



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

Oct 29, 2019 – 02:56 PM EDT

PDB ID : 6J2X  
EMDB ID: : EMD-9772  
Title : Yeast proteasome in resting state (C1-a)  
Authors : Cong, Y.  
Deposited on : 2019-01-03  
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

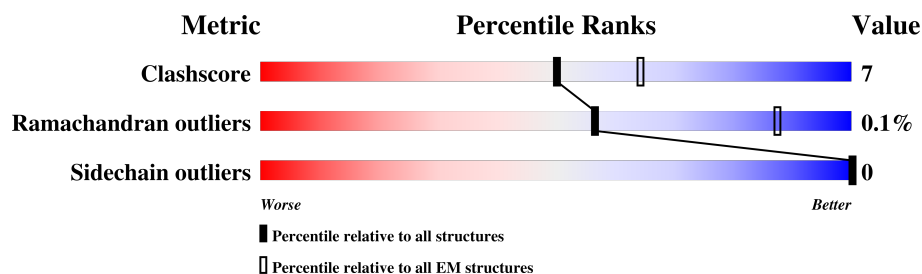
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.80 Å.

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









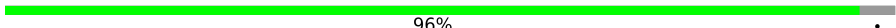

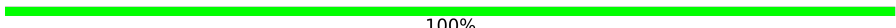

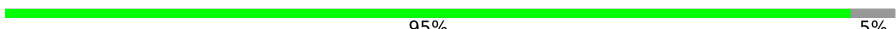

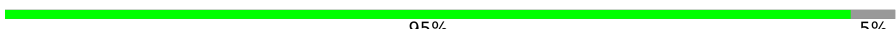



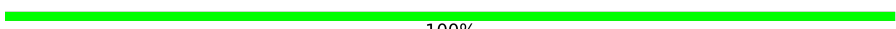








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	1	215	70% 25% 5%
1	b	215	95% 5%
2	2	261	74% 11% 15%
2	i	261	85% 15%
3	3	205	80% 20%
3	h	205	100%
4	4	198	79% 21%
4	g	198	100%
5	5	287	56% 18% 26%







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Mol	Chain	Length	Quality of chain
5	f	287	
6	6	241	
6	e	241	
7	7	266	
7	a	266	
8	A	252	
8	c	252	
9	B	250	
9	j	250	
10	C	258	
10	d	258	
11	D	254	
11	n	254	
12	E	260	
12	m	260	
13	F	234	
13	l	234	
14	G	288	
14	k	288	
15	H	467	
16	I	437	
17	J	405	
18	K	428	
19	L	437	
20	M	434	

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Mol	Chain	Length	Quality of chain
21	N	945	 76%14%10%
22	O	393	 84%14%.
23	P	445	 84%13%.
24	Q	434	 85%14%.
25	R	429	 76%17%7%
26	S	523	 78%13%9%
27	T	274	 89%11%.
28	U	338	 66%9%25%
29	V	306	 68%16%16%
30	W	268	 63%11%26%
31	X	156	 62%9%29%
32	Y	89	 25%. .70%
33	Z	993	 71%11%18%

## 2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 106176 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		
1	b	205	Total	C	N	O	S	0	0
			1576	996	261	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		
2	i	222	Total	C	N	O	S	0	0
			1684	1061	293	323	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		
3	h	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		
4	g	198	Total	C	N	O	S	0	0
			1585	1005	269	305	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
5	f	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 6 is a protein called PROTEASOME COMPONENT C5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
6	e	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		
7	a	233	Total	C	N	O	S	0	0
			1824	1154	312	351	7		

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	243	Total	C	N	O	S	0	0
			1921	1221	322	370	8		
8	c	243	Total	C	N	O	S	0	0
			1921	1221	322	370	8		

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
9	j	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		
11	n	241	Total	C	N	O	S	0	0
			1890	1181	331	374	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
12	m	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		

- Molecule 13 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		
13	l	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	243	Total	C	N	O	S	0	0
			1888	1201	328	355	4		
14	k	244	Total	C	N	O	S	0	0
			1896	1205	330	357	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	355	Total	C	N	O	S	0	0
			2787	1755	500	515	17		

- Molecule 16 is a protein called 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	362	Total	C	N	O	S	0	0
			2822	1773	471	563	15		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	373	Total	C	N	O	S	0	0
			2928	1837	527	547	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	381	Total	C	N	O	S	0	0
			3019	1898	530	581	10		

- Molecule 19 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	371	Total	C	N	O	S	0	0
			2937	1852	519	554	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	367	Total	C	N	O	S	0	0
			2866	1799	503	553	11		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	849	Total	C	N	O	S	0	0
			6562	4174	1099	1261	28		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	387	Total	C	N	O	S	0	0
			3182	2047	520	606	9		

- Molecule 23 is a protein called 26S PROTEASOME REGULATORY SUBUNIT RPN5.



Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	432	Total	C	N	O	S	0	0
			3545	2260	592	684	9		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	431	Total	C	N	O	S	0	0
			3471	2205	574	676	16		

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	400	Total	C	N	O	S	0	0
			3218	2051	527	630	10		

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	272	Total	C	N	O	S	0	0
			2235	1432	355	441	7		

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	255	Total	C	N	O	S	0	0
			2061	1312	352	391	6		

- Molecule 29 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	258	Total	C	N	O	S	0	0
			2025	1273	344	395	13		

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	111	Total	C	N	O	S	0	0
			906	586	148	169	3		

- Molecule 32 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	27	Total	C	N	O	0	0
			236	143	39	54		

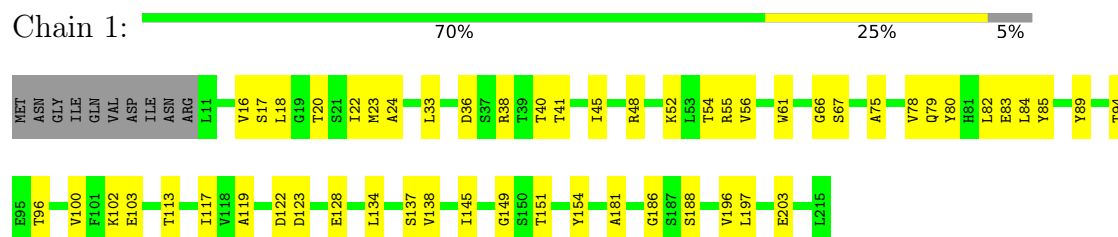
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	813	Total	C	N	O	S	0	0
			6290	3995	1029	1237	29		

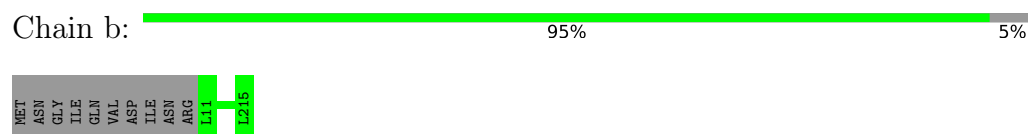
### 3 Residue-property plots

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

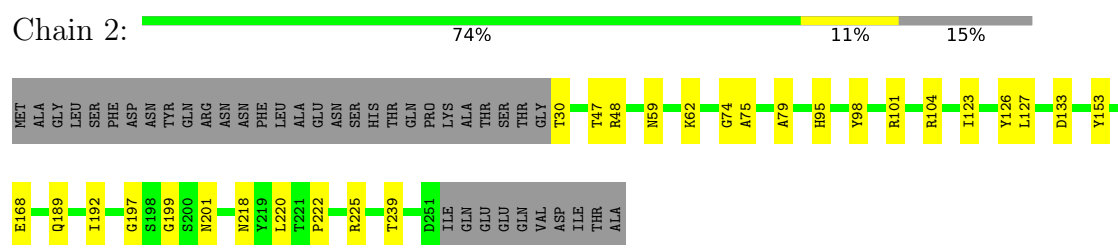
- Molecule 1: Proteasome subunit beta type-1



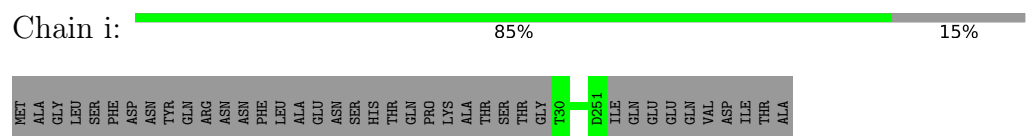
- Molecule 1: Proteasome subunit beta type-1



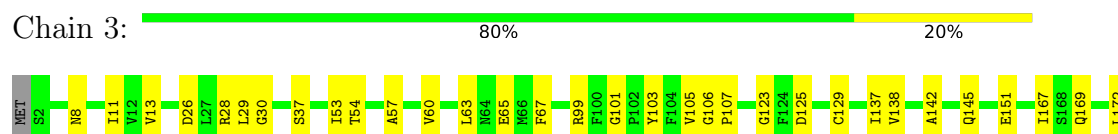
- Molecule 2: Proteasome subunit beta type-2

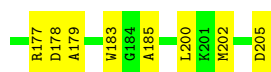


- Molecule 2: Proteasome subunit beta type-2



- Molecule 3: Proteasome subunit beta type-3





• Molecule 3: Proteasome subunit beta type-3

Chain h: 100%



• Molecule 4: Proteasome subunit beta type-4

Chain 4: 79% 21%



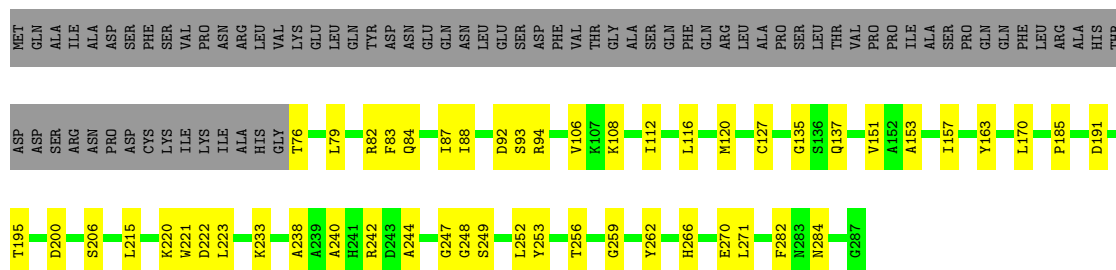
• Molecule 4: Proteasome subunit beta type-4

Chain g: 100%

There are no outlier residues recorded for this chain.

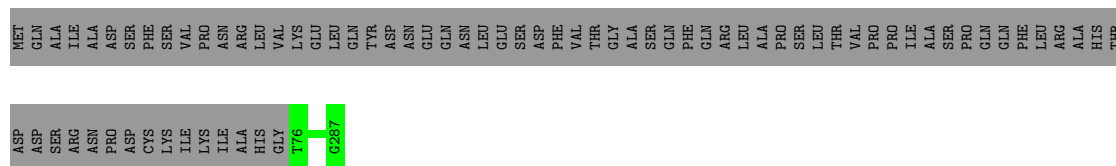
• Molecule 5: Proteasome subunit beta type-5

Chain 5: 56% 18% 26%



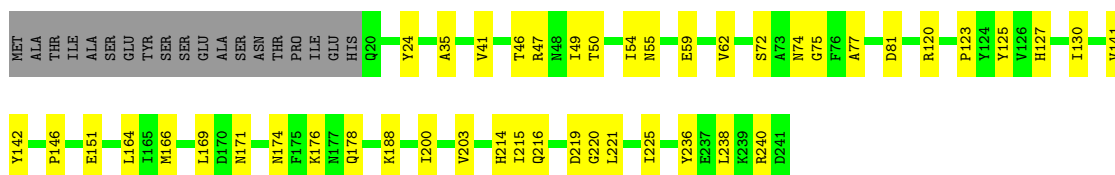
• Molecule 5: Proteasome subunit beta type-5

Chain f: 74% 26%



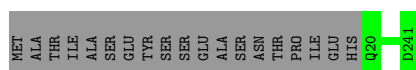
• Molecule 6: PROTEASOME COMPONENT C5

Chain 6: 73% 19% 8%



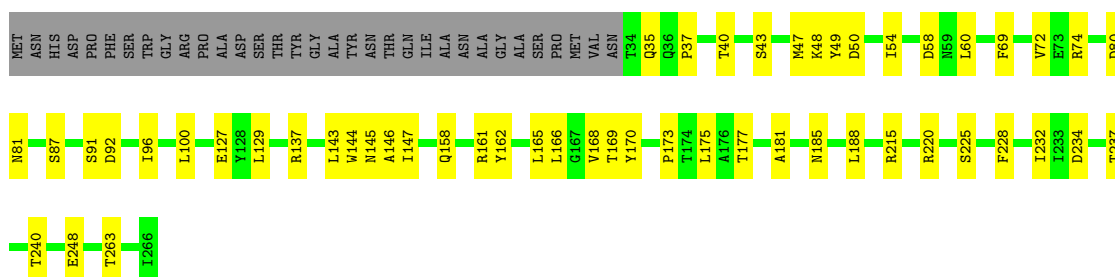
• Molecule 6: PROTEASOME COMPONENT C5

Chain e: 92% 8%



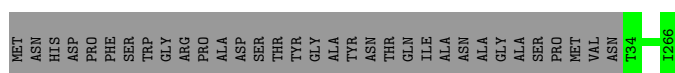
• Molecule 7: Proteasome subunit beta type-7

Chain 7: 68% 20% 12%



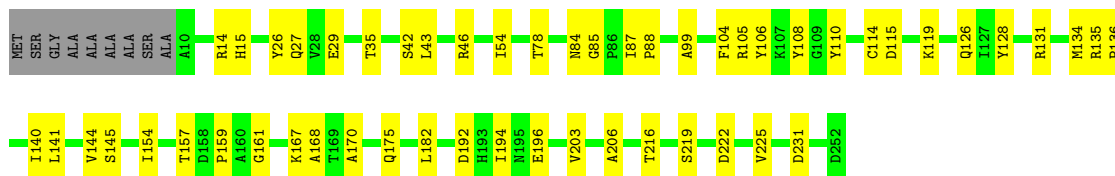
• Molecule 7: Proteasome subunit beta type-7

Chain a: 88% 12%



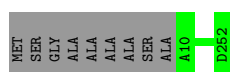
• Molecule 8: Proteasome subunit alpha type-1

Chain A: 75% 21% 4%




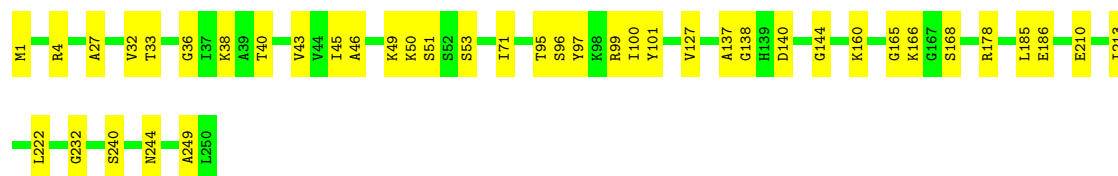
• Molecule 8: Proteasome subunit alpha type-1

Chain c: 96% 4%



• Molecule 9: Proteasome subunit alpha type-2

Chain B:  84% 16%




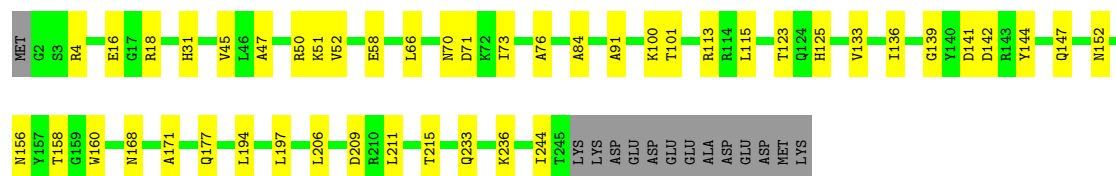
- Molecule 9: Proteasome subunit alpha type-2

Chain j:  100%

There are no outlier residues recorded for this chain.

