



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Apr 1, 2019 – 09:32 AM EDT

PDB ID : 6J2Q
EMDB ID: : EMD-9771
Title : Yeast proteasome in Ub-accepted state (C1-b)
Authors : Cong, Y.
Deposited on : 2019-01-02
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

A user guide is available at

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

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) : rb-20031633

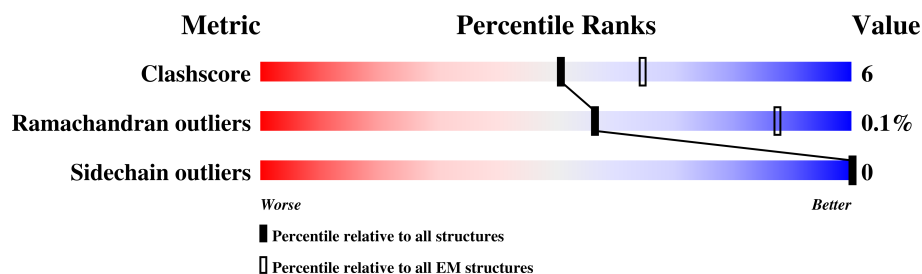
1 Overall quality at a glance

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.









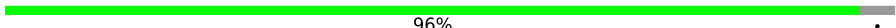

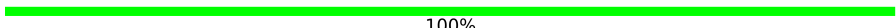

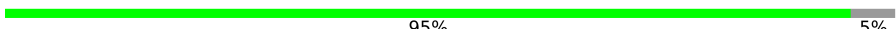

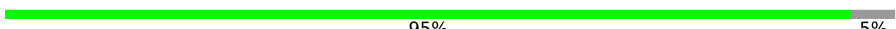



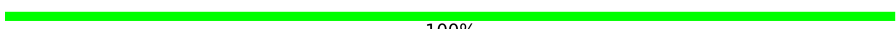








Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 ≥ 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	75% 20% 5%
1	b	215	95% 5%
2	2	261	72% 13% 15%
2	i	261	85% 15%
3	3	205	79% 20%
3	h	205	99%
4	4	198	80% 20%
4	g	198	100%
5	5	287	62% 12% 26%














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Mol	Chain	Length	Quality of chain
5	f	287	 74% 26%
6	6	241	 79% 13% 8%
6	e	241	 92% 8%
7	7	266	 72% 15% 12%
7	a	266	 88% 12%
8	A	252	 78% 19% .
8	c	252	 96% .
9	B	250	 80% 20%
9	j	250	 100%
10	C	258	 77% 18% 5%
10	d	258	 95% 5%
11	D	254	 79% 16% 5%
11	n	254	 95% 5%
12	E	260	 76% 17% 7%
12	m	260	 93% 7%
13	F	234	 76% 23%
13	l	234	 100%
14	G	288	 68% 16% 16%
14	k	288	 85% 15%
15	H	467	 58% 18% 24%
16	I	437	 69% 14% 17%
17	J	405	 73% 20% 8%
18	K	428	 71% 18% 11%
19	L	437	 68% 17% 15%
20	M	434	 67% 18% 15%

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Mol	Chain	Length	Quality of chain
21	N	945	 77%13%10%
22	O	393	 82%16%.
23	P	445	 81%16%.
24	Q	434	 91%9%.
25	R	429	 77%17%7%
26	S	523	 81%10%9%
27	T	274	 89%11%.
28	U	338	 64%12%25%
29	V	306	 64%20%16%
30	W	268	 56%17%26%
31	X	156	 68%13%19%
32	Y	89	 24%7%70%
33	Z	993	 70%12%18%

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 106311 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 subunit beta type-6.

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 protease 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	363	Total	C	N	O	S	0	0
			2831	1779	472	565	15		

- Molecule 17 is a protein called 26S protease 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 protease 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 protease 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 protease 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	127	Total	C	N	O	S	0	0
			1032	664	169	195	4		

- 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.

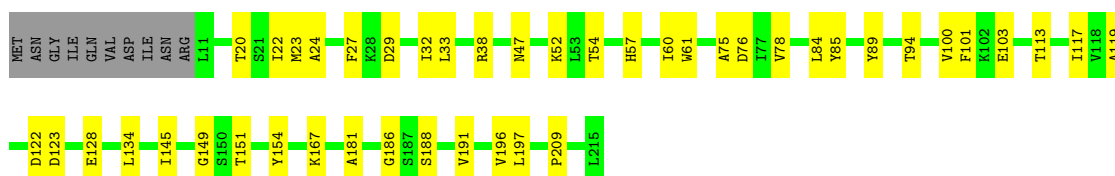
Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	813	Total	C	N	O	S	0	0
			6290	3995	1029	1237	29		

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.

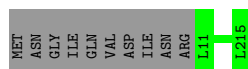
- Molecule 1: Proteasome subunit beta type-1

Chain 1: 



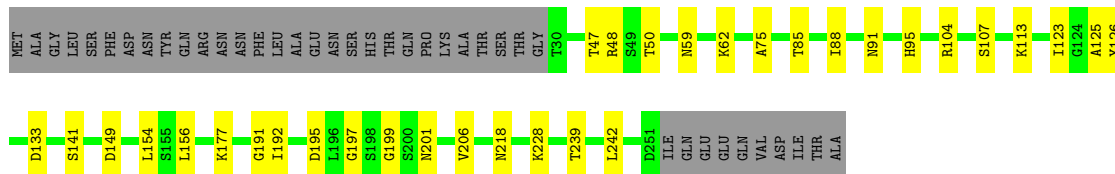
- Molecule 1: Proteasome subunit beta type-1

Chain b: 




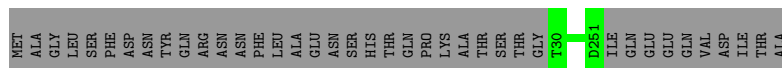
- Molecule 2: Proteasome subunit beta type-2

Chain 2: 




- Molecule 2: Proteasome subunit beta type-2

Chain i: 



- Molecule 3: Proteasome subunit beta type-3

Chain 3: 





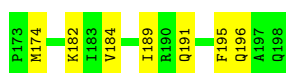
- Molecule 3: Proteasome subunit beta type-3

Chain h: 99%



- Molecule 4: Proteasome subunit beta type-4

Chain 4: 80% 20%



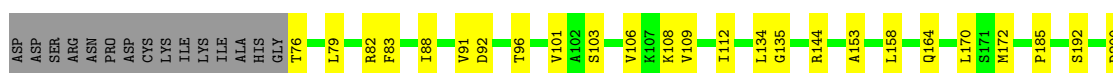
- Molecule 4: Proteasome subunit beta type-4

Chain g: 100%

There are no outlier residues recorded for this chain.

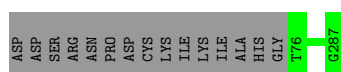
- Molecule 5: Proteasome subunit beta type-5

Chain 5: 62% 12% 26%



- Molecule 5: Proteasome subunit beta type-5

Chain f: 74% 26%



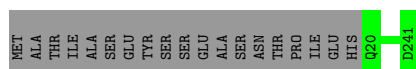
- Molecule 6: Proteasome subunit beta type-6

Chain 6: 79% 13% 8%



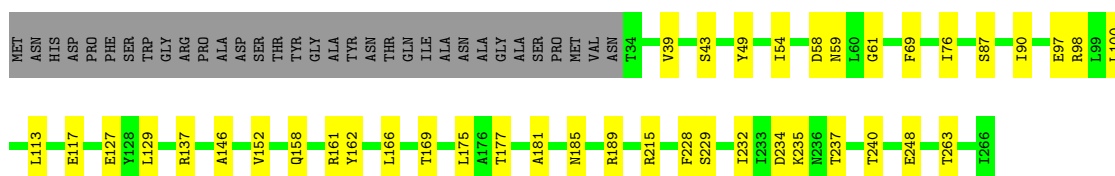
- Molecule 6: Proteasome subunit beta type-6

Chain e: 92% 8%



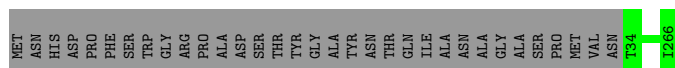
- Molecule 7: Proteasome subunit beta type-7

Chain 7: 72% 15% 12%



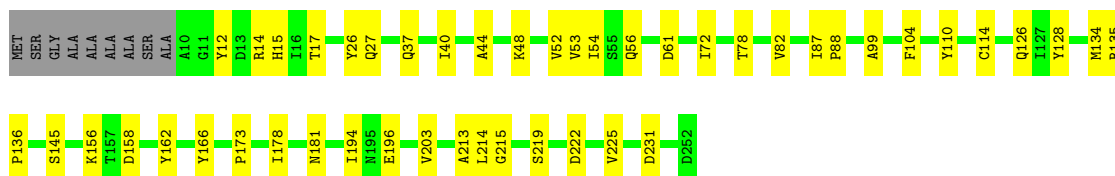
- Molecule 7: Proteasome subunit beta type-7

Chain a: 88% 12%



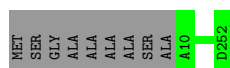
- Molecule 8: Proteasome subunit alpha type-1

Chain A: 78% 19% .



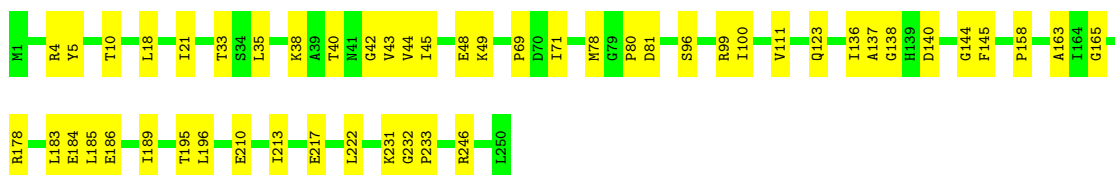
- Molecule 8: Proteasome subunit alpha type-1

Chain c: 96% .



- Molecule 9: Proteasome subunit alpha type-2

Chain B: 80% 20%



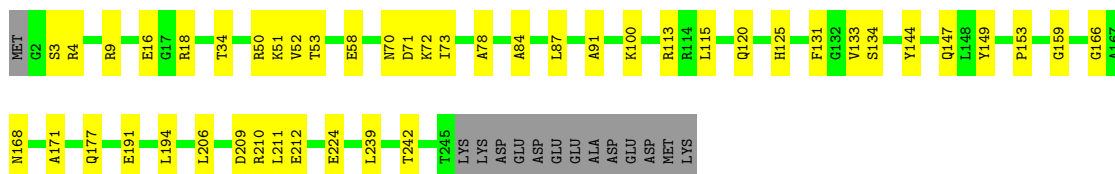
- Molecule 9: Proteasome subunit alpha type-2

Chain j:  100%

There are no outlier residues recorded for this chain.

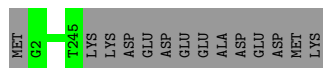
- Molecule 10: Proteasome subunit alpha type-3

Chain C:  77%  18%  5%






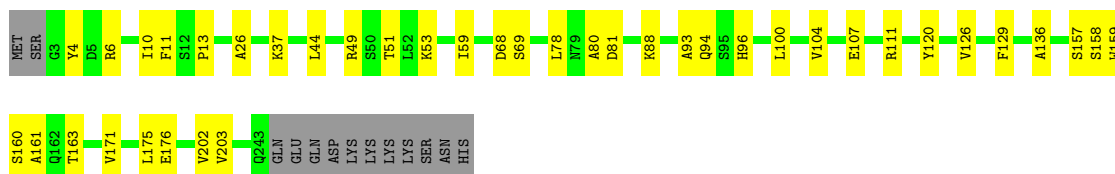
- Molecule 10: Proteasome subunit alpha type-3

Chain d:  95%  5%



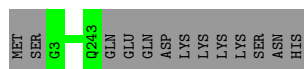
- Molecule 11: Proteasome subunit alpha type-4

Chain D:  79%  16%  5%





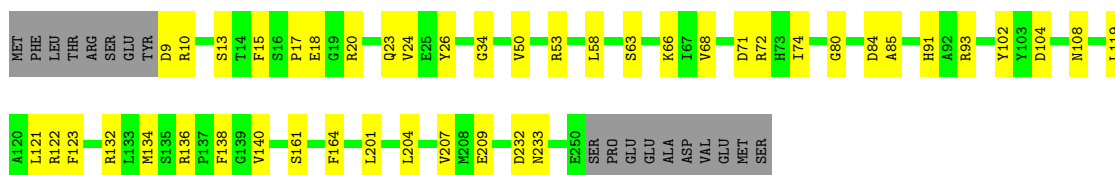
- Molecule 11: Proteasome subunit alpha type-4

Chain n:  95%  5%

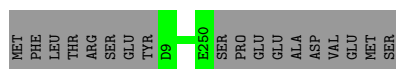


- Molecule 12: Proteasome subunit alpha type-5

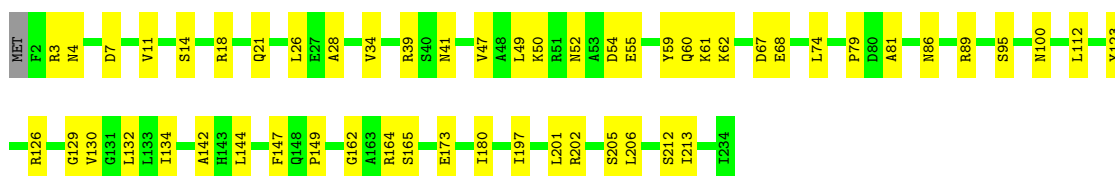
Chain E:  76%  17%  7%



- Molecule 12: Proteasome subunit alpha type-5



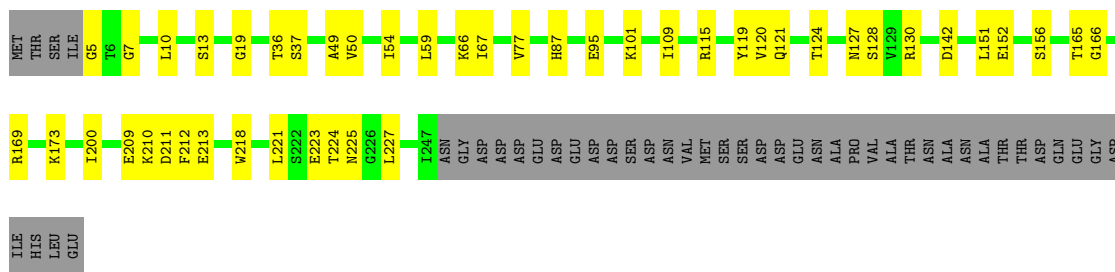
- Molecule 13: Proteasome subunit alpha type-6



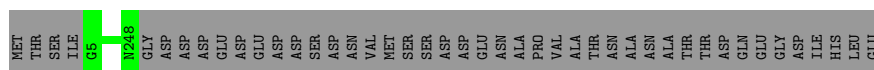
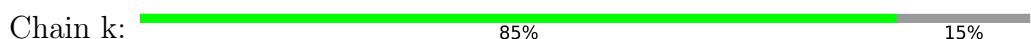
- Molecule 13: Proteasome subunit alpha type-6



