



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 12:17 PM UTC

PDB ID : 8D6X / pdb_00008d6x
EMDB ID : EMD-27225
Title : Structure of the Mycobacterium tuberculosis 20S proteasome bound to the ATP-bound Mpa ATPase
Authors : Xiao, X.; Li, H.
Deposited on : 2022-06-06
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

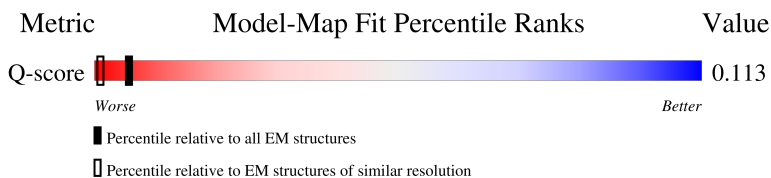
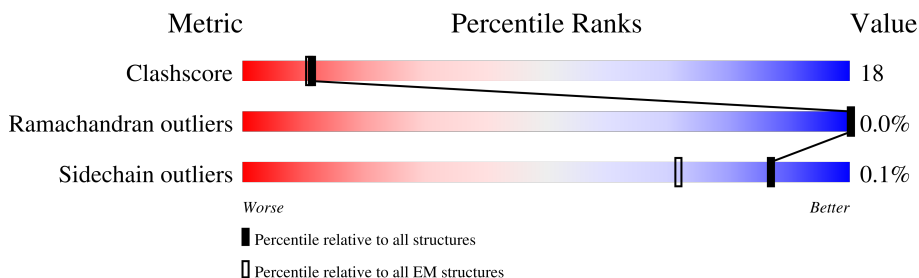
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	609	 52% 25% 23%
1	B	609	 55% 24% 22%
1	C	609	 50% 26% 24%
1	D	609	 46% 28% 26%

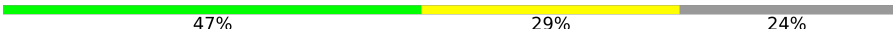
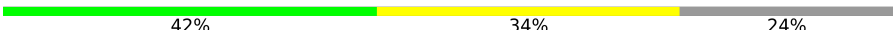
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Mol	Chain	Length	Quality of chain
1	E	609	
1	F	609	
2	G	248	
2	H	248	
2	I	248	
2	J	248	
2	K	248	
2	L	248	
2	M	248	
2	N	248	
2	O	248	
2	k	248	
2	l	248	
2	m	248	
2	n	248	
2	o	248	
3	P	291	
3	Q	291	
3	R	291	
3	S	291	
3	T	291	
3	U	291	
3	V	291	
3	W	291	
3	X	291	

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Mol	Chain	Length	Quality of chain
3	Y	291	
3	Z	291	
3	a	291	
3	b	291	
3	c	291	
4	d	4	
4	e	4	
4	f	4	
4	g	4	
4	h	4	
4	i	4	
4	j	4	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 68362 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 AAA ATPase forming ring-shaped complexes.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	466	Total	C	N	O	S	0	0
			3650	2306	630	703	11		
1	B	476	Total	C	N	O	S	0	0
			3719	2343	642	723	11		
1	C	464	Total	C	N	O	S	0	0
			3629	2291	625	702	11		
1	D	452	Total	C	N	O	S	0	0
			3542	2242	607	682	11		
1	E	476	Total	C	N	O	S	0	0
			3719	2343	642	723	11		
1	F	477	Total	C	N	O	S	0	0
			3723	2345	643	724	11		

- Molecule 2 is a protein called Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	l	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	m	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	n	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	o	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	G	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	H	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	I	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	J	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	L	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	M	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	N	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		
2	O	215	Total	C	N	O	S	0	0
			1658	1039	303	313	3		

- Molecule 3 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	Q	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	R	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	S	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	T	222	Total	C	N	O	S	0	0
			1636	1026	282	323	5		
3	U	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	V	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	W	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	X	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	Y	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	Z	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	a	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	b	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		
3	c	222	Total	C	N	O	S	0	0
			1638	1027	282	324	5		

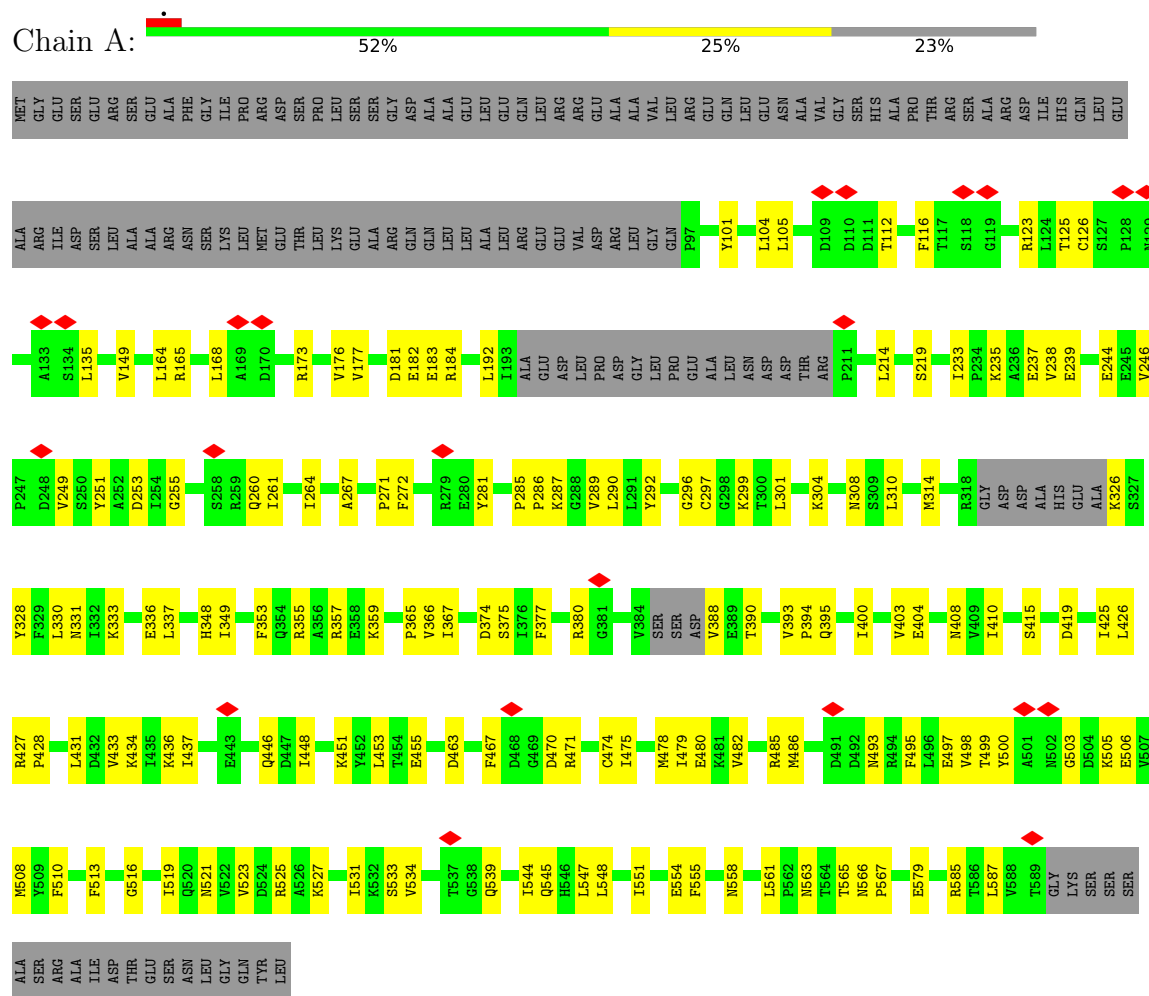
- Molecule 4 is a protein called Proteasome-associated ATPase.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	d	4	Total	C	N	O	0	0
			34	22	5	7		
4	e	4	Total	C	N	O	0	0
			34	22	5	7		
4	f	4	Total	C	N	O	0	0
			34	22	5	7		
4	g	4	Total	C	N	O	0	0
			34	22	5	7		
4	h	4	Total	C	N	O	0	0
			34	22	5	7		
4	i	4	Total	C	N	O	0	0
			34	22	5	7		
4	j	4	Total	C	N	O	0	0
			34	22	5	7		

