



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

Nov 21, 2016 – 04:32 PM EST

PDB ID : 5T0J  
EMDB ID: : EMD-8337  
Title : Structural basis for dynamic regulation of the human 26S proteasome  
Authors : Chen, S.; Wu, J.; Lu, Y.; Ma, Y.B.; Lee, B.H.; Yu, Z.; Ouyang, Q.; Finley, D.;  
Kirschner, M.W.; Mao, Y.  
Deposited on : 2016-08-16  
Resolution : 8.00 Å(reported)

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

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

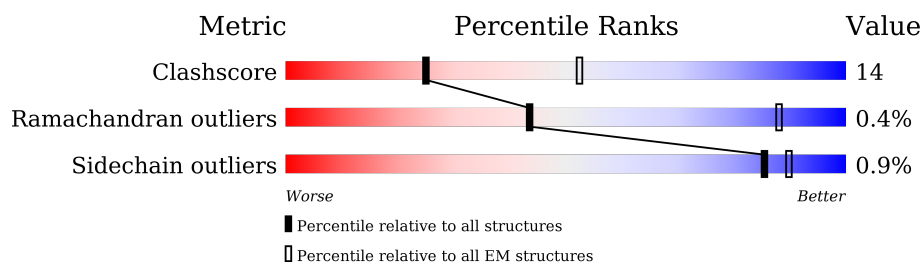
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.00 Å.

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














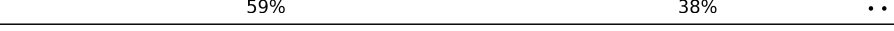

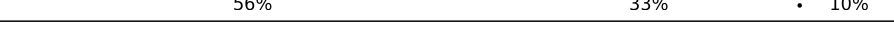

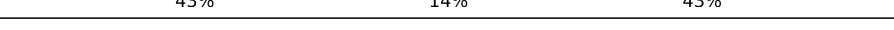


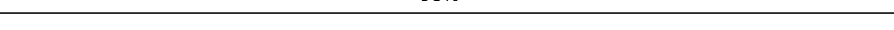


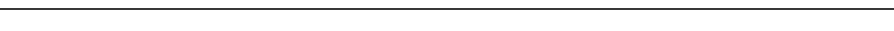

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	f	749	
2	G	245	
3	H	233	
4	I	260	
5	J	247	
6	K	240	
7	L	268	
8	M	254	
9	N	238	

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Mol	Chain	Length	Quality of chain
10	O	276	
11	P	204	
12	Q	201	
13	R	262	
14	S	240	
15	T	263	
16	A	433	
17	B	440	
18	D	418	
19	E	403	
20	F	439	
21	C	398	
22	U	953	
23	V	533	
24	W	456	
25	X	422	
26	Y	389	
27	Z	324	
28	a	376	
29	b	377	
30	c	309	
31	d	349	
32	e	70	

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 76674 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 proteasome non-ATPase regulatory subunit 2.

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

- Molecule 2 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 3 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

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

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

- Molecule 5 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 6 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 8 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 9 is a protein called Proteasome subunit beta type-6.

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

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

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

- Molecule 11 is a protein called Proteasome subunit beta type-3.

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

- Molecule 12 is a protein called Proteasome subunit beta type-2.

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

- Molecule 13 is a protein called Proteasome subunit beta type-5.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

- Molecule 15 is a protein called Proteasome subunit beta type-4.

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

- Molecule 16 is a protein called 26S protease regulatory subunit 7.

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

- Molecule 17 is a protein called 26S protease regulatory subunit 4.

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

- Molecule 18 is a protein called 26S protease regulatory subunit 6B.

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

- Molecule 19 is a protein called 26S protease regulatory subunit 10B.

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

- Molecule 20 is a protein called 26S protease regulatory subunit 6A.

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

- Molecule 21 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C	392	Total	C	N	O	S	0	0
			3078	1932	551	577	18		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

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

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

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

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	241	Total	C	N	O	S	0	0
			1905	1212	320	365	8		

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	278	Total	C	N	O	S	0	0
			2187	1389	374	406	18		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

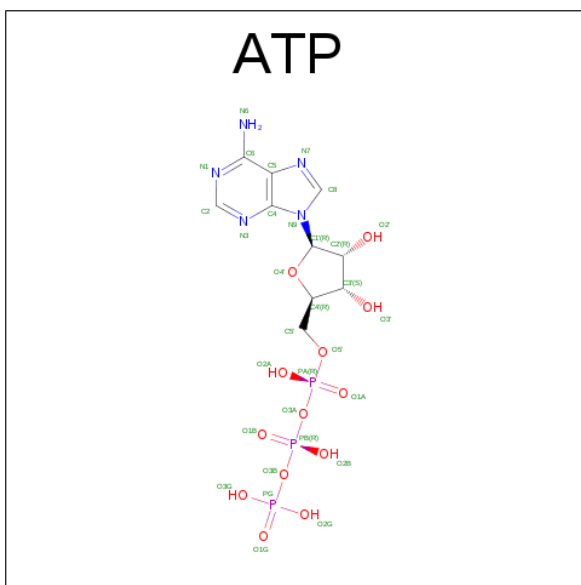
Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 32 is a protein called 26S proteasome complex subunit DSS1.

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

- Molecule 33 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).





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

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

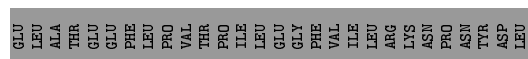
Mol	Chain	Residues	Atoms	AltConf
34	c	1	Total Zn 1 1	0

### 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.

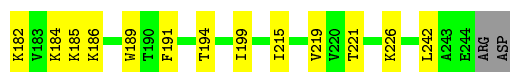
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 2

Chain f: 



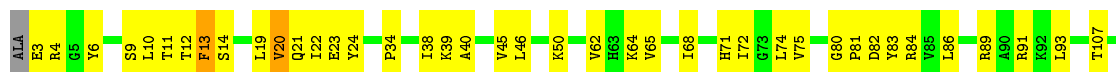
- Molecule 2: Proteasome subunit alpha type-6

Chain G: 



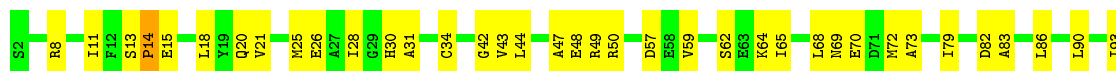
- Molecule 3: Proteasome subunit alpha type-2

Chain H: 



- Molecule 4: Proteasome subunit alpha type-4

Chain I: 

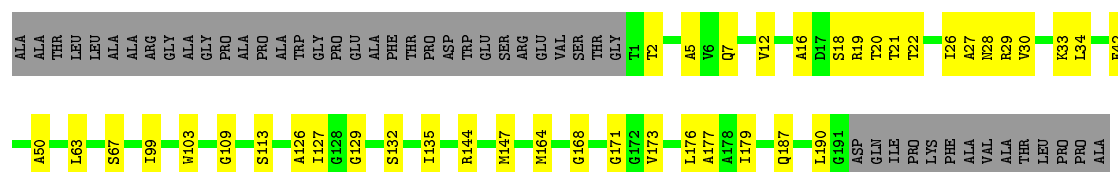






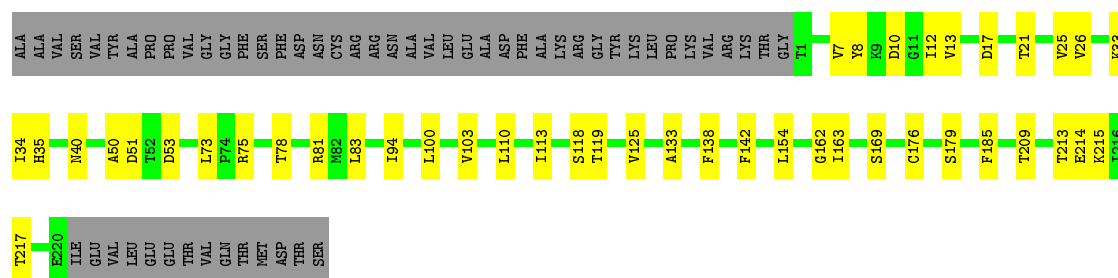
• Molecule 9: Proteasome subunit beta type-6

Chain N: 63% 17% 20%



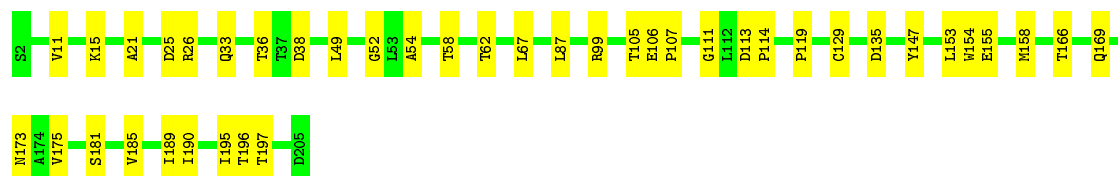
• Molecule 10: Proteasome subunit beta type-7

Chain O: 64% 16% 20%



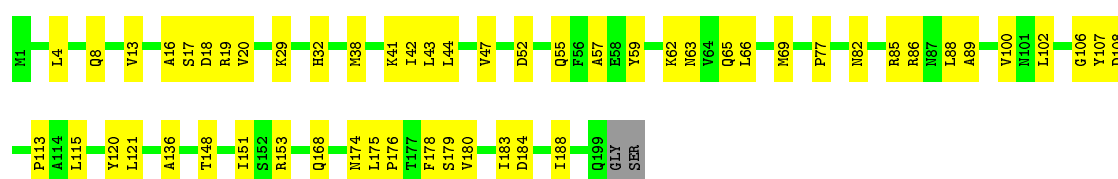
• Molecule 11: Proteasome subunit beta type-3

Chain P: 80% 20%



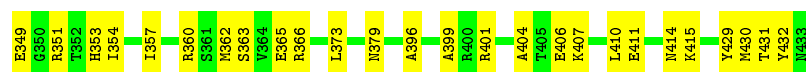
• Molecule 12: Proteasome subunit beta type-2

Chain Q: 72% 27%



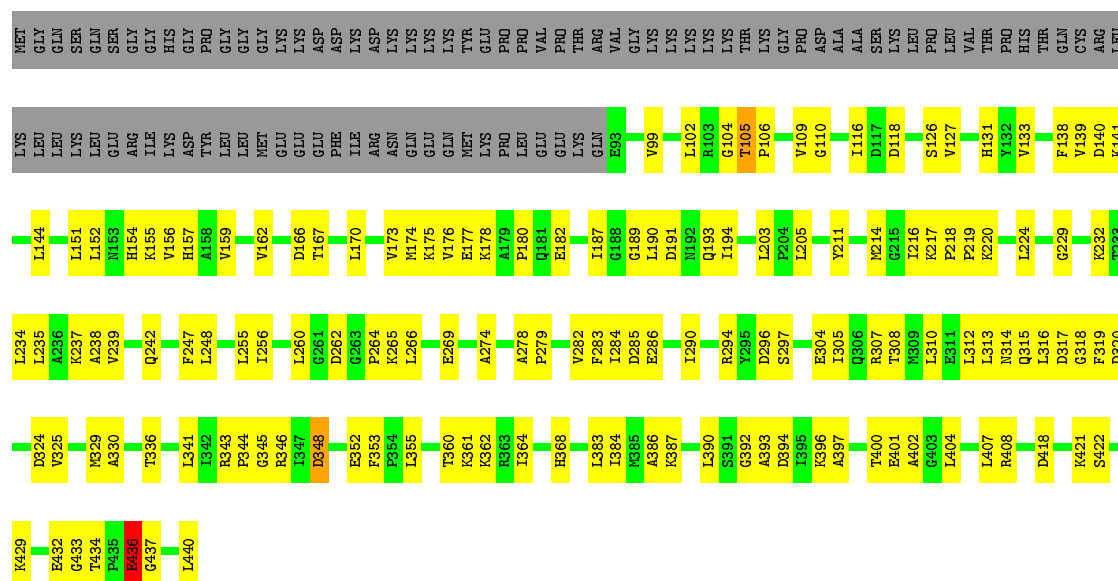
• Molecule 13: Proteasome subunit beta type-5





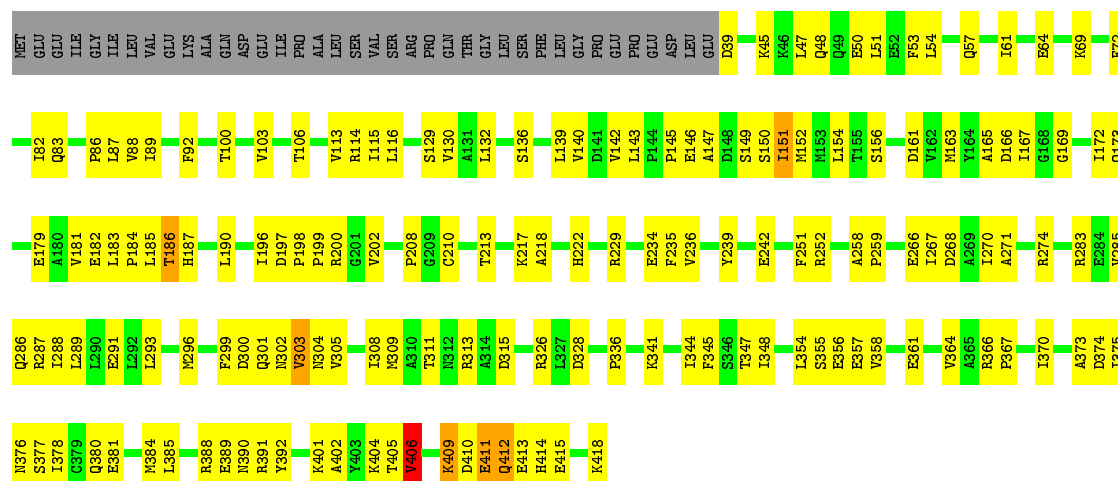
• Molecule 17: 26S protease regulatory subunit 4

Chain B: 47% 32% 21%



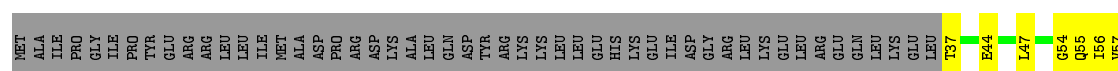
• Molecule 18: 26S protease regulatory subunit 6B

Chain D: 54% 36% 9%



• Molecule 19: 26S protease regulatory subunit 10B

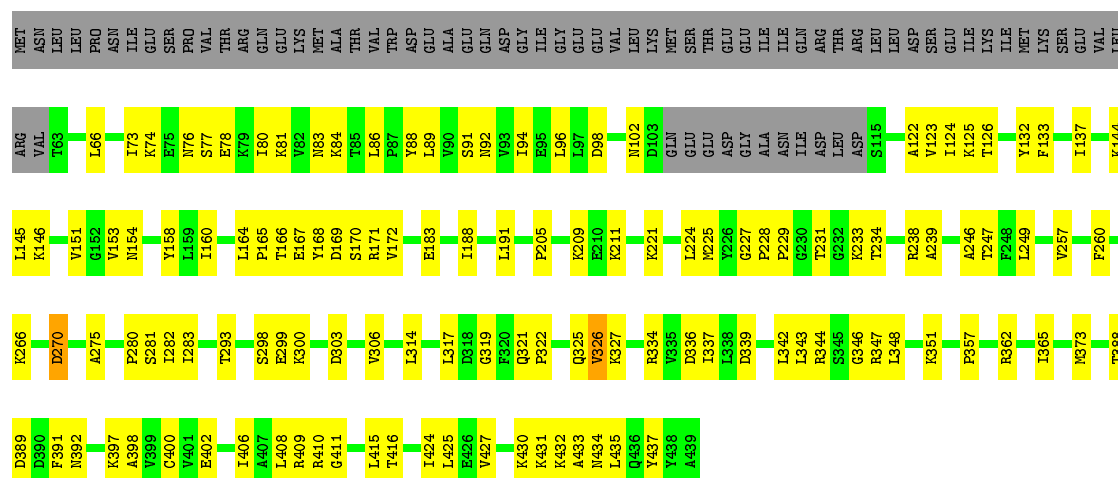
Chain E: 61% 26% 12%





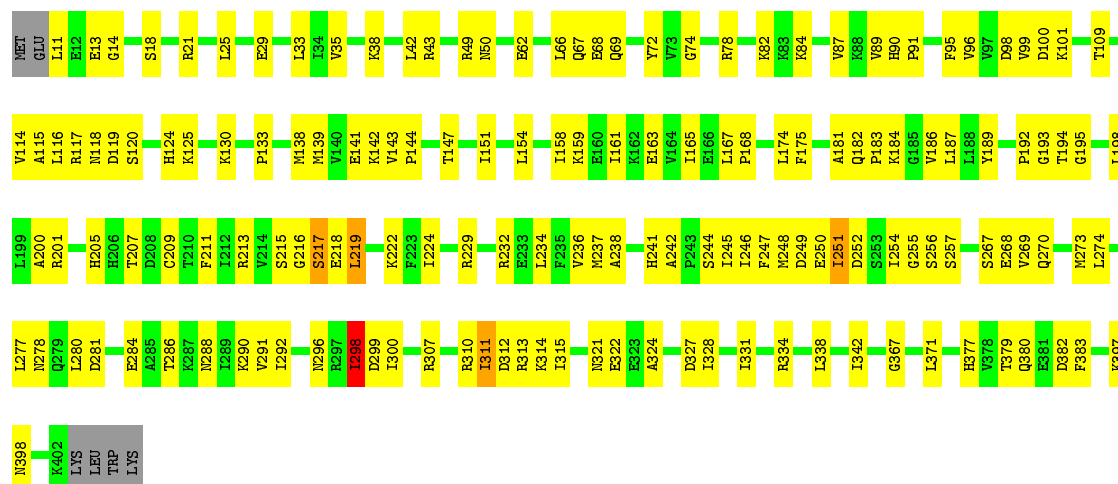
• Molecule 20: 26S protease regulatory subunit 6A

Chain F: 54% 28% 17%



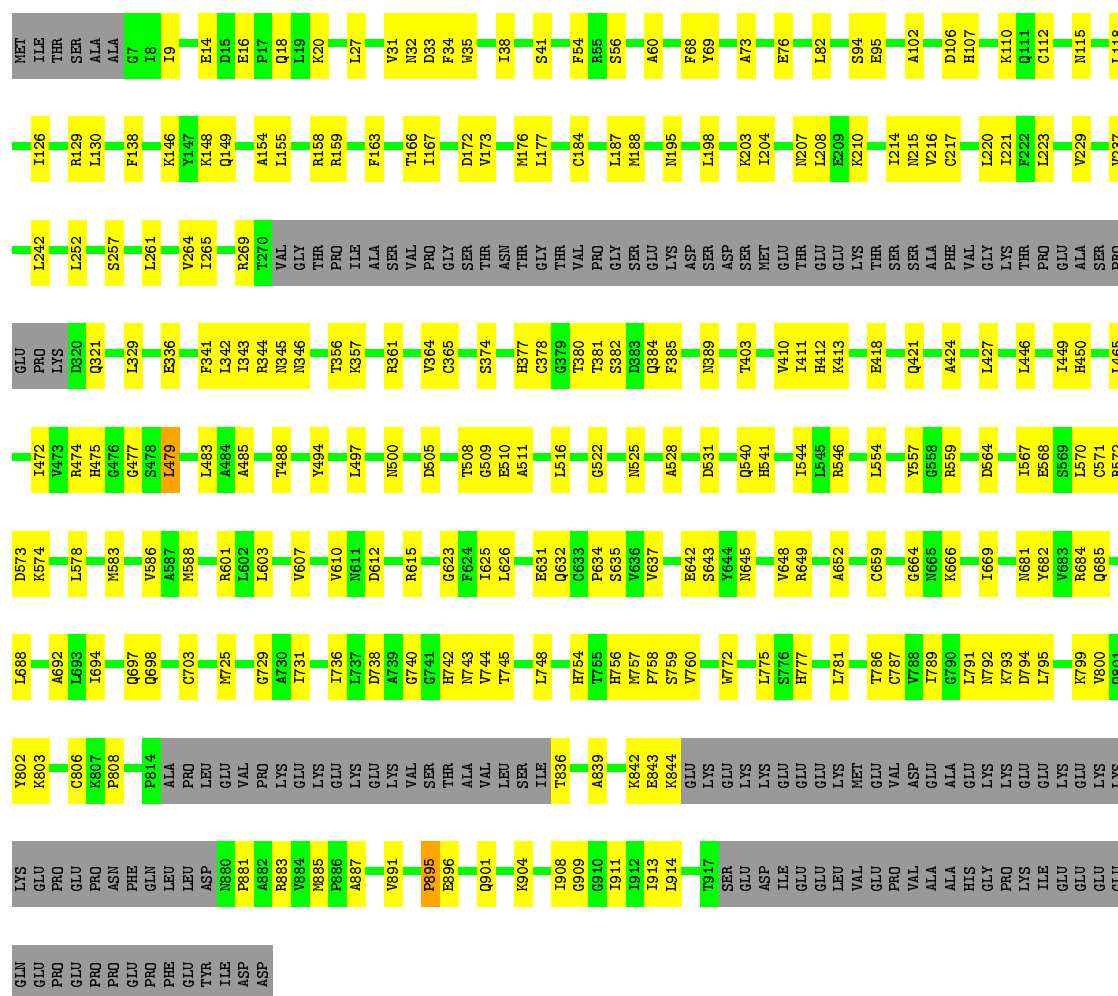
• Molecule 21: 26S protease regulatory subunit 8

Chain C: 59% 38% ..