- Molecule 14: Probable proteasome subunit alpha type-7

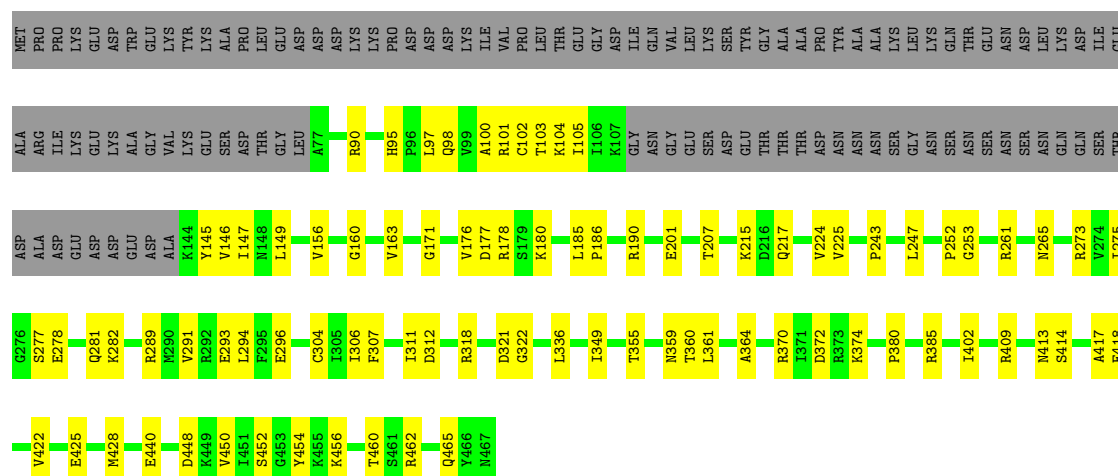


- Molecule 14: Probable proteasome subunit alpha type-7



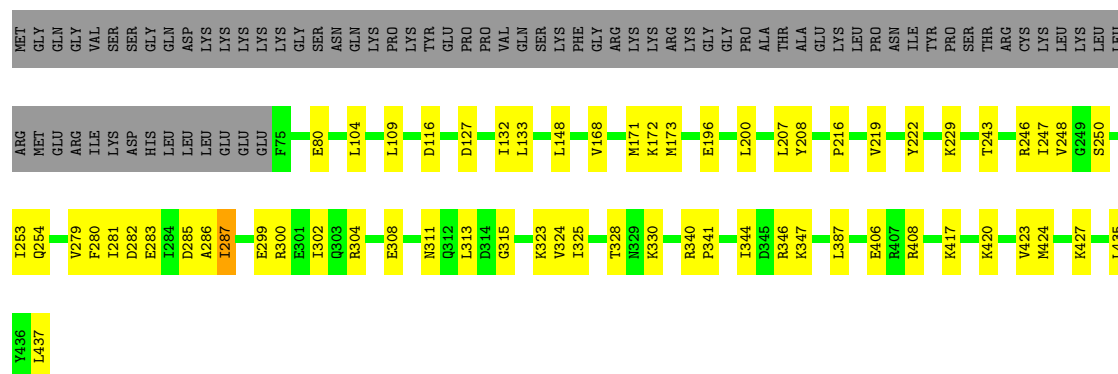
- Molecule 15: 26S protease regulatory subunit 7 homolog

Chain H:  58% 18% 24%



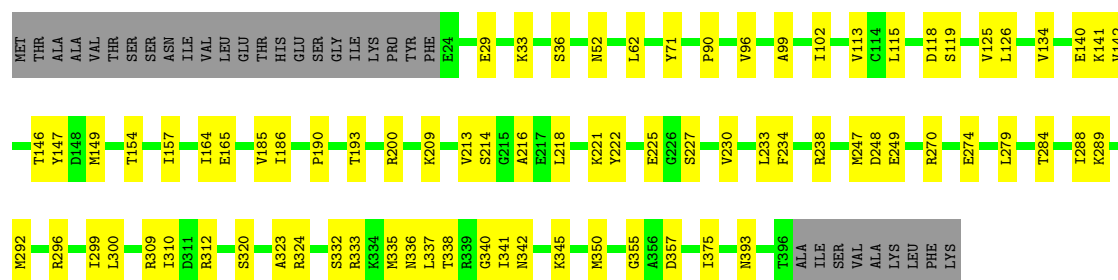
- Molecule 16: 26S protease regulatory subunit 4 homolog

Chain I:  69% 14% 17%



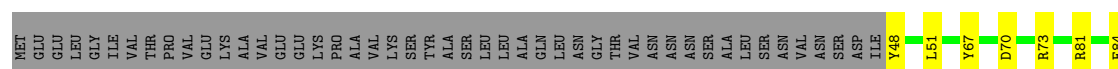
- Molecule 17: 26S protease regulatory subunit 8 homolog

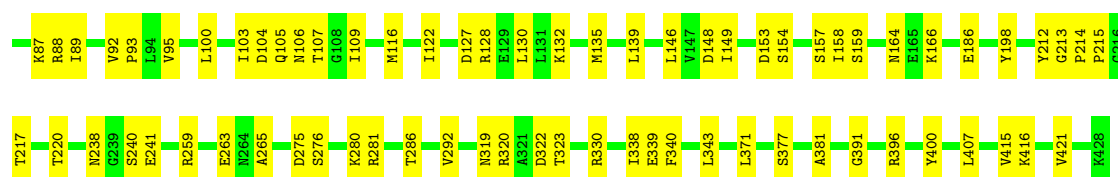
Chain J: 73% 20% 8%



- Molecule 18: 26S protease regulatory subunit 6B homolog

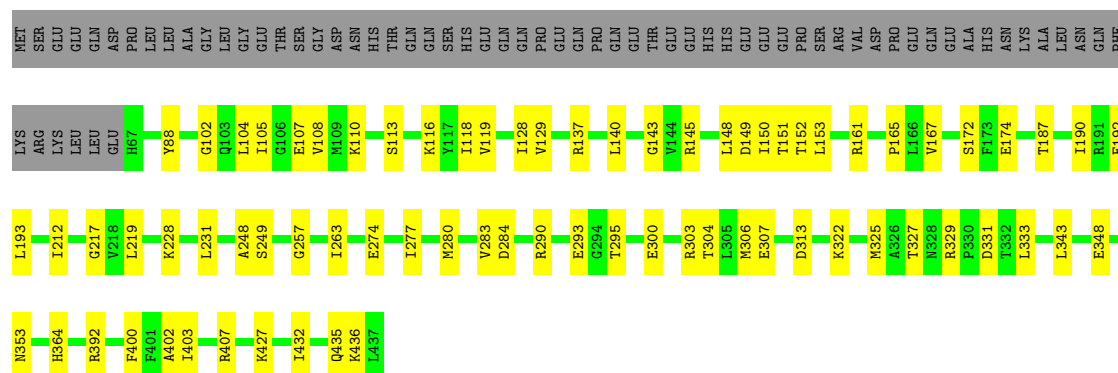
Chain K:  71% 18% 11%





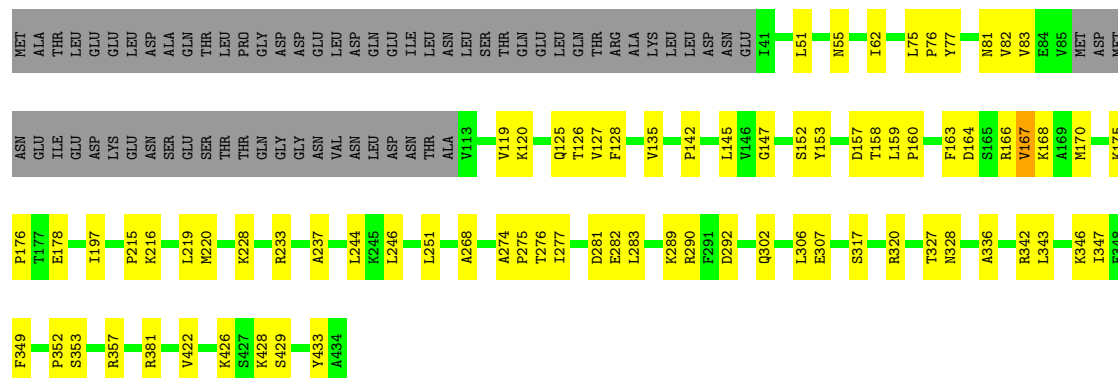
• Molecule 19: 26S protease subunit RPT4

Chain L: 68% 17% 15%



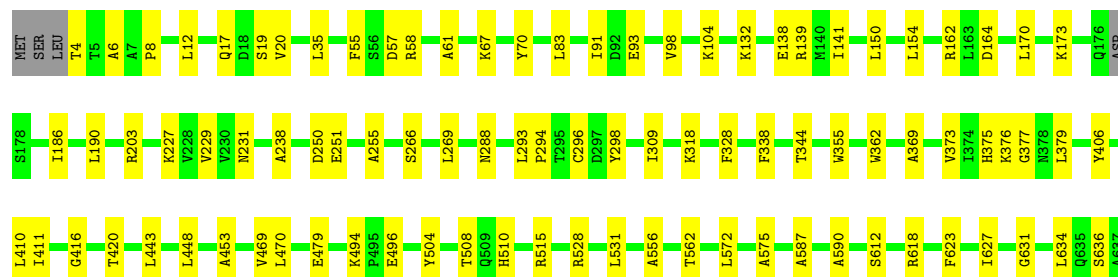
• Molecule 20: 26S protease regulatory subunit 6A

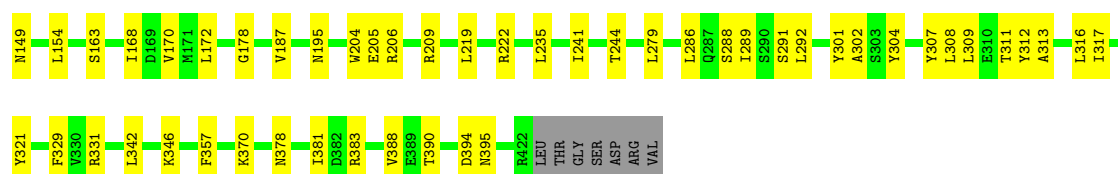
Chain M: 67% 18% 15%



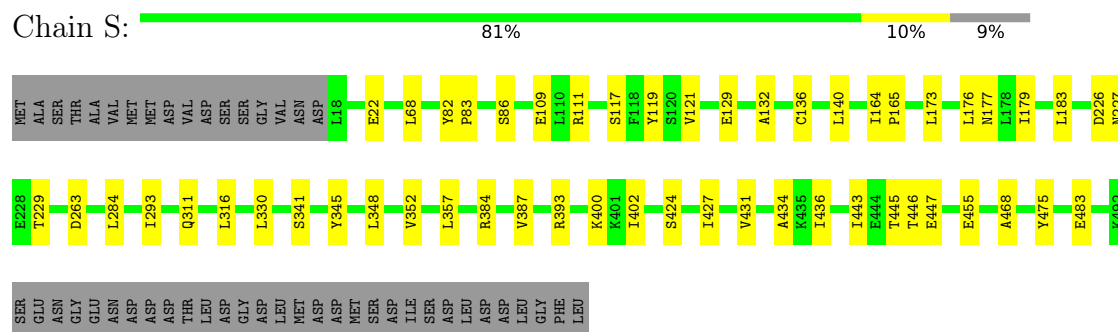
• Molecule 21: 26S proteasome regulatory subunit RPN2

Chain N: 77% 13% 10%

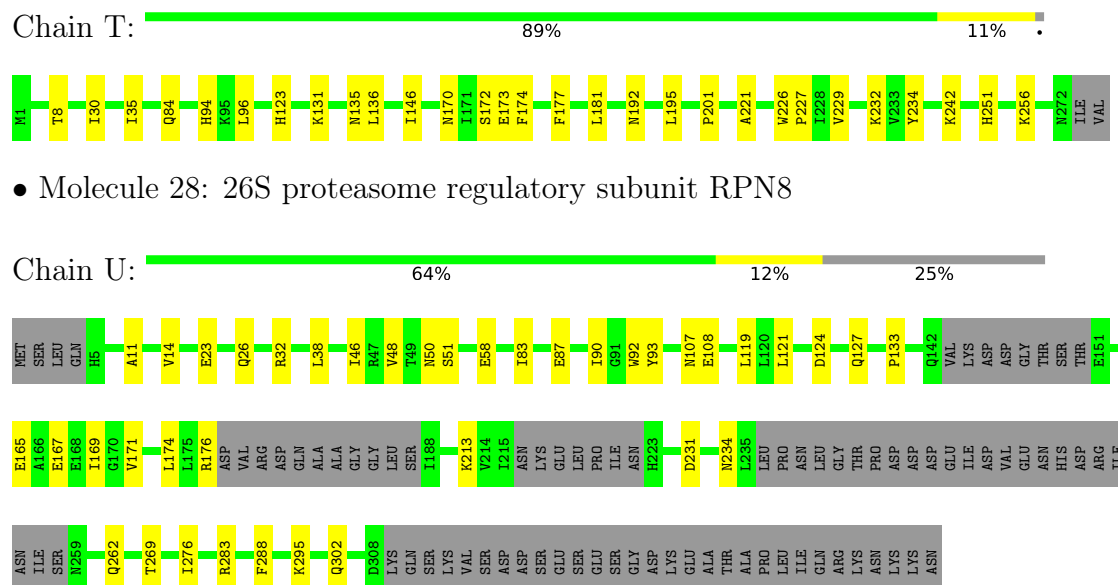




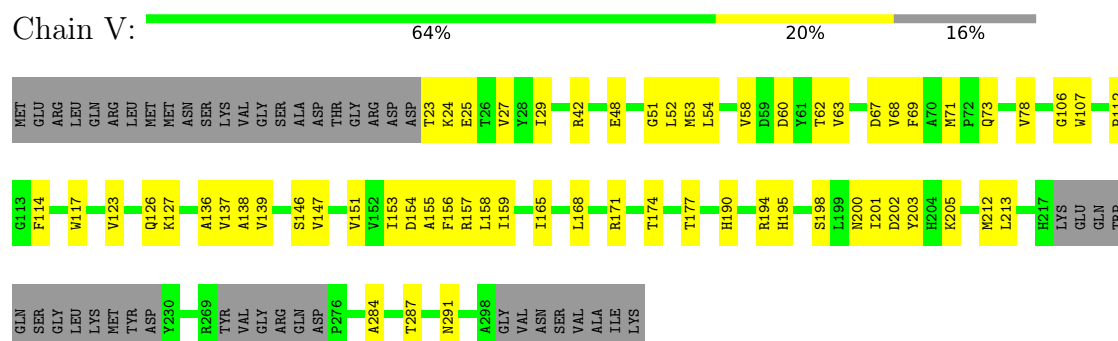
- Molecule 26: 26S proteasome regulatory subunit RPN3

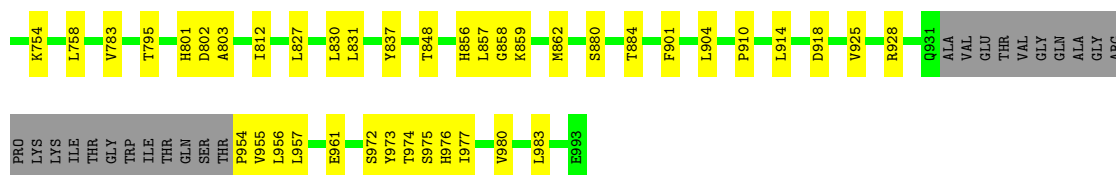


- Molecule 27: 26S proteasome regulatory subunit RPN12



- Molecule 28: 26S proteasome regulatory subunit RPN8





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	77729	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	0.23	0/1605	0.41	0/2171
1	b	0.23	0/1605	0.42	0/2171
10	C	0.23	0/1934	0.41	0/2618
10	d	0.23	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	0.40	0/2541
12	m	0.23	0/1886	0.39	0/2541
13	F	0.24	0/1823	0.42	0/2463
13	l	0.23	0/1823	0.41	0/2463
14	G	0.24	0/1928	0.40	0/2603
14	k	0.24	0/1936	0.40	0/2614
15	H	0.24	0/2834	0.41	0/3816
16	I	0.23	0/2869	0.41	0/3867
17	J	0.23	0/2964	0.39	0/3981
18	K	0.31	1/3062 (0.0%)	0.40	0/4132
19	L	0.33	1/2981 (0.0%)	0.39	0/4008
2	2	0.23	0/1715	0.41	0/2326
2	i	0.23	0/1715	0.41	0/2326
20	M	0.24	0/2903	0.42	0/3909
21	N	0.25	1/6670 (0.0%)	0.38	0/9023
22	O	0.25	1/3243 (0.0%)	0.39	0/4374
23	P	0.22	0/3599	0.37	0/4854
24	Q	0.23	0/3527	0.36	0/4748
25	R	0.23	0/3272	0.37	0/4412
26	S	0.23	0/3966	0.36	0/5355
27	T	0.23	0/2279	0.38	0/3077
28	U	0.22	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	0/1058	0.40	0/1432
32	Y	0.24	0/239	0.43	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	0.40	0/2173
4	g	0.23	0/1613	0.39	0/2173
5	5	0.23	0/1681	0.40	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	0.41	0/2514
7	a	0.23	0/1855	0.41	0/2514
8	A	0.23	0/1959	0.39	0/2652
8	c	0.24	0/1959	0.39	0/2652
9	B	0.24	0/1952	0.40	0/2642
9	j	0.24	0/1952	0.40	0/2642
All	All	0.24	4/108128 (0.0%)	0.39	0/146037