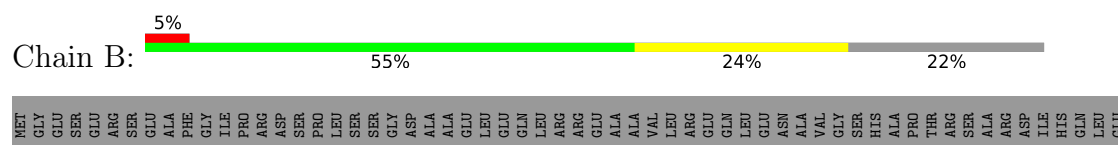
3 Residue-property plots

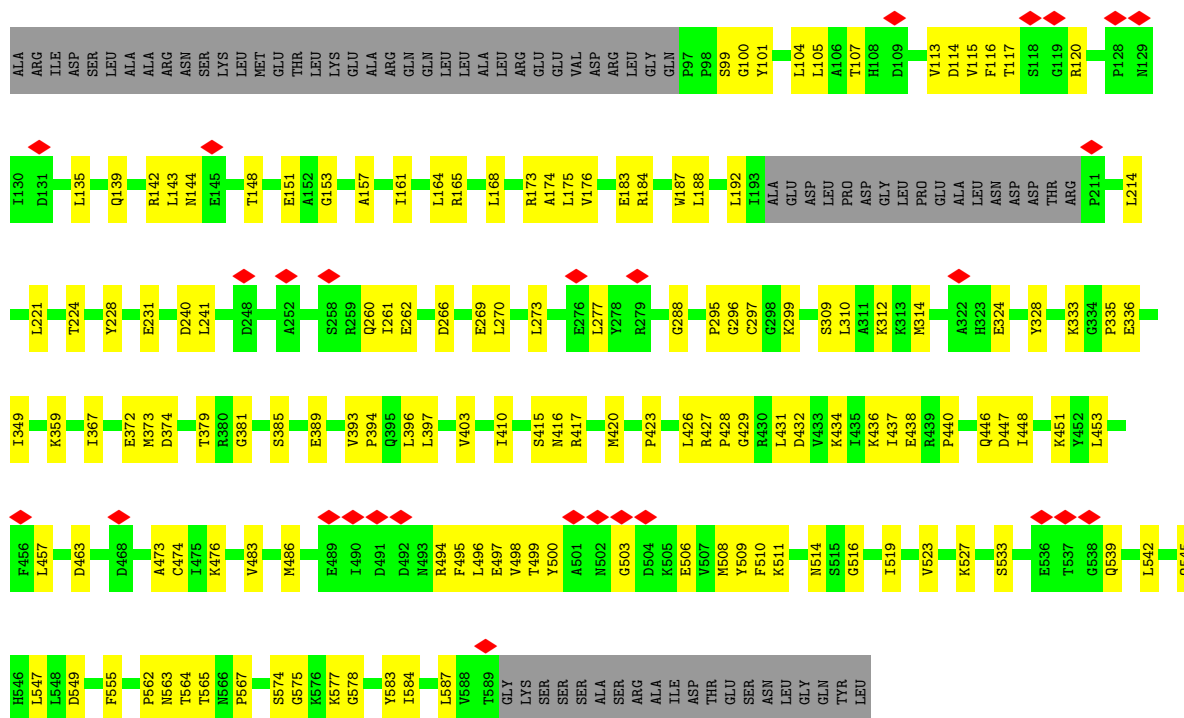
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: AAA ATPase forming ring-shaped complexes

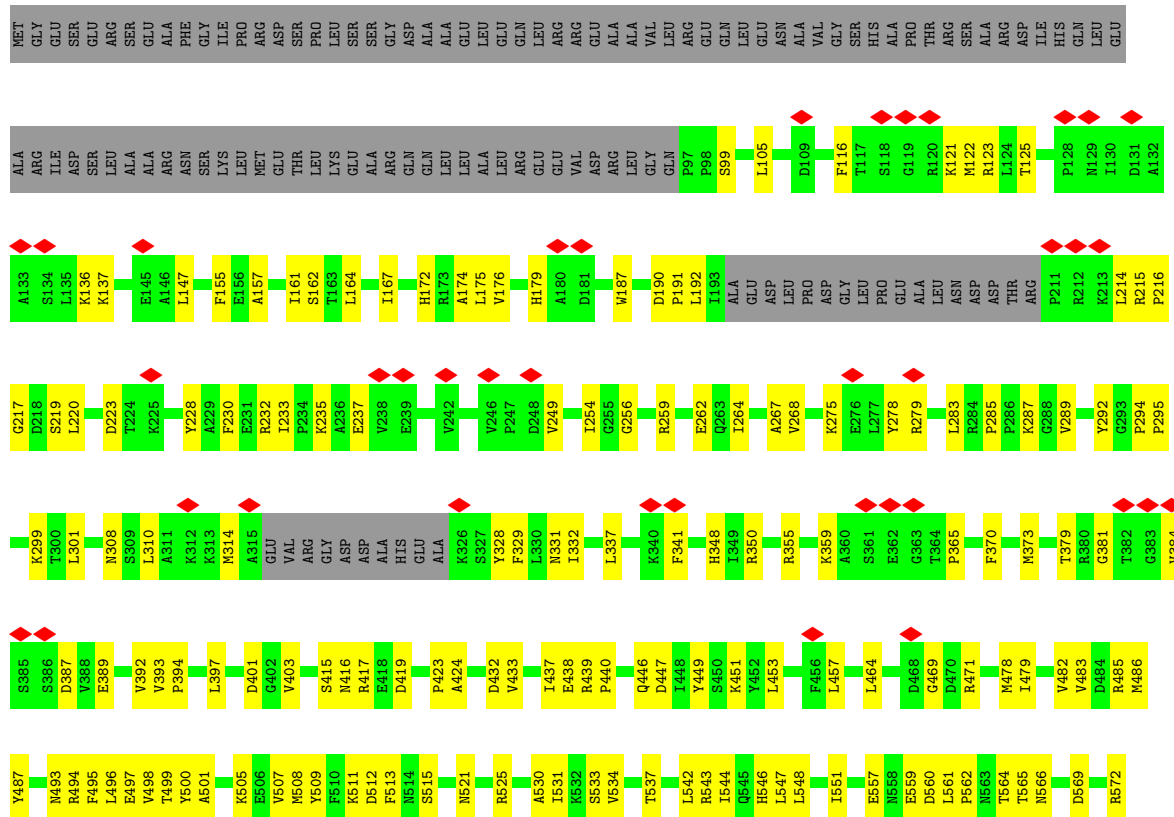


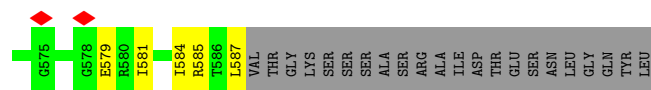
- Molecule 1: AAA ATPase forming ring-shaped complexes



