:A:246:VAL:HG21	2:B:307:ARG:HD2	1.87	0.57
2:B:119:ASN:O	2:B:134:SER:OG	2.19	0.57
2:B:269:GLU:HA	2:B:272:ARG:HG2	1.87	0.57
5:E:345:ASN:HB3	6:F:345:SER:HB2	1.87	0.57
17:Q:29:LYS:HE2	18:R:121:ILE:HB	1.87	0.57
22:V:441:ALA:HB1	22:V:446:VAL:HB	1.85	0.57
2:B:286:GLU:HA	2:B:331:THR:HA	1.87	0.57
5:E:151:LEU:HD11	5:E:158:LEU:HD12	1.87	0.57
6:F:301:ALA:HB3	6:F:304:ARG:HB2	1.87	0.57
25:Y:78:GLU:O	25:Y:82:LYS:N	2.33	0.57
1:A:358:HIS:HE1	1:A:386:ARG:HA	1.69	0.57
11:K:101:PHE:O	18:R:57:ARG:NH2	2.38	0.57
12:L:10:VAL:HG13	12:L:19:ILE:HG21	1.86	0.57
17:Q:20:VAL:HG21	17:Q:175:LEU:HA	1.87	0.57
22:V:419:LEU:HD22	22:V:431:PRO:HA	1.87	0.57
4:D:282:ASP:HA	4:D:285:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:385:ASP:OD1	6:F:340:PRO:HB2	2.04	0.56
10:J:201:SER:HB3	10:J:202:GLY:CA	2.35	0.56
21:U:203:LYS:O	21:U:207:ASN:ND2	2.38	0.56
21:U:908:ILE:HG12	21:U:909:GLY:H	1.70	0.56
22:V:227:VAL:HA	22:V:230:PHE:HB3	1.87	0.56
4:D:146:GLU:HG2	4:D:148:ASP:H	1.70	0.56
3:C:336:MET:HA	4:D:195:GLY:HA3	1.86	0.56
15:O:161:ALA:O	15:O:165:ASN:ND2	2.34	0.56
25:Y:182:VAL:HA	25:Y:201:PHE:HE1	1.70	0.56
2:B:139:VAL:HA	2:B:140:ASP:HB3	1.87	0.56
2:B:182:GLU:HB2	2:B:239:VAL:HG11	1.86	0.56
3:C:132:ASP:O	3:C:136:SER:N	2.29	0.56
4:D:411:GLU:HA	4:D:412:GLN:HB2	1.87	0.56
5:E:169:GLY:N	5:E:296:ASP:OD2	2.39	0.56
5:E:313:LEU:O	5:E:317:ALA:N	2.31	0.56
6:F:384:LEU:O	6:F:388:THR:N	2.38	0.56
8:H:119:GLN:NE2	8:H:152:SER:O	2.37	0.56
8:H:150:ASP:OD1	8:H:154:ALA:N	2.38	0.56
15:O:6:VAL:HG23	15:O:124:TYR:HB3	1.88	0.56
21:U:198:LEU:HD21	21:U:219:CYS:HA	1.86	0.56
22:V:173:ILE:O	22:V:177:ASN:ND2	2.38	0.56
5:E:187:VAL:HA	5:E:190:GLN:HB3	1.88	0.56
6:F:190:GLY:HA3	6:F:361:ALA:HB2	1.86	0.56
20:T:112:ILE:O	20:T:123:GLY:N	2.34	0.56
21:U:494:TYR:OH	21:U:531:ASP:OD2	2.24	0.56
5:E:305:ASN:O	5:E:309:ARG:N	2.33	0.56
15:O:177:VAL:HB	15:O:184:ASP:HB2	1.86	0.56
5:E:247:THR:OG1	5:E:248:SER:N	2.39	0.56
6:F:365:ILE:HG13	6:F:366:MET:H	1.70	0.56
11:K:199:LEU:HA	11:K:202:LEU:HB2	1.86	0.56
11:K:43:SER:HA	11:K:151:PRO:HG3	1.86	0.56
22:V:212:TYR:HE1	22:V:256:ARG:HE	1.52	0.56
25:Y:141:VAL:HG21	25:Y:164:ALA:HB2	1.88	0.56
3:C:340:ARG:HH11	25:Y:97:GLU:HB2	1.71	0.56
1:A:170:PRO:HA	1:A:229:VAL:HG12	1.87	0.56
2:B:133:VAL:HG13	2:B:135:ILE:HG23	1.86	0.56
4:D:405:THR:O	5:E:298:LYS:NZ	2.37	0.56
6:F:249:LEU:HD12	6:F:283:ILE:HD11	1.88	0.56
7:G:78:CYS:SG	7:G:79:VAL:N	2.78	0.56
24:X:351:SER:HA	24:X:354:ILE:HG22	1.88	0.56
4:D:243:GLY:O	4:D:247:VAL:N	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:285:VAL:HA	4:D:288:ILE:HD12	1.86	0.56
3:C:43:ARG:HG2	21:U:639:LEU:HD22	1.86	0.56
23:W:237:GLU:HG2	23:W:238:GLY:N	2.20	0.56
26:Z:241:SER:HB2	26:Z:242:LEU:HA	1.88	0.56
2:B:96:ARG:HH22	3:C:82:LYS:HB2	1.70	0.56
5:E:61:LEU:HD11	5:E:72:LYS:HB2	1.88	0.56
17:Q:59:TYR:O	17:Q:63:ASN:ND2	2.29	0.56
19:S:64:LEU:HD21	19:S:92:LEU:HD11	1.88	0.56
19:S:68:ILE:HD11	19:S:92:LEU:HD13	1.87	0.56
3:C:212:ILE:N	3:C:245:ILE:O	2.35	0.56
4:D:96:VAL:HG22	4:D:101:ALA:HA	1.87	0.56
16:P:58:THR:O	17:Q:85:ARG:NH2	2.39	0.56
3:C:266:ASP:O	3:C:270:GLN:N	2.27	0.56
7:G:71:LYS:O	7:G:95:ARG:NH2	2.39	0.56
9:I:69:ASN:OD1	9:I:70:GLU:N	2.38	0.56
9:I:91:ARG:HD3	16:P:76:LEU:HB3	1.87	0.56
20:T:45:VAL:HG11	20:T:71:VAL:HG21	1.88	0.56
3:C:297:ARG:HG3	3:C:298:ILE:H	1.72	0.55
5:E:221:TYR:HA	5:E:224:ASP:HB3	1.87	0.55
25:Y:102:ASP:HA	25:Y:105:MET:HG2	1.88	0.55
1:A:162:THR:O	1:A:166:VAL:N	2.28	0.55
6:F:176:GLU:HB2	6:F:250:LYS:HB2	1.88	0.55
10:J:132:LEU:HG	10:J:146:GLN:HA	1.88	0.55
14:N:45:ARG:HB2	14:N:52:THR:HG21	1.88	0.55
23:W:273:TYR:HA	23:W:276:LEU:HD13	1.87	0.55
26:Z:219:LYS:HG3	26:Z:220:LEU:HD23	1.88	0.55
1:A:73:ALA:O	1:A:77:LEU:N	2.36	0.55
3:C:350:LEU:HD23	3:C:387:VAL:HG11	1.88	0.55
4:D:287:ARG:HA	4:D:290:LEU:HB3	1.88	0.55
13:M:12:SER:OG	13:M:124:LEU:O	2.20	0.55
3:C:135:VAL:HG22	3:C:223:PHE:HE2	1.72	0.55
6:F:283:ILE:HG22	6:F:328:VAL:HG13	1.87	0.55
6:F:430:LYS:NZ	11:K:17:PRO:HB2	2.22	0.55
8:H:128:ARG:HG3	8:H:130:PHE:H	1.71	0.55
10:J:34:GLY:HA2	10:J:43:LEU:HA	1.87	0.55
10:J:157:LYS:N	11:K:58:LEU:O	2.39	0.55
12:L:166:GLN:OE1	12:L:169:ARG:NH1	2.39	0.55
21:U:225:ASP:OD1	21:U:225:ASP:N	2.39	0.55
22:V:56:ALA:O	22:V:59:ALA:HB3	2.07	0.55
24:X:346:GLN:HE21	24:X:349:HIS:HB2	1.71	0.55
1:A:324:PRO:HD3	1:A:432:TYR:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:PRO:HG2	2:B:154:HIS:CD2	2.41	0.55
3:C:115:ALA:HB3	3:C:125:LYS:H	1.71	0.55
11:K:154:PHE:HB3	11:K:162:PHE:HE1	1.72	0.55
1:A:232:ARG:NE	1:A:235:ALA:O	2.39	0.55
3:C:376:VAL:HG13	3:C:377:HIS:H	1.71	0.55
5:E:241:ARG:HD3	6:F:298:SER:HB2	1.88	0.55
6:F:91:SER:OG	6:F:125:LYS:O	2.17	0.55
6:F:208:HIS:HB3	6:F:211:LYS:HD3	1.89	0.55
6:F:376:SER:O	6:F:378:ASP:N	2.39	0.55
11:K:182:GLN:NE2	12:L:55:GLU:OE1	2.39	0.55
15:O:18:THR:HB	15:O:31:CYS:H	1.72	0.55
22:V:100:MET:HG2	22:V:102:PRO:HD2	1.88	0.55
22:V:394:LEU:HA	22:V:397:ARG:HG2	1.89	0.55
2:B:113:GLU:HB3	2:B:123:VAL:HA	1.89	0.55
2:B:133:VAL:HG21	2:B:159:VAL:H	1.71	0.55
3:C:35:VAL:HA	3:C:38:LYS:HD3	1.89	0.55
4:D:341:LYS:O	4:D:345:PHE:N	2.32	0.55
6:F:130:GLN:OE1	6:F:132:TYR:OH	2.17	0.55
22:V:210:CYS:HA	22:V:213:TYR:HB2	1.87	0.55
22:V:54:LYS:N	22:V:55:THR:OG1	2.39	0.55
22:V:79:VAL:HG13	22:V:80:LYS:H	1.72	0.55
3:C:247:PHE:HD1	3:C:292:ILE:HB	1.72	0.55
9:I:28:ILE:HG21	9:I:133:SER:HB2	1.87	0.55
9:I:218:ARG:NH1	9:I:223:THR:OG1	2.39	0.55
19:S:114:ASP:OD1	19:S:118:LYS:N	2.39	0.55
1:A:239:ARG:HD3	2:B:319:PHE:HD2	1.71	0.55
1:A:373:LEU:HD22	1:A:409:PHE:HE1	1.72	0.55
4:D:133:HIS:HE1	4:D:135:HIS:HB2	1.72	0.55
7:G:47:CYS:HB3	7:G:221:THR:HG23	1.89	0.55
12:L:171:TYR:O	12:L:175:HIS:ND1	2.40	0.55
1:A:143:ASP:H	1:A:148:GLN:HG2	1.72	0.55
5:E:312:ILE:HD12	5:E:315:ILE:HD11	1.89	0.55
17:Q:29:LYS:HD3	18:R:121:ILE:HD12	1.88	0.55
21:U:161:ASP:OD1	21:U:162:VAL:N	2.35	0.55
22:V:80:LYS:HA	22:V:81:GLN:HB2	1.88	0.55
1:A:355:PHE:HE1	1:A:385:ILE:HB	1.72	0.54
2:B:177:GLU:H	2:B:178:LYS:HA	1.72	0.54
2:B:374:LEU:HB2	2:B:378:VAL:HB	1.89	0.54
4:D:391:ARG:NE	4:D:393:ILE:O	2.35	0.54
8:H:7:SER:HA	8:H:125:GLY:HA3	1.88	0.54
12:L:50:LYS:HB3	12:L:59:HIS:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:320:THR:HG23	22:V:321:ALA:HB2	1.89	0.54
23:W:429:SER:O	23:W:433:ASN:HB2	2.07	0.54
2:B:313:LEU:HD22	2:B:341:LEU:HD23	1.89	0.54
7:G:141:ILE:HD13	7:G:220:VAL:HG11	1.90	0.54
13:M:8:ASP:HB2	13:M:21:PHE:HB2	1.88	0.54
17:Q:141:SER:O	17:Q:145:ARG:HB3	2.07	0.54
1:A:122:VAL:N	6:F:88:TYR:O	2.29	0.54
9:I:44:LEU:HA	9:I:215:THR:HA	1.89	0.54
11:K:215:ILE:HD12	11:K:234:LEU:HD11	1.88	0.54
12:L:204:ASP:HB3	12:L:205:LEU:C	2.28	0.54
2:B:303:ARG:HA	2:B:306:GLN:HB3	1.90	0.54
4:D:268:ASP:N	4:D:268:ASP:OD1	2.41	0.54
14:N:16:ALA:HB1	14:N:33:LYS:HB2	1.88	0.54
23:W:373:ILE:HG23	23:W:413:ILE:HG13	1.88	0.54
2:B:268:ARG:HA	2:B:315:GLN:HE22	1.73	0.54
2:B:251:VAL:HG11	3:C:271:ARG:HD2	1.89	0.54
3:C:373:GLU:HG2	3:C:375:ARG:NH1	2.22	0.54
5:E:212:ALA:HB2	5:E:256:THR:HA	1.88	0.54
5:E:356:ARG:NH2	6:F:197:GLU:OE1	2.40	0.54
7:G:127:GLN:HE22	8:H:130:PHE:HZ	1.56	0.54
8:H:139:TRP:HA	8:H:144:PRO:HA	1.89	0.54
8:H:66:GLU:HG3	8:H:91:ARG:HH22	1.71	0.54
1:A:159:PRO:O	1:A:162:THR:OG1	2.20	0.54
3:C:375:ARG:HH21	3:C:378:VAL:HG13	1.72	0.54
5:E:81:VAL:HG11	5:E:105:LEU:HB2	1.88	0.54
5:E:281:ARG:HH22	6:F:296:PHE:HD1	1.55	0.54
7:G:215:ILE:HD11	7:G:235:ILE:HG21	1.87	0.54
13:M:26:ALA:HB1	13:M:132:GLY:HA2	1.90	0.54
22:V:349:ARG:HB3	22:V:354:LYS:HB2	1.88	0.54
2:B:255:LEU:HD11	2:B:267:VAL:HG23	1.88	0.54
4:D:208:PRO:HD2	5:E:287:PRO:HB2	1.90	0.54
4:D:353:ASN:HB3	4:D:393:ILE:HG12	1.89	0.54
7:G:16:PHE:HB3	7:G:20:GLY:HA2	1.90	0.54
13:M:189:ILE:HA	13:M:192:GLU:HB2	1.89	0.54
18:R:2:THR:HA	18:R:129:GLY:HA3	1.88	0.54
22:V:254:LEU:O	22:V:258:TYR:HB2	2.08	0.54
25:Y:191:ILE:HG13	25:Y:192:ARG:H	1.72	0.54
25:Y:377:LEU:HA	25:Y:380:VAL:HG22	1.90	0.54
2:B:166:ASP:N	2:B:166:ASP:OD1	2.40	0.54
2:B:313:LEU:O	2:B:317:ASP:N	2.40	0.54
3:C:267:SER:O	3:C:271:ARG:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ARG:HB3	3:C:283:PHE:HE2	1.72	0.54
5:E:44:GLU:HB3	6:F:76:ASN:HD22	1.73	0.54
22:V:149:PRO:HG2	22:V:199:ASN:HB3	1.88	0.54
22:V:235:LEU:HD11	22:V:247:GLN:HG3	1.90	0.54
22:V:349:ARG:NH2	22:V:358:MET:SD	2.81	0.54
4:D:323:ARG:HE	4:D:326:ARG:NE	2.04	0.54
21:U:8:ILE:HD11	21:U:27:LEU:HG	1.90	0.54
22:V:455:LYS:N	22:V:456:GLY:HA2	2.22	0.54
26:Z:182:THR:N	26:Z:183:THR:HA	2.22	0.54
4:D:60:TYR:CG	21:U:603:LEU:HD11	2.42	0.54
4:D:92:PHE:HA	4:D:103:VAL:HG23	1.88	0.54
5:E:235:ILE:HG23	5:E:285:LEU:HD21	1.90	0.54
6:F:234:THR:HB	33:F:501:ADP:H3'	1.88	0.54
17:Q:29:LYS:HE3	17:Q:32:HIS:HB2	1.90	0.54
21:U:429:LYS:HB3	21:U:431:THR:HG23	1.89	0.54
22:V:81:GLN:HB3	22:V:83:GLU:N	2.22	0.54
23:W:412:ILE:HG22	24:X:344:ARG:HH22	1.73	0.54
25:Y:190:ALA:HA	25:Y:287:LEU:HD13	1.90	0.54
2:B:264:PRO:O	2:B:267:VAL:N	2.36	0.53
3:C:388:ALA:O	3:C:392:GLN:HG2	2.08	0.53
4:D:200:ARG:NH2	4:D:325:GLY:O	2.35	0.53
15:O:17:ASP:O	15:O:33:LYS:NZ	2.31	0.53
21:U:772:TRP:HB3	21:U:775:LEU:HG	1.88	0.53
22:V:357:LEU:O	22:V:360:TYR:N	2.41	0.53
4:D:225:ALA:HB1	4:D:260:ALA:HA	1.90	0.53
14:N:175:ARG:HG2	14:N:188:VAL:HG13	1.90	0.53
14:N:32:ASP:O	14:N:45:ARG:NH1	2.41	0.53
21:U:109:THR:OG1	21:U:156:GLU:O	2.18	0.53
22:V:195:ILE:HG13	22:V:196:SER:HB3	1.90	0.53
22:V:200:ARG:HH11	22:V:242:HIS:CE1	2.26	0.53
23:W:438:LEU:HD21	26:Z:237:LEU:HD21	1.89	0.53
1:A:420:TYR:HA	1:A:423:PHE:CE2	2.43	0.53
33:D:501:ADP:H1'	5:E:291:ARG:CZ	2.38	0.53
5:E:322:LYS:HD2	5:E:367:PHE:HE2	1.74	0.53
11:K:61:PRO:HB3	11:K:213:THR:HG22	1.90	0.53
17:Q:182:ILE:HG23	17:Q:189:HIS:HB2	1.91	0.53
21:U:403:THR:HG23	21:U:777:HIS:HE2	1.73	0.53
9:I:137:ILE:HG22	9:I:147:LEU:HD22	1.90	0.53
13:M:228:PRO:HB2	13:M:231:ILE:HB	1.90	0.53
19:S:38:ARG:HH22	20:T:151:ARG:HD3	1.74	0.53
23:W:274:VAL:O	23:W:283:GLN:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:229:ILE:HG23	25:Y:298:GLU:HG2	1.90	0.53
3:C:277:LEU:HD13	3:C:311:ILE:HG13	1.90	0.53
4:D:293:LEU:O	4:D:326:ARG:NH2	2.42	0.53
5:E:207:TYR:OH	6:F:129:ARG:NH1	2.41	0.53
22:V:419:LEU:HD21	22:V:456:GLY:H	1.73	0.53
22:V:59:ALA:N	22:V:60:ALA:HB3	2.24	0.53
3:C:276:LEU:O	3:C:280:LEU:N	2.42	0.53
3:C:286:THR:HG23	3:C:287:LYS:H	1.74	0.53
3:C:295:THR:HG21	3:C:299:ASP:HB2	1.90	0.53
6:F:195:ILE:HG12	6:F:199:VAL:HG23	1.90	0.53
6:F:359:GLU:HB2	6:F:385:ALA:HB1	1.91	0.53
9:I:72:MET:HG2	9:I:138:GLY:HA3	1.89	0.53
13:M:54:LEU:H	13:M:57:LEU:HD11	1.72	0.53
16:P:13:ALA:HA	16:P:22:ILE:HA	1.90	0.53
21:U:645:ASN:HD21	21:U:648:VAL:HG23	1.73	0.53
23:W:343:SER:HB2	23:W:346:GLU:HB3	1.91	0.53
24:X:404:ILE:HG12	25:Y:372:LYS:HE2	1.91	0.53
6:F:311:LEU:O	6:F:315:ASN:N	2.32	0.53
6:F:312:GLU:O	6:F:316:GLN:N	2.38	0.53
5:E:378:LYS:NZ	6:F:349:ASP:O	2.31	0.53
7:G:43:ARG:HA	7:G:48:ALA:HA	1.91	0.53
21:U:896:GLU:O	21:U:901:GLN:NE2	2.42	0.53
21:U:904:LYS:H	21:U:913:ILE:HD11	1.73	0.53