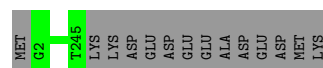
- Molecule 10: Proteasome subunit alpha type-3

Chain C:  77% 18% 5%




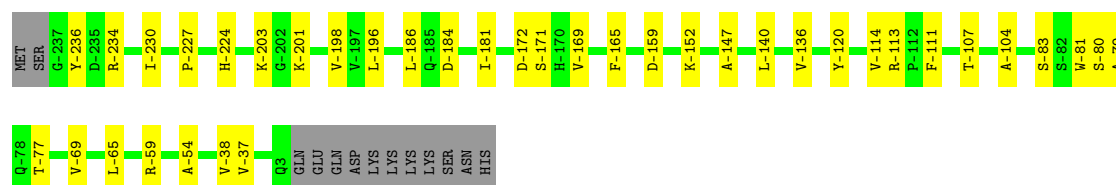
- Molecule 10: Proteasome subunit alpha type-3

Chain d:  95% 5%



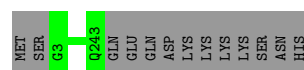
- Molecule 11: Proteasome subunit alpha type-4

Chain D:  80% 15% 5%




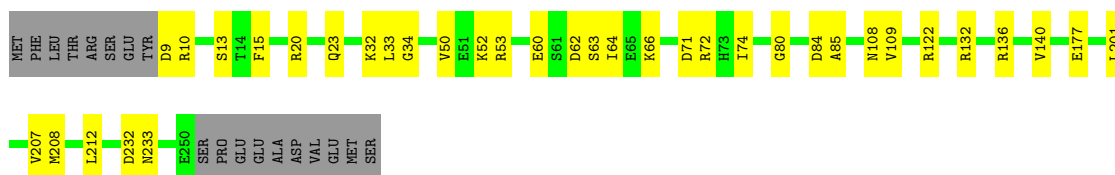
- Molecule 11: Proteasome subunit alpha type-4

Chain n:  95% 5%



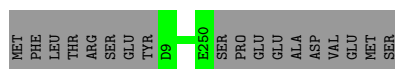
- Molecule 12: Proteasome subunit alpha type-5

Chain E:  79% 14% 7%



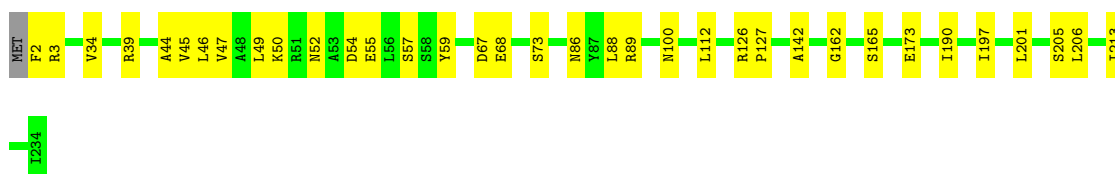
- Molecule 12: Proteasome subunit alpha type-5

Chain m: 93% 7%



- Molecule 13: Proteasome subunit alpha type-6

Chain F: 85% 15%



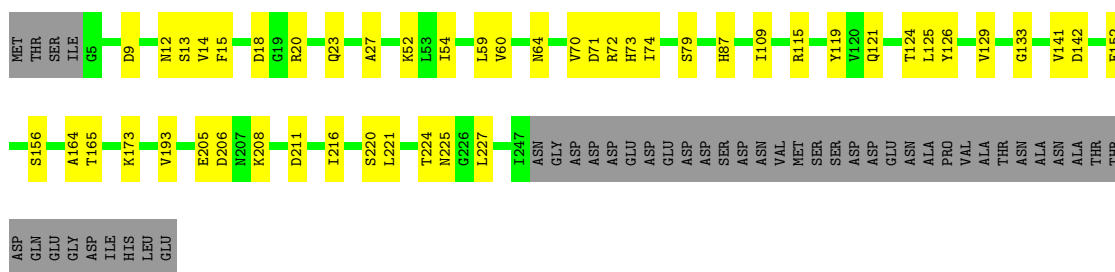
- Molecule 13: Proteasome subunit alpha type-6

Chain l: 100%



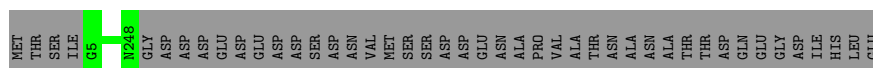
- Molecule 14: Probable proteasome subunit alpha type-7

Chain G: 68% 17% 16%



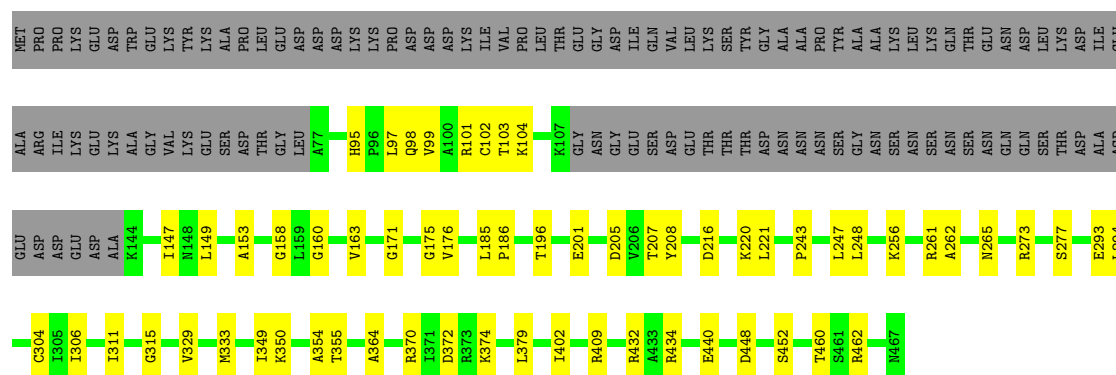
- Molecule 14: Probable proteasome subunit alpha type-7

Chain k: 85% 15%



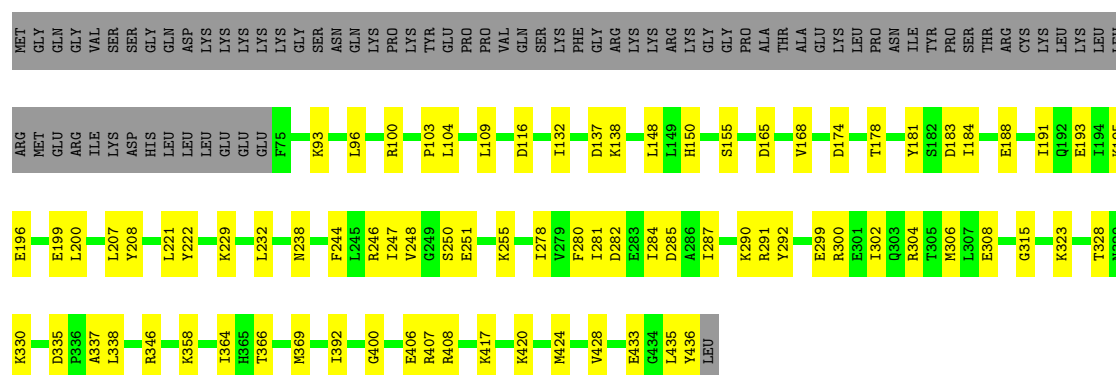
- Molecule 15: 26S proteasome regulatory subunit 7 homolog

Chain H:  63% 13% 24%




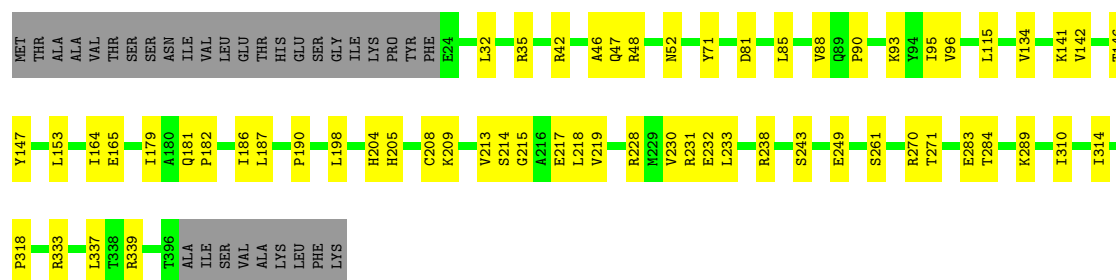
• Molecule 16: 26S PROTEASE REGULATORY SUBUNIT 4 HOMOLOG

Chain I:  64% 19% 17%



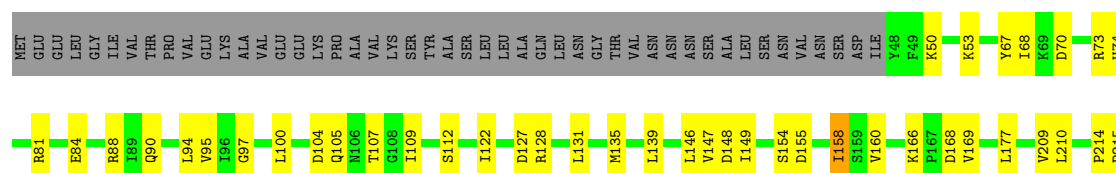
• Molecule 17: 26S proteasome regulatory subunit 8 homolog

Chain J:  77% 15% 8%

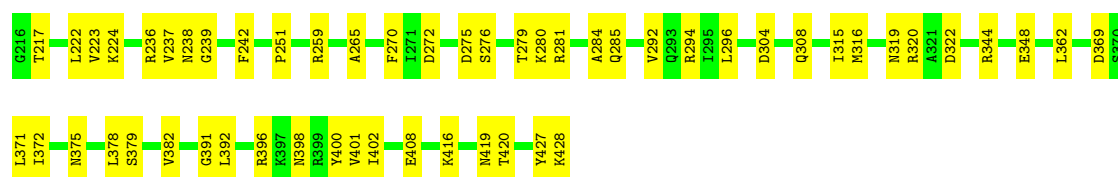


• Molecule 18: 26S proteasome regulatory subunit 6B homolog

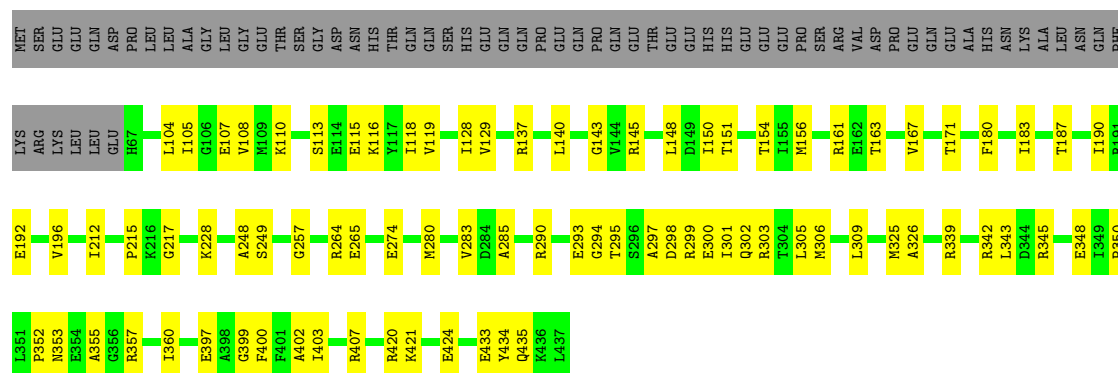
Chain K:  67% 22% 11%



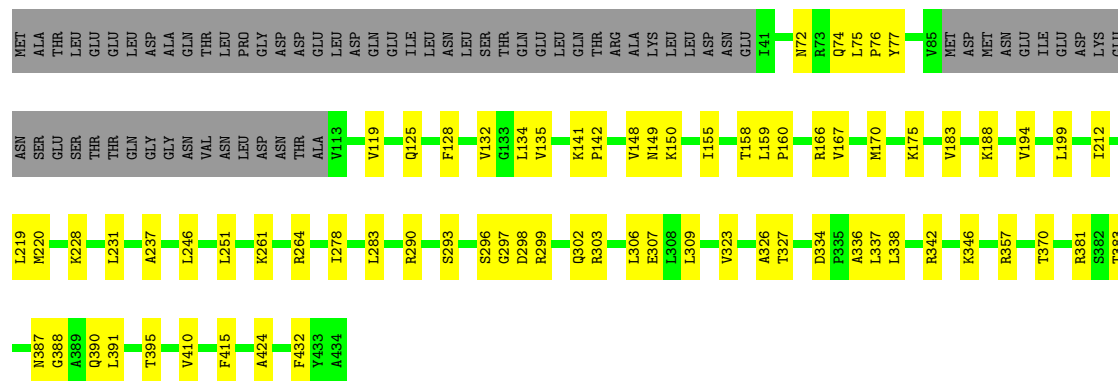




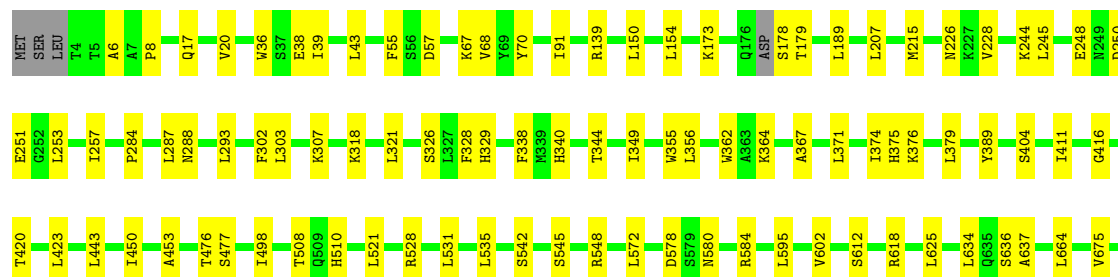
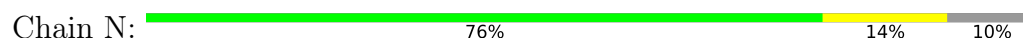
- Molecule 19: 26S proteasome subunit RPT4

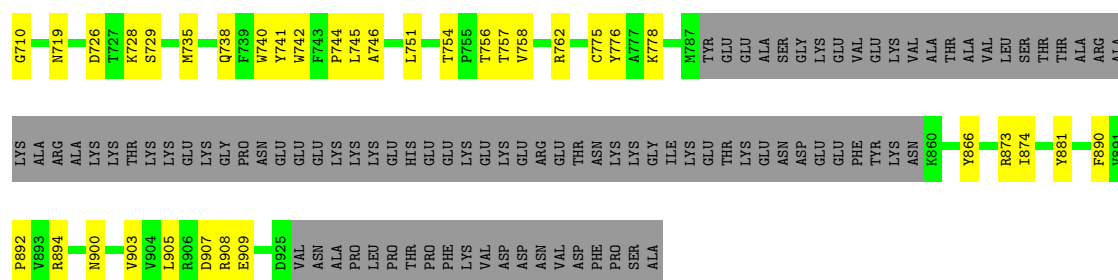


- Molecule 20: 26S proteasome regulatory subunit 6A

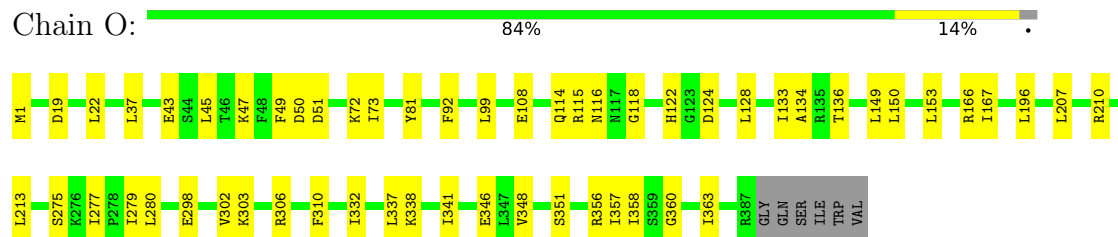


- Molecule 21: 26S proteasome regulatory subunit RPN2

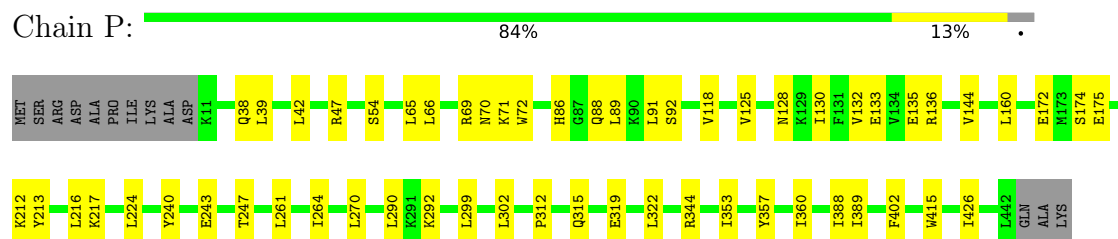




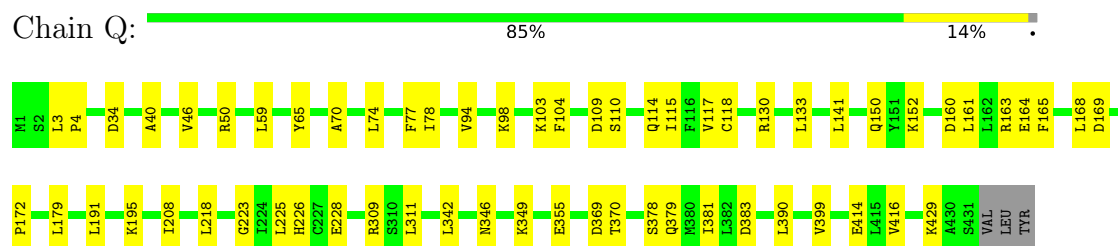
- Molecule 22: 26S proteasome regulatory subunit RPN9



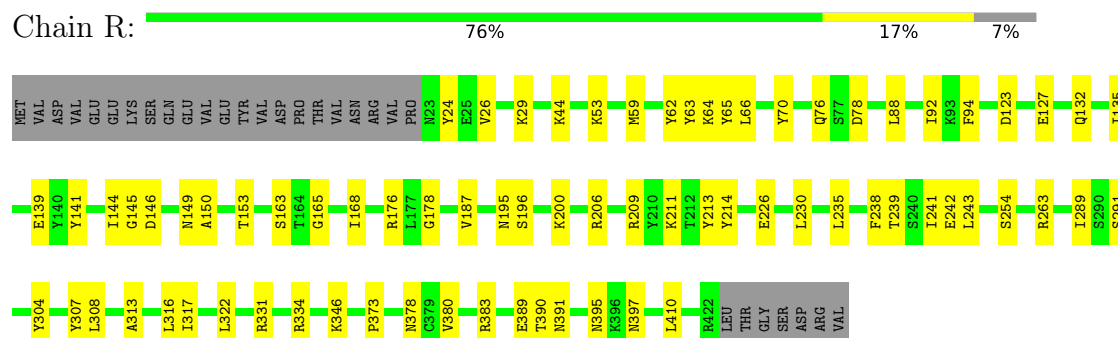
- Molecule 23: 26S PROTEASOME REGULATORY SUBUNIT RPN5



- Molecule 24: 26S proteasome regulatory subunit RPN6

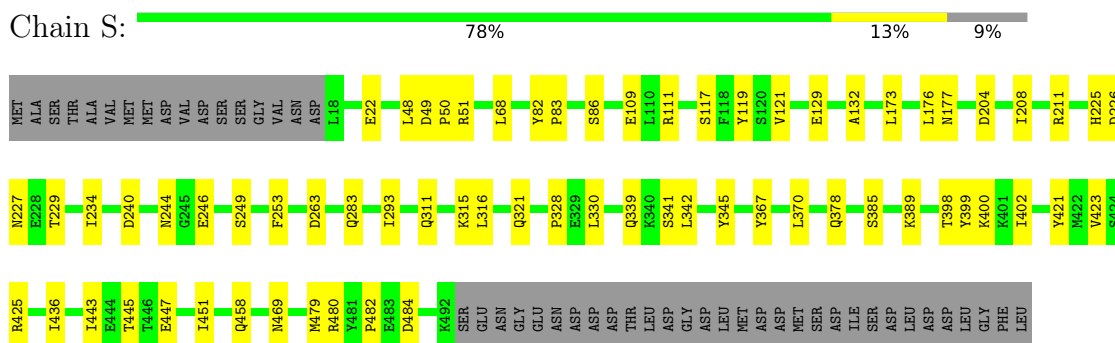


- Molecule 25: 26S proteasome regulatory subunit RPN7



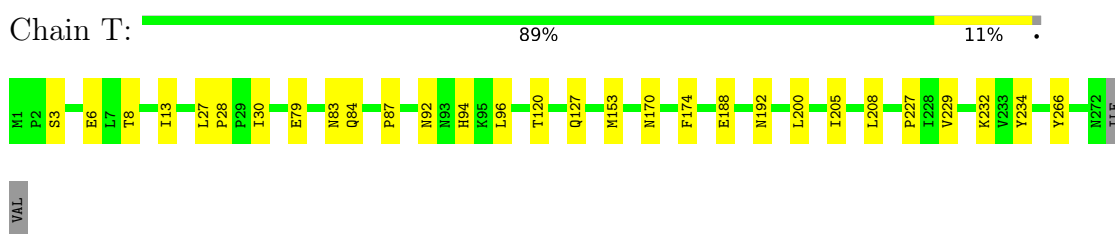
- Molecule 26: 26S proteasome regulatory subunit RPN3