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	L	274	GLU	C-N	12.44	1.57	1.34
18	K	265	ALA	C-N	11.26	1.55	1.34
21	N	743	PHE	C-N	6.50	1.46	1.34
22	O	55	THR	C-N	5.11	1.44	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	1576	0	1552	27	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	h	1581	0	1571	0	0
4	4	1585	0	1590	26	0
4	g	1585	0	1590	0	0
5	5	1644	0	1592	26	0
5	f	1644	0	1592	0	0
6	6	1757	0	1708	23	0
6	e	1757	0	1708	0	0
7	7	1824	0	1829	28	0
7	a	1824	0	1829	0	0
8	A	1921	0	1910	33	0
8	c	1921	0	1910	0	0
9	B	1915	0	1929	32	0
9	j	1915	0	1929	0	0
10	C	1904	0	1901	32	0
10	d	1904	0	1901	0	0
11	D	1890	0	1900	29	0
11	n	1890	0	1900	0	0
12	E	1861	0	1836	35	0
12	m	1861	0	1836	0	0
13	F	1795	0	1797	37	0
13	l	1795	0	1797	0	0
14	G	1888	0	1880	33	0
14	k	1896	0	1886	0	0
15	H	2787	0	2851	57	0
16	I	2831	0	2881	50	0
17	J	2928	0	3057	52	0
18	K	3019	0	3084	51	0
19	L	2937	0	3011	55	0
20	M	2866	0	2938	53	0
21	N	6562	0	6625	72	0
22	O	3182	0	3207	36	0
23	P	3545	0	3629	45	0
24	Q	3471	0	3495	20	0
25	R	3218	0	3216	44	0
26	S	3894	0	3938	33	0
27	T	2235	0	2207	19	0
28	U	2061	0	2116	31	0
29	V	2025	0	2035	44	0
30	W	1534	0	1542	28	0
31	X	1032	0	1015	12	0
32	Y	236	0	203	5	0
33	Z	6290	0	6236	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	106311	0	106652	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 6.

