



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 29, 2019 – 01:34 PM EDT

PDB ID : 6J2N
EMDB ID: : EMD-9770
Title : yeast proteasome in substrate-processing state (C3-b)
Authors : Cong, Y.
Deposited on : 2019-01-02
Resolution : 7.50 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) : 2.4

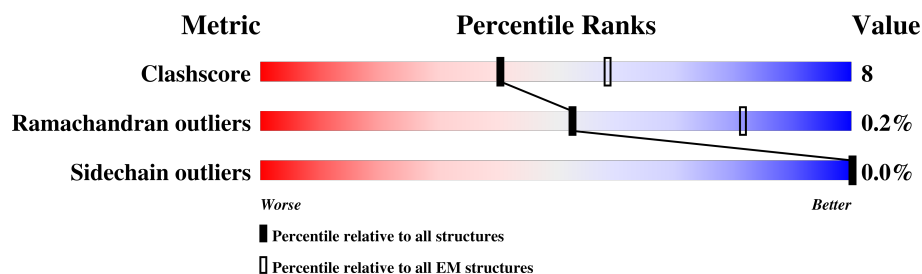
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY










The reported resolution of this entry is 7.50 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.









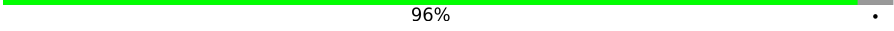

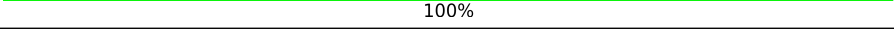

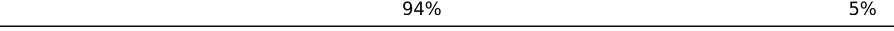
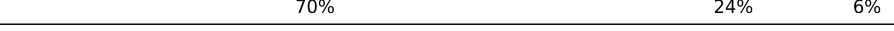
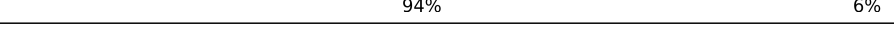

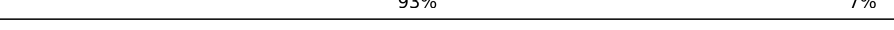

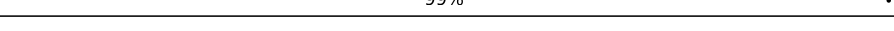


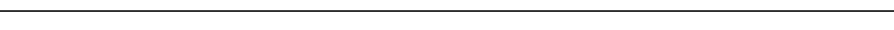

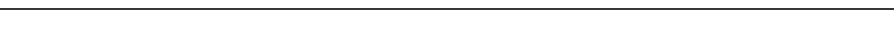
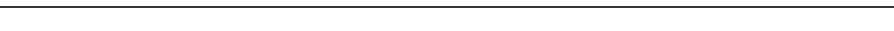


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	
1	b	215	
2	2	261	
2	i	261	
3	3	205	
3	h	205	
4	4	198	
4	g	198	
5	5	287	












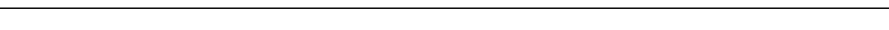
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Mol	Chain	Length	Quality of chain
5	f	287	 74%26%
6	6	241	 78%15%8%
6	e	241	 92%8%
7	7	266	 67%20%14%
7	a	266	 87%13%
8	A	252	 73%23%.
8	c	252	 96%.
9	B	250	 72%28%
9	j	250	 100%
10	C	258	 73%21%5%
10	d	258	 94%5%
11	D	254	 70%24%6%
11	n	254	 94%6%
12	E	260	 74%19%7%
12	m	260	 93%7%
13	F	234	 74%26%
13	l	234	 99%.
14	G	288	 66%18%16%
14	k	288	 84%16%
15	H	467	 57%20%23%
16	I	437	 61%22%17%
17	J	405	 70%22%8%
18	K	428	 64%25%11%
19	L	437	 64%19%17%
20	M	434	 62%22%15%

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Mol	Chain	Length	Quality of chain
21	N	945	
22	O	393	
23	P	445	
24	Q	434	
25	R	429	
26	S	523	
27	T	274	
28	U	338	
29	V	306	
30	W	268	
31	X	156	
32	Y	89	
33	Z	993	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 106100 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	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
1	b	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
2	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	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	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
4	g	195	Total	C	N	O	S	0	0
			1561	992	264	299	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	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		
7	a	232	Total	C	N	O	S	0	0
			1815	1148	311	349	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
8	c	241	Total	C	N	O	S	0	0
			1907	1214	320	365	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	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
11	n	240	Total	C	N	O	S	0	0
			1881	1176	329	372	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	231	Total	C	N	O	S	0	0
			1773	1114	307	348	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
			1892	1203	329	356	4		
14	k	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	359	Total	C	N	O	S	0	0
			2792	1755	499	523	15		

- 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	361	Total	C	N	O	S	0	0
			2853	1798	507	536	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	284	Total	C	N	O	S	0	0
			2236	1405	381	436	14		

- 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.

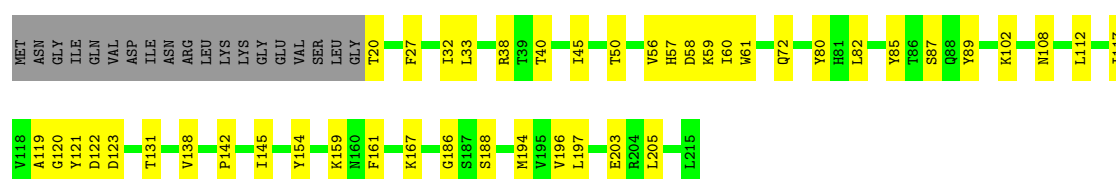
Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	813	Total	C	N	O	S	0	0
			6290	3995	1029	1237	29		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

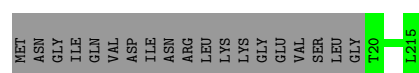
- Molecule 1: Proteasome subunit beta type-1

Chain 1: 



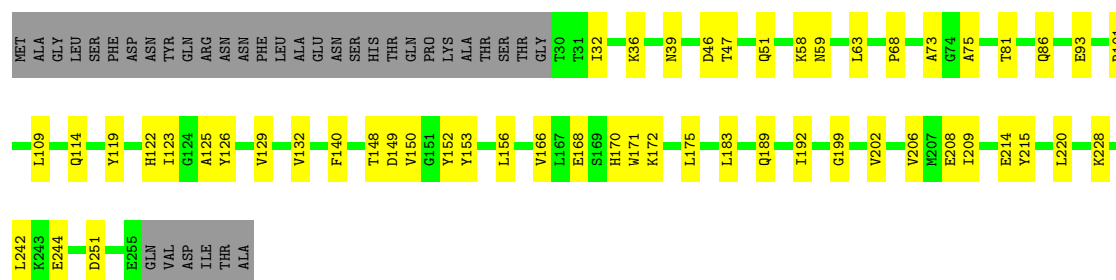
- Molecule 1: Proteasome subunit beta type-1

Chain b: 




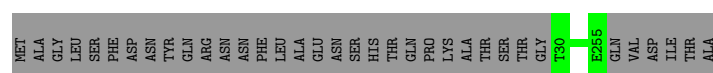
- Molecule 2: Proteasome subunit beta type-2

Chain 2: 



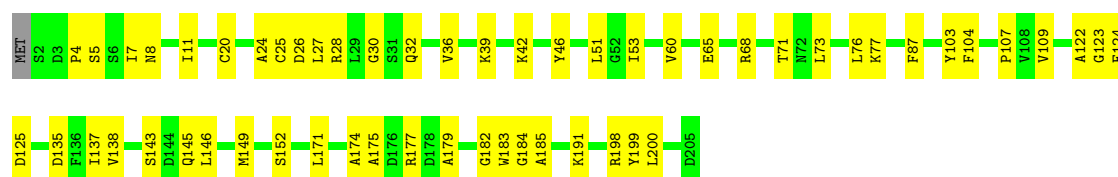
- Molecule 2: Proteasome subunit beta type-2

Chain i: 



- Molecule 3: Proteasome subunit beta type-3

Chain 3: 



- Molecule 3: Proteasome subunit beta type-3

Chain h: 100%



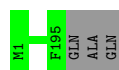
- Molecule 4: Proteasome subunit beta type-4

Chain 4: 78% 20%



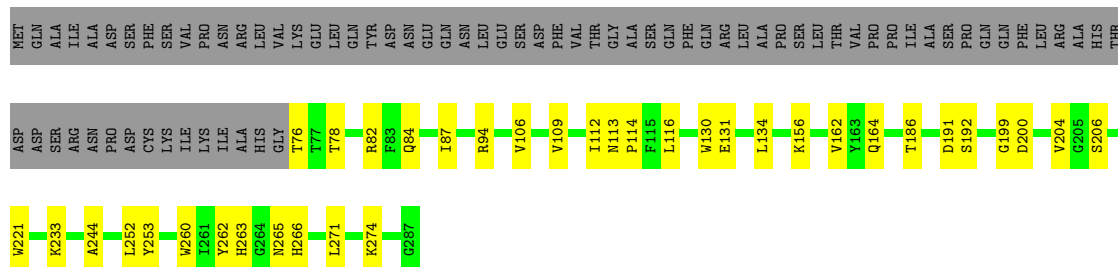
- Molecule 4: Proteasome subunit beta type-4

Chain g: 98%



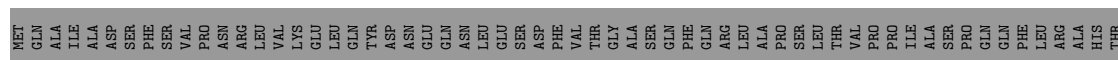
- Molecule 5: Proteasome subunit beta type-5

Chain 5: 61% 13% 26%



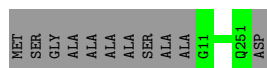
- Molecule 5: Proteasome subunit beta type-5

Chain f: 74% 26%



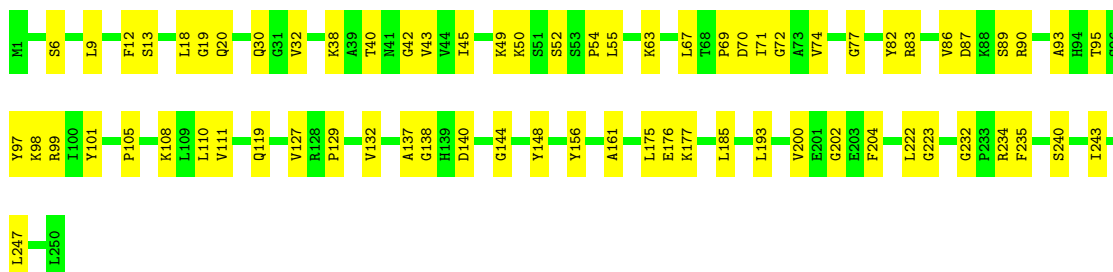


Chain c:  96%



- Molecule 9: Proteasome subunit alpha type-2

Chain B:  72% 28%



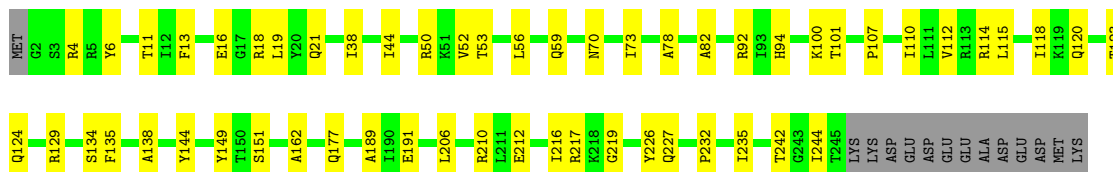
- Molecule 9: Proteasome subunit alpha type-2

Chain j:  100%

There are no outlier residues recorded for this chain.

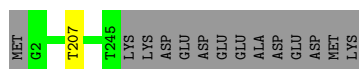
- Molecule 10: Proteasome subunit alpha type-3

Chain C:  73% 21% 5%



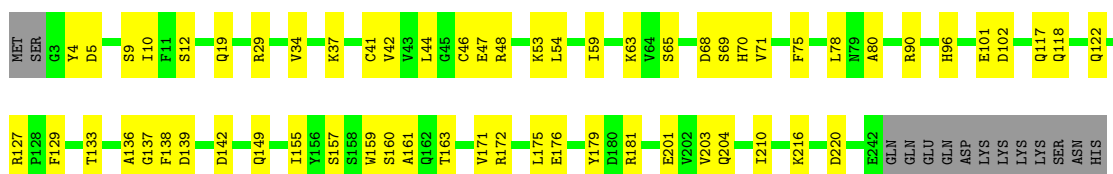
- Molecule 10: Proteasome subunit alpha type-3

Chain d:  94% 5%



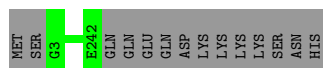
- Molecule 11: Proteasome subunit alpha type-4

Chain D:  70% 24% 6%



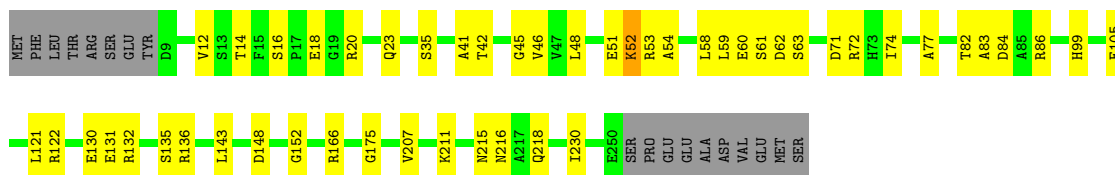
- Molecule 11: Proteasome subunit alpha type-4

Chain n:  94% 6%



- Molecule 12: Proteasome subunit alpha type-5

Chain E:  74% 19% 7%



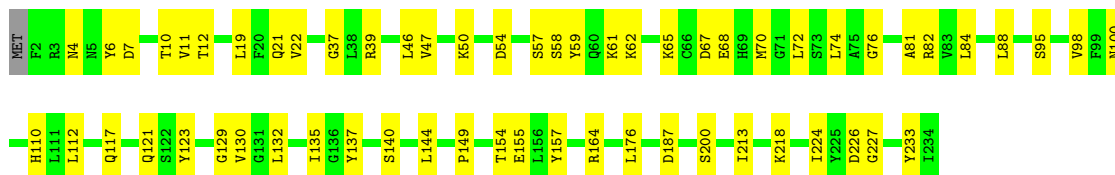
- Molecule 12: Proteasome subunit alpha type-5

Chain m:  93% 7%



- Molecule 13: Proteasome subunit alpha type-6

Chain F:  74% 26%



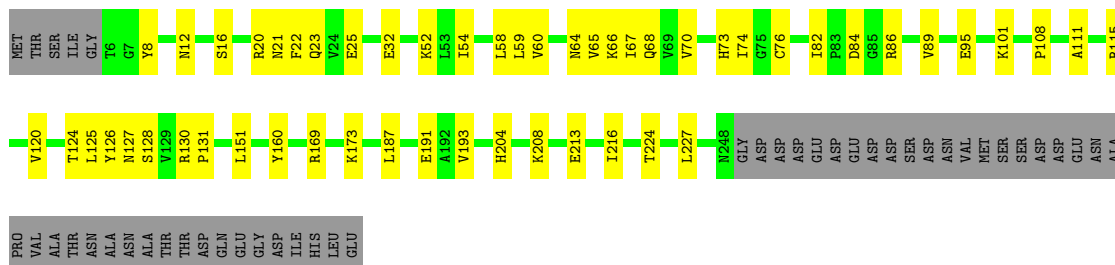
- Molecule 13: Proteasome subunit alpha type-6

Chain l:  99% .



- Molecule 14: Probable proteasome subunit alpha type-7

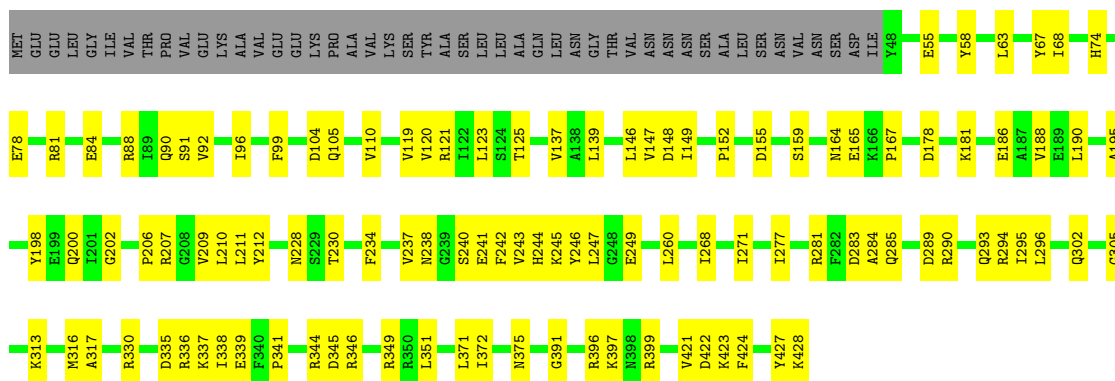
Chain G:  66% 18% 16%



- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|
| Met | Thr | Ala | Ala | Val | Thr | Thr | Ser | Ser | Asn | Ile | Ile | Val | Leu | Glu | Thr | His | Glu | Ser | Ser | Gly | Ile | Lys | Pro | Trp | Phe | E24 | I34 | R35 | T38 | R42 | R43 | L44 | E61 | S70 | V79 | S90 | D81 | L85 | K93 | V96 | D97 | Q111 | R116 | S117 | D118 | M121 | N128 | V134 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|

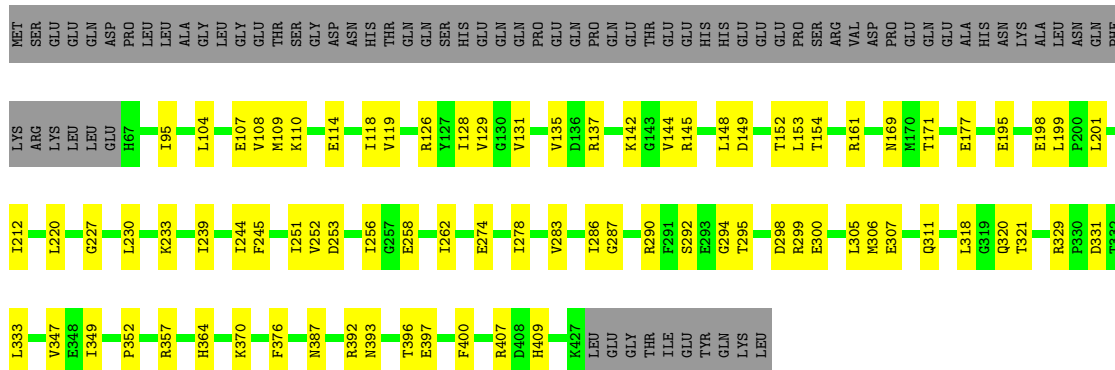
- Molecule 18: 26S protease regulatory subunit 6B homolog