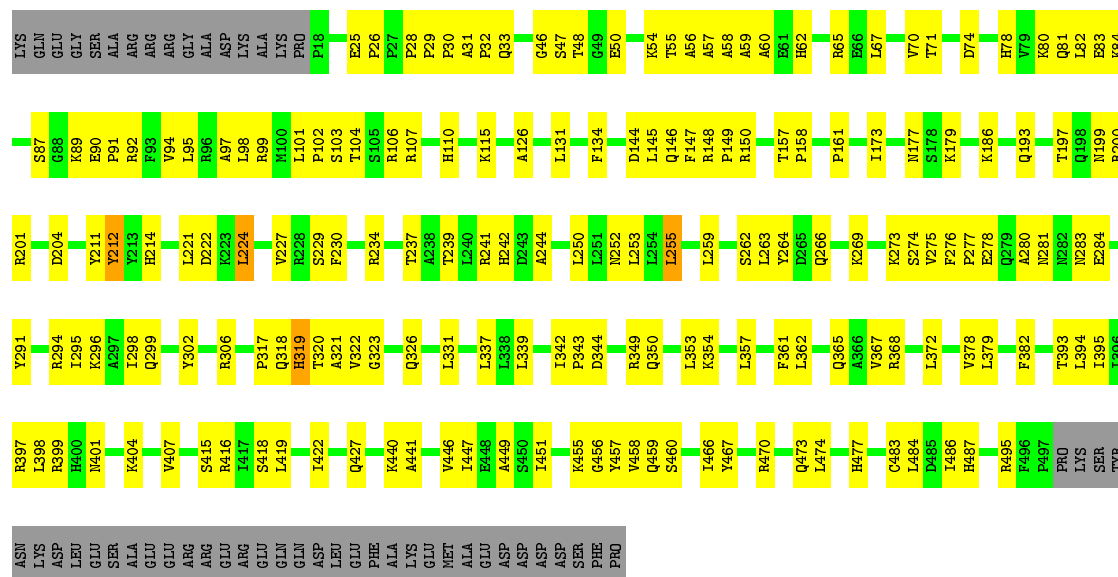
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 1

Chain U: 60% 25% 15%



- Molecule 23: 26S proteasome non-ATPase regulatory subunit 3

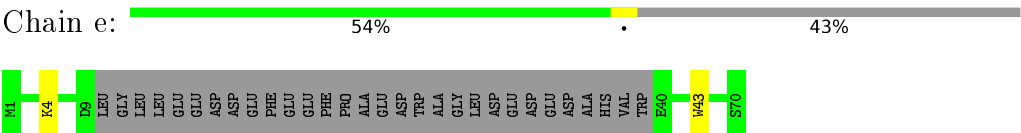
Chain V: 56% 33% 10%





- Molecule 27: 26S proteasome non-ATPase regulatory subunit 7





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	14382	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	f	0.24	0/5413	0.50	1/7317 (0.0%)
10	O	0.23	0/1670	0.43	0/2265
11	P	0.23	0/1614	0.40	0/2177
12	Q	0.24	0/1603	0.41	0/2174
13	R	0.23	0/1579	0.39	0/2134
14	S	0.24	0/1671	0.41	0/2253
15	T	0.24	0/1700	0.41	0/2305
16	A	0.25	0/2886	0.50	0/3899
17	B	0.25	0/2756	0.50	0/3721
18	D	0.25	0/3090	0.51	1/4168 (0.0%)
19	E	0.39	1/2835 (0.0%)	0.45	0/3821
2	G	0.24	0/1859	0.45	0/2523
20	F	0.26	0/2903	0.50	0/3912
21	C	0.27	1/3117 (0.0%)	0.50	2/4189 (0.0%)
22	U	0.23	0/6396	0.40	0/8646
23	V	1.26	6/3929 (0.2%)	0.50	0/5309
24	W	0.24	0/3751	0.47	2/5042 (0.0%)
25	X	0.23	0/1936	0.41	0/2614
26	Y	0.24	0/3173	0.47	2/4273 (0.0%)
27	Z	0.24	0/2324	0.48	0/3150
28	a	0.23	0/3053	0.42	0/4133
29	b	0.26	0/1478	0.44	0/2001
3	H	0.25	0/1743	0.49	0/2372
30	c	0.26	1/2226 (0.0%)	0.46	0/3007
31	d	0.25	0/2162	0.48	0/2919
32	e	3.67	1/338 (0.3%)	0.75	2/450 (0.4%)
4	I	0.60	1/1942 (0.1%)	0.59	4/2628 (0.2%)
5	J	3.05	6/1728 (0.3%)	0.48	0/2358
6	K	0.24	0/1747	0.43	0/2364
7	L	0.23	0/1885	0.43	0/2552
8	M	0.23	0/1891	0.40	0/2552
9	N	0.23	0/1454	0.41	0/1967

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
All	All	0.64	17/77852 (0.0%)	0.46	14/105195 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
17	B	0	1
18	D	0	3
23	V	0	1
24	W	0	1
26	Y	0	1
28	a	0	1
31	d	0	1
All	All	0	9

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	e	4	LYS	CD-CE	67.17	3.19	1.51
5	J	21	TYR	CD2-CE2	67.11	2.40	1.39
5	J	21	TYR	CD1-CE1	65.88	2.38	1.39
5	J	21	TYR	CE1-CZ	49.34	2.02	1.38
5	J	21	TYR	CE2-CZ	45.57	1.97	1.38
23	V	212	TYR	CD2-CE2	40.57	2.00	1.39
23	V	212	TYR	CD1-CE1	40.40	2.00	1.39
5	J	21	TYR	CG-CD2	36.47	1.86	1.39
5	J	21	TYR	CG-CD1	35.86	1.85	1.39
23	V	212	TYR	CE1-CZ	29.51	1.76	1.38
23	V	212	TYR	CE2-CZ	28.92	1.76	1.38
4	I	14	PRO	CA-C	23.61	2.00	1.52
23	V	212	TYR	CG-CD2	23.07	1.69	1.39
23	V	212	TYR	CG-CD1	22.77	1.68	1.39
19	E	175	PRO	C-N	16.65	1.65	1.34
21	C	242	ALA	C-N	7.00	1.47	1.34
30	c	104	ARG	C-N	5.89	1.45	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	14	PRO	O-C-N	-15.43	98.01	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	e	4	LYS	CD-CE-NZ	8.24	130.65	111.70
4	I	14	PRO	CA-C-N	7.71	134.15	117.20
32	e	4	LYS	CG-CD-CE	7.23	133.60	111.90
4	I	14	PRO	N-CA-CB	-7.13	94.75	103.30
1	f	459	GLU	N-CA-C	6.14	127.58	111.00
4	I	14	PRO	N-CA-C	6.01	127.73	112.10
21	C	217	SER	C-N-CA	5.74	136.05	121.70
26	Y	63	TRP	C-N-CA	5.73	136.03	121.70
26	Y	287	LEU	CA-CB-CG	5.41	127.73	115.30
24	W	92	LYS	C-N-CA	5.22	134.76	121.70
24	W	135	LYS	C-N-CA	5.21	134.72	121.70
18	D	409	LYS	C-N-CA	5.19	134.68	121.70
21	C	217	SER	CA-C-N	5.12	128.47	117.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	B	436	GLU	Peptide
18	D	258	ALA	Peptide
18	D	406	VAL	Peptide
18	D	412	GLN	Peptide
23	V	319	HIS	Peptide
24	W	416	GLN	Peptide
26	Y	357	ASN	Peptide
28	a	286	ALA	Peptide
31	d	3	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	f	5331	0	5344	0	0
2	G	1826	0	1796	71	0
3	H	1708	0	1594	58	0
4	I	1912	0	1851	86	0
5	J	1704	0	1517	90	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	1722	0	1673	51	0
7	L	1850	0	1822	51	0
8	M	1856	0	1814	47	0
9	N	1430	0	1398	23	0
10	O	1643	0	1644	30	0
11	P	1585	0	1598	29	0
12	Q	1570	0	1547	41	0
13	R	1548	0	1499	35	0
14	S	1641	0	1618	25	0
15	T	1667	0	1628	37	0
16	A	2835	0	2879	114	0
17	B	2717	0	2755	119	0
18	D	3040	0	3076	129	0
19	E	2790	0	2846	85	0
20	F	2863	0	2931	100	0
21	C	3078	0	3193	132	0
22	U	6287	0	6338	144	0
23	V	3852	0	3893	130	0
24	W	3703	0	3822	94	0
25	X	1905	0	1951	46	0
26	Y	3115	0	3120	102	0
27	Z	2281	0	2312	57	0
28	a	2995	0	3012	0	0
29	b	1458	0	1505	0	0
30	c	2187	0	2215	0	0
31	d	2116	0	2146	0	0
32	e	334	0	294	0	0
33	A	31	0	12	1	0
33	D	31	0	12	2	0
33	E	31	0	12	3	0
33	F	31	0	12	1	0
34	c	1	0	0	0	0
All	All	76674	0	76679	1703	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 14.