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)
22:O:147:ARG:HD3	23:P:288:ASN:HD21	1.47	0.78
29:V:24:LYS:H	29:V:174:THR:HG22	1.50	0.77
19:L:165:PRO:HD2	20:M:83:VAL:HB	1.67	0.75
9:B:78:MET:HG2	9:B:80:PRO:HD2	1.69	0.73
30:W:12:ASN:ND2	30:W:53:SER:OG	2.23	0.72
8:A:135:ARG:HB3	14:G:13:SER:HB2	1.71	0.71
13:F:34:VAL:HA	13:F:162:GLY:HA3	1.72	0.71
23:P:66:LEU:HD13	23:P:70:ASN:HD22	1.56	0.71
10:C:51:LYS:HG2	10:C:52:VAL:HG23	1.73	0.71
20:M:178:GLU:HG3	20:M:233:ARG:HE	1.57	0.70
29:V:52:LEU:HB2	29:V:69:PHE:HB3	1.74	0.70
6:6:101:LYS:HD2	12:E:108:ASN:HD21	1.57	0.69
15:H:243:PRO:HB3	15:H:372:ASP:HB2	1.74	0.69
18:K:275:ASP:OD2	18:K:319:ASN:ND2	2.24	0.69
19:L:118:ILE:HG12	19:L:128:ILE:HG12	1.75	0.68
19:L:280:MET:HB2	19:L:325:MET:HA	1.75	0.68
15:H:247:LEU:HB3	15:H:374:LYS:HA	1.75	0.68
28:U:32:ARG:NH2	28:U:58:GLU:OE1	2.27	0.68
10:C:34:THR:HA	10:C:166:GLY:HA3	1.76	0.68
11:D:10:ILE:HG23	12:E:23:GLN:HE22	1.59	0.67
25:R:346:LYS:NZ	25:R:390:THR:O	2.27	0.67
12:E:53:ARG:HH12	12:E:209:GLU:H	1.40	0.67
17:J:193:THR:HA	17:J:355:GLY:H	1.59	0.67
15:H:185:LEU:HD12	15:H:186:PRO:HD2	1.77	0.67
12:E:121:LEU:HD11	13:F:79:PRO:HB2	1.77	0.67
26:S:330:LEU:O	32:Y:63:ASN:ND2	2.27	0.67
5:5:220:LYS:HE2	5:5:222:ASP:HB2	1.77	0.67
22:O:41:LEU:HD22	22:O:62:TYR:HB2	1.77	0.67
3:3:28:ARG:NH2	3:3:205:ASP:OXT	2.27	0.66
28:U:169:ILE:HG21	29:V:147:VAL:HA	1.78	0.66
33:Z:928:ARG:HG3	33:Z:955:VAL:HG13	1.77	0.66
16:I:246:ARG:NH2	17:J:274:GLU:OE2	2.27	0.66
28:U:38:LEU:HB2	28:U:50:ASN:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:89:LEU:HG	23:P:91:LEU:H	1.61	0.66
1:I:47:ASN:HD22	2:2:149:ASP:HB3	1.61	0.66
18:K:276:SER:HB2	19:L:303:ARG:HG2	1.78	0.66
18:K:416:LYS:HE3	18:K:421:VAL:HG12	1.78	0.66
15:H:321:ASP:OD1	20:M:290:ARG:NH2	2.29	0.65
33:Z:362:LEU:HD13	33:Z:859:LYS:HD2	1.78	0.65
18:K:281:ARG:NH2	19:L:293:GLU:OE1	2.27	0.65
23:P:135:GLU:OE1	23:P:138:ARG:NH2	2.29	0.65
15:H:364:ALA:O	15:H:370:ARG:NH1	2.29	0.65
20:M:274:ALA:HA	20:M:320:ARG:HH21	1.59	0.65
22:O:225:ASP:O	22:O:290:LYS:NZ	2.29	0.65
10:C:84:ALA:HB2	10:C:133:VAL:HG21	1.79	0.65
19:L:248:ALA:HB2	19:L:283:VAL:HG22	1.78	0.65
9:B:71:ILE:HG12	9:B:138:GLY:HA3	1.79	0.64
13:F:52:ASN:ND2	13:F:54:ASP:O	2.30	0.64
19:L:329:ARG:NH2	19:L:435:GLN:OE1	2.29	0.64
25:R:383:ARG:HG3	26:S:402:ILE:HG13	1.78	0.64
16:I:104:LEU:HB3	16:I:148:LEU:HD11	1.79	0.64
22:O:118:GLY:HA3	22:O:128:LEU:HD22	1.80	0.64
28:U:48:VAL:HG22	28:U:90:ILE:HD11	1.80	0.64
8:A:14:ARG:O	8:A:27:GLN:NE2	2.29	0.64
10:C:91:ALA:HB2	10:C:115:LEU:HD11	1.79	0.64
19:L:219:LEU:HB2	19:L:343:LEU:HD13	1.80	0.64
15:H:103:THR:O	20:M:166:ARG:NH1	2.30	0.64
14:G:87:HIS:HE2	14:G:119:TYR:HH	1.42	0.64
25:R:219:LEU:O	25:R:222:ARG:NH1	2.30	0.64
21:N:190:LEU:HD22	21:N:227:LYS:HE2	1.79	0.64
29:V:23:THR:HG23	29:V:190:HIS:HE1	1.63	0.64
15:H:318:ARG:HB3	16:I:300:ARG:HH21	1.62	0.64
21:N:494:LYS:HE2	21:N:496:GLU:HB2	1.80	0.64
16:I:285:ASP:OD2	17:J:270:ARG:NH1	2.30	0.64
25:R:172:LEU:HD21	25:R:209:ARG:HD3	1.79	0.64
33:Z:387:ASN:O	33:Z:391:ASN:ND2	2.31	0.64
9:B:49:LYS:HE3	9:B:210:GLU:HB2	1.78	0.64
16:I:172:LYS:HG3	16:I:246:ARG:HB2	1.80	0.64
24:Q:40:ALA:HA	24:Q:46:VAL:HA	1.80	0.63
26:S:173:LEU:O	26:S:177:ASN:ND2	2.32	0.63
7:7:263:THR:HG23	16:I:109:LEU:HD22	156.43	0.63
10:C:9:ARG:NH1	12:E:9:ASP:OD2	2.32	0.63
17:J:29:GLU:OE2	21:N:104:LYS:NZ	2.31	0.63
21:N:203:ARG:HH22	21:N:562:THR:HG21	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:138:ARG:HE	33:Z:161:ILE:HD11	1.63	0.63
12:E:85:ALA:HB2	12:E:140:VAL:HG21	1.80	0.62
17:J:320:SER:H	17:J:323:ALA:HB3	1.64	0.62
26:S:227:ASN:HD22	26:S:263:ASP:HB2	1.63	0.62
28:U:127:GLN:HE22	29:V:212:MET:HA	1.64	0.62
20:M:336:ALA:O	20:M:342:ARG:NH2	2.31	0.62
22:O:269:LEU:HD23	22:O:270:ILE:HG13	1.82	0.62
30:W:20:ASP:HB2	30:W:25:ARG:HD2	1.80	0.62
20:M:246:LEU:HD11	20:M:251:LEU:HD21	1.81	0.62
10:C:50:ARG:NH2	10:C:209:ASP:O	2.33	0.62
20:M:82:VAL:HG22	20:M:119:VAL:HG12	1.82	0.62
29:V:287:THR:O	29:V:291:ASN:ND2	2.33	0.62
11:D:163:THR:HG21	11:D:171:VAL:HB	1.82	0.61
18:K:371:LEU:HD11	18:K:407:LEU:HB3	1.80	0.61
17:J:332:SER:HB2	17:J:337:LEU:HD21	1.82	0.61
24:Q:170:ASP:HB3	24:Q:173:SER:HB2	1.80	0.61
26:S:136:CYS:HB3	26:S:179:ILE:HG21	1.82	0.61
8:A:78:THR:HG22	8:A:231:ASP:HA	1.83	0.61
8:A:40:ILE:HG23	8:A:56:GLN:HB2	1.80	0.61
17:J:338:THR:HG22	17:J:340:GLY:H	1.65	0.61
26:S:475:TYR:HE1	28:U:295:LYS:HB2	1.66	0.61
33:Z:229:SER:HB2	33:Z:232:LYS:HB2	1.83	0.61
20:M:77:TYR:HB3	20:M:147:GLY:HA3	1.83	0.61
25:R:154:LEU:HB3	25:R:170:VAL:HG13	1.81	0.61
22:O:258:LEU:HD13	22:O:291:ILE:HG13	1.83	0.61
9:B:33:THR:HA	9:B:165:GLY:HA3	1.83	0.60
18:K:84:GLU:HA	18:K:87:LYS:HE2	1.82	0.60
22:O:207:LEU:HD23	22:O:210:ARG:HD2	1.83	0.60
23:P:147:LYS:HB3	23:P:152:LYS:HB2	1.83	0.60
31:X:87:PHE:HB2	31:X:99:PHE:HB2	1.83	0.60
13:F:173:GLU:OE2	20:M:381:ARG:NH1	2.33	0.60
25:R:178:GLY:HA3	25:R:187:VAL:HG21	1.83	0.60
25:R:76:GLN:HG3	25:R:78:ASP:H	1.65	0.60
28:U:14:VAL:HG21	28:U:48:VAL:HG12	1.83	0.60
10:C:144:TYR:HB2	10:C:147:GLN:HE21	1.67	0.60
17:J:149:MET:SD	17:J:333:ARG:NH2	2.74	0.60
26:S:311:GLN:NE2	26:S:341:SER:OG	2.34	0.60
31:X:34:GLU:HB3	31:X:51:ARG:HE	1.65	0.60
2:2:47:THR:HB	2:2:59:ASN:HA	1.83	0.60
4:4:184:VAL:HG22	4:4:189:ILE:HG12	1.82	0.60
8:A:114:CYS:HB2	8:A:145:SER:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:70:ASN:OD1	10:C:71:ASP:N	2.34	0.60
25:R:331:ARG:NH2	25:R:370:LYS:O	2.33	0.60
6:6:128:THR:HB	6:6:144:PHE:HB2	1.83	0.60
11:D:88:LYS:NZ	11:D:120:TYR:OH	2.34	0.60
23:P:38:GLN:O	23:P:88:GLN:NE2	2.35	0.60
33:Z:389:PHE:HB3	33:Z:857:LEU:HA	1.83	0.60
13:F:11:VAL:HA	14:G:130:ARG:HD3	1.84	0.59
13:F:50:LYS:HE2	13:F:61:LYS:HA	1.84	0.59
22:O:117:ASN:HB3	22:O:127:LEU:HB2	1.84	0.59
29:V:114:PHE:HB3	29:V:117:TRP:HE1	1.67	0.59
10:C:191:GLU:HG2	10:C:242:THR:HG22	1.83	0.59
16:I:247:ILE:HB	16:I:281:ILE:HG12	1.83	0.59
20:M:51:LEU:O	20:M:55:ASN:ND2	2.36	0.59
9:B:222:LEU:HD13	9:B:232:GLY:HA2	1.84	0.59
29:V:24:LYS:HB2	29:V:174:THR:HA	1.85	0.59
11:D:37:LYS:HE2	11:D:160:SER:HA	1.85	0.59
3:3:101:GLY:O	4:4:93:ARG:NH1	2.35	0.59
5:5:144:ARG:O	11:D:111:ARG:NH1	2.35	0.59
15:H:98:GLN:N	15:H:176:VAL:O	2.33	0.59
21:N:891:VAL:HB	21:N:906:ARG:HB2	1.85	0.59
7:7:232:ILE:HB	7:7:240:THR:HB	1.85	0.59
15:H:224:VAL:HG23	15:H:225:VAL:HG23	1.85	0.59
23:P:353:ILE:HG23	23:P:357:TYR:HB2	1.85	0.59
3:3:103:TYR:HA	4:4:93:ARG:HH22	1.68	0.59
12:E:34:GLY:HA3	12:E:80:GLY:HA2	1.85	0.59
7:7:58:ASP:HA	7:7:228:PHE:HA	1.84	0.58
30:W:150:ASN:OD1	30:W:151:THR:N	2.36	0.58
33:Z:351:PRO:HG2	33:Z:464:ASP:HB3	1.84	0.58
18:K:415:VAL:HG13	18:K:416:LYS:HG2	1.85	0.58
19:L:172:SER:OG	19:L:174:GLU:OE2	2.20	0.58
25:R:313:ALA:HA	25:R:317:ILE:HD12	1.86	0.58
27:T:170:ASN:HA	27:T:174:PHE:HB2	1.85	0.58
11:D:13:PRO:HB2	15:H:462:ARG:HB3	1.85	0.58
8:A:37:GLN:NE2	14:G:19:GLY:O	2.36	0.58
16:I:173:MET:HG3	16:I:243:THR:HG23	1.84	0.58
14:G:224:THR:HB	14:G:227:LEU:HB2	1.86	0.58
16:I:417:LYS:HA	16:I:420:LYS:HE2	1.85	0.58
30:W:161:VAL:O	30:W:163:ASN:ND2	2.36	0.58
7:7:54:ILE:HG12	7:7:232:ILE:HG12	1.83	0.58
29:V:146:SER:HB2	29:V:151:VAL:HA	1.85	0.58
29:V:153:ILE:HG23	29:V:201:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:112:ILE:HG23	5:5:135:GLY:HA2	1.85	0.58
1:1:103:GLU:OE2	7:7:98:ARG:NH1	2.36	0.58
33:Z:975:SER:HB3	33:Z:977:ILE:HG12	1.86	0.58
6:6:55:ASN:O	7:7:189:ARG:NH2	2.37	0.58
25:R:54:ILE:HG21	25:R:63:TYR:HB2	1.85	0.58
5:5:170:LEU:HD23	6:6:120:ARG:HH21	1.68	0.58
19:L:402:ALA:HB1	19:L:407:ARG:HB2	1.86	0.58
22:O:83:LEU:HD21	22:O:98:TYR:HB2	1.85	0.58
33:Z:972:SER:OG	33:Z:976:HIS:ND1	2.37	0.58
6:6:74:ASN:HB3	6:6:127:HIS:HB2	1.85	0.57
17:J:62:LEU:HD13	18:K:89:ILE:HD13	1.84	0.57
31:X:89:LEU:O	31:X:96:ARG:NE	2.37	0.57
12:E:207:VAL:HG12	15:H:409:ARG:HH12	1.69	0.57
27:T:172:SER:OG	27:T:173:GLU:OE1	2.22	0.57
3:3:65:GLU:OE1	3:3:68:ARG:NH2	2.37	0.57
19:L:228:LYS:NZ	19:L:327:THR:O	2.35	0.57
22:O:338:LYS:HB3	22:O:351:SER:HB3	1.87	0.57
4:4:4:ILE:HG13	4:4:47:ALA:HB2	1.85	0.57
23:P:212:LYS:HA	23:P:216:LEU:HD22	1.87	0.57
17:J:146:THR:HG21	25:R:163:SER:HB3	1.86	0.57
13:F:47:VAL:HG22	13:F:213:ILE:HG12	1.84	0.57
17:J:52:ASN:HD21	21:N:612:SER:HA	1.70	0.57
33:Z:233:LEU:HB3	33:Z:271:ILE:HD11	1.86	0.57
12:E:84:ASP:OD2	12:E:136:ARG:NH1	2.38	0.57
18:K:70:ASP:OD1	18:K:73:ARG:NH2	2.38	0.57
15:H:311:ILE:HG22	15:H:355:THR:HB	1.86	0.57
9:B:38:LYS:HG3	9:B:43:VAL:HG22	1.87	0.57
20:M:166:ARG:HD2	20:M:170:MET:HB3	1.87	0.57
29:V:126:GLN:HG2	29:V:158:LEU:HD21	1.85	0.57
8:A:53:VAL:HG21	8:A:82:VAL:HG21	1.87	0.57
10:C:168:ASN:HB3	10:C:171:ALA:HB3	1.86	0.57
21:N:344:THR:HG22	21:N:375:HIS:HA	1.87	0.57
31:X:120:GLU:HG2	31:X:124:LYS:HE3	1.86	0.57
33:Z:371:SER:HA	33:Z:387:ASN:HB3	1.87	0.57
14:G:120:VAL:HG21	14:G:151:LEU:HD21	1.87	0.56
14:G:210:LYS:HE3	20:M:353:SER:HB2	1.87	0.56
21:N:162:ARG:HE	21:N:164:ASP:HB3	1.69	0.56
25:R:292:LEU:HD11	25:R:311:THR:HG21	1.85	0.56
29:V:24:LYS:HD2	29:V:200:ASN:HD21	1.69	0.56
4:4:130:TYR:OH	4:4:145:ASP:OD1	2.22	0.56
21:N:650:ASP:HB3	21:N:694:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:180:LEU:O	30:W:184:ASN:ND2	2.37	0.56
8:A:126:GLN:HE22	9:B:81:ASP:HA	1.69	0.56
19:L:300:GLU:OE1	19:L:303:ARG:NH2	2.38	0.56
22:O:44:SER:O	22:O:47:LYS:NZ	2.37	0.56
1:1:54:THR:HG21	1:1:75:ALA:HB1	1.87	0.56
2:2:126:TYR:HB3	2:2:156:LEU:HD13	1.87	0.56
16:I:435:LEU:HG	16:I:437:LEU:H	1.70	0.56
23:P:70:ASN:OD1	23:P:71:LYS:N	2.38	0.56
28:U:50:ASN:OD1	28:U:51:SER:N	2.39	0.56
21:N:362:TRP:HZ3	29:V:168:LEU:HB3	1.70	0.56
3:3:105:VAL:HG23	3:3:107:PRO:HD3	1.86	0.56
29:V:58:VAL:HB	29:V:62:THR:HB	1.87	0.56
33:Z:309:GLN:NE2	33:Z:980:VAL:O	2.34	0.56
8:A:178:ILE:HD11	8:A:214:LEU:HD21	1.88	0.56
33:Z:453:LEU:HB2	33:Z:488:ALA:HB1	1.88	0.56
13:F:50:LYS:HE3	13:F:212:SER:HB2	1.88	0.56
14:G:152:GLU:OE1	14:G:156:SER:OG	2.24	0.56
30:W:28:ALA:HB1	30:W:181:LEU:HD22	1.87	0.56
30:W:1:MET:HG2	30:W:2:VAL:HG13	1.86	0.56
33:Z:282:ILE:HD11	33:Z:310:LEU:HD22	1.88	0.56
33:Z:925:VAL:HG12	33:Z:983:LEU:HD11	1.87	0.56
6:6:174:ASN:HB3	6:6:176:LYS:HE2	1.86	0.56
19:L:102:GLY:N	20:M:152:SER:O	2.39	0.56
3:3:54:THR:O	3:3:106:GLY:N	2.39	0.55
24:Q:389:VAL:HG12	24:Q:400:TYR:HB2	1.88	0.55
26:S:173:LEU:H	26:S:176:LEU:HD12	1.70	0.55
28:U:14:VAL:HG13	28:U:51:SER:HB3	1.88	0.55
6:6:214:HIS:HD2	6:6:217:VAL:HG23	1.71	0.55
15:H:294:LEU:HD13	15:H:306:ILE:HD11	1.87	0.55
14:G:7:GLY:HA2	14:G:10:LEU:HG	1.89	0.55
15:H:90:ARG:HE	16:I:133:LEU:HD22	1.71	0.55
16:I:287:ILE:HG12	16:I:302:ILE:HG23	1.88	0.55
18:K:100:LEU:HB2	18:K:109:ILE:HG23	1.89	0.55
4:4:36:ARG:HG3	4:4:57:ALA:HB1	1.89	0.55
13:F:201:LEU:HD11	13:F:206:LEU:HG	1.89	0.55
23:P:440:HIS:HB3	28:U:213:LYS:HE3	1.89	0.55
3:3:46:TYR:OH	3:3:64:ASN:OD1	2.24	0.55
17:J:96:VAL:HG11	17:J:115:LEU:HD11	1.89	0.55
21:N:634:LEU:HG	21:N:636:SER:H	1.72	0.55
25:R:146:ASP:HB3	25:R:149:ASN:HB2	1.88	0.55
21:N:742:TRP:CD2	21:N:744:PRO:HD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:249:ALA:HB1	23:P:252:SER:HB3	1.88	0.55
18:K:217:THR:HA	18:K:381:ALA:HB2	1.88	0.55
19:L:150:ILE:HG13	19:L:151:THR:HG23	1.88	0.55
20:M:220:MET:HB3	20:M:349:PHE:HE2	1.72	0.55
23:P:319:GLU:HB3	23:P:322:LEU:HB2	1.88	0.55
28:U:11:ALA:HB1	28:U:167:GLU:HG2	1.89	0.55
29:V:52:LEU:HD23	29:V:107:TRP:HB3	1.89	0.55
30:W:129:ALA:HB1	30:W:161:VAL:HB	1.87	0.55
32:Y:63:ASN:OD1	32:Y:64:TRP:N	2.36	0.55
4:4:149:ARG:HB2	4:4:152:MET:HG2	1.89	0.55
6:6:125:TYR:HA	6:6:146:PRO:HB3	1.89	0.55
4:4:71:GLU:OE2	10:C:113:ARG:NH1	2.37	0.55
5:5:256:THR:HG23	5:5:258:ASP:H	1.71	0.55
17:J:186:ILE:HD13	17:J:300:LEU:HD11	1.89	0.55
29:V:53:MET:HG2	29:V:68:VAL:HG12	1.89	0.54
15:H:318:ARG:NH1	15:H:360:THR:O	2.40	0.54
19:L:107:GLU:OE2	19:L:145:ARG:NH2	2.40	0.54
11:D:4:TYR:CZ	11:D:6:ARG:HB3	2.43	0.54
19:L:348:GLU:OE2	19:L:436:LYS:NZ	2.40	0.54
29:V:53:MET:HA	29:V:68:VAL:HA	1.88	0.54
16:I:200:LEU:HD11	16:I:207:LEU:HD22	1.89	0.54
20:M:244:LEU:HD12	20:M:276:THR:HG21	1.88	0.54
22:O:119:SER:HB2	22:O:166:ARG:HH11	1.73	0.54
29:V:106:GLY:HA3	29:V:137:VAL:H	1.73	0.54
8:A:52:VAL:HG21	8:A:203:VAL:HG22	1.90	0.54
8:A:72:ILE:HG12	8:A:82:VAL:HG22	1.90	0.54
16:I:229:LYS:NZ	16:I:328:THR:O	2.41	0.54
21:N:150:LEU:HD21	21:N:173:LYS:HG3	1.89	0.54
26:S:445:THR:HG22	26:S:447:GLU:H	1.72	0.54
28:U:23:GLU:O	28:U:26:GLN:NE2	2.40	0.54
28:U:276:ILE:HG23	29:V:291:ASN:HB3	1.89	0.54
30:W:14:GLU:HG2	30:W:82:GLU:HB2	1.90	0.54