Chain K:  64% 25% 11%



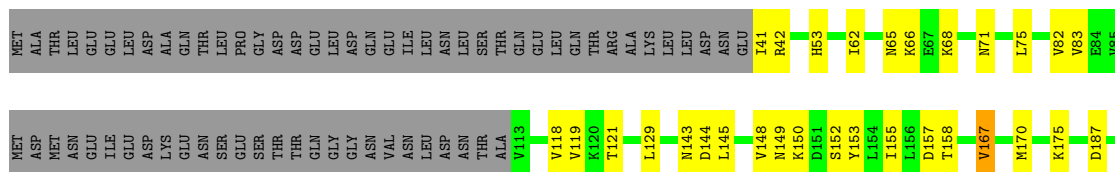
- Molecule 19: 26S protease subunit RPT4

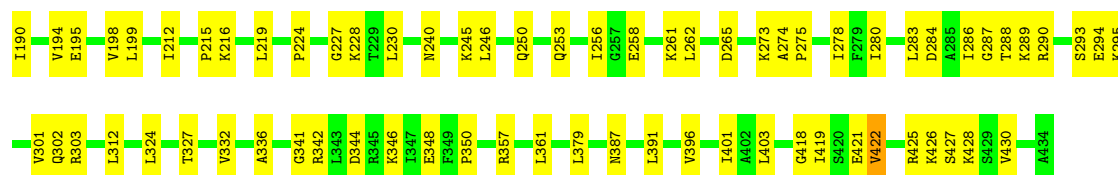
Chain L: 64% 19% 17%



- Molecule 20: 26S protease regulatory subunit 6A

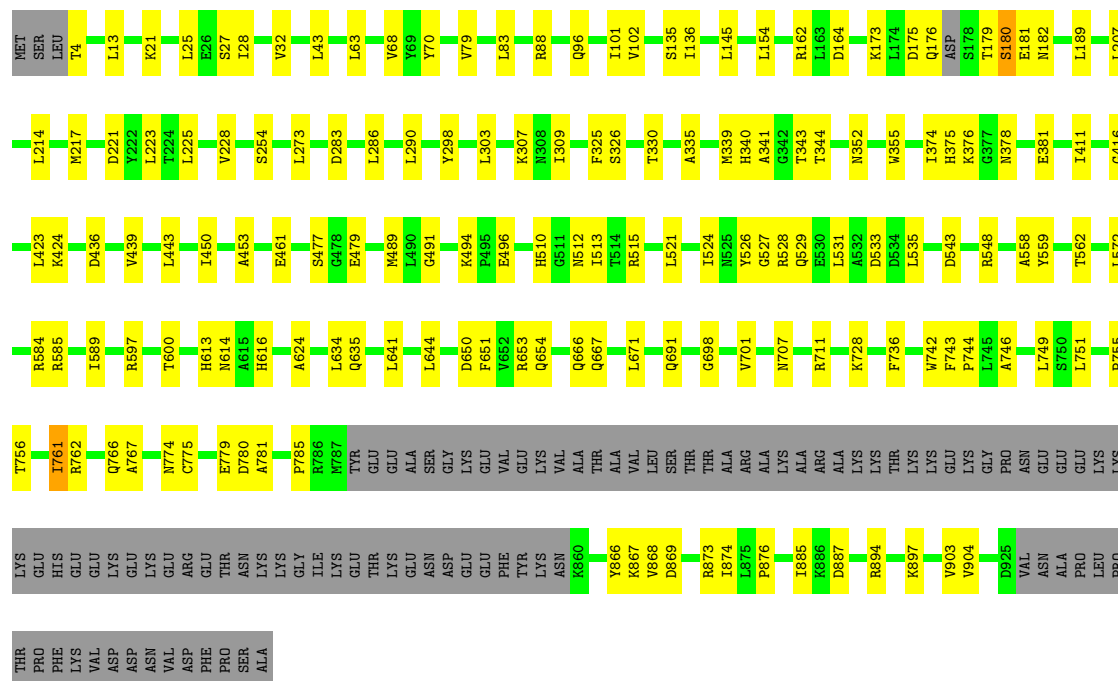
Chain M:  62% 22% 15%





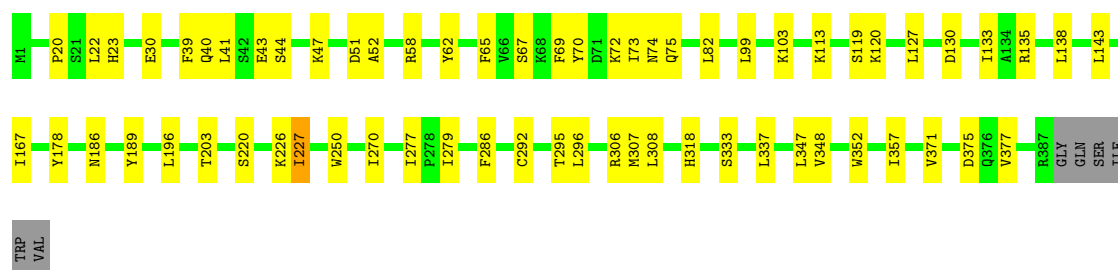
• Molecule 21: 26S proteasome regulatory subunit RPN2

Chain N: 73% 16% 10%



• Molecule 22: 26S proteasome regulatory subunit RPN9

Chain O: 82% 16% .

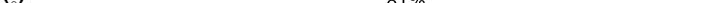


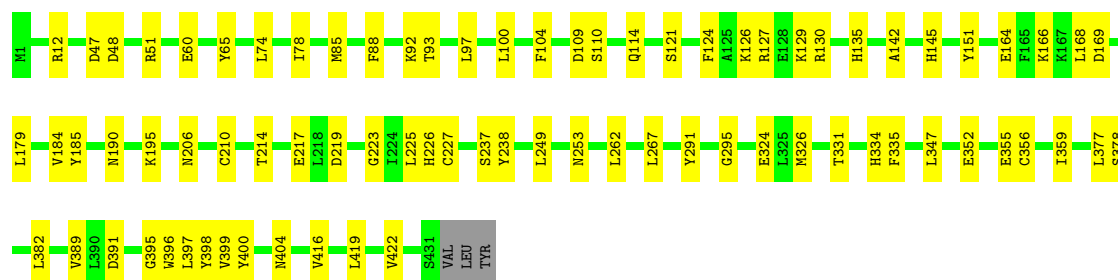
• Molecule 23: 26S proteasome regulatory subunit RPN5

Chain P: 83% 14% .



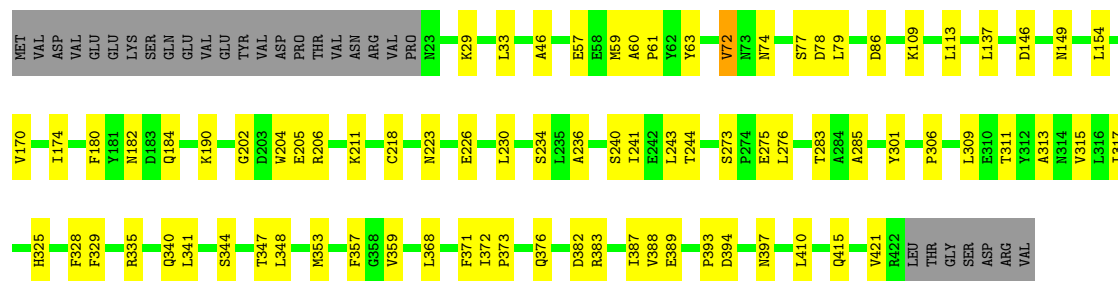
- Molecule 24: 26S proteasome regulatory subunit RPN6

Chain Q:  81% 18%



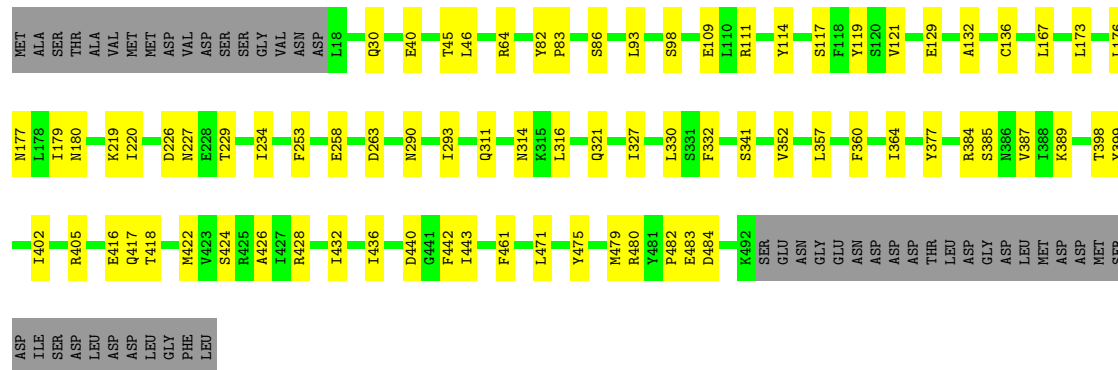
- Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R: 74% 19% 7%



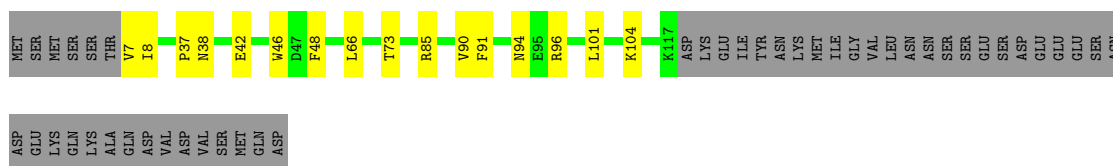
- Molecule 26: 26S proteasome regulatory subunit RPN3

Chain S:  76% 15% 9%



- Molecule 27: 26S proteasome regulatory subunit RPN12

Chain T: 81% 18%



- Molecule 32: 26S proteasome complex subunit SEM1

- Molecule 33: 26S proteasome regulatory subunit RPN1

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	6171	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	0/1541	0.41	0/2087
1	b	0.23	0/1541	0.41	0/2087
10	C	0.23	0/1934	0.39	0/2618
10	d	0.23	0/1934	0.41	0/2618
11	D	0.23	0/1910	0.39	0/2586
11	n	0.23	0/1910	0.40	0/2586
12	E	0.23	0/1886	0.41	0/2541
12	m	0.25	0/1886	0.40	0/2541
13	F	0.23	0/1823	0.41	0/2463
13	l	0.23	0/1800	0.41	0/2433
14	G	0.24	0/1932	0.38	0/2609
14	k	0.24	0/1932	0.39	0/2609
15	H	0.27	1/2831 (0.0%)	0.40	0/3808
16	I	0.25	0/2869	0.42	0/3867
17	J	0.23	0/2964	0.39	0/3981
18	K	0.23	0/3062	0.40	0/4132
19	L	0.24	0/2896	0.39	0/3895
2	2	0.23	0/1750	0.40	0/2373
2	i	0.23	0/1750	0.41	0/2373
20	M	0.23	0/2903	0.40	0/3909
21	N	0.24	1/6670 (0.0%)	0.39	0/9023
22	O	0.23	0/3243	0.39	0/4374
23	P	0.22	0/3599	0.37	0/4854
24	Q	0.23	0/3527	0.38	0/4748
25	R	0.23	0/3272	0.38	0/4412
26	S	0.23	0/3966	0.37	0/5355
27	T	0.24	0/2279	0.40	0/3077
28	U	0.23	0/2087	0.37	0/2811
29	V	0.23	0/2271	0.43	0/3064
3	3	0.24	0/1611	0.40	0/2174
3	h	0.24	0/1611	0.40	0/2174
30	W	0.26	0/1557	0.43	0/2111
31	X	0.23	0/931	0.41	0/1262
32	Y	0.23	0/239	0.39	0/322

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
33	Z	0.26	1/6404 (0.0%)	0.40	0/8686
4	4	0.23	0/1589	0.39	0/2142
4	g	0.23	0/1589	0.39	0/2142
5	5	0.23	0/1681	0.39	0/2274
5	f	0.23	0/1681	0.39	0/2274
6	6	0.24	0/1795	0.39	0/2420
6	e	0.24	0/1795	0.40	0/2420
7	7	0.24	0/1821	0.41	0/2470
7	a	0.24	0/1846	0.42	0/2503
8	A	0.24	0/1945	0.39	0/2634
8	c	0.24	0/1945	0.38	0/2634
9	B	0.24	0/1952	0.40	0/2642
9	j	0.24	0/1952	0.39	0/2642
All	All	0.24	3/107912 (0.0%)	0.40	0/145760

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	Z	468	GLU	C-N	8.44	1.50	1.34
15	H	192	ASP	C-N	6.36	1.46	1.34
21	N	217	MET	C-N	6.12	1.45	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	1512	0	1478	33	0
1	b	1512	0	1478	0	0
2	2	1719	0	1716	39	0
2	i	1719	0	1716	0	0
3	3	1581	0	1571	41	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	1561	0	1569	28	0
4	g	1561	0	1569	0	0
5	5	1644	0	1592	28	0
5	f	1644	0	1592	0	0
6	6	1757	0	1708	25	0
6	e	1757	0	1708	0	0
7	7	1790	0	1790	33	0
7	a	1815	0	1818	0	0
8	A	1907	0	1901	43	0
8	c	1907	0	1901	0	0
9	B	1915	0	1929	52	0
9	j	1915	0	1929	0	0
10	C	1904	0	1901	46	0
10	d	1904	0	1901	0	0
11	D	1881	0	1892	54	0
11	n	1881	0	1892	0	0
12	E	1861	0	1836	43	0
12	m	1861	0	1836	0	0
13	F	1795	0	1797	45	0
13	l	1773	0	1775	0	0
14	G	1892	0	1883	44	0
14	k	1892	0	1883	0	0
15	H	2792	0	2879	66	0
16	I	2831	0	2881	70	0
17	J	2928	0	3057	63	0
18	K	3019	0	3084	84	0
19	L	2853	0	2926	58	0
20	M	2866	0	2938	73	0
21	N	6562	0	6625	101	0
22	O	3182	0	3207	42	0
23	P	3545	0	3629	36	0
24	Q	3471	0	3495	48	0
25	R	3218	0	3216	53	0
26	S	3894	0	3938	56	0
27	T	2235	0	2207	35	0
28	U	2061	0	2116	54	0
29	V	2236	0	2242	64	0
30	W	1534	0	1542	28	0
31	X	906	0	888	10	0
32	Y	236	0	203	9	0
33	Z	6290	0	6236	81	0
All	All	106100	0	106441	1348	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 8.