23:W:449:GLU:O	23:W:453:HIS:ND1	2.39	0.53
2:B:316:LEU:HD11	2:B:327:VAL:HG21	1.91	0.53
6:F:308:ARG:O	6:F:312:GLU:N	2.29	0.53
7:G:43:ARG:HD2	7:G:149:PRO:HB2	1.90	0.53
8:H:50:LYS:NZ	8:H:62:VAL:O	2.42	0.53
9:I:154:GLY:HA3	10:J:78:ALA:HB2	1.90	0.53
14:N:132:SER:HA	14:N:135:ILE:HG12	1.89	0.53
22:V:416:ARG:HG2	22:V:457:TYR:HB3	1.91	0.53
23:W:320:LEU:HD21	23:W:354:LEU:HD21	1.90	0.53
25:Y:323:PHE:CD2	25:Y:326:GLY:HA3	2.44	0.53
22:V:462:GLU:HB3	25:Y:346:LYS:HG3	1.90	0.53
1:A:343:PHE:HB3	1:A:344:SER:C	2.29	0.53
2:B:111:THR:HA	2:B:149:SER:HA	1.90	0.53
3:C:285:ALA:HB1	3:C:286:THR:HB	1.91	0.53
4:D:133:HIS:CB	4:D:138:ALA:H	2.22	0.53
12:L:45:VAL:HG11	12:L:188:VAL:HA	1.90	0.53
2:B:424:GLU:O	2:B:428:TYR:N	2.29	0.53
4:D:217:LYS:NZ	5:E:266:GLY:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:50:LYS:HD2	8:H:64:LYS:HG2	1.91	0.53
13:M:15:SER:OG	13:M:19:ARG:O	2.27	0.53
20:T:138:ALA:HB3	20:T:147:GLN:HB2	1.91	0.53
21:U:485:ALA:HB3	21:U:519:VAL:HG12	1.91	0.53
22:V:273:LYS:HA	22:V:274:SER:HB2	1.91	0.53
22:V:319:HIS:HB2	22:V:320:THR:HA	1.90	0.53
23:W:393:LEU:HD23	23:W:406:VAL:HG11	1.91	0.53
23:W:412:ILE:O	24:X:344:ARG:NH2	2.42	0.53
15:O:3:ILE:HG13	15:O:127:MET:HB2	1.90	0.52
21:U:31:VAL:HA	21:U:34:PHE:HB2	1.91	0.52
22:V:495:ARG:NH1	26:Z:282:ASN:OD1	2.41	0.52
1:A:284:ARG:HG3	1:A:285:PHE:HD2	1.73	0.52
3:C:283:PHE:CD1	3:C:284:GLU:HG2	2.44	0.52
5:E:360:ASP:N	5:E:360:ASP:OD1	2.34	0.52
7:G:71:LYS:HE3	7:G:74:GLU:HA	1.91	0.52
23:W:259:GLU:HG2	23:W:262:LYS:HB3	1.89	0.52
26:Z:91:ILE:HD11	26:Z:115:TYR:HB3	1.90	0.52
3:C:74:GLY:N	3:C:114:VAL:O	2.39	0.52
22:V:33:GLN:HG2	22:V:86:VAL:HG21	1.90	0.52
26:Z:186:THR:HG23	26:Z:187:LEU:H	1.74	0.52
1:A:100:LYS:HG2	1:A:113:ILE:HG22	1.92	0.52
1:A:76:ALA:HA	1:A:79:ASP:HB2	1.92	0.52
3:C:71:SER:HA	3:C:118:ASN:HB3	1.91	0.52
3:C:143:VAL:HG11	3:C:197:THR:HG22	1.91	0.52
11:K:13:ASN:HD21	12:L:126:ARG:HH11	1.57	0.52
12:L:18:ARG:NH1	12:L:23:GLU:OE2	2.42	0.52
18:R:77:ALA:HA	18:R:120:ARG:HH22	1.74	0.52
22:V:349:ARG:HE	22:V:354:LYS:HG3	1.74	0.52
25:Y:304:TYR:OH	25:Y:333:GLU:OE2	2.28	0.52
25:Y:349:LYS:O	25:Y:350:VAL:HG22	2.09	0.52
26:Z:214:LYS:HB3	26:Z:222:ILE:HD13	1.90	0.52
26:Z:254:ASN:HA	26:Z:257:MET:HG3	1.91	0.52
2:B:230:THR:HG21	2:B:353:PHE:CE2	2.45	0.52
4:D:366:ARG:HB3	4:D:367:PRO:HD3	1.92	0.52
4:D:387:VAL:HG21	5:E:159:PHE:HE1	1.74	0.52
6:F:126:THR:OG1	6:F:130:GLN:N	2.42	0.52
6:F:253:GLY:H	6:F:287:GLU:HB2	1.74	0.52
21:U:325:MET:HA	21:U:328:ILE:HG12	1.91	0.52
21:U:765:VAL:HG12	21:U:775:LEU:HD22	1.91	0.52
22:V:193:GLN:HB3	22:V:194:LYS:CA	2.38	0.52
23:W:236:HIS:HB3	23:W:237:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:424:LEU:O	23:W:428:TRP:HB2	2.10	0.52
2:B:383:LEU:HD21	2:B:420:LYS:HG2	1.91	0.52
3:C:13:GLU:N	3:C:14:GLY:HA3	2.25	0.52
5:E:65:THR:HG22	5:E:66:GLU:H	1.75	0.52
6:F:310:MET:HA	6:F:313:LEU:HB3	1.90	0.52
13:M:231:ILE:HG22	13:M:232:ARG:HG3	1.92	0.52
14:N:40:ARG:NH1	14:N:180:ALA:O	2.42	0.52
18:R:25:TYR:OH	19:S:142:SER:O	2.27	0.52
22:V:318:GLN:O	22:V:319:HIS:ND1	2.42	0.52
1:A:297:ARG:O	1:A:301:GLU:N	2.31	0.52
1:A:274:PHE:HB2	1:A:319:MET:SD	2.50	0.52
3:C:166:GLU:OE2	3:C:207:THR:OG1	2.22	0.52
5:E:242:ARG:HB3	5:E:254:GLN:HG3	1.91	0.52
5:E:306:GLU:HA	5:E:309:ARG:HB3	1.91	0.52
6:F:195:ILE:HD12	6:F:236:LEU:HD21	1.92	0.52
7:G:210:PHE:CE1	7:G:215:ILE:HG23	2.45	0.52
11:K:32:LYS:NZ	11:K:172:SER:O	2.30	0.52
11:K:42:THR:HG22	11:K:44:GLU:H	1.73	0.52
11:K:37:ALA:HB2	11:K:50:VAL:HG23	1.92	0.52
12:L:155:ASP:HB3	13:M:62:SER:HB2	1.91	0.52
10:J:95:ARG:HG3	17:Q:62:LYS:HE3	1.91	0.52
22:V:342:ILE:HD12	22:V:343:PRO:HD2	1.91	0.52
25:Y:367:GLN:HG3	25:Y:371:LYS:HG2	1.92	0.52
1:A:106:SER:HB3	1:A:110:LYS:HD2	1.92	0.52
3:C:99:VAL:HG13	3:C:100:ASP:C	2.30	0.52
5:E:135:ILE:HD11	5:E:142:ILE:HG12	1.92	0.52
5:E:335:SER:HB3	5:E:338:PHE:HE2	1.74	0.52
9:I:73:ALA:HB3	9:I:137:ILE:HD11	1.91	0.52
10:J:115:LYS:NZ	10:J:129:ILE:O	2.42	0.52
21:U:522:GLY:O	21:U:559:ARG:NH2	2.43	0.52
21:U:774:PRO:HA	21:U:777:HIS:HD2	1.75	0.52
2:B:194:ILE:O	2:B:198:LYS:N	2.43	0.52
11:K:16:SER:O	11:K:19:GLY:HA3	2.09	0.52
18:R:100:MET:HG2	18:R:113:TYR:HD1	1.75	0.52
19:S:116:GLU:OE1	19:S:118:LYS:NZ	2.38	0.52
1:A:388:VAL:HG13	1:A:413:VAL:HG22	1.92	0.52
3:C:39:SER:O	3:C:43:ARG:HG3	2.10	0.52
5:E:329:GLU:O	5:E:333:LYS:N	2.37	0.52
1:A:297:ARG:NH1	6:F:303:ASP:OD1	2.41	0.52
6:F:430:LYS:HZ2	11:K:17:PRO:HB2	1.75	0.52
10:J:19:VAL:HG22	10:J:126:PRO:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:157:ASP:OD2	11:K:159:SER:OG	2.27	0.52
20:T:24:ALA:HB1	20:T:41:ARG:HH12	1.75	0.52
21:U:212:ASP:O	21:U:215:ASN:ND2	2.43	0.52
21:U:625:ILE:HG13	21:U:626:LEU:HG	1.91	0.52
22:V:451:ILE:HG12	22:V:458:VAL:HG22	1.91	0.52
4:D:281:ALA:O	4:D:285:VAL:HG13	2.09	0.51
12:L:15:PRO:O	13:M:28:LYS:NZ	2.32	0.51
14:N:7:GLN:HB3	14:N:111:VAL:HG23	1.92	0.51
25:Y:224:VAL:HG13	25:Y:256:VAL:HG11	1.92	0.51
25:Y:233:ARG:NH1	25:Y:306:GLN:OE1	2.43	0.51
25:Y:386:VAL:HG12	25:Y:387:ILE:HG23	1.92	0.51
1:A:316:LYS:O	1:A:317:VAL:HG13	2.11	0.51
3:C:189:TYR:O	3:C:317:PHE:N	2.31	0.51
3:C:298:ILE:O	3:C:301:LEU:N	2.42	0.51
5:E:176:PRO:HB2	5:E:302:ASP:HA	1.91	0.51
11:K:18:GLU:HB2	11:K:19:GLY:HA2	1.92	0.51
1:A:80:LEU:HD22	2:B:99:VAL:HG21	1.92	0.51
4:D:289:LEU:O	4:D:293:LEU:HB2	2.09	0.51
4:D:337:ASP:O	4:D:341:LYS:N	2.28	0.51
4:D:377:SER:O	4:D:381:GLU:N	2.42	0.51
5:E:115:VAL:HG22	5:E:117:PRO:HD2	1.92	0.51
10:J:137:ASP:N	10:J:141:THR:O	2.43	0.51
23:W:414:ASN:OD1	23:W:414:ASN:N	2.43	0.51
1:A:80:LEU:HG	2:B:137:SER:OG	2.10	0.51
2:B:224:LEU:HA	2:B:351:ILE:HG13	1.91	0.51
4:D:98:GLN:HG3	4:D:99:ASN:HD22	1.76	0.51
5:E:111:LEU:HD22	6:F:96:LEU:HD23	1.92	0.51
7:G:28:ALA:HB1	7:G:135:GLY:HA3	1.92	0.51
8:H:119:GLN:O	8:H:122:THR:OG1	2.28	0.51
11:K:79:SER:H	11:K:139:VAL:HG23	1.75	0.51
22:V:266:GLN:HG3	22:V:295:ILE:HG23	1.92	0.51
23:W:452:ILE:HG21	26:Z:226:ILE:H	1.75	0.51
25:Y:301:ILE:HG13	25:Y:343:LEU:HB2	1.92	0.51
26:Z:136:GLU:OE2	26:Z:157:HIS:ND1	2.40	0.51
26:Z:48:LEU:HD11	26:Z:92:VAL:HG21	1.93	0.51
1:A:126:SER:OG	1:A:149:ILE:O	2.23	0.51
3:C:254:ILE:HG23	3:C:296:ASN:HD22	1.76	0.51
3:C:307:ARG:HE	3:C:312:ASP:CB	2.23	0.51
3:C:337:ASN:ND2	4:D:193:GLN:O	2.43	0.51
7:G:138:MET:HB3	7:G:154:CYS:HB3	1.93	0.51
11:K:202:LEU:HA	11:K:205:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:52:GLY:N	16:P:108:VAL:O	2.39	0.51
21:U:45:ILE:HG21	21:U:64:ALA:HB2	1.93	0.51
22:V:26:PRO:O	22:V:29:PRO:HD2	2.10	0.51
1:A:261:PHE:O	1:A:265:ARG:N	2.38	0.51
5:E:126:ASP:OD1	5:E:185:ARG:NE	2.36	0.51
6:F:92:ASN:HB3	6:F:125:LYS:HB2	1.92	0.51
6:F:174:ALA:HB1	6:F:177:VAL:HG23	1.92	0.51
6:F:229:PRO:O	6:F:392:ASN:ND2	2.44	0.51
10:J:132:LEU:HD13	10:J:161:ILE:HG12	1.93	0.51
12:L:137:TYR:CZ	12:L:142:PRO:HB3	2.46	0.51
18:R:1:THR:N	18:R:17:ASP:OD2	2.34	0.51
21:U:154:ALA:HB2	21:U:166:THR:HG21	1.93	0.51
22:V:200:ARG:HA	22:V:203:LEU:HB2	1.93	0.51
25:Y:358:ARG:HH21	25:Y:359:PRO:HD2	1.76	0.51
1:A:279:ALA:O	2:B:307:ARG:NH1	2.43	0.51
3:C:131:VAL:HG13	3:C:132:ASP:H	1.76	0.51
4:D:311:THR:HG21	4:D:317:LEU:HD11	1.93	0.51
6:F:204:LEU:O	6:F:209:LYS:N	2.44	0.51
7:G:172:GLN:N	7:G:172:GLN:OE1	2.44	0.51
8:H:39:LYS:HE3	8:H:144:PRO:HG2	1.93	0.51
21:U:490:ARG:HH11	21:U:493:VAL:HB	1.75	0.51
2:B:235:LEU:HA	2:B:238:ALA:HB3	1.93	0.51
5:E:281:ARG:NE	5:E:283:ASP:OD2	2.35	0.51
8:H:44:VAL:O	8:H:213:CYS:N	2.39	0.51
11:K:146:VAL:HG11	11:K:222:PRO:HG3	1.93	0.51
22:V:79:VAL:HG22	22:V:80:LYS:HG2	1.93	0.51
25:Y:77:ASN:HD21	25:Y:114:ILE:HG13	1.74	0.51
2:B:180:PRO:HD2	2:B:242:GLN:NE2	2.26	0.51
3:C:117:ARG:N	3:C:122:THR:O	2.30	0.51
33:E:401:ADP:O1B	6:F:347:ARG:NH2	2.44	0.51
6:F:84:LYS:H	6:F:85:THR:HA	1.76	0.51
12:L:41:LYS:HG3	12:L:180:MET:HB3	1.91	0.51
13:M:15:SER:OG	13:M:17:ASP:OD1	2.19	0.51
13:M:39:ILE:HG21	13:M:193:VAL:HG21	1.93	0.51
17:Q:168:GLN:NE2	17:Q:174:ASN:O	2.44	0.51
22:V:148:ARG:NH2	22:V:192:MET:O	2.44	0.51
23:W:232:GLN:O	23:W:236:HIS:HB2	2.11	0.51
3:C:165:ILE:HG13	3:C:203:VAL:HG11	1.92	0.51
3:C:49:ARG:HA	3:C:52:LEU:HB2	1.93	0.51
6:F:246:ALA:HB3	6:F:282:ILE:HG12	1.92	0.51
7:G:206:LEU:HB3	7:G:208:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:210:PHE:HE1	7:G:215:ILE:HG23	1.74	0.51
10:J:98:VAL:HG12	10:J:100:ASP:OD1	2.11	0.51
13:M:37:ILE:HG22	13:M:164:ALA:HA	1.92	0.51
17:Q:148:THR:HB	17:Q:151:ILE:HB	1.93	0.51
18:R:164:THR:HG22	18:R:170:SER:HB3	1.93	0.51
26:Z:32:GLN:HG3	26:Z:33:LYS:H	1.75	0.51
1:A:100:LYS:HG3	1:A:115:VAL:HB	1.92	0.50
2:B:139:VAL:HB	2:B:141:LYS:N	2.26	0.50
2:B:364:ILE:HG12	33:B:501:ADP:N6	2.27	0.50
3:C:238:ALA:HB1	3:C:289:ILE:HD12	1.92	0.50
5:E:128:GLY:O	5:E:189:SER:OG	2.16	0.50
6:F:204:LEU:HD13	6:F:212:PHE:CE2	2.46	0.50
8:H:231:ALA:HB3	8:H:232:ALA:CB	2.39	0.50
9:I:75:SER:HB2	9:I:135:LEU:HB2	1.92	0.50
22:V:319:HIS:HB3	22:V:325:LYS:HD3	1.93	0.50
26:Z:164:ALA:HB1	26:Z:168:GLU:HG3	1.93	0.50
2:B:151:LEU:O	2:B:159:VAL:HA	2.10	0.50
2:B:151:LEU:HD11	2:B:163:LEU:HD13	1.93	0.50
5:E:157:GLU:HA	5:E:160:GLN:HG2	1.92	0.50
5:E:174:GLY:HA2	5:E:176:PRO:HD2	1.93	0.50
22:V:310:THR:HA	22:V:332:LEU:HD11	1.91	0.50
4:D:407:ILE:HG13	4:D:408:LYS:H	1.76	0.50
5:E:281:ARG:HD2	5:E:388:PRO:HD2	1.93	0.50
6:F:342:LEU:HA	6:F:347:ARG:HD3	1.92	0.50
6:F:80:ILE:HA	6:F:83:ASN:O	2.11	0.50
11:K:15:PHE:HE1	12:L:126:ARG:HD2	1.75	0.50
12:L:157:ARG:HD2	12:L:176:MET:HG3	1.94	0.50
19:S:99:ARG:HB3	19:S:103:PRO:HA	1.91	0.50
20:T:46:ASN:OD1	20:T:48:SER:N	2.41	0.50
22:V:311:ASN:HA	22:V:314:ARG:HG2	1.94	0.50
25:Y:232:GLU:O	25:Y:236:LEU:N	2.41	0.50
1:A:102:ILE:HG22	1:A:113:ILE:HG23	1.94	0.50
1:A:163:MET:SD	2:B:146:PRO:HG2	2.52	0.50
1:A:302:LEU:O	1:A:306:LEU:N	2.40	0.50
5:E:313:LEU:HD12	5:E:316:HIS:HB2	1.94	0.50
6:F:336:ASP:OD1	6:F:336:ASP:N	2.43	0.50
10:J:98:VAL:HG22	18:R:78:ALA:HB1	1.94	0.50
12:L:97:PHE:O	19:S:66:LYS:NZ	2.40	0.50
21:U:126:ILE:HG23	21:U:130:LEU:HD11	1.93	0.50
23:W:312:MET:SD	23:W:361:HIS:ND1	2.85	0.50
23:W:420:ASP:CG	23:W:421:PRO:HD2	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:314:ARG:HD2	25:Y:378:ASN:OD1	2.11	0.50
2:B:144:LEU:HD22	2:B:162:VAL:HG21	1.93	0.50
4:D:53:PHE:HB2	21:U:632:GLN:HE22	1.76	0.50
4:D:62:LYS:HA	4:D:65:GLN:HE21	1.77	0.50
6:F:225:MET:O	6:F:331:ALA:HA	2.11	0.50
10:J:131:ALA:H	10:J:147:THR:HG1	1.58	0.50
13:M:67:PHE:HB2	13:M:75:MET:HB2	1.92	0.50
16:P:70:ARG:NH2	16:P:97:GLU:OE2	2.45	0.50
21:U:436:ALA:HB1	21:U:472:ILE:HD13	1.93	0.50
21:U:62:LEU:HD12	21:U:84:ALA:HB1	1.94	0.50
22:V:38:LYS:HA	22:V:41:ALA:HB3	1.93	0.50
3:C:41:ASN:ND2	22:V:492:LYS:HD3	2.22	0.50
25:Y:179:ARG:NH2	25:Y:212:GLU:OE2	2.38	0.50
24:X:416:ASN:HB3	26:Z:283:ARG:HH21	1.76	0.50
1:A:328:ASP:HA	1:A:331:LEU:HG	1.93	0.50
3:C:130:LYS:HG3	3:C:133:PRO:HG2	1.92	0.50
4:D:207:PRO:HD2	4:D:312:ASN:HA	1.93	0.50
5:E:305:ASN:OD1	5:E:306:GLU:N	2.45	0.50
6:F:139:LEU:N	6:F:160:ILE:O	2.45	0.50