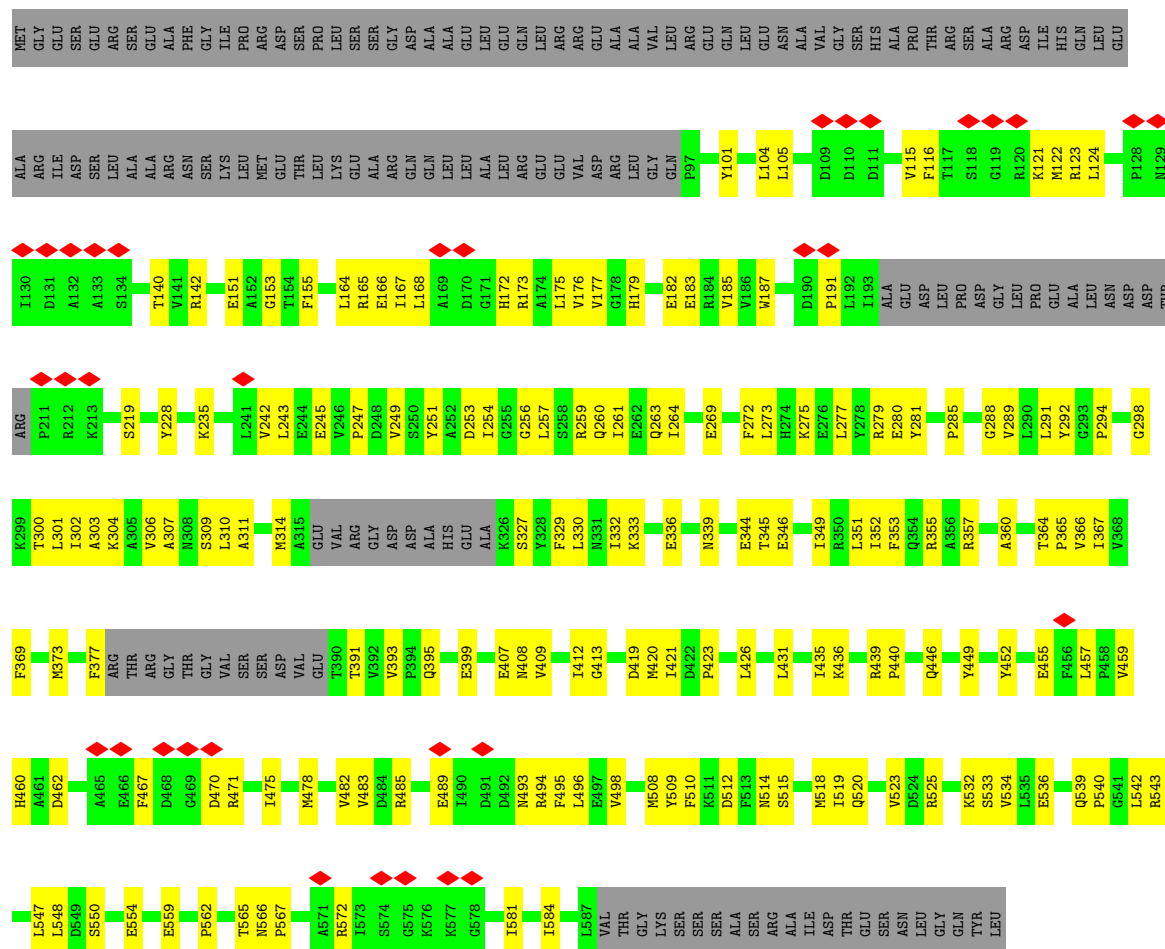


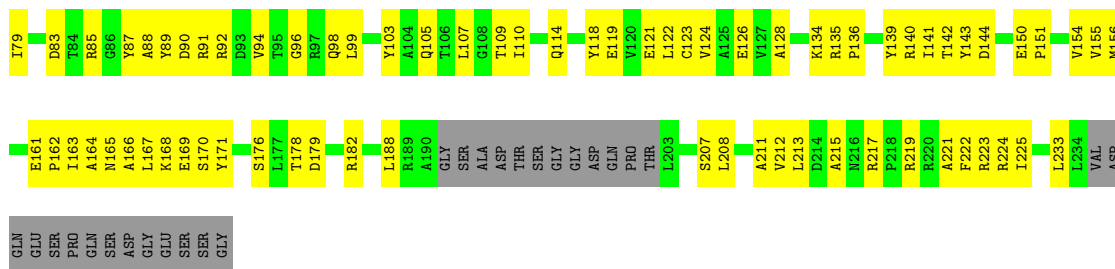
• Molecule 1: AAA ATPase forming ring-shaped complexes