All (1348) 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)
28:U:210:TYR:HH	28:U:223:HIS:N	1.59	0.99
21:N:510:HIS:HB3	21:N:513:ILE:HB	1.48	0.93
27:T:103:SER:HB2	27:T:142:LEU:HD23	1.53	0.89
21:N:742:TRP:HD1	29:V:61:TYR:HH	1.27	0.82
27:T:107:SER:HB3	27:T:142:LEU:HD13	1.62	0.81
27:T:141:LEU:O	27:T:142:LEU:HG	1.83	0.79
12:E:20:ARG:HG3	20:M:426:LYS:HD3	1.65	0.79
21:N:221:ASP:HA	21:N:894:ARG:HH22	1.49	0.77
12:E:60:GLU:OE1	12:E:63:SER:HB2	1.86	0.75
20:M:421:GLU:HG2	20:M:422:VAL:H	1.53	0.74
25:R:393:PRO:HB2	25:R:397:ASN:H	1.52	0.74
4:4:29:LYS:HD3	5:5:199:GLY:HA2	1.69	0.74
6:6:78:ALA:HB2	7:7:167:GLY:HA3	1.69	0.74
18:K:289:ASP:HA	19:L:299:ARG:HH21	1.53	0.72
19:L:290:ARG:NH2	19:L:292:SER:OG	2.23	0.72
1:1:20:THR:N	1:1:188:SER:HG	1.88	0.72
19:L:171:THR:HB	19:L:245:PHE:HB3	1.70	0.72
21:N:528:ARG:HB3	21:N:531:LEU:HB2	1.72	0.72
27:T:103:SER:HB2	27:T:142:LEU:CD2	2.20	0.71
25:R:359:VAL:HA	32:Y:81:LEU:HD22	1.73	0.71
18:K:244:HIS:O	19:L:299:ARG:NH1	2.24	0.71
30:W:162:ASN:HA	30:W:168:THR:HG21	1.73	0.70
17:J:79:VAL:HG12	17:J:81:ASP:H	1.56	0.70
33:Z:453:LEU:HB2	33:Z:488:ALA:HB1	1.73	0.70
11:D:37:LYS:HE2	11:D:160:SER:HA	1.73	0.70
21:N:512:ASN:ND2	29:V:61:TYR:CE2	2.60	0.70
33:Z:784:SER:O	33:Z:826:ARG:NH1	2.25	0.69
15:H:203:LYS:HE2	15:H:268:ASP:HB3	1.75	0.69
18:K:188:VAL:HG22	18:K:313:LYS:HE2	1.73	0.69
21:N:666:GLN:HA	21:N:873:ARG:HH21	1.57	0.69
17:J:252:SER:HB2	17:J:295:ASN:H	1.56	0.69
11:D:5:ASP:O	11:D:19:GLN:NE2	2.26	0.69
33:Z:914:LEU:H	33:Z:980:VAL:HG22	1.58	0.68
1:1:40:THR:HG22	1:1:45:ILE:HG12	1.74	0.68
11:D:118:GLN:HE22	12:E:86:ARG:HB2	1.59	0.68
12:E:77:ALA:HB3	12:E:143:LEU:HB2	1.76	0.68
15:H:217:GLN:HE21	15:H:378:SER:H	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:188:LEU:HB3	29:V:192:LEU:HA	1.76	0.68
8:A:46:ARG:HH21	8:A:167:LYS:HA	1.58	0.68
25:R:313:ALA:HA	25:R:317:ILE:HD12	1.76	0.68
1:1:80:TYR:HB2	8:A:102:ALA:HB1	1.76	0.67
2:2:58:LYS:NZ	3:3:135:ASP:OD2	2.27	0.67
19:L:253:ASP:HB3	20:M:293:SER:HB2	1.76	0.67
17:J:164:ILE:HG12	17:J:289:LYS:HE2	1.76	0.67
22:O:357:ILE:HB	28:U:223:HIS:HB2	1.77	0.67
16:I:387:LEU:HD23	16:I:391:ASP:HB3	1.76	0.66
17:J:335:MET:HA	18:K:202:GLY:HA3	1.76	0.66
9:B:176:GLU:HA	10:C:56:LEU:HD21	1.76	0.66
11:D:181:ARG:HH12	12:E:60:GLU:HA	1.59	0.66
19:L:195:GLU:HA	19:L:199:LEU:HD13	1.77	0.66
25:R:348:LEU:HB2	25:R:388:VAL:HB	1.77	0.66
24:Q:85:MET:HG3	24:Q:126:LYS:HG2	1.76	0.66
31:X:38:ASN:HD22	31:X:42:GLU:H	1.43	0.66
12:E:18:GLU:OE1	20:M:426:LYS:NZ	2.23	0.66
33:Z:284:LEU:HB3	33:Z:293:MET:HB3	1.77	0.66
3:3:5:SER:HB2	3:3:104:PHE:HB3	1.78	0.66
18:K:246:TYR:HB2	19:L:256:ILE:HG12	1.77	0.66
21:N:711:ARG:NH2	21:N:781:ALA:O	2.27	0.66
9:B:40:THR:HG22	9:B:45:ILE:HG12	16.54	0.66
24:Q:93:THR:H	24:Q:129:LYS:HG2	1.61	0.66
16:I:174:ASP:HB3	16:I:244:PHE:HB3	1.78	0.65
30:W:85:LEU:HD21	30:W:118:ILE:HG12	1.77	0.65
8:A:144:VAL:HG12	8:A:154:ILE:HG12	1.78	0.65
17:J:221:LYS:HB2	18:K:247:LEU:H	1.61	0.65
17:J:258:VAL:O	18:K:293:GLN:NE2	2.30	0.65
3:3:27:LEU:HB3	3:3:39:LYS:HA	1.77	0.65
21:N:207:LEU:HB3	21:N:228:VAL:HG13	1.78	0.65
1:1:57:HIS:HB3	1:1:60:ILE:HB	1.77	0.65
31:X:91:PHE:H	31:X:96:ARG:HD3	1.61	0.65
6:6:174:ASN:HB3	6:6:176:LYS:HE2	1.79	0.65
19:L:129:VAL:HG12	19:L:153:LEU:HB3	1.78	0.65
16:I:294:SER:HB3	16:I:300:ARG:HG3	1.78	0.65
21:N:83:LEU:HD11	21:N:136:ILE:HG13	1.79	0.64
21:N:307:LYS:HD3	21:N:343:THR:HG21	1.78	0.64
28:U:105:LYS:O	30:W:60:ARG:NH2	2.29	0.64
16:I:218:GLY:HA3	16:I:344:ILE:HG12	1.78	0.64
26:S:173:LEU:O	26:S:177:ASN:ND2	2.31	0.64
28:U:283:ARG:HB2	29:V:287:THR:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:82:ARG:HH11	5:5:186:THR:HA	1.62	0.64
29:V:60:ASP:O	29:V:61:TYR:HB2	1.98	0.64
18:K:123:LEU:H	18:K:146:LEU:HD23	1.61	0.64
18:K:155:ASP:OD2	19:L:142:LYS:NZ	2.31	0.64
12:E:52:LYS:HE2	12:E:218:GLN:HB2	1.78	0.64
11:D:163:THR:HG21	11:D:171:VAL:HB	1.79	0.64
16:I:401:LEU:HD11	17:J:162:GLU:HB3	1.80	0.64
20:M:253:GLN:HG3	20:M:258:GLU:HG3	1.79	0.64
2:2:51:GLN:NE2	3:3:125:ASP:OD2	2.31	0.64
13:F:155:GLU:H	14:G:64:ASN:HD21	1.46	0.63
21:N:96:GLN:HG3	26:S:220:ILE:HG12	1.80	0.63
33:Z:865:ASP:O	33:Z:909:ARG:NH1	2.29	0.63
7:7:161:ARG:HE	7:7:169:THR:HB	1.62	0.63
18:K:397:LYS:HB3	18:K:399:ARG:HH11	1.63	0.63
19:L:407:ARG:HG2	19:L:409:HIS:H	1.63	0.63
3:3:175:ALA:HB1	3:3:182:GLY:HA2	1.80	0.63
8:A:119:LYS:HE3	9:B:83:ARG:HD2	1.80	0.63
13:F:67:ASP:HB3	13:F:70:MET:HB3	1.80	0.63
21:N:494:LYS:HE2	21:N:496:GLU:HB3	1.81	0.63
7:7:87:SER:HB3	7:7:146:ALA:HB3	1.80	0.63
10:C:18:ARG:NH1	16:I:435:LEU:O	2.29	0.63
17:J:189:GLY:HA3	17:J:316:PHE:HB3	1.79	0.63
27:T:194:GLU:OE1	27:T:224:ARG:NH2	2.31	0.63
18:K:244:HIS:CE1	18:K:249:GLU:HB3	2.34	0.63
20:M:219:LEU:HD23	20:M:346:LYS:HG2	1.81	0.63
25:R:373:PRO:HB2	32:Y:64:TRP:HZ3	1.64	0.63
22:O:186:ASN:HB3	22:O:226:LYS:HD2	1.80	0.62
21:N:654:GLN:HG3	21:N:698:GLY:HA3	1.81	0.62
4:4:184:VAL:HG22	4:4:189:ILE:HG12	1.81	0.62
11:D:10:ILE:HG22	11:D:12:SER:H	1.65	0.62
21:N:273:LEU:HB3	21:N:290:LEU:HD13	1.80	0.62
21:N:584:ARG:NH1	21:N:614:ASN:OD1	2.32	0.62
21:N:736:PHE:HB2	21:N:749:LEU:HD11	1.80	0.62
25:R:113:LEU:HD22	25:R:137:LEU:HD13	1.81	0.62
3:3:145:GLN:HE22	3:3:177:ARG:HB2	1.65	0.62
3:3:28:ARG:NH1	3:3:179:ALA:O	2.33	0.62
15:H:96:PRO:HB3	15:H:191:ILE:HG21	1.82	0.62
16:I:195:LYS:HG3	16:I:199:GLU:HB3	1.82	0.62
14:G:224:THR:HB	14:G:227:LEU:HB2	1.80	0.62
17:J:160:ILE:HG23	17:J:164:ILE:HD12	1.80	0.62
21:N:562:THR:HA	21:N:597:ARG:HE	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:394:ASP:O	25:R:397:ASN:ND2	2.32	0.62
33:Z:577:GLN:HB3	33:Z:580:GLN:HB2	1.82	0.62
16:I:198:VAL:HG13	16:I:323:LYS:HG3	1.81	0.62
9:B:50:LYS:NZ	18:K:427:TYR:OH	2.33	0.62
19:L:352:PRO:O	19:L:357:ARG:NH1	2.32	0.62
22:O:73:ILE:HD12	30:W:17:ARG:HH11	1.64	0.62
5:5:94:ARG:NH1	5:5:244:ALA:O	2.33	0.62
20:M:246:LEU:HD12	20:M:280:ILE:HG12	1.80	0.62
5:5:76:THR:N	5:5:206:SER:HG	1.98	0.62
10:C:4:ARG:NH2	10:C:6:TYR:OH	2.33	0.62
21:N:510:HIS:CB	21:N:513:ILE:HD12	2.30	0.62
26:S:314:ASN:HB3	26:S:332:PHE:HZ	1.65	0.62
33:Z:802:ASP:HB3	33:Z:807:VAL:HG21	1.81	0.62
6:6:74:ASN:HB3	6:6:127:HIS:HB3	1.80	0.62
21:N:341:ALA:HA	21:N:374:ILE:HA	1.82	0.62
21:N:780:ASP:HB3	21:N:873:ARG:HD3	1.82	0.62
26:S:389:LYS:NZ	26:S:422:MET:O	2.32	0.62
8:A:72:ILE:HG12	8:A:82:VAL:HG22	1.82	0.61
27:T:193:THR:HA	27:T:197:TYR:HB3	1.82	0.61
1:1:145:ILE:HD11	1:1:154:TYR:HD1	1.65	0.61
21:N:728:LYS:HB3	21:N:751:LEU:HB3	1.82	0.61
28:U:32:ARG:NH2	28:U:58:GLU:OE2	2.31	0.61
19:L:393:ASN:ND2	20:M:344:ASP:OD2	2.32	0.61
33:Z:539:ASN:H	33:Z:577:GLN:HE22	1.45	0.61
13:F:81:ALA:HB2	13:F:130:VAL:HG21	1.82	0.61
17:J:277:ASN:HB2	17:J:309:ARG:HE	1.64	0.61
7:7:107:ASN:HD21	7:7:119:ALA:HA	1.66	0.61
10:C:44:ILE:HB	10:C:216:ILE:HD12	1.81	0.61
26:S:480:ARG:HD2	26:S:483:GLU:HB2	1.81	0.61
16:I:290:LYS:HD2	16:I:303:GLN:HG2	1.82	0.61
19:L:252:VAL:HG13	19:L:300:GLU:HB2	1.82	0.61
20:M:227:GLY:HA2	20:M:230:LEU:HB2	1.83	0.61
22:O:30:GLU:OE2	22:O:58:ARG:NH1	2.34	0.61
10:C:124:GLN:NE2	11:D:127:ARG:O	2.34	0.61
15:H:225:VAL:HA	15:H:350:LYS:HE2	1.82	0.61
21:N:867:LYS:HG2	21:N:868:VAL:HG23	1.83	0.61
10:C:11:THR:HA	11:D:127:ARG:HB2	1.81	0.61
16:I:388:SER:OG	17:J:306:ARG:NH1	2.33	0.61
21:N:742:TRP:HD1	29:V:61:TYR:OH	1.83	0.61
27:T:142:LEU:HD12	27:T:142:LEU:O	2.01	0.61
17:J:297:LEU:HD21	17:J:302:PRO:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:339:ARG:NH2	25:R:205:GLU:OE1	2.32	0.60
28:U:167:GLU:HG3	29:V:35:LEU:HD11	1.82	0.60
20:M:425:ARG:HG2	20:M:426:LYS:H	1.65	0.60
4:4:146:HIS:O	4:4:149:ARG:NH1	2.31	0.60
14:G:52:LYS:HE3	14:G:59:LEU:HD21	1.84	0.60
22:O:74:ASN:OD1	22:O:75:GLN:N	2.35	0.60
33:Z:117:ASP:OD1	33:Z:138:ARG:NH1	2.34	0.60
22:O:70:TYR:HD1	22:O:75:GLN:HB3	1.67	0.60
33:Z:915:ALA:HB2	33:Z:957:LEU:HG	1.82	0.60
3:3:76:LEU:O	10:C:92:ARG:NH1	2.34	0.60
16:I:423:VAL:HA	16:I:427:LYS:HB2	1.83	0.60
23:P:90:LYS:HG3	23:P:129:LYS:HB3	1.84	0.60
27:T:164:LEU:O	27:T:170:ASN:ND2	2.34	0.60
9:B:93:ALA:HB1	9:B:105:PRO:HG2	1.82	0.60
17:J:336:ASN:ND2	18:K:200:GLN:O	2.35	0.60
11:D:68:ASP:HB3	11:D:71:VAL:HB	1.83	0.60
17:J:188:TYR:HB2	17:J:315:GLU:HA	1.83	0.60
10:C:78:ALA:HB3	10:C:134:SER:HB3	1.83	0.60
12:E:71:ASP:HB3	12:E:74:ILE:HB	1.83	0.60
23:P:141:LYS:HE2	23:P:182:GLU:HG3	1.83	0.60
24:Q:355:GLU:HB2	24:Q:399:VAL:HG22	1.82	0.60
2:2:192:ILE:HG12	2:2:199:GLY:HA2	1.84	0.60
3:3:46:TYR:HB3	3:3:71:THR:HG21	1.84	0.60
14:G:120:VAL:HG21	14:G:151:LEU:HD21	1.83	0.60
16:I:110:GLU:HB2	16:I:119:ILE:HB	1.84	0.60
29:V:23:THR:HG21	29:V:171:ARG:HE	1.67	0.60
33:Z:133:ASP:OD1	33:Z:136:ARG:NH2	2.34	0.60
28:U:38:LEU:HB2	28:U:50:ASN:HB3	1.84	0.59
2:2:172:LYS:H	2:2:175:LEU:HD11	1.67	0.59
16:I:428:VAL:HG13	17:J:305:LEU:HD13	1.83	0.59
19:L:169:ASN:OD1	20:M:302:GLN:NE2	2.34	0.59
19:L:295:THR:OG1	19:L:298:ASP:O	2.20	0.59
4:4:29:LYS:HE3	4:4:31:SER:HB2	1.84	0.59
18:K:289:ASP:HA	19:L:299:ARG:NH2	2.16	0.59
33:Z:225:LEU:HD13	33:Z:256:LEU:HB2	1.84	0.59
3:3:138:VAL:HG11	3:3:146:LEU:HB2	1.85	0.59
10:C:44:ILE:H	10:C:216:ILE:HB	1.67	0.59
20:M:295:LYS:HB3	20:M:302:GLN:HB2	1.83	0.59
21:N:489:MET:HB3	21:N:524:ILE:HG13	1.84	0.59
22:O:40:GLN:O	22:O:58:ARG:NH2	2.29	0.59
4:4:149:ARG:HB2	4:4:152:MET:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:335:ALA:HB2	21:N:701:VAL:HA	1.85	0.59
25:R:306:PRO:HA	25:R:309:LEU:HD13	1.84	0.59
25:R:33:LEU:O	25:R:74:ASN:ND2	2.35	0.59
29:V:221:TRP:NE1	29:V:223:SER:OG	2.36	0.59
33:Z:574:TYR:HB2	33:Z:581:VAL:HG12	1.83	0.59
8:A:46:ARG:HD3	8:A:154:ILE:HG13	1.84	0.59
11:D:161:ALA:HB1	11:D:175:LEU:HD23	1.85	0.59
26:S:327:ILE:HG21	32:Y:64:TRP:HE1	1.66	0.59
1:1:194:MET:HB2	1:1:205:LEU:HB2	1.85	0.59
5:5:82:ARG:NH2	5:5:199:GLY:O	2.36	0.59
10:C:216:ILE:HG12	10:C:227:GLN:HG2	1.85	0.59
11:D:149:GLN:NE2	11:D:157:SER:OG	2.36	0.59
14:G:68:GLN:HG3	14:G:89:VAL:HG11	1.85	0.59
9:B:222:LEU:HD13	9:B:232:GLY:HA2	1.85	0.59
18:K:90:GLN:HG2	18:K:147:VAL:HG13	1.84	0.59
23:P:392:LYS:HD2	23:P:401:ASN:HB2	1.85	0.59
16:I:147:VAL:HG12	16:I:159:VAL:HG23	1.85	0.59
24:Q:378:SER:HB2	25:R:344:SER:HB2	1.85	0.59
27:T:79:GLU:O	27:T:83:ASN:ND2	2.34	0.59
3:3:11:ILE:HD12	3:3:146:LEU:HD11	1.85	0.58
13:F:47:VAL:HG22	13:F:213:ILE:HG12	1.85	0.58
16:I:161:GLN:NE2	16:I:163:ASP:OD2	2.36	0.58
21:N:43:LEU:HD21	21:N:68:VAL:HG11	1.84	0.58
33:Z:257:PRO:HB2	33:Z:259:PRO:HD2	1.85	0.58
12:E:54:ALA:HA	12:E:59:LEU:HD23	1.85	0.58
25:R:218:CYS:HB3	25:R:223:ASN:HB2	1.85	0.58
28:U:50:ASN:OD1	28:U:51:SER:N	2.36	0.58
33:Z:352:LYS:HB3	33:Z:466:GLU:HG3	1.83	0.58
3:3:109:VAL:HB	3:3:122:ALA:HB3	1.85	0.58
10:C:217:ARG:HG2	10:C:219:GLY:H	1.68	0.58
11:D:155:ILE:HG22	12:E:82:THR:HB	1.84	0.58
15:H:168:ILE:HD12	15:H:174:VAL:HG11	1.85	0.58
23:P:66:LEU:HD13	23:P:75:LEU:HA	1.86	0.58
33:Z:116:ALA:HB3	33:Z:141:SER:HB2	1.84	0.58
6:6:74:ASN:OD1	6:6:75:GLY:N	2.35	0.58
24:Q:142:ALA:HA	24:Q:145:HIS:HD2	1.68	0.58
25:R:347:THR:HG22	25:R:389:GLU:HG2	1.84	0.58
2:2:153:TYR:OH	2:2:168:GLU:OE1	2.22	0.58
9:B:87:ASP:OD1	9:B:90:ARG:NH2	2.37	0.58
21:N:742:TRP:CD1	29:V:61:TYR:OH	2.53	0.58
3:3:77:LYS:O	9:B:108:LYS:NZ	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:215:ARG:HG2	7:7:247:VAL:HG13	1.86	0.58
11:D:118:GLN:NE2	12:E:83:ALA:O	2.36	0.58
7:7:131:THR:HG21	13:F:98:VAL:HG22	1.86	0.58
24:Q:92:LYS:HA	24:Q:129:LYS:HE2	1.85	0.58
25:R:223:ASN:HB3	25:R:226:GLU:HB2	1.86	0.58
32:Y:69:VAL:HG12	32:Y:70:ASP:H	1.69	0.58
14:G:193:VAL:HG13	14:G:216:ILE:HG21	1.84	0.58
20:M:195:GLU:HA	20:M:199:LEU:HD12	1.85	0.58
29:V:54:LEU:HB3	29:V:102:GLN:HB2	1.85	0.58
1:1:131:THR:HG21	7:7:68:ARG:HH21	1.67	0.57
10:C:177:GLN:HE22	11:D:53:LYS:HD3	1.69	0.57
17:J:196:THR:HG21	18:K:305:GLY:HA2	1.86	0.57
33:Z:76:LYS:NZ	33:Z:149:TRP:O	2.31	0.57
33:Z:330:ILE:HG22	33:Z:341:TYR:HB2	1.85	0.57
33:Z:87:LYS:HE2	33:Z:89:LEU:HB2	1.85	0.57
3:3:185:ALA:HB3	3:3:200:LEU:HB2	1.86	0.57
3:3:53:ILE:HG22	3:3:60:VAL:HG22	1.86	0.57
7:7:98:ARG:HD2	14:G:101:LYS:HA	1.86	0.57
20:M:286:ILE:HG22	20:M:301:VAL:HG13	1.84	0.57
29:V:147:VAL:HG12	29:V:149:GLY:H	1.68	0.57
9:B:119:GLN:NE2	10:C:82:ALA:O	2.37	0.57
17:J:273:LEU:HD13	17:J:304:LEU:HD21	1.85	0.57
27:T:98:GLU:HB2	27:T:101:LYS:HG2	1.85	0.57
11:D:9:SER:HA	12:E:136:ARG:HD2	1.86	0.57
19:L:252:VAL:O	20:M:293:SER:N	2.35	0.57
9:B:32:VAL:HG21	9:B:63:LYS:HZ3	1.70	0.57
20:M:148:VAL:HG12	20:M:155:ILE:HA	1.84	0.57
26:S:109:GLU:OE2	26:S:111:ARG:NE	2.34	0.57
6:6:50:THR:OG1	6:6:55:ASN:ND2	2.33	0.57
11:D:159:TRP:CZ3	12:E:59:LEU:HB2	2.40	0.57
13:F:164:ARG:O	13:F:200:SER:OG	2.22	0.57
18:K:207:ARG:NH2	18:K:302:GLN:O	2.36	0.57
10:C:120:GLN:NE2	10:C:123:THR:OG1	2.37	0.57
14:G:68:GLN:O	14:G:76:CYS:N	2.35	0.57
28:U:286:ILE:HG23	29:V:280:LEU:HG	1.87	0.57
16:I:319:ARG:NH2	33:Z:825:ALA:O	2.37	0.57
6:6:49:ILE:HG22	6:6:54:ILE:HA	1.87	0.57
16:I:249:GLY:HA3	16:I:284:ILE:HG12	1.87	0.57
33:Z:770:GLU:HG2	33:Z:773:ARG:HD2	1.86	0.57
1:1:38:ARG:HD2	1:1:45:ILE:HD13	1.86	0.57
2:2:123:ILE:HG22	2:2:125:ALA:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:232:ILE:HB	7:7:240:THR:HB	1.86	0.57
16:I:384:LYS:NZ	16:I:386:ASP:OD1	2.35	0.57
21:N:589:ILE:HA	21:N:624:ALA:HB2	1.87	0.57
24:Q:185:TYR:HB3	24:Q:190:ASN:HB3	1.87	0.57
15:H:246:ILE:HB	15:H:352:MET:HG2	1.86	0.56
21:N:666:GLN:HG2	21:N:873:ARG:HE	1.70	0.56
30:W:21:PHE:HB2	30:W:22:PRO:HD3	1.87	0.56
10:C:50:ARG:HH21	10:C:212:GLU:HG2	1.71	0.56
25:R:240:SER:HB3	25:R:243:LEU:HB2	1.87	0.56
21:N:70:TYR:HE2	26:S:219:LYS:HD2	1.71	0.56
3:3:138:VAL:HG12	3:3:143:SER:HB2	1.86	0.56
15:H:380:PRO:O	15:H:385:ARG:NH1	2.38	0.56
21:N:521:LEU:HB3	21:N:535:LEU:HD21	1.86	0.56
2:2:93:GLU:OE1	9:B:98:LYS:NZ	2.38	0.56
10:C:112:VAL:HG21	10:C:149:TYR:HD2	1.70	0.56
17:J:301:ASP:HB3	17:J:304:LEU:HG	1.86	0.56
20:M:421:GLU:HG2	20:M:422:VAL:N	2.19	0.56
26:S:417:GLN:HE22	27:T:208:LEU:HD23	1.69	0.56
2:2:129:VAL:HB	2:2:140:PHE:HB2	1.87	0.56
24:Q:164:GLU:HA	24:Q:168:LEU:HD12	1.86	0.56
26:S:227:ASN:HD22	26:S:263:ASP:HB2	1.69	0.56
33:Z:183:LYS:NZ	33:Z:292:ASP:OD2	2.39	0.56
8:A:156:LYS:NZ	8:A:158:ASP:OD1	2.38	0.56
14:G:54:ILE:HD11	14:G:213:GLU:HG3	1.87	0.56
15:H:453:GLY:O	16:I:347:LYS:NZ	2.37	0.56
22:O:352:TRP:HE1	28:U:235:LEU:HD13	1.69	0.56
11:D:34:VAL:HG22	11:D:163:THR:HG23	1.88	0.56
17:J:70:SER:H	18:K:119:VAL:H	1.53	0.56
23:P:259:PRO:O	23:P:263:HIS:ND1	2.30	0.56
24:Q:97:LEU:HB3	24:Q:130:ARG:HH21	1.71	0.56
2:2:101:ARG:NH1	8:A:110:TYR:OH	2.35	0.56
9:B:111:VAL:HG21	9:B:148:TYR:HD2	1.70	0.56
23:P:225:VAL:HG11	23:P:328:ALA:HB1	1.88	0.56
29:V:52:LEU:HD21	29:V:104:VAL:HG22	1.88	0.56
11:D:122:GLN:HA	12:E:136:ARG:HE	1.70	0.56
15:H:247:LEU:HD23	15:H:374:LYS:HG2	1.87	0.56
21:N:543:ASP:OD1	21:N:548:ARG:NH2	2.39	0.55
23:P:126:THR:O	23:P:136:ARG:NH2	2.38	0.55
27:T:131:LYS:HD3	27:T:134:LYS:HB2	1.89	0.55
11:D:201:GLU:O	11:D:204:GLN:NE2	2.34	0.55
21:N:223:LEU:HD11	21:N:897:LYS:HE3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:325:HIS:HB2	25:R:329:PHE:CE2	2.41	0.55
33:Z:769:ASN:OD1	33:Z:770:GLU:N	2.39	0.55
8:A:54:ILE:HG12	8:A:225:VAL:HG22	1.88	0.55
9:B:176:GLU:HB2	10:C:56:LEU:HD11	1.87	0.55
17:J:267:GLU:OE1	18:K:290:ARG:NH1	2.39	0.55
31:X:91:PHE:HB3	31:X:94:ASN:HD22	1.70	0.55
9:B:13:SER:HB2	9:B:18:LEU:HD23	1.88	0.55
8:A:17:THR:HG23	8:A:27:GLN:HG3	1.89	0.55
19:L:290:ARG:HH21	19:L:294:GLY:H	1.53	0.55
23:P:137:ALA:HB2	23:P:167:THR:HG21	1.89	0.55
1:1:38:ARG:NH2	1:1:186:GLY:O	2.40	0.55
3:3:73:LEU:HD23	3:3:76:LEU:HD12	1.88	0.55
8:A:78:THR:H	8:A:233:PHE:HB2	1.72	0.55
19:L:109:MET:N	19:L:118:ILE:O	2.40	0.55
29:V:170:PRO:HB3	29:V:175:SER:OG	2.07	0.55
24:Q:223:GLY:HA2	24:Q:226:HIS:HD2	1.72	0.55
30:W:40:LYS:HE3	30:W:191:ILE:HG12	1.88	0.55
33:Z:225:LEU:HD21	33:Z:253:VAL:HA	1.89	0.55
33:Z:266:LYS:NZ	33:Z:290:GLU:OE1	2.40	0.55
14:G:73:HIS:ND1	14:G:74:ILE:HG13	2.22	0.55
18:K:209:VAL:HG23	18:K:336:ARG:HB2	1.89	0.55
18:K:84:GLU:HB3	18:K:88:ARG:HH12	1.72	0.55
19:L:329:ARG:HG2	19:L:331:ASP:H	1.71	0.55
24:Q:78:ILE:HG12	24:Q:100:LEU:HD13	1.88	0.55
7:7:187:LEU:HD11	7:7:216:VAL:HG11	1.90	0.54