6:F:223:VAL:HG23	6:F:350:ARG:HB2	1.94	0.50
5:E:47:LEU:HD13	6:F:80:ILE:HG12	1.93	0.50
11:K:97:GLN:HG2	18:R:61:ARG:HG3	1.94	0.50
15:O:14:LEU:HB2	15:O:176:CYS:HB3	1.92	0.50
17:Q:103:LEU:HB3	17:Q:118:MET:H	1.76	0.50
21:U:154:ALA:HB1	21:U:163:PHE:HD1	1.77	0.50
21:U:474:ARG:NH1	21:U:500:ASN:OD1	2.45	0.50
22:V:167:LEU:HD11	22:V:171:VAL:HB	1.92	0.50
1:A:402:LYS:N	1:A:402:LYS:HD2	2.27	0.50
3:C:43:ARG:HB3	21:U:639:LEU:HD13	1.94	0.50
5:E:216:ARG:HG3	5:E:263:GLN:HE21	1.77	0.50
11:K:11:GLY:C	11:K:13:ASN:H	2.14	0.50
13:M:57:LEU:HB2	13:M:58:TYR:CD1	2.47	0.50
16:P:91:VAL:HG21	16:P:109:ILE:HD11	1.93	0.50
17:Q:4:LEU:HD22	17:Q:17:SER:HA	1.92	0.50
21:U:427:LEU:HG	21:U:428:PRO:HD2	1.93	0.50
21:U:82:LEU:HD21	21:U:130:LEU:HB3	1.94	0.50
1:A:329:PRO:HA	1:A:332:MET:HB3	1.94	0.50
1:A:384:GLU:HA	2:B:347:ILE:HG12	1.94	0.50
3:C:295:THR:HB	3:C:300:ILE:HG12	1.94	0.50
4:D:83:GLN:HG2	4:D:84:SER:H	1.77	0.50
12:L:36:VAL:HG22	12:L:160:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:217:SER:HB3	3:C:218:GLU:CB	2.31	0.50
6:F:181:PRO:HG3	6:F:238:ARG:O	2.12	0.50
7:G:123:GLN:O	7:G:127:GLN:HG2	2.12	0.50
12:L:48:ALA:HB3	12:L:211:SER:HB2	1.94	0.50
14:N:15:GLY:HA2	14:N:176:LEU:HD22	1.94	0.50
15:O:40:ASN:ND2	15:O:104:ASP:OD1	2.37	0.50
16:P:160:PRO:HA	16:P:163:LEU:HB3	1.94	0.50
17:Q:164:LEU:HB3	17:Q:196:PHE:HE2	1.76	0.50
20:T:49:THR:HB	20:T:85:PRO:HG3	1.92	0.50
21:U:54:PHE:CZ	21:U:56:SER:HB2	2.46	0.50
2:B:406:ALA:O	2:B:411:ARG:N	2.44	0.49
5:E:63:GLN:HA	5:E:69:PHE:HA	1.93	0.49
9:I:245:ALA:O	9:I:249:ARG:NH2	2.44	0.49
11:K:157:ASP:OD1	11:K:161:THR:N	2.45	0.49
12:L:200:PRO:HD2	12:L:203:GLN:HE22	1.76	0.49
23:W:334:GLU:OE1	23:W:338:THR:OG1	2.29	0.49
25:Y:357:ASN:HB2	25:Y:359:PRO:HD3	1.92	0.49
4:D:49:GLN:N	4:D:49:GLN:OE1	2.45	0.49
5:E:121:ASN:HB3	5:E:197:LYS:O	2.13	0.49
6:F:194:GLN:HB2	6:F:352:ILE:HG21	1.94	0.49
21:U:367:THR:HG21	21:U:773:PHE:HB3	1.94	0.49
23:W:285:ASP:OD1	23:W:285:ASP:N	2.46	0.49
12:L:138:ASP:OD1	12:L:143:HIS:NE2	2.43	0.49
21:U:554:LEU:HG	21:U:588:MET:HE1	1.94	0.49
22:V:304:GLU:HA	22:V:307:ARG:HG2	1.93	0.49
23:W:447:ALA:O	23:W:451:MET:HG2	2.12	0.49
1:A:111:TYR:CE2	1:A:125:LEU:HD23	2.46	0.49
4:D:230:VAL:O	4:D:265:ASP:N	2.46	0.49
4:D:373:ALA:HB3	4:D:375:ILE:HG12	1.95	0.49
4:D:106:THR:HB	5:E:77:PRO:HA	1.95	0.49
6:F:169:ASP:N	6:F:173:LYS:HB2	2.26	0.49
12:L:50:LYS:N	12:L:209:ASN:O	2.41	0.49
13:M:106:ILE:HD12	13:M:107:PRO:HD2	1.93	0.49
20:T:124:TYR:HB2	20:T:137:LEU:HD13	1.95	0.49
20:T:41:ARG:NH2	20:T:53:ALA:O	2.46	0.49
1:A:190:VAL:HG23	1:A:209:PRO:HG2	1.93	0.49
1:A:328:ASP:HB3	1:A:329:PRO:HD3	1.94	0.49
2:B:224:LEU:N	2:B:329:MET:O	2.45	0.49
2:B:290:ILE:HG23	2:B:336:THR:HB	1.93	0.49
3:C:363:CYS:HA	3:C:366:ALA:HB3	1.95	0.49
4:D:344:ILE:HA	4:D:347:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:183:VAL:HG13	7:G:189:TRP:HZ2	1.77	0.49
13:M:229:LYS:HE2	13:M:235:ALA:HB3	1.94	0.49
23:W:420:ASP:OD2	23:W:425:LEU:HB3	2.12	0.49
22:V:487:HIS:HD1	26:Z:279:LYS:HD2	1.77	0.49
1:A:115:VAL:HG12	1:A:119:ALA:O	2.12	0.49
5:E:108:MET:HG2	5:E:109:ARG:HG3	1.95	0.49
5:E:170:CYS:SG	5:E:171:LEU:N	2.85	0.49
6:F:342:LEU:HB3	6:F:348:LEU:HG	1.93	0.49
7:G:218:GLY:HA2	7:G:230:LEU:HD13	1.93	0.49
8:H:69:THR:HG22	8:H:70:LYS:H	1.77	0.49
15:O:7:VAL:HG13	15:O:12:ILE:HG12	1.94	0.49
25:Y:356:THR:HA	25:Y:357:ASN:CG	2.32	0.49
26:Z:9:VAL:HG12	26:Z:48:LEU:HB3	1.94	0.49
1:A:271:LEU:HG	1:A:315:ILE:O	2.13	0.49
1:A:292:ASP:O	1:A:296:GLN:HG2	2.13	0.49
2:B:286:GLU:OE1	2:B:332:ASN:N	2.45	0.49
2:B:383:LEU:HB3	2:B:387:LYS:HZ1	1.78	0.49
3:C:257:SER:C	3:C:259:LEU:H	2.16	0.49
4:D:389:GLU:HB3	4:D:390:ASN:C	2.32	0.49
6:F:394:ALA:HB2	33:F:501:ADP:H1'	1.95	0.49
16:P:126:LEU:HD12	16:P:127:ILE:HG23	1.94	0.49
21:U:599:ILE:HD12	21:U:602:LEU:HD22	1.95	0.49
25:Y:312:ARG:HG3	25:Y:313:SER:N	2.28	0.49
25:Y:355:GLU:HG3	25:Y:357:ASN:ND2	2.27	0.49
23:W:452:ILE:HD13	26:Z:226:ILE:HG22	1.94	0.49
1:A:115:VAL:HG13	1:A:117:GLN:N	2.28	0.49
1:A:355:PHE:CE1	1:A:385:ILE:HB	2.48	0.49
1:A:79:ASP:HB3	2:B:137:SER:HA	1.95	0.49
2:B:307:ARG:O	2:B:311:GLU:N	2.33	0.49
5:E:227:PRO:HD3	5:E:272:ARG:HH11	1.78	0.49
21:U:27:LEU:O	21:U:31:VAL:HB	2.13	0.49
22:V:160:LEU:HB2	22:V:161:PRO:HD3	1.95	0.49
22:V:349:ARG:HH21	22:V:354:LYS:HG3	1.77	0.49
22:V:485:ASP:O	22:V:489:MET:HG2	2.13	0.49
26:Z:263:ALA:O	26:Z:267:ARG:HG2	2.13	0.49
1:A:218:PRO:O	1:A:221:GLY:N	2.45	0.49
1:A:295:VAL:HG21	2:B:303:ARG:HH12	1.78	0.49
2:B:394:ASP:O	2:B:398:ILE:N	2.45	0.49
3:C:157:GLN:HE22	3:C:318:PRO:HD3	1.77	0.49
3:C:194:THR:HG21	3:C:357:ALA:N	2.28	0.49
3:C:87:VAL:HG21	3:C:123:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:204:MET:SD	4:D:212:LYS:HA	2.53	0.49
4:D:374:ASP:HA	5:E:291:ARG:CZ	2.42	0.49
4:D:62:LYS:HD2	4:D:65:GLN:HE21	1.78	0.49
5:E:269:THR:OG1	5:E:271:HIS:ND1	2.41	0.49
5:E:228:CYS:O	5:E:273:VAL:HA	2.13	0.49
8:H:19:LEU:HD12	8:H:22:ILE:HD12	1.95	0.49
12:L:82:ARG:O	12:L:86:ASN:ND2	2.41	0.49
18:R:179:VAL:HA	18:R:184:TRP:HA	1.94	0.49
21:U:14:GLU:OE1	21:U:16:GLU:HG2	2.13	0.49
22:V:91:PRO:HA	22:V:94:VAL:HG12	1.94	0.49
22:V:97:ALA:N	22:V:98:LEU:HB2	2.27	0.49
25:Y:190:ALA:O	25:Y:291:HIS:NE2	2.36	0.49
1:A:96:ALA:HB3	2:B:132:TYR:CE2	2.47	0.49
2:B:394:ASP:O	2:B:398:ILE:HG23	2.13	0.49
5:E:253:ILE:O	5:E:256:THR:OG1	2.26	0.49
5:E:304:PRO:HD2	5:E:309:ARG:HH22	1.77	0.49
5:E:182:LEU:H	33:E:401:ADP:H3'	1.78	0.49
7:G:124:VAL:HA	7:G:127:GLN:HG3	1.94	0.49
10:J:201:SER:HB3	10:J:202:GLY:HA3	1.94	0.49
12:L:69:HIS:HE2	12:L:102:PRO:HB2	1.78	0.49
12:L:50:LYS:HE2	12:L:61:LYS:HA	1.95	0.49
21:U:396:ALA:O	21:U:401:LYS:NZ	2.45	0.49
23:W:372:ARG:HG2	23:W:414:ASN:HB3	1.94	0.49
22:V:413:SER:HB2	25:Y:339:ALA:HB2	1.95	0.49
26:Z:238:PRO:HB2	26:Z:239:ASP:HA	1.95	0.49
1:A:190:VAL:HG22	1:A:316:LYS:HD2	1.94	0.48
1:A:316:LYS:HG2	1:A:317:VAL:H	1.78	0.48
1:A:421:ALA:HA	1:A:424:SER:O	2.13	0.48
1:A:220:THR:HB	33:A:501:ADP:C4	2.47	0.48
4:D:375:ILE:HD13	4:D:378:ILE:HD12	1.93	0.48
4:D:82:ILE:HG23	4:D:83:GLN:HB3	1.95	0.48
7:G:208:ILE:HB	7:G:210:PHE:HD2	1.77	0.48
11:K:227:HIS:HA	11:K:228:MET:C	2.33	0.48
11:K:50:VAL:HG11	11:K:66:LYS:HB2	1.95	0.48
16:P:15:LYS:HE2	16:P:119:PRO:HB2	1.95	0.48
22:V:290:TYR:OH	22:V:294:ARG:NH2	2.46	0.48
24:X:414:LEU:HD23	25:Y:383:LEU:HD11	1.95	0.48
25:Y:51:ALA:HA	25:Y:54:TYR:HD2	1.78	0.48
1:A:333:ARG:O	1:A:337:LEU:N	2.46	0.48
1:A:392:ALA:HB2	1:A:409:PHE:HB3	1.95	0.48
3:C:117:ARG:O	3:C:121:TYR:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:349:GLU:O	5:E:353:PHE:N	2.35	0.48
7:G:73:THR:HG22	7:G:74:GLU:H	1.77	0.48
12:L:204:ASP:HA	12:L:205:LEU:HB3	1.95	0.48
21:U:724:VAL:HA	21:U:727:LYS:HG2	1.95	0.48
22:V:197:THR:HG21	22:V:200:ARG:HG3	1.94	0.48
22:V:410:ILE:HG23	22:V:414:TYR:CD2	2.47	0.48
26:Z:271:ALA:O	26:Z:275:LEU:HB2	2.13	0.48
1:A:105:ASP:N	1:A:105:ASP:OD1	2.46	0.48
1:A:184:ILE:HD12	1:A:187:LEU:HD21	1.94	0.48
6:F:272:PHE:HA	6:F:275:ALA:HB3	1.95	0.48
6:F:380:ASN:C	6:F:382:GLU:H	2.16	0.48
6:F:69:MET:HA	6:F:72:LYS:HG2	1.95	0.48
21:U:435:SER:O	21:U:437:TYR:N	2.45	0.48
22:V:263:LEU:HG	22:V:264:TYR:H	1.78	0.48
26:Z:181:ASP:N	26:Z:181:ASP:OD1	2.46	0.48
2:B:235:LEU:O	2:B:239:VAL:N	2.31	0.48
2:B:224:LEU:HD22	2:B:351:ILE:HG12	1.95	0.48
2:B:364:ILE:HG22	2:B:368:HIS:HE1	1.78	0.48
3:C:86:LEU:HD23	3:C:96:VAL:HB	1.94	0.48
6:F:164:LEU:HD12	6:F:165:PRO:HD2	1.96	0.48
7:G:54:LYS:HD3	7:G:66:VAL:HG13	1.96	0.48
1:A:429:TYR:CZ	10:J:12:PRO:HD2	2.48	0.48
12:L:172:LEU:O	12:L:176:MET:N	2.30	0.48
25:Y:292:TYR:HA	25:Y:295:TYR:HB3	1.95	0.48
26:Z:239:ASP:OD1	26:Z:239:ASP:N	2.47	0.48
1:A:157:ILE:CG2	1:A:158:ASP:HA	2.42	0.48
1:A:177:VAL:HG22	1:A:179:GLY:H	1.77	0.48
1:A:184:ILE:O	1:A:188:ARG:N	2.47	0.48
1:A:417:ILE:HG13	1:A:418:LYS:N	2.28	0.48
3:C:295:THR:HG22	3:C:296:ASN:H	1.78	0.48
4:D:288:ILE:O	4:D:292:LEU:N	2.30	0.48
6:F:315:ASN:O	6:F:320:PHE:N	2.47	0.48
7:G:24:GLN:OE1	13:M:14:PHE:N	2.41	0.48
7:G:43:ARG:HH21	7:G:164:LYS:HG3	1.79	0.48
21:U:340:GLN:HG3	21:U:880:ASN:HB3	1.96	0.48
22:V:194:LYS:HB3	22:V:195:ILE:HG23	1.96	0.48
22:V:322:VAL:HG13	22:V:323:GLY:H	1.78	0.48
22:V:480:ILE:HG13	26:Z:267:ARG:HB3	1.95	0.48
23:W:435:LEU:HG	23:W:438:LEU:HD12	1.96	0.48
1:A:180:CYS:SG	1:A:344:SER:HB2	2.54	0.48
2:B:283:PHE:HA	2:B:328:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:GLU:O	3:C:251:ILE:HG22	2.14	0.48
4:D:113:VAL:HB	4:D:139:LEU:HG	1.95	0.48
6:F:152:GLY:O	6:F:160:ILE:HA	2.14	0.48
6:F:223:VAL:HG13	6:F:329:ILE:HG23	1.96	0.48
7:G:79:VAL:HG13	7:G:139:ILE:HB	1.94	0.48
10:J:180:ALA:HA	10:J:181:ILE:HA	1.47	0.48
21:U:413:LYS:HA	21:U:449:ILE:HG12	1.94	0.48
22:V:27:PRO:O	22:V:30:PRO:HD2	2.14	0.48
22:V:416:ARG:CZ	22:V:457:TYR:HB2	2.44	0.48
1:A:384:GLU:O	1:A:388:VAL:N	2.45	0.48
2:B:318:GLY:O	2:B:320:ASP:HA	2.13	0.48
6:F:388:THR:HG22	6:F:391:PHE:CD2	2.47	0.48
9:I:34:CYS:HB2	9:I:164:ILE:HB	1.95	0.48
13:M:185:THR:O	13:M:189:ILE:HG12	2.13	0.48
19:S:192:ALA:HA	19:S:209:SER:HA	1.95	0.48
14:N:119:MET:HB2	20:T:57:TYR:HD2	1.79	0.48
21:U:253:TYR:CZ	21:U:331:GLY:HA3	2.49	0.48
21:U:388:ASP:OD1	21:U:389:ASN:N	2.47	0.48
21:U:403:THR:HG23	21:U:777:HIS:NE2	2.29	0.48
21:U:74:PHE:HD1	21:U:103:LYS:HD2	1.78	0.48
2:B:431:GLN:NE2	9:I:170:ALA:HA	2.28	0.48
3:C:167:LEU:HG	3:C:171:HIS:HB2	1.95	0.48
3:C:271:ARG:HA	3:C:274:LEU:HB2	1.94	0.48
5:E:204:VAL:HG13	6:F:308:ARG:HH22	1.79	0.48
8:H:111:VAL:HG22	8:H:136:ILE:HD12	1.95	0.48
12:L:104:PRO:HD2	12:L:107:ARG:HH12	1.77	0.48
16:P:189:ILE:HG23	16:P:196:THR:HB	1.94	0.48
22:V:210:CYS:HA	22:V:213:TYR:HD2	1.78	0.48
22:V:289:LEU:HA	22:V:292:THR:HG22	1.96	0.48
23:W:262:LYS:HA	23:W:265:GLN:HG2	1.95	0.48
1:A:215:PHE:HB3	1:A:321:THR:HG23	1.95	0.48
3:C:191:PRO:O	3:C:193:GLY:HA3	2.13	0.48
4:D:104:GLY:HA2	4:D:109:SER:O	2.14	0.48
4:D:303:VAL:CG2	4:D:304:ASN:HB2	2.44	0.48
4:D:315:ASP:N	4:D:315:ASP:OD1	2.45	0.48
5:E:139:SER:O	5:E:143:ARG:N	2.32	0.48
5:E:157:GLU:O	5:E:161:ARG:N	2.45	0.48
5:E:84:ARG:HD2	5:E:108:MET:HA	1.96	0.48
6:F:230:GLY:HA2	6:F:231:THR:HB	1.96	0.48
5:E:204:VAL:HB	6:F:261:ILE:HD12	1.95	0.48
8:H:45:VAL:HG22	8:H:212:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:120:GLN:O	11:K:134:SER:OG	2.25	0.48
12:L:69:HIS:HB2	12:L:137:TYR:HB2	1.96	0.48
2:B:151:LEU:HD13	3:C:96:VAL:HG11	1.96	0.48
4:D:162:VAL:O	4:D:221:HIS:NE2	2.44	0.48
4:D:244:PRO:HA	4:D:248:ARG:H	1.78	0.48
10:J:96:LEU:HA	17:Q:62:LYS:HE2	1.95	0.48
18:R:3:THR:O	18:R:127:SER:OG	2.21	0.48
21:U:689:ILE:HG12	21:U:732:LEU:HD22	1.95	0.48
21:U:759:SER:HA	21:U:782:ALA:HA	1.95	0.48
23:W:435:LEU:HA	23:W:438:LEU:HB2	1.96	0.48
1:A:194:PRO:HB3	1:A:201:PHE:HE2	1.78	0.47
3:C:256:SER:O	3:C:262:GLY:HA3	2.14	0.47
5:E:134:GLU:O	5:E:315:ILE:HD12	2.14	0.47
5:E:180:LYS:NZ	5:E:279:THR:O	2.43	0.47
6:F:88:TYR:HB2	6:F:154:ASN:OD1	2.14	0.47
6:F:195:ILE:HA	6:F:198:LEU:HB3	1.94	0.47
12:L:157:ARG:HG3	12:L:176:MET:HE2	1.96	0.47