All (1703) 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)
23:V:212:TYR:CE1	23:V:212:TYR:CZ	1.76	1.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:21:TYR:CD1	5:J:21:TYR:CG	1.85	1.64
5:J:21:TYR:CG	5:J:21:TYR:CD2	1.86	1.64
23:V:212:TYR:CZ	23:V:212:TYR:CE2	1.76	1.63
5:J:21:TYR:CE2	5:J:21:TYR:CZ	1.97	1.51
23:V:212:TYR:CD1	23:V:212:TYR:CE1	2.00	1.49
23:V:212:TYR:CD2	23:V:212:TYR:CE2	2.00	1.49
5:J:21:TYR:CE1	5:J:21:TYR:CZ	2.02	1.47
4:I:14:PRO:HA	5:J:21:TYR:CG	1.63	1.32
4:I:14:PRO:HA	5:J:21:TYR:CD1	1.63	1.31
4:I:14:PRO:C	4:I:14:PRO:CA	2.00	1.30
4:I:15:GLU:N	5:J:21:TYR:CZ	2.02	1.28
4:I:14:PRO:C	5:J:21:TYR:CE2	2.13	1.22
4:I:14:PRO:C	5:J:21:TYR:CE1	2.15	1.20
4:I:14:PRO:C	5:J:21:TYR:CD1	2.19	1.16
4:I:14:PRO:C	5:J:21:TYR:CZ	2.19	1.15
4:I:14:PRO:C	5:J:21:TYR:CD2	2.23	1.12
5:J:21:TYR:CE1	5:J:21:TYR:CD1	2.38	1.11
4:I:14:PRO:O	5:J:21:TYR:CG	2.03	1.11
5:J:21:TYR:CE2	5:J:21:TYR:CD2	2.40	1.10
4:I:15:GLU:N	5:J:21:TYR:CE1	2.20	1.09
4:I:14:PRO:CA	5:J:21:TYR:CD1	2.35	1.08
4:I:14:PRO:O	5:J:21:TYR:CD2	2.11	1.04
4:I:14:PRO:HB2	5:J:21:TYR:CE2	1.92	1.04
4:I:14:PRO:CA	5:J:21:TYR:CE1	2.42	1.03
4:I:14:PRO:C	5:J:21:TYR:CG	2.34	1.01
21:C:217:SER:HB3	21:C:218:GLU:HB3	1.40	1.00
4:I:14:PRO:CA	5:J:21:TYR:CG	2.45	0.98
4:I:14:PRO:CA	5:J:21:TYR:CZ	2.47	0.98
4:I:14:PRO:CA	5:J:21:TYR:CD2	2.48	0.97
4:I:14:PRO:CA	5:J:21:TYR:CE2	2.53	0.92
17:B:166:ASP:HB3	17:B:167:THR:HA	1.52	0.91
4:I:14:PRO:N	5:J:21:TYR:CE1	2.40	0.89
4:I:14:PRO:CB	5:J:21:TYR:CE2	2.54	0.89
24:W:40:LEU:HB2	24:W:41:GLN:HA	1.56	0.84
6:K:225:ASN:HA	6:K:227:HIS:HB3	1.59	0.84
24:W:416:GLN:HB3	24:W:417:ARG:HA	1.61	0.82
3:H:10:LEU:HB3	3:H:124:SER:HA	1.62	0.82
18:D:389:GLU:HA	18:D:390:ASN:HB2	1.62	0.81
19:E:266:GLY:HA2	19:E:267:PHE:HB3	1.62	0.81
18:D:166:ASP:HB3	33:D:501:ATP:HN61	1.46	0.81
2:G:159:TYR:HB3	3:H:81:PRO:HG3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:144:PRO:HD2	21:C:201:ARG:HG3	1.63	0.80
4:I:14:PRO:CB	5:J:21:TYR:CD2	2.65	0.80
18:D:303:VAL:HG23	18:D:304:ASN:HB2	1.62	0.80
21:C:158:ILE:HA	21:C:161:ILE:HG22	1.64	0.80
20:F:431:LYS:HD2	20:F:434:ASN:HB3	1.62	0.80
13:R:19:ARG:HE	13:R:29:GLN:HE22	1.29	0.79
26:Y:170:GLU:HG3	26:Y:171:GLY:HA3	1.63	0.79
18:D:100:THR:HB	18:D:114:ARG:HD2	1.64	0.78
17:B:220:LYS:HB3	17:B:346:ARG:HB3	1.64	0.78
19:E:174:GLY:HA2	19:E:176:PRO:HD2	1.63	0.78
18:D:283:ARG:HA	18:D:286:GLN:HE21	1.49	0.77
23:V:57:ALA:HB3	23:V:58:ALA:HB3	1.64	0.77
16:A:333:ARG:HB2	16:A:337:LEU:HB2	1.66	0.77
16:A:102:ILE:HA	16:A:113:ILE:HA	1.65	0.77
21:C:310:ARG:HG3	21:C:311:ILE:HG23	1.64	0.77
16:A:267:LYS:HB3	16:A:270:CYS:HB3	1.67	0.76
18:D:199:PRO:HG3	18:D:328:ASP:HB2	1.66	0.76
20:F:409:ARG:HB2	20:F:411:GLY:HA2	1.67	0.76
18:D:410:ASP:HB3	18:D:412:GLN:N	1.99	0.76
4:I:14:PRO:HA	4:I:14:PRO:C	2.02	0.76
4:I:15:GLU:N	5:J:21:TYR:CE2	2.53	0.76
21:C:195:GLY:HA2	21:C:198:LEU:HB2	1.66	0.75
23:V:80:LYS:HE2	23:V:87:SER:HA	1.68	0.75
17:B:177:GLU:H	17:B:178:LYS:HA	1.53	0.74
4:I:14:PRO:O	5:J:21:TYR:CD1	2.41	0.74
16:A:401:ARG:HD2	16:A:407:LYS:HE2	1.70	0.74
21:C:254:ILE:HG23	21:C:257:SER:HB3	1.69	0.74
24:W:92:LYS:H	24:W:93:ARG:HB3	1.52	0.73
20:F:299:GLU:HB3	20:F:300:LYS:HB3	1.71	0.73
19:E:245:GLU:HG2	19:E:250:ASP:HB3	1.69	0.73
33:E:401:ATP:H4'	20:F:344:ARG:HE	1.53	0.73
20:F:168:TYR:HB2	20:F:169:ASP:HB2	1.71	0.73
16:A:407:LYS:NZ	16:A:411:GLU:OE1	2.21	0.73
3:H:14:SER:HB3	3:H:19:LEU:HA	1.70	0.73
22:U:418:GLU:HG3	22:U:421:GLN:HE21	1.53	0.73
19:E:222:ALA:HB1	19:E:273:VAL:HG21	1.70	0.73
3:H:39:LYS:HE2	3:H:144:PRO:HG2	1.71	0.73
17:B:396:LYS:HD3	21:C:181:ALA:HB3	1.68	0.72
7:L:67:ASP:HB3	7:L:70:ILE:HB	1.69	0.72
18:D:208:PRO:HB3	19:E:291:ARG:HH12	1.53	0.72
27:Z:176:LEU:HD12	27:Z:177:ARG:H	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:33:ASN:HA	2:G:170:VAL:HG22	1.71	0.72
20:F:165:PRO:HB2	20:F:166:THR:HG22	1.72	0.72
12:Q:4:LEU:HD22	12:Q:17:SER:HA	1.70	0.71
24:W:257:GLN:HA	24:W:258:ALA:HB3	1.72	0.71
24:W:90:LEU:HA	24:W:94:ARG:HD2	1.72	0.71
18:D:210:CYS:SG	18:D:376:ASN:ND2	2.64	0.70
25:X:229:TYR:OH	25:X:258:LYS:NZ	2.23	0.70
20:F:357:PRO:O	20:F:362:ARG:NH1	2.25	0.70
21:C:313:ARG:NH1	21:C:314:LYS:O	2.24	0.70
27:Z:63:LYS:HB2	27:Z:64:ASP:HB2	1.74	0.70
22:U:261:LEU:HD22	22:U:329:LEU:HD22	1.73	0.69
16:A:140:VAL:HA	16:A:152:PRO:HA	1.74	0.69
23:V:255:LEU:HD22	23:V:291:TYR:HB3	1.74	0.69
26:Y:358:ARG:HD2	26:Y:359:PRO:HD2	1.73	0.69
21:C:72:TYR:HB2	21:C:116:LEU:HB3	1.74	0.69
16:A:172:VAL:HG13	33:A:501:ATP:H3'	1.74	0.69
6:K:50:VAL:HG11	6:K:66:LYS:HB2	1.74	0.69
26:Y:356:THR:OG1	26:Y:357:ASN:O	2.10	0.69
16:A:80:LEU:HB3	17:B:99:VAL:HG11	1.74	0.69
10:O:17:ASP:O	10:O:33:LYS:NZ	2.26	0.69
18:D:143:LEU:O	23:V:440:LYS:NZ	75.12	0.69
16:A:404:ALA:HA	16:A:407:LYS:HD3	1.73	0.69
2:G:159:TYR:H	18:D:418:LYS:HZ1	1.40	0.69
19:E:44:GLU:OE1	20:F:76:ASN:ND2	2.23	0.69
20:F:137:ILE:HG21	20:F:160:ILE:HB	1.75	0.69
26:Y:101:ARG:NH2	26:Y:126:LYS:O	2.23	0.68
8:M:190:VAL:HG11	8:M:232:ARG:HH11	1.57	0.68
19:E:81:VAL:HG11	19:E:105:LEU:HB2	1.73	0.68
17:B:285:ASP:HA	17:B:330:ALA:HB3	1.76	0.68
18:D:375:ILE:H	18:D:378:ILE:HD12	1.59	0.68
11:P:26:ARG:HH21	11:P:38:ASP:HA	1.59	0.68
23:V:455:LYS:N	23:V:456:GLY:HA2	2.09	0.68
23:V:81:GLN:HB3	23:V:82:LEU:C	2.14	0.68
2:G:109:ILE:HG12	2:G:111:VAL:H	1.58	0.68
22:U:842:LYS:HA	22:U:843:GLU:HB3	1.75	0.68
23:V:275:VAL:H	23:V:276:PHE:HA	1.58	0.68
23:V:80:LYS:HA	23:V:81:GLN:HB2	1.76	0.68
17:B:317:ASP:HB3	17:B:318:GLY:HA2	1.76	0.67
5:J:122:ASN:N	5:J:123:GLY:HA3	2.09	0.67
19:E:138:LEU:HD22	19:E:140:GLU:HG2	1.76	0.67
5:J:61:LYS:HG3	5:J:62:ILE:HD12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:99:ARG:HG3	15:T:105:PRO:HA	1.76	0.67
17:B:407:LEU:HB3	21:C:163:GLU:HG2	1.75	0.67
11:P:105:THR:HG23	11:P:107:PRO:HD3	1.76	0.67
8:M:41:CYS:HB3	8:M:189:ILE:HG13	1.76	0.66
22:U:155:LEU:O	22:U:158:ARG:NH1	2.27	0.66
26:Y:190:ALA:HA	26:Y:287:LEU:HD13	1.77	0.66
21:C:222:LYS:HE3	27:Z:179:ILE:HG12	59.70	0.66
4:I:8:ARG:HD3	4:I:11:ILE:HB	1.78	0.66
21:C:38:LYS:HG2	23:V:495:ARG:HB3	1.77	0.66
7:L:122:ARG:HG2	8:M:128:VAL:HG12	1.76	0.66
18:D:236:VAL:HG22	18:D:285:VAL:HG11	1.76	0.66
23:V:416:ARG:HG3	23:V:459:GLN:HA	1.77	0.66
20:F:321:GLN:HG3	20:F:322:PRO:HD3	1.78	0.65
3:H:68:ILE:HA	3:H:91:ARG:HE	1.60	0.65
7:L:85:CYS:SG	7:L:89:ARG:NH1	2.69	0.65
16:A:186:LYS:HB3	16:A:339:ARG:HD2	1.77	0.65
17:B:174:MET:HA	17:B:248:LEU:HD13	1.77	0.65
22:U:904:LYS:H	22:U:913:ILE:HD11	1.60	0.65
24:W:436:MET:O	24:W:440:ASN:ND2	2.27	0.65
16:A:113:ILE:O	16:A:121:PHE:N	2.28	0.65
18:D:198:PRO:HD2	18:D:302:ASN:HD21	1.62	0.65
20:F:424:ILE:HG22	20:F:425:LEU:HD12	1.77	0.65
16:A:147:TYR:HB3	20:F:86:LEU:HD13	1.78	0.65
18:D:182:GLU:HA	18:D:185:LEU:HD13	1.78	0.65
19:E:83:CYS:HB3	19:E:87:LEU:HD21	1.78	0.65
23:V:224:LEU:HD13	23:V:227:VAL:HB	1.79	0.65
18:D:293:LEU:O	18:D:326:ARG:NH1	2.30	0.65
4:I:174:MET:SD	4:I:195:LYS:NZ	2.70	0.65
7:L:52:ALA:HB2	7:L:59:HIS:HA	1.79	0.65
16:A:95:VAL:HG12	16:A:144:ARG:HG2	1.78	0.65
23:V:97:ALA:HB1	23:V:150:ARG:HH22	1.62	0.65
26:Y:349:LYS:HG3	26:Y:350:VAL:HG13	1.79	0.65
4:I:216:LEU:HD12	4:I:225:ILE:HG12	1.77	0.65
7:L:10:VAL:HG22	7:L:21:GLN:HG3	1.79	0.65
21:C:69:GLN:HB2	21:C:118:ASN:HB2	1.77	0.64
21:C:217:SER:HB3	21:C:218:GLU:CB	2.21	0.64
18:D:89:ILE:HD11	19:E:80:VAL:HG13	1.77	0.64
4:I:136:TYR:HB2	4:I:148:TYR:HB2	1.80	0.64
17:B:402:ALA:O	17:B:421:LYS:NZ	2.30	0.64
16:A:331:LEU:HD13	20:F:229:PRO:HB2	1.79	0.64
2:G:140:LEU:HB2	2:G:152:TYR:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:74:LEU:HD21	3:H:134:LEU:HD22	1.78	0.64
23:V:451:ILE:HG13	23:V:458:VAL:HG13	1.78	0.64
24:W:331:GLY:HA2	24:W:332:SER:HB3	1.79	0.64
22:U:221:ILE:HB	22:U:754:HIS:HB2	1.80	0.64
22:U:356:THR:HG21	22:U:731:ILE:HD13	1.80	0.64
4:I:14:PRO:HA	5:J:21:TYR:CD2	2.32	0.64
23:V:148:ARG:HG3	23:V:149:PRO:HD3	1.80	0.64
16:A:171:ASP:OD1	16:A:239:ARG:NH2	2.31	0.64
21:C:209:CYS:HB2	21:C:244:SER:HA	1.79	0.64
16:A:306:LEU:O	16:A:336:ARG:NH2	2.31	0.64
20:F:229:PRO:O	20:F:392:ASN:ND2	2.31	0.64
2:G:139:ILE:HG13	2:G:153:LYS:HG3	1.80	0.64
2:G:11:ARG:NH1	2:G:27:TYR:OH	2.31	0.64
4:I:121:TYR:HA	4:I:127:LYS:HE2	1.79	0.64
13:R:100:MET:HG2	13:R:113:TYR:HD1	1.63	0.64
4:I:228:LEU:HD11	4:I:232:GLU:HG2	1.80	0.63
7:L:48:ALA:HB3	7:L:211:SER:HB2	1.80	0.63
25:X:318:ILE:O	25:X:322:HIS:ND1	2.32	0.63
26:Y:64:GLN:HG2	26:Y:65:ILE:HG22	1.79	0.63
18:D:61:ILE:HD12	21:C:43:ARG:HG3	1.80	0.63
15:T:185:ASN:ND2	15:T:205:THR:OG1	2.31	0.63
26:Y:51:ALA:HA	26:Y:54:TYR:HB2	1.79	0.63
26:Y:77:ASN:O	26:Y:81:LEU:N	2.31	0.63
2:G:148:GLY:O	2:G:150:GLN:NE2	2.32	0.63
10:O:217:THR:HB	11:P:195:ILE:HB	1.81	0.63
22:U:789:ILE:HG23	22:U:844:LYS:HG2	1.81	0.63
4:I:72:MET:HG2	4:I:138:GLY:HA3	1.80	0.63
23:V:262:SER:HB2	23:V:263:LEU:HB2	1.80	0.63
16:A:165:GLN:HG2	16:A:240:VAL:HG13	1.81	0.63
16:A:280:ILE:HA	17:B:310:LEU:HD11	1.81	0.63
2:G:159:TYR:H	18:D:418:LYS:NZ	1.95	0.63
18:D:83:GLN:HG3	18:D:87:LEU:HD11	1.79	0.63
3:H:82:ASP:OD1	3:H:128:ARG:NH2	2.31	0.63
8:M:141:SER:HB3	8:M:144:ASP:HB2	1.81	0.63
26:Y:63:TRP:HB3	26:Y:64:GLN:HB3	1.81	0.63
20:F:434:ASN:OD1	20:F:435:LEU:N	2.32	0.63
2:G:105:TYR:HA	10:O:78:THR:HG23	1.80	0.63
2:G:182:LYS:O	2:G:185:LYS:NZ	2.30	0.63
4:I:159:TRP:HB3	5:J:54:GLN:HB3	1.81	0.63
9:N:22:THR:HG22	9:N:27:ALA:HB2	1.80	0.63
24:W:55:ARG:HH22	24:W:79:GLU:HG3	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:47:ALA:HB3	4:I:212:GLU:HB3	1.80	0.62
19:E:194:ASN:ND2	19:E:227:PRO:O	2.32	0.62
23:V:91:PRO:HG3	23:V:126:ALA:HB3	1.81	0.62
21:C:21:ARG:NH2	22:U:102:ALA:O	2.31	0.62
19:E:222:ALA:O	19:E:226:GLN:NE2	2.31	0.62
16:A:215:PHE:HB3	16:A:321:THR:HG23	1.80	0.62
16:A:248:LYS:HB3	17:B:260:LEU:HD21	1.80	0.62
20:F:164:LEU:HD12	20:F:165:PRO:HD2	1.82	0.62
8:M:194:ALA:HB1	8:M:238:TYR:HD1	1.64	0.62
23:V:393:THR:O	23:V:397:ARG:NH2	2.31	0.62
26:Y:346:LYS:HB2	26:Y:355:GLU:HB3	1.81	0.62
17:B:166:ASP:CB	17:B:167:THR:HA	2.29	0.62
18:D:286:GLN:NE2	21:C:218:GLU:OE2	2.32	0.62
18:D:197:ASP:OD2	18:D:301:GLN:NE2	2.33	0.62
19:E:233:ASP:HA	19:E:278:ALA:HB3	1.81	0.62
6:K:225:ASN:HB2	6:K:226:PHE:CG	2.34	0.62
23:V:266:GLN:O	23:V:269:LYS:NZ	2.33	0.62
4:I:48:GLU:HA	4:I:211:VAL:HA	1.82	0.62
5:J:116:GLN:OE1	6:K:135:ARG:NH2	2.33	0.62
2:G:145:GLU:OE2	10:O:75:ARG:NH2	2.33	0.62
24:W:259:GLU:HG2	24:W:262:LYS:HB3	1.80	0.62
26:Y:138:LEU:HD12	26:Y:141:VAL:HB	1.81	0.62
3:H:38:ILE:HB	3:H:45:VAL:HB	1.80	0.62
3:H:39:LYS:HB3	3:H:159:LYS:HA	1.82	0.61
22:U:252:LEU:HD21	22:U:264:VAL:HG11	1.81	0.61
5:J:115:LYS:HG3	5:J:127:PHE:HD2	1.65	0.61
16:A:194:PRO:HB3	16:A:200:ARG:HB2	1.82	0.61
17:B:264:PRO:HA	17:B:315:GLN:HG3	1.82	0.61
7:L:66:VAL:HG13	7:L:89:ARG:HD3	1.81	0.61
27:Z:33:LYS:NZ	27:Z:34:ARG:O	2.27	0.61
18:D:410:ASP:HB3	18:D:411:GLU:C	2.20	0.61
3:H:20:VAL:HG12	3:H:21:GLN:H	1.65	0.61
22:U:341:PHE:HB2	22:U:881:PRO:HD2	1.81	0.61
23:V:455:LYS:HD2	23:V:457:TYR:HE2	1.66	0.61
17:B:400:THR:HG21	21:C:183:PRO:HD3	1.82	0.61
7:L:164:ARG:HD2	7:L:199:LEU:HD23	1.82	0.61
26:Y:138:LEU:HD23	26:Y:176:ARG:HB2	1.82	0.61
17:B:313:LEU:HG	17:B:341:LEU:HD11	1.81	0.61
21:C:284:GLU:HG3	21:C:286:THR:H	1.66	0.61
12:Q:29:LYS:NZ	13:R:122:SER:O	2.31	0.61
23:V:321:ALA:HB1	23:V:322:VAL:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:252:LYS:HD3	25:X:287:LEU:HD21	1.81	0.61
18:D:392:TYR:HE1	19:E:161:ARG:HH22	1.49	0.61
5:J:137:ASP:N	5:J:141:THR:O	2.33	0.61
6:K:32:LYS:HD2	6:K:172:SER:HA	1.82	0.61
7:L:151:ALA:O	8:M:85:ARG:NH2	2.33	0.61
26:Y:145:LEU:HG	26:Y:160:ASN:HD21	1.65	0.61
7:L:33:SER:HB2	7:L:49:LEU:HB3	1.82	0.61
26:Y:357:ASN:HB2	26:Y:358:ARG:HA	1.83	0.61
17:B:404:LEU:HD12	21:C:163:GLU:HB2	1.83	0.60
20:F:247:THR:O	20:F:281:SER:OG	2.17	0.60
5:J:119:THR:HG22	5:J:126:PRO:HB3	1.83	0.60
4:I:14:PRO:HB3	5:J:21:TYR:CD2	2.35	0.60
23:V:379:LEU:HD13	23:V:395:ILE:HG12	1.83	0.60
18:D:169:GLY:HA3	18:D:173:GLN:HB3	1.82	0.60
9:N:19:ARG:NH1	9:N:168:GLY:O	2.33	0.60
10:O:142:PHE:HB2	10:O:154:LEU:HD21	1.83	0.60
13:R:91:LYS:NZ	13:R:117:GLU:OE1	2.31	0.60
24:W:219:THR:HA	24:W:220:GLU:HB2	1.82	0.60
17:B:390:LEU:HD13	17:B:432:GLU:HG3	1.83	0.60
21:C:213:ARG:NH2	21:C:249:ASP:OD2	2.34	0.60
5:J:115:LYS:HE2	5:J:149:PRO:HA	1.84	0.60
21:C:50:ASN:ND2	22:U:642:GLU:O	2.33	0.60
19:E:207:TYR:HB3	20:F:260:PHE:HB3	1.82	0.60
2:G:38:THR:H	2:G:53:GLN:HE22	1.47	0.60
17:B:361:LYS:HE2	17:B:390:LEU:H	1.67	0.60
11:P:153:LEU:HB3	11:P:166:THR:HG23	1.82	0.60
24:W:91:SER:HB2	24:W:92:LYS:HD2	1.82	0.60
17:B:294:ARG:NH1	17:B:297:SER:O	2.35	0.60
18:D:405:THR:HA	18:D:406:VAL:C	2.22	0.60
19:E:384:LEU:HD12	19:E:385:ASP:HA	1.82	0.60
20:F:362:ARG:NH2	20:F:388:THR:O	2.34	0.60
8:M:76:ALA:HB3	8:M:136:MET:HB2	1.83	0.60
25:X:203:PRO:HB3	25:X:206:LEU:HB2	1.83	0.60
16:A:123:VAL:HG22	16:A:124:ASP:O	2.02	0.60
17:B:383:LEU:O	17:B:387:LYS:NZ	2.34	0.60
20:F:433:ALA:HA	20:F:434:ASN:OD1	2.01	0.60
18:D:136:SER:HB3	21:C:67:GLN:HA	1.82	0.60
20:F:246:ALA:HB1	20:F:281:SER:HA	1.84	0.60
6:K:77:ALA:HB3	6:K:142:LEU:HB2	1.83	0.60
7:L:120:THR:O	8:M:129:ARG:NH1	2.35	0.60
27:Z:97:THR:HA	27:Z:124:ILE:HG13	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:18:GLU:HB2	6:K:19:GLY:HA2	1.83	0.60
23:V:252:ASN:ND2	23:V:284:GLU:OE2	2.29	0.60
20:F:257:VAL:HG22	20:F:306:VAL:HG21	1.83	0.59
9:N:5:ALA:HB3	9:N:126:ALA:HB3	1.83	0.59
14:S:27:THR:HB	14:S:40:SER:H	1.67	0.59
20:F:231:THR:OG1	20:F:233:LYS:NZ	2.27	0.59
3:H:231:ALA:H	3:H:232:ALA:HB3	1.67	0.59
6:K:143:PHE:HB2	6:K:154:PHE:HB2	1.82	0.59
19:E:305:ASN:O	19:E:309:ARG:N	2.28	0.59
7:L:107:ARG:NH2	15:T:79:ASP:OD2	2.35	0.59
22:U:742:HIS:HB2	22:U:883:ARG:HH12	1.68	0.59
21:C:255:GLY:H	21:C:256:SER:HB2	1.67	0.59
4:I:25:MET:HA	4:I:28:ILE:HD12	1.83	0.59
13:R:73:ARG:HH22	13:R:107:ARG:HG3	1.67	0.59
13:R:21:THR:HG22	13:R:27:ALA:H	1.68	0.59
25:X:242:ILE:HG22	25:X:243:ASP:H	1.67	0.59
16:A:357:ILE:HG13	16:A:360:ARG:HH21	1.68	0.59
20:F:280:PRO:HA	20:F:326:VAL:HG22	1.83	0.59
2:G:159:TYR:CG	18:D:418:LYS:HG3	2.37	0.59
4:I:20:GLN:HG2	4:I:129:PRO:HG3	1.84	0.59
22:U:237:VAL:HG13	22:U:321:GLN:HG3	1.82	0.59
27:Z:202:ASN:OD1	27:Z:203:SER:N	2.35	0.59
27:Z:245:PHE:O	27:Z:249:PHE:N	2.35	0.59
16:A:399:ALA:HB3	16:A:401:ARG:HE	1.68	0.59
18:D:163:MET:HG3	18:D:165:ALA:H	1.68	0.59
20:F:96:LEU:HB3	20:F:122:ALA:HA	1.83	0.59
20:F:409:ARG:HG3	20:F:410:ARG:HA	1.83	0.59
3:H:166:ASN:O	3:H:170:GLY:N	2.27	0.59
22:U:424:ALA:HA	22:U:427:LEU:HD13	1.84	0.59
24:W:66:ILE:HG23	24:W:67:LEU:HB2	1.83	0.59
9:N:144:ARG:H	9:N:147:MET:HE3	1.66	0.59
11:P:49:LEU:HG	11:P:111:GLY:HA3	1.85	0.59
23:V:237:THR:OG1	23:V:241:ARG:NH2	2.34	0.59
16:A:172:VAL:HG12	16:A:223:THR:HG23	1.83	0.59
19:E:269:THR:HG1	19:E:271:HIS:HD1	1.50	0.59
2:G:22:LEU:HD13	2:G:25:VAL:HB	1.83	0.59
4:I:31:ALA:O	4:I:50:ARG:NH2	2.36	0.59
13:R:97:MET:H	13:R:116:SER:HB3	1.68	0.59
6:K:104:ASN:ND2	14:S:86:GLY:O	2.36	0.59
23:V:323:GLY:HA2	23:V:326:GLN:HB2	1.83	0.59
27:Z:102:HIS:HD2	27:Z:104:ASN:HB3	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:87:VAL:HG11	21:C:116:LEU:HD13	1.84	0.59
20:F:280:PRO:HD3	20:F:325:GLN:HE21	1.66	0.59
26:Y:111:LEU:HA	26:Y:114:ILE:HD13	1.83	0.59
21:C:245:ILE:HG23	21:C:290:LYS:HB2	1.85	0.58
7:L:39:LYS:HD3	7:L:144:ILE:HG12	1.85	0.58
22:U:505:ASP:HB3	22:U:508:THR:HG22	1.84	0.58
25:X:354:ILE:HG21	25:X:361:VAL:HG11	1.85	0.58
23:V:173:ILE:O	23:V:177:ASN:ND2	2.35	0.58
21:C:119:ASP:OD1	21:C:119:ASP:N	2.37	0.58
22:U:474:ARG:HH21	22:U:500:ASN:HB2	1.68	0.58
23:V:349:ARG:HG3	23:V:357:LEU:HD21	1.85	0.58
24:W:13:ILE:HG22	24:W:54:THR:HG21	1.85	0.58
26:Y:190:ALA:O	26:Y:291:HIS:NE2	2.35	0.58
27:Z:96:HIS:HE1	27:Z:121:LEU:HD13	1.68	0.58
19:E:354:ALA:HB1	19:E:362:VAL:HG21	1.83	0.58
8:M:99:ARG:O	15:T:65:GLN:NE2	2.34	0.58
10:O:133:ALA:HB3	10:O:162:GLY:HA2	1.86	0.58
22:U:637:VAL:HG13	22:U:652:ALA:HB1	1.85	0.58
16:A:183:GLN:NE2	16:A:342:GLU:O	2.36	0.58
2:G:53:GLN:HA	2:G:215:ILE:HA	1.84	0.58
22:U:610:VAL:HG11	27:Z:177:ARG:HG3	1.86	0.58
5:J:137:ASP:OD1	5:J:143:ARG:NE	2.34	0.58
12:Q:148:THR:HB	12:Q:151:ILE:HB	1.86	0.58
22:U:14:GLU:O	22:U:20:LYS:NZ	2.37	0.58
23:V:337:LEU:O	23:V:401:ASN:ND2	2.37	0.58
25:X:414:LEU:HD23	25:X:417:LYS:HD2	1.83	0.58
26:Y:51:ALA:HB2	26:Y:116:ASP:H	1.68	0.58
21:C:42:LEU:HD13	27:Z:168:GLU:HA	40.39	0.58
16:A:351:ARG:HH11	16:A:379:ASN:H	1.52	0.58
21:C:14:GLY:O	21:C:18:SER:N	2.27	0.58
8:M:15:SER:OG	8:M:19:ARG:O	2.22	0.58
23:V:211:TYR:HB3	23:V:253:LEU:HD11	1.85	0.58
23:V:357:LEU:O	23:V:361:PHE:N	2.37	0.58
8:M:99:ARG:HB3	15:T:69:GLN:HE22	1.68	0.58
23:V:326:GLN:HB3	23:V:353:LEU:HD22	1.86	0.58
26:Y:179:ARG:NH2	26:Y:212:GLU:OE2	2.34	0.58
18:D:385:LEU:HD22	18:D:402:ALA:HB2	1.86	0.57
26:Y:194:PHE:HB3	26:Y:230:ALA:HB2	1.84	0.57
21:C:13:GLU:N	21:C:14:GLY:HA3	2.18	0.57
2:G:37:LEU:HD23	2:G:81:THR:HA	1.84	0.57
6:K:16:SER:HB3	6:K:20:ARG:H	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:96:LEU:HA	12:Q:62:LYS:HE2	1.86	0.57
22:U:215:ASN:OD1	22:U:216:VAL:N	2.36	0.57
25:X:223:LYS:NZ	26:Y:242:LYS:O	2.36	0.57
26:Y:192:ARG:NH2	26:Y:291:HIS:O	2.37	0.57
26:Y:301:ILE:HD12	26:Y:342:ARG:HB3	1.85	0.57
17:B:274:ALA:O	17:B:278:ALA:N	2.38	0.57
18:D:200:ARG:HE	18:D:305:VAL:HG11	1.70	0.57
2:G:119:ALA:HA	2:G:122:SER:HB2	1.87	0.57
4:I:154:GLY:O	5:J:81:ARG:NH1	2.37	0.57
13:R:12:VAL:H	13:R:179:VAL:HB	1.68	0.57
22:U:220:LEU:HD11	22:U:252:LEU:HD13	1.85	0.57
23:V:283:ASN:HB2	23:V:317:PRO:HD2	1.87	0.57
21:C:167:LEU:HD11	21:C:174:LEU:HD11	1.86	0.57
21:C:151:ILE:HD12	21:C:198:LEU:HB3	1.87	0.57
18:D:283:ARG:HE	21:C:222:LYS:HD3	1.69	0.57
18:D:179:GLU:HA	18:D:183:LEU:HD22	1.85	0.57
8:M:149:TYR:HD1	8:M:159:GLY:HA3	1.70	0.57
8:M:35:THR:HA	8:M:166:GLY:HA3	1.86	0.57
17:B:131:HIS:NE2	17:B:156:VAL:O	2.37	0.57
18:D:196:ILE:HD13	21:C:367:GLY:HA3	1.86	0.57
21:C:89:VAL:HG12	21:C:91:PRO:HD2	1.87	0.57
3:H:222:THR:OG1	3:H:225:GLU:OE1	2.22	0.57
4:I:13:SER:C	5:J:21:TYR:CE1	2.77	0.57
8:M:54:LEU:H	8:M:57:LEU:HD11	1.69	0.57
10:O:100:LEU:HB2	10:O:113:ILE:HD11	1.86	0.57
27:Z:138:TYR:HB3	27:Z:155:PHE:HB3	1.85	0.57
16:A:406:GLU:H	16:A:407:LYS:HB3	1.69	0.57
17:B:106:PRO:O	17:B:154:HIS:NE2	2.38	0.57
18:D:202:VAL:HB	18:D:308:ILE:HA	1.86	0.57
18:D:389:GLU:HB3	18:D:391:ARG:N	2.20	0.57
20:F:94:ILE:HB	20:F:123:VAL:HB	1.86	0.57
2:G:86:ASP:HB2	2:G:136:CYS:HB3	1.87	0.57
4:I:86:LEU:HD22	4:I:114:LEU:HD11	1.87	0.57
23:V:483:CYS:HA	23:V:486:ILE:HD12	1.87	0.57
16:A:339:ARG:NH2	20:F:402:GLU:OE1	2.38	0.57
12:Q:168:GLN:NE2	12:Q:174:ASN:O	2.38	0.57
14:S:35:ILE:O	15:T:151:ARG:NH2	2.37	0.57
24:W:136:ILE:H	24:W:141:GLU:HG2	1.70	0.57
24:W:440:ASN:O	24:W:443:THR:OG1	2.16	0.57
26:Y:68:ASP:HA	26:Y:71:ASN:HB2	1.85	0.57
17:B:219:PRO:O	17:B:346:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:62:SER:OG	4:I:65:ILE:O	2.18	0.56
8:M:15:SER:OG	8:M:17:ASP:OD1	2.17	0.56
15:T:112:ILE:O	15:T:123:GLY:N	2.35	0.56
24:W:223:LYS:HA	24:W:226:TYR:HB3	1.86	0.56
24:W:235:GLN:NE2	24:W:247:TYR:OH	2.37	0.56
19:E:97:ARG:HD2	19:E:111:LEU:HD11	1.88	0.56
3:H:34:PRO:HB3	3:H:165:LYS:H	1.70	0.56
18:D:388:ARG:O	18:D:390:ASN:ND2	2.38	0.56
19:E:241:ARG:HG2	19:E:243:PHE:H	1.71	0.56
3:H:46:LEU:O	3:H:211:GLY:N	2.33	0.56
4:I:83:ALA:HB2	4:I:132:VAL:HG11	1.87	0.56
22:U:800:VAL:HG21	22:U:914:LEU:HD21	1.86	0.56
25:X:255:LEU:HD12	25:X:287:LEU:HB3	1.88	0.56
27:Z:113:LYS:NZ	27:Z:117:PRO:O	2.31	0.56
14:S:46:LEU:HB3	14:S:72:LEU:HD11	1.88	0.56
24:W:44:ILE:HB	24:W:93:ARG:HD2	1.88	0.56
18:D:354:LEU:HA	18:D:355:SER:C	2.24	0.56
19:E:56:ILE:O	19:E:100:LEU:N	2.37	0.56
11:P:190:ILE:HG22	11:P:195:ILE:HG23	1.86	0.56
24:W:125:ILE:HD12	24:W:128:LEU:HD12	1.86	0.56
26:Y:13:LYS:O	26:Y:17:LEU:N	2.35	0.56
18:D:88:VAL:N	18:D:132:LEU:O	2.29	0.56
3:H:50:LYS:NZ	3:H:62:VAL:O	2.38	0.56
24:W:92:LYS:N	24:W:93:ARG:HB3	2.19	0.56
21:C:184:LYS:HD3	21:C:280:LEU:HB2	1.88	0.56
24:W:151:THR:O	24:W:155:GLN:NE2	2.38	0.56
15:T:136:SER:HB2	15:T:150:LEU:HD13	1.88	0.56
22:U:82:LEU:O	22:U:129:ARG:NE	2.39	0.56
22:U:522:GLY:O	22:U:559:ARG:NH2	2.39	0.56
23:V:148:ARG:HH22	23:V:193:GLN:HB2	1.71	0.56
23:V:415:SER:O	23:V:460:SER:OG	2.22	0.56
16:A:333:ARG:O	16:A:337:LEU:N	2.39	0.56
4:I:99:LEU:O	12:Q:86:ARG:NH2	2.39	0.56
25:X:258:LYS:HD3	25:X:267:VAL:HG22	1.88	0.56
16:A:140:VAL:HG12	16:A:152:PRO:HB3	1.88	0.56
16:A:210:LYS:HA	16:A:316:LYS:HG2	1.88	0.56
17:B:191:ASP:HA	17:B:194:ILE:HG22	1.88	0.56
18:D:251:PHE:HB3	18:D:299:PHE:HZ	1.70	0.56
20:F:415:LEU:HD23	20:F:416:THR:HG22	1.87	0.56
15:T:49:THR:HA	15:T:114:GLY:HA3	1.88	0.56
26:Y:174:TRP:O	26:Y:178:ASN:ND2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:248:MET:HG3	21:C:269:VAL:HG11	1.88	0.56
20:F:293:THR:HA	20:F:337:ILE:HG21	1.88	0.56
3:H:46:LEU:HD13	3:H:75:VAL:HG22	1.88	0.56
5:J:81:ARG:O	5:J:85:ASN:ND2	2.39	0.56
6:K:101:PHE:HA	13:R:57:ARG:HH21	1.70	0.56
7:L:152:ASN:HA	8:M:85:ARG:HH22	1.70	0.56
10:O:163:ILE:HG12	10:O:169:SER:HB3	1.88	0.56
22:U:799:LYS:HA	22:U:843:GLU:HG3	1.88	0.56
18:D:381:GLU:HA	18:D:384:MET:HB2	1.88	0.55
3:H:22:ILE:HG23	3:H:129:PRO:HB3	1.86	0.55
4:I:14:PRO:N	5:J:21:TYR:CZ	2.74	0.55
11:P:189:ILE:HG23	11:P:196:THR:HB	1.88	0.55
13:R:18:SER:OG	13:R:173:ALA:N	2.35	0.55
7:L:91:GLU:HB3	7:L:108:LEU:HD11	1.87	0.55
15:T:114:GLY:HA2	15:T:192:VAL:HG21	1.88	0.55
22:U:94:SER:OG	22:U:95:GLU:OE1	2.24	0.55
23:V:447:ILE:HG13	23:V:449:ALA:H	1.71	0.55
23:V:81:GLN:HB3	23:V:83:GLU:N	2.21	0.55
24:W:40:LEU:HB2	24:W:41:GLN:CA	2.32	0.55
17:B:182:GLU:HB2	17:B:239:VAL:HG21	1.87	0.55
18:D:208:PRO:HB2	18:D:375:ILE:HG12	1.88	0.55
19:E:182:LEU:HD21	33:E:401:ATP:H2'	1.88	0.55
20:F:92:ASN:HB3	20:F:125:LYS:HB2	1.88	0.55
22:U:73:ALA:HB1	22:U:76:GLU:HB3	1.89	0.55
17:B:284:ILE:HB	17:B:329:MET:HA	1.88	0.55
22:U:792:ASN:OD1	22:U:793:LYS:N	2.39	0.55
27:Z:224:HIS:CG	27:Z:225:GLN:HA	2.41	0.55
3:H:40:ALA:HB1	3:H:184:LEU:HA	1.89	0.55
12:Q:100:VAL:H	12:Q:120:TYR:HB3	1.71	0.55
18:D:376:ASN:HD22	19:E:291:ARG:HH21	1.55	0.55
15:T:54:SER:HB2	15:T:109:THR:HB	1.89	0.55
27:Z:186:THR:HG23	27:Z:187:LEU:H	1.71	0.55
17:B:116:ILE:HG22	17:B:118:ASP:H	1.72	0.55
18:D:283:ARG:HH11	21:C:222:LYS:HB2	1.70	0.55
4:I:15:GLU:O	5:J:28:LYS:NZ	2.37	0.55
8:M:34:SER:OG	8:M:65:ARG:NH2	2.39	0.55
12:Q:107:TYR:HA	12:Q:113:PRO:HA	1.88	0.55
23:V:241:ARG:HG3	23:V:242:HIS:H	1.72	0.55
2:G:47:CYS:HB3	2:G:221:THR:HG23	1.89	0.55
6:K:52:LYS:NZ	6:K:215:ILE:O	2.39	0.55
24:W:220:GLU:N	24:W:221:LYS:HA	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:165:ILE:HG23	21:C:207:THR:HG23	1.88	0.55
8:M:37:ILE:HD11	8:M:193:VAL:HG13	1.88	0.55
10:O:209:THR:OG1	11:P:169:GLN:NE2	2.40	0.55
21:C:21:ARG:HH22	22:U:106:ASP:HB2	1.71	0.55
23:V:322:VAL:HG13	23:V:323:GLY:H	1.72	0.55
2:G:63:SER:O	2:G:67:THR:OG1	2.17	0.55
7:L:137:TYR:HE1	7:L:215:VAL:HG13	1.72	0.55
12:Q:55:GLN:HE21	13:R:85:ASN:HD22	1.54	0.55
22:U:612:ASP:HA	22:U:615:ARG:HD3	1.89	0.55
23:V:54:LYS:N	23:V:55:THR:OG1	2.40	0.55
13:R:179:VAL:HA	13:R:184:TRP:HA	1.89	0.54
23:V:62:HIS:HA	23:V:65:ARG:HB3	1.89	0.54
17:B:386:ALA:O	17:B:429:LYS:NZ	2.40	0.54
19:E:269:THR:OG1	19:E:271:HIS:ND1	2.36	0.54
4:I:218:ARG:NH1	4:I:223:THR:OG1	2.39	0.54
13:R:167:ASP:HB3	13:R:170:SER:HB2	1.89	0.54
17:B:99:VAL:HA	17:B:102:LEU:HD13	1.89	0.54
15:T:92:LEU:HG	15:T:125:VAL:HG11	1.90	0.54
15:T:8:GLY:HA3	15:T:55:GLY:H	1.73	0.54
22:U:772:TRP:HB3	22:U:775:LEU:HG	1.90	0.54
24:W:186:ILE:O	24:W:189:GLN:NE2	2.40	0.54
18:D:336:PRO:HG2	18:D:375:ILE:HD11	1.89	0.54
19:E:61:LEU:HD11	19:E:72:LYS:HB2	1.90	0.54
20:F:89:LEU:HB3	20:F:153:VAL:HG13	1.89	0.54
2:G:96:TYR:O	2:G:100:ASN:ND2	2.41	0.54
7:L:69:HIS:HE2	7:L:102:PRO:HB2	1.72	0.54
22:U:380:THR:HG23	22:U:382:SER:H	1.72	0.54
16:A:176:ASP:HA	16:A:357:ILE:HD13	1.90	0.54
4:I:143:TYR:HB2	4:I:146:GLN:HE21	1.73	0.54
5:J:88:ARG:NH2	12:Q:66:LEU:O	2.40	0.54
8:M:123:THR:HG22	8:M:130:PRO:HB3	1.90	0.54
16:A:94:GLN:HE22	17:B:157:HIS:HB2	1.72	0.54
18:D:401:LYS:HA	18:D:404:LYS:HE2	1.90	0.54
7:L:72:ILE:HG22	7:L:134:ILE:HA	1.90	0.54
22:U:242:LEU:HB2	22:U:793:LYS:HD2	1.88	0.54
26:Y:92:GLU:HA	26:Y:100:ILE:HD13	1.90	0.54
17:B:110:GLY:H	17:B:152:LEU:HD13	1.72	0.54
17:B:220:LYS:HD3	17:B:346:ARG:HH21	1.71	0.54
20:F:431:LYS:HA	20:F:432:LYS:HB3	1.89	0.54
8:M:66:LEU:HD13	8:M:214:SER:HB2	1.90	0.54
22:U:173:VAL:HG13	22:U:176:MET:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:69:ASN:OD1	4:I:70:GLU:N	2.41	0.54
13:R:164:THR:HG22	13:R:170:SER:HB3	1.90	0.54
27:Z:225:GLN:HB2	27:Z:228:TYR:CE1	2.43	0.54
17:B:345:GLY:HA3	17:B:346:ARG:HD2	1.90	0.54
21:C:187:LEU:HD21	21:C:307:ARG:HB2	1.90	0.54
19:E:165:ILE:HD12	19:E:166:PRO:HD2	1.89	0.54
22:U:494:TYR:OH	22:U:531:ASP:OD2	2.25	0.54
22:U:740:GLY:HA3	22:U:744:VAL:HG22	1.90	0.54
17:B:105:THR:HG23	17:B:106:PRO:HD3	1.89	0.53
19:E:353:PHE:HA	19:E:356:ARG:HD3	1.89	0.53
2:G:184:LYS:HA	2:G:185:LYS:C	2.29	0.53
23:V:259:LEU:HD21	23:V:294:ARG:HD2	1.90	0.53
17:B:139:VAL:HA	17:B:140:ASP:HB3	1.90	0.53
9:N:127:ILE:O	15:T:35:ARG:NH2	2.41	0.53
23:V:30:PRO:HA	23:V:33:GLN:HB2	1.89	0.53
24:W:56:THR:HG21	24:W:103:LYS:HE3	1.91	0.53
2:G:86:ASP:OD1	8:M:120:HIS:NE2	2.41	0.53
3:H:19:LEU:O	3:H:23:GLU:HB2	2.08	0.53
4:I:26:GLU:O	4:I:30:HIS:ND1	2.30	0.53
8:M:99:ARG:HD3	8:M:103:GLY:HA2	1.90	0.53
17:B:397:ALA:HB3	21:C:311:ILE:HD12	1.90	0.53
18:D:72:PHE:HD2	21:C:49:ARG:HH21	1.56	0.53
18:D:151:ILE:HB	18:D:152:MET:HA	1.91	0.53
2:G:34:GLN:NE2	8:M:17:ASP:O	2.41	0.53
22:U:384:GLN:HG2	22:U:385:PHE:H	1.73	0.53
23:V:59:ALA:N	23:V:60:ALA:HB3	2.24	0.53
24:W:66:ILE:HD13	24:W:67:LEU:HD13	1.90	0.53
27:Z:33:LYS:HD3	27:Z:60:GLU:N	2.24	0.53
16:A:164:MET:HE3	17:B:319:PHE:HD2	1.73	0.53
8:M:100:SER:O	15:T:65:GLN:NE2	2.41	0.53
22:U:126:ILE:HG23	22:U:130:LEU:HD11	1.89	0.53
18:D:149:SER:HB3	19:E:61:LEU:HD13	1.90	0.53
20:F:172:VAL:HG21	20:F:266:LYS:HE3	1.91	0.53
8:M:195:LYS:HD2	8:M:241:GLU:HB2	1.91	0.53
27:Z:102:HIS:CD2	27:Z:104:ASN:HB3	2.44	0.53
27:Z:37:GLY:HA2	27:Z:56:VAL:HG12	1.90	0.53
17:B:133:VAL:HG11	17:B:159:VAL:HG12	1.91	0.53
2:G:179:LEU:HA	2:G:182:LYS:HB3	1.90	0.53
4:I:73:ALA:HB3	4:I:137:ILE:HD11	1.91	0.53
23:V:319:HIS:HB2	23:V:320:THR:HA	1.91	0.53
25:X:194:ARG:HD2	25:X:210:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:225:MET:HG2	20:F:233:LYS:HD2	1.90	0.53
3:H:150:ASP:OD2	3:H:152:SER:OG	2.26	0.53
23:V:441:ALA:HB1	23:V:446:VAL:HB	1.91	0.53
24:W:135:LYS:HB3	24:W:136:ILE:HB	1.90	0.53
26:Y:251:HIS:HA	26:Y:257:ARG:HD3	1.90	0.53