20:M:82:VAL:HA	20:M:119:VAL:HA	1.88	0.54
11:D:44:LEU:HD11	11:D:136:ALA:HB3	1.89	0.54
30:W:11:ASP:HA	30:W:55:ALA:HB3	1.88	0.54
1:1:117:ILE:HG12	1:1:131:THR:HG23	1.90	0.54
2:2:228:LYS:NZ	3:3:152:SER:O	2.39	0.54
21:N:512:ASN:OD1	21:N:515:ARG:NH2	2.33	0.54
26:S:475:TYR:OH	28:U:295:LYS:N	2.41	0.54
10:C:206:LEU:HD23	10:C:244:ILE:HG21	1.88	0.54
16:I:209:GLU:OE2	16:I:319:ARG:NH1	2.41	0.54
20:M:312:LEU:HD13	20:M:342:ARG:HG2	1.90	0.54
25:R:325:HIS:HB3	25:R:328:PHE:HB2	1.88	0.54
25:R:382:ASP:HB3	25:R:387:ILE:H	1.73	0.54
22:O:306:ARG:NH2	28:U:234:ASN:OD1	2.41	0.54
6:6:47:ARG:NH1	6:6:215:ILE:O	2.35	0.54
11:D:41:CYS:HA	11:D:138:PHE:HZ	1.73	0.54
19:L:230:LEU:HD11	19:L:387:ASN:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:62:ILE:HG13	20:M:66:LYS:HG3	1.88	0.54
21:N:154:LEU:HD22	21:N:189:LEU:HD21	1.88	0.54
15:H:318:ARG:NH2	15:H:328:GLU:OE1	2.39	0.54
15:H:330:GLN:NE2	20:M:250:GLN:OE1	2.41	0.54
17:J:61:GLU:OE2	18:K:121:ARG:NH2	2.40	0.54
22:O:189:TYR:HE2	22:O:227:ILE:HB	1.72	0.54
24:Q:391:ASP:HB3	24:Q:396:TRP:H	1.73	0.54
28:U:210:TYR:OH	28:U:223:HIS:N	2.34	0.54
8:A:133:TYR:HD1	14:G:127:ASN:HB3	1.73	0.54
2:2:109:LEU:HD21	2:2:148:THR:HB	1.89	0.54
2:2:166:VAL:O	2:2:170:HIS:ND1	2.37	0.54
7:7:48:LYS:HG2	7:7:53:VAL:HG12	1.89	0.54
14:G:124:THR:HG22	14:G:131:PRO:HB3	1.89	0.54
17:J:225:GLU:OE2	17:J:228:ARG:NH2	2.40	0.54
9:B:177:LYS:NZ	24:Q:206:ASN:O	2.41	0.54
13:F:72:LEU:HD13	13:F:132:LEU:HD22	1.89	0.54
14:G:124:THR:HA	14:G:131:PRO:HG3	1.89	0.54
21:N:378:ASN:HD21	21:N:381:GLU:HB2	1.72	0.54
7:7:49:TYR:O	7:7:158:GLN:NE2	2.32	0.53
21:N:83:LEU:HD13	21:N:135:SER:HB3	1.90	0.53
21:N:653:ARG:NH1	21:N:691:GLN:OE1	2.41	0.53
25:R:240:SER:HB2	25:R:244:THR:HG22	1.90	0.53
28:U:13:LEU:HD21	29:V:36:LYS:HG2	1.90	0.53
22:O:377:VAL:HG13	28:U:197:LEU:HD22	1.90	0.53
25:R:57:GLU:OE1	25:R:109:LYS:NZ	2.34	0.53
17:J:185:VAL:HB	17:J:289:LYS:HZ1	1.72	0.53
18:K:188:VAL:HG12	18:K:230:THR:HG21	1.91	0.53
15:H:223:GLU:HG2	20:M:403:LEU:HD23	1.89	0.53
24:Q:227:CYS:HB3	24:Q:334:HIS:HE2	1.72	0.53
24:Q:51:ARG:HD2	24:Q:88:PHE:HA	1.91	0.53
23:P:432:LEU:HD13	28:U:225:ILE:HG13	1.89	0.53
33:Z:68:LEU:HD23	33:Z:71:LEU:HD12	1.91	0.53
1:1:87:SER:O	8:A:98:LYS:NZ	2.38	0.53
11:D:4:TYR:HD1	11:D:10:ILE:HG21	1.72	0.53
18:K:211:LEU:HB2	18:K:317:ALA:HA	1.91	0.53
22:O:286:PHE:HE1	22:O:337:LEU:HD23	1.73	0.53
23:P:248:ASP:HA	23:P:252:SER:HB3	1.90	0.53
25:R:182:ASN:OD1	25:R:184:GLN:NE2	2.42	0.53
25:R:204:TRP:HE1	25:R:234:SER:HA	1.74	0.53
3:3:28:ARG:HB2	3:3:183:TRP:HB2	1.90	0.53
15:H:313:ALA:HA	16:I:304:ARG:HE	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:359:VAL:HG12	32:Y:81:LEU:HD13	1.90	0.53
33:Z:301:THR:O	33:Z:307:HIS:NE2	2.38	0.53
29:V:57:PHE:HB2	29:V:63:VAL:HA	1.90	0.53
20:M:53:HIS:CE1	30:W:70:GLY:HA3	2.44	0.53
1:1:27:PHE:HE2	1:1:32:ILE:HG13	1.73	0.53
3:3:8:ASN:ND2	3:3:30:GLY:O	2.32	0.53
15:H:314:VAL:HG13	15:H:329:VAL:HG22	1.91	0.53
20:M:175:LYS:HE2	20:M:240:ASN:HB3	1.90	0.53
22:O:143:LEU:HD13	22:O:178:TYR:HA	1.88	0.53
24:Q:404:ASN:O	25:R:397:ASN:ND2	2.42	0.53
11:D:78:LEU:HG	11:D:80:ALA:H	1.73	0.53
28:U:38:LEU:HD13	28:U:87:GLU:HB3	1.91	0.53
33:Z:441:TYR:HA	33:Z:448:LYS:HE2	1.89	0.53
15:H:164:SER:OG	15:H:167:ASP:O	2.27	0.53
15:H:418:GLU:HG2	16:I:341:PRO:HG2	1.90	0.53
16:I:294:SER:HA	16:I:299:GLU:HA	1.91	0.53
20:M:216:LYS:HD3	20:M:341:GLY:HA2	1.90	0.53
26:S:311:GLN:NE2	26:S:341:SER:OG	2.42	0.53
26:S:482:PRO:HG2	28:U:301:ILE:HD13	1.90	0.53
9:B:45:ILE:HD12	9:B:74:VAL:HB	1.90	0.53
11:D:159:TRP:CH2	12:E:59:LEU:HB2	2.44	0.53
18:K:99:PHE:HA	18:K:110:VAL:HG12	1.91	0.53
21:N:742:TRP:CE3	21:N:743:PHE:HB3	2.44	0.53
24:Q:104:PHE:HB3	24:Q:114:GLN:HE21	1.73	0.53
26:S:136:CYS:HB3	26:S:179:ILE:HG21	1.91	0.53
4:4:8:ARG:HG3	4:4:13:VAL:HG22	1.91	0.52
10:C:50:ARG:NH1	10:C:59:GLN:O	2.37	0.52
11:D:122:GLN:O	12:E:135:SER:OG	2.27	0.52
24:Q:12:ARG:HH22	24:Q:60:GLU:HG3	1.74	0.52
8:A:48:LYS:HG2	8:A:53:VAL:HG12	15.26	0.52
12:E:122:ARG:NH1	12:E:131:GLU:O	2.42	0.52
16:I:330:LYS:HG2	16:I:332:GLU:H	1.74	0.52
1:1:59:LYS:HD3	1:1:121:TYR:HD2	1.74	0.52
12:E:71:ASP:OD1	12:E:72:ARG:N	2.43	0.52
19:L:118:ILE:HG12	19:L:128:ILE:HG12	1.92	0.52
21:N:145:LEU:O	21:N:173:LYS:NZ	2.38	0.52
21:N:176:GLN:HG2	21:N:182:ASN:ND2	2.24	0.52
3:3:65:GLU:OE2	3:3:68:ARG:NH1	2.42	0.52
13:F:176:LEU:HD13	14:G:58:LEU:HD23	1.91	0.52
20:M:290:ARG:NH2	20:M:294:GLU:OE2	2.39	0.52
9:B:95:THR:HA	9:B:99:ARG:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:385:ARG:NH1	15:H:413:ASN:OD1	2.42	0.52
10:C:18:ARG:HH22	16:I:437:LEU:HD22	1.74	0.52
1:1:89:TYR:HD1	14:G:111:ALA:HB1	1.74	0.52
2:2:206:VAL:HB	2:2:214:GLU:HB2	1.92	0.52
7:7:137:ARG:HA	7:7:142:PRO:HG3	1.92	0.52
10:C:162:ALA:HB3	11:D:54:LEU:HD13	1.90	0.52
13:F:67:ASP:OD1	13:F:68:GLU:N	2.43	0.52
13:F:154:THR:OG1	14:G:64:ASN:ND2	2.42	0.52
14:G:68:GLN:HB2	14:G:76:CYS:HB3	1.92	0.52
18:K:396:ARG:HA	19:L:195:GLU:HG3	1.92	0.52
24:Q:127:ARG:HA	24:Q:130:ARG:HB2	1.91	0.52
28:U:48:VAL:HG22	28:U:90:ILE:HD11	1.90	0.52
4:4:63:ASN:HD22	4:4:83:PHE:HZ	1.56	0.52
9:B:30:GLN:HG2	18:K:428:LYS:HA	1.92	0.52
9:B:50:LYS:HE3	18:K:424:PHE:CG	2.45	0.52
15:H:276:GLY:N	15:H:309:ASP:O	2.40	0.52
33:Z:588:ILE:HG12	33:Z:596:THR:HB	1.92	0.52
3:3:28:ARG:HG3	3:3:183:TRP:CE3	2.45	0.52
3:3:65:GLU:HB3	10:C:100:LYS:HG3	1.91	0.52
16:I:181:TYR:HB3	16:I:191:ILE:HD13	1.91	0.52
21:N:491:GLY:H	21:N:526:TYR:HB3	1.74	0.52
24:Q:416:VAL:HA	25:R:410:LEU:HD21	1.91	0.52
16:I:102:ASN:N	16:I:103:PRO:CD	2.73	0.52
16:I:293:ASP:OD1	16:I:294:SER:N	2.41	0.52
19:L:144:VAL:HA	19:L:161:ARG:HG2	1.91	0.52
19:L:177:GLU:HB2	19:L:233:LYS:HD3	1.92	0.52
22:O:67:SER:HA	22:O:113:LYS:HE3	1.92	0.52
10:C:44:ILE:HG21	10:C:138:ALA:HB1	1.92	0.52
13:F:121:GLN:NE2	14:G:84:ASP:OD1	2.43	0.52
24:Q:391:ASP:OD1	25:R:347:THR:OG1	2.27	0.52
28:U:94:HIS:CE1	28:U:122:ILE:HG12	2.45	0.52
29:V:27:VAL:HA	29:V:63:VAL:HG11	1.92	0.52
31:X:48:PHE:HB2	31:X:66:LEU:HB3	1.92	0.52
11:D:172:ARG:NH1	11:D:176:GLU:OE2	2.43	0.51
20:M:284:ASP:O	20:M:288:THR:OG1	2.21	0.51
20:M:62:ILE:HD12	20:M:65:ASN:HB2	1.93	0.51
23:P:361:THR:HG22	23:P:363:LEU:H	1.75	0.51
26:S:418:THR:OG1	27:T:158:GLN:OE1	2.26	0.51
2:2:46:ASP:HA	2:2:202:VAL:HA	1.90	0.51
11:D:216:LYS:HB2	11:D:220:ASP:HB3	1.92	0.51
20:M:144:ASP:OD1	20:M:145:LEU:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:R:273:SER:HB3	25:R:276:LEU:HB2	1.92	0.51
29:V:73:GLN:HE21	29:V:77:GLY:HA2	1.74	0.51
2:2:119:TYR:HB3	2:2:122:HIS:HB3	1.90	0.51
9:B:200:VAL:HG22	9:B:202:GLY:H	1.75	0.51
15:H:253:GLY:HA2	15:H:256:LYS:HE2	1.92	0.51
15:H:327:ASN:O	15:H:331:ARG:NH2	2.43	0.51
18:K:123:LEU:HG	18:K:125:THR:H	1.74	0.51
22:O:43:GLU:HA	22:O:82:LEU:HD21	1.93	0.51
26:S:417:GLN:HE22	27:T:208:LEU:HA	1.74	0.51
6:6:55:ASN:HB3	7:7:170:TYR:CZ	2.45	0.51
8:A:14:ARG:NE	14:G:8:TYR:OH	2.30	0.51
18:K:120:VAL:HG11	18:K:139:LEU:HD22	1.92	0.51
24:Q:419:LEU:HD22	25:R:410:LEU:HD23	1.93	0.51
30:W:132:LEU:HB3	30:W:137:VAL:HB	1.92	0.51
33:Z:964:GLU:HG3	33:Z:965:LEU:HG	1.91	0.51
18:K:104:ASP:OD1	18:K:105:GLN:N	2.42	0.51
18:K:195:ALA:HA	18:K:198:TYR:HD2	1.74	0.51
20:M:278:ILE:O	20:M:324:LEU:N	2.38	0.51
25:R:202:GLY:HA3	25:R:206:ARG:HD2	1.93	0.51
26:S:330:LEU:HD12	32:Y:65:ASP:H	1.75	0.51
33:Z:139:LEU:HD21	33:Z:161:ILE:HG21	1.92	0.51
2:2:149:ASP:OD1	2:2:150:VAL:N	2.43	0.51
6:6:220:GLY:HA2	6:6:237:GLU:HA	1.93	0.51
16:I:219:VAL:HB	16:I:325:ILE:HG12	1.91	0.51
16:I:282:ASP:OD1	16:I:283:GLU:N	2.44	0.51
17:J:85:LEU:HD11	17:J:93:LYS:HB3	1.93	0.51
18:K:210:LEU:HD12	18:K:337:LYS:HG2	1.93	0.51
19:L:149:ASP:OD2	19:L:152:THR:OG1	2.21	0.51
24:Q:121:SER:HB3	24:Q:126:LYS:HD2	1.93	0.51
29:V:50:MET:HG3	29:V:71:MET:HB2	1.93	0.51
1:1:61:TRP:HD1	1:1:197:LEU:HD11	1.76	0.51
12:E:35:SER:OG	12:E:51:GLU:O	2.21	0.51
14:G:70:VAL:N	14:G:74:ILE:O	2.44	0.51
17:J:336:ASN:HB3	17:J:376:HIS:ND1	2.25	0.51
19:L:107:GLU:HB2	19:L:145:ARG:HD3	1.93	0.51
19:L:227:GLY:HA3	19:L:349:ILE:HG21	1.92	0.51
20:M:262:LEU:HA	20:M:265:ASP:HB2	1.93	0.51
20:M:274:ALA:HB3	20:M:275:PRO:HD3	1.92	0.51
8:A:218:PHE:HB3	8:A:222:ASP:HB2	1.93	0.51
20:M:149:ASN:OD1	20:M:150:LYS:N	2.43	0.51
21:N:635:GLN:NE2	21:N:667:GLN:OE1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:75:GLN:NE2	22:O:119:SER:O	2.43	0.51
5:5:252:LEU:HB2	5:5:263:HIS:HB2	1.93	0.51
8:A:135:ARG:HB2	14:G:125:LEU:HD22	1.92	0.51
16:I:136:VAL:HB	16:I:140:LEU:HD12	1.92	0.51
17:J:116:ARG:HG2	17:J:118:ASP:H	1.76	0.51
17:J:251:ASP:OD1	17:J:253:ILE:HG12	2.10	0.51
28:U:265:LEU:HB3	28:U:268:LYS:HE2	1.93	0.51
1:1:196:VAL:HB	1:1:203:GLU:HB3	1.91	0.51
15:H:227:LEU:HD22	20:M:403:LEU:HD22	1.93	0.51
26:S:129:GLU:OE2	26:S:132:ALA:N	2.44	0.51
26:S:167:LEU:HD13	26:S:180:ASN:HD22	1.76	0.51
29:V:27:VAL:HA	29:V:63:VAL:CG1	2.41	0.51
20:M:71:ASN:HB3	29:V:75:GLY:HA3	1.93	0.51
2:2:63:LEU:HD12	2:2:215:TYR:HE1	1.75	0.50
4:4:92:ILE:HA	4:4:97:PRO:HB3	1.93	0.50
10:C:19:LEU:HG	10:C:21:GLN:H	1.76	0.50
12:E:48:LEU:HD23	12:E:77:ALA:HB2	1.92	0.50
15:H:147:ILE:HD11	15:H:157:VAL:HG23	1.93	0.50
15:H:217:GLN:NE2	15:H:378:SER:OG	2.44	0.50
19:L:131:VAL:HB	19:L:135:VAL:HG21	1.93	0.50
25:R:33:LEU:HB3	25:R:74:ASN:HD22	1.76	0.50
29:V:57:PHE:CB	29:V:63:VAL:HA	2.40	0.50
15:H:57:LYS:HA	15:H:61:ALA:HB3	1.93	0.50
16:I:347:LYS:HE2	16:I:349:LEU:HD21	1.94	0.50
18:K:152:PRO:HG2	18:K:260:LEU:HB2	1.93	0.50
18:K:423:LYS:HE3	18:K:424:PHE:CE2	2.47	0.50
16:I:205:PRO:HD2	33:Z:826:ARG:HH21	1.77	0.50
7:7:77:PRO:HA	7:7:83:VAL:HA	1.94	0.50
12:E:166:ARG:HB3	13:F:58:SER:HB3	1.94	0.50
23:P:388:ILE:HG22	23:P:389:ILE:HG23	1.94	0.50
28:U:276:ILE:HD13	29:V:294:SER:HB2	1.94	0.50
8:A:220:LYS:HD3	8:A:242:GLU:HB2	1.93	0.50
9:B:71:ILE:HG12	9:B:138:GLY:HA3	1.93	0.50
15:H:54:ASN:HB2	16:I:96:LEU:HD23	1.92	0.50
18:K:148:ASP:OD1	18:K:149:ILE:N	2.45	0.50
23:P:271:SER:OG	23:P:277:GLN:NE2	2.41	0.50
27:T:206:LYS:HG3	27:T:211:PHE:HB2	1.94	0.50
11:D:65:SER:HB3	11:D:90:ARG:HH21	1.76	0.50
33:Z:169:VAL:HG22	33:Z:195:PHE:HD1	1.75	0.50
2:2:114:GLN:HE22	8:A:107:LYS:HA	1.76	0.50
5:5:78:THR:OG1	5:5:204:VAL:O	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:277:SER:OG	16:I:308:GLU:OE1	2.26	0.50
33:Z:446:GLU:HG2	33:Z:484:LYS:HG3	1.93	0.50
8:A:14:ARG:HE	14:G:8:TYR:HH	1.55	0.50
9:B:70:ASP:HA	9:B:234:ARG:HB2	1.94	0.50
13:F:226:ASP:OD1	13:F:227:GLY:N	2.45	0.50
15:H:244:LYS:HZ2	15:H:346:ARG:HD3	1.76	0.50
18:K:295:ILE:HG13	18:K:296:LEU:HD12	1.93	0.50
27:T:200:LEU:HB2	27:T:233:VAL:HB	1.94	0.50
4:4:29:LYS:HE3	4:4:32:ASP:H	1.76	0.50
13:F:76:GLY:HA3	13:F:130:VAL:HA	1.94	0.50
16:I:132:ILE:HG12	16:I:156:ILE:HD12	1.94	0.50
18:K:371:LEU:O	18:K:375:ASN:ND2	2.34	0.50
20:M:41:ILE:HG23	20:M:42:ARG:HG2	1.92	0.50
21:N:303:LEU:HD21	21:N:755:PRO:HB3	1.94	0.50
23:P:89:LEU:HG	23:P:91:LEU:H	1.77	0.50
27:T:85:LEU:HD23	27:T:88:TYR:HD2	1.77	0.50
7:7:151:GLY:HA2	7:7:233:ILE:HG21	1.94	0.50
10:C:52:VAL:HG23	10:C:59:GLN:HE21	1.77	0.50
17:J:139:VAL:HG22	17:J:211:ILE:HG12	1.94	0.50
18:K:391:GLY:HA3	19:L:212:ILE:HG21	1.93	0.50
18:K:63:LEU:HG	21:N:572:LEU:HD22	1.94	0.50
26:S:290:ASN:OD1	26:S:321:GLN:NE2	2.45	0.50
28:U:19:LEU:HG	29:V:208:LYS:HD3	1.93	0.50
33:Z:812:ILE:HD12	33:Z:847:ILE:HG22	1.93	0.50
3:3:25:CYS:HB2	3:3:42:LYS:NZ	2.27	0.49
4:4:96:ARG:HH12	5:5:164:GLN:HA	1.77	0.49
15:H:157:VAL:O	15:H:182:ASN:ND2	2.45	0.49
18:K:423:LYS:HE3	18:K:424:PHE:HE2	1.76	0.49
22:O:23:HIS:HB2	22:O:65:PHE:HZ	1.77	0.49
26:S:357:LEU:HA	26:S:384:ARG:HH22	1.77	0.49
30:W:2:VAL:HG13	30:W:196:SER:HB2	1.93	0.49
31:X:85:ARG:HD2	31:X:101:LEU:HD12	1.94	0.49
33:Z:515:SER:OG	33:Z:521:GLU:OE1	2.30	0.49
4:4:33:ASP:OD1	4:4:34:LYS:N	2.45	0.49
9:B:6:SER:HB3	9:B:19:GLY:H	1.77	0.49
15:H:254:THR:HG21	15:H:415:THR:HB	1.93	0.49
18:K:283:ASP:OD1	18:K:284:ALA:N	2.44	0.49
24:Q:109:ASP:OD1	24:Q:110:SER:N	2.45	0.49
27:T:205:ILE:HD13	27:T:208:LEU:HD12	1.93	0.49
2:2:39:ASN:HB3	2:2:208:GLU:HG3	1.93	0.49
6:6:100:ASP:OD2	13:F:65:LYS:NZ	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Q:295:GLY:N	24:Q:324:GLU:OE1	2.44	0.49
27:T:126:LEU:O	27:T:130:ASP:N	2.44	0.49
11:D:96:HIS:HE1	11:D:102:ASP:HB2	1.77	0.49
15:H:365:LEU:HA	15:H:370:ARG:HH21	1.78	0.49
17:J:169:LYS:HE3	17:J:206:THR:HG22	1.95	0.49
22:O:196:LEU:HB2	22:O:203:THR:HG21	1.94	0.49
24:Q:47:ASP:OD1	24:Q:48:ASP:N	2.46	0.49
25:R:61:PRO:HG2	25:R:180:PHE:HZ	1.77	0.49
33:Z:347:ASN:HB3	33:Z:353:VAL:HG23	1.93	0.49
13:F:123:TYR:HB2	14:G:128:SER:HA	1.94	0.49
18:K:397:LYS:HB3	18:K:399:ARG:NH1	2.27	0.49
23:P:409:SER:HB3	23:P:412:LEU:HD12	1.94	0.49
24:Q:356:CYS:HA	24:Q:397:LEU:HB3	1.95	0.49
21:N:510:HIS:CD2	29:V:62:THR:OG1	2.66	0.49
7:7:48:LYS:HD2	7:7:173:PRO:HA	1.95	0.49
17:J:134:VAL:HG22	17:J:137:MET:HE2	1.95	0.49
17:J:160:ILE:HD11	17:J:198:LEU:HD21	1.94	0.49
17:J:230:VAL:HG11	17:J:272:MET:HA	1.93	0.49
18:K:244:HIS:HE1	18:K:249:GLU:HB3	1.76	0.49
18:K:245:LYS:HA	19:L:299:ARG:NH1	2.27	0.49
5:5:82:ARG:HH21	5:5:200:ASP:HA	1.77	0.49
17:J:220:GLN:HB2	17:J:225:GLU:HG3	1.95	0.49
11:D:46:CYS:SG	11:D:47:GLU:N	2.85	0.49
18:K:167:PRO:O	18:K:228:ASN:ND2	2.42	0.49
33:Z:323:TYR:HB3	33:Z:537:THR:HG22	1.95	0.49
1:1:102:LYS:HD3	1:1:138:VAL:HG23	1.94	0.49
5:5:82:ARG:HG2	5:5:87:ILE:HG12	1.94	0.49
6:6:79:ASP:HB3	6:6:124:TYR:HB3	1.94	0.49
10:C:191:GLU:HG2	10:C:242:THR:HG22	1.94	0.49
12:E:99:HIS:HE1	12:E:105:GLU:HB3	1.77	0.49
12:E:14:THR:HA	13:F:21:GLN:HE22	1.78	0.49
15:H:414:SER:HB3	15:H:418:GLU:HB2	1.94	0.49
16:I:417:LYS:HA	16:I:420:LYS:HE2	1.95	0.49
15:H:57:LYS:HD3	16:I:99:ILE:HG22	1.94	0.49
20:M:283:LEU:H	20:M:327:THR:HB	1.78	0.49
22:O:296:LEU:HD11	22:O:308:LEU:HB2	1.95	0.49
23:P:147:LYS:HB3	23:P:152:LYS:HB2	1.93	0.49
25:R:154:LEU:HD11	25:R:170:VAL:HG22	1.95	0.49
25:R:301:TYR:HE2	25:R:341:LEU:HB2	1.77	0.49
26:S:293:ILE:HD13	26:S:316:LEU:HD23	1.95	0.49
28:U:108:GLU:HB2	30:W:60:ARG:HH22	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:V:26:THR:O	29:V:63:VAL:HB	2.12	0.49
10:C:53:THR:HA	10:C:210:ARG:HE	1.78	0.49
13:F:46:LEU:HG	13:F:135:ILE:HD13	1.93	0.49
15:H:228:PRO:HB3	15:H:242:PRO:HG2	1.94	0.49
18:K:211:LEU:HD23	18:K:338:ILE:HB	1.95	0.49
23:P:323:ASN:OD1	23:P:338:TRP:NE1	2.46	0.49
24:Q:135:HIS:ND1	24:Q:169:ASP:OD2	2.45	0.48
25:R:372:ILE:HB	26:S:398:THR:HG22	1.94	0.48
25:R:415:GLN:HE21	26:S:471:LEU:HD21	1.78	0.48
26:S:436:ILE:HG12	26:S:443:ILE:HG12	1.94	0.48
5:5:253:TYR:HE1	5:5:262:TYR:HD1	1.61	0.48
6:6:76:PHE:CE2	6:6:78:ALA:HB3	2.48	0.48
17:J:42:ARG:NE	26:S:484:ASP:OD2	2.46	0.48
6:6:221:LEU:N	6:6:236:TYR:O	2.40	0.48
14:G:187:LEU:HD23	14:G:191:GLU:HB3	1.95	0.48
14:G:32:GLU:OE2	14:G:169:ARG:NH2	2.45	0.48
17:J:279:LEU:O	17:J:284:THR:N	2.45	0.48
28:U:259:ASN:HA	28:U:262:GLN:HB2	1.96	0.48
33:Z:857:LEU:HD11	33:Z:908:ILE:HD11	1.95	0.48
1:1:72:GLN:HE22	2:2:148:THR:H	1.61	0.48
10:C:144:TYR:HB3	11:D:59:ILE:HG22	1.95	0.48
12:E:41:ALA:HA	12:E:46:VAL:HG22	1.96	0.48
15:H:311:ILE:HG23	15:H:361:LEU:HD21	1.94	0.48
17:J:193:THR:OG1	17:J:255:SER:OG	2.31	0.48
20:M:427:SER:OG	20:M:428:LYS:N	2.40	0.48
23:P:429:ILE:HD11	28:U:203:LYS:HG2	1.94	0.48
30:W:109:ARG:HH22	30:W:195:GLY:HA3	1.78	0.48
4:4:36:ARG:HG3	4:4:57:ALA:HB1	1.95	0.48
11:D:68:ASP:OD1	11:D:69:SER:N	2.42	0.48
18:K:212:TYR:HB2	18:K:339:GLU:HA	1.96	0.48
19:L:307:GLU:OE2	19:L:311:GLN:NE2	2.46	0.48
20:M:215:PRO:HA	20:M:341:GLY:H	1.79	0.48
20:M:401:ILE:HD11	20:M:422:VAL:HG21	1.96	0.48
21:N:774:ASN:ND2	21:N:866:TYR:O	2.37	0.48
21:N:885:ILE:HG12	21:N:887:ASP:H	1.79	0.48
23:P:286:ASN:HA	23:P:293:LEU:HD11	1.96	0.48
26:S:364:ILE:HB	26:S:377:TYR:HE1	1.77	0.48
27:T:143:SER:HA	27:T:146:ILE:HB	1.94	0.48
29:V:45:VAL:HA	29:V:144:ILE:HG21	1.95	0.48
29:V:61:TYR:O	29:V:62:THR:HB	2.13	0.48
33:Z:144:SER:HB3	33:Z:154:ILE:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:211:LYS:O	12:E:216:ASN:ND2	2.41	0.48
16:I:106:ILE:HD11	16:I:146:SER:HB3	1.93	0.48
16:I:358:LYS:HD3	16:I:381:VAL:HG12	1.93	0.48
2:2:101:ARG:NH2	8:A:147:ASP:OD2	2.47	0.48
3:3:51:LEU:HD22	3:3:87:PHE:HZ	1.77	0.48
7:7:176:ALA:HB3	7:7:185:ASN:HB2	1.95	0.48