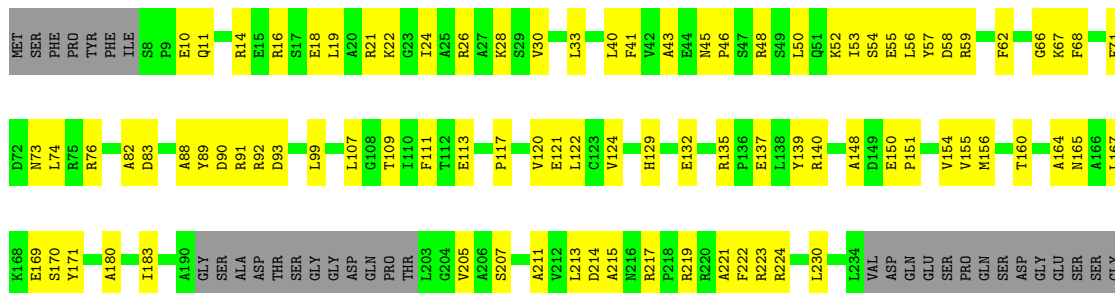


- Molecule 1: AAA ATPase forming ring-shaped complexes

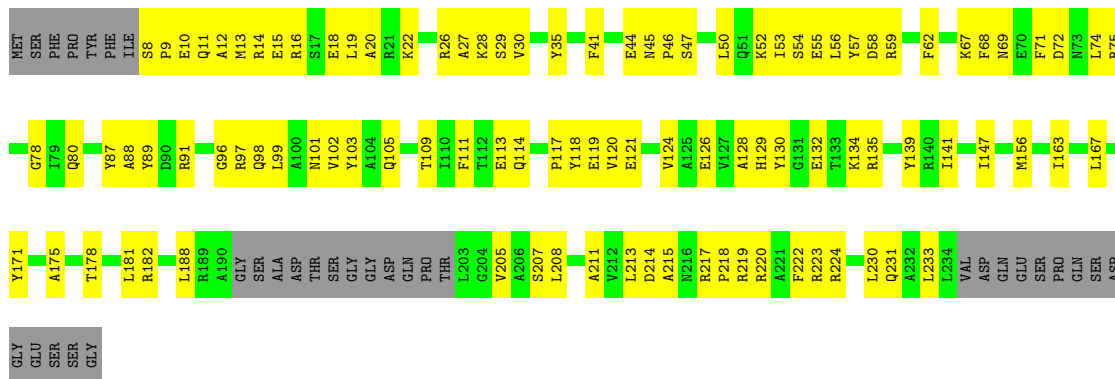




- Molecule 2: Proteasome subunit alpha



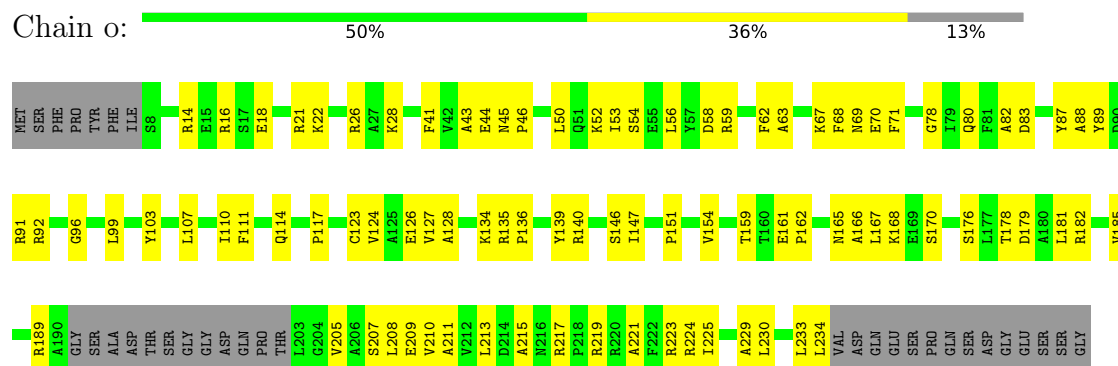
- Molecule 2: Proteasome subunit alpha



- Molecule 2: Proteasome subunit alpha



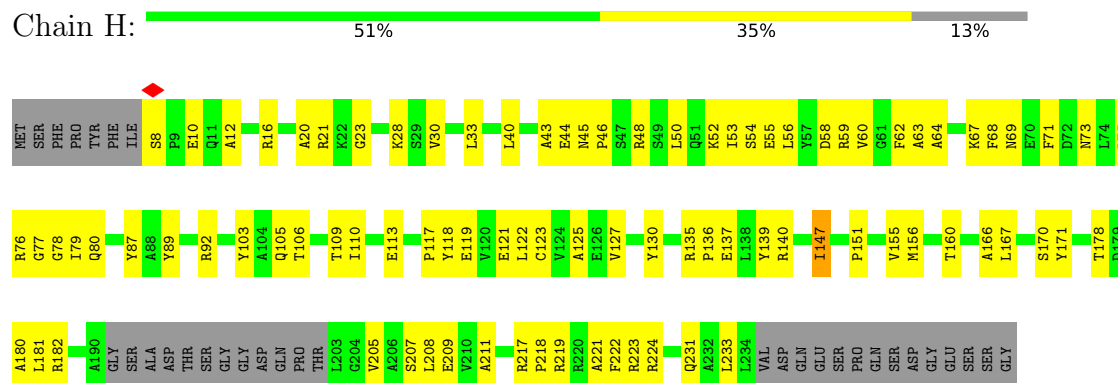
- Molecule 2: Proteasome subunit alpha



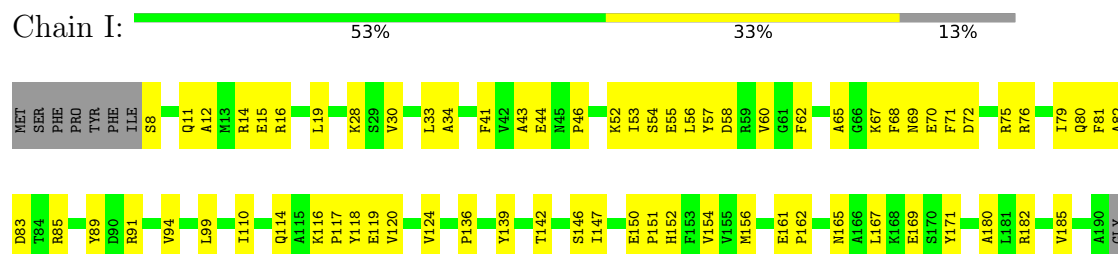
- Molecule 2: Proteasome subunit alpha



- Molecule 2: Proteasome subunit alpha

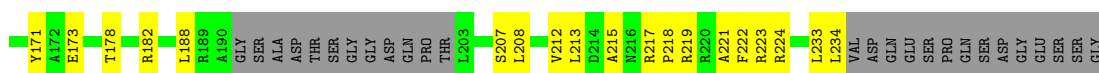


- Molecule 2: Proteasome subunit alpha

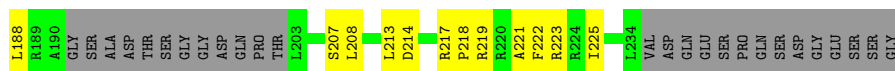
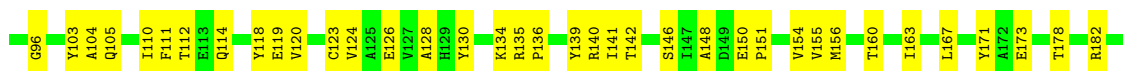
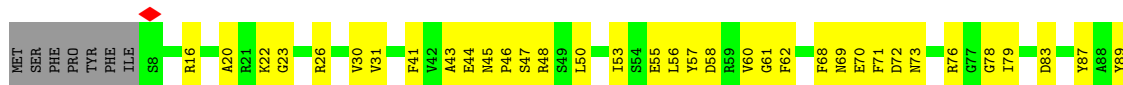