16:A:244:GLU:OE2	17:B:314:ASN:ND2	2.42	0.53
24:W:178:GLU:OE1	24:W:181:GLU:N	2.42	0.53
24:W:5:GLY:HA2	24:W:34:LEU:HD13	1.90	0.53
8:M:231:ILE:O	8:M:232:ARG:HG2	2.08	0.53
11:P:36:THR:OG1	11:P:38:ASP:OD1	2.22	0.53
12:Q:38:MET:O	12:Q:65:GLN:NE2	2.42	0.53
22:U:808:PRO:HD3	22:U:836:THR:HB	1.90	0.53
23:V:47:SER:HA	23:V:50:GLU:HB2	1.91	0.53
24:W:135:LYS:HB3	24:W:136:ILE:C	2.30	0.53
16:A:95:VAL:HB	16:A:144:ARG:H	1.74	0.52
20:F:391:PHE:CE2	20:F:424:ILE:HG23	2.44	0.52
2:G:172:GLN:OE1	2:G:172:GLN:N	2.40	0.52
11:P:11:VAL:HG11	11:P:52:GLY:HA3	1.90	0.52
12:Q:43:LEU:HD12	12:Q:183:ILE:HD11	1.91	0.52
12:Q:38:MET:HG3	12:Q:44:LEU:HB2	1.92	0.52
22:U:265:ILE:HG23	22:U:269:ARG:HH12	1.74	0.52
17:B:278:ALA:HB1	17:B:279:PRO:HA	1.92	0.52
20:F:153:VAL:HG23	20:F:158:TYR:HA	1.91	0.52
7:L:82:ARG:O	7:L:86:ASN:ND2	2.41	0.52
7:L:84:LEU:O	7:L:88:MET:N	2.42	0.52
12:Q:41:LYS:O	12:Q:107:TYR:N	2.43	0.52
22:U:446:LEU:O	22:U:450:HIS:ND1	2.38	0.52
22:U:497:LEU:HD23	22:U:516:LEU:HB2	1.91	0.52
21:C:90:HIS:HB2	21:C:91:PRO:HD3	1.91	0.52
20:F:124:ILE:O	20:F:132:TYR:N	2.36	0.52
7:L:196:ARG:HE	7:L:239:ARG:HH21	1.55	0.52
22:U:803:LYS:HA	22:U:839:ALA:H	1.74	0.52
24:W:187:LEU:HD22	24:W:226:TYR:CD1	2.45	0.52
24:W:372:ARG:HG2	24:W:414:ASN:HB3	1.92	0.52
26:Y:102:ASP:HA	26:Y:105:MET:HG2	1.91	0.52
26:Y:14:ASN:HA	26:Y:17:LEU:HB3	1.91	0.52
16:A:161:VAL:HG13	16:A:162:THR:HG23	1.92	0.52
17:B:286:GLU:N	17:B:330:ALA:O	2.43	0.52
18:D:54:LEU:HA	18:D:57:GLN:HB2	1.90	0.52
20:F:327:LYS:H	20:F:327:LYS:HD2	1.74	0.52
7:L:39:LYS:HE2	7:L:157:ARG:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:738:ASP:OD1	22:U:742:HIS:NE2	2.42	0.52
27:Z:222:ILE:HG23	27:Z:224:HIS:HB2	1.90	0.52
18:D:341:LYS:NZ	18:D:374:ASP:O	2.28	0.52
2:G:155:ASP:HB2	18:D:418:LYS:HE2	1.91	0.52
18:D:53:PHE:HB3	22:U:632:GLN:HE22	1.74	0.52
20:F:74:LYS:O	20:F:78:GLU:N	2.38	0.52
5:J:36:ARG:HE	5:J:157:LYS:HA	1.73	0.52
7:L:204:ASP:HA	7:L:205:LEU:HB3	1.92	0.52
8:M:56:LYS:H	8:M:57:LEU:HA	1.74	0.52
9:N:18:SER:HB2	9:N:30:VAL:HA	1.90	0.52
22:U:643:SER:O	22:U:649:ARG:NH1	2.38	0.52
18:D:47:LEU:HB2	21:C:25:LEU:HD23	1.92	0.52
20:F:91:SER:OG	20:F:124:ILE:HG23	2.10	0.52
10:O:51:ASP:HB3	10:O:94:ILE:HG23	1.92	0.52
15:T:5:MET:HB3	15:T:30:TYR:HE1	1.72	0.52
22:U:203:LYS:O	22:U:207:ASN:ND2	2.43	0.52
23:V:349:ARG:HH11	23:V:354:LYS:HB2	1.74	0.52
16:A:100:LYS:HB3	16:A:115:VAL:HG23	1.92	0.52
20:F:314:LEU:HD11	20:F:342:LEU:HD23	1.91	0.52
5:J:195:LEU:O	5:J:201:SER:OG	2.21	0.52
5:J:66:ASP:OD1	5:J:67:ASP:N	2.40	0.52
7:L:215:VAL:HB	7:L:221:PHE:HD1	1.75	0.52
14:S:166:LEU:HA	14:S:170:ARG:HD3	1.92	0.52
22:U:623:GLY:HA2	22:U:659:CYS:HB2	1.91	0.52
23:V:302:TYR:HB3	23:V:339:LEU:HD23	1.92	0.52
24:W:312:MET:SD	24:W:361:HIS:ND1	2.83	0.52
18:D:200:ARG:HH21	18:D:296:MET:HE2	1.75	0.52
7:L:104:PRO:HB3	7:L:138:ASP:HB3	1.91	0.52
14:S:4:PRO:O	15:T:100:ARG:NH2	2.42	0.52
23:V:56:ALA:O	23:V:59:ALA:HB3	2.10	0.52
17:B:170:LEU:HD13	17:B:255:LEU:HD21	1.92	0.52
17:B:265:LYS:O	17:B:269:GLU:N	2.32	0.52
19:E:312:ILE:HD11	33:E:401:ATP:HN62	1.75	0.52
23:V:197:THR:HG21	23:V:200:ARG:HG3	1.92	0.52
23:V:372:LEU:H	23:V:427:GLN:NE2	2.08	0.52
26:Y:330:ILE:HA	26:Y:333:GLU:HB3	1.92	0.52
26:Y:356:THR:HA	26:Y:357:ASN:CG	2.29	0.52
27:Z:182:THR:N	27:Z:183:THR:HA	2.25	0.52
18:D:218:ALA:O	18:D:222:HIS:ND1	2.36	0.52
19:E:171:LEU:N	19:E:297:ARG:O	2.38	0.52
20:F:249:LEU:HB2	20:F:283:ILE:HG13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:231:ALA:N	3:H:232:ALA:HB3	2.25	0.52
22:U:154:ALA:HB2	22:U:166:THR:HG21	1.91	0.52
22:U:483:LEU:HD11	22:U:781:LEU:HD11	1.91	0.52
23:V:404:LYS:HA	23:V:407:VAL:HG12	1.91	0.52
17:B:400:THR:O	17:B:404:LEU:N	2.39	0.51
21:C:232:ARG:O	21:C:236:VAL:N	2.34	0.51
6:K:209:LYS:O	6:K:214:ASN:ND2	2.43	0.51
10:O:50:ALA:HB2	11:P:129:CYS:HB2	1.90	0.51
9:N:164:MET:HB3	9:N:171:GLY:HA2	1.91	0.51
10:O:213:THR:HG22	10:O:214:GLU:H	1.75	0.51
14:S:169:ASP:OD2	14:S:173:ARG:NH2	2.44	0.51
22:U:510:GLU:OE2	22:U:546:ARG:NH2	2.43	0.51
27:Z:68:TRP:CD2	27:Z:108:ILE:HG13	2.45	0.51
16:A:164:MET:HG2	17:B:264:PRO:HD2	1.92	0.51
16:A:334:PRO:HB3	20:F:398:ALA:HB2	1.92	0.51
22:U:208:LEU:HD23	22:U:210:LYS:H	1.75	0.51
23:V:98:LEU:HD12	23:V:107:ARG:HH21	1.76	0.51
25:X:251:LEU:HA	25:X:254:MET:HG2	1.92	0.51
17:B:193:GLN:NE2	17:B:352:GLU:O	2.44	0.51
18:D:113:VAL:HA	21:C:66:LEU:HD11	1.92	0.51
18:D:64:GLU:HB2	22:U:603:LEU:HD11	1.92	0.51
6:K:36:THR:HA	6:K:171:GLY:HA3	1.91	0.51
6:K:45:GLY:HA3	6:K:221:GLN:HG3	1.92	0.51
22:U:154:ALA:HB1	22:U:163:PHE:HD1	1.74	0.51
17:B:232:LYS:HB3	21:C:278:ASN:HD22	1.76	0.51
21:C:321:ASN:OD1	21:C:322:GLU:N	2.42	0.51
4:I:156:TYR:HE1	5:J:58:THR:HB	1.75	0.51
5:J:77:THR:HA	5:J:80:ALA:HB3	1.92	0.51
6:K:74:ILE:HG12	6:K:109:VAL:HG22	1.93	0.51
11:P:155:GLU:HB2	11:P:158:MET:HG2	1.93	0.51
24:W:359:VAL:O	24:W:363:ILE:HG12	2.11	0.51
19:E:109:ARG:NH1	20:F:98:ASP:OD2	2.40	0.51
19:E:357:ALA:O	19:E:359:HIS:ND1	2.43	0.51
5:J:9:VAL:HG21	6:K:12:VAL:HG11	1.93	0.51
5:J:97:THR:HA	13:R:81:LYS:HG2	1.92	0.51
23:V:101:LEU:HB3	23:V:102:PRO:HD2	1.90	0.51
23:V:179:LYS:HD2	23:V:214:HIS:CE1	2.45	0.51
23:V:416:ARG:HH12	23:V:418:SER:HB2	1.75	0.51
25:X:225:TRP:HB3	25:X:261:LEU:HG	1.93	0.51
16:A:95:VAL:HB	16:A:143:ASP:HA	1.91	0.51
20:F:281:SER:H	20:F:326:VAL:HG13	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:90:LEU:HD12	4:I:114:LEU:HB2	1.93	0.51
11:P:175:VAL:HG13	11:P:181:SER:HB3	1.92	0.51
22:U:570:LEU:HD22	22:U:578:LEU:HD11	1.93	0.51
24:W:139:GLU:HG2	24:W:142:ARG:HD2	1.92	0.51
24:W:366:MET:HB3	24:W:370:TYR:CE2	2.45	0.51
16:A:210:LYS:HG2	16:A:336:ARG:HH11	1.76	0.51
17:B:305:ILE:HA	17:B:308:THR:HG22	1.93	0.51
20:F:406:ILE:HG22	20:F:410:ARG:HH21	1.76	0.51
2:G:52:THR:HG22	2:G:53:GLN:H	1.75	0.51
8:M:31:GLU:OE1	8:M:169:ARG:NH1	2.44	0.51
11:P:169:GLN:O	11:P:173:ASN:ND2	2.35	0.51
13:R:191:ASN:OD1	13:R:192:VAL:N	2.44	0.51
22:U:748:LEU:HD23	22:U:760:VAL:HG22	1.92	0.51
5:J:154:HIS:CE1	6:K:59:MET:HG3	2.45	0.51
5:J:11:SER:OG	5:J:15:HIS:O	2.29	0.51
10:O:7:VAL:HG22	10:O:12:ILE:HG12	1.91	0.51
15:T:51:LEU:HD11	15:T:110:MET:HB3	1.93	0.51
23:V:33:GLN:HB3	23:V:115:LYS:HD3	1.93	0.51
26:Y:74:LYS:HA	26:Y:77:ASN:HB3	1.92	0.51
11:P:54:ALA:HB3	11:P:106:GLU:HB2	1.93	0.51
23:V:372:LEU:HD13	23:V:427:GLN:HE21	1.76	0.51
25:X:356:LEU:HD13	25:X:359:ALA:HB3	1.93	0.51
17:B:264:PRO:HG3	17:B:315:GLN:HA	1.92	0.50
18:D:186:THR:HG23	18:D:187:HIS:H	1.76	0.50
5:J:20:GLU:N	5:J:20:GLU:OE1	2.40	0.50
11:P:135:ASP:N	11:P:135:ASP:OD1	2.43	0.50
12:Q:17:SER:OG	12:Q:179:SER:OG	2.22	0.50
22:U:112:CYS:SG	22:U:159:ARG:NH1	2.84	0.50
23:V:101:LEU:O	23:V:103:SER:N	2.44	0.50
23:V:294:ARG:HH21	23:V:331:LEU:HD23	1.76	0.50
17:B:189:GLY:HA3	17:B:360:THR:HG23	1.94	0.50
21:C:245:ILE:HG22	21:C:246:ILE:H	1.74	0.50
5:J:11:SER:OG	5:J:13:ASP:OD1	2.19	0.50
9:N:173:VAL:HG23	9:N:190:LEU:HB3	1.93	0.50
13:R:73:ARG:NH2	13:R:105:ASP:OD1	2.43	0.50
21:C:50:ASN:HD21	22:U:643:SER:HA	1.76	0.50
23:V:234:ARG:HG3	23:V:250:LEU:HD11	1.92	0.50
25:X:360:ASP:OD1	25:X:361:VAL:N	2.44	0.50
19:E:285:LEU:HB3	19:E:289:LEU:HB2	1.93	0.50
19:E:55:GLN:O	20:F:133:PHE:N	2.36	0.50
3:H:38:ILE:N	3:H:45:VAL:O	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:48:GLU:H	4:I:64:LYS:HD2	1.77	0.50
15:T:138:ALA:HB3	15:T:147:GLN:HB2	1.92	0.50
15:T:153:VAL:HG21	15:T:168:LEU:HD11	1.94	0.50
23:V:200:ARG:O	23:V:204:ASP:N	2.39	0.50
24:W:431:LYS:O	24:W:435:LEU:HB2	2.10	0.50
26:Y:144:LEU:HD22	26:Y:160:ASN:HB3	1.93	0.50
17:B:109:VAL:HG22	17:B:151:LEU:HD23	1.93	0.50
21:C:229:ARG:HH11	21:C:232:ARG:HD2	1.77	0.50
9:N:63:LEU:O	9:N:67:SER:N	2.43	0.50
12:Q:85:ARG:HA	12:Q:88:LEU:HB2	1.93	0.50
14:S:28:ARG:NH2	14:S:211:ARG:O	2.44	0.50
24:W:221:LYS:HG3	24:W:224:LEU:HB2	1.93	0.50
26:Y:191:ILE:HG13	26:Y:192:ARG:H	1.76	0.50
18:D:45:LYS:O	18:D:48:GLN:NE2	2.45	0.50
18:D:83:GLN:HE21	18:D:87:LEU:HD21	1.76	0.50
19:E:180:LYS:HG3	19:E:181:THR:H	1.77	0.50
12:Q:44:LEU:HD21	12:Q:57:ALA:HA	1.93	0.50
23:V:362:LEU:HB3	23:V:382:PHE:HE2	1.77	0.50
23:V:474:LEU:HA	23:V:477:HIS:HD2	1.77	0.50
26:Y:66:ASP:HB3	26:Y:70:LEU:HD12	1.92	0.50
27:Z:241:SER:HB2	27:Z:242:LEU:HD12	1.93	0.50
16:A:333:ARG:HH22	16:A:340:LYS:HD3	1.76	0.50
19:E:130:VAL:O	19:E:134:GLU:HG2	2.12	0.50
4:I:234:GLU:HA	4:I:237:ILE:HD12	1.93	0.50
9:N:103:TRP:HA	9:N:109:GLY:HA2	1.94	0.50
12:Q:47:VAL:HB	12:Q:102:LEU:HG	1.93	0.50
25:X:203:PRO:HB2	25:X:204:PRO:C	2.31	0.50
26:Y:301:ILE:HA	26:Y:304:TYR:HB2	1.92	0.50
26:Y:349:LYS:O	26:Y:350:VAL:HG22	2.11	0.50
21:C:238:ALA:O	21:C:244:SER:OG	2.30	0.50
21:C:84:LYS:HA	21:C:98:ASP:HA	1.93	0.50
12:Q:52:ASP:OD1	13:R:88:TYR:OH	2.22	0.50
16:A:183:GLN:HB3	16:A:341:ILE:HD12	1.93	0.50
3:H:72:ILE:HD11	3:H:107:THR:HG22	1.94	0.50
4:I:44:LEU:HD21	4:I:189:ALA:HB3	1.94	0.50
5:J:96:LEU:HD23	5:J:97:THR:HG23	1.93	0.50
6:K:79:SER:HB2	6:K:140:ALA:HB3	1.93	0.50
8:M:92:ARG:HH21	15:T:73:ASP:HA	1.76	0.50
12:Q:8:GLN:HE21	12:Q:115:LEU:HB2	1.77	0.50
23:V:99:ARG:HH22	23:V:146:GLN:HB3	1.76	0.50
24:W:436:MET:HA	24:W:439:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:316:LEU:HG	26:Y:352:GLU:HG3	1.93	0.50
17:B:242:GLN:HG2	17:B:247:PHE:CD2	2.47	0.50
3:H:74:LEU:HD11	3:H:134:LEU:HD13	1.94	0.50
7:L:41:LYS:NZ	7:L:180:MET:O	2.39	0.50
10:O:138:PHE:O	10:O:142:PHE:HB3	2.12	0.50
22:U:666:LYS:HZ3	22:U:703:CYS:HB2	1.76	0.50
16:A:183:GLN:HG3	16:A:341:ILE:HB	1.94	0.49
19:E:44:GLU:HG3	20:F:73:ILE:HG22	1.94	0.49
3:H:183:GLU:HB3	3:H:186:ASP:HB2	1.92	0.49
4:I:105:ILE:HG12	4:I:110:LEU:HD13	1.93	0.49
23:V:201:ARG:HG2	23:V:244:ALA:HB3	1.93	0.49
21:C:250:GLU:O	21:C:251:ILE:HG22	2.12	0.49
19:E:185:ARG:NH2	20:F:319:GLY:HA2	2.27	0.49
7:L:11:THR:HG23	8:M:129:ARG:HB3	1.94	0.49
15:T:89:HIS:CE1	15:T:131:ALA:HB1	2.47	0.49
22:U:115:ASN:HA	22:U:118:LEU:HD13	1.94	0.49
22:U:465:LEU:HD11	22:U:477:GLY:HA3	1.94	0.49
22:U:908:ILE:HG12	22:U:909:GLY:H	1.76	0.49
16:A:407:LYS:HA	16:A:410:LEU:HG	1.93	0.49
19:E:47:LEU:HD22	20:F:76:ASN:HD21	1.76	0.49
10:O:215:LYS:HB3	11:P:197:THR:HB	1.93	0.49
15:T:92:LEU:HD23	15:T:112:ILE:HD11	1.94	0.49
24:W:299:ILE:HG22	24:W:301:LYS:H	1.78	0.49
16:A:104:ALA:O	16:A:112:ILE:HG22	2.12	0.49
16:A:239:ARG:HA	16:A:273:PHE:HB3	1.94	0.49
16:A:406:GLU:N	16:A:407:LYS:HB3	2.28	0.49
21:C:247:PHE:HE2	21:C:249:ASP:HB2	1.77	0.49
6:K:94:VAL:O	6:K:98:ASN:ND2	2.44	0.49
12:Q:85:ARG:O	12:Q:89:ALA:N	2.34	0.49
14:S:145:LEU:O	14:S:149:LEU:N	2.37	0.49
22:U:184:CYS:O	22:U:188:MET:N	2.46	0.49
22:U:757:MET:HG3	22:U:758:PRO:HD3	1.94	0.49
24:W:91:SER:HB2	24:W:92:LYS:HA	1.94	0.49
21:C:74:GLY:N	21:C:114:VAL:O	2.42	0.49
14:S:16:ALA:HA	14:S:21:ALA:HA	1.93	0.49
22:U:571:CYS:HB2	22:U:601:ARG:HH21	1.78	0.49
23:V:106:ARG:O	23:V:110:HIS:ND1	2.32	0.49
18:D:45:LYS:HB2	22:U:187:LEU:HD22	1.93	0.49
19:E:76:GLY:N	19:E:77:PRO:HD2	2.28	0.49
6:K:181:LEU:HD23	6:K:182:GLN:HG3	1.93	0.49
25:X:410:VAL:HG11	26:Y:376:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:367:PRO:HA	18:D:370:ILE:HG22	1.95	0.49
9:N:176:LEU:HD12	9:N:187:GLN:HE21	1.76	0.49
15:T:23:ALA:HB3	15:T:169:VAL:HG11	1.94	0.49
22:U:541:HIS:HB2	22:U:544:ILE:HG22	1.94	0.49
23:V:320:THR:HG23	23:V:321:ALA:HB2	1.95	0.49
25:X:260:MET:HE3	25:X:322:HIS:HA	1.95	0.49
25:X:356:LEU:HD11	25:X:360:ASP:OD1	2.13	0.49
26:Y:101:ARG:HD3	26:Y:130:LYS:HD3	1.94	0.49
27:Z:106:ILE:HG13	27:Z:153:LYS:HD2	1.94	0.49
16:A:76:ALA:HA	17:B:138:PHE:HD1	1.78	0.49
21:C:267:SER:HA	21:C:270:GLN:HB2	1.95	0.49
2:G:159:TYR:HA	3:H:84:ARG:HH21	1.77	0.49
5:J:98:VAL:HG13	13:R:78:ALA:HB2	1.94	0.49
6:K:51:GLU:HA	6:K:215:ILE:HG22	1.94	0.49
9:N:34:LEU:HD22	9:N:177:ALA:HB2	1.94	0.49
10:O:35:HIS:NE2	10:O:53:ASP:OD1	2.46	0.49
23:V:237:THR:O	23:V:241:ARG:NE	2.36	0.49
27:Z:222:ILE:N	27:Z:223:ASN:HA	2.27	0.49
17:B:126:SER:HA	17:B:127:VAL:HA	1.54	0.49
6:K:16:SER:OG	6:K:18:GLU:OE1	2.25	0.49
8:M:106:ILE:HD12	8:M:107:PRO:HD2	1.93	0.49
7:L:123:TYR:N	8:M:127:ALA:O	2.44	0.49
25:X:228:ALA:HA	25:X:231:TYR:HD2	1.78	0.49
27:Z:256:GLN:HG3	27:Z:260:VAL:HG23	1.95	0.49
19:E:360:ASP:N	19:E:360:ASP:OD1	2.41	0.49
23:V:362:LEU:HD12	23:V:365:GLN:HB3	1.94	0.49
26:Y:197:ALA:HB3	26:Y:226:VAL:HG21	1.95	0.49
26:Y:346:LYS:O	26:Y:355:GLU:N	2.39	0.49
27:Z:238:PRO:HG2	27:Z:240:VAL:HG22	1.93	0.49
16:A:210:LYS:HB3	16:A:317:VAL:HG22	1.95	0.48
16:A:234:ASP:HA	16:A:235:ALA:HA	1.51	0.48
21:C:29:GLU:O	21:C:33:LEU:N	2.40	0.48
18:D:50:GLU:HA	18:D:53:PHE:HB2	1.94	0.48
19:E:266:GLY:HA3	19:E:268:ASP:H	1.77	0.48
20:F:77:SER:O	20:F:81:LYS:N	2.45	0.48
23:V:26:PRO:O	23:V:29:PRO:HD2	2.13	0.48
23:V:466:ILE:HG23	23:V:467:TYR:H	1.77	0.48
24:W:202:THR:HG21	24:W:233:LEU:HD11	1.95	0.48
25:X:200:ILE:HG22	25:X:201:TYR:H	1.77	0.48
25:X:262:ASN:O	25:X:297:ARG:NH2	2.37	0.48
25:X:370:LEU:HD13	26:Y:306:GLN:HB2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:48:ASN:ND2	26:Y:77:ASN:HB2	2.28	0.48
27:Z:82:PHE:HA	27:Z:85:VAL:HG12	1.95	0.48
21:C:183:PRO:HG2	21:C:290:LYS:HE3	1.95	0.48
18:D:200:ARG:NH1	18:D:296:MET:O	2.46	0.48
18:D:300:ASP:HA	18:D:301:GLN:HA	1.52	0.48
20:F:334:ARG:HG2	20:F:336:ASP:H	1.77	0.48
3:H:93:LEU:HD11	3:H:117:VAL:HB	1.95	0.48
22:U:27:LEU:O	22:U:31:VAL:HB	2.14	0.48
21:C:139:MET:HB3	21:C:211:PHE:HB3	1.94	0.48
21:C:312:ASP:OD1	21:C:313:ARG:N	2.41	0.48
21:C:397:LYS:HG2	21:C:398:ASN:HA	1.95	0.48
4:I:107:CYS:HA	4:I:110:LEU:HB3	1.95	0.48
6:K:73:HIS:ND1	6:K:146:VAL:O	2.46	0.48
7:L:157:ARG:HG3	7:L:176:MET:HE2	1.95	0.48
10:O:40:ASN:HB3	10:O:73:LEU:HD11	1.95	0.48
12:Q:20:VAL:HG21	12:Q:175:LEU:HA	1.95	0.48
23:V:25:GLU:HG2	23:V:84:LYS:HD2	1.95	0.48
17:B:248:LEU:HD23	17:B:282:VAL:HG13	1.95	0.48
19:E:385:ASP:HB3	19:E:386:TYR:HA	1.94	0.48
20:F:183:GLU:HG2	20:F:239:ALA:HB2	1.95	0.48
5:J:120:GLN:O	6:K:134:SER:OG	2.31	0.48
7:L:95:SER:O	7:L:100:ASP:N	2.46	0.48
14:S:2:PHE:H	15:T:2:GLN:HE22	1.62	0.48
2:G:17:SER:O	3:H:24:TYR:HB3	2.14	0.48
3:H:89:ARG:O	3:H:93:LEU:N	2.39	0.48
23:V:273:LYS:HA	23:V:274:SER:HB2	1.95	0.48
24:W:364:ARG:HG2	24:W:402:ILE:HD11	1.95	0.48
26:Y:380:VAL:HA	26:Y:383:LEU:HB2	1.96	0.48
21:C:255:GLY:N	21:C:256:SER:HB2	2.28	0.48
18:D:413:GLU:HG2	18:D:414:HIS:H	1.78	0.48
19:E:235:ILE:HG22	19:E:279:THR:HB	1.95	0.48
20:F:188:ILE:HA	20:F:365:ILE:HG22	1.95	0.48
2:G:189:TRP:HE3	2:G:194:THR:HG22	1.78	0.48
2:G:44:GLY:N	2:G:47:CYS:O	2.45	0.48
7:L:205:LEU:H	7:L:209:ASN:HD21	1.61	0.48
22:U:697:GLN:NE2	22:U:786:THR:OG1	2.47	0.48
22:U:802:TYR:HB3	22:U:895:PRO:HG3	1.95	0.48
24:W:243:ILE:HA	24:W:246:HIS:HB3	1.96	0.48
25:X:264:PRO:HG2	25:X:267:VAL:HG23	1.95	0.48
17:B:290:ILE:HG21	17:B:336:THR:HG21	1.94	0.48
18:D:366:ARG:HB3	18:D:367:PRO:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:28:ILE:HG21	20:F:437:TYR:HD1	1.78	0.48
5:J:94:HIS:CE1	5:J:103:THR:H	2.31	0.48
10:O:34:ILE:HD12	10:O:185:PHE:HE1	1.78	0.48
24:W:55:ARG:NH1	24:W:75:TYR:HB3	2.29	0.48
26:Y:16:ASP:HB2	26:Y:113:ARG:HE	1.79	0.48
26:Y:215:ASP:O	26:Y:218:THR:OG1	2.26	0.48
27:Z:34:ARG:NE	27:Z:98:GLY:O	2.39	0.48
17:B:262:ASP:OD1	17:B:262:ASP:N	2.47	0.48
6:K:94:VAL:HG22	13:R:65:ILE:HD13	1.94	0.48
22:U:16:GLU:HB3	22:U:18:GLN:HG2	1.95	0.48
22:U:9:ILE:HG12	22:U:41:SER:HB2	1.94	0.48
16:A:200:ARG:HA	16:A:204:LEU:HD13	1.95	0.48
16:A:219:GLY:HA2	16:A:220:THR:HA	1.58	0.48
18:D:69:LYS:HG3	21:C:49:ARG:HH22	1.79	0.48
19:E:260:LEU:HB3	19:E:264:MET:HE1	1.95	0.48
4:I:220:ASN:HA	4:I:221:GLY:HA2	1.54	0.48
5:J:92:GLN:HG3	12:Q:62:LYS:HB3	1.95	0.48
13:R:171:GLY:HA2	13:R:192:VAL:HG21	1.95	0.48
15:T:54:SER:O	15:T:108:ASN:ND2	2.39	0.48
25:X:206:LEU:O	25:X:210:LEU:N	2.37	0.48
25:X:299:LEU:HA	25:X:302:PHE:HB3	1.95	0.48
18:D:235:PHE:HZ	18:D:270:ILE:HD13	1.79	0.48
20:F:102:ASN:O	27:Z:45:LYS:NZ	2.29	0.48
20:F:233:LYS:N	33:F:501:ATP:O1B	2.47	0.48
5:J:34:GLY:HA2	5:J:43:LEU:HA	1.94	0.48
6:K:225:ASN:HB2	6:K:226:PHE:CD2	2.49	0.48
9:N:99:ILE:HG23	9:N:113:SER:HA	1.96	0.48
24:W:12:ARG:HA	24:W:15:LYS:HD3	1.96	0.48
24:W:409:LEU:HD23	25:X:384:VAL:HG21	1.95	0.48
16:A:217:PRO:HD2	16:A:343:PHE:HB2	1.96	0.47
16:A:362:MET:HG2	16:A:363:SER:H	1.79	0.47
18:D:242:GLU:OE1	19:E:78:ARG:NH1	2.39	0.47
19:E:196:LEU:HB3	19:E:230:ILE:HG12	1.96	0.47
4:I:49:ARG:N	4:I:210:LYS:O	2.41	0.47
5:J:121:SER:C	5:J:123:GLY:HA3	2.33	0.47
15:T:192:VAL:HG12	15:T:197:VAL:HG22	1.96	0.47
22:U:343:ILE:HG23	22:U:344:ARG:HG2	1.96	0.47
22:U:509:GLY:HA3	22:U:544:ILE:HD13	1.96	0.47
24:W:141:GLU:HB3	24:W:172:GLU:HG2	1.95	0.47
24:W:16:MET:HG2	24:W:27:ARG:HH22	1.79	0.47
24:W:247:TYR:HA	24:W:250:ILE:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:301:GLN:HA	18:D:302:ASN:HA	1.62	0.47
20:F:339:ASP:HB3	20:F:342:LEU:HG	1.94	0.47
6:K:40:ILE:HG23	6:K:185:TYR:HE1	1.79	0.47
12:Q:13:VAL:HB	12:Q:183:ILE:HD12	1.97	0.47
22:U:756:HIS:HD2	22:U:759:SER:HB2	1.79	0.47
25:X:366:SER:HA	25:X:369:ILE:HD12	1.96	0.47
26:Y:134:LEU:HB2	26:Y:168:ILE:HG23	1.95	0.47
19:E:135:ILE:HA	19:E:312:ILE:HD13	1.96	0.47
2:G:159:TYR:HA	3:H:84:ARG:NH2	2.29	0.47
13:R:7:LYS:O	13:R:143:TYR:OH	2.32	0.47
16:A:345:LEU:HG	16:A:346:PRO:HD2	1.96	0.47
21:C:147:THR:HA	21:C:205:HIS:CD2	2.48	0.47
21:C:241:HIS:HB2	21:C:244:SER:HB3	1.96	0.47
21:C:298:ILE:HG22	21:C:299:ASP:H	1.80	0.47
18:D:172:ILE:HG13	18:D:173:GLN:H	1.79	0.47
18:D:303:VAL:HA	18:D:304:ASN:HA	1.78	0.47
18:D:39:ASP:N	22:U:148:LYS:O	2.48	0.47
20:F:94:ILE:HD11	20:F:125:LYS:HG2	1.95	0.47
2:G:97:GLU:HA	2:G:100:ASN:HD22	1.78	0.47
6:K:212:ALA:HA	6:K:234:LEU:HD22	1.96	0.47
7:L:27:GLU:O	7:L:31:GLN:N	2.48	0.47
11:P:11:VAL:HG23	11:P:54:ALA:HB2	1.96	0.47
24:W:373:ILE:HG12	24:W:374:THR:N	2.29	0.47
17:B:106:PRO:HB3	21:C:120:SER:HB2	1.97	0.47
21:C:310:ARG:HA	21:C:311:ILE:HA	1.53	0.47
18:D:287:ARG:O	18:D:291:GLU:N	2.44	0.47
3:H:6:TYR:HB2	3:H:13:PHE:HB3	1.95	0.47
8:M:20:VAL:HG12	8:M:22:GLN:H	1.79	0.47
10:O:110:LEU:HD21	10:O:125:VAL:HG22	1.97	0.47
15:T:44:ARG:HA	15:T:50:MET:HG3	1.95	0.47
22:U:345:ASN:HD21	22:U:883:ARG:HG2	1.80	0.47
22:U:564:ASP:HA	22:U:567:ILE:HB	1.97	0.47
22:U:69:TYR:OH	23:V:239:THR:O	2.22	0.47
19:E:232:MET:O	19:E:278:ALA:N	2.48	0.47
19:E:309:ARG:HA	19:E:312:ILE:HG22	1.96	0.47
3:H:6:TYR:H	3:H:13:PHE:HB3	1.79	0.47
4:I:43:VAL:HG12	4:I:216:LEU:HB3	1.95	0.47
23:V:221:LEU:HD12	23:V:222:ASP:H	1.80	0.47
26:Y:173:ASP:N	26:Y:177:ARG:HD3	2.29	0.47
27:Z:142:GLU:OE2	27:Z:153:LYS:NZ	2.47	0.47
27:Z:240:VAL:O	27:Z:243:GLN:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A:115:VAL:HG13	16:A:117:GLN:H	1.79	0.47
4:I:143:TYR:HB2	4:I:146:GLN:NE2	2.30	0.47
4:I:93:ILE:HA	4:I:96:ARG:HG2	1.96	0.47
7:L:164:ARG:HH21	20:F:430:LYS:HE2	1.80	0.47
13:R:173:ALA:HA	13:R:191:ASN:HA	1.96	0.47
23:V:227:VAL:HA	23:V:230:PHE:HB3	1.97	0.47
23:V:394:LEU:HD13	23:V:398:LEU:HD13	1.96	0.47
26:Y:174:TRP:CE3	26:Y:175:ASP:HB2	2.49	0.47
16:A:210:LYS:HG2	16:A:336:ARG:NH1	2.30	0.47
17:B:262:ASP:H	17:B:266:LEU:HD11	1.80	0.47
8:M:80:LEU:HD23	8:M:83:ASP:H	1.80	0.47
26:Y:232:GLU:O	26:Y:236:LEU:N	2.39	0.47
27:Z:223:ASN:HB2	27:Z:227:ILE:HG12	1.97	0.47
16:A:273:PHE:CD1	16:A:318:LEU:HD22	2.49	0.47
21:C:252:ASP:CG	21:C:296:ASN:H	2.18	0.47
19:E:240:GLY:O	19:E:254:GLN:NE2	2.47	0.47
4:I:57:ASP:HB3	4:I:59:VAL:HG13	1.96	0.47
22:U:346:ASN:HA	22:U:743:ASN:HD21	1.79	0.47
22:U:787:CYS:HB2	22:U:881:PRO:HB2	1.97	0.47
23:V:280:ALA:HA	23:V:281:ASN:HA	1.54	0.47
26:Y:131:THR:O	26:Y:137:ARG:NH1	2.48	0.47
26:Y:286:TRP:O	26:Y:287:LEU:HG	2.14	0.47
26:Y:357:ASN:HB2	26:Y:359:PRO:HD3	1.97	0.47
16:A:365:GLU:HG2	16:A:366:ARG:H	1.80	0.47
21:C:213:ARG:NE	21:C:249:ASP:O	2.28	0.47
3:H:136:ILE:N	3:H:147:PHE:O	2.43	0.47
3:H:34:PRO:HB3	3:H:165:LYS:N	2.29	0.47
27:Z:39:LEU:HD11	27:Z:50:VAL:HG11	1.97	0.47
18:D:326:ARG:HH22	21:C:141:GLU:HB3	1.79	0.46
21:C:186:VAL:HG23	21:C:312:ASP:HB3	1.96	0.46
2:G:39:SER:H	2:G:172:GLN:NE2	2.13	0.46
5:J:211:MET:HB2	5:J:217:LEU:HB3	1.96	0.46
4:I:13:SER:O	5:J:21:TYR:CD1	2.68	0.46
14:S:68:ILE:O	14:S:72:LEU:N	2.47	0.46
22:U:896:GLU:O	22:U:901:GLN:NE2	2.49	0.46
24:W:422:ASN:OD1	24:W:423:ASN:N	2.48	0.46
2:G:77:GLY:H	2:G:141:ILE:HD11	1.80	0.46
4:I:140:ASP:OD1	4:I:144:GLY:N	2.49	0.46
14:S:193:LEU:HB3	14:S:208:VAL:HB	1.97	0.46
22:U:625:ILE:HG13	22:U:626:LEU:HG	1.97	0.46
23:V:221:LEU:HD12	23:V:222:ASP:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:89:LYS:HD3	23:V:92:ARG:HH11	1.81	0.46
24:W:169:LEU:HD22	24:W:186:ILE:HG13	1.97	0.46
16:A:343:PHE:HA	16:A:344:SER:OG	2.15	0.46
16:A:349:GLU:O	16:A:353:HIS:ND1	2.32	0.46
16:A:401:ARG:HH12	16:A:414:ASN:HD22	1.63	0.46
16:A:164:MET:HA	17:B:265:LYS:HE2	1.97	0.46
18:D:213:THR:HG22	18:D:217:LYS:HE3	1.96	0.46
2:G:71:LYS:HE2	2:G:74:GLU:HA	1.97	0.46
3:H:65:VAL:HG22	3:H:75:VAL:HG12	1.98	0.46
5:J:93:SER:O	5:J:97:THR:N	2.47	0.46
8:M:37:ILE:HG22	8:M:164:ALA:HA	1.96	0.46
22:U:214:ILE:HA	22:U:217:CYS:HB3	1.97	0.46
22:U:632:GLN:O	22:U:635:SER:OG	2.29	0.46
16:A:167:GLU:HB2	16:A:239:ARG:HG2	1.96	0.46
18:D:285:VAL:HA	18:D:288:ILE:HD12	1.96	0.46
18:D:274:ARG:NH1	19:E:248:SER:OG	2.49	0.46
2:G:56:VAL:HA	2:G:61:LEU:HD13	1.96	0.46
5:J:180:ALA:HA	5:J:181:ILE:HA	1.46	0.46
8:M:77:VAL:HG21	8:M:84:ALA:HB1	1.98	0.46
11:P:62:THR:OG1	12:Q:85:ARG:NH2	2.31	0.46
22:U:68:PHE:HB3	22:U:73:ALA:HB3	1.96	0.46
23:V:67:LEU:O	23:V:71:THR:OG1	2.22	0.46
26:Y:20:ALA:HB2	26:Y:150:PHE:HD1	1.80	0.46
27:Z:32:GLN:HG3	27:Z:33:LYS:H	1.79	0.46
17:B:203:LEU:HG	17:B:211:TYR:HD1	1.79	0.46
17:B:343:ARG:HB2	17:B:344:PRO:HD3	1.96	0.46
21:C:186:VAL:HG12	21:C:292:ILE:HG12	1.98	0.46
21:C:207:THR:HG21	21:C:245:ILE:HG12	1.97	0.46
21:C:192:PRO:HD3	21:C:296:ASN:O	2.16	0.46
3:H:136:ILE:HB	3:H:147:PHE:HB2	1.97	0.46
6:K:167:ALA:HB3	6:K:181:LEU:HD21	1.98	0.46
7:L:84:LEU:HA	7:L:87:PHE:HB3	1.98	0.46
22:U:195:ASN:HB2	22:U:223:LEU:HD13	1.98	0.46
22:U:664:GLY:HA2	22:U:698:GLN:HE22	1.81	0.46
23:V:148:ARG:NH1	23:V:193:GLN:OE1	2.36	0.46
17:B:324:ASP:N	17:B:324:ASP:OD1	2.49	0.46
19:E:223:ARG:HA	19:E:226:GLN:HE21	1.80	0.46
20:F:397:LYS:HA	20:F:400:CYS:HB3	1.97	0.46
5:J:45:VAL:HG13	5:J:46:GLU:H	1.80	0.46
9:N:42:PHE:HB2	9:N:179:ILE:HD11	1.98	0.46
22:U:789:ILE:HB	22:U:911:ILE:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:885:MET:HG2	22:U:887:ALA:H	1.80	0.46
17:B:144:LEU:HD11	17:B:162:VAL:HG21	1.98	0.46
19:E:264:MET:HB3	19:E:294:ARG:HA	1.98	0.46
19:E:57:VAL:HA	19:E:99:ALA:HA	1.98	0.46
20:F:298:SER:HB2	20:F:299:GLU:HG3	1.98	0.46
2:G:199:ILE:HD13	2:G:242:LEU:HD21	1.97	0.46
2:G:93:ARG:HH22	2:G:121:ILE:HB	1.80	0.46
6:K:46:VAL:HG23	6:K:151:PRO:HB2	1.97	0.46
13:R:55:TRP:O	13:R:59:LEU:N	2.39	0.46
13:R:95:LEU:HD21	14:S:100:ARG:HG2	1.97	0.46
15:T:11:VAL:HG13	15:T:24:ALA:HB2	1.97	0.46
23:V:263:LEU:HG	23:V:264:TYR:H	1.80	0.46
23:V:98:LEU:N	23:V:99:ARG:HA	2.31	0.46
24:W:370:TYR:OH	24:W:373:ILE:HD12	2.15	0.46
26:Y:181:LYS:HA	26:Y:200:LEU:HD23	1.97	0.46
27:Z:62:ASP:OD2	27:Z:63:LYS:NZ	2.39	0.46
21:C:99:VAL:HA	21:C:100:ASP:HB2	1.98	0.46
22:U:107:HIS:HA	22:U:110:LYS:HE3	1.98	0.46
23:V:486:ILE:HG21	26:Y:377:LEU:HD21	1.97	0.46
25:X:377:ILE:HG12	26:Y:312:ARG:HB3	1.96	0.46
16:A:107:GLU:HB2	16:A:110:LYS:HG2	1.97	0.46
16:A:253:GLY:HA3	16:A:298:THR:HG22	1.98	0.46
20:F:83:ASN:O	20:F:154:ASN:ND2	2.49	0.46
5:J:98:VAL:HG12	5:J:100:ASP:OD1	2.16	0.46
9:N:132:SER:HA	9:N:135:ILE:HG12	1.97	0.46
12:Q:20:VAL:HG21	12:Q:176:PRO:HD2	1.97	0.46
22:U:573:ASP:OD1	22:U:574:LYS:N	2.49	0.46
16:A:94:GLN:HA	17:B:131:HIS:CD2	2.50	0.46
18:D:116:LEU:HB2	18:D:140:VAL:HA	1.98	0.46
2:G:109:ILE:HD13	2:G:114:LEU:HB2	1.98	0.46
3:H:11:THR:HG22	3:H:12:THR:H	1.81	0.46
3:H:80:GLY:O	3:H:82:ASP:N	2.48	0.46
7:L:204:ASP:HB3	7:L:205:LEU:C	2.36	0.46
22:U:494:TYR:HD1	22:U:516:LEU:HD11	1.81	0.46
22:U:540:GLN:HG3	22:U:541:HIS:CD2	2.50	0.46
22:U:557:TYR:HD1	22:U:588:MET:HB3	1.79	0.46
27:Z:237:LEU:HB2	27:Z:239:ASP:OD1	2.16	0.46
16:A:97:ARG:HA	16:A:98:CYS:HA	1.66	0.45
17:B:176:VAL:HG23	17:B:177:GLU:HB2	1.97	0.45
18:D:267:ILE:HD13	18:D:309:MET:SD	2.55	0.45
18:D:345:PHE:HA	18:D:348:ILE:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:221:LYS:HD2	20:F:327:LYS:HG3	1.98	0.45
17:B:176:VAL:HA	17:B:177:GLU:HA	1.60	0.45
18:D:268:ASP:HA	18:D:271:ALA:HB3	1.98	0.45
2:G:157:ALA:HB3	18:D:418:LYS:HG2	1.97	0.45
7:L:148:CYS:SG	7:L:150:SER:OG	2.62	0.45
7:L:156:CYS:HA	8:M:59:GLU:H	1.80	0.45
26:Y:71:ASN:HA	26:Y:74:LYS:HG2	1.97	0.45
17:B:139:VAL:HA	17:B:140:ASP:CB	2.46	0.45
21:C:215:SER:HA	21:C:216:GLY:HA3	1.59	0.45
18:D:198:PRO:HD2	18:D:302:ASN:ND2	2.29	0.45
18:D:313:ARG:HH11	19:E:242:ARG:HG3	1.81	0.45
18:D:412:GLN:O	18:D:415:GLU:N	2.47	0.45
20:F:317:LEU:HD13	20:F:347:ARG:HA	1.98	0.45
6:K:17:PRO:HA	7:L:24:TYR:CZ	2.50	0.45
8:M:200:VAL:HG22	8:M:201:HIS:H	1.81	0.45
10:O:8:TYR:CE1	10:O:13:VAL:HG23	2.52	0.45
22:U:377:HIS:HB3	22:U:411:ILE:HG23	1.98	0.45
16:A:105:ASP:N	16:A:105:ASP:OD1	2.50	0.45
17:B:104:GLY:HA3	17:B:105:THR:HA	1.76	0.45
17:B:175:LYS:HB3	17:B:176:VAL:HB	1.99	0.45
21:C:224:ILE:HD13	21:C:237:MET:HG3	1.98	0.45
20:F:342:LEU:HD13	20:F:348:LEU:HD12	1.97	0.45
3:H:71:HIS:HA	3:H:217:GLY:HA2	1.97	0.45
5:J:22:ALA:HB1	5:J:128:GLY:HA2	1.99	0.45
22:U:32:ASN:OD1	22:U:33:ASP:N	2.49	0.45
26:Y:300:ARG:O	26:Y:304:TYR:N	2.41	0.45
27:Z:54:PHE:HB3	27:Z:82:PHE:HE2	1.82	0.45
17:B:362:LYS:HB2	17:B:384:ILE:HD13	1.99	0.45
21:C:161:ILE:HD13	21:C:315:ILE:HD11	1.98	0.45
21:C:338:LEU:HD21	21:C:342:ILE:HD13	1.99	0.45
2:G:184:LYS:HA	2:G:186:LYS:N	2.31	0.45
5:J:10:PHE:H	6:K:23:GLN:NE2	2.14	0.45
5:J:131:ALA:N	5:J:147:THR:OG1	2.44	0.45
13:R:25:TYR:OH	14:S:142:SER:O	2.29	0.45
22:U:568:GLU:OE2	22:U:572:ARG:NH2	2.48	0.45
23:V:31:ALA:HB3	23:V:32:PRO:HD3	1.98	0.45
23:V:372:LEU:HD21	23:V:399:ARG:HH22	1.80	0.45
23:V:78:HIS:HB3	23:V:161:PRO:HB3	1.99	0.45
18:D:145:PRO:O	18:D:252:ARG:NH1	2.49	0.45
6:K:68:VAL:HG23	6:K:76:CYS:HB3	1.99	0.45
23:V:419:LEU:HD23	23:V:458:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:85:ASP:O	26:Y:88:LEU:HG	2.15	0.45
21:C:11:LEU:HD23	22:U:149:GLN:HE21	1.82	0.45
19:E:226:GLN:HE22	19:E:273:VAL:HB	1.80	0.45
19:E:378:LYS:HE3	20:F:343:LEU:HD22	1.98	0.45
20:F:266:LYS:O	20:F:270:ASP:HB2	2.16	0.45
2:G:153:LYS:O	2:G:161:CYS:HB3	2.16	0.45
3:H:71:HIS:CD2	3:H:72:ILE:HG13	2.52	0.45
5:J:76:LEU:HB3	17:B:440:LEU:HD23	1.98	0.45
10:O:176:CYS:HB2	10:O:185:PHE:HD1	1.82	0.45
14:S:28:ARG:NH1	14:S:187:VAL:O	2.49	0.45
23:V:131:LEU:HD23	23:V:134:PHE:HD2	1.82	0.45
24:W:397:VAL:HG13	25:X:341:PRO:HB2	1.99	0.45