9:B:161:ALA:HB1	9:B:175:LEU:HB3	1.96	0.48
11:D:157:SER:HG	11:D:159:TRP:HE1	1.60	0.48
13:F:39:ARG:HD3	13:F:144:LEU:HB2	1.94	0.48
28:U:298:ASN:HA	28:U:301:ILE:HD12	1.95	0.48
16:I:188:GLU:HA	16:I:191:ILE:HD12	1.96	0.48
16:I:395:MET:HA	16:I:423:VAL:HG21	1.96	0.48
18:K:341:PRO:O	18:K:344:ARG:NH1	2.39	0.48
15:H:162:ARG:H	15:H:183:ILE:HG21	1.79	0.48
15:H:397:SER:HB3	15:H:437:VAL:HG12	1.96	0.48
27:T:163:LEU:O	27:T:167:GLY:N	2.46	0.48
28:U:57:GLU:OE2	29:V:97:GLN:NE2	2.32	0.48
28:U:171:VAL:HG11	29:V:217:HIS:HB3	1.95	0.48
4:4:36:ARG:HG2	4:4:46:PHE:HE2	1.78	0.48
6:6:112:ILE:HD13	6:6:128:THR:HG21	1.96	0.48
12:E:218:GLN:HE21	12:E:230:ILE:HG21	1.79	0.48
17:J:96:VAL:HB	17:J:121:MET:HA	1.95	0.48
19:L:318:LEU:HB3	19:L:321:THR:HB	1.96	0.48
20:M:143:ASN:HB3	20:M:261:LYS:HD3	1.96	0.48
21:N:533:ASP:OD1	21:N:559:TYR:OH	2.32	0.48
22:O:196:LEU:HD13	22:O:203:THR:HB	1.96	0.48
24:Q:179:LEU:HD21	24:Q:217:GLU:HG2	1.95	0.48
33:Z:256:LEU:HB3	33:Z:257:PRO:HD3	1.96	0.48
33:Z:498:ALA:HA	33:Z:533:VAL:HA	1.96	0.48
33:Z:596:THR:HA	33:Z:599:ILE:HD12	1.96	0.48
16:I:246:ARG:HE	17:J:278:GLN:HE21	1.62	0.47
21:N:179:THR:O	21:N:180:SER:HB3	2.13	0.47
21:N:762:ARG:NE	21:N:767:ALA:HB2	2.29	0.47
23:P:384:VAL:HG12	24:Q:352:GLU:HG3	1.94	0.47
1:1:82:LEU:HA	1:1:85:TYR:HB3	1.96	0.47
9:B:42:GLY:HA3	9:B:185:LEU:HD22	1.96	0.47
10:C:16:GLU:O	11:D:29:ARG:NH2	2.36	0.47
18:K:152:PRO:HD2	18:K:260:LEU:HD13	1.96	0.47
10:C:135:PHE:HB2	10:C:151:SER:HB3	1.96	0.47
11:D:37:LYS:HB3	11:D:42:VAL:HG23	1.96	0.47
12:E:61:SER:HB2	12:E:215:ASN:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:261:SER:HA	18:K:293:GLN:HG3	1.96	0.47
17:J:270:ARG:HG3	17:J:271:THR:HG23	1.95	0.47
17:J:379:GLN:HA	17:J:382:PHE:HD2	1.79	0.47
16:I:102:ASN:HB3	17:J:97:ASP:OD1	2.14	0.47
21:N:527:GLY:H	21:N:558:ALA:HA	1.79	0.47
32:Y:69:VAL:HG12	32:Y:70:ASP:N	2.29	0.47
33:Z:151:HIS:HB3	33:Z:153:TYR:HD2	1.78	0.47
1:I:58:ASP:OD2	8:A:77:ARG:NH2	2.47	0.47
7:7:54:ILE:HD11	7:7:230:LEU:HD21	1.96	0.47
9:B:49:LYS:HA	9:B:63:LYS:NZ	2.29	0.47
11:D:139:ASP:HB2	11:D:142:ASP:HB3	1.96	0.47
13:F:7:ASP:H	13:F:12:THR:HG21	1.79	0.47
19:L:149:ASP:HB3	19:L:154:THR:H	1.79	0.47
19:L:396:THR:HA	20:M:212:ILE:HD12	1.95	0.47
21:N:707:ASN:HD21	21:N:785:PRO:HG2	1.80	0.47
23:P:101:MET:HG3	23:P:139:VAL:HG12	1.96	0.47
24:Q:359:ILE:HD12	24:Q:395:GLY:HA2	1.97	0.47
29:V:225:LEU:HB3	29:V:228:TYR:HB2	1.95	0.47
12:E:52:LYS:NZ	12:E:215:ASN:O	2.46	0.47
17:J:383:GLU:OE1	24:Q:166:LYS:NZ	2.34	0.47
20:M:194:VAL:HG13	20:M:198:VAL:HB	1.97	0.47
25:R:60:ALA:HA	25:R:63:TYR:HB3	1.96	0.47
33:Z:914:LEU:HD22	33:Z:959:HIS:CD2	2.49	0.47
1:I:56:VAL:HB	1:I:82:LEU:HD12	1.95	0.47
11:D:117:GLN:HE21	11:D:129:PHE:HB2	1.79	0.47
15:H:100:ALA:HB3	15:H:149:LEU:HD13	1.96	0.47
21:N:479:GLU:HB2	21:N:512:ASN:HB3	1.97	0.47
26:S:475:TYR:CZ	28:U:294:ASN:HB2	2.50	0.47
28:U:14:VAL:HG21	28:U:48:VAL:HG12	1.95	0.47
29:V:173:THR:HG22	29:V:174:THR:HG23	1.96	0.47
21:N:512:ASN:ND2	29:V:61:TYR:CD2	2.82	0.47
30:W:98:LEU:HD13	30:W:108:GLN:HB3	1.96	0.47
30:W:54:GLY:HA3	30:W:90:ALA:HB2	1.95	0.47
2:2:126:TYR:HB3	2:2:156:LEU:HD21	1.97	0.47
15:H:178:ARG:HG2	15:H:284:VAL:HB	1.96	0.47
15:H:244:LYS:HZ1	15:H:346:ARG:HH11	1.61	0.47
17:J:155:LYS:HD3	17:J:317:PRO:HG3	1.95	0.47
17:J:34:ILE:O	17:J:38:THR:OG1	2.29	0.47
18:K:186:GLU:HA	18:K:190:LEU:HD13	1.97	0.47
19:L:370:LYS:HE3	19:L:376:PHE:HZ	1.78	0.47
21:N:175:ASP:O	21:N:176:GLN:C	2.53	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	2.49	0.47
7:7:77:PRO:HB3	7:7:83:VAL:HG22	1.97	0.47
9:B:240:SER:HA	9:B:243:ILE:HD12	1.97	0.47
15:H:77:ALA:HA	15:H:101:ARG:HE	1.80	0.47
16:I:353:PRO:HB3	16:I:357:THR:HG21	1.97	0.47
24:Q:326:MET:HA	24:Q:335:PHE:HE2	1.80	0.47
29:V:53:MET:HA	29:V:68:VAL:HG12	1.95	0.47
7:7:136:ARG:HB3	7:7:142:PRO:HA	1.97	0.47
8:A:170:ALA:HB3	8:A:175:GLN:HG3	1.96	0.47
13:F:22:VAL:HG13	13:F:149:PRO:HG2	1.95	0.47
14:G:20:ARG:HH21	14:G:25:GLU:HG2	1.80	0.47
18:K:91:SER:OG	18:K:92:VAL:N	2.45	0.47
21:N:756:THR:HG21	21:N:876:PRO:HG3	1.96	0.47
26:S:173:LEU:H	26:S:176:LEU:HD12	1.78	0.47
29:V:62:THR:HG22	29:V:62:THR:O	2.14	0.47
18:K:238:ASN:HB2	18:K:241:GLU:HG3	1.96	0.47
18:K:240:SER:HB2	19:L:306:MET:HB2	1.96	0.47
22:O:292:CYS:O	22:O:295:THR:OG1	2.24	0.47
23:P:144:VAL:HG12	23:P:148:LYS:HE3	1.97	0.47
33:Z:516:THR:HB	33:Z:562:TRP:HE3	1.80	0.47
7:7:144:TRP:HE3	7:7:165:LEU:HD21	1.79	0.47
11:D:48:ARG:HG3	11:D:63:LYS:HE2	1.96	0.47
15:H:399:GLU:HG2	15:H:401:GLY:H	1.80	0.47
18:K:277:ILE:HG12	18:K:295:ILE:HD12	1.96	0.47
21:N:510:HIS:HB3	21:N:513:ILE:CB	2.32	0.47
21:N:779:GLU:HG2	21:N:866:TYR:CE1	2.50	0.47
30:W:101:ARG:HE	30:W:108:GLN:HE21	1.60	0.47
33:Z:358:TYR:HE1	33:Z:962:ARG:HB2	1.80	0.47
8:A:147:ASP:OD1	8:A:148:GLU:N	2.48	0.46
11:D:70:HIS:ND1	11:D:71:VAL:HG23	2.30	0.46
15:H:224:VAL:HG21	15:H:373:ARG:HG3	1.96	0.46
18:K:345:ASP:OD1	18:K:346:ARG:N	2.48	0.46
21:N:436:ASP:HB2	21:N:439:VAL:HG23	1.97	0.46
21:N:529:GLN:H	21:N:558:ALA:HB1	1.78	0.46
26:S:418:THR:O	27:T:157:TYR:OH	2.32	0.46
28:U:174:LEU:HD13	29:V:31:SER:HB3	1.96	0.46
21:N:298:TYR:OH	21:N:766:GLN:NE2	2.45	0.46
28:U:276:ILE:HG23	29:V:290:ASN:HB3	1.98	0.46
3:3:30:GLY:HA2	3:3:36:VAL:HG23	1.95	0.46
3:3:7:ILE:HG23	3:3:32:GLN:HG3	1.96	0.46
12:E:130:GLU:HB3	12:E:132:ARG:HH12	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:D:161:ALA:HB3	12:E:58:LEU:HD13	1.97	0.46
14:G:12:ASN:ND2	14:G:126:TYR:O	2.41	0.46
21:N:424:LYS:NZ	21:N:461:GLU:OE1	2.48	0.46
21:N:667:GLN:O	21:N:671:LEU:HB2	2.16	0.46
23:P:249:ALA:HB1	23:P:285:GLN:HG3	1.97	0.46
24:Q:382:LEU:HD11	25:R:340:GLN:HB3	1.97	0.46
27:T:187:ASP:O	27:T:191:LYS:HG3	2.15	0.46
15:H:77:ALA:O	15:H:101:ARG:NH2	2.47	0.46
16:I:187:LEU:HD13	16:I:232:LEU:HD21	1.98	0.46
17:J:111:GLN:HE22	17:J:128:ASN:HB2	1.79	0.46
21:N:309:ILE:HG22	21:N:339:MET:HB3	1.96	0.46
26:S:82:TYR:CD2	26:S:86:SER:HB3	2.49	0.46
33:Z:151:HIS:HB3	33:Z:153:TYR:CD2	2.50	0.46
33:Z:228:GLU:HG2	33:Z:264:PHE:HZ	1.81	0.46
2:2:129:VAL:N	2:2:140:PHE:O	2.48	0.46
9:B:86:VAL:HA	9:B:89:SER:HB3	1.96	0.46
13:F:110:HIS:HB2	14:G:86:ARG:HH21	1.81	0.46
18:K:241:GLU:O	18:K:243:VAL:HG23	2.14	0.46
18:K:96:ILE:HD12	19:L:126:ARG:HB3	1.97	0.46
20:M:348:GLU:HG2	20:M:350:PRO:HD3	1.98	0.46
24:Q:151:TYR:HB3	24:Q:184:VAL:HG13	1.97	0.46
28:U:74:GLU:OE2	28:U:113:TYR:OH	2.33	0.46
1:1:89:TYR:CD1	14:G:111:ALA:HB1	2.51	0.46
6:6:47:ARG:HB2	6:6:219:ASP:HB2	1.97	0.46
9:B:97:TYR:O	9:B:101:TYR:N	2.46	0.46
11:D:175:LEU:HA	11:D:179:TYR:HD2	1.81	0.46
13:F:187:ASP:OD1	13:F:233:TYR:OH	2.33	0.46
16:I:247:ILE:HD13	16:I:279:VAL:HG13	1.98	0.46
18:K:421:VAL:HG12	18:K:422:ASP:O	2.16	0.46
21:N:283:ASP:HB3	21:N:286:LEU:HB2	1.97	0.46
21:N:352:ASN:HB3	21:N:355:TRP:CE3	2.51	0.46
19:L:258:GLU:O	19:L:262:ILE:HG12	2.16	0.46
30:W:25:ARG:HH11	30:W:26:PHE:H	1.63	0.46
31:X:73:THR:HG23	31:X:90:VAL:H	1.81	0.46
9:B:13:SER:HB2	9:B:18:LEU:HA	1.98	0.46
13:F:50:LYS:HB3	13:F:59:TYR:HB3	1.98	0.46
19:L:244:ILE:HB	19:L:278:ILE:HA	1.97	0.46
24:Q:121:SER:HA	24:Q:124:PHE:HD2	1.80	0.46
33:Z:506:LEU:HD22	33:Z:539:ASN:HD21	1.80	0.46
2:2:202:VAL:HB	2:2:220:LEU:HB3	1.97	0.46
3:3:20:CYS:HB3	3:3:191:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:156:LYS:HB3	8:A:166:TYR:HE2	1.81	0.46
30:W:186:ALA:HA	30:W:191:ILE:HD12	1.98	0.46
1:1:33:LEU:HD21	1:1:119:ALA:HB3	1.98	0.46
4:4:34:LYS:HB3	4:4:46:PHE:CE1	2.51	0.46
21:N:775:CYS:N	21:N:869:ASP:OD2	2.44	0.46
27:T:235:PHE:CZ	27:T:237:ASN:HB2	2.51	0.46
5:5:162:VAL:HG11	5:5:192:SER:HA	1.97	0.45
9:B:193:LEU:HD13	9:B:247:LEU:HD23	1.97	0.45
13:F:10:THR:HG22	13:F:21:GLN:HG3	1.97	0.45
15:H:149:LEU:HD21	15:H:175:GLY:HA3	1.97	0.45
15:H:173:ARG:NH2	16:I:129:TYR:H	2.14	0.45
16:I:200:LEU:HD11	16:I:207:LEU:HD22	1.98	0.45
15:H:150:LYS:HG2	15:H:152:ILE:H	1.82	0.45
25:R:368:LEU:HD23	25:R:371:PHE:HD2	1.80	0.45
26:S:352:VAL:HG13	26:S:387:VAL:HA	1.99	0.45
26:S:93:LEU:O	26:S:98:SER:OG	2.29	0.45
5:5:76:THR:O	5:5:206:SER:N	2.49	0.45
10:C:13:PHE:CD2	11:D:19:GLN:HB3	2.52	0.45
10:C:94:HIS:CD2	10:C:114:ARG:HG2	2.52	0.45
5:5:156:LYS:NZ	11:D:101:GLU:OE1	2.47	0.45
16:I:205:PRO:HD2	33:Z:826:ARG:NH2	2.30	0.45
33:Z:516:THR:HA	33:Z:523:ALA:HB3	1.99	0.45
33:Z:905:ASN:HA	33:Z:908:ILE:HD12	1.98	0.45
6:6:110:ARG:NH1	6:6:113:GLN:OE1	2.50	0.45
6:6:183:THR:HB	6:6:186:LYS:HB3	1.99	0.45
3:3:76:LEU:HB3	10:C:92:ARG:HD3	1.98	0.45
12:E:52:LYS:HZ2	12:E:216:ASN:C	2.20	0.45
13:F:54:ASP:H	13:F:57:SER:HB3	1.81	0.45
15:H:241:ASP:HB2	15:H:346:ARG:HH21	1.82	0.45
17:J:251:ASP:HA	17:J:293:ALA:O	2.17	0.45
18:K:74:HIS:NE2	18:K:78:GLU:OE2	2.49	0.45
28:U:16:LEU:HG	29:V:32:ILE:HG12	1.99	0.45
33:Z:145:ASP:OD1	33:Z:146:PHE:N	2.49	0.45
1:1:60:ILE:HA	1:1:120:GLY:HA2	1.99	0.45
4:4:80:VAL:HG12	4:4:104:ILE:HD13	1.98	0.45
9:B:38:LYS:HA	9:B:43:VAL:HG22	1.98	0.45
10:C:232:PRO:HA	10:C:235:ILE:HD12	1.98	0.45
17:J:202:VAL:HG12	17:J:244:ILE:HD13	1.98	0.45
18:K:351:LEU:HD21	24:Q:237:SER:HB3	1.98	0.45
22:O:307:MET:HG3	22:O:347:LEU:HD22	1.99	0.45
23:P:254:GLU:HA	23:P:257:TRP:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:W:143:ASN:HD21	30:W:149:GLN:H	1.64	0.45
3:3:107:PRO:HG2	3:3:124:PHE:HB2	1.98	0.45
5:5:84:GLN:OE1	5:5:221:TRP:NE1	2.47	0.45
5:5:106:VAL:HA	6:6:151:GLU:HG2	1.99	0.45
11:D:75:PHE:HB3	11:D:133:THR:HG22	1.99	0.45
26:S:234:ILE:HD11	26:S:258:GLU:HG2	1.98	0.45
26:S:352:VAL:HG22	26:S:387:VAL:HG22	1.98	0.45
24:Q:422:VAL:HG13	29:V:266:LEU:HD11	1.99	0.45
31:X:48:PHE:HD2	31:X:66:LEU:HD23	1.82	0.45
2:2:132:VAL:HG11	2:2:209:ILE:HA	1.98	0.45
4:4:135:TYR:HA	4:4:138:PHE:HE2	1.81	0.45
19:L:104:LEU:HB2	19:L:148:LEU:HB2	1.98	0.45
19:L:114:GLU:OE1	19:L:137:ARG:NH1	2.50	0.45
21:N:179:THR:O	21:N:179:THR:OG1	2.31	0.45
21:N:309:ILE:HG21	21:N:340:HIS:CE1	2.51	0.45
23:P:415:TRP:CH2	29:V:235:GLU:HB3	2.52	0.45
24:Q:262:LEU:HD13	24:Q:291:TYR:HB2	1.98	0.45
1:1:50:THR:OG1	2:2:149:ASP:OD2	2.34	0.45
5:5:112:ILE:HD11	5:5:131:GLU:HB3	1.98	0.45
2:2:86:GLN:NE2	9:B:98:LYS:O	2.42	0.45
13:F:19:LEU:HG	13:F:21:GLN:H	1.82	0.45
13:F:37:GLY:HA3	13:F:46:LEU:HD23	1.97	0.45
16:I:184:ILE:HD11	16:I:191:ILE:HD11	1.98	0.45
18:K:281:ARG:HH22	18:K:285:GLN:H	1.63	0.45
18:K:281:ARG:NH2	18:K:285:GLN:H	2.15	0.45
20:M:167:VAL:HB	20:M:262:LEU:HD21	1.98	0.45
13:F:84:LEU:HD13	13:F:112:LEU:HD11	1.98	0.45
14:G:65:VAL:HG12	14:G:67:ILE:H	1.82	0.45
18:K:206:PRO:HB3	18:K:335:ASP:HB2	1.99	0.45
19:L:201:LEU:HD12	19:L:239:ILE:HD13	1.98	0.45
23:P:23:LYS:HA	23:P:27:LEU:HD11	1.99	0.45
24:Q:195:LYS:HG2	24:Q:225:LEU:HD13	1.99	0.45
28:U:52:PHE:O	28:U:93:TYR:OH	2.28	0.45
1:1:122:ASP:OD1	1:1:123:ASP:N	2.49	0.45
6:6:183:THR:HG21	6:6:187:VAL:HB	1.99	0.45
8:A:114:CYS:SG	8:A:153:SER:OG	2.74	0.45
8:A:130:GLN:HG3	9:B:127:VAL:HG13	1.98	0.45
8:A:236:LEU:HD22	8:A:240:ASN:HB3	1.99	0.45
18:K:178:ASP:HA	18:K:181:LYS:HD3	1.99	0.45
1:1:159:LYS:HG2	9:B:156:TYR:HE1	81.43	0.44
15:H:215:LYS:HA	15:H:218:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:510:HIS:CG	21:N:513:ILE:HD12	2.52	0.44
29:V:127:LYS:HA	29:V:158:LEU:HD22	1.97	0.44
17:J:252:SER:HA	17:J:257:ARG:HG3	1.99	0.44
24:Q:249:LEU:HB2	24:Q:253:ASN:HB2	2.00	0.44
31:X:85:ARG:HH22	31:X:104:LYS:HG3	1.81	0.44
13:F:7:ASP:HA	13:F:12:THR:HB	1.99	0.44
5:5:94:ARG:NH2	15:H:205:ASP:OD2	104.91	0.44
18:K:268:ILE:HG12	18:K:313:LYS:HB3	1.99	0.44
21:N:254:SER:HB2	21:N:286:LEU:HD11	1.98	0.44
21:N:585:ARG:HB2	21:N:616:HIS:HB3	1.99	0.44
25:R:174:ILE:HD13	25:R:190:LYS:HB3	1.99	0.44
27:T:109:TYR:HE2	27:T:125:GLU:HG2	1.82	0.44
27:T:143:SER:HA	27:T:146:ILE:HD12	1.98	0.44
28:U:275:VAL:HG11	29:V:245:VAL:HG13	2.00	0.44
29:V:46:PRO:HA	29:V:112:PRO:HG3	1.98	0.44
30:W:143:ASN:ND2	30:W:149:GLN:O	2.51	0.44
33:Z:352:LYS:HG2	33:Z:462:VAL:HG23	1.98	0.44
10:C:70:ASN:OD1	10:C:73:ILE:N	2.50	0.44
15:H:100:ALA:HA	15:H:173:ARG:HB3	1.99	0.44
22:O:130:ASP:HA	22:O:133:ILE:HD12	1.99	0.44
33:Z:381:LEU:HD13	33:Z:414:GLY:HA2	1.99	0.44
10:C:107:PRO:HD2	10:C:110:ILE:HD12	1.99	0.44
15:H:251:PRO:HG2	15:H:254:THR:HB	1.99	0.44
16:I:184:ILE:HB	16:I:187:LEU:HD12	1.99	0.44
17:J:159:GLU:HB3	17:J:314:ILE:HG12	2.00	0.44
21:N:25:LEU:HD23	21:N:28:ILE:HD12	1.99	0.44
27:T:134:LYS:HA	27:T:138:ASP:HB3	1.99	0.44
6:6:127:HIS:HE1	6:6:129:ILE:HD11	1.83	0.44
4:4:82:SER:OG	10:C:101:THR:O	2.23	0.44
12:E:148:ASP:OD1	12:E:152:GLY:N	2.50	0.44
13:F:95:SER:O	13:F:100:ASN:N	2.50	0.44
14:G:95:GLU:HB3	14:G:115:ARG:HD3	2.00	0.44
14:G:204:HIS:NE2	14:G:208:LYS:HA	2.33	0.44
16:I:253:ILE:HG13	16:I:302:ILE:HG12	2.00	0.44
21:N:600:THR:HA	21:N:634:LEU:HD22	1.98	0.44
23:P:35:ALA:HB1	23:P:62:ILE:HG12	2.00	0.44
26:S:360:PHE:CD2	26:S:384:ARG:HD3	2.53	0.44
29:V:57:PHE:HE1	29:V:135:ARG:HD2	1.83	0.44
33:Z:120:SER:HB3	33:Z:138:ARG:NH2	2.32	0.44
33:Z:427:GLN:HA	33:Z:458:SER:HA	2.00	0.44
1:1:59:LYS:HB3	1:1:121:TYR:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:27:PHE:CE2	1:1:32:ILE:HG13	2.52	0.44
9:B:50:LYS:HE2	9:B:52:SER:HB2	2.00	0.44
10:C:13:PHE:HD2	11:D:19:GLN:HB3	1.83	0.44
16:I:167:MET:HB3	16:I:266:GLN:HB3	1.98	0.44
18:K:81:ARG:HH12	21:N:613:HIS:CD2	2.35	0.44
19:L:110:LYS:HA	19:L:142:LYS:HE2	1.99	0.44
23:P:83:SER:HB3	23:P:93:ILE:HG13	1.99	0.44
25:R:211:LYS:HD3	25:R:230:LEU:HD22	2.00	0.44
29:V:51:GLY:HA3	29:V:108:TYR:CZ	2.52	0.44
33:Z:134:SER:HA	33:Z:137:TYR:CD2	2.53	0.44
33:Z:295:ARG:HD3	33:Z:321:PHE:HZ	1.81	0.44
5:5:233:LYS:HG3	5:5:252:LEU:HD21	1.99	0.44
15:H:144:LYS:HE3	20:M:75:LEU:HG	1.99	0.44
16:I:118:ALA:HB2	16:I:132:ILE:HD11	1.99	0.44
17:J:327:ILE:HG22	17:J:358:VAL:HG11	1.98	0.44
20:M:157:ASP:OD1	20:M:158:THR:N	2.50	0.44
24:Q:400:TYR:OH	24:Q:404:ASN:ND2	2.33	0.44
27:T:248:GLU:H	27:T:252:GLU:HG3	1.83	0.44
15:H:105:ILE:HB	15:H:146:VAL:HG22	2.00	0.44
16:I:281:ILE:HB	16:I:326:MET:HG2	1.99	0.44
20:M:336:ALA:O	20:M:342:ARG:NH1	2.51	0.44
28:U:122:ILE:HD12	28:U:137:TYR:HE2	1.82	0.44
33:Z:181:GLY:HA2	33:Z:230:ILE:HD13	2.00	0.44
5:5:114:PRO:HA	5:5:260:TRP:CD1	2.52	0.43
12:E:207:VAL:HG12	15:H:409:ARG:HH12	1.82	0.43
13:F:117:GLN:HE21	13:F:121:GLN:HG3	1.82	0.43
20:M:119:VAL:HB	20:M:155:ILE:HD11	2.00	0.43
20:M:289:LYS:HG2	20:M:332:VAL:HG11	2.00	0.43
22:O:189:TYR:HB2	22:O:220:SER:HB2	1.99	0.43
25:R:236:ALA:HB3	25:R:275:GLU:HB3	2.00	0.43
26:S:226:ASP:OD2	26:S:229:THR:OG1	2.33	0.43
28:U:122:ILE:HD12	28:U:137:TYR:CE2	2.53	0.43
26:S:327:ILE:HG13	32:Y:64:TRP:HZ2	1.83	0.43
5:5:266:HIS:HB3	5:5:271:LEU:HD11	2.00	0.43
8:A:46:ARG:HH11	8:A:152:PRO:HB2	1.82	0.43
9:B:9:LEU:HD11	9:B:129:PRO:HD3	1.99	0.43
12:E:61:SER:O	12:E:62:ASP:OD1	2.36	0.43
14:G:54:ILE:HG12	14:G:59:LEU:HD23	1.99	0.43
15:H:221:LEU:O	15:H:225:VAL:HB	2.19	0.43
12:E:175:GLY:HA2	15:H:409:ARG:NH2	2.33	0.43
16:I:193:GLU:HB3	16:I:346:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:J:327:ILE:HA	17:J:330:ILE:HD12	1.99	0.43
21:N:762:ARG:NH2	21:N:766:GLN:O	2.50	0.43
22:O:250:TRP:CE2	22:O:270:ILE:HG22	2.53	0.43
31:X:37:PRO:HB3	31:X:46:TRP:HD1	1.83	0.43
33:Z:262:VAL:HG11	33:Z:287:ARG:HD3	2.00	0.43
33:Z:415:MET:HG2	33:Z:447:VAL:HA	1.99	0.43
15:H:399:GLU:HB3	15:H:402:ILE:HG23	2.00	0.43
16:I:135:PHE:CD2	16:I:136:VAL:HG13	2.53	0.43
16:I:399:ALA:HB1	16:I:411:VAL:HG11	2.00	0.43
17:J:262:GLY:H	18:K:281:ARG:HD3	1.82	0.43
19:L:198:GLU:HG3	19:L:239:ILE:HG12	2.00	0.43
19:L:397:GLU:HA	19:L:400:PHE:HD2	1.83	0.43
20:M:167:VAL:HG11	20:M:262:LEU:HD11	2.00	0.43
3:3:149:MET:HG3	3:3:174:ALA:HB2	2.00	0.43
7:7:198:ILE:HB	7:7:199:PRO:HD3	2.00	0.43
11:D:10:ILE:HG12	12:E:23:GLN:HE22	1.84	0.43
14:G:108:PRO:HG2	14:G:111:ALA:HB3	1.99	0.43
15:H:200:VAL:HG22	15:H:272:ILE:HG12	2.01	0.43
16:I:278:ILE:HG23	16:I:323:LYS:H	1.84	0.43
16:I:190:GLN:NE2	16:I:349:LEU:O	2.51	0.43
16:I:371:LEU:HD22	16:I:375:VAL:HG11	2.00	0.43
20:M:224:PRO:HA	20:M:228:LYS:HE2	1.99	0.43
30:W:163:ASN:HB3	30:W:164:PRO:HD3	2.01	0.43
8:A:63:LEU:HD11	14:G:173:LYS:HG3	2.00	0.43
11:D:96:HIS:ND1	11:D:102:ASP:O	2.48	0.43
13:F:88:LEU:HD21	13:F:112:LEU:HB2	1.99	0.43
13:F:65:LYS:HE3	13:F:224:ILE:HD12	2.01	0.43
19:L:119:VAL:HG21	19:L:148:LEU:HD21	2.01	0.43
21:N:175:ASP:HB2	21:N:181:GLU:HB2	2.00	0.43