• Molecule 2: Proteasome subunit alpha



• Molecule 2: Proteasome subunit alpha

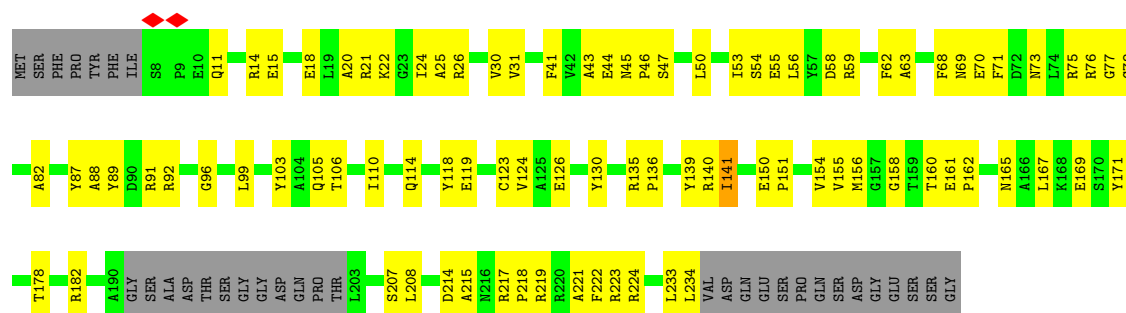


• Molecule 2: Proteasome subunit alpha



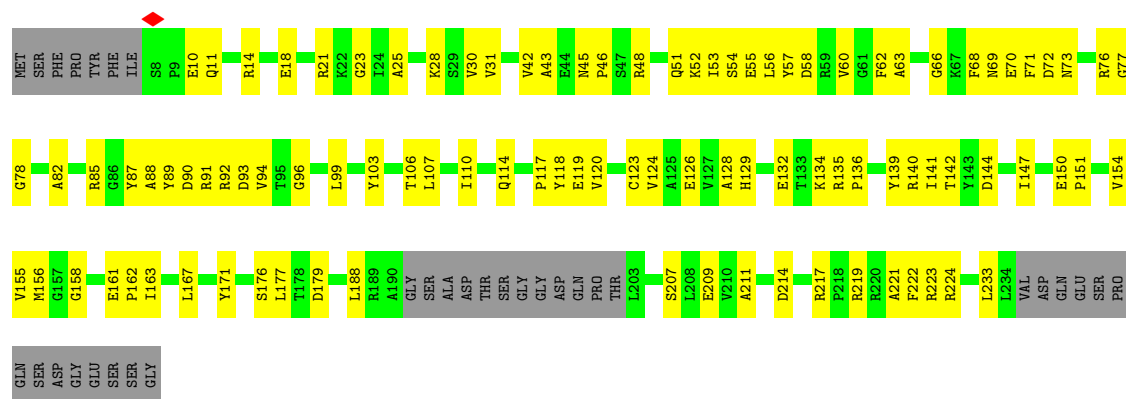
• Molecule 2: Proteasome subunit alpha





• Molecule 2: Proteasome subunit alpha

Chain N: 47% 40% 13%



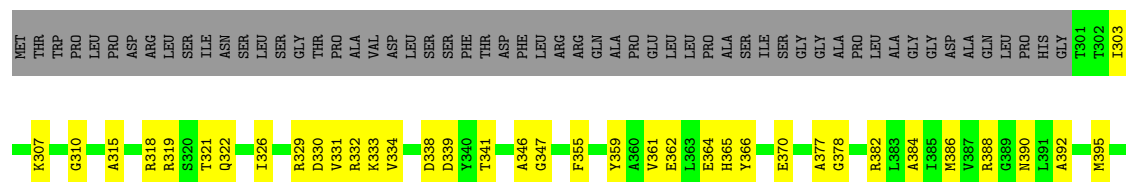
• Molecule 2: Proteasome subunit alpha

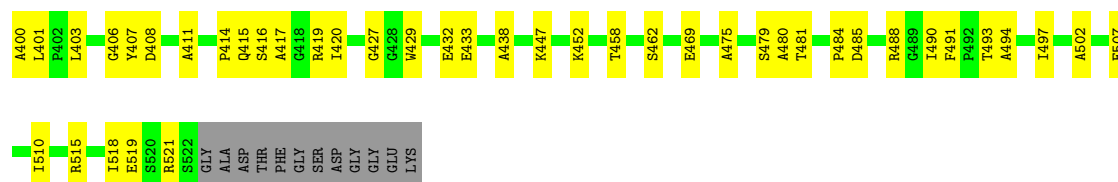
Chain O: 49% 38% 13%



• Molecule 3: Proteasome subunit beta

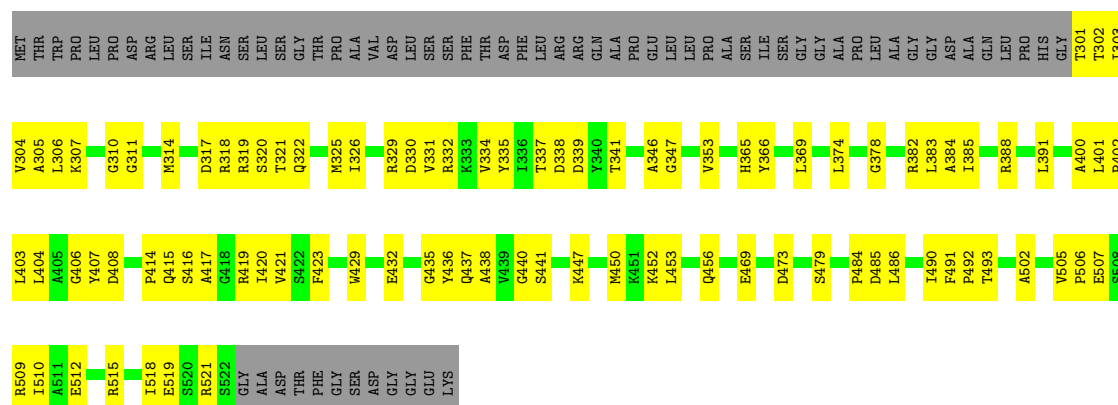
Chain P: 49% 27% 24%





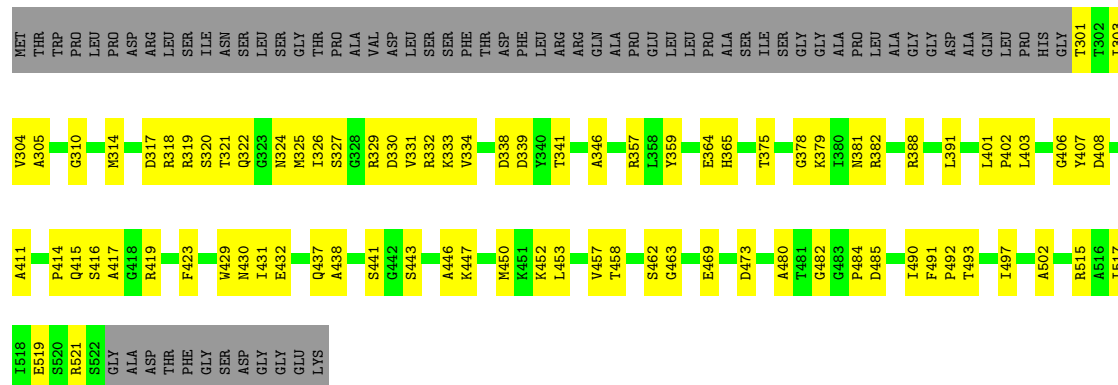
• Molecule 3: Proteasome subunit beta

Chain Q: 45% 32% 24%



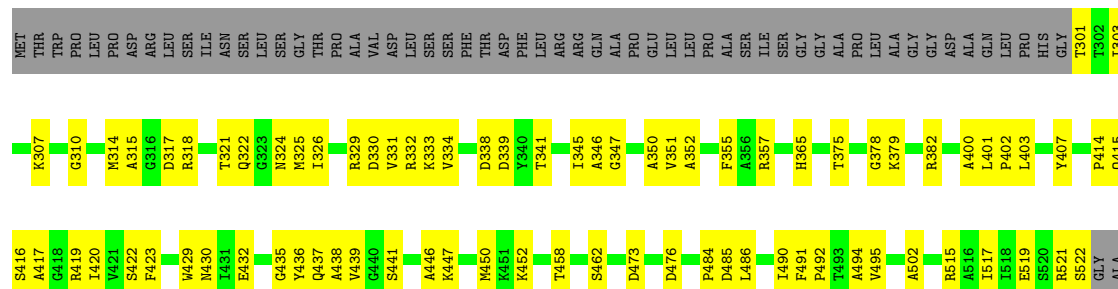
• Molecule 3: Proteasome subunit beta

Chain R: 48% 29% 24%



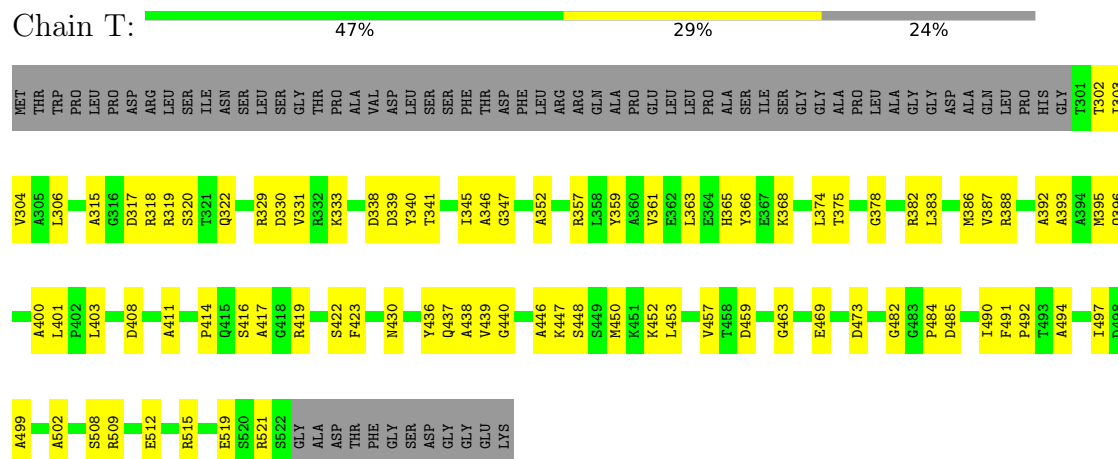
• Molecule 3: Proteasome subunit beta