18:R:50:ALA:HB2	19:S:129:SER:HB2	1.96	0.47
24:X:407:MET:HE2	25:Y:372:LYS:HE3	1.96	0.47
25:Y:178:ASN:HB3	25:Y:207:THR:HG22	1.96	0.47
3:C:233:GLU:O	3:C:237:MET:HG2	2.13	0.47
4:D:244:PRO:O	4:D:248:ARG:HB3	2.14	0.47
4:D:231:VAL:HA	4:D:265:ASP:O	2.14	0.47
6:F:170:SER:OG	6:F:171:ARG:N	2.47	0.47
7:G:54:LYS:HG2	7:G:214:GLU:O	2.15	0.47
9:I:76:VAL:HG21	9:I:83:ALA:HB1	1.96	0.47
12:L:11:THR:HG23	13:M:129:ARG:HB3	1.95	0.47
14:N:76:VAL:HG23	14:N:104:ASP:HB2	1.96	0.47
21:U:586:VAL:HG11	21:U:601:ARG:HH12	1.78	0.47
1:A:193:THR:O	1:A:200:ARG:NH1	2.47	0.47
2:B:155:LYS:HA	2:B:156:VAL:HA	1.55	0.47
4:D:147:ALA:O	5:E:62:LYS:HD2	2.14	0.47
5:E:346:VAL:HA	5:E:349:GLU:HB3	1.96	0.47
6:F:428:GLN:HG2	6:F:429:ALA:HB2	1.96	0.47
7:G:185:LYS:HB3	7:G:186:LYS:H	1.44	0.47
9:I:122:THR:O	10:J:125:ARG:NH1	2.47	0.47
21:U:541:HIS:HB2	21:U:544:ILE:HG22	1.96	0.47
22:V:96:ARG:HB2	22:V:107:ARG:HD2	1.96	0.47
25:Y:89:GLU:HA	25:Y:92:GLU:HG2	1.96	0.47
26:Z:63:LYS:CB	26:Z:64:ASP:HB2	2.33	0.47
2:B:167:THR:OG1	2:B:168:ASP:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:PRO:HB3	3:C:228:ALA:HB2	1.96	0.47
4:D:83:GLN:NE2	4:D:140:VAL:HG21	2.23	0.47
5:E:44:GLU:HB3	6:F:76:ASN:ND2	2.29	0.47
6:F:368:ILE:O	6:F:371:ARG:HG2	2.14	0.47
11:K:117:SER:HB3	12:L:82:ARG:HH22	1.79	0.47
13:M:40:ARG:HH11	13:M:148:LEU:HB3	1.78	0.47
13:M:80:LEU:HD23	13:M:82:ALA:H	1.80	0.47
17:Q:17:SER:OG	17:Q:179:SER:OG	2.25	0.47
21:U:241:ASN:HD21	21:U:244:MET:HG3	1.80	0.47
23:W:403:PHE:CD2	23:W:419:LYS:HE3	2.49	0.47
26:Z:96:HIS:HE1	26:Z:121:LEU:HD13	1.79	0.47
1:A:111:TYR:O	1:A:123:VAL:N	2.47	0.47
1:A:187:LEU:O	1:A:191:VAL:HG12	2.14	0.47
1:A:97:ARG:HD3	2:B:130:GLU:O	2.15	0.47
2:B:375:ALA:HA	2:B:413:LYS:HD2	1.96	0.47
3:C:172:PRO:O	3:C:175:PHE:HB2	2.14	0.47
5:E:268:ASP:OD1	5:E:269:THR:N	2.47	0.47
14:N:7:GLN:HA	14:N:12:VAL:HG12	1.97	0.47
21:U:610:VAL:O	26:Z:177:ARG:NH2	2.47	0.47
26:Z:262:LEU:O	26:Z:266:ILE:HD12	2.13	0.47
2:B:178:LYS:HE2	3:C:285:ALA:HB2	1.97	0.47
2:B:274:ALA:HB1	2:B:325:VAL:HB	1.95	0.47
3:C:194:THR:HB	33:C:501:ADP:C8	2.49	0.47
3:C:229:ARG:NH1	3:C:279:GLN:HE22	2.13	0.47
4:D:417:TYR:OH	7:G:22:LEU:HG	2.14	0.47
8:H:9:SER:O	8:H:11:THR:N	2.47	0.47
8:H:221:LEU:HD13	8:H:225:GLU:HB2	1.96	0.47
21:U:89:ASN:HB3	21:U:136:LYS:NZ	2.29	0.47
22:V:224:LEU:HD13	22:V:227:VAL:HB	1.96	0.47
26:Z:102:HIS:CD2	26:Z:104:ASN:HB3	2.49	0.47
1:A:237:PHE:HB2	1:A:271:LEU:O	2.14	0.47
3:C:214:VAL:HG22	3:C:215:SER:H	1.80	0.47
5:E:215:ILE:HB	5:E:263:GLN:HE22	1.79	0.47
5:E:44:GLU:OE2	6:F:77:SER:OG	2.33	0.47
4:D:86:PRO:HB3	5:E:81:VAL:HG12	1.96	0.47
6:F:428:GLN:HA	6:F:429:ALA:HA	1.69	0.47
17:Q:117:TYR:N	17:Q:125:ALA:O	2.47	0.47
21:U:738:ASP:OD1	21:U:742:HIS:NE2	2.47	0.47
3:C:117:ARG:HD3	3:C:122:THR:OG1	2.15	0.47
3:C:194:THR:OG1	3:C:356:GLY:HA3	2.15	0.47
4:D:282:ASP:OD1	5:E:251:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:GLN:N	6:F:133:PHE:O	2.48	0.47
5:E:62:LYS:O	5:E:70:ILE:N	2.47	0.47
7:G:132:ARG:HB2	13:M:124:LEU:HA	1.96	0.47
11:K:68:VAL:HG21	11:K:89:ILE:HG13	1.97	0.47
15:O:217:THR:HB	16:P:195:ILE:HB	1.97	0.47
18:R:127:SER:N	18:R:136:TYR:OH	2.43	0.47
19:S:110:ILE:HG13	19:S:124:PHE:HE2	1.79	0.47
19:S:11:THR:N	19:S:26:ASP:OD1	2.48	0.47
12:L:101:ARG:HH12	20:T:87:ALA:HB2	1.80	0.47
22:V:336:GLU:HA	22:V:339:LEU:HD12	1.96	0.47
1:A:243:SER:HB3	2:B:264:PRO:HD3	1.96	0.47
2:B:314:ASN:HA	2:B:317:ASP:HB2	1.96	0.47
2:B:363:ARG:NH1	2:B:363:ARG:O	2.48	0.47
4:D:277:ALA:C	4:D:280:GLY:H	2.18	0.47
4:D:300:ASP:HA	4:D:301:GLN:HA	1.51	0.47
5:E:289:LEU:HD23	5:E:294:ARG:HD3	1.96	0.47
7:G:110:PRO:O	7:G:111:VAL:HG12	2.14	0.47
10:J:73:PHE:HA	10:J:131:ALA:HA	1.96	0.47
21:U:92:ASP:N	21:U:92:ASP:OD1	2.48	0.47
22:V:344:ASP:HB2	22:V:368:ARG:NH1	2.29	0.47
1:A:288:GLY:HA2	1:A:289:ALA:HA	1.65	0.47
1:A:384:GLU:H	2:B:343:ARG:NH1	2.09	0.47
3:C:184:LYS:HG3	3:C:311:ILE:HD12	1.96	0.47
4:D:133:HIS:CE1	4:D:135:HIS:HB2	2.49	0.47
5:E:47:LEU:HA	5:E:50:LEU:CD1	2.45	0.47
6:F:93:VAL:HG22	6:F:151:VAL:HG21	1.97	0.47
14:N:80:ALA:HA	14:N:83:PHE:HD2	1.80	0.47
17:Q:5:ILE:HG13	17:Q:7:ILE:HG13	1.96	0.47
21:U:118:LEU:HD23	21:U:121:GLY:O	2.15	0.47
21:U:167:ILE:HD12	21:U:204:ILE:HG21	1.97	0.47
21:U:581:SER:O	21:U:585:THR:OG1	2.27	0.47
25:Y:221:THR:HA	25:Y:224:VAL:HG12	1.97	0.47
25:Y:204:THR:HB	25:Y:246:ILE:HD13	1.96	0.47
1:A:104:ALA:H	1:A:112:ILE:HG23	1.80	0.47
1:A:83:ASP:HA	1:A:86:THR:HB	1.97	0.47
6:F:222:GLY:O	6:F:349:ASP:HB3	2.15	0.47
6:F:299:GLU:CG	6:F:300:LYS:HB3	2.40	0.47
6:F:344:ARG:HB3	6:F:347:ARG:HG3	1.97	0.47
7:G:17:SER:OG	7:G:21:ARG:HG2	2.15	0.47
10:J:84:ILE:O	10:J:88:ARG:HG3	2.14	0.47
13:M:34:SER:OG	13:M:65:ARG:NH2	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:211:ARG:NH2	19:S:213:ASP:OD2	2.46	0.47
22:V:244:ALA:C	22:V:246:GLY:H	2.18	0.47
22:V:280:ALA:HB1	22:V:281:ASN:ND2	2.30	0.47
25:Y:240:VAL:HG23	25:Y:241:ILE:HG13	1.97	0.47
2:B:223:ILE:O	2:B:350:LYS:HA	2.15	0.46
2:B:365:PHE:HD2	2:B:380:LEU:HD12	1.79	0.46
4:D:205:TYR:HA	4:D:311:THR:O	2.15	0.46
4:D:202:VAL:HG11	4:D:308:ILE:HG22	1.96	0.46
4:D:401:LYS:HA	4:D:404:LYS:HG2	1.96	0.46
7:G:190:THR:H	7:G:193:GLN:HB3	1.80	0.46
10:J:154:HIS:CE1	11:K:59:MET:HG3	2.50	0.46
11:K:11:GLY:O	11:K:12:VAL:HG22	2.14	0.46
11:K:203:LYS:HA	11:K:206:MET:HG2	1.96	0.46
13:M:20:VAL:HG12	13:M:22:GLN:H	1.80	0.46
10:J:85:ASN:OD1	17:Q:70:ARG:NH1	2.48	0.46
21:U:32:ASN:OD1	21:U:33:ASP:N	2.44	0.46
25:Y:101:ARG:HA	25:Y:104:MET:HG2	1.96	0.46
25:Y:311:TYR:HD2	25:Y:314:LEU:HG	1.80	0.46
1:A:380:SER:HB3	1:A:385:ILE:CG2	2.45	0.46
2:B:187:ILE:HB	2:B:190:LEU:HD21	1.98	0.46
3:C:78:ARG:HB3	3:C:86:LEU:HD12	1.97	0.46
4:D:280:GLY:HA2	4:D:283:ARG:HD3	1.97	0.46
3:C:219:LEU:HD21	4:D:287:ARG:HG2	1.97	0.46
4:D:192:LYS:NZ	4:D:302:ASN:OD1	2.40	0.46
5:E:83:CYS:HA	5:E:107:ILE:HB	1.97	0.46
6:F:93:VAL:HA	6:F:124:ILE:HD12	1.97	0.46
10:J:10:PHE:HD2	11:K:23:GLN:HE21	1.62	0.46
13:M:197:ILE:HA	13:M:200:VAL:HG12	1.97	0.46
20:T:186:ARG:HE	20:T:202:PRO:HB2	1.81	0.46
22:V:58:ALA:HB2	22:V:201:ARG:HD2	1.97	0.46
23:W:299:ILE:HG22	23:W:301:LYS:H	1.79	0.46
1:A:125:LEU:HB3	1:A:149:ILE:HD12	1.98	0.46
1:A:388:VAL:HG13	1:A:413:VAL:CG2	2.45	0.46
2:B:111:THR:H	2:B:125:THR:HB	1.79	0.46
3:C:271:ARG:O	3:C:275:GLU:HG2	2.15	0.46
5:E:356:ARG:NE	6:F:200:GLU:OE2	2.48	0.46
16:P:26:ARG:HD3	16:P:186:ILE:HB	1.98	0.46
19:S:93:SER:OG	19:S:128:GLY:O	2.28	0.46
22:V:250:LEU:HA	22:V:253:LEU:HD12	1.95	0.46
23:W:444:HIS:O	23:W:448:LYS:NZ	2.46	0.46
25:Y:357:ASN:OD1	25:Y:358:ARG:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:ARG:HG3	2:B:283:PHE:HD2	1.80	0.46
4:D:82:ILE:HA	4:D:83:GLN:HA	1.47	0.46
5:E:146:ARG:HH22	5:E:190:GLN:HG2	1.80	0.46
11:K:77:ALA:HB3	11:K:142:LEU:HB2	1.97	0.46
12:L:10:VAL:HG22	12:L:21:GLN:HG3	1.97	0.46
12:L:89:ARG:HE	19:S:77:HIS:CD2	2.33	0.46
21:U:49:TYR:O	21:U:57:ARG:NH2	2.48	0.46
22:V:241:ARG:HG3	22:V:242:HIS:H	1.81	0.46
3:C:37:ASP:OD2	22:V:496:PHE:N	2.49	0.46
23:W:431:LYS:O	23:W:434:SER:OG	2.21	0.46
25:Y:78:GLU:HA	25:Y:81:LEU:HB3	1.96	0.46
1:A:382:GLY:HA3	33:A:501:ADP:C8	2.51	0.46
2:B:126:SER:HA	2:B:127:VAL:HA	1.42	0.46
6:F:334:ARG:HD3	6:F:336:ASP:HB3	1.97	0.46
6:F:92:ASN:OD1	6:F:93:VAL:N	2.43	0.46
8:H:93:LEU:HD11	8:H:113:ARG:HB3	1.97	0.46
13:M:57:LEU:HB2	13:M:58:TYR:HD1	1.81	0.46
16:P:135:ASP:OD1	16:P:136:PHE:N	2.44	0.46
17:Q:11:ASP:N	17:Q:11:ASP:OD1	2.47	0.46
17:Q:47:VAL:HB	17:Q:102:LEU:HG	1.97	0.46
22:V:100:MET:O	22:V:104:THR:HG23	2.15	0.46
25:Y:324:GLY:N	25:Y:325:VAL:HA	2.30	0.46
26:Z:193:ASN:HA	26:Z:196:HIS:CE1	2.49	0.46
26:Z:197:GLY:O	26:Z:201:LEU:HG	2.15	0.46
1:A:343:PHE:HA	1:A:344:SER:OG	2.15	0.46
1:A:429:TYR:CE1	10:J:12:PRO:HD2	2.50	0.46
2:B:220:LYS:HB2	2:B:346:ARG:NH2	2.30	0.46
4:D:269:ALA:HB1	5:E:255:ARG:HG2	1.97	0.46
6:F:102:ASN:HA	6:F:103:ASP:HA	1.69	0.46
10:J:88:ARG:NH2	17:Q:66:LEU:O	2.49	0.46
19:S:27:THR:HB	19:S:39:ASP:HA	1.96	0.46
22:V:363:LEU:HA	22:V:378:VAL:HG11	1.97	0.46
24:X:365:LEU:O	24:X:369:ILE:HD12	2.16	0.46
24:X:378:LEU:HA	24:X:385:LEU:HA	1.97	0.46
2:B:117:ASP:OD1	2:B:117:ASP:N	2.49	0.46
4:D:408:LYS:HB3	4:D:409:LYS:CB	2.45	0.46
4:D:413:GLU:HA	4:D:416:PHE:CG	2.50	0.46
6:F:358:ASN:HA	6:F:362:ARG:NH1	2.30	0.46
10:J:198:VAL:HA	10:J:199:VAL:HA	1.62	0.46
22:V:286:ALA:HB2	22:V:315:LYS:HB3	1.98	0.46
22:V:469:THR:HG21	26:Z:257:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:108:ALA:HA	25:Y:111:LEU:HB2	1.97	0.46
26:Z:138:TYR:HB3	26:Z:155:PHE:HB3	1.98	0.46
2:B:166:ASP:HB2	2:B:167:THR:O	2.16	0.46
3:C:97:VAL:HG11	3:C:122:THR:HA	1.97	0.46
4:D:244:PRO:HD3	4:D:288:ILE:CD1	2.45	0.46
5:E:128:GLY:HA3	5:E:131:SER:H	1.81	0.46
5:E:375:ALA:O	5:E:379:LYS:N	2.46	0.46
5:E:55:GLN:NE2	5:E:108:MET:SD	2.89	0.46
6:F:138:GLY:O	6:F:159:LEU:HB2	2.16	0.46
12:L:52:ALA:HB2	12:L:59:HIS:HA	1.98	0.46
21:U:524:LYS:HB3	21:U:559:ARG:HE	1.81	0.46
23:W:420:ASP:HB3	23:W:422:ASN:CB	2.44	0.46
1:A:100:LYS:HE2	1:A:115:VAL:HB	1.97	0.46
1:A:129:VAL:HG21	1:A:149:ILE:HG22	1.98	0.46
3:C:146:SER:HB2	3:C:150:MET:HB2	1.97	0.46
3:C:151:ILE:HD11	33:C:501:ADP:N7	2.31	0.46
4:D:105:SER:HB3	4:D:111:TYR:HE2	1.80	0.46
4:D:231:VAL:HG12	4:D:232:GLY:H	1.81	0.46
4:D:263:PHE:HB2	4:D:308:ILE:HD11	1.97	0.46
4:D:91:GLN:N	4:D:104:GLY:O	2.49	0.46
7:G:109:ILE:HG12	7:G:111:VAL:H	1.80	0.46
9:I:108:GLU:OE2	9:I:148:TYR:OH	2.33	0.46
12:L:107:ARG:HE	20:T:77:LEU:HD13	1.79	0.46
12:L:33:SER:HB2	12:L:49:LEU:HD23	1.97	0.46
13:M:83:ASP:HB2	13:M:133:CYS:SG	2.56	0.46
18:R:37:ILE:HG23	18:R:60:ALA:HB2	1.98	0.46
4:D:60:TYR:HB2	21:U:603:LEU:HD21	1.98	0.46
21:U:885:MET:HG2	21:U:887:ALA:H	1.81	0.46
22:V:258:TYR:HB3	22:V:265:ASP:OD2	2.15	0.46
25:Y:77:ASN:O	25:Y:81:LEU:N	2.49	0.46
3:C:338:LEU:HD21	3:C:342:ILE:HG21	1.98	0.46
4:D:414:HIS:CE1	7:G:21:ARG:HB2	2.50	0.46
6:F:314:LEU:HG	6:F:347:ARG:HE	1.80	0.46
2:B:110:GLY:N	2:B:150:VAL:O	2.47	0.45
6:F:122:ALA:N	6:F:134:LEU:O	2.43	0.45
10:J:119:THR:HG22	10:J:126:PRO:HG3	1.99	0.45
12:L:137:TYR:CZ	12:L:216:GLY:HA2	2.51	0.45
13:M:58:TYR:CE2	13:M:62:SER:HB3	2.51	0.45
14:N:19:ARG:HH21	14:N:26:ILE:HG12	1.82	0.45
26:Z:45:LYS:HG3	26:Z:46:LYS:H	1.80	0.45
1:A:338:ASP:OD1	1:A:339:ARG:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLU:HA	1:A:414:ASN:HD21	1.82	0.45
4:D:45:LYS:O	4:D:48:GLN:NE2	2.49	0.45
6:F:231:THR:HG22	6:F:233:LYS:HG3	1.99	0.45
6:F:310:MET:O	6:F:314:LEU:N	2.44	0.45
7:G:139:ILE:HG13	7:G:153:LYS:HG3	1.98	0.45
14:N:92:GLU:OE1	20:T:3:ASN:ND2	2.49	0.45
17:Q:47:VAL:O	17:Q:101:ASN:N	2.48	0.45
17:Q:91:CYS:SG	17:Q:98:TYR:HB2	2.56	0.45
20:T:27:LEU:HD13	20:T:184:TYR:HB3	1.98	0.45
21:U:20:LYS:HG2	21:U:48:LEU:HD21	1.97	0.45
22:V:156:SER:HB2	22:V:160:LEU:HG	1.98	0.45
25:Y:387:ILE:HA	25:Y:388:ASN:HA	1.70	0.45
2:B:115:ILE:HA	2:B:121:ALA:HA	1.98	0.45
2:B:140:ASP:O	2:B:144:LEU:HG	2.17	0.45
3:C:378:VAL:HG12	3:C:379:THR:H	1.81	0.45
4:D:272:THR:HB	5:E:251:ARG:HE	1.81	0.45