5:5:253:TYR:HE1	5:5:262:TYR:HD1	1.55	0.54
17:J:147:TYR:OH	17:J:165:GLU:OE1	2.26	0.54
27:T:136:LEU:HD22	27:T:146:ILE:HD11	1.90	0.54
15:H:448:ASP:HA	15:H:452:SER:HB2	1.90	0.54
17:J:279:LEU:HD11	17:J:288:ILE:HD12	1.90	0.54
27:T:177:PHE:HB3	27:T:181:LEU:HD13	1.90	0.54
1:1:85:TYR:HA	1:1:89:TYR:HD2	1.73	0.54
6:6:74:ASN:O	6:6:127:HIS:N	2.39	0.54
8:A:194:ILE:HG22	8:A:196:GLU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:248:ASP:OD2	18:K:330:ARG:NH2	2.33	0.54
17:J:296:ARG:H	17:J:299:ILE:HD12	1.73	0.54
17:J:185:VAL:HG22	17:J:312:ARG:HB3	1.88	0.54
25:R:309:LEU:HD11	32:Y:77:LEU:HB2	1.90	0.54
33:Z:405:ASN:HB3	33:Z:409:LYS:HE3	1.90	0.54
15:H:428:MET:HG3	16:I:346:ARG:HH22	1.72	0.54
23:P:89:LEU:HB3	23:P:92:SER:HB3	1.89	0.54
12:E:68:VAL:HB	12:E:93:ARG:HH21	1.71	0.54
15:H:275:ILE:HG23	16:I:311:ASN:HD22	1.73	0.54
16:I:80:GLU:HG3	33:Z:625:THR:HG21	1.90	0.54
18:K:95:VAL:O	18:K:139:LEU:N	2.40	0.54
25:R:36:SER:HB3	25:R:43:ARG:HE	1.73	0.54
6:6:46:THR:OG1	6:6:219:ASP:O	2.27	0.53
17:J:141:LYS:HG2	17:J:142:VAL:HG23	1.88	0.53
19:L:104:LEU:O	19:L:148:LEU:N	2.39	0.53
1:1:57:HIS:HB3	1:1:60:ILE:HB	1.90	0.53
17:J:324:ARG:NH2	17:J:350:MET:O	2.41	0.53
17:J:221:LYS:HE2	18:K:286:THR:HG21	1.90	0.53
21:N:4:THR:HG22	21:N:35:LEU:HD21	1.89	0.53
26:S:393:ARG:NH1	26:S:431:VAL:O	2.42	0.53
1:1:181:ALA:O	1:1:188:SER:OG	2.27	0.53
14:G:121:GLN:OE1	14:G:124:THR:OG1	2.26	0.53
30:W:20:ASP:HB3	30:W:144:PHE:HE2	1.72	0.53
5:5:83:PHE:HE2	5:5:88:ILE:HG12	1.73	0.53
7:7:181:ALA:O	7:7:185:ASN:ND2	2.40	0.53
26:S:424:SER:HB3	27:T:192:ASN:HB3	1.89	0.53
16:I:216:PRO:O	16:I:323:LYS:NZ	2.37	0.53
15:H:402:ILE:HD12	15:H:440:GLU:HB2	1.91	0.53
19:L:105:ILE:HD11	20:M:128:PHE:HB2	1.90	0.53
29:V:138:ALA:N	29:V:156:PHE:O	2.37	0.53
4:4:38:LEU:HB3	4:4:64:ILE:HG21	1.91	0.53
18:K:400:TYR:HB3	23:P:128:ASN:HB3	1.90	0.53
4:4:8:ARG:NH2	4:4:114:PRO:O	2.40	0.53
5:5:106:VAL:HA	6:6:151:GLU:HG2	1.91	0.53
8:A:126:GLN:NE2	9:B:81:ASP:OD1	2.41	0.53
30:W:1:MET:N	30:W:194:GLU:OE1	2.40	0.53
11:D:157:SER:HG	11:D:159:TRP:HE1	1.56	0.53
20:M:422:VAL:HA	20:M:426:LYS:HB2	1.91	0.53
25:R:38:VAL:HG11	25:R:313:ALA:HB1	1.89	0.52
28:U:171:VAL:HG13	29:V:213:LEU:HD13	1.89	0.52
30:W:3:LEU:HB3	30:W:106:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:36:THR:HA	14:G:166:GLY:HA3	1.91	0.52
17:J:190:PRO:HG2	17:J:193:THR:HG21	1.91	0.52
21:N:508:THR:HG22	21:N:510:HIS:H	1.73	0.52
22:O:16:MET:HG2	22:O:20:PRO:HD3	1.91	0.52
15:H:160:GLY:H	15:H:163:VAL:HB	1.74	0.52
21:N:250:ASP:OD1	21:N:251:GLU:N	2.41	0.52
33:Z:862:MET:HG2	33:Z:910:PRO:HB3	1.92	0.52
8:A:44:ALA:HB2	8:A:53:VAL:HG23	1.91	0.52
18:K:240:SER:OG	19:L:307:GLU:OE2	2.24	0.52
23:P:181:LEU:HD13	23:P:219:GLU:HB2	1.91	0.52
31:X:10:PHE:HD2	31:X:33:ILE:HD11	1.74	0.52
33:Z:186:GLY:HA2	33:Z:201:LEU:HD13	1.91	0.52
33:Z:166:ASN:ND2	33:Z:226:GLU:O	2.42	0.52
3:3:172:LEU:HD22	3:3:202:MET:HB3	1.91	0.52
12:E:71:ASP:OD1	12:E:72:ARG:N	2.42	0.52
2:2:107:SER:HB3	8:A:110:TYR:HE2	1.73	0.52
2:2:201:ASN:ND2	2:2:218:ASN:OD1	2.43	0.52
3:3:50:PHE:HE2	3:3:195:VAL:HG11	1.75	0.52
26:S:82:TYR:CD1	26:S:86:SER:HB3	2.44	0.52
4:4:47:ALA:HB3	4:4:101:ASN:HB2	1.91	0.52
9:B:40:THR:HG22	9:B:45:ILE:HG12	16.12	0.52
13:F:54:ASP:OD1	13:F:55:GLU:N	2.43	0.52
15:H:355:THR:HG21	15:H:361:LEU:HD21	1.91	0.52
15:H:456:LYS:O	16:I:347:LYS:NZ	2.30	0.52
13:F:81:ALA:HB2	13:F:130:VAL:HG21	1.91	0.52
33:Z:460:SER:HA	33:Z:496:ALA:HA	1.91	0.52
3:3:125:ASP:OD1	3:3:129:CYS:N	2.36	0.52
4:4:32:ASP:OD1	4:4:33:ASP:N	2.43	0.52
22:O:76:LEU:HB3	22:O:122:HIS:HB3	1.92	0.52
5:5:134:LEU:HD21	5:5:158:LEU:HB2	1.91	0.52
12:E:232:ASP:OD1	12:E:233:ASN:N	2.42	0.52
16:I:279:VAL:HB	16:I:324:VAL:HA	1.91	0.52
20:M:159:LEU:HD12	20:M:160:PRO:HD2	1.91	0.52
20:M:228:LYS:NZ	20:M:327:THR:O	2.33	0.52
26:S:436:ILE:HG12	26:S:443:ILE:HG12	1.91	0.52
17:J:248:ASP:OD1	17:J:249:GLU:N	2.41	0.51
22:O:135:ARG:NH1	22:O:174:THR:OG1	2.39	0.51
25:R:195:ASN:O	25:R:206:ARG:NH2	2.42	0.51
33:Z:827:LEU:HD23	33:Z:830:LEU:HD12	1.91	0.51
3:3:67:PHE:HE1	3:3:91:VAL:HA	1.74	0.51
7:7:113:LEU:HB3	7:7:117:GLU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:54:ILE:HG12	8:A:225:VAL:HG22	1.93	0.51
10:C:194:LEU:HD11	10:C:239:LEU:HD23	1.92	0.51
33:Z:390:LEU:HD21	33:Z:856:HIS:HB3	1.91	0.51
1:1:167:LYS:HE3	1:1:196:VAL:HG11	1.92	0.51
1:1:38:ARG:O	1:1:52:LYS:NZ	2.44	0.51
25:R:342:LEU:HD21	25:R:378:ASN:HB2	1.92	0.51
27:T:8:THR:HG23	27:T:30:ILE:HG23	1.91	0.51
29:V:177:THR:OG1	29:V:200:ASN:OD1	2.29	0.51
33:Z:802:ASP:OD1	33:Z:803:ALA:N	2.43	0.51
33:Z:954:PRO:HG2	33:Z:961:GLU:HG2	1.91	0.51
6:6:47:ARG:NH1	6:6:215:ILE:O	2.44	0.51
7:7:137:ARG:HD3	7:7:166:LEU:HA	1.91	0.51
9:B:69:PRO:HB3	9:B:233:PRO:HB3	1.92	0.51
14:G:54:ILE:HG23	14:G:59:LEU:HD22	1.92	0.51
18:K:213:GLY:HA3	18:K:340:PHE:HB3	1.92	0.51
20:M:219:LEU:HB2	20:M:343:LEU:HD13	1.93	0.51
20:M:75:LEU:HB2	20:M:76:PRO:HD3	1.91	0.51
25:R:222:ARG:NH2	25:R:321:TYR:O	2.36	0.51
29:V:60:ASP:O	29:V:157:ARG:NH1	2.42	0.51
18:K:276:SER:HB3	19:L:306:MET:HG3	1.91	0.51
24:Q:109:ASP:OD1	24:Q:110:SER:N	2.42	0.51
30:W:24:THR:HG22	30:W:26:PHE:H	1.74	0.51
2:2:50:THR:HG21	2:2:197:GLY:HA2	1.92	0.51
10:C:125:HIS:HB3	11:D:126:VAL:HG12	1.92	0.51
26:S:427:ILE:HD12	27:T:195:LEU:HD23	1.92	0.51
10:C:50:ARG:NH1	10:C:212:GLU:OE2	2.41	0.51
10:C:72:LYS:HE2	10:C:224:GLU:HA	1.92	0.51
22:O:277:ILE:HG22	22:O:279:ILE:H	1.74	0.51
26:S:109:GLU:OE2	26:S:111:ARG:NE	2.38	0.51
29:V:67:ASP:OD1	29:V:68:VAL:N	2.43	0.51
33:Z:391:ASN:HB2	33:Z:425:ILE:HG12	1.92	0.51
11:D:44:LEU:HD11	11:D:136:ALA:HB3	1.93	0.51
24:Q:369:ASP:OD1	24:Q:370:THR:N	2.43	0.51
30:W:52:ILE:HG12	30:W:61:VAL:HG22	1.92	0.51
1:1:33:LEU:HD11	1:1:119:ALA:HB3	1.93	0.51
2:2:239:THR:OG1	3:3:169:GLN:NE2	2.44	0.51
13:F:164:ARG:HH11	13:F:202:ARG:HG3	1.74	0.51
19:L:284:ASP:HB2	20:M:306:LEU:HD21	1.91	0.51
21:N:170:LEU:HD11	21:N:186:ILE:HG12	1.92	0.51
29:V:25:GLU:OE2	29:V:157:ARG:NH1	2.43	0.51
2:2:91:ASN:OD1	9:B:99:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:76:PHE:HZ	7:7:166:LEU:HB3	1.76	0.51
7:7:98:ARG:HD2	14:G:101:LYS:HA	1.91	0.51
16:I:406:GLU:O	16:I:408:ARG:NH1	2.44	0.51
4:4:182:LYS:HE2	4:4:191:GLN:HE21	1.76	0.50
20:M:157:ASP:OD1	20:M:158:THR:N	2.43	0.50
24:Q:104:PHE:HE2	24:Q:114:GLN:HA	1.76	0.50
28:U:174:LEU:O	29:V:205:LYS:NZ	2.31	0.50
33:Z:189:ALA:HB2	33:Z:198:GLU:HB2	1.93	0.50
7:7:59:ASN:ND2	7:7:229:SER:OG	2.37	0.50
18:K:104:ASP:OD1	18:K:105:GLN:N	2.42	0.50
31:X:38:ASN:HD22	31:X:42:GLU:H	1.59	0.50
33:Z:914:LEU:HB3	33:Z:980:VAL:HG22	1.94	0.50
3:3:78:GLU:HG2	3:3:80:ARG:HG2	1.94	0.50
5:5:79:LEU:HD13	5:5:215:LEU:HD11	1.93	0.50
6:6:76:PHE:CZ	7:7:166:LEU:HB3	2.47	0.50
10:C:159:GLY:HA3	11:D:59:ILE:HG13	1.93	0.50
11:D:93:ALA:HA	11:D:104:VAL:HG11	1.92	0.50
17:J:336:ASN:ND2	17:J:375:ILE:O	2.44	0.50
19:L:104:LEU:HD21	20:M:125:GLN:HE21	1.76	0.50
23:P:253:ASP:OD1	23:P:254:GLU:N	2.44	0.50
3:3:29:LEU:HD11	3:3:57:ALA:HB2	1.92	0.50
13:F:86:ASN:OD1	13:F:89:ARG:NH2	2.44	0.50
15:H:146:VAL:HG22	15:H:156:VAL:HG22	1.94	0.50
15:H:207:THR:HA	15:H:265:ASN:HD22	1.76	0.50
21:N:470:LEU:O	21:N:504:TYR:OH	2.22	0.50
14:G:54:ILE:HD11	14:G:213:GLU:HB2	1.93	0.50
16:I:423:VAL:HG22	16:I:427:LYS:HD2	1.92	0.50
18:K:104:ASP:HB3	18:K:107:THR:HB	1.92	0.50
23:P:415:TRP:HE1	28:U:262:GLN:HG2	1.77	0.50
6:6:62:VAL:HG22	6:6:72:SER:HB2	1.92	0.50
14:G:49:ALA:HB1	14:G:200:ILE:HD11	1.94	0.50
16:I:286:ALA:HB1	16:I:287:ILE:HD12	1.94	0.50
17:J:90:PRO:HG3	18:K:116:MET:HA	1.94	0.50
22:O:169:ASN:HD22	22:O:203:THR:HB	1.77	0.50
25:R:279:LEU:HD23	25:R:289:ILE:HD13	1.93	0.50
10:C:16:GLU:OE1	10:C:18:ARG:NH2	2.36	0.50
15:H:177:ASP:OD1	15:H:178:ARG:N	2.45	0.50
18:K:343:LEU:HD22	18:K:377:SER:HB3	1.93	0.50
19:L:149:ASP:OD2	19:L:152:THR:N	2.43	0.50
20:M:289:LYS:HA	20:M:302:GLN:HE21	1.77	0.50
21:N:556:ALA:HB2	21:N:590:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:631:GLY:HA2	21:N:716:GLN:HG2	1.93	0.50
23:P:346:ILE:HG23	23:P:369:LEU:HD22	1.93	0.50
26:S:455:GLU:HB3	27:T:256:LYS:HE2	1.94	0.50
28:U:83:ILE:HA	29:V:73:GLN:HG2	1.93	0.50
33:Z:812:ILE:HG21	33:Z:848:THR:HA	1.94	0.50
33:Z:858:GLY:HA3	33:Z:862:MET:HB2	1.92	0.50
33:Z:884:THR:HG21	33:Z:904:LEU:HG	1.94	0.50
1:1:22:ILE:HG13	1:1:117:ILE:HD12	1.93	0.50
5:5:153:ALA:HB1	11:D:100:LEU:HD22	1.94	0.50
9:B:158:PRO:HB2	10:C:58:GLU:HB3	1.94	0.50
9:B:4:ARG:HE	14:G:128:SER:HB2	1.76	0.50
15:H:425:GLU:OE1	16:I:346:ARG:NH1	2.45	0.50
18:K:132:LYS:NZ	18:K:263:GLU:OE2	2.44	0.50
21:N:190:LEU:HD11	21:N:231:ASN:HD22	1.77	0.50
21:N:266:SER:H	21:N:269:LEU:HD12	1.76	0.50
7:7:100:LEU:HD21	7:7:129:LEU:HD11	1.93	0.50
20:M:352:PRO:O	20:M:357:ARG:NH1	2.45	0.50
9:B:4:ARG:NH2	13:F:123:TYR:O	2.45	0.49
14:G:54:ILE:HB	14:G:211:ASP:HB3	1.93	0.49
21:N:575:ALA:HB2	21:N:587:ALA:HB3	1.94	0.49
22:O:20:PRO:HG3	22:O:71:ASP:HB2	1.93	0.49
25:R:168:ILE:HD13	25:R:205:GLU:HB3	1.94	0.49
26:S:284:LEU:HD11	27:T:123:HIS:HE1	1.77	0.49
24:Q:388:GLY:HA2	24:Q:400:TYR:HB3	1.95	0.49
33:Z:880:SER:HB3	33:Z:904:LEU:HD23	1.95	0.49
6:6:203:VAL:HG11	6:6:223:ILE:HD12	1.94	0.49
7:7:162:TYR:HB2	7:7:175:LEU:HD13	1.95	0.49
9:B:96:SER:HA	9:B:100:ILE:HD12	1.94	0.49
19:L:329:ARG:HG2	19:L:331:ASP:H	1.78	0.49
23:P:125:VAL:HG12	23:P:136:ARG:HB2	1.94	0.49
26:S:129:GLU:OE2	26:S:132:ALA:N	2.44	0.49
2:2:48:ARG:O	2:2:62:LYS:NZ	2.33	0.49
5:5:82:ARG:HE	5:5:185:PRO:HB2	1.76	0.49
6:6:47:ARG:HB2	6:6:219:ASP:HB2	1.94	0.49
12:E:17:PRO:HG2	13:F:3:ARG:HG2	1.94	0.49
26:S:226:ASP:OD2	26:S:229:THR:OG1	2.28	0.49
11:D:68:ASP:OD1	11:D:69:SER:N	2.42	0.49
33:Z:444:GLU:HB2	33:Z:447:VAL:HG23	1.95	0.49
7:7:161:ARG:HE	7:7:169:THR:HB	1.78	0.49
12:E:123:PHE:HA	12:E:134:MET:HB3	1.95	0.49
14:G:109:ILE:H	14:G:142:ASP:HB3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:99:LEU:HD22	22:O:129:ILE:HG23	1.95	0.49
9:B:178:ARG:NH1	9:B:195:THR:OG1	2.45	0.49
10:C:70:ASN:HB3	10:C:73:ILE:HB	1.94	0.49
13:F:28:ALA:O	20:M:433:TYR:OH	2.30	0.49
31:X:91:PHE:H	31:X:96:ARG:HH21	1.61	0.49
4:4:195:PHE:CE1	4:4:196:GLN:HG3	2.48	0.49
5:5:220:LYS:HB3	5:5:223:LEU:HG	1.93	0.49
8:A:48:LYS:HD3	8:A:173:PRO:HA	32.47	0.49
15:H:380:PRO:O	15:H:385:ARG:NH1	2.45	0.49
17:J:213:VAL:HG22	17:J:233:LEU:HD13	1.94	0.49
21:N:255:ALA:HB3	21:N:904:VAL:HG11	1.94	0.49
25:R:141:TYR:HA	25:R:144:ILE:HG12	1.94	0.49
5:5:82:ARG:NH1	5:5:200:ASP:OD1	2.41	0.49
7:7:87:SER:HB3	7:7:146:ALA:HB3	1.93	0.49
33:Z:319:THR:HG21	33:Z:535:VAL:HB	1.95	0.49
10:C:120:GLN:NE2	11:D:80:ALA:O	2.46	0.49
22:O:360:GLY:HA2	22:O:363:ILE:HD12	1.93	0.49
2:2:75:ALA:HB3	2:2:126:TYR:HB2	1.95	0.48
18:K:135:MET:HA	18:K:259:ARG:HH21	1.78	0.48
18:K:280:LYS:N	18:K:323:THR:O	2.46	0.48
23:P:299:LEU:HD23	23:P:302:LEU:HD12	1.95	0.48
29:V:136:ALA:HB3	29:V:158:LEU:HD12	1.94	0.48
1:1:122:ASP:OD1	1:1:123:ASP:N	2.46	0.48
11:D:176:GLU:HG2	12:E:58:LEU:HD13	1.94	0.48
12:E:84:ASP:HB3	12:E:138:PHE:HD1	1.78	0.48
15:H:282:LYS:HD2	17:J:221:LYS:HD2	1.95	0.48
26:S:119:TYR:CE2	26:S:121:VAL:HB	2.48	0.48
7:7:152:VAL:HG22	7:7:158:GLN:HG3	1.95	0.48
12:E:71:ASP:HB3	12:E:74:ILE:HB	1.94	0.48
22:O:354:GLN:NE2	22:O:355:PRO:HD2	2.27	0.48
4:4:66:LEU:HB2	11:D:94:GLN:HG3	1.94	0.48
23:P:20:GLU:HB3	23:P:23:LYS:HB2	1.95	0.48
27:T:229:VAL:HG23	27:T:232:LYS:HB2	1.95	0.48
8:A:128:TYR:HB3	8:A:136:PRO:HA	1.96	0.48
11:D:81:ASP:HB3	11:D:129:PHE:HD1	1.78	0.48
20:M:145:LEU:HD12	20:M:164:ASP:H	1.77	0.48
24:Q:74:LEU:HD23	24:Q:77:PHE:HD2	1.79	0.48
22:O:306:ARG:NH2	28:U:234:ASN:OD1	2.35	0.48
33:Z:758:LEU:HD11	33:Z:795:THR:HG21	1.95	0.48
11:D:6:ARG:NH2	12:E:9:ASP:OD1	2.47	0.48
17:J:141:LYS:HD2	17:J:209:LYS:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:396:ARG:NH2	19:L:192:GLU:OE2	2.36	0.48
25:R:36:SER:O	25:R:43:ARG:NH2	2.46	0.48
22:O:352:TRP:NE1	28:U:231:ASP:OD1	2.41	0.48
15:H:190:ARG:HG3	15:H:296:GLU:HG2	1.94	0.48
15:H:278:GLU:O	15:H:281:GLN:NE2	2.47	0.48
17:J:33:LYS:HA	17:J:36:SER:HB3	1.95	0.48
23:P:76:ASN:HD21	23:P:118:VAL:HG22	1.78	0.48
24:Q:59:LEU:HD22	24:Q:103:LYS:HG3	1.96	0.48
8:A:12:TYR:HA	8:A:15:HIS:HD1	1.77	0.48
10:C:206:LEU:HD11	10:C:211:LEU:HD21	1.96	0.48
17:J:216:ALA:HB1	18:K:281:ARG:HD3	1.95	0.48
23:P:94:GLN:HG3	23:P:133:GLU:HG2	1.96	0.48
30:W:111:VAL:HA	30:W:140:ASP:HB3	1.95	0.48
4:4:96:ARG:NH1	5:5:164:GLN:O	2.47	0.48
33:Z:60:ASP:OD1	33:Z:61:SER:N	2.47	0.48
17:J:222:TYR:HB2	17:J:225:GLU:HB2	1.94	0.48
23:P:220:TYR:HD1	23:P:224:LEU:HD11	1.79	0.48