Chain S: 49% 27% 24%

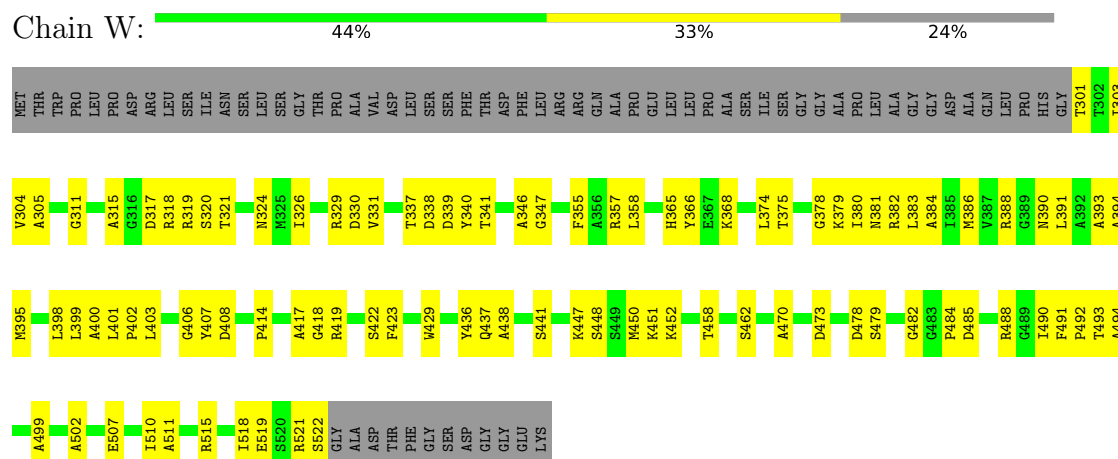


ASP
THR
TRP
PHE
GLY
SER
ASP
GLY
GLY
LYS

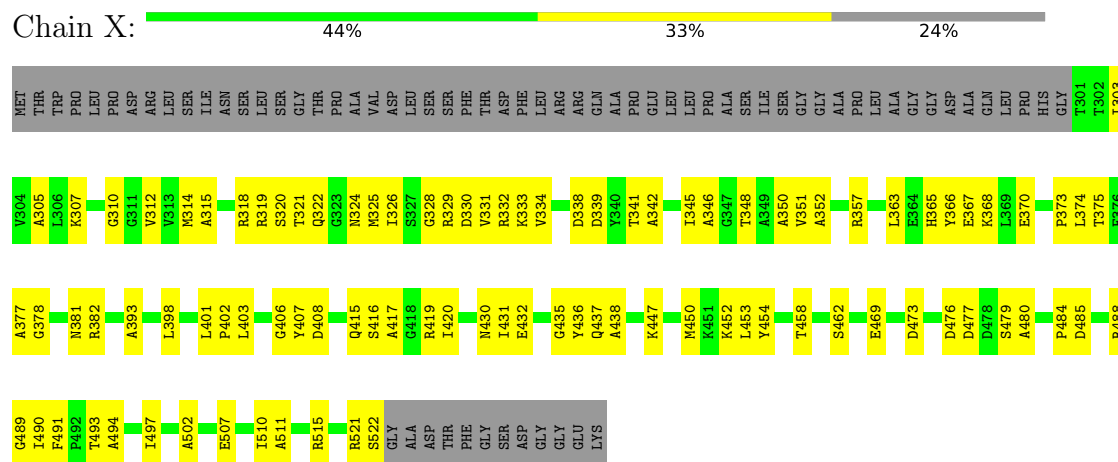
● Molecule 3: Proteasome subunit beta



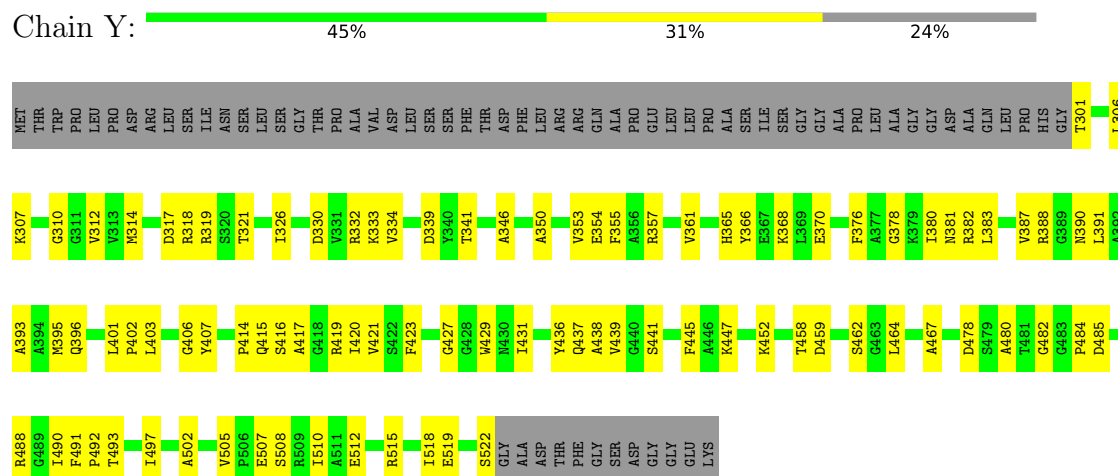
- Molecule 3: Proteasome subunit beta



- Molecule 3: Proteasome subunit beta



- Molecule 3: Proteasome subunit beta



- Molecule 3: Proteasome subunit beta

Digital Tool Type	Percentage
Digital tools for learning	52%
Digital tools for teaching	24%
Digital tools for assessment	24%



Response	Percentage
Best for the country	47%
Not the best for the country	29%
Don't know	24%

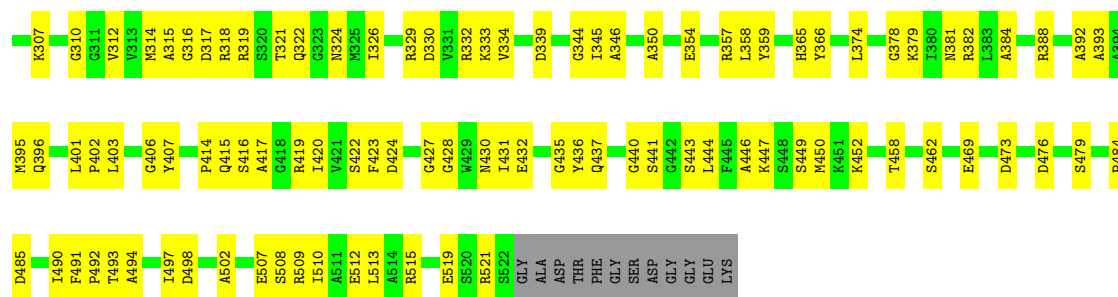


Response	Percentage
Best for the country	51%
Not the best for the country	26%
Don't know	24%



Digital Tool Type	Percentage
Green Segment	42%
Yellow Segment	34%
Grey Segment	24%