13:M:72:HIS:CD2	13:M:73:VAL:HG23	2.52	0.45
21:U:900:TYR:HB3	21:U:914:LEU:HG	1.97	0.45
22:V:62:HIS:HA	22:V:65:ARG:HB3	1.98	0.45
26:Z:68:TRP:CE3	26:Z:108:ILE:HG13	2.51	0.45
2:B:112:LEU:N	2:B:148:CYS:O	2.49	0.45
2:B:222:VAL:HA	2:B:346:ARG:HG2	1.98	0.45
3:C:114:VAL:HG21	3:C:123:LEU:HD13	1.97	0.45
6:F:312:GLU:HA	6:F:315:ASN:HB3	1.98	0.45
6:F:70:LYS:HD2	6:F:73:ILE:HD11	1.98	0.45
10:J:132:LEU:HD22	10:J:159:ASN:OD1	2.17	0.45
10:J:172:LEU:HD22	10:J:175:ASN:HD22	1.81	0.45
11:K:85:ALA:HB2	11:K:139:VAL:HG21	1.99	0.45
21:U:447:GLY:HA3	21:U:480:GLY:HA2	1.97	0.45
21:U:697:GLN:HG3	21:U:745:THR:HB	1.99	0.45
21:U:794:ASP:OD1	21:U:795:LEU:N	2.49	0.45
21:U:65:SER:HB3	21:U:96:TYR:OH	2.16	0.45
22:V:305:ALA:HB1	22:V:335:VAL:HG11	1.99	0.45
22:V:31:ALA:HB3	22:V:32:PRO:HD3	1.97	0.45
26:Z:34:ARG:HB2	26:Z:97:THR:HG22	1.97	0.45
1:A:299:MET:O	1:A:303:ILE:HG12	2.16	0.45
1:A:261:PHE:HD2	1:A:305:GLN:HE21	1.64	0.45
2:B:166:ASP:HA	2:B:167:THR:OG1	2.17	0.45
2:B:349:ARG:NE	2:B:351:ILE:HG22	2.32	0.45
2:B:365:PHE:HD1	2:B:395:ILE:HG12	1.82	0.45
3:C:209:CYS:HB3	3:C:243:PRO:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:168:LYS:NZ	5:E:293:GLY:HA2	2.31	0.45
5:E:62:LYS:HA	5:E:94:PRO:HB3	1.98	0.45
6:F:425:LEU:HA	6:F:428:GLN:O	2.17	0.45
7:G:12:HIS:HD2	13:M:7:TYR:HA	1.81	0.45
11:K:225:ASN:HB2	11:K:226:PHE:CD1	2.51	0.45
11:K:236:GLU:HG3	11:K:239:LYS:HE3	1.99	0.45
13:M:186:CYS:HA	13:M:189:ILE:HB	1.98	0.45
17:Q:81:ALA:HA	17:Q:104:LEU:HD12	1.98	0.45
18:R:80:SER:OG	18:R:120:ARG:NH2	2.36	0.45
21:U:342:LEU:O	21:U:346:ASN:HB2	2.16	0.45
21:U:415:HIS:NE2	21:U:418:GLU:HB3	2.32	0.45
21:U:563:ALA:O	21:U:567:ILE:HG12	2.17	0.45
22:V:192:MET:O	22:V:200:ARG:NH2	2.49	0.45
23:W:247:TYR:HB3	23:W:270:VAL:HG23	1.97	0.45
25:Y:356:THR:OG1	25:Y:357:ASN:O	2.19	0.45
1:A:168:GLU:HG2	1:A:169:LYS:HG2	1.97	0.45
3:C:268:GLU:O	3:C:272:THR:OG1	2.22	0.45
3:C:82:LYS:HG3	3:C:84:LYS:HG3	1.98	0.45
4:D:275:PHE:O	4:D:283:ARG:HD2	2.17	0.45
4:D:280:GLY:HA2	4:D:283:ARG:HB2	1.99	0.45
4:D:87:LEU:HD12	4:D:87:LEU:HA	1.81	0.45
5:E:40:TYR:O	5:E:44:GLU:HG2	2.17	0.45
6:F:84:LYS:NZ	6:F:139:LEU:HD23	2.31	0.45
6:F:233:LYS:HA	6:F:236:LEU:HB3	1.97	0.45
9:I:182:GLY:N	9:I:183:GLU:HB2	2.31	0.45
13:M:150:MET:N	13:M:158:TYR:O	2.34	0.45
13:M:214:SER:HA	13:M:226:ILE:HA	1.98	0.45
21:U:152:GLY:O	21:U:156:GLU:HG2	2.16	0.45
22:V:309:MET:HB3	22:V:332:LEU:HG	1.99	0.45
22:V:416:ARG:CB	25:Y:349:LYS:HB3	2.47	0.45
25:Y:357:ASN:CB	25:Y:358:ARG:HA	2.46	0.45
26:Z:181:ASP:HA	26:Z:182:THR:HA	1.72	0.45
1:A:187:LEU:O	1:A:190:VAL:HG12	2.16	0.45
1:A:298:THR:HA	1:A:301:GLU:HB3	1.98	0.45
1:A:428:ARG:HD3	1:A:431:THR:OG1	2.17	0.45
2:B:283:PHE:HB2	2:B:328:ILE:HB	1.99	0.45
2:B:294:ARG:HD2	2:B:295:TYR:H	1.82	0.45
7:G:138:MET:O	7:G:154:CYS:N	2.49	0.45
9:I:197:LEU:HB3	9:I:206:LEU:HD11	1.99	0.45
17:Q:38:MET:HE2	17:Q:38:MET:HB3	1.86	0.45
23:W:428:TRP:HE1	26:Z:252:LYS:HD3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:165:GLU:H	26:Z:168:GLU:HG3	1.81	0.45
1:A:222:LYS:HZ2	2:B:319:PHE:HB2	1.82	0.45
5:E:188:ALA:HB2	5:E:231:PHE:CE2	2.52	0.45
10:J:115:LYS:O	10:J:119:THR:HG23	2.17	0.45
20:T:136:SER:HB2	20:T:150:LEU:HD13	1.99	0.45
12:L:107:ARG:NH2	20:T:79:ASP:OD2	2.50	0.45
22:V:416:ARG:HA	22:V:458:VAL:O	2.17	0.45
23:W:268:LYS:HA	23:W:271:VAL:HG12	1.98	0.45
2:B:131:HIS:CD2	2:B:157:HIS:HB2	2.52	0.45
2:B:95:GLU:O	2:B:99:VAL:HG22	2.16	0.45
3:C:76:VAL:HG22	3:C:110:PRO:HA	1.98	0.45
3:C:229:ARG:HH11	3:C:279:GLN:HE22	1.63	0.45
4:D:375:ILE:O	4:D:379:CYS:N	2.36	0.45
5:E:84:ARG:HH22	6:F:117:ARG:HH12	1.65	0.45
6:F:161:LEU:HG	6:F:162:GLU:N	2.32	0.45
7:G:88:ARG:NH1	13:M:156:VAL:HA	2.32	0.45
13:M:140:TYR:HE2	13:M:218:GLU:HB2	1.82	0.45
13:M:71:ARG:O	13:M:224:HIS:N	2.47	0.45
14:N:26:ILE:HG21	14:N:29:ARG:HE	1.82	0.45
18:R:34:VAL:HG11	18:R:177:TYR:HD2	1.82	0.45
22:V:94:VAL:HG22	22:V:138:PRO:HD3	1.99	0.45
25:Y:131:THR:O	25:Y:137:ARG:NH1	2.50	0.45
1:A:112:ILE:HB	1:A:122:VAL:HG13	1.98	0.45
1:A:164:MET:O	1:A:239:ARG:NH2	2.50	0.45
1:A:96:ALA:HB3	2:B:132:TYR:HE2	1.79	0.45
3:C:11:LEU:HD23	3:C:14:GLY:HA2	1.99	0.45
4:D:240:LEU:HB2	4:D:284:GLU:OE1	2.16	0.45
6:F:365:ILE:HG13	6:F:366:MET:N	2.31	0.45
15:O:98:LEU:HB2	15:O:113:ILE:HD12	1.98	0.45
21:U:505:ASP:HB3	21:U:508:THR:HG22	1.99	0.45
21:U:607:VAL:O	21:U:615:ARG:NH1	2.49	0.45
21:U:742:HIS:HB2	21:U:883:ARG:HH12	1.82	0.45
22:V:225:ASP:HA	22:V:228:ARG:HG3	1.98	0.45
22:V:451:ILE:HB	22:V:453:HIS:CE1	2.52	0.45
25:Y:101:ARG:HD3	25:Y:130:LYS:HD3	1.99	0.45
25:Y:286:TRP:O	25:Y:287:LEU:HG	2.17	0.45
26:Z:185:GLY:O	26:Z:189:GLN:NE2	2.50	0.45
26:Z:253:THR:O	26:Z:257:MET:HG2	2.17	0.45
3:C:274:LEU:HD21	3:C:306:LEU:HD23	1.99	0.44
4:D:362:ASP:OD1	4:D:363:TYR:N	2.50	0.44
4:D:418:LYS:HE2	8:H:33:ALA:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:327:LYS:N	6:F:327:LYS:HD2	2.32	0.44
6:F:423:GLY:HA2	6:F:426:GLU:HB3	1.98	0.44
7:G:212:PRO:HG3	7:G:236:ASP:HB2	1.99	0.44
11:K:169:ALA:HB3	11:K:178:GLN:HG2	1.99	0.44
13:M:110:HIS:NE2	14:N:70:LEU:HA	2.32	0.44
14:N:177:ALA:HA	14:N:186:ARG:HA	1.98	0.44
16:P:93:ASN:O	16:P:97:GLU:HG3	2.17	0.44
21:U:501:LEU:HD11	21:U:544:ILE:HD11	1.98	0.44
22:V:98:LEU:HA	22:V:99:ARG:HA	1.69	0.44
26:Z:258:VAL:O	26:Z:262:LEU:HG	2.17	0.44
26:Z:68:TRP:HD1	26:Z:104:ASN:HD21	1.64	0.44
1:A:166:VAL:HG22	1:A:238:ILE:HG12	2.00	0.44
3:C:161:ILE:HD12	3:C:164:VAL:HB	1.99	0.44
4:D:289:LEU:HA	4:D:292:LEU:HG	1.99	0.44
6:F:300:LYS:HD2	6:F:304:ARG:HH21	1.82	0.44
9:I:220:ASN:HA	9:I:221:GLY:HA2	1.55	0.44
14:N:21:THR:HG22	14:N:26:ILE:HG13	1.98	0.44
18:R:157:ARG:HD3	18:R:195:LEU:HD22	1.99	0.44
18:R:55:TRP:CD2	18:R:87:VAL:HG22	2.53	0.44
20:T:122:LEU:HG	20:T:137:LEU:HD12	1.98	0.44
20:T:145:LEU:HD13	20:T:175:VAL:HG12	2.00	0.44
21:U:9:ILE:HG12	21:U:38:ILE:HG23	1.99	0.44
22:V:266:GLN:HB3	22:V:299:GLN:HE22	1.83	0.44
22:V:25:GLU:O	22:V:28:PRO:HD2	2.17	0.44
25:Y:318:TYR:HA	25:Y:321:GLU:HG3	1.99	0.44
1:A:174:TYR:OH	1:A:192:GLU:OE1	2.28	0.44
2:B:153:ASN:O	2:B:157:HIS:HA	2.17	0.44
3:C:268:GLU:O	3:C:272:THR:N	2.47	0.44
2:B:249:ARG:NH1	3:C:278:ASN:O	2.50	0.44
6:F:255:GLN:O	6:F:258:GLN:NE2	2.50	0.44
7:G:168:ALA:O	7:G:172:GLN:NE2	2.50	0.44
9:I:68:LEU:HD12	9:I:69:ASN:HB2	1.99	0.44
11:K:117:SER:HB2	12:L:82:ARG:HH12	1.82	0.44
21:U:424:ALA:HA	21:U:427:LEU:HD13	2.00	0.44
21:U:889:LEU:HD23	21:U:892:LEU:HD21	1.98	0.44
22:V:188:SER:O	22:V:200:ARG:NH2	2.40	0.44
22:V:194:LYS:HA	22:V:195:ILE:HA	1.54	0.44
23:W:367:ALA:HB1	23:W:416:GLN:OE1	2.18	0.44
1:A:301:GLU:HG3	6:F:254:PRO:HG3	1.98	0.44
2:B:184:TYR:HD2	2:B:240:ALA:HB1	1.82	0.44
3:C:73:VAL:HA	3:C:115:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:216:GLY:O	3:C:220:VAL:HG22	2.16	0.44
3:C:363:CYS:O	3:C:367:GLY:N	2.43	0.44
4:D:201:GLY:O	4:D:329:ARG:HB2	2.17	0.44
4:D:274:ARG:HD2	4:D:274:ARG:HA	1.76	0.44
3:C:28:ILE:HG22	4:D:51:LEU:HD11	1.99	0.44
5:E:117:PRO:HG2	5:E:214:LEU:HD11	1.98	0.44
7:G:52:THR:O	7:G:216:GLU:N	2.37	0.44
7:G:62:ASP:O	7:G:66:VAL:HG23	2.17	0.44
9:I:156:TYR:HE2	10:J:58:THR:HB	1.82	0.44
21:U:407:SER:O	21:U:411:ILE:HG13	2.17	0.44
25:Y:268:TYR:CZ	25:Y:307:LEU:HD12	2.52	0.44
25:Y:363:ASN:O	25:Y:367:GLN:HB2	2.17	0.44
25:Y:80:GLU:HA	25:Y:83:ARG:HG2	2.00	0.44
26:Z:96:HIS:CE1	26:Z:123:ILE:HG12	2.53	0.44
1:A:170:PRO:HB2	1:A:230:ALA:HA	2.00	0.44
1:A:206:ILE:HG23	1:A:207:GLU:N	2.29	0.44
2:B:313:LEU:HD22	2:B:341:LEU:HA	1.98	0.44
3:C:380:GLN:O	3:C:384:GLU:N	2.40	0.44
4:D:105:SER:OG	4:D:107:THR:OG1	2.25	0.44
4:D:186:THR:HG23	4:D:187:HIS:CD2	2.53	0.44
4:D:263:PHE:CD1	4:D:308:ILE:HG13	2.52	0.44
4:D:371:SER:HA	4:D:372:GLY:HA3	1.72	0.44
6:F:338:LEU:HD13	6:F:342:LEU:HD12	2.00	0.44
8:H:87:VAL:O	8:H:91:ARG:HG2	2.17	0.44
10:J:173:GLU:HA	10:J:176:TYR:HD2	1.82	0.44
16:P:53:LEU:HD23	16:P:107:PRO:HA	2.00	0.44
16:P:190:ILE:HG22	16:P:195:ILE:HG23	2.00	0.44
13:M:92:ARG:CZ	20:T:76:LEU:HD12	2.48	0.44
24:X:411:VAL:HA	24:X:414:LEU:HD12	1.97	0.44
25:Y:283:LYS:HE2	25:Y:292:TYR:CZ	2.53	0.44
1:A:143:ASP:O	1:A:147:TYR:N	2.46	0.44
2:B:203:LEU:HD21	2:B:211:TYR:HB2	2.00	0.44
2:B:230:THR:HA	33:B:501:ADP:O2A	2.17	0.44
1:A:244:GLU:HG2	2:B:268:ARG:NH2	2.32	0.44
2:B:343:ARG:HA	2:B:347:ILE:HD13	2.00	0.44
3:C:115:ALA:O	3:C:124:HIS:N	2.33	0.44
3:C:203:VAL:HA	3:C:206:HIS:HB2	2.00	0.44
3:C:228:ALA:O	3:C:230:MET:HG2	2.18	0.44
3:C:300:ILE:HA	3:C:300:ILE:HD13	1.84	0.44
5:E:270:LEU:O	5:E:273:VAL:HG12	2.16	0.44
5:E:349:GLU:OE2	6:F:350:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:76:ASN:O	6:F:80:ILE:HG13	2.18	0.44
7:G:16:PHE:CZ	8:H:130:PHE:HB3	2.53	0.44
7:G:86:ASP:OD1	13:M:120:HIS:NE2	2.50	0.44
11:K:219:THR:O	11:K:228:MET:N	2.50	0.44
12:L:168:ALA:HB1	12:L:194:ALA:HB1	2.00	0.44
15:O:110:LEU:HD21	15:O:125:VAL:HG22	1.98	0.44
20:T:45:VAL:HG12	20:T:46:ASN:ND2	2.33	0.44
21:U:107:HIS:HA	21:U:110:LYS:HE3	1.99	0.44
25:Y:238:GLU:O	25:Y:242:LYS:HB2	2.18	0.44
25:Y:34:ASP:OD1	25:Y:34:ASP:N	2.47	0.44
26:Z:176:LEU:HD12	26:Z:177:ARG:N	2.33	0.44
1:A:306:LEU:HA	1:A:312:ARG:NE	2.33	0.44
2:B:178:LYS:HB3	2:B:180:PRO:HD3	1.99	0.44
3:C:113:ARG:HG2	3:C:127:LEU:HB2	2.00	0.44
3:C:151:ILE:HA	3:C:151:ILE:HD12	1.88	0.44
3:C:243:PRO:HA	3:C:288:ASN:HB3	1.99	0.44
4:D:145:PRO:HB2	4:D:146:GLU:HB2	1.99	0.44
4:D:232:GLY:HA3	4:D:269:ALA:HB3	1.99	0.44
5:E:289:LEU:HA	5:E:294:ARG:HD2	1.99	0.44
6:F:145:LEU:HG	6:F:146:LYS:HG2	2.00	0.44
7:G:165:ALA:HB3	8:H:56:LEU:HD22	2.00	0.44
11:K:146:VAL:HG22	11:K:151:PRO:HA	1.99	0.44
11:K:154:PHE:HB3	11:K:162:PHE:CE1	2.50	0.44
17:Q:85:ARG:HD2	17:Q:124:LEU:HD11	1.99	0.44
22:V:239:THR:HA	22:V:240:LEU:HA	1.65	0.44
22:V:328:VAL:O	22:V:332:LEU:HB2	2.18	0.44
23:W:306:LEU:O	23:W:310:THR:HG22	2.17	0.44
4:D:263:PHE:HD1	4:D:308:ILE:HG13	1.83	0.44
4:D:348:ILE:HG12	4:D:379:CYS:HB3	1.99	0.44
5:E:257:LEU:O	5:E:261:LEU:HG	2.18	0.44
4:D:229:ARG:CZ	5:E:267:PHE:HB3	2.47	0.44
5:E:232:MET:N	5:E:276:ILE:O	2.47	0.44
6:F:93:VAL:HB	6:F:147:PRO:HB3	1.99	0.44
7:G:183:VAL:HG13	7:G:189:TRP:CZ2	2.52	0.44
8:H:191:ALA:HA	8:H:194:THR:HG22	1.99	0.44
12:L:197:GLU:N	12:L:197:GLU:OE1	2.51	0.44
19:S:206:GLU:HG2	19:S:207:THR:H	1.83	0.44
21:U:74:PHE:CD1	21:U:103:LYS:HD2	2.53	0.44
21:U:554:LEU:HD11	21:U:761:VAL:HG13	1.99	0.44
23:W:407:ASP:HB2	24:X:344:ARG:HG2	1.99	0.44
1:A:262:GLU:O	1:A:266:THR:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:211:TYR:CD1	2:B:218:PRO:HD2	2.52	0.44
2:B:427:LEU:HD12	2:B:430:LYS:HD2	1.99	0.44
4:D:355:SER:HB3	4:D:358:VAL:HG23	2.00	0.44
5:E:124:HIS:CE1	6:F:320:PHE:HA	2.53	0.44
7:G:27:TYR:HD1	7:G:30:LYS:HE2	1.83	0.44
10:J:92:GLN:HG3	17:Q:62:LYS:HB3	1.99	0.44
12:L:91:GLU:HB3	12:L:108:LEU:HD11	2.00	0.44
13:M:140:TYR:HB3	13:M:217:GLY:HA2	2.00	0.44
22:V:416:ARG:HB3	25:Y:349:LYS:HB3	1.99	0.44
1:A:311:PRO:N	1:A:312:ARG:HA	2.33	0.43
1:A:214:LEU:HB2	1:A:320:ALA:HA	2.00	0.43
2:B:194:ILE:HA	2:B:197:ILE:HG22	2.00	0.43