Chain S:



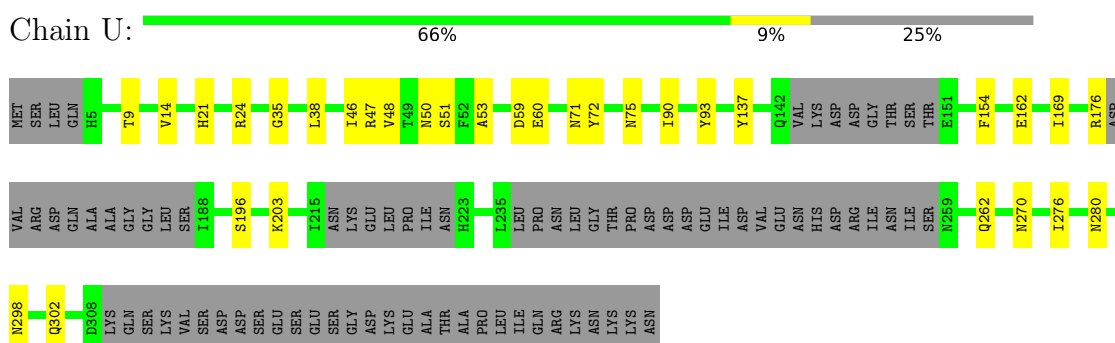
- Molecule 27: 26S proteasome regulatory subunit RPN12

Chain T:



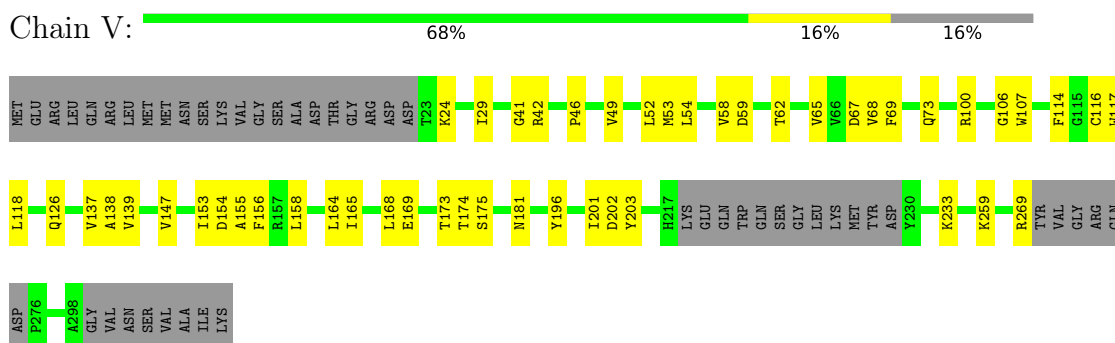
- Molecule 28: 26S proteasome regulatory subunit RPN8

Chain U:



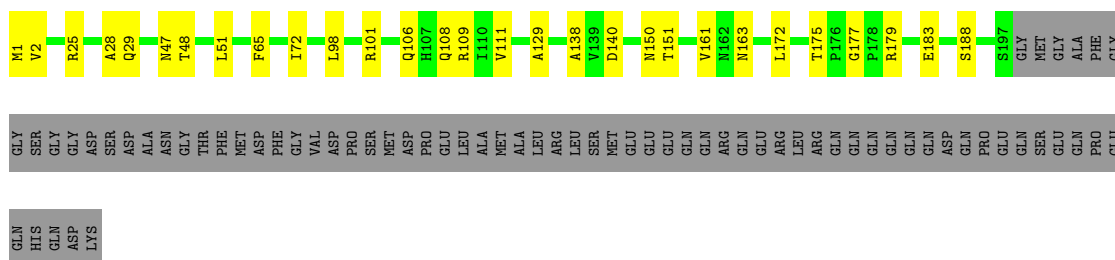
- Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:



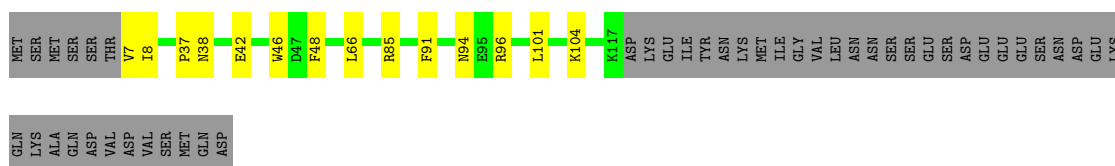
- Molecule 30: 26S proteasome regulatory subunit RPN10

Chain W:



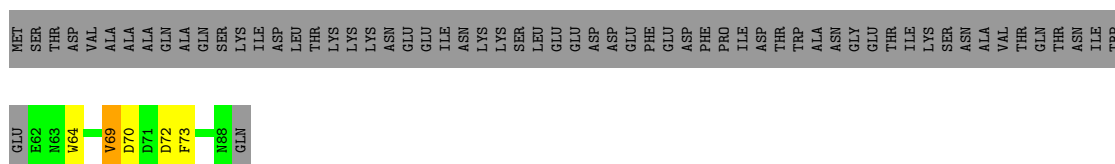
- Molecule 31: 26S proteasome regulatory subunit RPN13

Chain X:



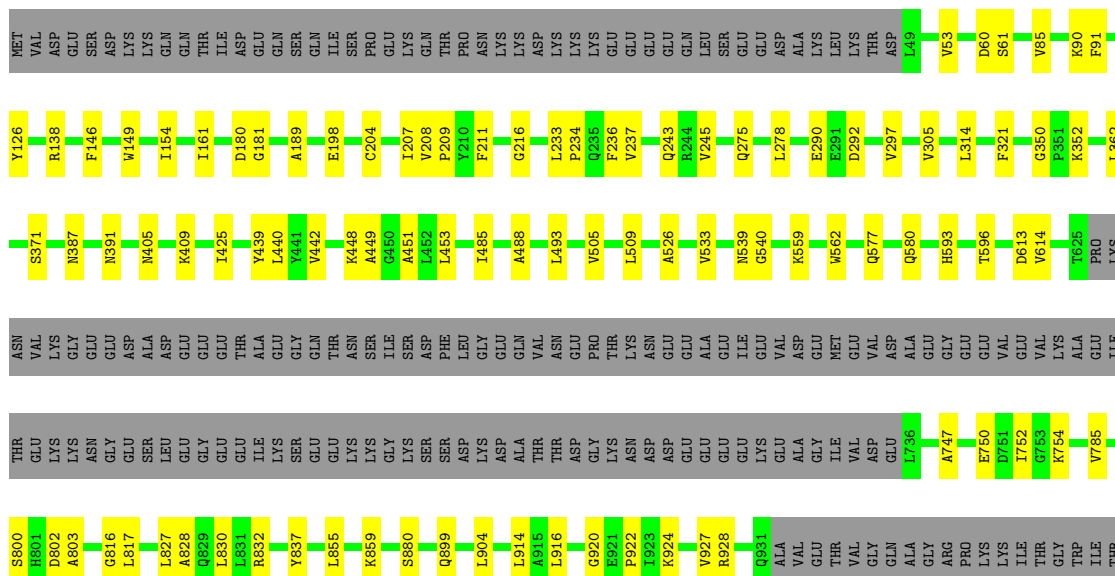
- Molecule 32: 26S proteasome complex subunit SEM1

Chain Y:



- Molecule 33: 26S proteasome regulatory subunit RPN1

Chain Z:



GLN	SER	THR	P954	V955	L956	L957	N958	H959	I971	S972	H976	V980	V981	L982	L983	E993
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	49507	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	38	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	1	0.24	0/1605	0.42	0/2171
1	b	0.23	0/1605	0.43	0/2171
10	C	0.23	0/1934	0.40	0/2618
10	d	0.24	0/1934	0.40	0/2618
11	D	0.22	0/1919	0.39	0/2598
11	n	0.23	0/1919	0.39	0/2598
12	E	0.23	0/1886	0.39	0/2541
12	m	0.23	0/1886	0.40	0/2541
13	F	0.24	0/1823	0.41	0/2463
13	l	0.24	0/1823	0.43	0/2463
14	G	0.24	0/1928	0.39	0/2603
14	k	0.23	0/1936	0.39	0/2614
15	H	0.24	0/2834	0.40	0/3816
16	I	0.26	1/2860 (0.0%)	0.41	0/3856
17	J	0.23	0/2964	0.39	0/3981
18	K	0.33	1/3062 (0.0%)	0.41	0/4132
19	L	0.32	1/2981 (0.0%)	0.40	0/4008
2	2	0.23	0/1715	0.42	0/2326
2	i	0.23	0/1715	0.42	0/2326
20	M	0.24	0/2903	0.41	0/3909
21	N	0.23	0/6670	0.39	0/9023
22	O	0.23	0/3243	0.39	0/4374
23	P	0.23	0/3599	0.38	0/4854
24	Q	0.23	0/3527	0.36	0/4748
25	R	0.23	0/3272	0.38	0/4412
26	S	0.23	0/3966	0.37	0/5355
27	T	0.23	0/2279	0.38	0/3077
28	U	0.23	0/2087	0.37	0/2811
29	V	0.23	0/2054	0.42	0/2770
3	3	0.24	0/1611	0.40	0/2174
3	h	0.24	0/1611	0.41	0/2174
30	W	0.23	0/1557	0.40	0/2111
31	X	0.23	0/931	0.40	0/1262
32	Y	0.22	0/239	0.37	0/322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
33	Z	0.23	0/6404	0.39	0/8686
4	4	0.23	0/1613	0.39	0/2173
4	g	0.23	0/1613	0.39	0/2173
5	5	0.23	0/1681	0.39	0/2274
5	f	0.23	0/1681	0.40	0/2274
6	6	0.24	0/1795	0.40	0/2420
6	e	0.24	0/1795	0.40	0/2420
7	7	0.24	0/1855	0.42	0/2514
7	a	0.24	0/1855	0.41	0/2514
8	A	0.24	0/1959	0.39	0/2652
8	c	0.24	0/1959	0.39	0/2652
9	B	0.24	0/1952	0.41	0/2642
9	j	0.24	0/1952	0.40	0/2642
All	All	0.24	3/107992 (0.0%)	0.40	0/145856

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	K	265	ALA	C-N	12.60	1.58	1.34
19	L	274	GLU	C-N	11.88	1.56	1.34
16	I	165	ASP	C-N	6.37	1.46	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1576	0	1552	34	0
1	b	1576	0	1552	0	0
2	2	1684	0	1685	21	0
2	i	1684	0	1685	0	0
3	3	1581	0	1571	27	0
3	h	1581	0	1571	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	4	1585	0	1590	27	0
4	g	1585	0	1590	0	0
5	5	1644	0	1592	33	0
5	f	1644	0	1592	0	0
6	6	1757	0	1708	33	0
6	e	1757	0	1708	0	0
7	7	1824	0	1829	31	0
7	a	1824	0	1829	0	0
8	A	1921	0	1910	42	0
8	c	1921	0	1910	0	0
9	B	1915	0	1929	27	0
9	j	1915	0	1929	0	0
10	C	1904	0	1901	31	0
10	d	1904	0	1901	0	0
11	D	1890	0	1903	26	0
11	n	1890	0	1900	0	0
12	E	1861	0	1836	25	0
12	m	1861	0	1836	0	0
13	F	1795	0	1797	24	0
13	l	1795	0	1797	0	0
14	G	1888	0	1880	34	0
14	k	1896	0	1886	0	0
15	H	2787	0	2851	38	0
16	I	2822	0	2870	55	0
17	J	2928	0	3057	45	0
18	K	3019	0	3084	65	0
19	L	2937	0	3011	62	0
20	M	2866	0	2938	56	0
21	N	6562	0	6625	79	0
22	O	3182	0	3207	31	0
23	P	3545	0	3629	36	0
24	Q	3471	0	3495	37	0
25	R	3218	0	3216	47	0
26	S	3894	0	3938	48	0
27	T	2235	0	2207	19	0
28	U	2061	0	2116	23	0
29	V	2025	0	2035	37	0
30	W	1534	0	1542	20	0
31	X	906	0	888	10	0
32	Y	236	0	203	4	0
33	Z	6290	0	6236	60	0
All	All	106176	0	106517	1029	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 7.