16:A:113:ILE:HB	16:A:121:PHE:HB3	1.98	0.45
21:C:35:VAL:HA	21:C:38:LYS:HB2	1.99	0.45
18:D:190:LEU:HD21	21:C:371:LEU:HG	1.98	0.45
19:E:65:THR:HG22	19:E:66:GLU:H	1.81	0.45
2:G:43:ARG:HG3	2:G:48:ALA:HB2	1.99	0.45
3:H:183:GLU:OE1	3:H:186:ASP:N	2.38	0.45
4:I:100:GLN:HG3	12:Q:86:ARG:HG3	1.98	0.45
5:J:104:VAL:HB	5:J:143:ARG:HD3	1.98	0.45
6:K:167:ALA:HB1	6:K:181:LEU:HD11	1.99	0.45
14:S:108:ASN:HB2	14:S:124:PHE:HD2	1.81	0.45
15:T:49:THR:HB	15:T:85:PRO:HG3	1.98	0.45
22:U:31:VAL:HG22	22:U:35:TRP:CD1	2.51	0.45
24:W:403:PHE:HB3	24:W:416:GLN:HG3	1.97	0.45
21:C:130:LYS:HB2	21:C:133:PRO:HG2	1.99	0.45
21:C:321:ASN:H	21:C:324:ALA:HB3	1.82	0.45
18:D:380:GLN:O	18:D:384:MET:N	2.46	0.45
18:D:45:LYS:HE3	22:U:158:ARG:HH12	1.82	0.45
19:E:55:GLN:HA	19:E:102:MET:HG2	1.98	0.45
20:F:205:PRO:O	20:F:209:LYS:HB2	2.16	0.45
2:G:144:ASP:HB3	2:G:147:GLN:HB2	1.99	0.45
2:G:191:PHE:HE1	2:G:219:VAL:HG21	1.82	0.45
2:G:61:LEU:HG	2:G:66:VAL:HG21	1.98	0.45
2:G:128:ASN:HA	3:H:127:VAL:HG11	1.99	0.45
3:H:9:SER:HA	3:H:10:LEU:HA	1.72	0.45
4:I:105:ILE:HD12	4:I:106:PRO:HD2	1.99	0.45
7:L:160:SER:O	7:L:169:ARG:NH2	2.50	0.45
7:L:229:VAL:HG12	7:L:233:LEU:HG	1.98	0.45
10:O:103:VAL:HG21	10:O:179:SER:HA	1.99	0.45
14:S:60:ASP:HB3	14:S:104:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:150:ASP:O	14:S:155:PHE:N	2.50	0.45
15:T:41:ARG:HH21	15:T:54:SER:HA	1.82	0.45
23:V:378:VAL:HG13	23:V:382:PHE:HD2	1.81	0.45
24:W:234:ASP:OD2	24:W:246:HIS:NE2	2.50	0.45
25:X:410:VAL:HB	26:Y:376:LEU:HD11	1.99	0.45
21:C:247:PHE:CE2	21:C:249:ASP:HB2	2.51	0.45
18:D:197:ASP:O	18:D:199:PRO:HD3	2.17	0.45
3:H:45:VAL:HG22	3:H:212:ILE:HG22	1.99	0.45
4:I:232:GLU:O	4:I:235:GLN:HG2	2.17	0.45
5:J:94:HIS:HE1	5:J:103:THR:H	1.63	0.45
5:J:158:ALA:HB3	5:J:172:LEU:HD13	1.97	0.45
6:K:174:SER:HA	6:K:177:ALA:HB3	1.99	0.45
8:M:197:ILE:HG21	8:M:211:LEU:HD13	1.98	0.45
8:M:40:ARG:HA	8:M:45:VAL:HA	2.00	0.45
15:T:20:VAL:HG11	15:T:122:LEU:HD13	1.99	0.45
15:T:51:LEU:HD13	15:T:112:ILE:HG12	1.98	0.45
22:U:682:TYR:HB3	22:U:725:MET:SD	2.57	0.45
22:U:842:LYS:HE3	22:U:843:GLU:O	2.17	0.45
24:W:78:LYS:HA	24:W:81:ASP:HB3	1.99	0.45
26:Y:387:ILE:HA	26:Y:388:ASN:HA	1.56	0.45
17:B:205:LEU:HG	17:B:279:PRO:HG3	1.99	0.44
17:B:436:GLU:CB	17:B:437:GLY:HA2	2.47	0.44
18:D:151:ILE:HB	18:D:152:MET:CA	2.46	0.44
18:D:161:ASP:OD2	18:D:229:ARG:NH2	2.50	0.44
24:W:76:GLU:HA	24:W:79:GLU:HB2	1.99	0.44
25:X:346:GLN:HA	25:X:384:VAL:HA	1.99	0.44
26:Y:43:ALA:O	26:Y:49:ASN:ND2	2.40	0.44
16:A:351:ARG:HA	16:A:354:ILE:HD12	1.98	0.44
17:B:256:ILE:HD12	17:B:312:LEU:HD13	1.98	0.44
16:A:164:MET:SD	17:B:265:LYS:HG3	2.57	0.44
17:B:319:PHE:HA	17:B:320:ASP:HA	1.55	0.44
17:B:397:ALA:HB3	21:C:311:ILE:HB	2.00	0.44
21:C:229:ARG:HE	21:C:232:ARG:HB3	1.81	0.44
7:L:50:LYS:HB2	7:L:209:ASN:HA	1.99	0.44
5:J:88:ARG:HH22	12:Q:69:MET:HB2	1.82	0.44
27:Z:58:PHE:CZ	27:Z:68:TRP:HB2	2.51	0.44
18:D:89:ILE:O	18:D:106:THR:OG1	2.28	0.44
3:H:50:LYS:HD2	3:H:64:LYS:HG2	1.99	0.44
14:S:21:ALA:HB3	14:S:198:VAL:HB	2.00	0.44
22:U:361:ARG:HG3	22:U:365:CYS:HB2	1.99	0.44
26:Y:46:ARG:C	26:Y:48:ASN:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:408:ARG:NH2	21:C:159:LYS:HD2	2.33	0.44
16:A:80:LEU:HD13	17:B:99:VAL:HG21	1.99	0.44
21:C:117:ARG:HG3	21:C:124:HIS:HB2	1.99	0.44
21:C:99:VAL:HG13	21:C:101:LYS:N	2.32	0.44
18:D:136:SER:HB2	21:C:66:LEU:HD23	1.99	0.44
18:D:356:GLU:C	18:D:358:VAL:H	2.19	0.44
20:F:336:ASP:OD1	20:F:337:ILE:N	2.49	0.44
7:L:171:TYR:O	7:L:175:HIS:ND1	2.50	0.44
8:M:185:THR:O	8:M:189:ILE:HG12	2.18	0.44
12:Q:77:PRO:HG2	12:Q:108:ASP:HB2	1.99	0.44
12:Q:19:ARG:HD2	12:Q:179:SER:HB3	1.99	0.44
22:U:195:ASN:HA	22:U:198:LEU:HB3	2.00	0.44
26:Y:357:ASN:OD1	26:Y:358:ARG:N	2.50	0.44
25:X:395:LYS:NZ	26:Y:366:TYR:OH	2.43	0.44
18:D:129:SER:HB3	18:D:143:LEU:HD12	1.99	0.44
18:D:266:GLU:HA	18:D:311:THR:HA	2.00	0.44
7:L:184:LEU:HD12	7:L:184:LEU:H	1.82	0.44
11:P:33:GLN:HE22	12:Q:136:ALA:HB1	1.82	0.44
23:V:94:VAL:HG13	23:V:95:LEU:HD12	1.99	0.44
26:Y:138:LEU:HD23	26:Y:176:ARG:HD3	1.99	0.44
26:Y:210:SER:H	26:Y:213:LEU:HB2	1.83	0.44
18:D:86:PRO:O	18:D:87:LEU:HD12	2.17	0.44
2:G:93:ARG:NH2	2:G:97:GLU:OE2	2.43	0.44
5:J:96:LEU:HG	13:R:81:LYS:HZ1	1.82	0.44
22:U:167:ILE:HB	22:U:177:LEU:HD21	2.00	0.44
24:W:316:ARG:O	24:W:319:THR:OG1	2.25	0.44
24:W:397:VAL:HG22	25:X:341:PRO:HB2	1.99	0.44
17:B:177:GLU:N	17:B:178:LYS:HA	2.22	0.44
21:C:130:LYS:HB2	21:C:133:PRO:HD2	1.98	0.44
21:C:273:MET:HB2	21:C:307:ARG:NH1	2.31	0.44
21:C:35:VAL:HA	21:C:38:LYS:HD3	2.00	0.44
18:D:270:ILE:HD12	18:D:289:LEU:HB2	1.98	0.44
19:E:171:LEU:HD22	19:E:295:LEU:HD13	2.00	0.44
5:J:132:LEU:HA	5:J:146:GLN:HA	1.99	0.44
26:Y:186:LEU:HA	26:Y:189:VAL:HG12	2.00	0.44
25:X:421:LEU:HD13	26:Y:386:VAL:HG21	2.00	0.44
16:A:269:ALA:H	16:A:315:ILE:HG22	1.83	0.44
17:B:229:GLY:HA2	21:C:274:LEU:HD13	1.99	0.44
18:D:409:LYS:NZ	18:D:413:GLU:OE1	2.49	0.44
18:D:167:ILE:HG23	33:D:501:ATP:HN62	1.83	0.44
20:F:344:ARG:HH11	20:F:346:GLY:H	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:F:91:SER:HB3	20:F:151:VAL:HG23	1.99	0.44
2:G:86:ASP:HA	8:M:120:HIS:CE1	2.52	0.44
4:I:42:GLY:HA3	4:I:186:LEU:HD21	2.00	0.44
27:Z:10:VAL:N	27:Z:48:LEU:O	2.50	0.44
18:D:361:GLU:O	18:D:364:VAL:HG12	2.17	0.44
19:E:384:LEU:HG	19:E:385:ASP:OD1	2.18	0.44
4:I:184:MET:HA	4:I:185:THR:OG1	2.18	0.44
22:U:806:CYS:SG	22:U:891:VAL:HG21	2.57	0.44
23:V:104:THR:HA	23:V:107:ARG:HG2	2.00	0.44
26:Y:116:ASP:HB2	26:Y:118:GLU:OE1	2.18	0.44
26:Y:50:MET:HA	26:Y:53:TYR:CE2	2.53	0.44
16:A:191:VAL:HG23	16:A:316:LYS:HE2	2.00	0.43
21:C:186:VAL:HG22	21:C:187:LEU:H	1.83	0.43
21:C:84:LYS:HZ2	21:C:98:ASP:N	2.16	0.43
2:G:159:TYR:CE1	18:D:418:LYS:HD2	2.53	0.43
2:G:43:ARG:HA	2:G:48:ALA:HA	2.00	0.43
3:H:83:TYR:N	3:H:132:VAL:HG21	2.33	0.43
10:O:113:ILE:HA	10:O:119:THR:HG22	1.98	0.43
15:T:50:MET:N	15:T:113:GLY:O	2.50	0.43
22:U:685:GLN:HG3	22:U:729:GLY:HA3	1.99	0.43
23:V:144:ASP:N	23:V:145:LEU:HA	2.32	0.43
23:V:46:GLY:HA3	23:V:62:HIS:HE1	1.83	0.43
23:V:80:LYS:HA	23:V:80:LYS:HD3	1.84	0.43
24:W:418:PRO:O	24:W:421:PRO:HD3	2.17	0.43
16:A:313:GLY:C	16:A:315:ILE:H	2.21	0.43
16:A:210:LYS:HD3	16:A:336:ARG:HG3	2.00	0.43
17:B:178:LYS:HG3	17:B:180:PRO:HG3	2.00	0.43
21:C:380:GLN:HA	21:C:383:PHE:HD1	1.83	0.43
20:F:80:ILE:O	20:F:84:LYS:N	2.51	0.43
5:J:88:ARG:HB3	12:Q:66:LEU:HD11	2.00	0.43
10:O:8:TYR:HE2	10:O:10:ASP:HB2	1.83	0.43
4:I:100:GLN:O	12:Q:82:ASN:ND2	2.51	0.43
22:U:167:ILE:HD12	22:U:204:ILE:HG21	2.00	0.43
22:U:789:ILE:HG22	22:U:791:LEU:H	1.83	0.43
23:V:97:ALA:N	23:V:98:LEU:HA	2.33	0.43
16:A:100:LYS:NZ	16:A:142:VAL:HB	2.33	0.43
16:A:159:PRO:HD2	16:A:162:THR:OG1	2.18	0.43
19:E:359:HIS:HB2	19:E:362:VAL:HG22	2.01	0.43
20:F:188:ILE:HD13	20:F:191:LEU:HB2	2.00	0.43
4:I:47:ALA:HB2	4:I:65:ILE:HD11	2.00	0.43
22:U:645:ASN:HD21	22:U:648:VAL:HG23	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:794:ASP:OD1	22:U:795:LEU:N	2.52	0.43
24:W:417:ARG:O	24:W:419:LYS:N	2.51	0.43
27:Z:33:LYS:HB3	27:Z:33:LYS:HE3	1.83	0.43
21:C:184:LYS:HB2	21:C:277:LEU:HD23	2.00	0.43
18:D:239:TYR:CE2	19:E:76:GLY:HA3	2.54	0.43
22:U:146:LYS:HE2	22:U:148:LYS:HD3	2.00	0.43
22:U:472:ILE:HA	22:U:475:HIS:CE1	2.53	0.43
22:U:20:LYS:HG3	22:U:54:PHE:HE1	1.84	0.43
23:V:419:LEU:HA	23:V:422:ILE:HG22	1.99	0.43
23:V:80:LYS:HB3	23:V:81:GLN:C	2.38	0.43
21:C:142:LYS:HB3	21:C:213:ARG:NH1	2.33	0.43
21:C:255:GLY:CA	21:C:256:SER:HB2	2.48	0.43
20:F:144:LYS:HA	20:F:145:LEU:HA	1.68	0.43
20:F:167:GLU:HB3	20:F:168:TYR:H	1.60	0.43
11:P:15:LYS:HD3	11:P:119:PRO:HG2	2.00	0.43
14:S:63:THR:HG23	15:T:94:ARG:HH12	1.82	0.43
23:V:372:LEU:H	23:V:427:GLN:HE22	1.65	0.43
17:B:320:ASP:N	17:B:320:ASP:OD1	2.50	0.43
21:C:189:TYR:HD2	21:C:300:ILE:HG23	1.82	0.43
20:F:281:SER:OG	20:F:282:ILE:N	2.51	0.43
4:I:228:LEU:HB3	4:I:229:LYS:HA	1.99	0.43
5:J:79:ASP:HB3	5:J:127:PHE:CE1	2.54	0.43
12:Q:42:ILE:HA	12:Q:106:GLY:HA2	1.99	0.43
12:Q:59:TYR:O	12:Q:63:ASN:ND2	2.47	0.43
24:W:370:TYR:HA	24:W:371:THR:HB	2.01	0.43
26:Y:384:SER:HB2	27:Z:279:LYS:HD3	2.00	0.43
26:Y:387:ILE:HD13	27:Z:283:ARG:HG3	2.00	0.43
16:A:303:ILE:HA	16:A:306:LEU:HB2	2.01	0.43
19:E:355:ILE:HD11	20:F:211:LYS:HE3	1.99	0.43
2:G:9:PHE:O	2:G:13:ILE:HG12	2.18	0.43
3:H:182:LEU:HD23	3:H:183:GLU:H	1.83	0.43
4:I:228:LEU:HB3	4:I:229:LYS:CA	2.48	0.43
6:K:157:ASP:OD1	6:K:161:THR:N	2.48	0.43
7:L:82:ARG:HA	7:L:85:CYS:HB3	2.00	0.43
9:N:16:ALA:HB1	9:N:33:LYS:HB2	2.01	0.43
11:P:21:ALA:HB2	11:P:189:ILE:HD13	2.00	0.43
22:U:138:PHE:CZ	22:U:166:THR:HG22	2.54	0.43
26:Y:67:VAL:O	26:Y:71:ASN:N	2.50	0.43
21:C:246:ILE:HB	21:C:291:VAL:HG12	2.00	0.43
19:E:385:ASP:HB3	19:E:386:TYR:CD1	2.54	0.43
20:F:433:ALA:HA	20:F:434:ASN:CG	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:86:LYS:HA	6:K:89:ILE:HB	2.01	0.43
9:N:2:THR:HA	9:N:129:GLY:HA3	1.99	0.43
13:R:167:ASP:OD1	13:R:168:ALA:N	2.52	0.43
22:U:154:ALA:HB1	22:U:163:PHE:CD1	2.52	0.43
22:U:172:ASP:HA	22:U:173:VAL:HB	2.01	0.43
23:V:266:GLN:HG3	23:V:295:ILE:HD12	2.01	0.43
24:W:135:LYS:HB3	24:W:136:ILE:CA	2.49	0.43
24:W:435:LEU:HA	24:W:438:LEU:HG	2.00	0.43
24:W:419:LYS:HE2	25:X:388:PHE:HA	2.01	0.43
26:Y:203:ASP:N	26:Y:203:ASP:OD1	2.52	0.43
26:Y:47:ASP:HB3	26:Y:49:ASN:ND2	2.33	0.43
27:Z:191:ILE:O	27:Z:195:VAL:HG23	2.18	0.43
16:A:203:ASN:HB3	16:A:204:LEU:HD12	2.01	0.43
17:B:187:ILE:HD12	17:B:190:LEU:HD21	2.01	0.43
21:C:249:ASP:HA	21:C:250:GLU:HA	1.72	0.43
21:C:84:LYS:HE3	21:C:96:VAL:HG22	2.01	0.43
4:I:44:LEU:HD22	4:I:190:LEU:HG	2.00	0.43
23:V:48:THR:HG23	23:V:147:PHE:HE2	1.83	0.43
23:V:186:LYS:NZ	23:V:234:ARG:HD3	2.33	0.43
26:Y:268:TYR:CZ	26:Y:307:LEU:HD12	2.54	0.43
27:Z:39:LEU:HB2	27:Z:95:TYR:HD2	1.82	0.43
16:A:249:TYR:N	17:B:304:GLU:OE2	2.38	0.43
21:C:194:THR:HG22	21:C:195:GLY:H	1.83	0.43
18:D:181:VAL:C	18:D:184:PRO:HD2	2.39	0.43
19:E:349:GLU:HG2	19:E:374:VAL:HG11	1.99	0.43
2:G:119:ALA:HB1	2:G:158:GLY:C	2.38	0.43
3:H:111:VAL:HG22	3:H:136:ILE:HG21	2.00	0.43
4:I:18:LEU:HD13	4:I:21:VAL:HG21	2.00	0.43
6:K:236:GLU:HA	6:K:239:LYS:HE3	2.00	0.43
10:O:25:VAL:HG11	11:P:147:TYR:CZ	2.54	0.43
23:V:484:LEU:HA	23:V:487:HIS:HD2	1.83	0.43
24:W:215:GLN:NE2	24:W:227:TYR:OH	2.44	0.43
25:X:223:LYS:HD3	26:Y:244:ALA:HA	2.01	0.43
16:A:291:GLY:H	16:A:294:GLU:HG2	1.83	0.42
16:A:316:LYS:O	16:A:317:VAL:HG13	2.19	0.42
16:A:373:LEU:HD23	16:A:415:LYS:HG2	2.01	0.42
18:D:356:GLU:HG2	18:D:357:GLU:H	1.83	0.42
20:F:170:SER:OG	20:F:171:ARG:N	2.50	0.42
19:E:381:GLU:OE1	20:F:351:LYS:HE3	2.19	0.42
2:G:140:LEU:N	2:G:152:TYR:O	2.37	0.42
3:H:86:LEU:HD13	3:H:134:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:R:13:ILE:HD12	13:R:176:LEU:HD11	2.01	0.42
15:T:24:ALA:H	15:T:42:ILE:HD11	1.84	0.42
23:V:91:PRO:HA	23:V:94:VAL:HG12	2.00	0.42
26:Y:324:GLY:N	26:Y:325:VAL:HA	2.33	0.42
21:C:277:LEU:HD22	21:C:311:ILE:HD11	2.01	0.42
18:D:146:GLU:CD	18:D:147:ALA:H	2.22	0.42
18:D:92:PHE:HA	18:D:103:VAL:HG23	2.01	0.42
19:E:37:THR:HG21	20:F:66:LEU:HD22	2.00	0.42
4:I:187:LYS:HA	4:I:190:LEU:HB2	2.00	0.42
6:K:96:THR:HG22	6:K:107:MET:HB3	2.01	0.42
6:K:227:HIS:HA	6:K:228:MET:C	2.39	0.42
8:M:49:VAL:O	8:M:212:GLU:N	2.44	0.42
8:M:8:ASP:O	8:M:22:GLN:NE2	2.32	0.42
11:P:113:ASP:OD1	11:P:114:PRO:HD2	2.19	0.42
22:U:525:ASN:HB3	22:U:528:ALA:HB2	2.01	0.42
22:U:681:ASN:OD1	22:U:681:ASN:N	2.51	0.42
23:V:197:THR:C	23:V:199:ASN:H	2.22	0.42
23:V:367:VAL:HG22	23:V:398:LEU:HD21	2.01	0.42
26:Y:289:ALA:HB3	26:Y:290:PRO:HD3	2.01	0.42
18:D:114:ARG:NH2	21:C:62:GLU:HG2	2.34	0.42
4:I:47:ALA:HB1	4:I:64:LYS:HB3	2.01	0.42
12:Q:43:LEU:HD21	12:Q:188:ILE:HG12	2.02	0.42
23:V:455:LYS:H	23:V:456:GLY:HA2	1.80	0.42
24:W:406:VAL:HA	24:W:413:ILE:HG22	2.01	0.42
25:X:366:SER:HB2	26:Y:310:SER:HB3	2.02	0.42
26:Y:42:MET:HG3	26:Y:46:ARG:HH12	1.84	0.42
27:Z:68:TRP:HH2	27:Z:111:LEU:HD22	1.84	0.42
16:A:180:CYS:HB3	16:A:184:ILE:HB	2.00	0.42
16:A:292:ASP:O	16:A:296:GLN:HG2	2.19	0.42
17:B:166:ASP:OD1	21:C:78:ARG:NH1	2.52	0.42
17:B:296:ASP:HA	17:B:297:SER:HA	1.56	0.42
21:C:175:PHE:CE2	21:C:182:GLN:HG3	2.55	0.42
2:G:110:PRO:O	2:G:111:VAL:HG12	2.19	0.42
8:M:68:ASN:ND2	8:M:224:HIS:O	2.53	0.42
11:P:58:THR:OG1	12:Q:121:LEU:O	2.23	0.42
24:W:162:ALA:O	24:W:166:LEU:HG	2.20	0.42
25:X:245:PRO:HA	25:X:248:ILE:HG22	2.02	0.42
26:Y:80:GLU:O	26:Y:84:LEU:HG	2.20	0.42
16:A:121:PHE:CE1	20:F:86:LEU:HD22	2.55	0.42
17:B:144:LEU:HD21	17:B:162:VAL:HB	2.02	0.42
17:B:224:LEU:O	17:B:330:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:219:LEU:HD23	21:C:219:LEU:O	2.19	0.42
18:D:381:GLU:O	18:D:385:LEU:N	2.47	0.42
19:E:264:MET:HE3	19:E:294:ARG:HB3	2.01	0.42
20:F:293:THR:HG23	20:F:337:ILE:HG21	2.01	0.42
2:G:155:ASP:HB3	2:G:156:PRO:HD2	2.02	0.42
6:K:114:GLN:HA	6:K:117:SER:HB2	2.00	0.42
22:U:257:SER:O	22:U:261:LEU:HG	2.20	0.42
22:U:479:LEU:HD13	22:U:511:ALA:HA	2.02	0.42
22:U:607:VAL:O	22:U:615:ARG:NH1	2.53	0.42
23:V:306:ARG:HB3	23:V:339:LEU:HD21	2.00	0.42
24:W:216:GLU:CD	24:W:217:GLU:H	2.23	0.42
26:Y:63:TRP:HB3	26:Y:64:GLN:CB	2.49	0.42
16:A:344:SER:O	16:A:344:SER:OG	2.19	0.42
16:A:94:GLN:NE2	17:B:157:HIS:HB2	2.34	0.42
20:F:234:THR:HG22	20:F:238:ARG:HH22	1.85	0.42
2:G:159:TYR:CD2	18:D:418:LYS:HG3	2.54	0.42
3:H:115:ALA:HA	3:H:118:MET:HB3	2.01	0.42
22:U:357:LYS:NZ	22:U:389:ASN:HD22	2.18	0.42
22:U:792:ASN:HA	22:U:914:LEU:HB3	2.01	0.42
24:W:347:GLY:O	24:W:351:TRP:N	2.51	0.42
24:W:92:LYS:HB2	24:W:93:ARG:HB2	2.02	0.42
26:Y:192:ARG:NH2	26:Y:294:TYR:HB3	2.33	0.42
26:Y:356:THR:HA	26:Y:357:ASN:OD1	2.19	0.42
27:Z:210:SER:O	27:Z:214:LYS:HG2	2.18	0.42
18:D:130:VAL:HB	18:D:142:VAL:HG12	2.01	0.42
18:D:82:ILE:HA	18:D:83:GLN:HA	1.68	0.42
19:E:54:GLY:H	20:F:158:TYR:HB2	1.85	0.42
4:I:79:ILE:HG22	4:I:82:ASP:H	1.85	0.42
22:U:56:SER:O	22:U:60:ALA:N	2.45	0.42
23:V:157:THR:OG1	23:V:158:PRO:HD3	2.20	0.42
23:V:90:GLU:N	23:V:90:GLU:OE1	2.46	0.42
25:X:391:PRO:HG2	25:X:392:PRO:HD3	2.02	0.42
26:Y:170:GLU:CG	26:Y:171:GLY:HA3	2.43	0.42
26:Y:84:LEU:HD12	26:Y:111:LEU:HD11	2.02	0.42
21:C:200:ALA:HB1	21:C:211:PHE:CZ	2.55	0.42
19:E:228:CYS:HB3	19:E:273:VAL:HG23	2.01	0.42
2:G:43:ARG:HD2	2:G:149:PRO:HG2	2.02	0.42
3:H:3:GLU:HA	3:H:4:ARG:HB2	2.01	0.42
5:J:109:ARG:NH2	13:R:69:ARG:HH11	2.18	0.42
24:W:353:ASP:OD1	24:W:357:ARG:NH2	2.52	0.42
25:X:332:GLU:HA	25:X:335:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:389:ASP:HB2	25:X:391:PRO:HD3	2.01	0.42
26:Y:191:ILE:HA	26:Y:191:ILE:HD12	1.91	0.42
21:C:168:PRO:HB2	21:C:288:ASN:ND2	2.35	0.42
10:O:83:LEU:HD13	10:O:113:ILE:HD13	2.02	0.42
12:Q:16:ALA:HA	12:Q:180:VAL:HA	2.02	0.42
12:Q:29:LYS:HE3	12:Q:32:HIS:HA	2.02	0.42
23:V:470:ARG:O	23:V:473:GLN:HG2	2.19	0.42
16:A:121:PHE:CD2	16:A:123:VAL:HB	2.54	0.42
17:B:217:LYS:HG2	17:B:219:PRO:HD3	2.00	0.42
17:B:364:ILE:O	17:B:368:HIS:ND1	2.48	0.42
21:C:268:GLU:HG3	25:X:409:LYS:HG3	63.01	0.42
19:E:309:ARG:HD2	19:E:332:VAL:HG13	2.02	0.42
19:E:61:LEU:HD12	19:E:70:ILE:HG22	2.01	0.42
20:F:228:PRO:O	20:F:231:THR:HG23	2.19	0.42
14:S:71:ARG:NE	14:S:91:MET:SD	2.75	0.42
23:V:295:ILE:O	23:V:298:ILE:HG22	2.20	0.42
24:W:306:LEU:O	24:W:310:THR:HG22	2.20	0.42
24:W:455:LEU:HD12	24:W:456:GLN:N	2.35	0.42
24:W:70:VAL:O	24:W:73:MET:HG2	2.20	0.42
27:Z:187:LEU:HA	27:Z:190:ARG:HG2	2.02	0.42
27:Z:199:LYS:HA	27:Z:202:ASN:ND2	2.35	0.42
16:A:237:PHE:HA	16:A:270:CYS:SG	2.60	0.41
16:A:293:ASN:ND2	20:F:303:ASP:HB2	2.35	0.41
5:J:20:GLU:HG3	16:A:430:MET:HE1	2.02	0.41
17:B:155:LYS:HA	17:B:156:VAL:HA	1.61	0.41
17:B:394:ASP:HA	21:C:311:ILE:HD13	2.02	0.41
21:C:192:PRO:HA	21:C:193:GLY:HA3	1.67	0.41
20:F:275:ALA:HB1	20:F:326:VAL:HG21	2.02	0.41
20:F:397:LYS:HE3	20:F:397:LYS:HB3	1.95	0.41
2:G:11:ARG:O	2:G:24:GLN:NE2	2.35	0.41
6:K:33:LEU:HB2	16:A:431:THR:HB	2.02	0.41
7:L:95:SER:HB3	7:L:103:LEU:HG	2.01	0.41
22:U:381:THR:HG22	22:U:412:HIS:HA	2.02	0.41
24:W:417:ARG:HG3	24:W:420:ASP:OD1	2.21	0.41
26:Y:357:ASN:CB	26:Y:358:ARG:HA	2.47	0.41
16:A:316:LYS:HB3	16:A:316:LYS:HE3	1.84	0.41
16:A:325:ASP:HA	16:A:326:THR:HA	1.57	0.41
16:A:401:ARG:HH12	16:A:414:ASN:ND2	2.18	0.41
21:C:331:ILE:HD13	21:C:334:ARG:HE	1.83	0.41
20:F:362:ARG:NH2	20:F:389:ASP:HA	2.35	0.41
2:G:101:TRP:CD2	2:G:105:TYR:HD2	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:67:LEU:HD21	11:P:87:LEU:HD11	2.02	0.41
23:V:277:PRO:HA	23:V:278:GLU:HA	1.74	0.41
24:W:135:LYS:CB	24:W:136:ILE:HB	2.50	0.41
24:W:155:GLN:HE21	24:W:161:GLU:HG3	1.85	0.41
24:W:428:TRP:O	24:W:432:LEU:HB2	2.19	0.41
24:W:59:ASP:HA	24:W:63:THR:HG23	2.02	0.41
26:Y:14:ASN:HD21	26:Y:214:MET:HA	1.85	0.41
21:C:377:HIS:HB3	26:Y:174:TRP:CD1	2.56	0.41
27:Z:225:GLN:NE2	27:Z:229:GLN:OE1	2.49	0.41
16:A:204:LEU:HB3	16:A:205:GLY:HA3	2.02	0.41
16:A:429:TYR:HA	16:A:432:TYR:CZ	2.55	0.41
17:B:220:LYS:HB2	17:B:348:ASP:HB2	2.02	0.41
17:B:256:ILE:HG21	17:B:312:LEU:HD22	2.03	0.41
17:B:393:ALA:HB2	21:C:281:ASP:HB2	2.02	0.41
21:C:379:THR:HG23	21:C:382:ASP:H	1.84	0.41
19:E:91:LYS:HD2	19:E:107:ILE:HB	2.02	0.41
2:G:103:TYR:O	10:O:81:ARG:HG2	2.21	0.41
2:G:12:HIS:HB3	8:M:13:THR:HG21	2.01	0.41
3:H:38:ILE:HD13	3:H:188:ILE:HA	2.01	0.41
5:J:43:LEU:HD23	5:J:134:VAL:HG11	2.02	0.41
5:J:36:ARG:HB3	5:J:144:LEU:HD23	2.03	0.41
12:Q:153:ARG:HH22	12:Q:184:ASP:HB3	1.85	0.41
22:U:692:ALA:HB1	22:U:736:ILE:HB	2.03	0.41
23:V:296:LYS:HA	23:V:299:GLN:HB2	2.01	0.41
16:A:199:GLU:HA	20:F:408:LEU:HD22	2.02	0.41
16:A:206:ILE:HG13	20:F:373:MET:HB3	2.02	0.41
16:A:328:ASP:HB3	16:A:329:PRO:HD3	2.02	0.41
17:B:214:MET:HG3	17:B:216:ILE:HG12	2.02	0.41
17:B:283:PHE:HE2	17:B:285:ASP:HB2	1.84	0.41
19:E:251:ARG:NH1	19:E:255:ARG:HD3	2.36	0.41
7:L:130:VAL:HG22	7:L:132:LEU:H	1.84	0.41
14:S:211:ARG:NE	14:S:213:ASP:O	2.54	0.41
15:T:174:ARG:NH2	15:T:206:GLU:OE1	2.53	0.41
22:U:34:PHE:O	22:U:38:ILE:HG12	2.21	0.41
23:V:25:GLU:O	23:V:28:PRO:HD2	2.19	0.41
27:Z:205:LEU:HA	27:Z:208:ILE:HG22	2.02	0.41
16:A:312:ARG:HA	16:A:313:GLY:HA2	1.58	0.41
16:A:321:THR:OG1	16:A:322:ASN:N	2.54	0.41
17:B:139:VAL:HB	17:B:141:LYS:N	2.35	0.41
17:B:139:VAL:HB	17:B:141:LYS:H	1.85	0.41
17:B:238:ALA:O	17:B:242:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B:283:PHE:CE2	17:B:285:ASP:HB2	2.55	0.41
17:B:433:GLY:O	17:B:434:THR:OG1	2.34	0.41
21:C:115:ALA:HB3	21:C:125:LYS:H	1.85	0.41
18:D:373:ALA:HB1	18:D:375:ILE:HB	2.03	0.41
18:D:409:LYS:HB2	18:D:410:ASP:C	2.41	0.41
19:E:60:VAL:O	19:E:95:GLY:HA2	2.20	0.41
2:G:91:VAL:HG12	2:G:95:ARG:HE	1.86	0.41
7:L:50:LYS:HD2	7:L:208:LYS:O	2.21	0.41
9:N:7:GLN:HA	9:N:12:VAL:HA	2.03	0.41
13:R:67:GLU:O	13:R:71:LYS:N	2.53	0.41
23:V:326:GLN:NE2	23:V:350:GLN:HE21	2.18	0.41
24:W:423:ASN:N	24:W:423:ASN:OD1	2.53	0.41
26:Y:40:GLU:O	26:Y:44:ALA:N	2.54	0.41
19:E:101:ASP:N	19:E:106:THR:O	2.54	0.41
2:G:61:LEU:HA	8:M:160:TYR:CD1	2.56	0.41
7:L:85:CYS:HG	7:L:89:ARG:HH12	1.67	0.41
9:N:20:THR:HB	9:N:28:ASN:HB3	2.03	0.41
10:O:94:ILE:HA	11:P:99:ARG:HH21	1.85	0.41
22:U:342:LEU:HD13	22:U:378:CYS:O	2.21	0.41
22:U:697:GLN:HG3	22:U:745:THR:HB	2.03	0.41
23:V:318:GLN:O	23:V:319:HIS:CG	2.74	0.41
21:C:151:ILE:HG21	21:C:154:LEU:HD13	2.03	0.41
18:D:296:MET:HA	18:D:299:PHE:CD2	2.56	0.41
3:H:4:ARG:HA	3:H:13:PHE:CG	2.55	0.41
7:L:137:TYR:CZ	7:L:142:PRO:HB3	2.56	0.41
7:L:212:ILE:HD13	7:L:229:VAL:HG13	2.03	0.41
13:R:178:HIS:O	13:R:185:ILE:N	2.51	0.41
22:U:403:THR:HG23	22:U:777:HIS:HE2	1.85	0.41
23:V:344:ASP:HB2	23:V:368:ARG:HH11	1.86	0.41
24:W:397:VAL:HG11	25:X:342:PHE:HD2	1.84	0.41
24:W:402:ILE:HG23	24:W:416:GLN:HE22	1.85	0.41
24:W:375:MET:N	24:W:411:GLY:O	2.47	0.41
16:A:250:VAL:HB	16:A:297:ARG:NH2	2.36	0.41
16:A:396:ALA:HA	16:A:401:ARG:HG3	2.01	0.41
20:F:145:LEU:HG	20:F:146:LYS:H	1.84	0.41
20:F:224:LEU:HB3	20:F:351:LYS:HG2	2.02	0.41
6:K:85:ALA:O	6:K:89:ILE:HG12	2.20	0.41
25:X:339:ILE:HG21	25:X:374:PHE:HE1	1.86	0.41
26:Y:349:LYS:C	26:Y:351:ASN:H	2.24	0.41
16:A:187:LEU:O	16:A:191:VAL:HG12	2.21	0.41
16:A:188:ARG:HG3	16:A:192:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:344:ILE:HA	18:D:347:THR:HG22	2.03	0.41
10:O:21:THR:HG22	10:O:26:VAL:HA	2.03	0.41
22:U:413:LYS:HA	22:U:449:ILE:HG12	2.03	0.41
22:U:684:ARG:O	22:U:688:LEU:HG	2.21	0.41
23:V:298:ILE:HA	23:V:298:ILE:HD12	1.96	0.41
23:V:318:GLN:O	23:V:319:HIS:ND1	2.54	0.41
24:W:455:LEU:HD12	24:W:456:GLN:H	1.86	0.41
17:B:364:ILE:HG21	17:B:392:GLY:HA3	2.02	0.41
21:C:139:MET:O	21:C:143:VAL:HG12	2.21	0.41
21:C:165:ILE:HD12	21:C:207:THR:HG23	2.03	0.41
18:D:115:ILE:HA	18:D:139:LEU:HB2	2.02	0.41
18:D:268:ASP:OD1	18:D:268:ASP:N	2.54	0.41
18:D:293:LEU:O	18:D:296:MET:HG2	2.20	0.41
18:D:313:ARG:NH2	18:D:315:ASP:OD2	2.40	0.41
18:D:48:GLN:HA	18:D:51:LEU:HB3	2.03	0.41
4:I:122:THR:HG22	4:I:129:PRO:HB3	2.03	0.41
14:S:193:LEU:N	14:S:208:VAL:O	2.49	0.41
22:U:374:SER:HB2	22:U:410:VAL:HB	2.01	0.41
23:V:70:VAL:O	23:V:74:ASP:N	2.46	0.41
21:C:234:LEU:HD21	21:C:246:ILE:HG21	2.03	0.41
18:D:150:SER:OG	18:D:151:ILE:N	2.54	0.41
18:D:154:LEU:C	18:D:156:SER:H	2.25	0.41
19:E:100:LEU:HD23	19:E:107:ILE:HG13	2.02	0.41
2:G:32:ILE:HG12	2:G:137:CYS:HB2	2.03	0.41
3:H:14:SER:HA	3:H:20:VAL:HG23	2.03	0.41
6:K:178:GLN:OE1	6:K:182:GLN:NE2	2.54	0.41
6:K:227:HIS:N	6:K:228:MET:HB3	2.36	0.41
6:K:73:HIS:HA	6:K:226:PHE:CZ	2.55	0.41
13:R:113:TYR:O	13:R:120:ARG:HA	2.21	0.41
22:U:631:GLU:O	22:U:634:PRO:HD2	2.21	0.41
24:W:205:ILE:O	24:W:209:ILE:HG12	2.21	0.41
27:Z:227:ILE:HD13	27:Z:227:ILE:HA	1.96	0.41
27:Z:34:ARG:HB2	27:Z:97:THR:HG22	2.02	0.41
21:C:87:VAL:O	21:C:95:PHE:N	2.49	0.40
19:E:135:ILE:HG13	19:E:135:ILE:H	1.70	0.40
3:H:111:VAL:HG21	3:H:147:PHE:HD2	1.86	0.40
9:N:21:THR:HG22	9:N:26:ILE:HA	2.02	0.40
9:N:50:ALA:N	10:O:118:SER:HB3	2.36	0.40
11:P:25:ASP:HA	11:P:185:VAL:HA	2.03	0.40
12:Q:18:ASP:HA	12:Q:178:PHE:HD1	1.86	0.40
22:U:229:VAL:HG21	22:U:252:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:135:LYS:HB3	24:W:137:TYR:N	2.37	0.40
24:W:75:TYR:HD1	24:W:78:LYS:HE2	1.86	0.40
17:B:191:ASP:N	17:B:191:ASP:OD1	2.53	0.40
17:B:234:LEU:HD21	17:B:353:PHE:HB2	2.01	0.40
17:B:418:ASP:O	17:B:422:SER:N	2.50	0.40
4:I:119:GLN:HE22	5:J:79:ASP:HA	1.86	0.40
13:R:40:TYR:CD2	13:R:41:LEU:HG	2.56	0.40
22:U:574:LYS:HG2	22:U:574:LYS:H	1.66	0.40
22:U:583:MET:HA	22:U:586:VAL:HG12	2.02	0.40
23:V:224:LEU:HD12	23:V:224:LEU:O	2.21	0.40
26:Y:355:GLU:HG3	26:Y:357:ASN:ND2	2.36	0.40
26:Y:48:ASN:HA	26:Y:73:MET:HE2	2.03	0.40
27:Z:199:LYS:HA	27:Z:202:ASN:HD21	1.86	0.40
17:B:390:LEU:HA	17:B:390:LEU:HD12	1.81	0.40
21:C:327:ASP:OD1	21:C:328:ILE:N	2.55	0.40
18:D:389:GLU:HB3	18:D:391:ARG:H	1.86	0.40
20:F:434:ASN:CG	20:F:435:LEU:H	2.23	0.40
2:G:74:GLU:HB3	2:G:226:LYS:HG3	2.03	0.40
5:J:76:LEU:HD13	5:J:78:ALA:HB3	2.02	0.40
6:K:211:ASN:OD1	6:K:214:ASN:N	2.55	0.40
9:N:21:THR:HA	9:N:27:ALA:H	1.87	0.40
22:U:742:HIS:O	22:U:883:ARG:NH2	2.55	0.40
24:W:365:ILE:HG13	24:W:366:MET:N	2.36	0.40
24:W:451:MET:HE1	27:Z:157:HIS:H	1.85	0.40
26:Y:367:GLN:HG3	26:Y:371:LYS:HG2	2.03	0.40
27:Z:118:ASN:N	27:Z:118:ASN:OD1	2.55	0.40
16:A:327:LEU:O	16:A:331:LEU:HG	2.21	0.40
17:B:151:LEU:HD21	21:C:82:LYS:HE2	2.03	0.40
17:B:170:LEU:O	17:B:173:VAL:HG22	2.21	0.40
17:B:175:LYS:HA	17:B:176:VAL:HA	1.87	0.40
17:B:194:ILE:HG13	17:B:237:LYS:HD3	2.03	0.40
19:E:101:ASP:O	19:E:105:LEU:HA	2.21	0.40
18:D:377:SER:HB3	19:E:292:PRO:HB2	2.02	0.40
19:E:55:GLN:HB3	19:E:100:LEU:O	2.20	0.40
2:G:80:MET:HG3	2:G:87:SER:HB2	2.04	0.40
3:H:171:LYS:HD2	3:H:171:LYS:HA	1.94	0.40
4:I:68:LEU:HD22	4:I:90:LEU:HD22	2.02	0.40
6:K:152:GLN:OE1	6:K:164:GLN:NE2	2.55	0.40
11:P:135:ASP:OD2	11:P:154:TRP:NE1	2.48	0.40
14:S:136:LYS:HA	14:S:136:LYS:HD3	1.96	0.40
22:U:669:ILE:HG12	22:U:694:ILE:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:8:ARG:HD2	24:W:34:LEU:HD21	2.02	0.40
24:W:405:LYS:HG3	25:X:344:ARG:HG2	2.04	0.40
16:A:108:ASP:HB2	16:A:109:PRO:HD3	2.04	0.40
17:B:220:LYS:HA	17:B:346:ARG:NH2	2.37	0.40
17:B:224:LEU:HD13	17:B:234:LEU:HB3	2.03	0.40
17:B:401:GLU:HA	17:B:404:LEU:HB3	2.03	0.40
19:E:87:LEU:H	19:E:87:LEU:HG	1.73	0.40
20:F:227:GLY:HA3	20:F:231:THR:HG21	2.02	0.40
20:F:89:LEU:HD11	20:F:126:THR:HB	2.04	0.40
2:G:10:ASP:HB3	2:G:15:ILE:HD11	2.03	0.40
3:H:86:LEU:HA	3:H:89:ARG:HB3	2.03	0.40
6:K:125:GLU:O	6:K:134:SER:N	2.54	0.40
7:L:205:LEU:N	7:L:209:ASN:HD21	2.18	0.40
9:N:26:ILE:HG21	9:N:29:ARG:HD3	2.03	0.40
13:R:54:PHE:O	13:R:58:LEU:N	2.47	0.40
22:U:485:ALA:O	22:U:488:THR:OG1	2.31	0.40
22:U:32:ASN:ND2	23:V:229:SER:OG	2.55	0.40
23:V:342:ILE:HG12	23:V:343:PRO:O	2.22	0.40
26:Y:145:LEU:HD13	26:Y:183:TYR:CD1	2.56	0.40
26:Y:301:ILE:HG13	26:Y:343:LEU:HD12	2.04	0.40
27:Z:223:ASN:HD22	27:Z:227:ILE:HG12	1.86	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	f	686/749 (92%)	575 (84%)	107 (16%)	4 (1%)	30	74
2	G	238/245 (97%)	221 (93%)	15 (6%)	2 (1%)	24	69
3	H	230/233 (99%)	200 (87%)	28 (12%)	2 (1%)	21	67
4	I	248/260 (95%)	223 (90%)	25 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	J	237/247 (96%)	214 (90%)	21 (9%)	2 (1%)	24	69
6	K	224/240 (93%)	196 (88%)	27 (12%)	1 (0%)	39	80
7	L	236/268 (88%)	221 (94%)	15 (6%)	0	100	100
8	M	238/254 (94%)	221 (93%)	17 (7%)	0	100	100
9	N	189/238 (79%)	179 (95%)	10 (5%)	0	100	100
10	O	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
11	P	202/204 (99%)	187 (93%)	15 (7%)	0	100	100
12	Q	197/201 (98%)	183 (93%)	14 (7%)	0	100	100
13	R	199/262 (76%)	185 (93%)	14 (7%)	0	100	100
14	S	211/240 (88%)	199 (94%)	12 (6%)	0	100	100
15	T	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
16	A	359/433 (83%)	307 (86%)	51 (14%)	1 (0%)	46	83
17	B	344/440 (78%)	304 (88%)	38 (11%)	2 (1%)	30	74
18	D	378/418 (90%)	323 (85%)	51 (14%)	4 (1%)	17	63
19	E	351/403 (87%)	317 (90%)	34 (10%)	0	100	100
20	F	362/439 (82%)	327 (90%)	34 (9%)	1 (0%)	46	83
21	C	390/398 (98%)	344 (88%)	42 (11%)	4 (1%)	19	65
22	U	798/953 (84%)	738 (92%)	59 (7%)	1 (0%)	56	90
23	V	478/533 (90%)	421 (88%)	57 (12%)	0	100	100
24	W	454/456 (100%)	407 (90%)	44 (10%)	3 (1%)	26	71
25	X	239/422 (57%)	213 (89%)	26 (11%)	0	100	100
26	Y	376/389 (97%)	332 (88%)	42 (11%)	2 (0%)	34	77
27	Z	284/324 (88%)	253 (89%)	30 (11%)	1 (0%)	39	80
28	a	371/376 (99%)	331 (89%)	38 (10%)	2 (0%)	34	77
29	b	189/377 (50%)	175 (93%)	14 (7%)	0	100	100
30	c	274/309 (89%)	246 (90%)	25 (9%)	3 (1%)	17	63
31	d	255/349 (73%)	229 (90%)	26 (10%)	0	100	100
32	e	36/70 (51%)	31 (86%)	5 (14%)	0	100	100
All	All	9704/11269 (86%)	8711 (90%)	958 (10%)	35 (0%)	43	80