8:A:158:ASP:OD1	8:A:162:TYR:N	2.46	0.47
15:H:454:TYR:CD1	16:I:347:LYS:HD3	2.49	0.47
21:N:91:ILE:HD11	21:N:139:ARG:HH11	1.80	0.47
21:N:775:CYS:O	21:N:866:TYR:N	2.43	0.47
29:V:123:VAL:HG12	29:V:127:LYS:HE3	1.96	0.47
33:Z:204:CYS:HA	33:Z:207:ILE:HD12	1.96	0.47
9:B:185:LEU:HD11	9:B:213:ILE:HB	1.95	0.47
13:F:95:SER:O	13:F:100:ASN:N	2.46	0.47
13:F:62:LYS:O	13:F:74:LEU:N	2.45	0.47
17:J:164:ILE:HG12	17:J:289:LYS:HE2	1.95	0.47
26:S:140:LEU:HA	26:S:183:LEU:HD21	1.96	0.47
26:S:22:GLU:HB3	26:S:68:LEU:HD22	1.97	0.47
1:1:38:ARG:NH1	1:1:186:GLY:O	2.47	0.47
6:6:49:ILE:HG22	6:6:54:ILE:HA	1.95	0.47
17:J:218:LEU:HB3	17:J:230:VAL:HA	1.95	0.47
21:N:376:LYS:HA	21:N:411:ILE:HG12	1.95	0.47
30:W:58:ASN:O	30:W:60:ARG:N	2.48	0.47
33:Z:260:GLU:HB2	33:Z:579:GLU:HB3	1.96	0.47
8:A:156:LYS:HD3	8:A:166:TYR:HE2	1.80	0.47
29:V:154:ASP:OD1	29:V:155:ALA:N	2.47	0.47
30:W:139:VAL:HG11	30:W:157:PHE:HE2	1.79	0.47
33:Z:234:PRO:HG3	33:Z:270:SER:HB2	1.96	0.47
3:3:63:LEU:HD12	3:3:105:VAL:HG11	1.96	0.47
16:I:116:ASP:HA	16:I:132:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:117:ASN:HB2	22:O:128:LEU:HB2	1.95	0.47
25:R:44:LYS:HB2	25:R:88:LEU:HD12	1.96	0.47
1:1:78:VAL:HG22	1:1:100:VAL:HG12	1.95	0.47
7:7:215:ARG:NH2	7:7:248:GLU:O	2.46	0.47
10:C:87:LEU:HD22	10:C:115:LEU:HD22	1.96	0.47
20:M:274:ALA:HB1	20:M:275:PRO:HD2	1.96	0.47
19:L:249:SER:OG	20:M:307:GLU:OE1	2.26	0.47
22:O:72:LYS:HG2	22:O:73:ILE:HG13	1.96	0.47
25:R:36:SER:H	25:R:43:ARG:HH21	1.63	0.47
26:S:483:GLU:HG3	28:U:302:GLN:HE21	1.79	0.47
33:Z:308:LYS:NZ	33:Z:918:ASP:O	2.37	0.47
1:1:113:THR:HG22	1:1:134:LEU:HD22	1.95	0.47
7:7:234:ASP:OD2	7:7:237:THR:N	2.42	0.47
9:B:10:THR:HG22	9:B:18:LEU:HD22	1.96	0.47
15:H:105:ILE:HG23	15:H:145:TYR:CE1	2.50	0.47
19:L:290:ARG:NH1	20:M:292:ASP:OD2	2.47	0.47
23:P:144:VAL:HG13	23:P:156:ALA:HB1	1.96	0.47
25:R:59:MET:HB3	25:R:62:TYR:HD2	1.79	0.47
32:Y:72:ASP:OD1	32:Y:73:PHE:N	2.47	0.47
3:3:53:ILE:HG22	3:3:60:VAL:HG22	1.95	0.47
14:G:209:GLU:HG2	14:G:210:LYS:HG3	1.96	0.47
27:T:221:ALA:HB1	27:T:226:TRP:HB2	1.97	0.47
31:X:78:ILE:HG12	31:X:80:SER:H	1.79	0.47
1:1:151:THR:HA	1:1:154:TYR:HE2	1.79	0.47
10:C:4:ARG:HD2	12:E:10:ARG:HA	1.97	0.47
30:W:15:TYR:HB2	30:W:116:SER:HB3	1.97	0.47
3:3:11:ILE:HG22	3:3:142:ALA:HB3	1.96	0.47
4:4:60:ILE:HD13	4:4:84:VAL:HG22	1.96	0.47
8:A:61:ASP:OD2	14:G:173:LYS:NZ	2.37	0.47
13:F:4:ASN:ND2	15:H:359:ASN:O	2.48	0.47
19:L:432:ILE:HG12	19:L:436:LYS:HB2	1.96	0.47
23:P:24:ILE:O	23:P:69:ARG:NH1	2.48	0.47
29:V:138:ALA:O	29:V:156:PHE:N	2.48	0.47
1:1:76:ASP:OD2	2:2:113:LYS:NZ	2.42	0.47
11:D:161:ALA:HB1	11:D:175:LEU:HD13	1.98	0.47
18:K:320:ARG:NH2	18:K:322:ASP:OD2	2.47	0.47
23:P:217:LYS:HA	23:P:220:TYR:HD2	1.80	0.47
25:R:302:ALA:HB2	25:R:357:PHE:HA	1.96	0.47
33:Z:827:LEU:HB3	33:Z:831:LEU:HD13	1.96	0.47
11:D:107:GLU:OE2	11:D:111:ARG:NH2	2.48	0.46
21:N:138:GLU:HA	21:N:141:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:736:PHE:HD1	21:N:746:ALA:HA	1.80	0.46
22:O:23:HIS:CE1	22:O:25:LEU:HB2	2.50	0.46
17:J:279:LEU:O	17:J:284:THR:N	2.48	0.46
19:L:277:ILE:HG23	19:L:322:LYS:HB2	1.97	0.46
21:N:17:GLN:HB3	21:N:20:VAL:HB	1.98	0.46
29:V:54:LEU:N	29:V:67:ASP:O	2.48	0.46
33:Z:92:LEU:HD12	33:Z:122:LEU:HD21	1.97	0.46
33:Z:138:ARG:HH22	33:Z:146:PHE:HZ	1.62	0.46
33:Z:531:ALA:HB1	33:Z:572:ILE:HB	1.97	0.46
9:B:18:LEU:HD12	9:B:21:ILE:HD12	1.97	0.46
9:B:5:TYR:HE1	10:C:3:SER:HA	1.80	0.46
17:J:71:TYR:N	17:J:115:LEU:O	2.40	0.46
19:L:137:ARG:HA	19:L:140:LEU:HD12	1.95	0.46
21:N:416:GLY:HA3	21:N:453:ALA:HB1	1.96	0.46
5:5:92:ASP:HB2	5:5:247:GLY:O	2.15	0.46
12:E:122:ARG:HG2	12:E:132:ARG:HH21	1.79	0.46
17:J:99:ALA:HB3	17:J:102:ILE:HG12	1.96	0.46
20:M:281:ASP:OD1	20:M:282:GLU:N	2.49	0.46
22:O:308:LEU:O	22:O:348:VAL:N	2.42	0.46
14:G:165:THR:HA	14:G:169:ARG:HD3	1.97	0.46
12:E:26:TYR:OH	15:H:465:GLN:OE1	2.32	0.46
17:J:247:MET:HG3	17:J:292:MET:HG2	1.96	0.46
20:M:175:LYS:HG3	20:M:237:ALA:HA	1.97	0.46
22:O:132:GLU:OE2	22:O:135:ARG:NH2	2.48	0.46
22:O:189:TYR:HE2	22:O:227:ILE:HB	1.81	0.46
30:W:12:ASN:H	30:W:55:ALA:HB3	1.81	0.46
33:Z:126:TYR:HD2	33:Z:128:GLU:HB2	1.81	0.46
2:2:242:LEU:HA	3:3:201:LYS:HE3	1.98	0.46
5:5:109:VAL:HG21	5:5:253:TYR:HE2	1.80	0.46
9:B:140:ASP:OD1	9:B:144:GLY:N	2.44	0.46
12:E:50:VAL:HG21	12:E:66:LYS:HB2	1.98	0.46
13:F:7:ASP:O	13:F:21:GLN:NE2	2.49	0.46
14:G:5:GLY:HA2	15:H:322:GLY:HA3	1.96	0.46
19:L:105:ILE:HD12	20:M:126:THR:HG22	1.98	0.46
20:M:220:MET:HG2	20:M:347:ILE:HB	1.98	0.46
5:5:103:SER:HB3	5:5:106:VAL:HG23	1.97	0.46
15:H:277:SER:OG	16:I:308:GLU:OE1	2.33	0.46
27:T:94:HIS:NE2	27:T:96:LEU:HB2	2.31	0.46
16:I:299:GLU:HA	16:I:302:ILE:HD12	1.96	0.46
21:N:713:VAL:HG12	21:N:755:PRO:HB3	1.97	0.46
27:T:201:PRO:HA	27:T:232:LYS:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:246:CYS:HB2	33:Z:250:VAL:HG23	1.98	0.46
7:7:49:TYR:HE2	7:7:54:ILE:HG13	1.80	0.46
9:B:123:GLN:HE22	10:C:131:PHE:HE1	1.64	0.46
13:F:201:LEU:HD13	13:F:205:SER:HA	1.97	0.46
16:I:254:GLN:NE2	17:J:227:SER:OG	2.49	0.46
19:L:167:VAL:HB	20:M:142:PRO:HG2	1.97	0.46
30:W:181:LEU:HA	30:W:184:ASN:HD22	1.81	0.46
8:A:219:SER:H	8:A:222:ASP:HB2	1.80	0.46
11:D:11:PHE:CE2	12:E:136:ARG:HB2	2.51	0.46
16:I:248:VAL:HG12	16:I:250:SER:H	1.81	0.46
20:M:274:ALA:O	20:M:276:THR:N	2.48	0.46
20:M:282:GLU:OE1	20:M:328:ASN:ND2	2.49	0.46
29:V:48:GLU:HG2	29:V:112:PRO:HD2	1.98	0.46
33:Z:441:TYR:CD2	33:Z:442:VAL:HG22	2.51	0.46
3:3:11:ILE:HD11	3:3:26:ASP:HB3	1.96	0.45
11:D:26:ALA:HB1	11:D:78:LEU:HG	1.96	0.45
15:H:414:SER:OG	15:H:418:GLU:OE1	2.29	0.45
19:L:263:ILE:HD11	19:L:304:THR:HG23	1.98	0.45
19:L:400:PHE:HZ	20:M:215:PRO:HD3	1.81	0.45
21:N:373:VAL:HG23	21:N:410:LEU:HD13	1.98	0.45
27:T:242:LYS:HB3	27:T:251:HIS:HD2	1.80	0.45
18:K:153:ASP:OD1	19:L:110:LYS:NZ	2.50	0.45
4:4:70:ARG:HE	10:C:113:ARG:CZ	2.28	0.45
12:E:201:LEU:HD23	12:E:204:LEU:HD12	1.99	0.45
21:N:67:LYS:HA	21:N:70:TYR:HB3	1.98	0.45
9:B:111:VAL:HG23	9:B:136:ILE:HD12	1.98	0.45
15:H:312:ASP:O	15:H:318:ARG:NH2	2.49	0.45
18:K:127:ASP:OD1	18:K:128:ARG:N	2.49	0.45
18:K:164:ASN:H	18:K:166:LYS:HG2	1.81	0.45
19:L:364:HIS:CE1	19:L:392:ARG:HE	2.34	0.45
33:Z:149:TRP:HA	33:Z:154:ILE:HD12	1.98	0.45
12:E:204:LEU:HA	12:E:207:VAL:HG22	1.99	0.45
15:H:101:ARG:HE	15:H:171:GLY:HA2	1.82	0.45
15:H:98:GLN:NE2	16:I:127:ASP:O	2.49	0.45
25:R:312:TYR:HD1	25:R:316:LEU:HD22	1.82	0.45
25:R:346:LYS:HD2	25:R:390:THR:HB	1.99	0.45
28:U:46:ILE:HG21	28:U:119:LEU:HD22	1.97	0.45
16:I:253:ILE:HG22	16:I:254:GLN:H	1.82	0.45
21:N:296:CYS:HB3	21:N:377:GLY:HA2	1.98	0.45
23:P:270:LEU:O	23:P:344:ARG:NE	2.50	0.45
26:S:293:ILE:HD13	26:S:316:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:141:SER:HB2	2:2:154:LEU:HD13	1.99	0.45
15:H:291:VAL:HG11	15:H:336:LEU:HA	1.99	0.45
15:H:385:ARG:NH1	15:H:413:ASN:OD1	2.41	0.45
19:L:113:SER:HB3	19:L:116:LYS:HB2	1.97	0.45
23:P:97:ILE:HG21	23:P:136:ARG:HB3	1.97	0.45
28:U:165:GLU:OE2	29:V:42:ARG:NH2	2.35	0.45
29:V:29:ILE:HD12	29:V:201:ILE:HG23	1.98	0.45
9:B:217:GLU:OE1	9:B:231:LYS:HB2	2.17	0.45
25:R:62:TYR:HE2	25:R:145:GLY:HA2	1.81	0.45
1:1:23:MET:HB3	1:1:145:ILE:HG22	1.98	0.44
8:A:14:ARG:HG2	8:A:26:TYR:CG	2.52	0.44
9:B:43:VAL:HG11	9:B:137:ALA:HB1	1.99	0.44
13:F:26:LEU:HD23	13:F:149:PRO:HD2	1.98	0.44
14:G:109:ILE:HG12	14:G:142:ASP:HB3	1.99	0.44
30:W:1:MET:H2	30:W:195:GLY:H	1.65	0.44
1:1:94:THR:OG1	1:1:128:GLU:OE1	2.30	0.44
14:G:95:GLU:HB3	14:G:115:ARG:HH11	1.83	0.44
17:J:154:THR:HA	17:J:157:ILE:HD12	1.99	0.44
19:L:88:TYR:HD1	20:M:62:ILE:HG13	1.83	0.44
21:N:742:TRP:CH2	21:N:744:PRO:HG2	2.51	0.44
31:X:117:LYS:HE2	31:X:119:LYS:HB2	1.98	0.44
33:Z:445:PRO:HB2	33:Z:485:ILE:HD11	2.00	0.44
33:Z:577:GLN:NE2	33:Z:580:GLN:OE1	2.51	0.44
9:B:186:GLU:OE1	9:B:246:ARG:NE	2.50	0.44
16:I:222:TYR:HE1	16:I:330:LYS:HA	1.82	0.44
22:O:138:LEU:HD11	22:O:178:TYR:HA	1.99	0.44
23:P:361:THR:HG22	23:P:399:ILE:HG22	1.98	0.44
30:W:98:LEU:HD13	30:W:108:GLN:HB3	1.99	0.44
5:5:220:LYS:HG2	5:5:222:ASP:H	1.82	0.44
7:7:61:GLY:N	7:7:69:PHE:O	2.37	0.44
15:H:422:VAL:HA	15:H:450:VAL:HG21	1.98	0.44
19:L:143:GLY:O	19:L:161:ARG:NH2	2.50	0.44
21:N:294:PRO:HB2	21:N:298:TYR:CZ	2.53	0.44
21:N:717:LEU:HD22	21:N:730:VAL:HA	1.99	0.44
24:Q:223:GLY:HA2	24:Q:226:HIS:HD2	1.82	0.44
25:R:61:PRO:HB2	25:R:65:TYR:CZ	2.53	0.44
16:I:196:GLU:O	16:I:208:TYR:OH	2.28	0.44
18:K:157:SER:C	18:K:159:SER:H	2.20	0.44
24:Q:92:LYS:HE3	24:Q:95:LYS:HZ2	1.82	0.44
26:S:111:ARG:HA	26:S:117:SER:HB3	2.00	0.44
21:N:8:PRO:HB3	27:T:84:GLN:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:202:ASP:OD1	29:V:203:TYR:N	2.50	0.44
30:W:47:ASN:OD1	30:W:48:THR:N	2.50	0.44
16:I:300:ARG:HB3	16:I:304:ARG:HH12	1.83	0.44
16:I:340:ARG:NH1	16:I:341:PRO:O	2.51	0.44
18:K:67:TYR:HB2	21:N:572:LEU:HD13	2.00	0.44
20:M:127:VAL:HG11	20:M:153:TYR:HB3	2.00	0.44
19:L:427:LYS:HD2	20:M:346:LYS:HE2	1.99	0.44
24:Q:15:VAL:HG13	24:Q:20:TYR:HB3	1.98	0.44
26:S:357:LEU:HB3	26:S:384:ARG:HH22	1.83	0.44
28:U:108:GLU:OE1	30:W:60:ARG:NH2	2.50	0.44
15:H:261:ARG:NH2	16:I:315:GLY:O	2.33	0.44
2:2:104:ARG:HG2	2:2:133:ASP:HB2	2.00	0.44
5:5:96:THR:HG22	5:5:101:VAL:HG22	2.00	0.44
5:5:172:MET:H	5:5:192:SER:HB3	1.82	0.44
13:F:41:ASN:ND2	13:F:180:ILE:O	2.51	0.44
21:N:406:TYR:HD1	21:N:448:LEU:HB3	1.82	0.44
23:P:144:VAL:HG12	23:P:148:LYS:HE3	1.99	0.44
2:2:123:ILE:HG22	2:2:125:ALA:H	1.83	0.44
10:C:53:THR:OG1	10:C:210:ARG:NE	2.51	0.44
14:G:37:SER:HB3	14:G:50:VAL:HG23	2.00	0.44
15:H:247:LEU:HD13	15:H:374:LYS:HG2	2.00	0.44
15:H:304:CYS:SG	15:H:349:ILE:HG21	2.58	0.44
16:I:104:LEU:HD22	16:I:148:LEU:HD21	2.00	0.44
30:W:36:ILE:HD11	30:W:185:ILE:HD12	1.98	0.44
15:H:102:CYS:HA	15:H:147:ILE:HA	2.01	0.43
16:I:253:ILE:HG22	16:I:254:GLN:N	2.33	0.43
19:L:107:GLU:HA	19:L:145:ARG:HA	2.00	0.43
27:T:227:PRO:HG2	27:T:234:TYR:HB3	2.00	0.43
30:W:91:LEU:HB2	30:W:128:LEU:HD21	1.99	0.43
14:G:13:SER:OG	14:G:127:ASN:ND2	2.45	0.43
15:H:273:ARG:HG3	15:H:307:PHE:HD2	1.83	0.43
19:L:129:VAL:HG11	19:L:148:LEU:HD22	1.99	0.43
19:L:257:GLY:HA2	19:L:303:ARG:HH22	1.82	0.43
7:7:39:VAL:HB	7:7:90:ILE:HG22	2.00	0.43
19:L:293:GLU:O	19:L:295:THR:HG23	2.19	0.43
21:N:6:ALA:HB2	21:N:35:LEU:HB3	1.99	0.43
23:P:131:PHE:HA	23:P:136:ARG:HH21	1.83	0.43
23:P:218:LEU:HD23	23:P:251:LYS:HE2	2.01	0.43
28:U:93:TYR:HB3	28:U:121:LEU:HD23	2.00	0.43
2:2:85:THR:HA	2:2:88:ILE:HG22	1.99	0.43
8:A:88:PRO:HD3	14:G:156:SER:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:666:GLN:HG2	21:N:873:ARG:HH21	1.83	0.43
22:O:332:ILE:HG12	22:O:337:LEU:HB2	2.00	0.43
25:R:394:ASP:OD1	25:R:395:ASN:N	2.52	0.43
26:S:434:ALA:HA	26:S:446:THR:H	1.83	0.43
28:U:124:ASP:HB3	28:U:133:PRO:HB2	2.00	0.43
33:Z:116:ALA:HB2	33:Z:140:LEU:HD23	2.01	0.43
10:C:177:GLN:HE22	11:D:53:LYS:HD2	1.83	0.43
16:I:313:LEU:HD21	16:I:324:VAL:HG21	2.00	0.43
18:K:212:TYR:HB2	18:K:339:GLU:HA	2.00	0.43
18:K:48:TYR:HA	18:K:51:LEU:HD12	2.00	0.43
20:M:283:LEU:HB2	20:M:327:THR:HB	2.00	0.43
24:Q:162:LEU:HD22	24:Q:166:LYS:HE3	2.00	0.43
25:R:286:LEU:HG	25:R:288:SER:H	1.82	0.43
30:W:117:PRO:HD3	30:W:146:GLU:HB2	2.01	0.43
7:7:152:VAL:HG11	7:7:235:LYS:HB3	2.00	0.43
17:J:118:ASP:OD1	17:J:119:SER:N	2.49	0.43
17:J:126:LEU:HD22	18:K:103:ILE:HD13	2.01	0.43
19:L:193:LEU:HD11	19:L:231:LEU:HD13	2.00	0.43
31:X:7:VAL:HG12	31:X:8:ILE:HG13	2.00	0.43
33:Z:957:LEU:HD22	33:Z:961:GLU:HB2	2.00	0.43
12:E:15:PHE:CE2	13:F:126:ARG:HB2	2.53	0.43
14:G:50:VAL:HG11	14:G:66:LYS:HB2	2.00	0.43
16:I:280:PHE:CE2	16:I:282:ASP:HB2	2.53	0.43
18:K:148:ASP:OD1	18:K:149:ILE:N	2.51	0.43
21:N:19:SER:HB3	27:T:35:ILE:HG21	2.01	0.43
4:4:59:TYR:O	4:4:63:ASN:ND2	2.52	0.43
8:A:181:ASN:HD22	8:A:213:ALA:HB2	1.84	0.43
13:F:39:ARG:NH1	13:F:142:ALA:O	2.52	0.43
25:R:309:LEU:HD21	32:Y:77:LEU:HD12	2.01	0.43
25:R:381:ILE:HA	25:R:388:VAL:HA	2.00	0.43
2:2:228:LYS:HE2	3:3:152:SER:HA	1.99	0.43
12:E:119:LEU:HB3	12:E:138:PHE:CE2	2.54	0.43
13:F:14:SER:HG	13:F:18:ARG:H	1.67	0.43
8:A:135:ARG:HD3	14:G:13:SER:HA	2.01	0.43
17:J:342:ASN:HB3	17:J:345:LYS:HB3	2.01	0.43
18:K:92:VAL:HB	18:K:93:PRO:HD2	2.01	0.43
26:S:468:ALA:HA	28:U:288:PHE:HZ	1.84	0.43
31:X:91:PHE:HB3	31:X:94:ASN:HD22	1.84	0.43
16:I:387:LEU:HD21	16:I:424:MET:HG2	2.00	0.43
17:J:113:VAL:HG12	17:J:125:VAL:HA	2.01	0.43
21:N:338:PHE:HZ	21:N:746:ALA:HB1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:222:LEU:HD23	22:O:254:LEU:HD22	2.01	0.43