All (1029) 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)
19:L:290:ARG:HH21	19:L:298:ASP:HB3	1.49	0.78
16:I:104:LEU:HB3	16:I:148:LEU:HD11	1.67	0.77
27:T:170:ASN:HA	27:T:174:PHE:HB2	1.68	0.75
18:K:238:ASN:HD22	19:L:264:ARG:HH22	1.32	0.75
21:N:8:PRO:HB3	27:T:84:GLN:HA	1.69	0.74
6:6:47:ARG:HB2	6:6:219:ASP:HB2	1.70	0.73
15:H:243:PRO:HB3	15:H:372:ASP:HB2	1.72	0.72
30:W:101:ARG:HH12	30:W:108:GLN:HE21	1.39	0.71
20:M:336:ALA:O	20:M:342:ARG:NH2	2.24	0.70
22:O:338:LYS:HB3	22:O:351:SER:HB3	1.74	0.70
29:V:24:LYS:H	29:V:174:THR:HG22	1.57	0.69
31:X:38:ASN:HD22	31:X:42:GLU:H	1.40	0.69
18:K:276:SER:HB3	19:L:306:MET:HG3	1.73	0.69
30:W:179:ARG:HH21	30:W:183:GLU:HB3	1.57	0.69
17:J:47:GLN:HE21	26:S:480:ARG:HD3	1.58	0.69
2:2:101:ARG:HH22	8:A:115:ASP:HB3	1.57	0.69
17:J:215:GLY:H	17:J:249:GLU:HG2	1.58	0.69
33:Z:453:LEU:HB2	33:Z:488:ALA:HB1	1.75	0.69
21:N:778:LYS:HB2	21:N:866:TYR:HB2	1.76	0.68
25:R:176:ARG:HG2	25:R:243:LEU:HD21	1.76	0.68
22:O:19:ASP:HB3	22:O:22:LEU:HB3	1.76	0.68
12:E:34:GLY:HA3	12:E:80:GLY:HA2	1.76	0.68
29:V:153:ILE:HG23	29:V:201:ILE:HG13	1.76	0.68
10:C:76:ALA:HB3	10:C:136:ILE:HB	1.76	0.68
15:H:185:LEU:HD12	15:H:186:PRO:HD2	1.76	0.67
9:B:49:LYS:HE3	9:B:210:GLU:HB2	1.75	0.67
20:M:74:GLN:HG3	20:M:76:PRO:HD2	1.76	0.67
17:J:52:ASN:HD21	21:N:612:SER:HA	1.58	0.67
13:F:34:VAL:HA	13:F:162:GLY:HA3	1.76	0.67
21:N:443:LEU:HD22	21:N:477:SER:HB2	1.75	0.67
25:R:397:ASN:HD22	26:S:451:ILE:HG12	1.60	0.67
12:E:85:ALA:HB2	12:E:140:VAL:HG21	1.74	0.67
18:K:400:TYR:HB3	23:P:128:ASN:HB3	1.76	0.66
23:P:125:VAL:HA	23:P:136:ARG:HE	1.60	0.66
25:R:146:ASP:HB3	25:R:149:ASN:HB2	1.78	0.66
10:C:51:LYS:HG2	10:C:52:VAL:HG23	1.76	0.66
14:G:52:LYS:NZ	14:G:64:ASN:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:114:CYS:HB2	8:A:145:SER:HB3	1.77	0.66
16:I:285:ASP:OD2	17:J:270:ARG:NH1	2.29	0.66
5:5:220:LYS:HE2	5:5:222:ASP:HB2	1.79	0.65
6:6:74:ASN:HB3	6:6:127:HIS:HB2	1.78	0.65
11:D:-152:LYS:NZ	11:D:-120:TYR:OH	2.30	0.65
20:M:246:LEU:HD11	20:M:251:LEU:HD21	1.77	0.65
23:P:89:LEU:HB3	23:P:92:SER:HB3	1.78	0.65
6:6:220:GLY:HA2	6:6:238:LEU:H	1.61	0.65
28:U:72:TYR:HA	28:U:75:ASN:HD22	1.62	0.64
4:4:14:ILE:HG12	4:4:183:ILE:HG12	1.78	0.64
10:C:50:ARG:NH2	10:C:209:ASP:O	2.30	0.64
12:E:13:SER:HB2	13:F:126:ARG:HB3	1.79	0.64
15:H:364:ALA:O	15:H:370:ARG:NH1	2.30	0.64
11:D:-203:LYS:HE2	11:D:-80:SER:HA	1.80	0.64
19:L:118:ILE:HG12	19:L:128:ILE:HG12	1.78	0.64
17:J:146:THR:HG21	25:R:163:SER:HB3	1.80	0.64
26:S:173:LEU:O	26:S:177:ASN:ND2	2.31	0.64
5:5:106:VAL:HA	6:6:151:GLU:HG2	1.80	0.64
20:M:290:ARG:HH21	20:M:297:GLY:C	2.01	0.63
22:O:357:ILE:HG12	22:O:358:ILE:HG13	1.80	0.63
6:6:219:ASP:HA	6:6:240:ARG:HD3	1.79	0.63
9:B:186:GLU:HB2	24:Q:130:ARG:HH12	1.63	0.63
25:R:44:LYS:HB2	25:R:88:LEU:HD12	1.80	0.63
14:G:164:ALA:HB3	14:G:173:LYS:HB2	1.80	0.63
21:N:710:GLY:O	21:N:873:ARG:NH2	2.31	0.63
27:T:188:GLU:O	27:T:192:ASN:ND2	2.31	0.63
19:L:280:MET:HB2	19:L:325:MET:HA	1.81	0.63
18:K:90:GLN:HB3	18:K:94:LEU:HD21	1.79	0.63
8:A:88:PRO:O	14:G:121:GLN:NE2	2.31	0.63
5:5:112:ILE:HG23	5:5:135:GLY:HA2	1.81	0.63
31:X:91:PHE:H	31:X:96:ARG:HD3	1.64	0.62
14:G:87:HIS:HE2	14:G:119:TYR:HH	1.45	0.62
19:L:293:GLU:HB2	20:M:296:SER:HB3	1.80	0.62
22:O:99:LEU:HD13	22:O:133:ILE:HG12	1.81	0.62
15:H:261:ARG:NH2	16:I:315:GLY:O	2.32	0.62
19:L:352:PRO:O	19:L:357:ARG:NH1	2.33	0.62
20:M:283:LEU:HB3	20:M:327:THR:HB	1.81	0.62
11:D:-196:LEU:HD11	11:D:-104:ALA:HB3	1.82	0.61
13:F:46:LEU:HD21	13:F:73:SER:HB3	1.81	0.61
17:J:333:ARG:HG2	17:J:337:LEU:HD12	1.82	0.61
18:K:67:TYR:HB2	21:N:572:LEU:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:313:ALA:HA	25:R:317:ILE:HD12	1.80	0.61
6:6:74:ASN:OD1	6:6:75:GLY:N	2.31	0.61
20:M:387:ASN:OD1	20:M:388:GLY:N	2.34	0.61
6:6:221:LEU:HB3	6:6:236:TYR:HB3	1.83	0.61
29:V:53:MET:HG2	29:V:68:VAL:HG12	1.82	0.61
26:S:425:ARG:HH21	27:T:153:MET:HG2	1.65	0.61
10:C:125:HIS:HB3	11:D:-114:VAL:HG12	1.83	0.61
18:K:236:ARG:HG3	18:K:270:PHE:HD2	1.65	0.61
33:Z:387:ASN:O	33:Z:391:ASN:ND2	2.34	0.61
7:7:263:THR:HG23	16:I:109:LEU:HD22	156.14	0.60
30:W:172:LEU:HD13	30:W:188:SER:HB3	1.83	0.60
11:D:-230:ILE:HG23	12:E:23:GLN:HE22	1.66	0.60
22:O:341:ILE:HG23	22:O:348:VAL:HG22	1.83	0.60
33:Z:371:SER:HA	33:Z:387:ASN:HB3	1.82	0.60
19:L:192:GLU:OE1	19:L:345:ARG:NH2	2.35	0.60
30:W:150:ASN:OD1	30:W:151:THR:N	2.34	0.60
8:A:216:THR:OG1	19:L:353:ASN:ND2	2.35	0.60
13:F:173:GLU:OE2	20:M:381:ARG:NH1	2.35	0.60
8:A:140:ILE:HG12	8:A:159:PRO:HD3	1.83	0.60
9:B:71:ILE:HG12	9:B:138:GLY:HA3	1.82	0.60
18:K:416:LYS:HD3	18:K:420:THR:HA	1.84	0.60
10:C:70:ASN:OD1	10:C:71:ASP:N	2.33	0.60
25:R:211:LYS:HG2	25:R:230:LEU:HD22	1.83	0.60
29:V:52:LEU:HB2	29:V:69:PHE:HB3	1.83	0.60
33:Z:972:SER:HA	33:Z:983:LEU:HA	1.82	0.60
1:1:36:ASP:O	1:1:52:LYS:NZ	2.31	0.60
16:I:278:ILE:HG12	16:I:323:LYS:HB2	1.83	0.60
19:L:248:ALA:HB2	19:L:283:VAL:HG22	1.83	0.60
20:M:132:VAL:HG12	20:M:134:LEU:H	1.67	0.60
26:S:48:LEU:HD22	26:S:51:ARG:HH21	1.67	0.60
8:A:203:VAL:HG13	8:A:225:VAL:HG11	1.83	0.60
17:J:141:LYS:HG2	17:J:142:VAL:HG23	1.84	0.60
18:K:215:PRO:O	19:L:339:ARG:NH1	2.34	0.60
20:M:159:LEU:HD12	20:M:160:PRO:HD2	1.83	0.60
14:G:9:ASP:O	14:G:23:GLN:NE2	2.34	0.59
17:J:217:GLU:OE2	18:K:280:LYS:NZ	2.31	0.59
23:P:144:VAL:HG21	23:P:160:LEU:HG	1.82	0.59
6:6:47:ARG:NH1	6:6:215:ILE:O	2.35	0.59
21:N:150:LEU:HD21	21:N:173:LYS:HG3	1.84	0.59
23:P:89:LEU:HG	23:P:91:LEU:H	1.67	0.59
6:6:49:ILE:HG22	6:6:54:ILE:HA	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:46:ARG:HE	8:A:167:LYS:HA	1.68	0.59
19:L:299:ARG:HG3	19:L:303:ARG:HH12	1.67	0.59
23:P:66:LEU:HD13	23:P:70:ASN:HD22	1.66	0.59
32:Y:69:VAL:HG12	32:Y:70:ASP:H	1.67	0.59
11:D:-77:THR:HG21	11:D:-69:VAL:HB	1.85	0.59
22:O:298:GLU:OE1	22:O:356:ARG:NH2	2.36	0.59
26:S:227:ASN:HD22	26:S:263:ASP:HB2	1.66	0.59
16:I:100:ARG:NH2	17:J:81:ASP:OD2	2.36	0.59
5:5:94:ARG:NH1	5:5:244:ALA:O	2.36	0.59
14:G:109:ILE:H	14:G:142:ASP:HB3	1.68	0.59
16:I:229:LYS:NZ	16:I:328:THR:O	2.35	0.59
18:K:378:LEU:HD22	18:K:382:VAL:HG11	1.83	0.59
6:6:174:ASN:HB3	6:6:176:LYS:HE2	1.85	0.59
8:A:219:SER:H	8:A:222:ASP:HB2	1.66	0.59
19:L:167:VAL:HG21	20:M:141:LYS:HE2	1.84	0.59
20:M:299:ARG:O	20:M:303:ARG:NH1	2.36	0.59
7:7:87:SER:HB3	7:7:146:ALA:HB3	1.85	0.58
2:2:201:ASN:ND2	2:2:218:ASN:OD1	2.35	0.58
1:1:89:TYR:OH	14:G:115:ARG:NH2	2.37	0.58
24:Q:34:ASP:OD1	24:Q:50:ARG:NH1	2.31	0.58
13:F:201:LEU:HD11	13:F:206:LEU:HG	1.85	0.58
13:F:52:ASN:ND2	13:F:54:ASP:O	2.36	0.58
15:H:432:ARG:NH1	16:I:196:GLU:OE1	2.35	0.58
23:P:319:GLU:HB3	23:P:322:LEU:HB2	1.84	0.58
26:S:480:ARG:NH1	26:S:484:ASP:OD1	2.37	0.58
17:J:42:ARG:O	26:S:480:ARG:NH2	2.36	0.58
8:A:144:VAL:HG12	8:A:154:ILE:HG12	1.85	0.58
20:M:299:ARG:HA	20:M:302:GLN:HG2	1.86	0.58
4:4:146:HIS:O	4:4:149:ARG:NH1	2.33	0.58
30:W:98:LEU:O	30:W:101:ARG:NH1	2.37	0.58
24:Q:40:ALA:HA	24:Q:46:VAL:HA	1.86	0.58
26:S:311:GLN:NE2	26:S:341:SER:OG	2.36	0.58
13:F:47:VAL:HG22	13:F:213:ILE:HG12	1.85	0.58
16:I:247:ILE:HB	16:I:281:ILE:HG12	1.86	0.58
22:O:341:ILE:HG12	22:O:348:VAL:HG13	1.86	0.58
21:N:738:GLN:HE21	21:N:741:TYR:HD2	1.52	0.58
24:Q:223:GLY:HA2	24:Q:226:HIS:HD2	1.69	0.58
9:B:160:LYS:HE2	10:C:58:GLU:HA	1.86	0.58
19:L:402:ALA:HB1	19:L:407:ARG:HB2	1.86	0.58
21:N:508:THR:HG22	21:N:510:HIS:H	1.69	0.58
25:R:383:ARG:HD3	26:S:402:ILE:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:493:LEU:HD23	33:Z:509:LEU:HD21	1.86	0.58
4:4:102:VAL:O	4:4:133:HIS:NE2	2.36	0.57
10:C:144:TYR:HB2	10:C:147:GLN:HE21	1.69	0.57
15:H:95:HIS:O	15:H:97:LEU:N	2.37	0.57
21:N:892:PRO:HA	21:N:905:LEU:HG	1.86	0.57
15:H:402:ILE:HD12	15:H:440:GLU:HB2	1.86	0.57
7:7:60:LEU:HD22	7:7:225:SER:HB3	1.86	0.57
25:R:64:LYS:HA	25:R:94:PHE:HB2	1.85	0.57
1:1:196:VAL:HB	1:1:203:GLU:HB3	1.86	0.57
18:K:236:ARG:NH2	18:K:272:ASP:OD2	2.37	0.57
22:O:275:SER:HA	22:O:280:LEU:HD23	1.87	0.57
8:A:135:ARG:HB3	14:G:13:SER:HB2	1.85	0.57
15:H:102:CYS:HA	15:H:147:ILE:HG12	1.86	0.57
20:M:298:ASP:OD1	20:M:299:ARG:N	2.38	0.57
4:4:149:ARG:HB2	4:4:152:MET:HG3	1.86	0.57
5:5:270:GLU:OE2	6:6:188:LYS:NZ	2.37	0.57
31:X:91:PHE:HB3	31:X:94:ASN:HD22	1.68	0.57
3:3:13:VAL:HA	3:3:138:VAL:HG12	1.87	0.57
6:6:214:HIS:HE1	6:6:216:GLN:HB2	1.68	0.57
22:O:1:MET:HG3	22:O:37:LEU:HD23	1.85	0.57
28:U:47:ARG:NH1	28:U:162:GLU:OE1	2.35	0.57
6:6:171:ASN:OD1	6:6:178:GLN:NE2	2.37	0.57
22:O:47:LYS:O	22:O:81:TYR:OH	2.23	0.57
7:7:50:ASP:O	7:7:158:GLN:NE2	2.37	0.57
21:N:521:LEU:HB3	21:N:535:LEU:HD21	1.87	0.57
3:3:8:ASN:ND2	3:3:30:GLY:O	2.37	0.56
16:I:200:LEU:HD11	16:I:207:LEU:HD22	1.87	0.56
20:M:357:ARG:NH2	20:M:383:THR:O	2.38	0.56
17:J:205:HIS:HD2	25:R:127:GLU:HB2	1.70	0.56
28:U:137:TYR:HB3	28:U:154:PHE:HB3	1.86	0.56
28:U:276:ILE:O	28:U:280:ASN:ND2	2.38	0.56
11:D:-59:ARG:HH22	12:E:60:GLU:HA	1.70	0.56
17:J:339:ARG:NH1	25:R:239:THR:O	2.38	0.56
17:J:85:LEU:HD11	17:J:93:LYS:HB3	1.86	0.56
18:K:398:ASN:HA	23:P:130:ILE:HB	1.87	0.56
18:K:70:ASP:OD1	18:K:73:ARG:NH2	2.38	0.56
22:O:332:ILE:HG12	22:O:337:LEU:HB2	1.87	0.56
23:P:415:TRP:HE1	28:U:262:GLN:HG2	1.70	0.56
24:Q:355:GLU:HG2	24:Q:399:VAL:HA	1.86	0.56
33:Z:747:ALA:HB1	33:Z:754:LYS:HA	1.87	0.56
3:3:101:GLY:O	4:4:93:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:222:LEU:HD13	9:B:232:GLY:HA2	1.86	0.56
22:O:207:LEU:HD23	22:O:210:ARG:HD2	1.87	0.56
15:H:207:THR:HA	15:H:265:ASN:HD22	1.70	0.56
1:1:181:ALA:O	1:1:188:SER:OG	2.23	0.56
15:H:221:LEU:HD21	15:H:248:LEU:HD21	1.86	0.56
21:N:207:LEU:HD22	21:N:228:VAL:HA	1.87	0.56
18:K:50:LYS:HA	18:K:53:LYS:HD3	1.87	0.56
19:L:105:ILE:HD11	20:M:128:PHE:HB2	1.88	0.56
6:6:214:HIS:CE1	6:6:216:GLN:HB2	2.41	0.56
6:6:41:VAL:HG12	6:6:225:ILE:HA	1.87	0.56
12:E:84:ASP:OD2	12:E:136:ARG:NH1	2.39	0.56
21:N:728:LYS:HD3	21:N:751:LEU:HD13	1.87	0.56
18:K:122:ILE:HA	18:K:146:LEU:HD23	1.86	0.56
31:X:85:ARG:HD2	31:X:101:LEU:HD12	1.87	0.56
10:C:177:GLN:HA	11:D:-186:LEU:HD11	1.87	0.56
14:G:173:LYS:HD3	19:L:420:ARG:HH22	1.70	0.56
24:Q:429:LYS:HG3	29:V:269:ARG:HH22	1.71	0.56
4:4:36:ARG:HG3	4:4:57:ALA:HB1	1.88	0.56
8:A:104:PHE:HA	8:A:108:TYR:HD2	1.71	0.56
11:D:-184:ASP:HB3	11:D:-181:ILE:HG12	1.87	0.56
19:L:309:LEU:HA	19:L:342:ARG:HE	1.71	0.56
26:S:469:ASN:HD22	27:T:266:TYR:HB3	1.71	0.56
2:2:192:ILE:HG23	2:2:199:GLY:HA2	1.87	0.55
2:2:123:ILE:HG12	3:3:99:ARG:HE	1.69	0.55
7:7:232:ILE:HB	7:7:240:THR:HB	1.88	0.55
10:C:84:ALA:HB2	10:C:133:VAL:HG21	1.88	0.55
4:4:184:VAL:HG22	4:4:189:ILE:HG12	1.88	0.55
1:1:38:ARG:NH1	1:1:186:GLY:O	2.39	0.55
3:3:28:ARG:NH2	3:3:205:ASP:OXT	2.40	0.55
8:A:141:LEU:HB2	8:A:157:THR:HB	1.88	0.55
8:A:194:ILE:HG22	8:A:196:GLU:H	1.71	0.55
29:V:54:LEU:N	29:V:67:ASP:O	2.38	0.55
4:4:181:VAL:HB	4:4:192:VAL:HB	1.89	0.55
7:7:181:ALA:O	7:7:185:ASN:ND2	2.39	0.55
3:3:65:GLU:HB3	10:C:100:LYS:HG3	1.87	0.55
30:W:98:LEU:HD13	30:W:108:GLN:HB3	1.89	0.55
15:H:247:LEU:HB3	15:H:374:LYS:HA	1.87	0.55
18:K:100:LEU:HB3	18:K:109:ILE:HG23	1.89	0.55
22:O:118:GLY:HA3	22:O:128:LEU:HD22	1.88	0.55
23:P:388:ILE:HG22	23:P:389:ILE:HG13	1.88	0.55
23:P:39:LEU:HD12	23:P:88:GLN:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:209:ARG:NH1	25:R:213:TYR:OH	2.40	0.55
26:S:445:THR:HG22	26:S:447:GLU:H	1.72	0.55
5:5:82:ARG:HD3	5:5:200:ASP:HA	1.88	0.55
14:G:224:THR:HB	14:G:227:LEU:HB2	1.88	0.55
15:H:99:VAL:HA	15:H:175:GLY:HA2	1.88	0.55
29:V:53:MET:HA	29:V:68:VAL:HA	1.89	0.55
10:C:73:ILE:HG12	10:C:139:GLY:HA3	1.89	0.55
23:P:38:GLN:O	23:P:88:GLN:NE2	2.39	0.55
6:6:203:VAL:HG12	6:6:221:LEU:HD21	1.89	0.55
17:J:186:ILE:HG22	17:J:310:ILE:HG21	1.88	0.55
18:K:275:ASP:OD2	18:K:319:ASN:ND2	2.40	0.55
6:6:49:ILE:HD11	6:6:216:GLN:HE21	1.72	0.54
16:I:193:GLU:OE1	16:I:346:ARG:NH2	2.35	0.54
25:R:70:TYR:O	25:R:76:GLN:NE2	2.40	0.54
26:S:173:LEU:H	26:S:176:LEU:HD12	1.71	0.54
21:N:476:THR:OG1	29:V:59:ASP:OD2	2.24	0.54
15:H:294:LEU:HD13	15:H:306:ILE:HD11	1.89	0.54
18:K:344:ARG:HH11	18:K:348:GLU:HB3	1.71	0.54
19:L:104:LEU:HD21	20:M:125:GLN:HE21	1.72	0.54
21:N:758:VAL:H	21:N:874:ILE:HD12	1.73	0.54
24:Q:416:VAL:HG13	25:R:410:LEU:HD11	1.90	0.54
26:S:482:PRO:HG2	28:U:302:GLN:HE22	1.71	0.54
11:D:-159:ASP:HB3	11:D:-111:PHE:HD1	1.72	0.54
14:G:152:GLU:OE1	14:G:156:SER:OG	2.25	0.54
17:J:48:ARG:HD3	18:K:68:ILE:HG23	1.88	0.54
19:L:143:GLY:O	19:L:161:ARG:NH2	2.40	0.54
21:N:67:LYS:HA	21:N:70:TYR:HB3	1.89	0.54
26:S:283:GLN:HE22	27:T:120:THR:HG23	1.72	0.54
3:3:125:ASP:OD1	3:3:129:CYS:N	2.40	0.54
25:R:195:ASN:HA	25:R:206:ARG:HD2	1.89	0.54
33:Z:138:ARG:HE	33:Z:161:ILE:HD11	1.72	0.54
1:1:48:ARG:NH2	2:2:153:TYR:OH	2.40	0.54
21:N:344:THR:HG22	21:N:375:HIS:HA	1.90	0.54
21:N:376:LYS:HA	21:N:411:ILE:HG12	1.88	0.54
10:C:70:ASN:HB3	10:C:73:ILE:HB	1.89	0.54
15:H:434:ARG:HG3	33:Z:956:LEU:HD13	1.90	0.54
30:W:1:MET:HG2	30:W:2:VAL:HG13	1.90	0.54
3:3:29:LEU:HD11	3:3:57:ALA:HB2	1.90	0.54
4:4:46:PHE:HA	4:4:102:VAL:HA	1.89	0.54
19:L:285:ALA:O	20:M:299:ARG:NH2	2.40	0.54
5:5:93:SER:OG	5:5:249:SER:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:52:LYS:NZ	12:E:64:ILE:O	2.40	0.54
17:J:182:PRO:O	17:J:289:LYS:NZ	2.40	0.54
22:O:108:GLU:HB3	22:O:124:ASP:HB2	1.90	0.54
33:Z:880:SER:HB3	33:Z:904:LEU:HD23	1.88	0.54
1:1:113:THR:HG22	1:1:134:LEU:HD22	1.91	0.53
2:2:239:THR:OG1	3:3:169:GLN:NE2	2.42	0.53
4:4:38:LEU:HB3	4:4:64:ILE:HG21	1.90	0.53
10:C:4:ARG:NH1	12:E:9:ASP:O	2.41	0.53
16:I:255:LYS:HB3	17:J:219:VAL:HG11	1.89	0.53
25:R:316:LEU:HD23	25:R:322:LEU:HD13	1.90	0.53
2:2:220:LEU:HG	2:2:222:PRO:HD3	1.88	0.53
15:H:448:ASP:HA	15:H:452:SER:HB2	1.89	0.53
18:K:135:MET:HA	18:K:259:ARG:HH21	1.73	0.53
15:H:104:LYS:NZ	20:M:160:PRO:O	2.41	0.53
21:N:719:ASN:HD21	21:N:754:THR:HG21	1.73	0.53
8:A:126:GLN:NE2	8:A:161:GLY:O	2.42	0.53
23:P:125:VAL:HG23	23:P:136:ARG:HB2	1.90	0.53
27:T:3:SER:H	27:T:13:ILE:HD11	1.73	0.53
9:B:240:SER:O	9:B:244:ASN:ND2	2.40	0.53
11:D:-236:TYR:CZ	11:D:-234:ARG:HB3	2.44	0.53
21:N:756:THR:HG22	21:N:900:ASN:HD22	1.72	0.53
23:P:70:ASN:OD1	23:P:71:LYS:N	2.41	0.53
24:Q:150:GLN:HE21	24:Q:152:LYS:HD2	1.74	0.53
5:5:266:HIS:HB3	5:5:271:LEU:HD11	1.90	0.53
8:A:14:ARG:O	8:A:27:GLN:NE2	2.39	0.53
16:I:188:GLU:HA	16:I:191:ILE:HB	1.91	0.53
16:I:300:ARG:HB3	16:I:304:ARG:HH12	1.72	0.53
21:N:757:THR:HA	21:N:874:ILE:HB	1.90	0.53
23:P:270:LEU:O	23:P:344:ARG:NE	2.37	0.53
4:4:38:LEU:O	4:4:65:GLN:NE2	2.42	0.53
4:4:71:GLU:OE2	10:C:113:ARG:NH1	2.41	0.53
23:P:270:LEU:HA	23:P:344:ARG:HG3	1.91	0.53
33:Z:305:VAL:HG13	33:Z:982:ILE:HD12	1.91	0.53
4:4:32:ASP:OD1	4:4:33:ASP:N	2.41	0.53
7:7:215:ARG:NH2	7:7:248:GLU:O	2.38	0.53
12:E:71:ASP:OD1	12:E:72:ARG:N	2.41	0.53
15:H:149:LEU:HD12	15:H:153:ALA:HB3	1.91	0.53
17:J:214:SER:HB3	17:J:217:GLU:HG2	1.89	0.53
20:M:119:VAL:HG11	20:M:155:ILE:HD11	1.90	0.53
26:S:423:VAL:HB	26:S:436:ILE:HD11	1.90	0.53
1:1:18:LEU:N	1:1:66:GLY:O	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:49:TYR:HE2	7:7:54:ILE:HG13	1.74	0.53
13:F:50:LYS:HB3	13:F:59:TYR:HB3	1.89	0.53
15:H:315:GLY:HA2	15:H:333:MET:HG3	1.91	0.53
18:K:81:ARG:HH21	28:U:176:ARG:HG2	1.72	0.53
7:7:48:LYS:HD3	7:7:173:PRO:HA	1.91	0.53
18:K:104:ASP:OD1	18:K:105:GLN:N	2.41	0.53
12:E:232:ASP:OD1	12:E:233:ASN:N	2.42	0.53
22:O:115:ARG:HH21	22:O:122:HIS:CD2	2.27	0.53
25:R:380:VAL:HB	25:R:389:GLU:HB2	1.91	0.53
33:Z:209:PRO:HD3	33:Z:236:PHE:HD1	1.74	0.53
11:D:-172:ASP:OD1	11:D:-171:SER:N	2.41	0.52
18:K:396:ARG:NH1	19:L:192:GLU:OE2	2.33	0.52
25:R:196:SER:HA	25:R:200:LYS:HG2	1.92	0.52
30:W:47:ASN:OD1	30:W:48:THR:N	2.42	0.52
1:1:102:LYS:NZ	1:1:103:GLU:OE2	2.40	0.52
10:C:152:ASN:OD1	10:C:156:ASN:N	2.34	0.52
21:N:215:MET:O	21:N:244:LYS:NZ	2.33	0.52
24:Q:3:LEU:HD12	24:Q:4:PRO:HD2	1.90	0.52
28:U:196:SER:HB3	29:V:233:LYS:HE3	1.91	0.52
1:1:17:SER:HA	1:1:67:SER:HA	1.91	0.52
23:P:213:TYR:HB2	23:P:216:LEU:HD13	1.90	0.52
25:R:139:GLU:HG2	25:R:176:ARG:HH12	1.75	0.52
25:R:346:LYS:NZ	25:R:390:THR:O	2.38	0.52
16:I:406:GLU:O	16:I:408:ARG:NH1	2.42	0.52
20:M:183:VAL:HG21	20:M:231:LEU:HD21	1.92	0.52
12:E:60:GLU:HG2	12:E:62:ASP:H	1.74	0.52
13:F:86:ASN:OD1	13:F:89:ARG:NH2	2.42	0.52
19:L:156:MET:HG2	29:V:46:PRO:HG3	1.92	0.52
33:Z:449:ALA:HB2	33:Z:485:ILE:HG23	1.92	0.52
7:7:220:ARG:NH1	9:B:46:ALA:O	94.32	0.52
8:A:131:ARG:HG2	9:B:127:VAL:HG12	1.91	0.52
21:N:634:LEU:HG	21:N:636:SER:H	1.74	0.52
23:P:65:LEU:O	23:P:69:ARG:NH2	2.36	0.52
25:R:178:GLY:HA3	25:R:187:VAL:HG21	1.90	0.52
33:Z:785:VAL:HG12	33:Z:817:LEU:HB3	1.90	0.52
6:6:46:THR:HB	6:6:59:GLU:H	1.74	0.52
24:Q:311:LEU:HG	24:Q:346:ASN:HD22	1.74	0.52