2:B:295:TYR:CG	2:B:299:SER:HB3	2.53	0.43
3:C:229:ARG:NH1	3:C:232:ARG:HB2	2.33	0.43
3:C:61:GLU:O	3:C:65:LEU:N	2.44	0.43
4:D:89:ILE:HG12	4:D:143:LEU:HD21	1.99	0.43
4:D:164:TYR:HE2	4:D:222:HIS:HE1	1.65	0.43
4:D:260:ALA:H	4:D:304:ASN:ND2	2.12	0.43
5:E:178:THR:HG23	33:E:401:ADP:H8	1.82	0.43
9:I:24:ALA:O	9:I:28:ILE:HD12	2.18	0.43
22:V:137:GLU:N	22:V:138:PRO:HD2	2.33	0.43
22:V:167:LEU:HD12	22:V:168:GLN:N	2.33	0.43
22:V:265:ASP:HA	22:V:268:GLU:HB3	2.00	0.43
22:V:451:ILE:HG23	22:V:458:VAL:HA	1.99	0.43
22:V:455:LYS:HD2	22:V:457:TYR:HE2	1.83	0.43
22:V:495:ARG:HH12	26:Z:282:ASN:HA	1.82	0.43
1:A:217:PRO:HA	1:A:428:ARG:NE	2.33	0.43
2:B:116:ILE:O	2:B:119:ASN:N	2.47	0.43
1:A:384:GLU:HB2	2:B:347:ILE:HD11	2.00	0.43
3:C:369:TYR:O	3:C:373:GLU:N	2.49	0.43
6:F:366:MET:HA	6:F:369:HIS:HB2	2.00	0.43
9:I:99:LEU:HD13	16:P:69:PHE:HB2	1.99	0.43
13:M:11:ALA:HA	13:M:20:VAL:HG11	2.00	0.43
21:U:570:LEU:HD22	21:U:578:LEU:HD11	2.00	0.43
26:Z:30:GLY:HA3	26:Z:31:ASN:OD1	2.18	0.43
2:B:249:ARG:HG3	2:B:283:PHE:CD2	2.53	0.43
3:C:41:ASN:ND2	22:V:492:LYS:HA	2.34	0.43
4:D:274:ARG:HE	5:E:248:SER:HB3	1.82	0.43
7:G:130:GLU:HG3	8:H:4:ARG:HD3	2.01	0.43
13:M:51:LYS:HB3	13:M:210:GLU:HB3	2.00	0.43
19:S:112:GLY:HA2	19:S:198:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:20:VAL:HG23	20:T:120:SER:HB3	2.00	0.43
21:U:681:ASN:OD1	21:U:681:ASN:N	2.51	0.43
25:Y:295:TYR:O	25:Y:299:MET:HG2	2.18	0.43
26:Z:105:ASP:HA	26:Z:108:ILE:HD13	1.99	0.43
23:W:423:ASN:HB2	26:Z:255:ASP:OD1	2.18	0.43
2:B:302:GLU:O	2:B:306:GLN:N	2.44	0.43
3:C:196:LYS:HE3	3:C:252:ASP:OD2	2.18	0.43
3:C:43:ARG:HD3	21:U:639:LEU:HB2	1.99	0.43
4:D:143:LEU:HB3	4:D:144:PRO:HD2	2.00	0.43
6:F:222:GLY:HA3	6:F:347:ARG:O	2.18	0.43
6:F:300:LYS:HD2	6:F:304:ARG:NH2	2.33	0.43
10:J:96:LEU:HG	17:Q:58:GLU:HB3	2.00	0.43
21:U:764:LEU:HA	21:U:767:THR:HG23	2.00	0.43
23:W:312:MET:HG3	23:W:365:ILE:HD13	2.00	0.43
24:X:406:ASN:HA	24:X:409:LYS:HB2	1.99	0.43
1:A:173:THR:OG1	1:A:174:TYR:N	2.50	0.43
1:A:417:ILE:O	1:A:421:ALA:N	2.51	0.43
2:B:288:ASP:OD2	3:C:271:ARG:NH2	2.52	0.43
4:D:341:LYS:HA	4:D:344:ILE:HG22	2.00	0.43
5:E:135:ILE:HD12	5:E:183:LEU:HD12	1.99	0.43
9:I:57:ASP:HB3	9:I:59:VAL:HG13	2.00	0.43
7:G:12:HIS:CD2	13:M:7:TYR:HA	2.54	0.43
19:S:193:LEU:N	19:S:208:VAL:O	2.41	0.43
21:U:742:HIS:O	21:U:883:ARG:NH2	2.52	0.43
21:U:842:LYS:HE3	21:U:843:GLU:O	2.18	0.43
22:V:32:PRO:O	22:V:36:GLU:HB3	2.19	0.43
23:W:276:LEU:HD21	23:W:350:ARG:NH1	2.34	0.43
25:Y:63:TRP:HB3	25:Y:64:GLN:CB	2.47	0.43
22:V:487:HIS:ND1	26:Z:279:LYS:HD2	2.33	0.43
1:A:102:ILE:HD11	1:A:136:GLU:HA	2.00	0.43
1:A:134:ILE:HD12	1:A:152:PRO:HG3	1.99	0.43
1:A:299:MET:HG3	1:A:300:LEU:H	1.83	0.43
1:A:322:ASN:OD1	1:A:428:ARG:NH2	2.52	0.43
3:C:42:LEU:HD12	3:C:45:LEU:HB2	2.00	0.43
4:D:293:LEU:HG	4:D:326:ARG:CZ	2.49	0.43
4:D:303:VAL:HG23	4:D:304:ASN:HB2	2.01	0.43
6:F:188:ILE:HD11	6:F:236:LEU:HD13	2.01	0.43
6:F:229:PRO:HA	6:F:230:GLY:HA2	1.77	0.43
1:A:335:GLY:HA2	6:F:394:ALA:HB3	1.99	0.43
7:G:88:ARG:CZ	13:M:157:SER:H	2.31	0.43
14:N:19:ARG:HE	14:N:26:ILE:HG12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:31:ALA:O	22:V:35:VAL:HG22	2.18	0.43
22:V:329:HIS:HD2	22:V:353:LEU:HD21	1.84	0.43
22:V:90:GLU:N	22:V:90:GLU:OE1	2.50	0.43
24:X:405:GLN:O	24:X:409:LYS:HD3	2.19	0.43
2:B:114:GLU:HG3	2:B:122:ILE:HB	2.00	0.43
2:B:304:GLU:HA	2:B:307:ARG:HG2	2.00	0.43
2:B:93:GLU:HG3	2:B:94:GLU:H	1.82	0.43
4:D:99:ASN:O	4:D:115:ILE:N	2.36	0.43
5:E:309:ARG:O	5:E:312:ILE:HG22	2.19	0.43
5:E:60:VAL:N	5:E:96:THR:O	2.49	0.43
7:G:142:GLY:N	7:G:150:GLN:O	2.52	0.43
18:R:53:SER:O	18:R:57:ARG:HG2	2.18	0.43
20:T:15:LYS:HE2	20:T:122:LEU:H	1.83	0.43
21:U:163:PHE:CE2	21:U:201:LEU:HD21	2.54	0.43
21:U:338:HIS:CE1	21:U:785:PRO:HB3	2.54	0.43
21:U:356:THR:HG22	21:U:717:ILE:HD13	2.00	0.43
22:V:25:GLU:HB2	22:V:26:PRO:HD3	2.00	0.43
22:V:275:VAL:N	22:V:276:PHE:HA	2.32	0.43
23:W:244:CYS:HA	23:W:273:TYR:CE1	2.54	0.43
25:Y:145:LEU:HD13	25:Y:183:TYR:CD1	2.54	0.43
1:A:283:ALA:HA	1:A:284:ARG:HA	1.69	0.43
3:C:213:ARG:HH21	3:C:249:ASP:CG	2.22	0.43
3:C:215:SER:HA	3:C:216:GLY:HA3	1.51	0.43
12:L:84:LEU:HA	12:L:87:PHE:HB3	2.01	0.43
19:S:21:ALA:HB3	19:S:198:VAL:HB	2.00	0.43
22:V:290:TYR:HB2	22:V:312:ALA:HB1	2.01	0.43
22:V:359:PRO:HB3	22:V:382:PHE:CG	2.53	0.43
22:V:435:GLU:HG2	22:V:453:HIS:NE2	2.32	0.43
23:W:340:VAL:HG22	23:W:350:ARG:HH11	1.82	0.43
1:A:222:LYS:HD2	2:B:319:PHE:HB2	2.00	0.43
4:D:396:ALA:HA	4:D:399:PHE:CD2	2.54	0.43
5:E:379:LYS:HD2	5:E:379:LYS:HA	1.83	0.43
6:F:187:ASP:HB3	6:F:368:ILE:HG21	2.00	0.43
7:G:74:GLU:HB3	7:G:226:LYS:HD2	2.00	0.43
8:H:156:PHE:HB2	8:H:158:TRP:CZ3	2.53	0.43
9:I:45:LEU:HD21	9:I:137:ILE:HG21	2.01	0.43
11:K:60:GLU:OE1	11:K:63:SER:N	2.52	0.43
13:M:179:LEU:HD13	13:M:189:ILE:HG23	2.00	0.43
15:O:35:HIS:NE2	15:O:53:ASP:OD1	2.52	0.43
17:Q:131:ALA:O	17:Q:132:HIS:ND1	2.52	0.43
19:S:190:GLY:HA2	19:S:210:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:429:LYS:HA	21:U:430:ASP:CB	2.46	0.43
22:V:438:VAL:O	22:V:442:ILE:HG13	2.19	0.43
25:Y:210:SER:HB3	25:Y:213:LEU:HG	2.01	0.43
26:Z:254:ASN:HA	26:Z:257:MET:CG	2.49	0.43
1:A:309:PHE:HZ	6:F:235:LEU:HA	1.84	0.43
2:B:108:SER:N	2:B:152:LEU:O	2.37	0.43
2:B:209:GLU:HG2	2:B:210:TYR:N	2.34	0.43
6:F:395:GLN:O	6:F:399:VAL:HG23	2.19	0.43
9:I:213:ILE:HG22	9:I:228:LEU:HD21	2.01	0.43
16:P:21:ALA:HB2	16:P:189:ILE:HD13	2.01	0.43
21:U:173:VAL:N	21:U:174:PRO:HD3	2.34	0.43
21:U:385:PHE:CE2	21:U:411:ILE:HD13	2.54	0.43
21:U:451:ALA:HB2	21:U:483:LEU:HG	2.01	0.43
22:V:80:LYS:HB3	22:V:81:GLN:O	2.19	0.43
26:Z:96:HIS:NE2	26:Z:123:ILE:HG12	2.34	0.43
26:Z:40:LEU:HD22	26:Z:89:GLU:HG3	2.00	0.43
1:A:241:ILE:HD12	2:B:268:ARG:CZ	2.49	0.42
1:A:312:ARG:HA	1:A:313:GLY:HA2	1.64	0.42
2:B:387:LYS:HE3	2:B:423:LYS:HE3	2.01	0.42
3:C:115:ALA:HB3	3:C:124:HIS:HB3	2.00	0.42
4:D:74:HIS:O	4:D:78:GLU:HG2	2.19	0.42
6:F:89:LEU:HG	6:F:153:VAL:O	2.19	0.42
11:K:143:PHE:HB2	11:K:154:PHE:HB2	2.00	0.42
21:U:362:ASN:HA	21:U:395:ARG:NH1	2.34	0.42
3:C:50:ASN:HD21	21:U:644:TYR:N	2.17	0.42
26:Z:109:ASN:O	26:Z:113:LYS:HG3	2.19	0.42
26:Z:241:SER:HB2	26:Z:246:VAL:HG23	2.01	0.42
23:W:428:TRP:CH2	26:Z:255:ASP:HB3	2.54	0.42
26:Z:54:PHE:HB3	26:Z:82:PHE:HE2	1.84	0.42
1:A:174:TYR:HE1	1:A:227:ARG:HH21	1.68	0.42
1:A:409:PHE:O	1:A:413:VAL:HG23	2.19	0.42
3:C:155:ASP:HA	3:C:158:ILE:HG12	2.02	0.42
3:C:324:ALA:O	3:C:328:ILE:HG22	2.19	0.42
3:C:75:GLU:HG2	3:C:90:HIS:NE2	2.34	0.42
4:D:163:MET:HA	4:D:221:HIS:NE2	2.34	0.42
5:E:83:CYS:SG	5:E:107:ILE:HD13	2.60	0.42
6:F:283:ILE:O	6:F:328:VAL:HA	2.19	0.42
8:H:46:LEU:HD11	8:H:137:CYS:SG	2.59	0.42
12:L:135:ALA:HA	12:L:143:HIS:O	2.19	0.42
16:P:12:MET:HA	16:P:138:VAL:HG12	2.00	0.42
20:T:136:SER:HB2	20:T:150:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:600:ARG:HA	21:U:600:ARG:HD3	1.75	0.42
22:V:398:LEU:O	22:V:402:VAL:HG23	2.19	0.42
23:W:337:ALA:O	23:W:342:GLY:N	2.51	0.42
1:A:392:ALA:HB2	1:A:409:PHE:CD2	2.54	0.42
2:B:254:GLU:HA	2:B:257:GLN:HG2	2.01	0.42
3:C:219:LEU:HD11	4:D:287:ARG:HG3	2.01	0.42
4:D:297:ASP:OD2	4:D:326:ARG:NH2	2.52	0.42
4:D:375:ILE:HA	4:D:378:ILE:HB	2.00	0.42
21:U:444:TYR:CE1	21:U:479:LEU:HD23	2.54	0.42
21:U:596:ASN:O	21:U:600:ARG:HG2	2.19	0.42
22:V:30:PRO:HA	22:V:33:GLN:HB2	2.01	0.42
22:V:345:ARG:HH12	22:V:357:LEU:HD22	1.85	0.42
23:W:433:ASN:HA	23:W:436:MET:HG3	2.00	0.42
26:Z:126:VAL:HG23	26:Z:127:LYS:HG3	2.02	0.42
26:Z:247:LYS:HA	26:Z:250:TYR:CE2	2.54	0.42
1:A:243:SER:CB	2:B:264:PRO:HD3	2.49	0.42
1:A:261:PHE:HE2	1:A:305:GLN:HB3	1.84	0.42
1:A:84:LYS:O	1:A:87:LEU:HG	2.19	0.42
2:B:187:ILE:HA	33:B:501:ADP:N6	2.34	0.42
2:B:316:LEU:HD11	2:B:327:VAL:HG11	2.01	0.42
4:D:233:SER:HB2	5:E:255:ARG:HB3	2.00	0.42
4:D:313:ARG:NH2	5:E:242:ARG:O	2.52	0.42
5:E:115:VAL:HG22	5:E:117:PRO:CD	2.50	0.42
5:E:132:TYR:O	5:E:135:ILE:HG12	2.19	0.42
5:E:69:PHE:O	5:E:80:VAL:HA	2.20	0.42
5:E:320:ILE:HD12	6:F:215:LEU:HB3	2.01	0.42
1:A:123:VAL:HG23	6:F:88:TYR:CE1	2.54	0.42
11:K:85:ALA:O	11:K:89:ILE:HG12	2.19	0.42
14:N:87:CYS:O	14:N:91:ARG:N	2.52	0.42
21:U:789:ILE:HG23	21:U:844:LYS:HG2	2.01	0.42
23:W:370:TYR:HA	23:W:371:THR:HB	2.02	0.42
26:Z:15:VAL:O	26:Z:19:VAL:HG23	2.19	0.42
1:A:122:VAL:HG23	6:F:90:VAL:HG22	2.01	0.42
2:B:138:PHE:HE2	2:B:162:VAL:H	1.67	0.42
3:C:249:ASP:HA	3:C:250:GLU:HA	1.56	0.42
3:C:157:GLN:NE2	3:C:318:PRO:HD3	2.34	0.42
4:D:208:PRO:HA	4:D:209:GLY:C	2.39	0.42
5:E:111:LEU:HD23	6:F:133:PHE:HE1	1.84	0.42
5:E:120:TYR:OH	6:F:147:PRO:HD2	2.20	0.42
5:E:149:ILE:HG12	5:E:274:LYS:HE2	2.01	0.42
5:E:314:LYS:O	5:E:318:GLY:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:381:GLU:HG2	6:F:351:LYS:HZ2	1.84	0.42
5:E:124:HIS:NE2	6:F:319:GLY:O	2.52	0.42
10:J:137:ASP:HA	10:J:143:ARG:HH21	1.84	0.42
12:L:137:TYR:HE1	12:L:215:VAL:HG13	1.85	0.42
13:M:125:TYR:HB2	13:M:128:VAL:HG22	2.01	0.42
17:Q:38:MET:SD	17:Q:44:LEU:HB2	2.59	0.42
19:S:4:PRO:O	20:T:100:ARG:NH2	2.51	0.42
22:V:144:ASP:N	22:V:145:LEU:HA	2.34	0.42
23:W:227:TYR:O	23:W:231:ILE:HG23	2.20	0.42
23:W:440:ASN:O	23:W:444:HIS:ND1	2.53	0.42
25:Y:237:ARG:HB2	25:Y:241:ILE:HD12	2.00	0.42
1:A:170:PRO:CB	1:A:230:ALA:HA	2.50	0.42
1:A:414:ASN:HA	1:A:417:ILE:HG12	2.00	0.42
2:B:175:LYS:HZ2	2:B:246:THR:HG22	1.84	0.42
2:B:393:ALA:HB2	33:B:501:ADP:H4'	2.02	0.42
4:D:201:GLY:HA2	4:D:327:LEU:HA	2.01	0.42
4:D:203:LEU:HB3	4:D:330:LYS:HA	2.02	0.42
4:D:207:PRO:HG2	4:D:312:ASN:HB3	2.01	0.42
5:E:261:LEU:O	5:E:265:ASP:N	2.52	0.42
6:F:204:LEU:HA	6:F:208:HIS:HB2	2.02	0.42
6:F:246:ALA:HB1	6:F:281:SER:HA	2.01	0.42
7:G:100:ASN:O	7:G:104:LYS:HG2	2.19	0.42
8:H:74:LEU:HD12	8:H:136:ILE:HG12	2.01	0.42
11:K:231:LYS:C	11:K:233:GLU:H	2.23	0.42
17:Q:157:VAL:O	17:Q:161:ARG:HG2	2.20	0.42
21:U:24:LEU:HA	21:U:27:LEU:HB2	2.01	0.42
21:U:603:LEU:O	21:U:607:VAL:HG23	2.20	0.42
22:V:346:LEU:HB3	22:V:361:PHE:CE1	2.54	0.42
25:Y:52:PRO:HD3	25:Y:115:GLY:HA2	2.02	0.42
25:Y:356:THR:HA	25:Y:357:ASN:OD1	2.18	0.42
1:A:101:ILE:HA	1:A:138:MET:O	2.20	0.42
1:A:354:ILE:O	1:A:357:ILE:HG22	2.19	0.42
1:A:220:THR:HB	33:A:501:ADP:C5	2.55	0.42
2:B:249:ARG:HB3	3:C:283:PHE:CE2	2.53	0.42
6:F:317:LEU:HD13	6:F:346:GLY:O	2.20	0.42
7:G:163:PHE:CD2	8:H:57:TYR:HA	2.54	0.42
11:K:225:ASN:HA	11:K:226:PHE:HA	1.82	0.42
12:L:67:ASP:HB3	12:L:70:ILE:HB	2.00	0.42
13:M:120:HIS:O	13:M:124:LEU:HG	2.20	0.42
17:Q:7:ILE:HG21	17:Q:156:ALA:HB1	2.01	0.42
20:T:92:LEU:HG	20:T:125:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:378:VAL:HG13	22:V:382:PHE:CD2	2.55	0.42
23:W:449:GLU:HG3	26:Z:211:TYR:HE1	1.85	0.42
22:V:494:MET:SD	26:Z:282:ASN:ND2	2.92	0.42
1:A:351:ARG:O	1:A:355:PHE:N	2.50	0.42
1:A:393:GLY:HA2	1:A:396:ALA:HB3	2.01	0.42
3:C:180:ILE:HA	3:C:180:ILE:HD12	1.95	0.42
3:C:327:ASP:O	3:C:331:ILE:N	2.49	0.42
4:D:103:VAL:HG11	4:D:139:LEU:HD21	2.01	0.42
4:D:130:VAL:HB	4:D:142:VAL:HG12	2.02	0.42
4:D:267:ILE:HG12	4:D:309:MET:HG3	2.01	0.42