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	f	62	ILE
1	f	447	VAL
2	G	111	VAL
22	U	364	VAL
24	W	68	VAL
24	W	136	ILE
26	Y	350	VAL
1	f	131	VAL
30	c	157	ILE
1	f	281	ILE
5	J	199	VAL
21	C	298	ILE
28	a	340	VAL
3	H	127	VAL
6	K	12	VAL
18	D	151	ILE
21	C	68	GLU
21	C	219	LEU
24	W	138	VAL
26	Y	67	VAL
27	Z	144	VAL
30	c	156	VAL
17	B	218	PRO
18	D	411	GLU
18	D	406	VAL
18	D	259	PRO
28	a	336	VAL
30	c	189	ILE
2	G	170	VAL
3	H	20	VAL
21	C	251	ILE
16	A	206	ILE
17	B	325	VAL
20	F	326	VAL
5	J	98	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	f	582/628 (93%)	572 (98%)	10 (2%)	68	87
2	G	193/209 (92%)	189 (98%)	4 (2%)	61	84
3	H	164/190 (86%)	162 (99%)	2 (1%)	78	90
4	I	193/220 (88%)	191 (99%)	2 (1%)	82	92
5	J	152/210 (72%)	151 (99%)	1 (1%)	88	94
6	K	186/202 (92%)	184 (99%)	2 (1%)	80	91
7	L	198/229 (86%)	198 (100%)	0	100	100
8	M	192/211 (91%)	192 (100%)	0	100	100
9	N	148/180 (82%)	148 (100%)	0	100	100
10	O	177/227 (78%)	177 (100%)	0	100	100
11	P	172/173 (99%)	172 (100%)	0	100	100
12	Q	164/171 (96%)	164 (100%)	0	100	100
13	R	153/201 (76%)	153 (100%)	0	100	100
14	S	174/198 (88%)	174 (100%)	0	100	100
15	T	175/214 (82%)	175 (100%)	0	100	100
16	A	308/372 (83%)	302 (98%)	6 (2%)	65	86
17	B	304/385 (79%)	297 (98%)	7 (2%)	58	83
18	D	333/366 (91%)	330 (99%)	3 (1%)	84	93
19	E	308/353 (87%)	302 (98%)	6 (2%)	65	86
20	F	312/379 (82%)	309 (99%)	3 (1%)	82	92
21	C	340/346 (98%)	336 (99%)	4 (1%)	78	90
22	U	685/816 (84%)	681 (99%)	4 (1%)	90	95
23	V	414/459 (90%)	412 (100%)	2 (0%)	92	96
24	W	416/416 (100%)	412 (99%)	4 (1%)	82	92
25	X	208/362 (58%)	207 (100%)	1 (0%)	92	96
26	Y	334/344 (97%)	332 (99%)	2 (1%)	90	95
27	Z	257/295 (87%)	255 (99%)	2 (1%)	86	94
28	a	333/336 (99%)	331 (99%)	2 (1%)	90	95
29	b	167/312 (54%)	167 (100%)	0	100	100
30	c	243/267 (91%)	239 (98%)	4 (2%)	70	88
31	d	231/293 (79%)	228 (99%)	3 (1%)	76	89
32	e	38/63 (60%)	37 (97%)	1 (3%)	54	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	8254/9627 (86%)	8179 (99%)	75 (1%)	85	93