26:S:426:ALA:HB1	26:S:432:ILE:HG12	2.00	0.43
26:S:40:GLU:HA	26:S:46:LEU:HD12	2.01	0.43
27:T:27:LEU:HB2	27:T:28:PRO:HD3	2.01	0.43
33:Z:99:LEU:HD23	33:Z:102:ILE:HD12	1.99	0.43
6:6:56:SER:HB2	7:7:170:TYR:CD1	2.53	0.43
8:A:179:THR:HG21	9:B:54:PRO:HD2	2.00	0.43
8:A:56:GLN:HA	8:A:223:LEU:HD23	2.00	0.43
9:B:140:ASP:OD1	9:B:144:GLY:N	2.52	0.43
10:C:59:GLN:HE22	10:C:210:ARG:HG2	1.84	0.43
11:D:122:GLN:HE21	12:E:84:ASP:HA	1.82	0.43
11:D:175:LEU:HA	11:D:179:TYR:CD2	2.54	0.43
17:J:218:LEU:HG	17:J:229:MET:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Z:295:ARG:HD3	33:Z:321:PHE:CZ	2.53	0.43
4:4:41:HIS:NE2	4:4:186:LYS:O	2.52	0.43
8:A:82:VAL:HB	8:A:142:THR:HB	2.01	0.43
12:E:42:THR:OG1	12:E:45:GLY:O	2.26	0.43
22:O:51:ASP:OD1	22:O:52:ALA:N	2.51	0.43
29:V:95:LEU:HB3	29:V:100:ARG:HB2	1.99	0.43
13:F:137:TYR:CZ	13:F:218:LYS:HG2	2.54	0.43
22:O:135:ARG:HA	22:O:138:LEU:HD12	2.01	0.43
25:R:59:MET:O	25:R:63:TYR:N	2.39	0.43
29:V:202:ASP:OD1	29:V:203:TYR:N	2.52	0.43
28:U:192:ASN:HB2	29:V:230:TYR:HD2	1.83	0.43
30:W:21:PHE:H	30:W:25:ARG:HB2	1.84	0.43
33:Z:518:LEU:HB2	33:Z:562:TRP:HH2	1.84	0.43
2:2:75:ALA:HB3	2:2:126:TYR:HB2	2.01	0.43
21:N:326:SER:N	29:V:168:LEU:HD11	2.34	0.43
21:N:746:ALA:HA	21:N:749:LEU:HD13	2.00	0.43
21:N:761:ILE:HG13	21:N:904:VAL:HG22	2.01	0.43
29:V:114:PHE:H	29:V:118:LEU:HD23	1.83	0.43
6:6:224:LEU:HG	6:6:233:LYS:HG2	2.00	0.43
7:7:148:ILE:HG23	7:7:175:LEU:HD23	2.00	0.43
2:2:68:PRO:HB3	9:B:223:GLY:HA3	2.00	0.43
16:I:280:PHE:CE1	16:I:325:ILE:HD12	2.54	0.43
20:M:357:ARG:HD2	20:M:391:LEU:HD21	2.00	0.43
24:Q:267:LEU:HD13	24:Q:331:THR:HG22	2.01	0.43
26:S:114:TYR:HB2	26:S:117:SER:HB2	2.00	0.43
26:S:399:TYR:CD2	26:S:402:ILE:HD12	2.54	0.43
26:S:330:LEU:N	32:Y:62:GLU:O	2.52	0.43
7:7:60:LEU:HD11	7:7:62:SER:HB3	2.01	0.42
8:A:64:LEU:HG	14:G:160:TYR:CE1	2.54	0.42
10:C:115:LEU:HD23	10:C:118:ILE:HD12	2.01	0.42
11:D:37:LYS:HA	11:D:42:VAL:HA	2.00	0.42
16:I:391:ASP:OD2	17:J:306:ARG:NH1	2.52	0.42
17:J:35:ARG:HH22	26:S:45:THR:HG21	1.84	0.42
21:N:443:LEU:HD22	21:N:477:SER:HB2	2.00	0.42
24:Q:65:TYR:HD2	24:Q:74:LEU:HD13	1.84	0.42
25:R:283:THR:HG22	25:R:285:ALA:H	1.83	0.42
27:T:191:LYS:HG2	27:T:224:ARG:HH22	1.83	0.42
3:3:103:TYR:OH	4:4:93:ARG:NH1	2.42	0.42
4:4:135:TYR:HA	4:4:138:PHE:CE2	2.54	0.42
7:7:62:SER:HB3	7:7:67:LEU:HD23	2.00	0.42
9:B:12:PHE:HB3	10:C:21:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:121:LEU:HB2	13:F:82:ARG:HH21	1.84	0.42
17:J:141:LYS:HG2	17:J:142:VAL:HG22	2.00	0.42
20:M:379:LEU:HD22	20:M:419:ILE:HD12	2.01	0.42
23:P:371:LEU:HD22	23:P:375:GLN:HB3	2.01	0.42
26:S:405:ARG:HG2	26:S:416:GLU:HG2	2.02	0.42
4:4:99:GLN:HB3	4:4:121:TYR:HB2	2.01	0.42
6:6:46:THR:HB	6:6:59:GLU:H	1.84	0.42
8:A:156:LYS:HE3	8:A:166:TYR:HE2	1.84	0.42
9:B:67:LEU:HD13	9:B:110:LEU:HD21	2.00	0.42
9:B:9:LEU:HD21	9:B:20:GLN:HG2	2.00	0.42
17:J:324:ARG:HA	17:J:327:ILE:HD12	2.00	0.42
23:P:319:GLU:OE1	23:P:323:ASN:HB3	2.19	0.42
24:Q:210:CYS:HB3	24:Q:214:THR:HB	2.01	0.42
26:S:234:ILE:HG23	26:S:253:PHE:HE2	1.84	0.42
31:X:7:VAL:HG12	31:X:8:ILE:HG13	2.00	0.42
3:3:24:ALA:HB1	3:3:171:LEU:HD22	2.02	0.42
4:4:22:THR:HA	4:4:27:VAL:HA	2.02	0.42
5:5:109:VAL:HG21	5:5:253:TYR:HE2	1.84	0.42
13:F:62:LYS:O	13:F:74:LEU:N	2.51	0.42
15:H:249:TYR:N	15:H:375:VAL:O	2.52	0.42
16:I:221:LEU:HD12	16:I:327:ALA:HB2	2.01	0.42
20:M:361:LEU:HD21	20:M:391:LEU:HD22	2.00	0.42
23:P:244:ILE:HD12	23:P:247:THR:HB	2.01	0.42
28:U:174:LEU:HD21	29:V:34:LEU:HD23	2.02	0.42
28:U:72:TYR:HB3	29:V:94:MET:SD	2.60	0.42
2:2:244:GLU:HG3	3:3:198:ARG:HG2	2.00	0.42
4:4:192:VAL:HG12	4:4:194:ASP:H	1.83	0.42
13:F:157:TYR:CZ	14:G:60:VAL:HG22	2.54	0.42
18:K:349:ARG:NH2	18:K:372:ILE:O	2.49	0.42
25:R:29:LYS:HB3	25:R:46:ALA:HB1	2.02	0.42
27:T:63:GLU:HG3	27:T:105:LEU:HD22	2.01	0.42
30:W:22:PRO:HD2	30:W:24:THR:O	2.20	0.42
33:Z:307:HIS:CE1	33:Z:340:LEU:HD12	2.54	0.42
1:1:61:TRP:CD1	1:1:197:LEU:HD21	2.55	0.42
3:3:123:GLY:HA3	3:3:137:ILE:HG21	2.01	0.42
4:4:38:LEU:HD23	4:4:61:GLN:HG3	2.02	0.42
4:4:4:ILE:HG12	4:4:103:LEU:HD12	2.00	0.42
7:7:58:ASP:HA	7:7:228:PHE:HA	2.02	0.42
8:A:156:LYS:HE3	8:A:166:TYR:CE2	2.55	0.42
13:F:39:ARG:NH2	13:F:155:GLU:OE2	2.52	0.42
15:H:244:LYS:NZ	15:H:346:ARG:HD3	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:174:ASP:O	16:I:244:PHE:N	2.44	0.42
19:L:274:GLU:HB3	19:L:320:GLN:HG3	2.01	0.42
20:M:83:VAL:N	20:M:118:VAL:O	2.52	0.42
19:L:251:ILE:N	20:M:293:SER:OG	2.53	0.42
23:P:421:GLU:HB2	28:U:235:LEU:HD23	2.00	0.42
33:Z:878:LEU:HD23	33:Z:881:ILE:HD12	2.01	0.42
5:5:113:ASN:OD1	5:5:116:LEU:N	2.53	0.42
7:7:185:ASN:HB3	7:7:186:PRO:HD3	2.02	0.42
11:D:117:GLN:HG2	11:D:129:PHE:HB2	2.00	0.42
11:D:71:VAL:HG22	11:D:137:GLY:HA3	2.01	0.42
13:F:12:THR:HG23	14:G:23:GLN:HE21	1.84	0.42
15:H:173:ARG:NE	16:I:129:TYR:HB3	2.35	0.42
15:H:357:ARG:HG2	15:H:359:ASN:H	1.85	0.42
16:I:193:GLU:HB3	16:I:346:ARG:HH12	1.83	0.42
20:M:175:LYS:HE3	20:M:273:LYS:NZ	2.35	0.42
20:M:187:ASP:HA	20:M:190:ILE:HB	2.01	0.42
26:S:440:ASP:HB3	26:S:442:PHE:CE2	2.54	0.42
28:U:121:LEU:HD23	28:U:136:ALA:HA	2.00	0.42
30:W:25:ARG:HG3	30:W:26:PHE:CD2	2.54	0.42
33:Z:621:LEU:O	33:Z:625:THR:OG1	2.29	0.42
2:2:75:ALA:H	2:2:81:THR:HG21	1.85	0.42
7:7:117:GLU:HG2	13:F:140:SER:HA	2.01	0.42
18:K:190:LEU:O	18:K:195:ALA:N	2.53	0.42
21:N:761:ILE:HG23	21:N:767:ALA:H	1.85	0.42
21:N:96:GLN:HB2	26:S:219:LYS:HE3	2.01	0.42
26:S:479:MET:O	26:S:482:PRO:HD2	2.20	0.42
28:U:171:VAL:HB	29:V:217:HIS:HD2	1.85	0.42
29:V:238:LEU:HD22	29:V:242:LYS:HB2	2.01	0.42
33:Z:911:LYS:HE3	33:Z:964:GLU:HB3	2.00	0.42
2:2:242:LEU:N	3:3:199:TYR:O	2.46	0.42
4:4:22:THR:HB	4:4:27:VAL:HG22	2.00	0.42
15:H:70:LYS:O	15:H:74:THR:OG1	2.26	0.42
17:J:393:ASN:OD1	18:K:330:ARG:NH1	2.35	0.42
19:L:290:ARG:HH21	19:L:294:GLY:N	2.16	0.42
29:V:197:TYR:CE2	29:V:199:LEU:HB2	2.54	0.42
29:V:67:ASP:OD1	29:V:68:VAL:N	2.52	0.42
33:Z:598:ALA:HB3	33:Z:738:TYR:HB3	2.02	0.42
5:5:265:ASN:OD1	5:5:266:HIS:N	2.53	0.42
7:7:61:GLY:HA3	7:7:69:PHE:HB2	2.02	0.42
9:B:77:GLY:HA3	9:B:132:VAL:HG12	2.02	0.42
12:E:16:SER:C	12:E:18:GLU:H	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:K:137:VAL:HG12	18:K:149:ILE:HA	2.02	0.42
21:N:102:VAL:HA	21:N:136:ILE:HG21	2.02	0.42
22:O:41:LEU:O	22:O:43:GLU:HG3	2.20	0.42
22:O:44:SER:O	22:O:47:LYS:N	2.53	0.42
25:R:211:LYS:HB3	25:R:230:LEU:HB3	2.02	0.42
28:U:16:LEU:HD22	29:V:213:LEU:HD21	2.01	0.42
2:2:251:ASP:HB3	10:C:226:TYR:CE1	2.55	0.41
7:7:179:PHE:CE2	7:7:221:ASP:HB2	2.55	0.41
9:B:72:GLY:N	9:B:137:ALA:O	2.43	0.41
18:K:237:VAL:O	18:K:271:ILE:HA	2.19	0.41
23:P:268:LEU:HD11	23:P:277:GLN:HG2	2.02	0.41
21:N:325:PHE:HB3	29:V:168:LEU:HD11	2.02	0.41
28:U:71:ASN:ND2	30:W:64:THR:OG1	2.53	0.41
1:1:142:PRO:HB2	1:1:161:PHE:CZ	2.55	0.41
5:5:130:TRP:O	5:5:134:LEU:N	2.49	0.41
9:B:69:PRO:O	9:B:235:PHE:N	2.52	0.41
13:F:129:GLY:HA2	13:F:149:PRO:HB3	2.01	0.41
13:F:11:VAL:HA	14:G:130:ARG:HD3	2.03	0.41
18:K:159:SER:HA	18:K:242:PHE:HA	2.03	0.41
17:J:44:LEU:HD21	18:K:67:TYR:HD2	1.85	0.41
19:L:220:LEU:HD23	19:L:347:VAL:HB	2.02	0.41
21:N:330:THR:HG21	21:N:744:PRO:HG2	2.03	0.41
25:R:78:ASP:OD1	25:R:79:LEU:N	2.53	0.41
26:S:385:SER:O	26:S:389:LYS:HG2	2.20	0.41
30:W:98:LEU:HB3	30:W:108:GLN:NE2	2.35	0.41
33:Z:277:GLU:HG3	33:Z:279:THR:H	1.85	0.41
8:A:19:PHE:O	8:A:20:SER:OG	2.31	0.41
18:K:164:ASN:HB3	18:K:234:PHE:HD2	1.85	0.41
19:L:108:VAL:HA	19:L:119:VAL:HG12	2.02	0.41
20:M:149:ASN:ND2	20:M:152:SER:OG	2.54	0.41
20:M:418:GLY:HA2	20:M:422:VAL:HG11	2.03	0.41
21:N:79:VAL:HG22	21:N:101:ILE:HG23	2.02	0.41
22:O:20:PRO:HD2	22:O:22:LEU:HG	2.01	0.41
23:P:418:ASN:HA	28:U:235:LEU:HD21	2.03	0.41
33:Z:146:PHE:HD2	33:Z:147:GLU:HG3	1.85	0.41
33:Z:869:ASP:OD2	33:Z:978:GLU:N	2.52	0.41
7:7:115:ASP:OD1	7:7:116:ALA:N	2.53	0.41
13:F:4:ASN:C	13:F:6:TYR:H	2.22	0.41
13:F:50:LYS:HG2	13:F:61:LYS:HA	2.02	0.41
20:M:224:PRO:O	20:M:387:ASN:ND2	2.54	0.41
21:N:63:LEU:HD22	21:N:88:ARG:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:127:LEU:HB2	22:O:167:ILE:HG12	2.01	0.41
22:O:308:LEU:HB3	22:O:348:VAL:HB	2.01	0.41
26:S:377:TYR:CE2	27:T:133:ILE:HG21	2.55	0.41
27:T:54:ASP:O	27:T:58:THR:HG23	2.21	0.41
30:W:101:ARG:HH22	30:W:106:GLN:HB2	1.86	0.41
10:C:38:ILE:HG21	10:C:189:ALA:HB1	2.03	0.41
11:D:203:VAL:HG21	11:D:210:ILE:HG12	2.02	0.41
12:E:20:ARG:HG2	20:M:430:VAL:HB	2.03	0.41
15:H:403:ARG:HE	15:H:405:GLU:HB2	1.86	0.41
18:K:159:SER:HG	18:K:244:HIS:HE2	1.68	0.41
18:K:290:ARG:HB3	18:K:294:ARG:HH12	1.84	0.41
18:K:55:GLU:HA	18:K:58:TYR:HD2	1.86	0.41
25:R:77:SER:OG	25:R:86:ASP:N	2.54	0.41
26:S:424:SER:O	26:S:428:ARG:HG2	2.20	0.41
3:3:25:CYS:HB2	3:3:42:LYS:HZ3	1.85	0.41
9:B:32:VAL:HG21	9:B:63:LYS:NZ	2.34	0.41
19:L:129:VAL:HG11	19:L:148:LEU:HD22	2.02	0.41
19:L:252:VAL:HG23	19:L:286:ILE:HG22	2.03	0.41
20:M:170:MET:HG3	20:M:245:LYS:O	2.21	0.41
25:R:311:THR:O	25:R:315:VAL:HB	2.21	0.41
27:T:132:HIS:O	27:T:136:LEU:HB3	2.19	0.41
33:Z:87:LYS:HD3	33:Z:90:LYS:HG3	2.02	0.41
8:A:168:ALA:HB3	9:B:55:LEU:HD13	2.01	0.41
8:A:30:TYR:HD1	8:A:33:LYS:HD2	1.86	0.41
14:G:12:ASN:HB3	14:G:127:ASN:HA	2.02	0.41
15:H:243:PRO:HG3	20:M:396:VAL:HG11	2.03	0.41
20:M:290:ARG:H	20:M:332:VAL:HG21	1.86	0.41
19:L:95:ILE:HD13	20:M:68:LYS:HE3	2.02	0.41
21:N:376:LYS:HA	21:N:411:ILE:HG12	2.02	0.41
21:N:641:LEU:HD23	21:N:644:LEU:HD12	2.03	0.41
25:R:335:ARG:CZ	25:R:376:GLN:HB3	2.50	0.41
28:U:192:ASN:HB2	29:V:230:TYR:CD2	2.56	0.41
33:Z:599:ILE:O	33:Z:603:VAL:HG13	2.20	0.41
33:Z:911:LYS:HG3	33:Z:964:GLU:HB2	2.02	0.41
3:3:27:LEU:HD12	3:3:184:GLY:HA3	2.02	0.41
8:A:50:CYS:SG	8:A:51:THR:N	2.94	0.41
9:B:82:TYR:CZ	9:B:86:VAL:HG21	2.56	0.41
8:A:135:ARG:HD3	14:G:125:LEU:HA	2.03	0.41
14:G:21:ASN:OD1	14:G:22:PHE:N	2.53	0.41
16:I:361:ILE:HG13	16:I:389:GLY:HA2	2.03	0.41
18:K:271:ILE:HD12	18:K:316:MET:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:M:256:ILE:HG21	20:M:303:ARG:NH1	2.35	0.41
21:N:162:ARG:HE	21:N:164:ASP:HB3	1.86	0.41
22:O:72:LYS:HG2	22:O:73:ILE:HG12	2.03	0.41
22:O:333:SER:HB2	23:P:304:THR:HG22	2.03	0.41
26:S:461:PHE:HB3	28:U:277:TYR:CE1	2.56	0.41
1:1:108:ASN:O	1:1:112:LEU:N	2.54	0.41
2:2:171:TRP:HB2	2:2:183:LEU:HD21	2.02	0.41
4:4:23:ARG:NH2	5:5:191:ASP:OD2	2.54	0.41
5:5:271:LEU:HD23	5:5:274:LYS:HD2	2.03	0.41
9:B:204:PHE:HD1	9:B:247:LEU:HD13	1.85	0.41
9:B:71:ILE:HA	9:B:138:GLY:HA2	2.02	0.41
17:J:219:VAL:HG22	17:J:268:VAL:HG11	2.02	0.41
18:K:164:ASN:OD1	18:K:165:GLU:N	2.54	0.41
20:M:129:LEU:HD11	20:M:155:ILE:HD12	2.02	0.41
21:N:214:LEU:HB2	21:N:225:LEU:HD21	2.02	0.41
22:O:318:HIS:ND1	22:O:318:HIS:O	2.54	0.41
22:O:371:VAL:O	22:O:375:ASP:N	2.49	0.41
22:O:62:TYR:HB2	22:O:69:PHE:HZ	1.85	0.41
28:U:56:PHE:CE2	28:U:58:GLU:HB2	2.56	0.41
33:Z:211:PHE:CG	33:Z:220:ALA:HB2	2.56	0.41
2:2:36:LYS:HD2	2:2:152:TYR:HA	2.03	0.41
3:3:4:PRO:HA	3:3:7:ILE:HD12	2.01	0.41
8:A:87:ILE:N	8:A:88:PRO:HD2	2.36	0.41
12:E:52:LYS:O	12:E:53:ARG:HB2	2.21	0.41
22:O:39:PHE:HB2	22:O:52:ALA:HB2	2.01	0.41
24:Q:347:LEU:HD22	24:Q:377:LEU:HD13	2.03	0.41
26:S:30:GLN:OE1	26:S:64:ARG:NH2	2.54	0.41
22:O:120:LYS:HG2	30:W:81:ILE:HB	2.02	0.41
33:Z:181:GLY:HA3	33:Z:266:LYS:HG3	2.03	0.41
2:2:206:VAL:N	2:2:214:GLU:O	2.37	0.41
3:3:26:ASP:OD1	3:3:42:LYS:NZ	2.54	0.41
10:C:70:ASN:HD21	10:C:73:ILE:HD12	1.85	0.41
18:K:290:ARG:CB	18:K:294:ARG:HH12	2.34	0.41
19:L:364:HIS:CD2	19:L:392:ARG:HE	2.38	0.41
22:O:41:LEU:HD22	22:O:82:LEU:HA	2.03	0.41
23:P:283:LYS:HD2	23:P:286:ASN:HD21	1.85	0.41
25:R:146:ASP:OD2	25:R:149:ASN:ND2	2.36	0.41
25:R:382:ASP:OD1	25:R:383:ARG:N	2.53	0.41
25:R:72:VAL:O	25:R:72:VAL:HG12	2.20	0.41
28:U:21:HIS:NE2	29:V:100:ARG:HD2	2.35	0.41
28:U:79:MET:HG3	29:V:72:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:510:HIS:CE1	29:V:61:TYR:HB3	2.56	0.41
2:2:32:ILE:HD13	2:2:73:ALA:HB1	2.02	0.40
4:4:41:HIS:HB2	4:4:74:GLU:OE2	2.21	0.40
14:G:66:LYS:HE2	14:G:82:ILE:HG12	2.02	0.40
19:L:287:GLY:HA2	19:L:305:LEU:HD21	2.03	0.40
19:L:283:VAL:HG23	19:L:333:LEU:HD21	2.02	0.40
21:N:28:ILE:O	21:N:32:VAL:HG13	2.21	0.40
22:O:99:LEU:O	22:O:103:LYS:HB3	2.21	0.40
26:S:417:GLN:NE2	27:T:208:LEU:HA	2.35	0.40
29:V:57:PHE:CG	29:V:63:VAL:HA	2.55	0.40
30:W:38:GLN:HG3	30:W:42:ASN:HD22	1.86	0.40
33:Z:290:GLU:HB3	33:Z:293:MET:HG3	2.02	0.40
6:6:46:THR:OG1	6:6:219:ASP:O	2.39	0.40
12:E:18:GLU:HB3	20:M:426:LYS:HD2	2.03	0.40
21:N:416:GLY:HA3	21:N:453:ALA:HB1	2.03	0.40
24:Q:389:VAL:HG23	24:Q:398:TYR:HB2	2.03	0.40
33:Z:217:GLU:HA	33:Z:220:ALA:HB3	2.02	0.40
1:1:167:LYS:HD2	1:1:196:VAL:HG11	2.02	0.40
2:2:47:THR:HB	2:2:59:ASN:HA	2.03	0.40
3:3:76:LEU:HD13	10:C:92:ARG:HD3	2.04	0.40
8:A:86:PRO:HD2	8:A:139:VAL:HG12	2.04	0.40
14:G:16:SER:OG	14:G:20:ARG:O	2.37	0.40
20:M:246:LEU:HD22	20:M:262:LEU:HD13	2.03	0.40
21:N:4:THR:HG22	21:N:27:SER:HB3	2.04	0.40
21:N:650:ASP:OD1	21:N:651:PHE:N	2.53	0.40
22:O:277:ILE:HG22	22:O:279:ILE:H	1.85	0.40
25:R:353:MET:HA	25:R:357:PHE:CD2	2.56	0.40
5:5:106:VAL:HG22	6:6:151:GLU:HG2	2.03	0.40
15:H:357:ARG:HH21	15:H:359:ASN:HD22	1.67	0.40
16:I:206:GLU:HA	16:I:209:GLU:HB2	2.02	0.40
20:M:283:LEU:O	20:M:287:GLY:N	2.53	0.40
21:N:13:LEU:HA	21:N:21:LYS:HE2	2.03	0.40
21:N:344:THR:HG22	21:N:375:HIS:HA	2.03	0.40
24:Q:219:ASP:HB3	24:Q:238:TYR:HB3	2.03	0.40
2:2:189:GLN:HB2	2:2:220:LEU:HD21	2.02	0.40
9:B:9:LEU:O	10:C:129:ARG:HD3	2.22	0.40
17:J:44:LEU:HD13	18:K:68:ILE:HG12	2.03	0.40
20:M:121:THR:HG21	20:M:153:TYR:HD1	1.86	0.40
21:N:423:LEU:HB2	21:N:450:ILE:HD13	2.04	0.40
28:U:20:ASP:OD2	28:U:24:ARG:NH2	2.55	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	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
1	b	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
2	2	224/261 (86%)	215 (96%)	9 (4%)	0	100	100
2	i	224/261 (86%)	217 (97%)	7 (3%)	0	100	100
3	3	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
3	h	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
4	4	193/198 (98%)	189 (98%)	4 (2%)	0	100	100
4	g	193/198 (98%)	186 (96%)	7 (4%)	0	100	100
5	5	210/287 (73%)	205 (98%)	5 (2%)	0	100	100
5	f	210/287 (73%)	203 (97%)	7 (3%)	0	100	100
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	227/266 (85%)	218 (96%)	9 (4%)	0	100	100
7	a	230/266 (86%)	221 (96%)	9 (4%)	0	100	100
8	A	239/252 (95%)	229 (96%)	10 (4%)	0	100	100
8	c	239/252 (95%)	234 (98%)	5 (2%)	0	100	100
9	B	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
9	j	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
10	C	242/258 (94%)	235 (97%)	7 (3%)	0	100	100
10	d	242/258 (94%)	231 (96%)	10 (4%)	1 (0%)	36	77
11	D	238/254 (94%)	226 (95%)	12 (5%)	0	100	100
11	n	238/254 (94%)	228 (96%)	10 (4%)	0	100	100
12	E	240/260 (92%)	226 (94%)	13 (5%)	1 (0%)	36	77
12	m	240/260 (92%)	230 (96%)	9 (4%)	1 (0%)	36	77
13	F	231/234 (99%)	218 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	l	229/234 (98%)	225 (98%)	4 (2%)	0	100	100
14	G	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
14	k	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
15	H	353/467 (76%)	316 (90%)	37 (10%)	0	100	100
16	I	361/437 (83%)	333 (92%)	28 (8%)	0	100	100
17	J	371/405 (92%)	351 (95%)	20 (5%)	0	100	100
18	K	379/428 (89%)	347 (92%)	32 (8%)	0	100	100
19	L	359/437 (82%)	334 (93%)	25 (7%)	0	100	100
20	M	363/434 (84%)	332 (92%)	29 (8%)	2 (1%)	27	70
21	N	843/945 (89%)	793 (94%)	46 (6%)	4 (0%)	31	74
22	O	385/393 (98%)	342 (89%)	42 (11%)	1 (0%)	43	81
23	P	430/445 (97%)	391 (91%)	39 (9%)	0	100	100
24	Q	429/434 (99%)	397 (92%)	32 (8%)	0	100	100
25	R	398/429 (93%)	357 (90%)	38 (10%)	3 (1%)	21	65
26	S	473/523 (90%)	451 (95%)	21 (4%)	1 (0%)	49	85
27	T	270/274 (98%)	238 (88%)	32 (12%)	0	100	100
28	U	245/338 (72%)	242 (99%)	2 (1%)	1 (0%)	36	77
29	V	282/306 (92%)	242 (86%)	37 (13%)	3 (1%)	16	58
30	W	195/268 (73%)	176 (90%)	16 (8%)	3 (2%)	11	51
31	X	109/156 (70%)	96 (88%)	13 (12%)	0	100	100
32	Y	25/89 (28%)	18 (72%)	6 (24%)	1 (4%)	3	29
33	Z	807/993 (81%)	740 (92%)	67 (8%)	0	100	100
All	All	13376/15139 (88%)	12565 (94%)	789 (6%)	22 (0%)	53	85