4:D:357:GLU:OE2	4:D:396:ALA:N	2.52	0.42
5:E:170:CYS:HB3	5:E:276:ILE:CD1	2.50	0.42
5:E:76:GLY:N	5:E:77:PRO:HD2	2.35	0.42
5:E:83:CYS:HB3	5:E:87:LEU:HD21	2.01	0.42
6:F:256:LEU:HD13	6:F:291:ILE:HD13	2.01	0.42
18:R:191:ASN:OD1	18:R:192:VAL:N	2.53	0.42
20:T:41:ARG:HH21	20:T:54:SER:HA	1.84	0.42
21:U:474:ARG:O	21:U:478:SER:OG	2.23	0.42
21:U:494:TYR:O	21:U:498:LYS:HG3	2.20	0.42
21:U:510:GLU:HA	21:U:547:GLY:HA3	2.01	0.42
21:U:579:ARG:O	21:U:583:MET:HG2	2.19	0.42
23:W:285:ASP:O	23:W:289:ARG:HG3	2.20	0.42
26:Z:33:LYS:HB3	26:Z:33:LYS:HE3	1.81	0.42
2:B:197:ILE:HG13	2:B:222:VAL:HG11	2.01	0.42
2:B:231:GLY:HA2	2:B:234:LEU:HD12	2.02	0.42
2:B:343:ARG:HB2	2:B:344:PRO:HD3	2.02	0.42
4:D:205:TYR:O	4:D:333:PHE:HB2	2.20	0.42
5:E:83:CYS:SG	5:E:87:LEU:HD11	2.60	0.42
6:F:248:PHE:CE1	6:F:284:PHE:HB3	2.55	0.42
1:A:289:ALA:HB1	6:F:295:ARG:HD3	2.01	0.42
9:I:111:VAL:HG22	9:I:136:TYR:CE1	2.54	0.42
9:I:49:ARG:H	9:I:211:VAL:HA	1.85	0.42
9:I:83:ALA:O	9:I:87:THR:HG23	2.19	0.42
12:L:50:LYS:HB2	12:L:209:ASN:HA	2.01	0.42
13:M:40:ARG:HD2	13:M:146:ALA:HB1	2.01	0.42
13:M:64:LYS:HD2	13:M:212:GLU:HG2	2.02	0.42
15:O:7:VAL:HG22	15:O:12:ILE:HG23	2.02	0.42
18:R:1:THR:N	18:R:169:TYR:O	2.45	0.42
19:S:63:THR:OG1	20:T:94:ARG:NH1	2.45	0.42
21:U:15:ASP:O	21:U:20:LYS:NZ	2.53	0.42
21:U:252:LEU:O	21:U:256:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:474:ARG:HG2	21:U:500:ASN:HD21	1.85	0.42
21:U:42:VAL:HG11	21:U:68:PHE:CZ	2.55	0.42
21:U:713:TYR:HB2	21:U:734:GLN:HE21	1.84	0.42
2:B:152:LEU:HD23	2:B:157:HIS:HB3	2.02	0.42
2:B:180:PRO:HD2	2:B:242:GLN:HE22	1.83	0.42
2:B:211:TYR:CZ	2:B:217:LYS:HA	2.55	0.42
3:C:243:PRO:HB3	3:C:288:ASN:HB3	2.02	0.42
3:C:184:LYS:HZ1	3:C:280:LEU:HB3	1.85	0.42
3:C:388:ALA:O	3:C:392:GLN:N	2.52	0.42
4:D:267:ILE:HG12	4:D:309:MET:CG	2.50	0.42
5:E:250:ASP:O	5:E:254:GLN:HG2	2.20	0.42
9:I:112:THR:HB	10:J:81:ARG:HD3	2.01	0.42
9:I:8:ARG:HB3	9:I:11:ILE:HB	2.02	0.42
20:T:74:GLU:HA	20:T:77:LEU:HD12	2.01	0.42
12:L:101:ARG:NH1	20:T:87:ALA:HB2	2.35	0.42
21:U:338:HIS:NE2	21:U:342:LEU:HD11	2.34	0.42
22:V:350:GLN:HB3	22:V:351:PRO:HD2	2.02	0.42
22:V:466:ILE:HG23	22:V:467:TYR:HB2	2.01	0.42
25:Y:14:ASN:HA	25:Y:17:LEU:HB3	2.02	0.42
1:A:165:GLN:HE21	1:A:240:VAL:HG13	1.85	0.41
1:A:418:LYS:O	1:A:422:LYS:N	2.52	0.41
2:B:214:MET:HB3	2:B:216:ILE:HG12	2.01	0.41
1:A:222:LYS:HG2	2:B:319:PHE:CD1	2.55	0.41
3:C:214:VAL:HG23	3:C:272:THR:HG21	2.02	0.41
4:D:159:LYS:HB3	4:D:160:PRO:HA	2.02	0.41
4:D:361:GLU:O	4:D:364:VAL:HG12	2.19	0.41
5:E:234:GLU:OE1	6:F:308:ARG:HD3	2.20	0.41
9:I:11:ILE:HD12	9:I:11:ILE:H	1.85	0.41
13:M:61:GLY:O	13:M:64:LYS:NZ	2.52	0.41
21:U:195:ASN:HB2	21:U:223:LEU:HD13	2.01	0.41
21:U:11:LEU:HB3	21:U:19:LEU:HG	2.02	0.41
21:U:408:LEU:O	21:U:412:HIS:ND1	2.53	0.41
21:U:457:ILE:H	21:U:457:ILE:HD12	1.86	0.41
21:U:684:ARG:O	21:U:688:LEU:HG	2.20	0.41
22:V:55:THR:HB	22:V:198:GLN:CD	2.41	0.41
25:Y:203:ASP:HB2	25:Y:206:SER:OG	2.20	0.41
24:X:378:LEU:O	25:Y:312:ARG:HG2	2.19	0.41
1:A:212:VAL:HG12	1:A:339:ARG:HB3	2.02	0.41
2:B:226:GLY:HA3	2:B:353:PHE:HB3	2.01	0.41
1:A:381:THR:HG1	2:B:343:ARG:NH1	2.18	0.41
4:D:191:TYR:HB3	4:D:198:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:124:HIS:NE2	5:E:185:ARG:HD2	2.35	0.41
5:E:341:ALA:HB2	33:E:401:ADP:N3	2.35	0.41
6:F:392:ASN:H	6:F:395:GLN:CD	2.23	0.41
13:M:189:ILE:HG22	13:M:193:VAL:HG23	2.02	0.41
17:Q:181:ARG:NH1	17:Q:190:ASP:OD1	2.52	0.41
22:V:96:ARG:HA	22:V:98:LEU:HB2	2.02	0.41
23:W:264:GLN:NE2	23:W:299:ILE:HD11	2.35	0.41
1:A:115:VAL:HG22	1:A:116:LYS:H	1.85	0.41
1:A:141:GLY:C	1:A:150:HIS:HB3	2.41	0.41
2:B:123:VAL:O	2:B:130:GLU:HA	2.20	0.41
2:B:175:LYS:NZ	2:B:247:PHE:O	2.52	0.41
3:C:306:LEU:O	3:C:307:ARG:NH2	2.49	0.41
3:C:80:MET:HB3	3:C:82:LYS:HG2	2.02	0.41
3:C:97:VAL:HG22	3:C:98:ASP:H	1.85	0.41
4:D:200:ARG:O	4:D:307:VAL:HB	2.19	0.41
4:D:203:LEU:HB3	4:D:331:ILE:H	1.85	0.41
4:D:370:ILE:HG23	4:D:371:SER:H	1.84	0.41
4:D:54:LEU:O	4:D:58:GLU:HG2	2.20	0.41
5:E:141:GLN:HE22	5:E:301:ILE:HA	1.85	0.41
5:E:84:ARG:HG2	5:E:87:LEU:HD23	2.02	0.41
8:H:50:LYS:HD3	8:H:59:GLU:OE1	2.20	0.41
9:I:64:LYS:O	9:I:76:VAL:HG12	2.19	0.41
10:J:114:LEU:HA	10:J:117:ARG:HG2	2.02	0.41
20:T:92:LEU:HD21	20:T:110:MET:SD	2.60	0.41
21:U:574:LYS:H	21:U:574:LYS:HG2	1.70	0.41
21:U:806:CYS:SG	21:U:891:VAL:HG21	2.60	0.41
22:V:487:HIS:CG	26:Z:275:LEU:HG	2.55	0.41
1:A:221:GLY:C	1:A:223:THR:H	2.23	0.41
1:A:304:ASN:HD22	6:F:254:PRO:CG	2.31	0.41
1:A:367:ASP:O	1:A:369:ARG:NH1	2.53	0.41
3:C:161:ILE:O	3:C:165:ILE:HG12	2.21	0.41
4:D:297:ASP:OD1	4:D:326:ARG:NH1	2.54	0.41
10:J:137:ASP:OD1	10:J:143:ARG:NE	2.54	0.41
18:R:127:SER:HB3	18:R:136:TYR:CE2	2.56	0.41
20:T:157:GLN:HG2	20:T:159:VAL:O	2.21	0.41
20:T:22:ILE:HB	20:T:50:MET:HE3	2.02	0.41
4:D:40:LEU:HB2	21:U:149:GLN:OE1	2.20	0.41
22:V:207:ALA:HA	22:V:210:CYS:SG	2.60	0.41
22:V:353:LEU:HG	22:V:357:LEU:HD23	2.00	0.41
23:W:340:VAL:HG13	23:W:350:ARG:HD2	2.02	0.41
25:Y:367:GLN:HG3	25:Y:371:LYS:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:CYS:O	1:A:229:VAL:HG23	2.20	0.41
3:C:310:ARG:HA	3:C:311:ILE:HA	1.77	0.41
4:D:159:LYS:HD3	4:D:159:LYS:HA	1.89	0.41
7:G:203:SER:O	7:G:207:SER:HB3	2.21	0.41
11:K:24:VAL:O	11:K:28:ILE:HG12	2.20	0.41
14:N:42:PHE:CE2	14:N:184:VAL:HG11	2.55	0.41
15:O:215:LYS:N	16:P:197:THR:O	2.41	0.41
20:T:20:VAL:HG11	20:T:122:LEU:HD13	2.03	0.41
21:U:342:LEU:HD13	21:U:378:CYS:O	2.19	0.41
21:U:59:PHE:HA	21:U:62:LEU:HD13	2.02	0.41
21:U:766:PHE:CD1	21:U:776:SER:HA	2.56	0.41
21:U:842:LYS:HA	21:U:843:GLU:CB	2.46	0.41
22:V:195:ILE:HG13	22:V:195:ILE:H	1.73	0.41
22:V:43:THR:HG23	22:V:62:HIS:HB3	2.01	0.41
25:Y:101:ARG:HH21	25:Y:126:LYS:HG3	1.86	0.41
1:A:123:VAL:HG22	1:A:124:ASP:H	1.86	0.41
1:A:278:ASP:HB3	1:A:321:THR:OG1	2.21	0.41
1:A:94:GLN:OE1	2:B:131:HIS:NE2	2.53	0.41
3:C:158:ILE:HA	3:C:161:ILE:HG22	2.02	0.41
3:C:163:GLU:OE1	3:C:163:GLU:N	2.49	0.41
4:D:116:LEU:HB2	4:D:140:VAL:HA	2.02	0.41
4:D:182:GLU:HG3	4:D:183:LEU:H	1.85	0.41
4:D:258:ALA:HA	4:D:259:PRO:C	2.41	0.41
5:E:216:ARG:HA	5:E:219:PHE:HB2	2.02	0.41
5:E:170:CYS:SG	5:E:299:ILE:HD13	2.60	0.41
5:E:321:THR:HG23	6:F:215:LEU:HD22	2.03	0.41
6:F:402:GLU:HA	6:F:405:MET:HB2	2.01	0.41
6:F:405:MET:O	6:F:408:LEU:HB3	2.20	0.41
6:F:431:LYS:HB2	6:F:432:LYS:HA	2.02	0.41
10:J:109:ARG:O	10:J:113:SER:OG	2.32	0.41
10:J:20:GLU:N	10:J:20:GLU:OE1	2.52	0.41
11:K:225:ASN:HB2	11:K:226:PHE:CD2	2.55	0.41
12:L:173:GLU:HA	12:L:176:MET:SD	2.61	0.41
12:L:82:ARG:HA	12:L:85:CYS:HB3	2.03	0.41
17:Q:84:THR:HG21	17:Q:104:LEU:HD11	2.02	0.41
17:Q:5:ILE:HD12	17:Q:5:ILE:HA	1.97	0.41
18:R:178:HIS:O	18:R:185:ILE:N	2.52	0.41
10:J:97:THR:HG22	18:R:82:LEU:HD21	2.03	0.41
21:U:363:SER:C	21:U:365:CYS:H	2.24	0.41
21:U:682:TYR:HB3	21:U:725:MET:SD	2.61	0.41
25:Y:236:LEU:O	25:Y:240:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:221:PRO:CB	26:Z:222:ILE:HA	2.50	0.41
1:A:262:GLU:HA	1:A:265:ARG:HB2	2.02	0.41
1:A:387:SER:O	1:A:391:GLU:HG2	2.20	0.41
2:B:208:PRO:O	2:B:211:TYR:HB3	2.21	0.41
3:C:99:VAL:HG13	3:C:101:LYS:HA	2.02	0.41
4:D:102:ILE:HA	4:D:111:TYR:O	2.21	0.41
4:D:146:GLU:CG	4:D:148:ASP:H	2.33	0.41
4:D:241:GLY:O	4:D:244:PRO:HD2	2.20	0.41
5:E:215:ILE:O	5:E:219:PHE:N	2.42	0.41
5:E:46:ASP:O	5:E:50:LEU:HG	2.20	0.41
6:F:144:LYS:HA	6:F:145:LEU:HA	1.70	0.41
6:F:140:VAL:HG13	6:F:161:LEU:O	2.21	0.41
6:F:357:PRO:O	6:F:362:ARG:NH1	2.53	0.41
9:I:109:GLN:HE22	17:Q:67:TYR:HE2	1.69	0.41
10:J:56:GLU:O	10:J:59:VAL:HG12	2.20	0.41
11:K:10:ARG:O	11:K:14:THR:OG1	2.27	0.41
11:K:123:PHE:HB2	11:K:134:SER:C	2.41	0.41
7:G:28:ALA:HB2	13:M:14:PHE:HE2	1.85	0.41
22:V:273:LYS:HB3	22:V:274:SER:O	2.21	0.41
3:C:33:LEU:HG	22:V:496:PHE:CZ	2.56	0.41
26:Z:195:VAL:O	26:Z:199:LYS:HB2	2.20	0.41
26:Z:229:GLN:O	26:Z:233:VAL:HG23	2.20	0.41
2:B:186:ASP:O	33:B:501:ADP:N6	2.53	0.41
6:F:317:LEU:HG	6:F:323:ASN:ND2	2.36	0.41
7:G:215:ILE:H	7:G:215:ILE:HG13	1.63	0.41
12:L:64:LEU:HG	12:L:72:ILE:HD11	2.03	0.41
15:O:175:LEU:HB2	15:O:186:LEU:HB2	2.03	0.41
3:C:21:ARG:NH2	21:U:102:ALA:HA	2.36	0.41
21:U:173:VAL:HG13	21:U:176:MET:HB2	2.03	0.41
1:A:292:ASP:HB3	1:A:296:GLN:HE21	1.86	0.41
2:B:303:ARG:HH21	2:B:307:ARG:NH1	2.19	0.41
2:B:346:ARG:HG3	2:B:349:ARG:H	1.85	0.41
2:B:346:ARG:CZ	2:B:348:ASP:HB3	2.51	0.41
3:C:100:ASP:OD1	3:C:122:THR:HB	2.21	0.41
3:C:328:ILE:O	3:C:332:HIS:ND1	2.31	0.41
6:F:321:GLN:O	6:F:324:THR:HG23	2.21	0.41
6:F:436:GLN:C	6:F:438:TYR:H	2.23	0.41
7:G:158:GLY:O	8:H:84:ARG:NH2	2.54	0.41
8:H:45:VAL:HG11	8:H:188:ILE:HG12	2.03	0.41
13:M:113:ASP:O	13:M:117:MET:HG2	2.21	0.41
21:U:357:LYS:HE2	21:U:389:ASN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:774:PRO:HA	21:U:777:HIS:CD2	2.54	0.41
22:V:447:ILE:HG13	22:V:449:ALA:H	1.86	0.41
26:Z:23:PHE:HA	26:Z:35:VAL:HG21	2.02	0.41
1:A:119:ALA:HB1	1:A:121:PHE:CE2	2.52	0.41
1:A:191:VAL:HG13	1:A:192:GLU:N	2.33	0.41
5:E:285:LEU:HB3	5:E:289:LEU:HD12	2.01	0.41
12:L:65:HIS:O	12:L:89:ARG:NH2	2.54	0.41
20:T:29:SER:HA	20:T:36:PHE:H	1.85	0.41
21:U:373:ASN:HB2	21:U:385:PHE:CE1	2.56	0.41
21:U:537:GLN:N	21:U:537:GLN:OE1	2.54	0.41
21:U:643:SER:O	21:U:649:ARG:NH1	2.42	0.41
25:Y:141:VAL:HG22	25:Y:160:ASN:HB2	2.02	0.41
25:Y:323:PHE:HA	25:Y:323:PHE:HD1	1.73	0.41
26:Z:58:PHE:CZ	26:Z:60:GLU:HB2	2.56	0.41
1:A:138:MET:O	1:A:140:VAL:HG13	2.21	0.41
1:A:283:ALA:HB3	1:A:326:THR:HB	2.03	0.41
1:A:413:VAL:O	1:A:417:ILE:HG12	2.19	0.41
2:B:224:LEU:HB2	2:B:330:ALA:CB	2.51	0.41
3:C:182:GLN:H	3:C:182:GLN:CD	2.24	0.41
4:D:180:ALA:C	4:D:184:PRO:HG2	2.41	0.41
4:D:409:LYS:O	4:D:411:GLU:HB2	2.21	0.41
5:E:55:GLN:HB3	5:E:100:LEU:O	2.21	0.41
5:E:141:GLN:NE2	5:E:301:ILE:HA	2.36	0.41
5:E:174:GLY:C	5:E:176:PRO:HD2	2.42	0.41
6:F:230:GLY:HA2	6:F:231:THR:CB	2.51	0.41
6:F:231:THR:HG21	6:F:233:LYS:NZ	2.36	0.41
9:I:2:SER:HB3	12:L:123:TYR:CZ	2.56	0.41
11:K:104:ASN:HD21	19:S:90:ALA:HB2	1.86	0.41
22:V:185:GLN:O	22:V:189:ASP:HB2	2.21	0.41
22:V:253:LEU:HD23	22:V:256:ARG:HH21	1.86	0.41
22:V:400:HIS:O	22:V:403:ILE:HG22	2.20	0.41
22:V:430:SER:HB2	22:V:431:PRO:HD2	2.02	0.41
26:Z:72:HIS:NE2	26:Z:111:LEU:HD21	2.36	0.41
26:Z:166:GLU:O	26:Z:170:VAL:HG23	2.20	0.41
1:A:123:VAL:HG11	1:A:147:TYR:HB3	2.02	0.40
2:B:175:LYS:NZ	2:B:246:THR:HG22	2.36	0.40
3:C:147:THR:HG22	3:C:150:MET:HG2	2.02	0.40
4:D:167:ILE:HD13	33:D:501:ADP:HN62	1.85	0.40
5:E:182:LEU:HD12	33:E:401:ADP:H2'	2.02	0.40
6:F:307:GLN:HG2	6:F:308:ARG:N	2.35	0.40
6:F:344:ARG:O	6:F:349:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:200:VAL:HG22	13:M:201:HIS:H	1.85	0.40
22:V:108:LEU:HD23	22:V:111:TYR:HE2	1.85	0.40
22:V:310:THR:HG22	22:V:314:ARG:HD3	2.03	0.40
23:W:407:ASP:N	23:W:413:ILE:HG22	2.32	0.40
1:A:386:ARG:NH1	33:A:501:ADP:O3'	2.49	0.40
3:C:135:VAL:O	3:C:139:MET:HG2	2.21	0.40
3:C:42:LEU:HD12	3:C:42:LEU:HA	1.84	0.40
4:D:163:MET:HA	4:D:221:HIS:HE2	1.86	0.40