1:1:137:SER:HB3	7:7:91:SER:HA	1.91	0.52
7:7:162:TYR:HB2	7:7:175:LEU:HD13	1.92	0.52
24:Q:383:ASP:OD1	25:R:263:ARG:NH1	2.33	0.52
24:Q:379:GLN:HE22	25:R:263:ARG:HH22	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:161:VAL:O	30:W:163:ASN:ND2	2.43	0.52
8:A:43:LEU:HA	8:A:170:ALA:HA	1.91	0.52
20:M:357:ARG:HD2	20:M:391:LEU:HD21	1.92	0.52
24:Q:309:ARG:HD2	24:Q:349:LYS:HE2	1.91	0.52
26:S:111:ARG:HA	26:S:117:SER:HB3	1.92	0.52
12:E:50:VAL:HG21	12:E:66:LYS:HB2	1.92	0.52
33:Z:505:VAL:HG11	33:Z:533:VAL:HG21	1.92	0.52
3:3:105:VAL:HG23	3:3:107:PRO:HD3	1.92	0.51
7:7:58:ASP:HA	7:7:228:PHE:HA	1.92	0.51
16:I:195:LYS:NZ	16:I:199:GLU:OE1	2.36	0.51
17:J:209:LYS:H	17:J:243:SER:HA	1.75	0.51
8:A:170:ALA:HB3	8:A:175:GLN:HG3	1.92	0.51
9:B:165:GLY:H	9:B:168:SER:HB3	1.75	0.51
17:J:228:ARG:O	17:J:232:GLU:N	2.43	0.51
19:L:301:ILE:HD13	20:M:299:ARG:HD2	1.93	0.51
11:D:-227:PRO:HB2	15:H:462:ARG:HB3	1.91	0.51
16:I:407:ARG:NH2	25:R:123:ASP:OD2	2.44	0.51
20:M:261:LYS:HG2	20:M:264:ARG:HH21	1.75	0.51
21:N:307:LYS:HG3	21:N:710:GLY:HA3	1.91	0.51
5:5:83:PHE:HE1	5:5:88:ILE:HG12	1.76	0.51
14:G:206:ASP:O	20:M:188:LYS:NZ	2.35	0.51
25:R:165:GLY:HA2	25:R:168:ILE:HD12	1.91	0.51
27:T:8:THR:HG23	27:T:30:ILE:HG23	1.93	0.51
30:W:129:ALA:HB1	30:W:161:VAL:HB	1.92	0.51
3:3:37:SER:HA	4:4:128:LEU:HD21	1.93	0.51
9:B:140:ASP:OD1	9:B:144:GLY:N	2.43	0.51
15:H:101:ARG:HE	15:H:171:GLY:HA2	1.75	0.51
19:L:150:ILE:HG13	19:L:151:THR:HG23	1.92	0.51
21:N:250:ASP:HB3	21:N:253:LEU:HB2	1.93	0.51
25:R:62:TYR:HE2	25:R:145:GLY:HA2	1.74	0.51
27:T:3:SER:OG	27:T:6:GLU:O	2.23	0.51
3:3:183:TRP:NE1	3:3:205:ASP:OXT	2.44	0.51
5:5:137:GLN:HG2	5:5:157:ILE:HG21	1.91	0.51
16:I:287:ILE:HD13	16:I:302:ILE:HA	1.92	0.51
33:Z:53:VAL:HG11	33:Z:91:PHE:HE2	1.74	0.51
3:3:11:ILE:HG22	3:3:142:ALA:HB3	1.92	0.51
20:M:334:ASP:HB3	20:M:337:LEU:HG	1.92	0.51
5:5:242:ARG:HH22	5:5:284:ASN:HD21	1.57	0.51
1:1:83:GLU:OE1	8:A:105:ARG:NH1	2.44	0.51
14:G:54:ILE:HG23	14:G:59:LEU:HD22	1.92	0.51
19:L:115:GLU:OE1	29:V:42:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:109:GLU:OE2	26:S:111:ARG:NE	2.38	0.51
30:W:25:ARG:HA	30:W:28:ALA:HB3	1.93	0.51
19:L:104:LEU:O	19:L:148:LEU:N	2.37	0.51
19:L:257:GLY:N	19:L:300:GLU:OE2	2.44	0.51
25:R:78:ASP:HB2	25:R:92:ILE:HD11	1.93	0.51
33:Z:914:LEU:HB2	33:Z:980:VAL:HG22	1.92	0.51
6:6:35:ALA:HB2	6:6:141:VAL:HG23	1.93	0.50
13:F:88:LEU:HD21	13:F:112:LEU:HB2	1.93	0.50
20:M:306:LEU:HD23	20:M:309:LEU:HD12	1.92	0.50
21:N:302:PHE:HD2	21:N:303:LEU:HD12	1.76	0.50
30:W:48:THR:HB	30:W:65:PHE:HB3	1.94	0.50
7:7:137:ARG:HD3	7:7:166:LEU:HA	1.92	0.50
18:K:104:ASP:HB3	18:K:107:THR:HB	1.93	0.50
18:K:95:VAL:O	18:K:139:LEU:N	2.40	0.50
21:N:735:MET:HB3	21:N:745:LEU:HB3	1.94	0.50
5:5:220:LYS:HB3	5:5:223:LEU:HG	1.93	0.50
6:6:164:LEU:HD12	6:6:214:HIS:HB2	1.94	0.50
12:E:71:ASP:HB3	12:E:74:ILE:HB	1.93	0.50
21:N:250:ASP:OD1	21:N:251:GLU:N	2.42	0.50
29:V:139:VAL:HA	29:V:155:ALA:HA	1.92	0.50
2:2:30:THR:N	2:2:197:GLY:O	2.45	0.50
7:7:96:ILE:HD13	7:7:147:ILE:HD11	1.94	0.50
15:H:158:GLY:HA3	20:M:75:LEU:HD13	1.93	0.50
15:H:201:GLU:HG3	15:H:273:ARG:HH12	1.77	0.50
17:J:46:ALA:H	26:S:480:ARG:HH21	1.57	0.50
18:K:304:ASP:O	18:K:308:GLN:NE2	2.45	0.50
24:Q:109:ASP:OD1	24:Q:110:SER:N	2.42	0.50
29:V:164:LEU:HA	29:V:168:LEU:HB2	1.93	0.50
29:V:52:LEU:HD23	29:V:107:TRP:HB3	1.93	0.50
8:A:15:HIS:HD2	14:G:14:VAL:HG11	1.76	0.50
21:N:226:ASN:HD21	21:N:257:ILE:HB	1.77	0.50
21:N:379:LEU:HD23	21:N:411:ILE:HG22	1.93	0.50
21:N:420:THR:HG23	21:N:450:ILE:HD11	1.93	0.50
21:N:612:SER:O	21:N:618:ARG:NH1	2.40	0.50
9:B:249:ALA:O	24:Q:98:LYS:NZ	2.43	0.50
25:R:373:PRO:HD3	26:S:398:THR:HG22	1.92	0.50
27:T:229:VAL:HG23	27:T:232:LYS:HB2	1.92	0.50
8:A:84:ASN:OD1	8:A:85:GLY:N	2.44	0.50
16:I:250:SER:HB3	17:J:270:ARG:HH21	1.76	0.50
21:N:321:LEU:HD13	21:N:328:PHE:HE2	1.75	0.50
26:S:129:GLU:OE2	26:S:132:ALA:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:399:TYR:HD2	26:S:402:ILE:HD12	1.76	0.50
26:S:22:GLU:HB3	26:S:68:LEU:HD22	1.94	0.50
28:U:48:VAL:HG22	28:U:90:ILE:HD11	1.93	0.50
33:Z:916:LEU:HD22	33:Z:920:GLY:HA2	1.92	0.50
10:C:168:ASN:HB3	10:C:171:ALA:HB3	1.93	0.50
14:G:221:LEU:HA	14:G:225:ASN:HA	1.94	0.50
15:H:160:GLY:H	15:H:163:VAL:HB	1.76	0.50
17:J:208:CYS:HB3	17:J:243:SER:HA	1.94	0.50
16:I:196:GLU:O	16:I:208:TYR:OH	2.27	0.50
21:N:8:PRO:HG3	27:T:87:PRO:HG3	1.94	0.50
29:V:58:VAL:HB	29:V:62:THR:HB	1.93	0.50
32:Y:72:ASP:OD1	32:Y:73:PHE:N	2.42	0.50
16:I:168:VAL:HG13	17:J:228:ARG:HD2	1.93	0.49
19:L:113:SER:HB3	19:L:116:LYS:HB3	1.93	0.49
23:P:172:GLU:HB3	23:P:175:GLU:HB3	1.94	0.49
28:U:38:LEU:HB2	28:U:50:ASN:HB3	1.94	0.49
1:1:55:ARG:O	1:1:79:GLN:NE2	2.45	0.49
3:3:54:THR:O	3:3:106:GLY:N	2.41	0.49
9:B:95:THR:HA	9:B:99:ARG:HD3	1.92	0.49
15:H:329:VAL:HG21	16:I:300:ARG:HD2	1.95	0.49
17:J:238:ARG:NH2	17:J:283:GLU:O	2.45	0.49
25:R:66:LEU:HB3	25:R:92:ILE:HD12	1.94	0.49
30:W:25:ARG:HD2	30:W:28:ALA:HB3	1.94	0.49
31:X:48:PHE:HB2	31:X:66:LEU:HB3	1.93	0.49
18:K:217:THR:HG22	18:K:379:SER:HB2	1.94	0.49
21:N:894:ARG:HB3	21:N:903:VAL:HG13	1.93	0.49
24:Q:115:ILE:HG23	24:Q:141:LEU:HD11	1.94	0.49
26:S:400:LYS:HG3	26:S:445:THR:HB	1.94	0.49
12:E:108:ASN:OD1	12:E:109:VAL:N	2.45	0.49
15:H:379:LEU:HG	15:H:462:ARG:HH21	1.76	0.49
17:J:147:TYR:OH	17:J:165:GLU:OE1	2.29	0.49
1:1:16:VAL:HA	1:1:41:THR:HG21	1.93	0.49
3:3:53:ILE:HG22	3:3:60:VAL:HG22	1.95	0.49
9:B:36:GLY:HA2	9:B:45:ILE:HA	1.94	0.49
10:C:47:ALA:HB1	10:C:197:LEU:HD11	1.93	0.49
11:D:-79:ALA:HB1	11:D:-65:LEU:HD13	1.95	0.49
15:H:311:ILE:HG22	15:H:355:THR:HB	1.94	0.49
22:O:310:PHE:HE2	22:O:346:GLU:HA	1.77	0.49
10:C:123:THR:O	11:D:-113:ARG:NE	2.36	0.49
10:C:16:GLU:OE1	10:C:18:ARG:NH2	2.32	0.49
16:I:400:GLY:HA3	17:J:179:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:114:PHE:HB3	29:V:117:TRP:HE1	1.76	0.49
1:1:151:THR:HA	1:1:154:TYR:HE2	1.77	0.49
24:Q:130:ARG:HD2	24:Q:133:LEU:HD12	1.94	0.49
20:M:72:ASN:O	20:M:77:TYR:OH	2.29	0.49
30:W:175:THR:HG22	30:W:177:GLY:H	1.78	0.49
17:J:181:GLN:HE21	17:J:289:LYS:HD2	1.78	0.49
21:N:775:CYS:O	21:N:866:TYR:N	2.45	0.49
22:O:43:GLU:HA	22:O:47:LYS:HD3	1.94	0.49
1:1:40:THR:OG1	1:1:45:ILE:HG12	2.13	0.49
13:F:39:ARG:HH21	14:G:60:VAL:HG21	1.78	0.49
21:N:318:LYS:HD2	21:N:355:TRP:CD1	2.48	0.49
21:N:36:TRP:HA	21:N:39:ILE:HD12	1.95	0.49
28:U:35:GLY:HA3	28:U:93:TYR:CZ	2.47	0.49
33:Z:613:ASP:OD1	33:Z:614:VAL:N	2.46	0.49
33:Z:927:VAL:HB	33:Z:957:LEU:HG	1.95	0.49
9:B:38:LYS:HG3	9:B:43:VAL:HG22	1.95	0.48
18:K:148:ASP:OD1	18:K:149:ILE:N	2.46	0.48
14:G:54:ILE:HB	14:G:211:ASP:HB3	1.95	0.48
18:K:166:LYS:O	18:K:168:ASP:N	2.45	0.48
9:B:178:ARG:HG2	24:Q:169:ASP:HB3	1.95	0.48
28:U:50:ASN:OD1	28:U:51:SER:N	2.47	0.48
2:2:48:ARG:O	2:2:62:LYS:NZ	2.35	0.48
9:B:51:SER:OG	9:B:53:SER:O	2.28	0.48
10:C:206:LEU:HD21	10:C:211:LEU:HD11	1.96	0.48
20:M:149:ASN:OD1	20:M:150:LYS:N	2.46	0.48
26:S:436:ILE:HG12	26:S:443:ILE:HG12	1.95	0.48
28:U:9:THR:N	28:U:46:ILE:O	2.41	0.48
7:7:47:MET:HB2	7:7:188:LEU:HD13	1.94	0.48
13:F:201:LEU:HD13	13:F:205:SER:HA	1.96	0.48
14:G:73:HIS:CD2	14:G:74:ILE:HG13	2.48	0.48
16:I:174:ASP:OD1	16:I:246:ARG:NH1	2.47	0.48
1:1:122:ASP:OD1	1:1:123:ASP:N	2.46	0.48
3:3:63:LEU:HB3	3:3:67:PHE:CE2	2.49	0.48
20:M:175:LYS:HG3	20:M:237:ALA:HA	1.96	0.48
29:V:154:ASP:OD1	29:V:155:ALA:N	2.45	0.48
29:V:67:ASP:OD1	29:V:68:VAL:N	2.47	0.48
5:5:82:ARG:NH1	5:5:200:ASP:OD1	2.47	0.48
21:N:545:SER:HB2	21:N:580:ASN:HD22	1.79	0.48
25:R:378:ASN:HB3	25:R:391:ASN:HB3	1.95	0.48
19:L:108:VAL:HA	19:L:119:VAL:HG22	1.95	0.48
5:5:79:LEU:HD13	5:5:215:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:137:ASP:OD1	16:I:138:LYS:N	2.47	0.48
16:I:424:MET:HA	16:I:428:VAL:HB	1.96	0.48
18:K:251:PRO:HD3	18:K:294:ARG:HB3	1.95	0.48
25:R:395:ASN:ND2	25:R:397:ASN:OD1	2.46	0.48
33:Z:290:GLU:HG2	33:Z:292:ASP:H	1.79	0.48
8:A:46:ARG:NH2	8:A:192:ASP:O	2.47	0.48
12:E:122:ARG:HB3	12:E:132:ARG:HD3	1.95	0.48
22:O:306:ARG:HH21	22:O:351:SER:HA	1.78	0.48
24:Q:369:ASP:OD1	24:Q:370:THR:N	2.47	0.48
33:Z:928:ARG:HG2	33:Z:955:VAL:HG13	1.95	0.48
2:2:95:HIS:CE1	8:A:104:PHE:HE1	2.32	0.48
2:2:98:TYR:O	8:A:119:LYS:NZ	2.39	0.48
18:K:94:LEU:HD22	18:K:147:VAL:HG21	1.95	0.48
20:M:219:LEU:HD23	20:M:346:LYS:HG3	1.96	0.48
24:Q:414:GLU:OE1	29:V:259:LYS:NZ	2.40	0.48
5:5:253:TYR:HE1	5:5:262:TYR:HD1	1.62	0.47
7:7:234:ASP:OD2	7:7:237:THR:N	2.42	0.47
13:F:54:ASP:OD1	13:F:55:GLU:N	2.47	0.47
8:A:135:ARG:HD3	14:G:13:SER:HA	1.96	0.47
16:I:103:PRO:O	17:J:95:ILE:N	2.46	0.47
21:N:321:LEU:HD22	21:N:328:PHE:HD2	1.79	0.47
33:Z:802:ASP:OD1	33:Z:803:ALA:N	2.47	0.47
5:5:76:THR:O	5:5:206:SER:N	2.47	0.47
22:O:196:LEU:HD13	22:O:213:LEU:HD22	1.97	0.47
1:1:24:ALA:HB2	1:1:33:LEU:HG	1.95	0.47
13:F:52:ASN:ND2	13:F:57:SER:OG	2.47	0.47
19:L:163:THR:HG22	19:L:265:GLU:HG2	1.97	0.47
21:N:154:LEU:HB3	21:N:189:LEU:HD21	1.96	0.47
33:Z:488:ALA:HA	33:Z:899:GLN:HG2	1.96	0.47
24:Q:74:LEU:HD23	24:Q:77:PHE:HD2	1.79	0.47
33:Z:539:ASN:OD1	33:Z:540:GLY:N	2.47	0.47
14:G:109:ILE:HG12	14:G:142:ASP:HB3	1.96	0.47
15:H:256:LYS:HE3	15:H:354:ALA:HB1	1.96	0.47
19:L:420:ARG:HG2	19:L:424:GLU:HG3	1.96	0.47
28:U:71:ASN:O	28:U:75:ASN:ND2	2.47	0.47
3:3:11:ILE:HD11	3:3:26:ASP:HB3	1.96	0.47
5:5:170:LEU:HD23	6:6:120:ARG:HH21	1.79	0.47
13:F:67:ASP:OD1	13:F:68:GLU:N	2.44	0.47
20:M:220:MET:HB3	20:M:326:ALA:HA	1.95	0.47
21:N:726:ASP:HB3	21:N:729:SER:HB2	1.97	0.47
21:N:894:ARG:HD3	21:N:903:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:S:119:TYR:CE2	26:S:121:VAL:HB	2.48	0.47
16:I:284:ILE:H	16:I:328:THR:HB	1.80	0.47
16:I:93:LYS:HA	16:I:96:LEU:HD13	1.96	0.47
18:K:169:VAL:HG22	18:K:224:LYS:HE2	1.97	0.47
21:N:423:LEU:HB2	21:N:450:ILE:HD13	1.95	0.47
21:N:741:TYR:HA	29:V:173:THR:HG23	1.95	0.47
30:W:25:ARG:O	30:W:29:GLN:N	2.32	0.47
33:Z:149:TRP:HA	33:Z:154:ILE:HD12	1.96	0.47
11:D:-165:PHE:HB3	11:D:-107:THR:HG22	1.96	0.47
16:I:116:ASP:HA	16:I:132:ILE:HD12	1.96	0.47
23:P:42:LEU:HD23	23:P:54:SER:HB2	1.95	0.47
5:5:82:ARG:HE	5:5:185:PRO:HB2	1.80	0.47
7:7:58:ASP:OD1	7:7:74:ARG:NH2	2.36	0.47
4:4:86:GLN:HG3	10:C:101:THR:HG23	1.96	0.47
10:C:158:THR:OG1	10:C:160:TRP:NE1	2.47	0.47
30:W:101:ARG:HD2	30:W:106:GLN:HB2	1.96	0.47
7:7:127:GLU:HG2	13:F:100:ASN:HB2	1.96	0.47
14:G:27:ALA:HB1	14:G:133:GLY:HA2	1.97	0.47
19:L:104:LEU:HB2	19:L:148:LEU:HB2	1.96	0.47
19:L:357:ARG:HA	19:L:360:ILE:HD12	1.96	0.47
20:M:290:ARG:HG3	20:M:290:ARG:O	2.13	0.47
23:P:47:ARG:HA	23:P:86:HIS:HE1	1.80	0.47
2:2:47:THR:HB	2:2:59:ASN:HA	1.95	0.47
4:4:3:ILE:HB	4:4:18:SER:HB3	1.97	0.47
9:B:27:ALA:HB1	18:K:428:LYS:HE3	1.97	0.47
19:L:137:ARG:HA	19:L:140:LEU:HD12	1.97	0.47
20:M:290:ARG:NE	20:M:298:ASP:HA	2.30	0.47
21:N:364:LYS:HA	21:N:367:ALA:HB3	1.97	0.47
26:S:293:ILE:HD13	26:S:316:LEU:HD23	1.97	0.47
31:X:85:ARG:HH22	31:X:104:LYS:HG3	1.79	0.47
33:Z:750:GLU:HG2	33:Z:752:ILE:H	1.80	0.47
33:Z:924:LYS:HA	33:Z:958:ASN:HB3	1.96	0.47
15:H:216:ASP:HB3	15:H:220:LYS:HE3	1.96	0.46
18:K:210:LEU:HD23	18:K:316:MET:HB2	1.96	0.46
30:W:25:ARG:HG3	30:W:29:GLN:HG3	1.97	0.46
5:5:240:ALA:HB1	5:5:247:GLY:HA2	1.97	0.46
7:7:43:SER:HA	7:7:177:THR:HB	1.97	0.46
8:A:42:SER:OG	8:A:54:ILE:O	2.26	0.46
11:D:-172:ASP:HB3	11:D:-169:VAL:HG12	1.97	0.46
14:G:126:TYR:HB2	14:G:129:VAL:HG22	1.97	0.46
14:G:141:VAL:HG21	14:G:220:SER:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:181:TYR:HD1	16:I:184:ILE:HD11	1.81	0.46
16:I:290:LYS:HG2	16:I:292:TYR:H	1.80	0.46
17:J:238:ARG:NH2	17:J:284:THR:OG1	2.47	0.46
18:K:214:PRO:HG2	18:K:217:THR:HG21	1.97	0.46
20:M:135:VAL:HG12	20:M:158:THR:HG22	1.97	0.46
23:P:261:LEU:HA	23:P:264:ILE:HD12	1.97	0.46
16:I:221:LEU:HD21	16:I:232:LEU:HD23	1.96	0.46
21:N:416:GLY:HA3	21:N:453:ALA:HB1	1.98	0.46
20:M:290:ARG:NH1	20:M:293:SER:OG	2.44	0.46
21:N:595:LEU:HD13	21:N:602:VAL:HA	1.97	0.46
22:O:150:LEU:HD23	22:O:153:LEU:HD12	1.97	0.46
22:O:92:PHE:HD1	22:O:136:THR:HG23	1.81	0.46
33:Z:971:ILE:HG23	33:Z:976:HIS:HE1	1.80	0.46
14:G:87:HIS:NE2	14:G:119:TYR:OH	2.39	0.46
15:H:196:THR:HG21	15:H:293:GLU:HB3	1.96	0.46
19:L:294:GLY:O	19:L:295:THR:OG1	2.31	0.46
21:N:245:LEU:HA	21:N:248:GLU:HB2	1.97	0.46
21:N:349:ILE:HG23	21:N:356:LEU:HD21	1.96	0.46
25:R:62:TYR:HA	25:R:65:TYR:HD2	1.80	0.46
29:V:138:ALA:N	29:V:156:PHE:O	2.32	0.46
1:1:78:VAL:HG22	1:1:100:VAL:HG12	1.98	0.46
17:J:190:PRO:HG2	17:J:318:PRO:HB3	1.96	0.46
21:N:288:ASN:HB3	21:N:293:LEU:HB2	1.97	0.46
22:O:134:ALA:HB2	22:O:149:LEU:HB2	1.98	0.46
24:Q:78:ILE:HD12	24:Q:117:VAL:HG11	1.98	0.46
24:Q:118:CYS:HB2	24:Q:141:LEU:HD13	1.96	0.46
24:Q:195:LYS:HG2	24:Q:225:LEU:HD13	1.96	0.46
27:T:94:HIS:NE2	27:T:96:LEU:HB2	2.30	0.46
14:G:18:ASP:OD2	14:G:20:ARG:NH2	2.45	0.46
17:J:153:LEU:HD13	17:J:198:LEU:HD11	1.98	0.46
29:V:126:GLN:HE21	29:V:158:LEU:HG	1.81	0.46
33:Z:439:TYR:HB2	33:Z:451:ALA:HB2	1.98	0.46
5:5:233:LYS:HB2	5:5:252:LEU:HD11	1.97	0.46
6:6:125:TYR:HA	6:6:146:PRO:HB3	1.98	0.46
19:L:107:GLU:HA	19:L:145:ARG:HA	1.97	0.46
24:Q:342:LEU:O	24:Q:346:ASN:N	2.47	0.46
30:W:111:VAL:HA	30:W:140:ASP:HB3	1.96	0.46
12:E:53:ARG:HH12	12:E:208:MET:HA	1.80	0.46
13:F:34:VAL:HG23	13:F:165:SER:HB3	1.97	0.46
14:G:79:SER:HB3	14:G:165:THR:HG23	1.97	0.46
16:I:300:ARG:HB3	16:I:304:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:235:LEU:H	25:R:238:PHE:HE2	1.63	0.46
25:R:331:ARG:HG2	25:R:334:ARG:HH21	1.81	0.46
3:3:185:ALA:HB3	3:3:200:LEU:HD12	1.98	0.46
6:6:200:ILE:HD11	6:6:225:ILE:HD11	1.98	0.46
15:H:208:TYR:HA	15:H:262:ALA:HB1	1.98	0.46
18:K:320:ARG:NH2	18:K:322:ASP:OD2	2.49	0.46
20:M:370:THR:HG22	20:M:410:VAL:HB	1.97	0.46
25:R:141:TYR:HA	25:R:144:ILE:HG12	1.98	0.46
33:Z:243:GLN:HB2	33:Z:275:GLN:HE22	1.80	0.46
6:6:166:MET:HA	6:6:169:LEU:HD12	1.97	0.45
16:I:251:GLU:OE2	17:J:231:ARG:NE	2.49	0.45
28:U:9:THR:HB	28:U:47:ARG:HG2	1.98	0.45
33:Z:278:LEU:HD22	33:Z:297:VAL:HB	1.98	0.45
33:Z:371:SER:HB2	33:Z:391:ASN:HD21	1.80	0.45
16:I:433:GLU:OE2	16:I:435:LEU:HB3	2.16	0.45
22:O:72:LYS:HG2	22:O:73:ILE:HG23	1.97	0.45
33:Z:816:GLY:HA2	33:Z:855:LEU:HD12	1.97	0.45
13:F:39:ARG:NH1	13:F:142:ALA:O	2.49	0.45
14:G:12:ASN:HD21	14:G:124:THR:HA	1.81	0.45
16:I:150:HIS:HB3	16:I:155:SER:H	1.81	0.45
33:Z:440:LEU:HA	33:Z:448:LYS:HG2	1.97	0.45
18:K:84:GLU:O	18:K:88:ARG:NE	2.46	0.45
19:L:167:VAL:HG13	20:M:142:PRO:HB2	1.98	0.45
21:N:528:ARG:HB3	21:N:531:LEU:HB2	1.97	0.45
33:Z:828:ALA:O	33:Z:832:ARG:NE	2.49	0.45
6:6:77:ALA:O	6:6:81:ASP:N	2.46	0.45
7:7:69:PHE:HB3	7:7:72:VAL:HG23	1.99	0.45
15:H:98:GLN:N	15:H:176:VAL:O	2.33	0.45
8:A:216:THR:HG23	19:L:355:ALA:HB2	1.98	0.45
12:E:20:ARG:HG3	20:M:432:PHE:HE2	1.80	0.45
28:U:14:VAL:HG21	28:U:48:VAL:HG12	1.98	0.45
19:L:433:GLU:HB3	19:L:435:GLN:HE22	1.82	0.45
20:M:228:LYS:HE3	20:M:231:LEU:HD12	1.99	0.45
3:3:178:ASP:OD1	3:3:179:ALA:N	2.50	0.45
9:B:96:SER:HA	9:B:100:ILE:HD12	1.99	0.45
18:K:154:SER:HB3	18:K:259:ARG:NH1	2.31	0.45
22:O:114:GLN:HG2	22:O:116:ASN:H	1.80	0.45
24:Q:179:LEU:HD13	24:Q:218:LEU:HD23	1.98	0.45
1:1:84:LEU:HD21	8:A:99:ALA:HA	1.98	0.45
11:D:-201:LYS:HD2	11:D:-54:ALA:HB2	1.99	0.45
10:C:4:ARG:HD2	12:E:10:ARG:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:277:SER:OG	16:I:308:GLU:OE1	2.35	0.45
17:J:213:VAL:HG13	17:J:233:LEU:HD12	1.99	0.45
19:L:228:LYS:HE3	19:L:326:ALA:HB1	1.99	0.45
19:L:249:SER:OG	20:M:307:GLU:OE2	2.29	0.45
23:P:174:SER:HB2	23:P:216:LEU:HD11	1.98	0.45
25:R:59:MET:HB3	25:R:62:TYR:HD2	1.80	0.45
26:S:479:MET:SD	28:U:298:ASN:ND2	2.80	0.45
29:V:106:GLY:HA3	29:V:137:VAL:H	1.81	0.45
29:V:138:ALA:O	29:V:156:PHE:N	2.46	0.45
33:Z:208:VAL:HB	33:Z:236:PHE:CD1	2.52	0.45
18:K:158:ILE:HG21	18:K:237:VAL:HA	1.99	0.45
19:L:348:GLU:HG2	19:L:350:PRO:HD3	1.98	0.45
29:V:202:ASP:OD1	29:V:203:TYR:N	2.50	0.45
10:C:45:VAL:HA	10:C:215:THR:HG22	1.99	0.45
12:E:15:PHE:CE2	13:F:126:ARG:HB2	2.51	0.45
20:M:290:ARG:HH21	20:M:297:GLY:CA	2.30	0.45
20:M:299:ARG:O	20:M:303:ARG:HG3	2.17	0.45
23:P:299:LEU:HD23	23:P:302:LEU:HD12	1.99	0.45
24:Q:164:GLU:HB3	24:Q:168:LEU:HD12	1.99	0.45
24:Q:65:TYR:HB3	24:Q:70:ALA:HB3	1.98	0.45
11:D:-83:SER:HG	11:D:-81:TRP:HE1	1.65	0.44
19:L:180:PHE:HA	19:L:183:ILE:HG12	1.99	0.44
20:M:219:LEU:HD22	20:M:338:LEU:HD21	2.00	0.44
21:N:578:ASP:O	21:N:584:ARG:NE	2.42	0.44
24:Q:390:LEU:O	25:R:346:LYS:N	2.50	0.44
5:5:82:ARG:HG2	5:5:87:ILE:HG12	2.00	0.44
8:A:29:GLU:HG2	18:K:427:TYR:HE2	1.81	0.44
9:B:1:MET:HG2	9:B:4:ARG:HH21	1.81	0.44
12:E:15:PHE:HE2	13:F:127:PRO:HD2	1.81	0.44
19:L:217:GLY:HA3	19:L:343:LEU:HD23	1.99	0.44