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	f	15	ASP
1	f	33	VAL
1	f	301	ASP
1	f	334	ASN
1	f	339	LEU
1	f	342	LEU
1	f	371	CYS
1	f	391	LEU
1	f	526	THR
1	f	659	LEU
2	G	22	LEU
2	G	34	GLN
2	G	111	VAL
2	G	159	TYR
3	H	13	PHE
3	H	182	LEU
4	I	34	CYS
4	I	107	CYS
5	J	3	TYR
6	K	36	THR
6	K	42	THR
16	A	94	GLN
16	A	125	LEU
16	A	153	LEU
16	A	316	LYS
16	A	331	LEU
16	A	344	SER
17	B	105	THR
17	B	235	LEU
17	B	307	ARG
17	B	316	LEU
17	B	348	ASP
17	B	355	LEU
17	B	436	GLU
18	D	186	THR
18	D	234	GLU
18	D	303	VAL

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Mol	Chain	Res	Type
19	E	65	THR
19	E	87	LEU
19	E	104	THR
19	E	265	ASP
19	E	269	THR
19	E	358	ASP
20	F	88	TYR
20	F	270	ASP
20	F	427	VAL
21	C	109	THR
21	C	138	MET
21	C	298	ILE
21	C	311	ILE
22	U	336	GLU
22	U	479	LEU
22	U	554	LEU
22	U	895	PRO
23	V	224	LEU
23	V	255	LEU
24	W	250	ILE
24	W	371	THR
24	W	417	ARG
24	W	444	HIS
25	X	331	LEU
26	Y	315	THR
26	Y	352	GLU
27	Z	176	LEU
27	Z	186	THR
28	a	28	LEU
28	a	158	LEU
30	c	194	HIS
30	c	229	LEU
30	c	273	LYS
30	c	309	PHE
31	d	158	ILE
31	d	190	LEU
31	d	193	GLU
32	e	43	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	f	246	HIS
1	f	269	GLN
1	f	293	ASN
1	f	491	GLN
1	f	565	ASN
2	G	53	GLN
2	G	100	ASN
4	I	95	GLN
4	I	109	GLN
4	I	119	GLN
6	K	23	GLN
6	K	97	GLN
6	K	164	GLN
7	L	166	GLN
7	L	190	HIS
9	N	187	GLN
11	P	33	GLN
12	Q	8	GLN
12	Q	99	HIS
13	R	29	GLN
13	R	85	ASN
15	T	2	GLN
15	T	69	GLN
16	A	414	ASN
17	B	157	HIS
17	B	314	ASN
18	D	57	GLN
18	D	137	ASN
18	D	286	GLN
18	D	301	GLN
18	D	302	ASN
18	D	304	ASN
18	D	376	ASN
19	E	190	GLN
19	E	316	HIS
20	F	194	GLN
21	C	50	ASN
21	C	129	ASN
21	C	205	HIS
21	C	270	GLN
21	C	278	ASN
21	C	288	ASN
22	U	189	GLN