4:D:341:LYS:NZ	4:D:375:ILE:HG13	2.36	0.40
4:D:412:GLN:HB3	4:D:414:HIS:HB3	2.02	0.40
5:E:266:GLY:CA	5:E:267:PHE:HB2	2.46	0.40
11:K:73:HIS:HA	11:K:226:PHE:CE1	2.56	0.40
12:L:184:LEU:O	12:L:188:VAL:HG23	2.21	0.40
12:L:13:TRP:NE1	13:M:129:ARG:HD2	2.36	0.40
13:M:51:LYS:HE2	13:M:212:GLU:OE2	2.22	0.40
15:O:3:ILE:HD12	15:O:99:VAL:HG23	2.02	0.40
21:U:14:GLU:HB3	21:U:19:LEU:HD23	2.03	0.40
21:U:479:LEU:HD13	21:U:511:ALA:HA	2.02	0.40
22:V:469:THR:O	22:V:473:GLN:HG2	2.21	0.40
24:X:394:ASP:N	24:X:394:ASP:OD1	2.54	0.40
25:Y:122:THR:O	25:Y:126:LYS:HB2	2.21	0.40
25:Y:186:LEU:HA	25:Y:189:VAL:HG12	2.04	0.40
25:Y:71:ASN:HA	25:Y:74:LYS:HG2	2.04	0.40
1:A:290:GLY:HA2	1:A:291:GLY:HA3	1.82	0.40
2:B:211:TYR:OH	2:B:217:LYS:HG3	2.21	0.40
3:C:321:ASN:OD1	3:C:322:GLU:N	2.50	0.40
3:C:36:ASN:O	3:C:40:GLN:HG2	2.21	0.40
4:D:207:PRO:HG3	4:D:212:LYS:NZ	2.37	0.40
6:F:405:MET:HB3	6:F:409:ARG:HH22	1.85	0.40
7:G:159:TYR:HB3	8:H:81:PRO:HG3	2.03	0.40
8:H:118:MET:HG3	8:H:129:PRO:HB3	2.03	0.40
13:M:39:ILE:HG23	13:M:46:VAL:HB	2.02	0.40
21:U:13:ASP:OD1	21:U:44:LYS:NZ	2.38	0.40
21:U:362:ASN:HA	21:U:395:ARG:HH11	1.85	0.40
21:U:802:TYR:HB3	21:U:895:PRO:HD3	2.02	0.40
24:X:344:ARG:HA	24:X:385:LEU:O	2.21	0.40
25:Y:349:LYS:C	25:Y:351:ASN:H	2.23	0.40
26:Z:221:PRO:HB2	26:Z:224:HIS:O	2.22	0.40
1:A:199:GLU:HA	1:A:202:VAL:HG23	2.04	0.40
1:A:232:ARG:NH1	1:A:271:LEU:HD13	2.30	0.40
1:A:327:LEU:HD12	1:A:328:ASP:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:TYR:HA	2:B:213:GLU:HB2	2.03	0.40
2:B:232:LYS:HB2	33:B:501:ADP:O1B	2.21	0.40
2:B:349:ARG:HA	2:B:349:ARG:HD2	1.84	0.40
3:C:386:ALA:O	3:C:390:VAL:HG22	2.21	0.40
4:D:313:ARG:NH1	5:E:241:ARG:O	2.55	0.40
5:E:62:LYS:H	5:E:70:ILE:HB	1.86	0.40
6:F:144:LYS:HB2	6:F:145:LEU:HB2	2.04	0.40
6:F:172:VAL:HG13	6:F:267:LEU:HG	2.02	0.40
7:G:62:ASP:CG	13:M:40:ARG:HH22	2.25	0.40
8:H:103:GLU:HG2	8:H:104:PRO:HD2	2.04	0.40
11:K:155:HIS:CG	11:K:168:ARG:HG2	2.56	0.40
14:N:51:ASP:HB3	14:N:94:LEU:HD13	2.04	0.40
21:U:202:VAL:HG11	21:U:219:CYS:SG	2.61	0.40
21:U:472:ILE:HA	21:U:475:HIS:CE1	2.56	0.40
22:V:470:ARG:HA	22:V:470:ARG:HD3	1.96	0.40
26:Z:39:LEU:HB2	26:Z:95:TYR:HD2	1.87	0.40
1:A:140:VAL:HG12	1:A:152:PRO:HB3	2.03	0.40
2:B:232:LYS:HD2	33:B:501:ADP:O3'	2.21	0.40
3:C:264:GLY:HA2	3:C:267:SER:HB3	2.04	0.40
3:C:338:LEU:HG	3:C:339:THR:O	2.21	0.40
4:D:241:GLY:O	4:D:245:ARG:HG3	2.21	0.40
33:D:501:ADP:O3B	5:E:294:ARG:NH2	2.48	0.40
5:E:174:GLY:HA3	5:E:175:PRO:HA	1.86	0.40
6:F:299:GLU:HA	6:F:300:LYS:HA	1.92	0.40
6:F:77:SER:HA	6:F:80:ILE:HB	2.03	0.40
11:K:173:ALA:O	11:K:177:ALA:N	2.36	0.40
13:M:192:GLU:O	13:M:195:LYS:HG2	2.21	0.40
17:Q:51:GLY:HA3	18:R:88:TYR:CE1	2.57	0.40
21:U:350:LEU:O	21:U:354:LYS:HG2	2.22	0.40
21:U:609:ASP:O	21:U:615:ARG:HD2	2.21	0.40
21:U:688:LEU:HD22	21:U:713:TYR:HE1	1.86	0.40
22:V:135:LEU:HB3	22:V:181:TYR:HE2	1.85	0.40
25:Y:347:ILE:HG13	25:Y:354:VAL:HG22	2.02	0.40
26:Z:176:LEU:HD12	26:Z:177:ARG:H	1.87	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	304 (85%)	53 (15%)	2 (1%)	30	74
2	B	339/440 (77%)	298 (88%)	38 (11%)	3 (1%)	21	67
3	C	382/398 (96%)	317 (83%)	62 (16%)	3 (1%)	24	69
4	D	378/418 (90%)	328 (87%)	49 (13%)	1 (0%)	46	83
5	E	351/403 (87%)	299 (85%)	51 (14%)	1 (0%)	46	83
6	F	362/439 (82%)	316 (87%)	45 (12%)	1 (0%)	46	83
7	G	238/245 (97%)	221 (93%)	16 (7%)	1 (0%)	39	80
8	H	230/233 (99%)	210 (91%)	19 (8%)	1 (0%)	39	80
9	I	248/260 (95%)	230 (93%)	18 (7%)	0	100	100
10	J	237/247 (96%)	221 (93%)	15 (6%)	1 (0%)	39	80
11	K	224/240 (93%)	203 (91%)	20 (9%)	1 (0%)	39	80
12	L	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
13	M	238/254 (94%)	218 (92%)	20 (8%)	0	100	100
14	N	189/238 (79%)	175 (93%)	14 (7%)	0	100	100
15	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
16	P	202/204 (99%)	188 (93%)	14 (7%)	0	100	100
17	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
18	R	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
19	S	211/240 (88%)	199 (94%)	12 (6%)	0	100	100
20	T	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
21	U	798/953 (84%)	729 (91%)	67 (8%)	2 (0%)	46	83
22	V	478/533 (90%)	416 (87%)	60 (13%)	2 (0%)	39	80
23	W	234/456 (51%)	213 (91%)	21 (9%)	0	100	100
24	X	79/422 (19%)	75 (95%)	4 (5%)	0	100	100
25	Y	376/389 (97%)	336 (89%)	38 (10%)	2 (0%)	34	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	284/324 (88%)	251 (88%)	32 (11%)	1 (0%)	39	80
27	a	369/376 (98%)	340 (92%)	27 (7%)	2 (0%)	34	77
28	b	189/377 (50%)	178 (94%)	11 (6%)	0	100	100
29	c	285/309 (92%)	242 (85%)	39 (14%)	4 (1%)	14	58
30	d	255/349 (73%)	219 (86%)	34 (13%)	2 (1%)	24	69
31	e	20/70 (29%)	16 (80%)	4 (20%)	0	100	100
32	f	686/749 (92%)	574 (84%)	108 (16%)	4 (1%)	30	74
All	All	9304/11269 (83%)	8324 (90%)	946 (10%)	34 (0%)	43	80

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	111	VAL
11	K	12	VAL
21	U	364	VAL
25	Y	350	VAL
29	c	244	VAL
32	f	62	ILE
32	f	447	VAL
1	A	206	ILE
32	f	131	VAL
3	C	298	ILE
29	c	157	ILE
4	D	151	ILE
8	H	10	LEU
25	Y	67	VAL
26	Z	144	VAL
27	a	336	VAL
27	a	340	VAL
29	c	156	VAL
32	f	281	ILE
30	d	121	ARG
22	V	466	ILE
30	d	213	ARG
21	U	433	PRO
2	B	218	PRO
2	B	219	PRO
2	B	325	VAL
5	E	208	ILE
22	V	86	VAL

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Mol	Chain	Res	Type
3	C	192	PRO
3	C	251	ILE
10	J	98	VAL
29	c	189	ILE
1	A	172	VAL
6	F	326	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	305 (99%)	3 (1%)	82	92
2	B	298/385 (77%)	294 (99%)	4 (1%)	76	89
3	C	332/346 (96%)	324 (98%)	8 (2%)	57	82
4	D	333/366 (91%)	329 (99%)	4 (1%)	78	90
5	E	308/353 (87%)	306 (99%)	2 (1%)	90	95
6	F	312/379 (82%)	303 (97%)	9 (3%)	50	78
7	G	193/209 (92%)	192 (100%)	1 (0%)	92	96
8	H	164/190 (86%)	162 (99%)	2 (1%)	78	90
9	I	193/220 (88%)	193 (100%)	0	100	100
10	J	152/210 (72%)	151 (99%)	1 (1%)	88	94
11	K	186/202 (92%)	185 (100%)	1 (0%)	92	96
12	L	198/229 (86%)	197 (100%)	1 (0%)	92	96
13	M	192/211 (91%)	191 (100%)	1 (0%)	92	96
14	N	148/180 (82%)	148 (100%)	0	100	100
15	O	177/227 (78%)	177 (100%)	0	100	100
16	P	172/173 (99%)	172 (100%)	0	100	100
17	Q	164/171 (96%)	164 (100%)	0	100	100
18	R	153/201 (76%)	153 (100%)	0	100	100
19	S	174/198 (88%)	174 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	175/214 (82%)	174 (99%)	1 (1%)	90	95
21	U	685/816 (84%)	679 (99%)	6 (1%)	84	93
22	V	414/459 (90%)	408 (99%)	6 (1%)	74	89
23	W	218/416 (52%)	215 (99%)	3 (1%)	74	89
24	X	74/362 (20%)	74 (100%)	0	100	100
25	Y	334/344 (97%)	330 (99%)	4 (1%)	78	90
26	Z	257/295 (87%)	254 (99%)	3 (1%)	78	90
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	166 (99%)	1 (1%)	90	95
29	c	252/267 (94%)	249 (99%)	3 (1%)	78	90
30	d	231/293 (79%)	229 (99%)	2 (1%)	84	93
31	e	22/63 (35%)	22 (100%)	0	100	100
32	f	582/628 (93%)	574 (99%)	8 (1%)	74	89
All	All	7901/9627 (82%)	7827 (99%)	74 (1%)	85	93

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ASP
1	A	113	ILE
1	A	317	VAL
2	B	105	THR
2	B	137	SER
2	B	174	MET
2	B	320	ASP
3	C	66	LEU
3	C	69	GLN
3	C	118	ASN
3	C	175	PHE
3	C	182	GLN
3	C	219	LEU
3	C	286	THR
3	C	295	THR
4	D	82	ILE
4	D	124	LEU
4	D	230	VAL
4	D	282	ASP

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Mol	Chain	Res	Type
5	E	182	LEU
5	E	269	THR
6	F	93	VAL
6	F	150	LEU
6	F	151	VAL
6	F	161	LEU
6	F	166	THR
6	F	283	ILE
6	F	307	GLN
6	F	347	ARG
6	F	430	LYS
7	G	111	VAL
8	H	129	PRO
8	H	130	PHE
10	J	114	LEU
11	K	101	PHE
12	L	46	LEU
13	M	227	VAL
20	T	168	LEU
21	U	9	ILE
21	U	217	CYS
21	U	479	LEU
21	U	554	LEU
21	U	603	LEU
21	U	629	THR
22	V	94	VAL
22	V	167	LEU
22	V	197	THR
22	V	320	THR
22	V	391	THR
22	V	392	TYR
23	W	333	LEU
23	W	361	HIS
23	W	371	THR
25	Y	315	THR
25	Y	323	PHE
25	Y	343	LEU
25	Y	356	THR
26	Z	133	LEU
26	Z	186	THR
26	Z	191	ILE
28	b	53	THR

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Mol	Chain	Res	Type
29	c	194	HIS
29	c	227	GLU
29	c	229	LEU
30	d	107	LEU
30	d	116	HIS
32	f	107	LEU
32	f	317	THR
32	f	371	CYS
32	f	391	LEU
32	f	526	THR
32	f	600	LEU
32	f	686	ARG
32	f	689	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	304	ASN
1	A	305	GLN
1	A	358	HIS
1	A	414	ASN
2	B	119	ASN
2	B	154	HIS
2	B	193	GLN
2	B	314	ASN
3	C	32	GLN
3	C	40	GLN
3	C	182	GLN
3	C	279	GLN
3	C	296	ASN
4	D	65	GLN
4	D	91	GLN
4	D	99	ASN
4	D	193	GLN
4	D	222	HIS
4	D	304	ASN
4	D	376	ASN
5	E	55	GLN
5	E	141	GLN
6	F	83	ASN
6	F	207	ASN

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Mol	Chain	Res	Type
6	F	258	GLN
6	F	323	ASN
6	F	392	ASN
7	G	123	GLN
7	G	127	GLN
11	K	23	GLN
19	S	108	ASN
21	U	107	HIS
21	U	115	ASN
21	U	421	GLN
21	U	685	GLN
21	U	734	GLN
22	V	177	ASN
22	V	242	HIS
22	V	329	HIS
22	V	400	HIS
23	W	264	GLN
23	W	444	HIS
24	X	406	ASN
25	Y	77	ASN
25	Y	351	ASN
26	Z	235	ASN
27	a	86	GLN
27	a	193	GLN
28	b	76	HIS
29	c	44	HIS
29	c	101	GLN
29	c	172	HIS
29	c	190	GLN
29	c	241	ASN
29	c	287	HIS
30	d	245	GLN
32	f	86	ASN
32	f	246	HIS
32	f	269	GLN
32	f	372	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
33	ADP	A	501	-	24,29,29	1.03	1 (4%)	23,45,45	1.67	1 (4%)
33	ADP	B	501	-	24,29,29	0.99	1 (4%)	23,45,45	1.82	2 (8%)
33	ADP	C	501	-	24,29,29	1.01	1 (4%)	23,45,45	1.65	1 (4%)
33	ADP	D	501	-	24,29,29	0.96	1 (4%)	23,45,45	1.71	1 (4%)
33	ADP	E	401	-	24,29,29	1.02	1 (4%)	23,45,45	2.07	6 (26%)
33	ADP	F	501	-	24,29,29	1.04	1 (4%)	23,45,45	1.74	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	ADP	A	501	-	-	0/12/32/32	0/3/3/3
33	ADP	B	501	-	-	0/12/32/32	0/3/3/3
33	ADP	C	501	-	-	0/12/32/32	0/3/3/3
33	ADP	D	501	-	-	0/12/32/32	0/3/3/3
33	ADP	E	401	-	-	0/12/32/32	0/3/3/3
33	ADP	F	501	-	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	501	ADP	C5-C4	3.04	1.47	1.40
33	B	501	ADP	C5-C4	3.06	1.47	1.40
33	E	401	ADP	C5-C4	3.10	1.47	1.40
33	F	501	ADP	C5-C4	3.19	1.47	1.40
33	C	501	ADP	C5-C4	3.20	1.47	1.40
33	A	501	ADP	C5-C4	3.28	1.47	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	E	401	ADP	N3-C2-N1	-6.73	123.59	128.87
33	B	501	ADP	N3-C2-N1	-6.70	123.61	128.87
33	D	501	ADP	N3-C2-N1	-6.57	123.71	128.87
33	F	501	ADP	N3-C2-N1	-6.56	123.72	128.87
33	A	501	ADP	N3-C2-N1	-6.31	123.92	128.87
33	C	501	ADP	N3-C2-N1	-6.25	123.96	128.87
33	E	401	ADP	C1'-N9-C4	-2.52	124.00	126.81
33	E	401	ADP	C4'-O4'-C1'	-2.47	107.03	109.64
33	E	401	ADP	C2'-C1'-N9	-2.42	106.98	113.47
33	E	401	ADP	O3B-PB-O2B	2.01	114.81	107.44
33	B	501	ADP	O4'-C1'-N9	2.21	112.28	108.11
33	F	501	ADP	O4'-C1'-N9	2.25	112.36	108.11
33	E	401	ADP	O4'-C1'-N9	3.87	115.42	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	A	501	ADP	5	0
33	B	501	ADP	8	0
33	C	501	ADP	2	0
33	D	501	ADP	4	0
33	E	401	ADP	7	0
33	F	501	ADP	4	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	f	3
27	a	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	8.67
1	f	79:ASN	C	80:TYR	N	7.26
1	f	348:ASP	C	349:SER	N	6.44
1	a	341:LEU	C	342:ASP	N	5.77