27:T:79:GLU:O	27:T:83:ASN:ND2	2.51	0.44
1:1:33:LEU:HD11	1:1:119:ALA:HB3	1.99	0.44
2:2:104:ARG:HG2	2:2:133:ASP:HB2	2.00	0.44
5:5:116:LEU:HD21	5:5:151:VAL:HG22	1.98	0.44
5:5:191:ASP:OD1	5:5:195:THR:N	2.47	0.44
8:A:35:THR:HG21	8:A:140:ILE:HG13	1.99	0.44
10:C:66:LEU:HD23	10:C:76:ALA:HA	2.00	0.44
16:I:178:THR:HG23	16:I:238:ASN:HD21	1.81	0.44
16:I:299:GLU:HA	16:I:302:ILE:HD12	1.99	0.44
16:I:417:LYS:HA	16:I:420:LYS:HE2	1.99	0.44
33:Z:208:VAL:HA	33:Z:211:PHE:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:405:ASN:HB3	33:Z:409:LYS:HE3	2.00	0.44
8:A:128:TYR:CD1	8:A:134:MET:HG2	2.53	0.44
17:J:71:TYR:N	17:J:115:LEU:O	2.46	0.44
23:P:72:TRP:HE3	23:P:118:VAL:HG21	1.83	0.44
24:Q:104:PHE:HE2	24:Q:114:GLN:HA	1.83	0.44
28:U:21:HIS:CE1	28:U:53:ALA:HB2	2.52	0.44
33:Z:577:GLN:NE2	33:Z:580:GLN:OE1	2.50	0.44
2:2:104:ARG:HD2	8:A:110:TYR:CE1	2.52	0.44
17:J:35:ARG:HH22	26:S:48:LEU:HD11	1.83	0.44
21:N:326:SER:HB3	21:N:329:HIS:HD2	1.82	0.44
29:V:116:CYS:HB2	29:V:181:ASN:HD22	1.82	0.44
29:V:29:ILE:HA	29:V:65:VAL:HB	1.99	0.44
5:5:84:GLN:OE1	5:5:221:TRP:NE1	2.50	0.44
6:6:24:TYR:OH	6:6:123:PRO:O	2.24	0.44
7:7:92:ASP:HB3	7:7:145:ASN:HD21	1.82	0.44
18:K:131:LEU:HB3	18:K:149:ILE:HD13	1.99	0.44
24:Q:172:PRO:HB3	24:Q:208:ILE:HG21	1.99	0.44
4:4:77:PRO:HG2	4:4:115:GLU:HB2	2.00	0.44
4:4:46:PHE:HE1	4:4:53:THR:HB	1.83	0.44
7:7:144:TRP:HA	7:7:165:LEU:HD23	2.00	0.44
23:P:353:ILE:HG23	23:P:357:TYR:HB2	2.00	0.44
33:Z:204:CYS:HA	33:Z:207:ILE:HD12	1.99	0.44
15:H:103:THR:O	20:M:166:ARG:NH1	2.35	0.44
16:I:335:ASP:HB3	16:I:338:LEU:HG	1.99	0.44
21:N:250:ASP:HB3	21:N:253:LEU:HD13	1.99	0.44
21:N:738:GLN:O	21:N:745:LEU:HD12	2.18	0.44
23:P:212:LYS:HB2	23:P:217:LYS:HE3	2.00	0.44
23:P:243:GLU:O	23:P:247:THR:OG1	2.27	0.44
1:1:82:LEU:HA	1:1:85:TYR:HB3	2.00	0.44
3:3:63:LEU:HD12	3:3:105:VAL:HG11	1.98	0.44
4:4:8:ARG:HH11	4:4:116:LEU:H	1.65	0.44
5:5:153:ALA:HB1	11:D:-140:LEU:HD22	1.99	0.44
9:B:43:VAL:HG11	9:B:137:ALA:HB1	1.99	0.44
15:H:304:CYS:SG	15:H:349:ILE:HG21	2.58	0.44
31:X:7:VAL:HG12	31:X:8:ILE:HG13	2.00	0.44
16:I:248:VAL:HG21	17:J:271:THR:HG23	2.00	0.43
21:N:890:PHE:HB3	21:N:905:LEU:HD23	2.00	0.43
26:S:234:ILE:HG23	26:S:253:PHE:HE2	1.83	0.43
26:S:82:TYR:CD2	26:S:86:SER:HB3	2.53	0.43
29:V:24:LYS:HB2	29:V:174:THR:HA	1.98	0.43
33:Z:314:LEU:O	33:Z:321:PHE:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:233:GLN:HA	10:C:236:LYS:HE2	2.00	0.43
11:D:-147:ALA:HA	11:D:-136:VAL:HG11	1.99	0.43
12:E:201:LEU:HD22	12:E:212:LEU:HD21	1.99	0.43
14:G:70:VAL:HB	14:G:74:ILE:HB	2.00	0.43
17:J:146:THR:HG22	17:J:204:HIS:CD2	2.52	0.43
21:N:625:LEU:HD13	21:N:637:ALA:HB1	2.00	0.43
29:V:154:ASP:OD2	29:V:181:ASN:ND2	2.50	0.43
1:1:22:ILE:HG13	1:1:117:ILE:HD12	1.99	0.43
2:2:225:ARG:HH12	3:3:151:GLU:HG3	1.83	0.43
4:4:172:MET:HG2	4:4:174:MET:H	1.84	0.43
4:4:70:ARG:HE	10:C:113:ARG:CZ	2.32	0.43
5:5:76:THR:HG23	5:5:108:LYS:HZ3	1.82	0.43
5:5:220:LYS:HG2	5:5:222:ASP:H	1.83	0.43
6:6:50:THR:OG1	6:6:55:ASN:ND2	2.42	0.43
6:6:62:VAL:HG22	6:6:72:SER:HB3	2.00	0.43
9:B:33:THR:HA	9:B:165:GLY:HA3	2.01	0.43
19:L:400:PHE:HA	19:L:403:ILE:HD12	2.00	0.43
21:N:362:TRP:HB2	29:V:169:GLU:HB2	1.99	0.43
10:C:194:LEU:HB3	10:C:244:ILE:HG13	2.00	0.43
16:I:280:PHE:CE2	16:I:282:ASP:HB2	2.53	0.43
16:I:291:ARG:HB3	17:J:261:SER:HB3	2.01	0.43
18:K:127:ASP:OD1	18:K:128:ARG:N	2.52	0.43
18:K:177:LEU:HD13	18:K:222:LEU:HD11	1.99	0.43
20:M:194:VAL:HG12	20:M:199:LEU:HG	1.99	0.43
22:O:302:VAL:HG12	22:O:303:LYS:HG2	1.99	0.43
23:P:312:PRO:HA	23:P:315:GLN:HB3	2.00	0.43
27:T:200:LEU:HD13	27:T:205:ILE:HB	2.01	0.43
28:U:59:ASP:OD1	28:U:60:GLU:N	2.51	0.43
33:Z:233:LEU:HB2	33:Z:234:PRO:HD3	1.99	0.43
1:1:23:MET:HB3	1:1:145:ILE:HG22	2.00	0.43
7:7:100:LEU:HD21	7:7:129:LEU:HD11	2.00	0.43
21:N:17:GLN:HB3	21:N:20:VAL:HB	2.00	0.43
25:R:254:SER:HB3	25:R:289:ILE:HG22	2.00	0.43
26:S:458:GLN:NE2	28:U:270:ASN:OD1	2.44	0.43
33:Z:189:ALA:HB2	33:Z:198:GLU:HG3	2.01	0.43
7:7:35:GLN:HE22	7:7:143:LEU:HD23	1.83	0.43
13:F:2:PHE:CD2	13:F:3:ARG:HG3	2.53	0.43
18:K:362:LEU:HG	18:K:402:ILE:HB	2.00	0.43
18:K:285:GLN:HE22	19:L:297:ALA:HB2	1.83	0.43
21:N:91:ILE:HD11	21:N:139:ARG:HH11	1.84	0.43
22:O:50:ASP:OD1	22:O:51:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:138:ARG:HH12	33:Z:146:PHE:HZ	1.65	0.43
33:Z:391:ASN:HB2	33:Z:425:ILE:HG12	2.01	0.43
4:4:55:GLN:HG3	5:5:163:TYR:CG	2.54	0.43
10:C:141:ASP:OD1	10:C:142:ASP:N	2.51	0.43
13:F:45:VAL:HG11	13:F:190:ILE:HA	2.01	0.43
26:S:49:ASP:HB2	26:S:50:PRO:HD3	2.00	0.43
21:N:740:TRP:HE3	29:V:175:SER:HB2	1.84	0.43
18:K:372:ILE:HA	18:K:375:ASN:ND2	2.34	0.43
19:L:295:THR:HB	19:L:298:ASP:OD1	2.19	0.43
18:K:419:ASN:HB3	19:L:435:GLN:HA	2.01	0.43
20:M:278:ILE:HB	20:M:323:VAL:HG22	2.01	0.43
22:O:166:ARG:HG3	22:O:167:ILE:H	1.83	0.43
33:Z:593:HIS:O	33:Z:596:THR:HG22	2.19	0.43
33:Z:800:SER:O	33:Z:837:TYR:OH	2.26	0.43
14:G:70:VAL:N	14:G:74:ILE:O	2.43	0.43
16:I:287:ILE:HG21	16:I:302:ILE:HG23	1.99	0.43
25:R:29:LYS:HE3	25:R:53:LYS:HB2	2.00	0.43
33:Z:971:ILE:HA	33:Z:976:HIS:CE1	2.54	0.43
1:1:61:TRP:CD1	1:1:197:LEU:HD21	2.54	0.43
1:1:56:VAL:HA	1:1:79:GLN:HG2	2.00	0.43
5:5:120:MET:HG2	5:5:127:CYS:HB3	2.01	0.43
8:A:43:LEU:HD11	8:A:206:ALA:HB1	2.01	0.43
11:D:-198:VAL:HG11	11:D:-104:ALA:HB1	2.01	0.43
11:D:-38:VAL:HG13	11:D:-37:VAL:H	1.83	0.43
12:E:207:VAL:HG12	15:H:409:ARG:HH12	1.84	0.43
15:H:460:THR:HG21	16:I:337:ALA:HA	2.01	0.43
18:K:158:ILE:HG21	18:K:237:VAL:HG22	2.00	0.43
18:K:279:THR:C	18:K:281:ARG:H	2.22	0.43
18:K:97:GLY:HA2	18:K:112:SER:HA	2.01	0.43
4:4:3:ILE:HD12	4:4:176:PHE:HB3	2.00	0.42
18:K:369:ASP:HA	18:K:372:ILE:HD12	2.01	0.42
19:L:397:GLU:OE1	19:L:421:LYS:NZ	2.43	0.42
19:L:399:GLY:HA3	20:M:212:ILE:HD13	2.01	0.42
1:1:85:TYR:CZ	1:1:96:THR:HG21	2.54	0.42
2:2:75:ALA:HB3	2:2:126:TYR:HB2	2.01	0.42
15:H:243:PRO:O	15:H:350:LYS:NZ	2.48	0.42
18:K:155:ASP:HB2	19:L:110:LYS:HB3	2.01	0.42
33:Z:211:PHE:HD1	33:Z:216:GLY:HA3	1.84	0.42
33:Z:350:GLY:O	33:Z:352:LYS:N	2.51	0.42
33:Z:60:ASP:OD1	33:Z:61:SER:N	2.52	0.42
2:2:189:GLN:HA	2:2:192:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:249:ALA:HB1	24:Q:94:VAL:HG11	2.01	0.42
18:K:223:VAL:HG21	18:K:270:PHE:CE1	2.54	0.42
18:K:284:ALA:HB1	18:K:292:VAL:HG21	2.01	0.42
19:L:293:GLU:HG2	20:M:296:SER:H	1.84	0.42
20:M:395:THR:HG22	20:M:415:PHE:HE1	1.85	0.42
21:N:776:TYR:HD2	21:N:881:TYR:HB3	1.85	0.42
29:V:118:LEU:HD12	29:V:196:TYR:HB3	2.01	0.42
31:X:37:PRO:HB3	31:X:46:TRP:HD1	1.84	0.42
9:B:33:THR:OG1	9:B:166:LYS:N	2.52	0.42
11:D:-83:SER:HB2	12:E:63:SER:HB3	2.01	0.42
11:D:-224:HIS:CE1	12:E:33:LEU:HD13	2.54	0.42
25:R:132:GLN:HA	25:R:135:ILE:HD12	2.01	0.42
33:Z:362:LEU:HD13	33:Z:859:LYS:HD2	2.01	0.42
2:2:74:GLY:HA2	2:2:127:LEU:HD23	2.01	0.42
4:4:118:GLN:NE2	4:4:132:ALA:O	2.52	0.42
4:4:130:TYR:OH	4:4:145:ASP:OD1	2.33	0.42
21:N:498:ILE:HG23	21:N:535:LEU:HD13	2.01	0.42
21:N:664:LEU:HD13	21:N:675:VAL:HG23	2.02	0.42
24:Q:161:LEU:HD22	24:Q:165:PHE:CZ	2.55	0.42
26:S:385:SER:O	26:S:389:LYS:HG2	2.20	0.42
8:A:54:ILE:HG22	8:A:225:VAL:HG13	2.01	0.42
24:Q:59:LEU:HD22	24:Q:103:LYS:HG3	2.02	0.42
26:S:321:GLN:HG3	26:S:328:PRO:HB3	2.01	0.42
26:S:330:LEU:HD13	32:Y:64:TRP:CD1	2.55	0.42
2:2:79:ALA:HB2	3:3:129:CYS:HB2	2.01	0.42
3:3:145:GLN:HG2	3:3:177:ARG:HB2	2.02	0.42
13:F:39:ARG:HA	13:F:44:ALA:HA	2.01	0.42
25:R:150:ALA:O	25:R:153:THR:OG1	2.30	0.42
29:V:126:GLN:HG2	29:V:158:LEU:HD21	2.01	0.42
30:W:109:ARG:HA	30:W:138:ALA:HB3	2.02	0.42
1:1:20:THR:HA	1:1:188:SER:HB3	2.01	0.42
1:1:54:THR:HG21	1:1:75:ALA:HB1	2.01	0.42
5:5:92:ASP:HB2	5:5:247:GLY:O	2.19	0.42
7:7:54:ILE:HG12	7:7:232:ILE:HG12	2.02	0.42
8:A:78:THR:HG22	8:A:231:ASP:HA	2.02	0.42
9:B:32:VAL:HG23	9:B:50:LYS:HE2	2.02	0.42
13:F:49:LEU:HB2	13:F:197:ILE:HD11	2.01	0.42
26:S:421:TYR:CE2	27:T:208:LEU:HD13	2.55	0.42
31:X:48:PHE:HD2	31:X:66:LEU:HD23	1.84	0.42
31:X:91:PHE:HB3	31:X:94:ASN:ND2	2.34	0.42
33:Z:90:LYS:HG2	33:Z:126:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:205:GLU:HA	14:G:208:LYS:HE3	2.01	0.42
16:I:358:LYS:HG2	16:I:392:ILE:HD11	2.00	0.42
19:L:290:ARG:HG2	20:M:296:SER:HA	2.00	0.42
26:S:378:GLN:HB2	27:T:127:GLN:HE21	1.85	0.42
6:6:77:ALA:HB3	7:7:168:VAL:HG22	2.02	0.42
8:A:104:PHE:HA	8:A:108:TYR:CD2	2.54	0.42
18:K:391:GLY:HA3	19:L:212:ILE:HG21	2.02	0.42
22:O:277:ILE:HG12	22:O:279:ILE:H	1.85	0.42
33:Z:922:PRO:HB3	33:Z:959:HIS:HB3	2.02	0.42
6:6:47:ARG:HD2	6:6:216:GLN:O	2.20	0.41
19:L:290:ARG:HD2	20:M:298:ASP:HB3	2.02	0.41
21:N:338:PHE:HZ	21:N:746:ALA:HB1	1.85	0.41
25:R:235:LEU:N	25:R:238:PHE:HE2	2.18	0.41
26:S:226:ASP:OD2	26:S:229:THR:OG1	2.31	0.41
29:V:49:VAL:HG12	29:V:73:GLN:HE22	1.85	0.41
14:G:193:VAL:HG13	14:G:216:ILE:HG21	2.01	0.41
17:J:96:VAL:HG11	17:J:115:LEU:HD11	2.02	0.41
17:J:32:LEU:HD11	26:S:225:HIS:HB2	2.01	0.41
26:S:315:LYS:HG2	26:S:345:TYR:HE2	1.85	0.41
26:S:367:TYR:HD1	26:S:370:LEU:HD12	1.85	0.41
33:Z:827:LEU:HD23	33:Z:830:LEU:HD12	2.02	0.41
1:1:20:THR:O	1:1:149:GLY:N	2.50	0.41
3:3:172:LEU:HD22	3:3:202:MET:HB3	2.02	0.41
3:3:103:TYR:HA	4:4:93:ARG:HH22	1.84	0.41
8:A:168:ALA:HB1	8:A:182:LEU:HD13	2.01	0.41
9:B:97:TYR:O	9:B:101:TYR:N	2.54	0.41
9:B:185:LEU:HD21	9:B:213:ILE:HD12	2.02	0.41
12:E:32:LYS:NZ	12:E:177:GLU:OE2	2.46	0.41
16:I:306:MET:HB3	16:I:338:LEU:HD11	2.02	0.41
20:M:166:ARG:HB2	20:M:170:MET:HB2	2.02	0.41
21:N:6:ALA:HB3	21:N:38:GLU:HB2	2.02	0.41
22:O:45:LEU:HG	22:O:49:PHE:HE2	1.85	0.41
33:Z:180:ASP:OD1	33:Z:181:GLY:N	2.53	0.41
8:A:134:MET:SD	14:G:125:LEU:HB3	2.60	0.41
18:K:239:GLY:HA2	18:K:242:PHE:HE2	1.85	0.41
19:L:302:GLN:HE22	19:L:305:LEU:HD23	1.85	0.41
21:N:389:TYR:HB3	21:N:404:SER:HB3	2.02	0.41
21:N:43:LEU:HD13	21:N:68:VAL:HG21	2.02	0.41
25:R:304:TYR:CZ	25:R:308:LEU:HD21	2.56	0.41
1:1:80:TYR:HB2	8:A:106:TYR:HB2	2.03	0.41
2:2:192:ILE:HG12	2:2:199:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:13:VAL:HG13	3:3:167:ILE:HD11	2.03	0.41
6:6:130:ILE:HD11	6:6:142:TYR:HD2	1.86	0.41
8:A:87:ILE:N	8:A:88:PRO:HD2	2.35	0.41
21:N:542:SER:O	21:N:548:ARG:NE	2.47	0.41
33:Z:85:VAL:HB	33:Z:90:LYS:HD2	2.02	0.41
8:A:136:PRO:HD2	14:G:15:PHE:HE2	1.86	0.41
14:G:71:ASP:CG	14:G:72:ARG:H	2.24	0.41
18:K:280:LYS:HB2	18:K:296:LEU:HD13	2.03	0.41
19:L:187:THR:HA	19:L:190:ILE:HD12	2.02	0.41
23:P:130:ILE:HG23	23:P:132:VAL:HG13	2.03	0.41
25:R:63:TYR:CE2	25:R:94:PHE:HA	2.56	0.41
26:S:339:GLN:HA	26:S:342:LEU:HB2	2.01	0.41
33:Z:237:VAL:HG21	33:Z:245:VAL:HG21	2.02	0.41
16:I:183:ASP:HA	16:I:364:ILE:HG21	2.03	0.41
16:I:248:VAL:HG12	16:I:250:SER:H	1.85	0.41
16:I:435:LEU:HG	16:I:436:TYR:CD2	2.56	0.41
23:P:290:LEU:HG	23:P:292:LYS:H	1.86	0.41
26:S:204:ASP:O	27:T:92:ASN:ND2	2.54	0.41
1:1:94:THR:OG1	1:1:128:GLU:OE1	2.31	0.41
7:7:161:ARG:HE	7:7:169:THR:HB	1.85	0.41
6:6:55:ASN:HB3	7:7:170:TYR:CZ	2.55	0.41
18:K:90:GLN:HG3	18:K:147:VAL:HG13	2.03	0.41
22:O:166:ARG:HG3	22:O:167:ILE:N	2.36	0.41
25:R:214:TYR:OH	25:R:226:GLU:OE1	2.31	0.41
27:T:227:PRO:HB2	27:T:234:TYR:HB3	2.03	0.41
3:3:123:GLY:HA3	3:3:137:ILE:HG21	2.03	0.41
6:6:220:GLY:H	6:6:238:LEU:HB2	1.85	0.41
10:C:91:ALA:HA	10:C:115:LEU:HD21	2.01	0.41
16:I:174:ASP:OD2	16:I:244:PHE:HB3	2.20	0.41
16:I:366:THR:HA	16:I:369:MET:HB2	2.03	0.41
17:J:164:ILE:HG12	17:J:289:LYS:HE2	2.03	0.41
19:L:167:VAL:O	19:L:171:THR:OG1	2.30	0.41
20:M:390:GLN:HB3	20:M:424:ALA:HB2	2.02	0.41
21:N:340:HIS:HB2	21:N:374:ILE:HG12	2.03	0.41
22:O:360:GLY:HA2	22:O:363:ILE:HD12	2.02	0.41
25:R:291:SER:HB3	25:R:307:TYR:CG	2.56	0.41
1:1:48:ARG:NH1	2:2:168:GLU:OE2	2.38	0.41
4:4:4:ILE:HG13	4:4:47:ALA:HB2	2.02	0.41
10:C:31:HIS:O	10:C:51:LYS:NZ	2.37	0.41
16:I:222:TYR:HE1	16:I:330:LYS:HA	1.86	0.41
18:K:209:VAL:HB	18:K:315:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:L:129:VAL:HB	19:L:154:THR:HA	2.02	0.41
21:N:178:SER:OG	21:N:179:THR:N	2.52	0.41
28:U:24:ARG:HD3	29:V:100:ARG:NH1	2.35	0.41
32:Y:69:VAL:HG12	32:Y:70:ASP:N	2.31	0.41
7:7:80:ASP:OD1	7:7:81:ASN:N	2.54	0.41
17:J:218:LEU:HB3	17:J:230:VAL:HG22	2.02	0.41
23:P:360:ILE:HG22	23:P:402:PHE:HE2	1.85	0.41
23:P:426:ILE:HA	28:U:203:LYS:HZ1	1.86	0.41
24:Q:378:SER:HA	24:Q:381:ILE:HD12	2.03	0.41
26:S:208:ILE:HG12	26:S:211:ARG:HH21	1.86	0.41
8:A:14:ARG:HG2	8:A:26:TYR:CD2	2.56	0.40
9:B:40:THR:OG1	9:B:45:ILE:HG12	15.63	0.40
19:L:196:VAL:HG12	19:L:215:PRO:HG2	2.04	0.40
21:N:55:PHE:CZ	21:N:57:ASP:HB2	2.56	0.40
21:N:742:TRP:CH2	21:N:744:PRO:HG2	2.57	0.40
21:N:762:ARG:NH2	21:N:907:ASP:OD2	2.43	0.40
33:Z:509:LEU:HB3	33:Z:526:ALA:HB1	2.03	0.40
5:5:238:ALA:HA	5:5:282:PHE:HZ	1.86	0.40
11:D:-38:VAL:HG13	11:D:-37:VAL:N	2.36	0.40
17:J:187:LEU:HG	17:J:314:ILE:HB	2.03	0.40
17:J:88:VAL:HG12	17:J:90:PRO:HD2	2.02	0.40
23:P:224:LEU:HD13	23:P:240:TYR:HB3	2.03	0.40
24:Q:191:LEU:HD11	24:Q:228:GLU:HG3	2.02	0.40
25:R:24:TYR:CE1	25:R:242:GLU:HG2	2.56	0.40
33:Z:559:LYS:O	33:Z:562:TRP:NE1	2.55	0.40
21:N:17:GLN:HG2	21:N:20:VAL:HG23	2.03	0.40
21:N:908:ARG:HG2	21:N:909:GLU:HG3	2.03	0.40
23:P:133:GLU:O	23:P:135:GLU:HG2	2.22	0.40
26:S:234:ILE:HG12	26:S:253:PHE:HZ	1.87	0.40
27:T:27:LEU:HB2	27:T:28:PRO:HD3	2.03	0.40
30:W:51:LEU:HD22	30:W:72:ILE:HG23	2.03	0.40
1:1:102:LYS:HD3	1:1:138:VAL:HG12	2.04	0.40
5:5:248:GLY:N	15:H:205:ASP:OD2	102.84	0.40
18:K:177:LEU:HD21	18:K:344:ARG:HH22	1.86	0.40
18:K:401:VAL:HG22	23:P:128:ASN:HB2	2.02	0.40
18:K:371:LEU:HD21	18:K:408:GLU:HG2	2.02	0.40
18:K:70:ASP:O	18:K:74:HIS:ND1	2.31	0.40
20:M:148:VAL:HG12	20:M:155:ILE:HG12	2.04	0.40
21:N:284:PRO:HA	21:N:287:LEU:HG	2.04	0.40
26:S:240:ASP:OD2	26:S:244:ASN:ND2	2.55	0.40
28:U:169:ILE:HD11	29:V:147:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:256:THR:OG1	5:5:259:GLY:O	2.26	0.40
7:7:37:PRO:HB2	7:7:40:THR:HG22	2.04	0.40
18:K:392:LEU:HD13	19:L:345:ARG:HH11	1.86	0.40
18:K:419:ASN:HB3	19:L:434:TYR:O	2.22	0.40
21:N:371:LEU:HD22	21:N:375:HIS:HE1	1.87	0.40
24:Q:160:ASP:OD1	24:Q:163:ARG:NH2	2.54	0.40
26:S:246:GLU:HG3	26:S:249:SER:H	1.87	0.40
29:V:41:GLY:HA2	29:V:49:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	203/215 (94%)	194 (96%)	9 (4%)	0	100	100
1	b	203/215 (94%)	191 (94%)	12 (6%)	0	100	100
2	2	220/261 (84%)	214 (97%)	6 (3%)	0	100	100
2	i	220/261 (84%)	211 (96%)	9 (4%)	0	100	100
3	3	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
3	h	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
4	4	196/198 (99%)	187 (95%)	9 (5%)	0	100	100
4	g	196/198 (99%)	190 (97%)	6 (3%)	0	100	100
5	5	210/287 (73%)	200 (95%)	10 (5%)	0	100	100
5	f	210/287 (73%)	201 (96%)	9 (4%)	0	100	100
6	6	220/241 (91%)	213 (97%)	7 (3%)	0	100	100
6	e	220/241 (91%)	212 (96%)	8 (4%)	0	100	100
7	7	231/266 (87%)	219 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	a	231/266 (87%)	226 (98%)	5 (2%)	0	100	100
8	A	241/252 (96%)	235 (98%)	6 (2%)	0	100	100
8	c	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
9	B	248/250 (99%)	240 (97%)	8 (3%)	0	100	100
9	j	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
10	C	242/258 (94%)	233 (96%)	9 (4%)	0	100	100
10	d	242/258 (94%)	234 (97%)	8 (3%)	0	100	100
11	D	239/254 (94%)	232 (97%)	7 (3%)	0	100	100
11	n	239/254 (94%)	231 (97%)	8 (3%)	0	100	100
12	E	240/260 (92%)	230 (96%)	10 (4%)	0	100	100
12	m	240/260 (92%)	230 (96%)	10 (4%)	0	100	100
13	F	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
13	l	231/234 (99%)	217 (94%)	14 (6%)	0	100	100
14	G	241/288 (84%)	232 (96%)	9 (4%)	0	100	100
14	k	242/288 (84%)	233 (96%)	9 (4%)	0	100	100
15	H	351/467 (75%)	313 (89%)	38 (11%)	0	100	100
16	I	360/437 (82%)	324 (90%)	36 (10%)	0	100	100
17	J	371/405 (92%)	344 (93%)	26 (7%)	1 (0%)	43	79
18	K	379/428 (89%)	338 (89%)	39 (10%)	2 (0%)	31	71
19	L	369/437 (84%)	339 (92%)	30 (8%)	0	100	100
20	M	363/434 (84%)	325 (90%)	37 (10%)	1 (0%)	43	79
21	N	843/945 (89%)	810 (96%)	33 (4%)	0	100	100
22	O	385/393 (98%)	342 (89%)	43 (11%)	0	100	100
23	P	430/445 (97%)	395 (92%)	35 (8%)	0	100	100
24	Q	429/434 (99%)	404 (94%)	25 (6%)	0	100	100
25	R	398/429 (93%)	355 (89%)	41 (10%)	2 (0%)	31	71
26	S	473/523 (90%)	452 (96%)	20 (4%)	1 (0%)	49	83
27	T	270/274 (98%)	245 (91%)	25 (9%)	0	100	100
28	U	245/338 (72%)	238 (97%)	7 (3%)	0	100	100
29	V	252/306 (82%)	231 (92%)	20 (8%)	1 (0%)	36	75
30	W	195/268 (73%)	183 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	X	109/156 (70%)	96 (88%)	13 (12%)	0	100	100
32	Y	25/89 (28%)	20 (80%)	4 (16%)	1 (4%)	3	32
33	Z	807/993 (81%)	753 (93%)	53 (7%)	1 (0%)	53	87
All	All	13383/15139 (88%)	12596 (94%)	777 (6%)	10 (0%)	56	87