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Mol	Chain	Res	Type
22	U	345	ASN
22	U	389	ASN
22	U	421	GLN
22	U	698	GLN
22	U	756	HIS
23	V	62	HIS
23	V	299	GLN
23	V	326	GLN
23	V	427	GLN
23	V	459	GLN
23	V	477	HIS
23	V	487	HIS
24	W	155	GLN
24	W	235	GLN
24	W	362	ASN
24	W	430	GLN
25	X	406	ASN
26	Y	136	HIS
26	Y	363	ASN
26	Y	378	ASN
27	Z	44	GLN
27	Z	102	HIS
27	Z	223	ASN
27	Z	224	HIS
28	a	23	HIS
28	a	257	GLN
28	a	273	GLN
28	a	290	GLN
28	a	337	GLN
30	c	115	HIS
32	e	6	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
33	ATP	A	501	-	26,33,33	0.95	1 (3%)	26,52,52	1.65	1 (3%)
33	ATP	D	501	-	26,33,33	0.95	1 (3%)	26,52,52	1.68	2 (7%)
33	ATP	E	401	-	26,33,33	0.96	1 (3%)	26,52,52	1.65	1 (3%)
33	ATP	F	501	-	26,33,33	0.96	1 (3%)	26,52,52	1.66	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	ATP	A	501	-	-	0/18/38/38	0/3/3/3
33	ATP	D	501	-	-	0/18/38/38	0/3/3/3
33	ATP	E	401	-	-	0/18/38/38	0/3/3/3
33	ATP	F	501	-	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	501	ATP	C5-C4	3.07	1.47	1.40
33	A	501	ATP	C5-C4	3.09	1.47	1.40
33	E	401	ATP	C5-C4	3.12	1.47	1.40
33	F	501	ATP	C5-C4	3.13	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	D	501	ATP	N3-C2-N1	-6.76	123.56	128.87
33	F	501	ATP	N3-C2-N1	-6.65	123.65	128.87
33	A	501	ATP	N3-C2-N1	-6.57	123.71	128.87
33	E	401	ATP	N3-C2-N1	-6.49	123.77	128.87
33	D	501	ATP	O4'-C1'-N9	2.36	112.57	108.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	f	3
17	B	1
19	E	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	8.87
1	f	79:ASN	C	80:TYR	N	7.82
1	f	348:ASP	C	349:SER	N	6.24
1	B	216:ILE	C	217:LYS	N	4.90
1	E	175:PRO	C	176:PRO	N	1.65