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	N	180	SER
21	N	874	ILE
28	U	130	VAL
30	W	22	PRO
10	d	207	THR
12	m	53	ARG
32	Y	69	VAL

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Mol	Chain	Res	Type
12	E	12	VAL
21	N	761	ILE
21	N	903	VAL
25	R	241	ILE
25	R	421	VAL
29	V	189	ILE
29	V	305	ILE
30	W	147	ILE
20	M	167	VAL
25	R	72	VAL
26	S	83	PRO
20	M	422	VAL
22	O	227	ILE
29	V	271	VAL
30	W	118	ILE

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	162/178 (91%)	162 (100%)	0	100	100
1	b	162/178 (91%)	162 (100%)	0	100	100
2	2	185/214 (86%)	185 (100%)	0	100	100
2	i	185/214 (86%)	185 (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	173/175 (99%)	173 (100%)	0	100	100
4	g	173/175 (99%)	173 (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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	7	195/224 (87%)	195 (100%)	0	100	100
7	a	198/224 (88%)	198 (100%)	0	100	100
8	A	206/210 (98%)	206 (100%)	0	100	100
8	c	206/210 (98%)	206 (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	212/226 (94%)	212 (100%)	0	100	100
11	n	212/226 (94%)	212 (100%)	0	100	100
12	E	198/215 (92%)	197 (100%)	1 (0%)	90	95
12	m	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	l	190/193 (98%)	190 (100%)	0	100	100
14	G	201/239 (84%)	201 (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	308/377 (82%)	308 (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
27	T	254/256 (99%)	254 (100%)	0	100	100
28	U	234/308 (76%)	234 (100%)	0	100	100
29	V	249/268 (93%)	249 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	11624/13054 (89%)	11623 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	E	52	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	47	ASN
2	2	95	HIS
2	2	114	GLN
2	2	120	GLN
3	3	145	GLN
3	3	169	GLN
4	4	63	ASN
6	6	55	ASN
6	6	127	HIS
7	7	35	GLN
7	7	95	HIS
7	7	107	ASN
2	i	114	GLN
2	i	115	HIS
2	i	122	HIS
4	g	55	GLN
4	g	61	GLN
4	g	86	GLN
4	g	147	HIS
4	g	191	GLN
5	f	104	GLN
5	f	208	GLN
6	e	171	ASN
6	e	177	ASN
7	a	59	ASN
7	a	111	ASN