25:R:304:TYR:CZ	25:R:308:LEU:HD21	2.54	0.43
29:V:139:VAL:HA	29:V:155:ALA:HA	2.00	0.43
13:F:67:ASP:OD1	13:F:68:GLU:N	2.45	0.42
29:V:137:VAL:HG22	29:V:157:ARG:HG3	2.01	0.42
33:Z:422:ILE:HA	33:Z:425:ILE:HD12	1.99	0.42
3:3:27:LEU:HB3	3:3:38:ASN:O	2.18	0.42
4:4:84:VAL:HG11	4:4:102:VAL:HG21	2.01	0.42
9:B:35:LEU:HA	9:B:163:ALA:HA	1.99	0.42
3:3:65:GLU:HB3	10:C:100:LYS:HG3	2.01	0.42
13:F:112:LEU:HD12	13:F:134:ILE:HD11	2.01	0.42
13:F:39:ARG:HD3	13:F:144:LEU:HB2	2.00	0.42
18:K:122:ILE:HA	18:K:146:LEU:HD23	2.01	0.42
18:K:238:ASN:HB3	18:K:241:GLU:HB2	2.00	0.42
20:M:216:LYS:HG2	20:M:317:SER:HB3	2.01	0.42
20:M:81:ASN:O	20:M:120:LYS:N	2.47	0.42
21:N:653:ARG:NH1	21:N:691:GLN:OE1	2.52	0.42
23:P:393:VAL:HG13	23:P:400:VAL:HG22	1.99	0.42
9:B:48:GLU:HB2	9:B:196:LEU:HD11	2.02	0.42
10:C:131:PHE:O	10:C:153:PRO:HB3	2.19	0.42
12:E:13:SER:HB2	13:F:126:ARG:HD3	2.01	0.42
13:F:50:LYS:HB3	13:F:59:TYR:HB3	2.02	0.42
17:J:214:SER:O	17:J:218:LEU:HG	2.19	0.42
17:J:234:PHE:O	17:J:238:ARG:HG3	2.19	0.42
21:N:309:ILE:HD13	21:N:707:ASN:HB3	2.01	0.42
23:P:290:LEU:HD21	23:P:292:LYS:HE3	2.01	0.42
33:Z:974:THR:HG23	33:Z:975:SER:N	2.34	0.42
8:A:215:GLY:O	19:L:353:ASN:ND2	2.52	0.42
12:E:24:VAL:HG11	12:E:161:SER:HA	2.00	0.42
13:F:49:LEU:HB2	13:F:197:ILE:HD11	2.01	0.42
14:G:67:ILE:HG12	14:G:77:VAL:HB	2.01	0.42
17:J:357:ASP:OD2	17:J:393:ASN:ND2	2.48	0.42
19:L:187:THR:HA	19:L:190:ILE:HD12	2.01	0.42
18:K:220:THR:HG21	19:L:313:ASP:OD1	2.18	0.42
19:L:327:THR:HG21	19:L:333:LEU:HD11	2.02	0.42
19:L:400:PHE:HA	19:L:403:ILE:HD12	2.01	0.42
20:M:428:LYS:HG3	20:M:429:SER:H	1.84	0.42
24:Q:390:LEU:O	25:R:346:LYS:N	2.52	0.42
26:S:345:TYR:HD1	26:S:348:LEU:HD12	1.85	0.42
26:S:400:LYS:HG3	26:S:445:THR:HB	2.00	0.42
28:U:92:TRP:CH2	28:U:107:ASN:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:171:ARG:NH1	29:V:198:SER:O	2.53	0.42
33:Z:928:ARG:HA	33:Z:956:LEU:H	1.84	0.42
2:2:95:HIS:HE1	8:A:104:PHE:HE1	1.67	0.42
11:D:202:VAL:HG13	11:D:203:VAL:H	1.84	0.42
16:I:219:VAL:HG12	16:I:346:ARG:HB2	2.00	0.42
16:I:279:VAL:O	16:I:325:ILE:N	2.45	0.42
17:J:186:ILE:HG22	17:J:310:ILE:HG21	2.02	0.42
20:M:135:VAL:HG12	20:M:158:THR:HG22	2.00	0.42
21:N:288:ASN:HB3	21:N:293:LEU:HB2	2.01	0.42
23:P:412:LEU:HD21	28:U:269:THR:HA	2.00	0.42
33:Z:180:ASP:OD1	33:Z:181:GLY:N	2.53	0.42
33:Z:539:ASN:OD1	33:Z:540:GLY:N	2.52	0.42
33:Z:884:THR:HG22	33:Z:901:PHE:HA	2.02	0.42
4:4:172:MET:HG2	4:4:174:MET:H	1.85	0.42
5:5:92:ASP:OD1	5:5:108:LYS:NZ	2.51	0.42
10:C:78:ALA:O	10:C:134:SER:OG	2.35	0.42
12:E:164:PHE:O	13:F:60:GLN:NE2	2.51	0.42
28:U:38:LEU:HD23	28:U:87:GLU:HB3	2.02	0.42
29:V:127:LYS:HE2	29:V:195:HIS:CE1	2.55	0.42
30:W:98:LEU:O	30:W:101:ARG:NH1	2.49	0.42
15:H:100:ALA:HB2	15:H:149:LEU:HD23	2.00	0.42
15:H:95:HIS:O	15:H:97:LEU:N	2.53	0.42
21:N:328:PHE:HE1	21:N:696:LYS:HB2	1.84	0.42
21:N:379:LEU:HD23	21:N:411:ILE:HG22	2.02	0.42
21:N:623:PHE:O	21:N:627:ILE:HG12	2.20	0.42
1:1:191:VAL:HG12	1:1:209:PRO:HD3	2.02	0.42
15:H:252:PRO:HB2	15:H:460:THR:HG21	2.01	0.42
18:K:212:TYR:N	18:K:338:ILE:O	2.52	0.42
19:L:217:GLY:HA3	19:L:343:LEU:HD23	2.02	0.42
28:U:283:ARG:NE	29:V:284:ALA:O	2.53	0.42
11:D:96:HIS:NE2	11:D:100:LEU:HD12	2.35	0.42
11:D:158:SER:HB3	12:E:63:SER:HB2	2.02	0.42
13:F:129:GLY:HA2	13:F:149:PRO:HG3	2.01	0.42
13:F:132:LEU:HB2	13:F:147:PHE:HB3	2.01	0.42
16:I:219:VAL:HG22	16:I:325:ILE:HG12	2.00	0.42
16:I:287:ILE:HG12	16:I:302:ILE:HG12	2.02	0.42
17:J:274:GLU:OE1	17:J:309:ARG:NH2	2.45	0.42
18:K:106:ASN:O	18:K:122:ILE:N	2.49	0.42
21:N:251:GLU:HB3	21:N:763:GLY:HA3	2.02	0.42
23:P:357:TYR:CG	23:P:360:ILE:HD11	2.55	0.42
25:R:204:TRP:CZ3	25:R:235:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:303:ASP:OD2	33:Z:973:TYR:OH	2.27	0.42
4:4:96:ARG:HH22	5:5:164:GLN:HE22	1.67	0.42
11:D:49:ARG:HG2	11:D:51:THR:H	1.84	0.42
13:F:34:VAL:HG23	13:F:165:SER:HB3	2.02	0.42
18:K:127:ASP:HB3	18:K:130:LEU:HG	2.02	0.42
18:K:154:SER:HB3	18:K:259:ARG:NH1	2.35	0.42
21:N:612:SER:O	21:N:618:ARG:NH1	2.48	0.42
5:5:91:VAL:HG21	5:5:109:VAL:HG23	2.02	0.41
1:1:84:LEU:HD21	8:A:99:ALA:HA	2.02	0.41
14:G:221:LEU:HA	14:G:225:ASN:HA	2.02	0.41
16:I:168:VAL:HG13	16:I:171:MET:HB2	2.01	0.41
18:K:93:PRO:HG2	19:L:153:LEU:HB2	2.02	0.41
21:N:369:ALA:HB1	21:N:406:TYR:HD2	1.85	0.41
23:P:235:LEU:HD23	23:P:271:SER:HB2	2.00	0.41
18:K:81:ARG:NH2	28:U:176:ARG:O	2.53	0.41
31:X:68:LEU:HD21	31:X:89:LEU:HD13	2.01	0.41
2:2:192:ILE:HG12	2:2:199:GLY:HA2	2.01	0.41
6:6:110:ARG:HG2	12:E:104:ASP:HB2	2.01	0.41
9:B:42:GLY:HA2	9:B:145:PHE:CE1	2.55	0.41
12:E:18:GLU:OE1	12:E:20:ARG:NH2	2.38	0.41
15:H:201:GLU:HG3	15:H:273:ARG:HH12	1.85	0.41
21:N:229:VAL:HG11	21:N:238:ALA:HB2	2.01	0.41
21:N:416:GLY:O	21:N:420:THR:N	2.52	0.41
21:N:528:ARG:HB3	21:N:531:LEU:HB2	2.02	0.41
25:R:291:SER:HB3	25:R:307:TYR:CD2	2.55	0.41
29:V:159:ILE:HG13	29:V:194:ARG:HA	2.02	0.41
1:1:27:PHE:HE1	1:1:29:ASP:HB2	1.85	0.41
18:K:186:GLU:O	18:K:198:TYR:OH	2.38	0.41
17:J:52:ASN:ND2	21:N:612:SER:HA	2.34	0.41
24:Q:391:ASP:HB3	24:Q:396:TRP:H	1.85	0.41
25:R:35:GLN:HG3	25:R:74:ASN:HB2	2.00	0.41
29:V:27:VAL:HG13	29:V:63:VAL:HB	2.02	0.41
3:3:42:LYS:HD3	3:3:54:THR:HG22	2.02	0.41
7:7:49:TYR:CE2	7:7:54:ILE:HG13	2.55	0.41
6:6:114:HIS:CD2	12:E:102:TYR:HA	2.55	0.41
14:G:211:ASP:OD1	14:G:212:PHE:N	2.53	0.41
21:N:743:PHE:HB2	21:N:744:PRO:HD3	2.01	0.41
22:O:40:GLN:HA	22:O:52:ALA:HA	2.02	0.41
22:O:99:LEU:HD13	22:O:133:ILE:HG12	2.01	0.41
23:P:202:LYS:HA	23:P:205:LYS:HE2	2.03	0.41
24:Q:85:MET:HA	24:Q:88:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:332:SER:HA	17:J:335:MET:HE3	2.01	0.41
20:M:163:PHE:HZ	20:M:268:ALA:HB1	1.85	0.41
21:N:55:PHE:CZ	21:N:57:ASP:HB2	2.55	0.41
21:N:58:ARG:HA	21:N:61:ALA:HB3	2.03	0.41
21:N:762:ARG:HH21	21:N:765:ASP:HB2	1.85	0.41
22:O:80:LYS:O	22:O:84:ALA:HB3	2.21	0.41
23:P:353:ILE:HA	23:P:357:TYR:HD2	1.86	0.41
25:R:301:TYR:HD2	25:R:357:PHE:HB3	1.85	0.41
2:2:177:LYS:HE3	2:2:206:VAL:HG11	2.03	0.41
3:3:143:SER:HA	3:3:146:LEU:HD12	2.03	0.41
4:4:101:ASN:HB3	4:4:133:HIS:CG	2.56	0.41
7:7:43:SER:HA	7:7:177:THR:HB	2.02	0.41
8:A:17:THR:HG22	8:A:27:GLN:HB2	2.01	0.41
19:L:108:VAL:HG22	19:L:119:VAL:HG22	2.01	0.41
21:N:443:LEU:HD21	21:N:469:VAL:HG13	2.01	0.41
21:N:638:ILE:HD11	21:N:672:ASN:HD21	1.86	0.41
26:S:357:LEU:HA	26:S:384:ARG:HH12	1.85	0.41
1:1:61:TRP:CD1	1:1:197:LEU:HD21	2.55	0.41
4:4:9:VAL:HG11	4:4:157:GLY:HA3	2.03	0.41
8:A:87:ILE:N	8:A:88:PRO:HD2	2.35	0.41
15:H:177:ASP:HB3	15:H:180:LYS:O	2.21	0.41
15:H:253:GLY:O	15:H:417:ALA:N	2.51	0.41
21:N:93:GLU:HB3	21:N:98:VAL:HG21	2.03	0.41
23:P:359:ARG:HD3	23:P:399:ILE:HD12	2.02	0.41
25:R:24:TYR:CD1	25:R:244:THR:HA	2.56	0.41
1:1:78:VAL:HG21	1:1:101:PHE:CE1	2.56	0.41
6:6:179:TYR:HD1	6:6:188:LYS:HA	1.85	0.41
6:6:226:VAL:HG22	6:6:231:VAL:HG22	2.03	0.41
7:7:127:GLU:HG2	13:F:100:ASN:HB2	2.02	0.41
8:A:128:TYR:HA	8:A:134:MET:HG3	2.03	0.41
16:I:219:VAL:HA	16:I:344:ILE:HG23	2.02	0.41
23:P:260:VAL:HG22	23:P:327:LEU:HB3	2.02	0.41
9:B:184:GLU:HG3	24:Q:129:LYS:HB2	2.02	0.41
25:R:222:ARG:HE	25:R:329:PHE:HZ	1.68	0.41
27:T:131:LYS:HB2	27:T:135:ASN:ND2	2.36	0.41
33:Z:801:HIS:ND1	33:Z:837:TYR:OH	2.39	0.41
1:1:24:ALA:HB2	1:1:33:LEU:HG	2.02	0.41
9:B:44:VAL:HG11	9:B:189:ILE:HA	2.03	0.41
20:M:176:PRO:HG2	20:M:237:ALA:HB2	2.03	0.41
21:N:154:LEU:HD21	21:N:170:LEU:HD12	2.03	0.41
24:Q:350:ILE:HD13	24:Q:362:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:12:LEU:HD21	27:T:84:GLN:HE22	1.86	0.41
1:1:61:TRP:HD1	1:1:197:LEU:HD11	1.86	0.41
4:4:49:GLU:O	4:4:53:THR:HG23	2.21	0.41
12:E:91:HIS:CD2	12:E:119:LEU:HD11	2.56	0.41
18:K:214:PRO:HA	18:K:215:PRO:HD3	1.90	0.41
20:M:167:VAL:HG12	20:M:168:LYS:HG3	2.02	0.41
21:N:479:GLU:OE2	21:N:515:ARG:NH2	2.54	0.41
3:3:145:GLN:HG2	3:3:177:ARG:HB2	2.02	0.41
10:C:147:GLN:HB3	10:C:149:TYR:CE2	2.56	0.41
16:I:282:ASP:OD1	16:I:283:GLU:N	2.54	0.41
17:J:338:THR:O	17:J:341:ILE:HG12	2.21	0.41
18:K:84:GLU:O	18:K:88:ARG:NE	2.48	0.41
21:N:726:ASP:HB3	21:N:729:SER:HB3	2.03	0.41
23:P:164:GLN:HE22	23:P:195:GLN:NE2	2.19	0.41
24:Q:275:ILE:HD11	24:Q:306:TYR:HD2	1.85	0.41
33:Z:124:MET:O	33:Z:156:HIS:ND1	2.53	0.41
33:Z:463:HIS:HB2	33:Z:496:ALA:HB1	2.03	0.41
33:Z:568:LEU:HD21	33:Z:738:TYR:CZ	2.55	0.41
1:1:20:THR:O	1:1:149:GLY:N	2.52	0.40
2:2:191:GLY:O	2:2:195:ASP:HB3	2.22	0.40
16:I:423:VAL:HA	16:I:427:LYS:HB2	2.03	0.40
19:L:88:TYR:CD1	20:M:62:ILE:HG13	2.56	0.40
21:N:83:LEU:HD13	21:N:132:LYS:HB3	2.03	0.40
26:S:352:VAL:HG22	26:S:387:VAL:HG22	2.03	0.40
3:3:13:VAL:HG13	3:3:167:ILE:HD11	2.03	0.40
9:B:40:THR:OG1	9:B:183:LEU:O	2.30	0.40
14:G:218:TRP:HH2	14:G:223:GLU:HB3	1.86	0.40
15:H:104:LYS:HB3	15:H:146:VAL:HB	2.03	0.40
18:K:391:GLY:HA3	19:L:212:ILE:HG21	2.02	0.40
21:N:318:LYS:HD2	21:N:355:TRP:CD1	2.57	0.40
23:P:61:LYS:O	23:P:65:LEU:HG	2.21	0.40
26:S:164:ILE:HB	26:S:165:PRO:HD3	2.03	0.40
33:Z:185:ASP:HB3	33:Z:230:ILE:HD12	2.02	0.40
33:Z:427:GLN:HA	33:Z:458:SER:HA	2.02	0.40
4:4:35:THR:HB	4:4:43:LEU:HD11	2.03	0.40
5:5:76:THR:HG23	5:5:108:LYS:HZ3	1.86	0.40
5:5:96:THR:HG21	5:5:245:TYR:HA	2.03	0.40
15:H:215:LYS:HB3	15:H:217:GLN:OE1	2.20	0.40
15:H:289:ARG:O	15:H:293:GLU:HG3	2.21	0.40
20:M:197:ILE:HB	20:M:277:ILE:HD13	2.03	0.40
21:N:328:PHE:HZ	21:N:693:GLY:HA2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:P:147:LYS:HB2	23:P:156:ALA:HB2	2.03	0.40
3:3:63:LEU:HB3	3:3:67:PHE:CE2	2.56	0.40
6:6:76:PHE:HD2	6:6:79:ASP:H	1.69	0.40
11:D:202:VAL:HG13	11:D:203:VAL:N	2.36	0.40
17:J:140:GLU:OE2	17:J:200:ARG:NH2	2.52	0.40
24:Q:161:LEU:HD22	24:Q:165:PHE:CZ	2.56	0.40
33:Z:754:LYS:HG3	33:Z:783:VAL:HB	2.03	0.40
1:1:32:ILE:HG12	1:1:196:VAL:HA	2.03	0.40
7:7:76:ILE:HG21	7:7:97:GLU:HG3	2.03	0.40
22:O:41:LEU:HD23	22:O:59:LEU:HD23	2.03	0.40
25:R:26:VAL:HG22	25:R:53:LYS:HG2	2.03	0.40
29:V:51:GLY:HA2	29:V:71:MET:HG2	2.04	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	1	203/215 (94%)	191 (94%)	12 (6%)	0	100	100
1	b	203/215 (94%)	193 (95%)	10 (5%)	0	100	100
2	2	220/261 (84%)	213 (97%)	7 (3%)	0	100	100
2	i	220/261 (84%)	214 (97%)	6 (3%)	0	100	100
3	3	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
3	h	202/205 (98%)	192 (95%)	9 (4%)	1 (0%)	31	71
4	4	196/198 (99%)	190 (97%)	6 (3%)	0	100	100
4	g	196/198 (99%)	188 (96%)	8 (4%)	0	100	100
5	5	210/287 (73%)	204 (97%)	6 (3%)	0	100	100
5	f	210/287 (73%)	203 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	6	220/241 (91%)	212 (96%)	8 (4%)	0	100	100
6	e	220/241 (91%)	211 (96%)	9 (4%)	0	100	100
7	7	231/266 (87%)	220 (95%)	11 (5%)	0	100	100
7	a	231/266 (87%)	221 (96%)	10 (4%)	0	100	100
8	A	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
8	c	241/252 (96%)	234 (97%)	7 (3%)	0	100	100
9	B	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
9	j	248/250 (99%)	238 (96%)	10 (4%)	0	100	100
10	C	242/258 (94%)	232 (96%)	10 (4%)	0	100	100
10	d	242/258 (94%)	233 (96%)	9 (4%)	0	100	100
11	D	239/254 (94%)	229 (96%)	10 (4%)	0	100	100
11	n	239/254 (94%)	230 (96%)	9 (4%)	0	100	100
12	E	240/260 (92%)	227 (95%)	13 (5%)	0	100	100
12	m	240/260 (92%)	234 (98%)	6 (2%)	0	100	100
13	F	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
13	l	231/234 (99%)	222 (96%)	9 (4%)	0	100	100
14	G	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
14	k	242/288 (84%)	235 (97%)	7 (3%)	0	100	100
15	H	351/467 (75%)	319 (91%)	32 (9%)	0	100	100
16	I	361/437 (83%)	331 (92%)	29 (8%)	1 (0%)	43	79
17	J	371/405 (92%)	338 (91%)	32 (9%)	1 (0%)	43	79
18	K	379/428 (89%)	340 (90%)	37 (10%)	2 (0%)	31	71
19	L	369/437 (84%)	336 (91%)	33 (9%)	0	100	100
20	M	363/434 (84%)	326 (90%)	36 (10%)	1 (0%)	43	79
21	N	843/945 (89%)	814 (97%)	29 (3%)	0	100	100
22	O	385/393 (98%)	352 (91%)	33 (9%)	0	100	100
23	P	430/445 (97%)	398 (93%)	32 (7%)	0	100	100
24	Q	429/434 (99%)	407 (95%)	22 (5%)	0	100	100
25	R	398/429 (93%)	360 (90%)	37 (9%)	1 (0%)	43	79
26	S	473/523 (90%)	453 (96%)	19 (4%)	1 (0%)	49	83
27	T	270/274 (98%)	246 (91%)	24 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	U	245/338 (72%)	241 (98%)	4 (2%)	0	100	100
29	V	252/306 (82%)	227 (90%)	23 (9%)	2 (1%)	21	62
30	W	195/268 (73%)	181 (93%)	14 (7%)	0	100	100
31	X	125/156 (80%)	113 (90%)	12 (10%)	0	100	100
32	Y	25/89 (28%)	19 (76%)	5 (20%)	1 (4%)	3	32
33	Z	807/993 (81%)	757 (94%)	49 (6%)	1 (0%)	53	87
All	All	13400/15139 (88%)	12648 (94%)	740 (6%)	12 (0%)	56	87