- Molecule 4: Proteasome-associated ATPase



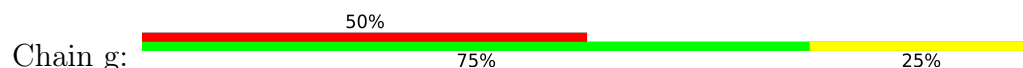
- Molecule 4: Proteasome-associated ATPase



- Molecule 4: Proteasome-associated ATPase



- Molecule 4: Proteasome-associated ATPase



- Molecule 4: Proteasome-associated ATPase

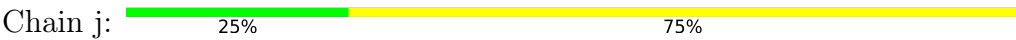


- Molecule 4: Proteasome-associated ATPase





● Molecule 4: Proteasome-associated ATPase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	213000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.2	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	25.608	Depositor
Minimum map value	-13.771	Depositor
Average map value	-0.122	Depositor
Map value standard deviation	1.501	Depositor
Recommended contour level	3.2	Depositor
Map size ($\text{\AA}$)	440.832, 440.832, 440.832	wwPDB
Map dimensions	96, 96, 96	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	4.592, 4.592, 4.592	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 >5	RMSZ	# Z >5
1	A	0.14	0/3709	0.32	0/5015
1	B	0.11	0/3781	0.31	0/5116
1	C	0.13	0/3689	0.32	0/4989
1	D	0.18	0/3601	0.37	0/4869
1	E	0.12	0/3781	0.28	0/5116
1	F	0.11	0/3785	0.28	0/5121
2	G	0.24	0/1683	0.43	0/2274
2	H	0.31	0/1683	0.47	0/2274
2	I	0.22	0/1683	0.43	0/2274
2	J	0.12	0/1683	0.33	0/2274
2	K	0.25	0/1683	0.40	0/2274
2	L	0.13	0/1683	0.35	0/2274
2	M	0.20	0/1683	0.38	0/2274
2	N	0.24	0/1683	0.42	0/2274
2	O	0.14	0/1683	0.36	0/2274
2	k	0.12	0/1683	0.33	0/2274
2	l	0.22	0/1683	0.41	0/2274
2	m	0.22	0/1683	0.44	0/2274
2	n	0.19	0/1683	0.41	0/2274
2	o	0.26	0/1683	0.41	0/2274
3	P	0.17	0/1662	0.38	0/2254
3	Q	0.13	0/1662	0.38	0/2254
3	R	0.14	0/1662	0.36	0/2254
3	S	0.14	0/1662	0.36	0/2254
3	T	0.15	0/1660	0.40	0/2251
3	U	0.19	0/1662	0.37	0/2254
3	V	0.24	0/1662	0.44	0/2254
3	W	0.23	0/1662	0.43	0/2254
3	X	0.17	0/1662	0.42	0/2254
3	Y	0.15	0/1662	0.37	0/2254
3	Z	0.33	0/1662	0.51	0/2254
3	a	0.13	0/1662	0.33	0/2254
3	b	0.15	0/1662	0.38	0/2254
3	c	0.14	0/1662	0.36	0/2254

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	d	0.14	0/34	0.32	0/43
4	e	0.15	0/34	0.36	0/43
4	f	0.11	0/34	0.26	0/43
4	g	0.12	0/34	0.32	0/43
4	h	0.21	0/34	0.47	0/43
4	i	0.12	0/34	0.33	0/43
4	j	0.14	0/34	0.46	0/43
All	All	0.18	0/69412	0.37	0/93916

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3650	0	3678	113	0
1	B	3719	0	3728	104	0
1	C	3629	0	3649	125	0
1	D	3542	0	3564	141	0
1	E	3719	0	3728	112	0
1	F	3723	0	3731	101	0
2	G	1658	0	1659	69	0
2	H	1658	0	1659	67	0
2	I	1658	0	1659	64	0
2	J	1658	0	1659	64	0
2	K	1658	0	1659	72	0
2	L	1658	0	1659	66	0
2	M	1658	0	1659	67	0
2	N	1658	0	1659	77	0
2	O	1658	0	1659	70	0
2	k	1658	0	1659	85	0
2	l	1658	0	1659	70	0
2	m	1658	0	1659	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	n	1658	0	1659	81	0
2	o	1658	0	1659	73	0
3	P	1638	0	1630	56	0
3	Q	1638	0	1630	70	0
3	R	1638	0	1630	60	0
3	S	1638	0	1630	68	0
3	T	1636	0	1625	65	0
3	U	1638	0	1630	70	0
3	V	1638	0	1630	62	0
3	W	1638	0	1630	78	0
3	X	1638	0	1630	77	0
3	Y	1638	0	1630	68	0
3	Z	1638	0	1630	56	0
3	a	1638	0	1630	61	0
3	b	1638	0	1630	59	0
3	c	1638	0	1630	81	0
4	d	34	0	30	4	0
4	e	34	0	30	5	0
4	f	34	0	30	2	0
4	g	34	0	30	2	0
4	h	34	0	30	2	0
4	i	34	0	30	2	0
4	j	34	0	30	6	0
All	All	68362	0	68329	2452	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 18.