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Mol	Chain	Res	Type
7	a	145	ASN
9	B	119	GLN
10	C	120	GLN
10	C	227	GLN
11	D	79	ASN
11	D	117	GLN
11	D	122	GLN
11	D	178	ASN
12	E	147	HIS
12	E	180	GLN
13	F	4	ASN
13	F	21	GLN
13	F	117	GLN
14	G	23	GLN
14	G	64	ASN
14	G	182	HIS
9	j	123	GLN
11	n	117	GLN
11	n	118	GLN
11	n	204	GLN
12	m	180	GLN
14	k	204	HIS
15	H	217	GLN
17	J	66	GLN
17	J	111	GLN
17	J	240	HIS
17	J	278	GLN
20	M	53	HIS
20	M	74	GLN
21	N	329	HIS
21	N	340	HIS
21	N	375	HIS
21	N	707	ASN
21	N	738	GLN
22	O	4	ASN
22	O	354	GLN
23	P	286	ASN
23	P	337	HIS
24	Q	54	GLN
24	Q	145	HIS
24	Q	178	HIS
24	Q	226	HIS

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Mol	Chain	Res	Type
24	Q	404	ASN
25	R	397	ASN
25	R	415	GLN
26	S	135	ASN
26	S	227	ASN
26	S	290	ASN
26	S	311	GLN
26	S	317	HIS
26	S	321	GLN
26	S	334	HIS
26	S	347	HIS
26	S	417	GLN
27	T	236	ASN
29	V	73	GLN
30	W	170	HIS
31	X	38	ASN
31	X	94	ASN
33	Z	577	GLN
33	Z	899	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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.