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	I	287	ILE
18	K	158	ILE
18	K	292	VAL
25	R	241	ILE
3	h	105	VAL
17	J	134	VAL
20	M	167	VAL
29	V	165	ILE
32	Y	69	VAL
33	Z	442	VAL
26	S	83	PRO
29	V	78	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	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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	320/385 (83%)	320 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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	116/144 (81%)	116 (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	11646/13054 (89%)	11646 (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 (87) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	95	HIS
3	3	169	GLN
4	4	191	GLN
5	5	164	GLN
5	5	263	HIS
6	6	55	ASN
6	6	214	HIS
7	7	59	ASN
2	i	122	HIS
2	i	173	GLN
4	g	191	GLN
5	f	283	ASN
6	e	55	ASN
6	e	111	ASN
7	a	145	ASN
7	a	153	GLN
8	A	84	ASN
8	A	126	GLN
8	A	181	ASN

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Mol	Chain	Res	Type
10	C	177	GLN
11	D	16	HIS
12	E	23	GLN
12	E	73	HIS
12	E	91	HIS
13	F	4	ASN
13	F	41	ASN
13	F	60	GLN
14	G	33	ASN
8	c	37	GLN
10	d	94	HIS
10	d	120	GLN
12	m	180	GLN
13	l	43	HIS
13	l	210	ASN
14	k	121	GLN
15	H	98	GLN
15	H	265	ASN
15	H	359	ASN
16	I	254	GLN
17	J	52	ASN
17	J	205	HIS
17	J	376	HIS
17	J	379	GLN
18	K	98	GLN
18	K	182	GLN
19	L	364	HIS
20	M	125	GLN
20	M	149	ASN
21	N	34	GLN
21	N	231	ASN
21	N	719	ASN
22	O	169	ASN
22	O	282	GLN
22	O	354	GLN
23	P	78	GLN
23	P	88	GLN
23	P	195	GLN
23	P	288	ASN
23	P	348	HIS
23	P	349	ASN
24	Q	54	GLN

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Mol	Chain	Res	Type
24	Q	226	HIS
24	Q	247	HIS
24	Q	379	GLN
25	R	73	ASN
25	R	76	GLN
25	R	217	HIS
26	S	177	ASN
26	S	207	ASN
26	S	227	ASN
26	S	244	ASN
26	S	311	GLN
26	S	321	GLN
26	S	488	GLN
27	T	123	HIS
27	T	132	HIS
27	T	251	HIS
28	U	26	GLN
28	U	71	ASN
28	U	84	ASN
28	U	127	GLN
28	U	302	GLN
29	V	190	HIS
30	W	12	ASN
30	W	95	GLN
33	Z	435	GLN
33	Z	622	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.