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	J	134	VAL
18	K	158	ILE
18	K	160	VAL
20	M	167	VAL
25	R	26	VAL
25	R	241	ILE
29	V	165	ILE
32	Y	69	VAL
33	Z	442	VAL
26	S	83	PRO

### 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	1	169/178 (95%)	169 (100%)	0	100	100
1	b	169/178 (95%)	169 (100%)	0	100	100
2	2	181/214 (85%)	181 (100%)	0	100	100
2	i	181/214 (85%)	181 (100%)	0	100	100
3	3	172/173 (99%)	172 (100%)	0	100	100
3	h	172/173 (99%)	172 (100%)	0	100	100
4	4	175/175 (100%)	175 (100%)	0	100	100
4	g	175/175 (100%)	175 (100%)	0	100	100
5	5	169/235 (72%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	f	169/235 (72%)	169 (100%)	0	100	100
6	6	185/201 (92%)	185 (100%)	0	100	100
6	e	185/201 (92%)	185 (100%)	0	100	100
7	7	199/224 (89%)	199 (100%)	0	100	100
7	a	199/224 (89%)	199 (100%)	0	100	100
8	A	207/210 (99%)	207 (100%)	0	100	100
8	c	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
9	j	209/209 (100%)	209 (100%)	0	100	100
10	C	203/216 (94%)	203 (100%)	0	100	100
10	d	203/216 (94%)	203 (100%)	0	100	100
11	D	213/226 (94%)	213 (100%)	0	100	100
11	n	213/226 (94%)	213 (100%)	0	100	100
12	E	198/215 (92%)	198 (100%)	0	100	100
12	m	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	l	192/193 (100%)	192 (100%)	0	100	100
14	G	200/239 (84%)	200 (100%)	0	100	100
14	k	201/239 (84%)	201 (100%)	0	100	100
15	H	303/399 (76%)	303 (100%)	0	100	100
16	I	319/385 (83%)	319 (100%)	0	100	100
17	J	325/352 (92%)	325 (100%)	0	100	100
18	K	334/374 (89%)	334 (100%)	0	100	100
19	L	317/377 (84%)	317 (100%)	0	100	100
20	M	315/375 (84%)	315 (100%)	0	100	100
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	363/368 (99%)	363 (100%)	0	100	100
23	P	405/415 (98%)	405 (100%)	0	100	100
24	Q	388/391 (99%)	388 (100%)	0	100	100
25	R	351/379 (93%)	351 (100%)	0	100	100
26	S	447/489 (91%)	447 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	234 (100%)	0	100	100
29	V	227/268 (85%)	227 (100%)	0	100	100
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	101/144 (70%)	101 (100%)	0	100	100
32	Y	26/81 (32%)	26 (100%)	0	100	100
33	Z	692/850 (81%)	692 (100%)	0	100	100
All	All	11630/13054 (89%)	11630 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	95	HIS
2	2	115	HIS
3	3	169	GLN
4	4	65	GLN
5	5	263	HIS
6	6	55	ASN
6	6	178	GLN
6	6	216	GLN
7	7	35	GLN
7	7	145	ASN
2	i	115	HIS
2	i	122	HIS
2	i	143	HIS
3	h	169	GLN
4	g	112	ASN
4	g	191	GLN
5	f	254	HIS
6	e	55	ASN
6	e	216	GLN
7	a	153	GLN
10	C	147	GLN
11	D	-224	HIS
12	E	23	GLN
13	F	41	ASN
13	F	52	ASN

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Mol	Chain	Res	Type
14	G	90	ASN
14	G	127	ASN
14	G	182	HIS
14	G	183	HIS
8	c	37	GLN
8	c	181	ASN
10	d	120	GLN
11	n	16	HIS
13	l	117	GLN
13	l	210	ASN
14	k	121	GLN
14	k	183	HIS
15	H	95	HIS
15	H	98	GLN
15	H	265	ASN
17	J	25	GLN
17	J	47	GLN
17	J	52	ASN
17	J	181	GLN
17	J	278	GLN
18	K	238	ASN
18	K	285	GLN
18	K	302	GLN
18	K	375	ASN
19	L	302	GLN
20	M	125	GLN
21	N	34	GLN
21	N	226	ASN
21	N	267	GLN
21	N	375	HIS
21	N	564	ASN
21	N	719	ASN
21	N	738	GLN
21	N	747	HIS
22	O	122	HIS
22	O	354	GLN
23	P	78	GLN
23	P	348	HIS
23	P	349	ASN
23	P	417	HIS
24	Q	106	GLN
24	Q	145	HIS

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Mol	Chain	Res	Type
24	Q	150	GLN
24	Q	226	HIS
24	Q	346	ASN
24	Q	379	GLN
25	R	73	ASN
26	S	177	ASN
26	S	227	ASN
26	S	283	GLN
26	S	311	GLN
26	S	321	GLN
26	S	334	HIS
26	S	450	ASN
26	S	459	GLN
26	S	469	ASN
27	T	92	ASN
27	T	127	GLN
28	U	75	ASN
28	U	193	GLN
28	U	302	GLN
29	V	73	GLN
29	V	126	GLN
29	V	181	ASN
29	V	190	HIS
29	V	279	HIS
30	W	108	GLN
30	W	184	ASN
31	X	38	ASN
31	X	94	ASN
33	Z	391	ASN
33	Z	532	HIS
33	Z	763	HIS
33	Z	810	ASN
33	Z	976	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.