All (2452) 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)
1:F:478:MET:HB2	1:F:544:ILE:HD13	1.59	0.83
1:A:314:MET:SD	1:A:326:LYS:N	2.51	0.83
1:F:486:MET:HE3	1:F:551:ILE:HG12	1.61	0.82
1:C:373:MET:HB2	1:C:415:SER:HB2	1.59	0.82
1:A:337:LEU:HD23	1:A:349:ILE:HG12	1.61	0.82
2:k:56:LEU:HG	2:k:62:PHE:HB2	1.60	0.81
1:D:249:VAL:HG11	1:D:301:LEU:HB3	1.63	0.81
2:k:107:LEU:HD23	2:k:110:ILE:HD11	1.63	0.81
3:X:432:GLU:HG3	3:X:437:GLN:HG3	1.61	0.81
2:O:46:PRO:HA	2:O:207:SER:HA	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:59:ARG:HG2	2:n:91:ARG:HH22	1.46	0.80
3:R:429:TRP:HZ3	3:R:431:ILE:HG13	1.46	0.80
3:b:341:THR:HG21	3:b:379:LYS:HE3	1.64	0.80
3:T:319:ARG:HH22	3:T:485:ASP:HB2	1.44	0.80
3:X:332:ARG:HH11	3:X:493:THR:HB	1.47	0.80
1:B:429:GLY:H	1:B:432:ASP:HB3	1.46	0.79
1:C:161:ILE:HD11	1:D:185:VAL:HG23	1.63	0.79
1:E:373:MET:HB2	1:E:415:SER:HB2	1.64	0.79
2:n:41:PHE:HB3	2:n:53:ILE:HD13	1.65	0.79
1:C:494:ARG:HG2	1:C:507:VAL:HG11	1.64	0.78
2:J:20:ALA:HA	2:J:119:GLU:HG2	1.65	0.78
3:T:359:TYR:HD1	3:T:386:MET:HE1	1.47	0.78
1:B:373:MET:HB3	1:B:415:SER:HB3	1.66	0.78
2:m:178:THR:HA	2:m:233:LEU:HD21	1.65	0.78
1:B:105:LEU:HD21	1:B:116:PHE:HB2	1.65	0.77
2:m:181:LEU:HD23	2:m:233:LEU:HD22	1.65	0.77
2:H:46:PRO:HA	2:H:207:SER:HA	1.67	0.77
1:A:486:MET:HG3	1:A:551:ILE:HD12	1.65	0.77
3:a:301:THR:N	3:a:441:SER:HG	1.82	0.77
2:l:56:LEU:HG	2:l:62:PHE:HB2	1.67	0.77
2:N:46:PRO:HA	2:N:207:SER:HA	1.67	0.77
3:R:303:ILE:HG22	3:R:403:LEU:HD23	1.66	0.77
2:l:46:PRO:HA	2:l:207:SER:HA	1.68	0.76
1:E:464:LEU:HB3	1:E:469:GLY:HA2	1.66	0.76
1:E:310:LEU:HD11	1:E:365:PRO:HG2	1.68	0.76
3:R:452:LYS:HG3	3:b:452:LYS:HG3	1.67	0.76
1:C:453:LEU:HD13	1:C:478:MET:HE1	1.66	0.76
2:I:68:PHE:H	4:h:172:GLN:HB2	1.51	0.75
2:N:91:ARG:HH22	3:b:361:VAL:HG22	1.51	0.75
1:E:481:LYS:HD2	1:E:544:ILE:HG12	1.68	0.75
2:H:135:ARG:NH2	2:H:151:PRO:O	2.20	0.75
2:J:46:PRO:HA	2:J:207:SER:HA	1.69	0.75
1:A:446:GLN:HE22	1:A:480:GLU:HA	1.50	0.75
2:n:124:VAL:HB	2:n:139:TYR:HB2	1.67	0.75
1:A:249:VAL:HG11	1:A:304:LYS:HG3	1.69	0.75
2:m:45:ASN:ND2	2:m:50:LEU:O	2.20	0.75
2:n:140:ARG:HH21	2:n:155:VAL:H	1.34	0.74
3:c:301:THR:N	3:c:441:SER:HG	1.85	0.74
2:O:20:ALA:HA	2:O:119:GLU:HG2	1.69	0.74
2:K:70:GLU:HG2	2:K:118:TYR:HD1	1.51	0.74
2:N:63:ALA:HB3	2:N:123:CYS:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:403:LEU:HD11	3:Y:437:GLN:HG3	1.70	0.74
1:B:494:ARG:NH2	1:B:506:GLU:O	2.21	0.74
3:W:436:TYR:HB2	3:W:450:MET:HE1	1.69	0.74
2:M:124:VAL:HB	2:M:139:TYR:HB2	1.70	0.73
2:m:124:VAL:HB	2:m:139:TYR:HB2	1.67	0.73
2:H:63:ALA:HB3	2:H:123:CYS:HB3	1.70	0.73
1:E:486:MET:HB3	1:E:551:ILE:HD13	1.70	0.73
2:M:46:PRO:HA	2:M:207:SER:HA	1.71	0.73
1:C:256:GLY:O	1:C:259:ARG:NH1	2.21	0.73
1:D:366:VAL:HB	1:D:409:VAL:HG22	1.70	0.73
1:B:314:MET:HE1	1:B:328:TYR:HB2	1.70	0.73
2:G:46:PRO:HA	2:G:207:SER:HA	1.71	0.73
3:S:332:ARG:HH21	3:S:334:VAL:HB	1.54	0.72
1:A:328:TYR:HD1	1:A:359:LYS:HB3	1.54	0.72
2:H:178:THR:HA	2:H:233:LEU:HD21	1.71	0.72
1:E:372:GLU:HG2	1:F:394:PRO:HB3	1.72	0.72
2:K:124:VAL:HB	2:K:139:TYR:HB2	1.71	0.72
2:J:113:GLU:OE2	2:K:114:GLN:NE2	2.22	0.72
3:S:350:ALA:HB1	3:T:388:ARG:HH21	1.54	0.72
3:X:367:GLU:HG3	3:X:373:PRO:HA	1.72	0.72
3:Z:332:ARG:HH11	3:Z:493:THR:HB	1.55	0.72
2:G:45:ASN:ND2	2:G:50:LEU:O	2.23	0.72
2:I:53:ILE:O	2:I:224:ARG:NH2	2.20	0.72
2:M:18:GLU:OE1	2:M:21:ARG:NH2	2.23	0.71
2:M:63:ALA:HB3	2:M:123:CYS:HB3	1.71	0.71
2:J:56:LEU:HG	2:J:62:PHE:HB2	1.72	0.71
2:G:11:GLN:HA	2:G:14:ARG:HG2	1.72	0.71
3:U:452:LYS:HG3	3:Y:452:LYS:HG3	1.72	0.71
1:A:554:GLU:OE2	1:A:558:ASN:ND2	2.24	0.71
2:n:46:PRO:HA	2:n:207:SER:HA	1.71	0.71
2:H:45:ASN:O	2:H:48:ARG:NH2	2.23	0.71
1:A:521:ASN:ND2	1:A:554:GLU:OE1	2.24	0.71
1:C:287:LYS:NZ	1:C:401:ASP:OD1	2.23	0.71
2:k:56:LEU:HD13	2:k:99:LEU:HD21	1.70	0.71
2:G:45:ASN:ND2	2:G:47:SER:O	2.24	0.71
3:T:521:ARG:O	3:Y:488:ARG:NH2	2.22	0.71
2:K:41:PHE:HB3	2:K:53:ILE:HD13	1.73	0.71
2:N:124:VAL:HB	2:N:139:TYR:HB2	1.73	0.71
3:Q:416:SER:O	3:Q:419:ARG:NH1	2.20	0.70
2:N:10:GLU:HG2	2:O:19:LEU:HD12	1.72	0.70
2:O:124:VAL:HB	2:O:139:TYR:HB2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:16:ARG:NH2	2:G:114:GLN:O	2.23	0.70
2:O:63:ALA:HB3	2:O:123:CYS:HB3	1.74	0.70
2:J:45:ASN:O	2:J:48:ARG:NH2	2.25	0.70
2:k:48:ARG:HH12	2:k:207:SER:H	1.40	0.70
2:N:107:LEU:HD23	2:N:110:ILE:HD11	1.73	0.70
3:Z:332:ARG:NH1	3:Z:493:THR:HB	2.06	0.70
3:b:461:ASP:OD1	3:b:462:SER:N	2.25	0.70
1:E:497:GLU:HB2	1:E:587:LEU:HD11	1.74	0.70
2:n:56:LEU:HG	2:n:62:PHE:HB2	1.73	0.70
2:J:124:VAL:HB	2:J:139:TYR:HB2	1.72	0.70
2:K:56:LEU:HG	2:K:62:PHE:HB2	1.72	0.70
3:R:321:THR:HG22	3:R:326:ILE:HA	1.74	0.70
3:c:388:ARG:HG2	3:c:427:GLY:HA3	1.71	0.70
2:l:45:ASN:O	2:l:48:ARG:NH2	2.24	0.70
3:c:469:GLU:OE2	3:c:521:ARG:NH2	2.25	0.70
1:D:534:VAL:HG22	1:D:540:PRO:HA	1.73	0.69
1:E:163:THR:HA	1:E:219:SER:HA	1.72	0.69
1:D:365:PRO:HA	1:D:408:ASN:HB2	1.74	0.69
2:N:45:ASN:O	2:N:48:ARG:NH2	2.23	0.69
2:O:56:LEU:HG	2:O:62:PHE:HB2	1.73	0.69
1:A:235:LYS:HE3	1:B:165:ARG:HE	1.57	0.69
3:S:447:LYS:HA	3:S:450:MET:HE2	1.74	0.69
2:n:45:ASN:ND2	2:n:50:LEU:O	2.23	0.69
1:D:256:GLY:O	1:D:259:ARG:NH1	2.25	0.69
2:J:134:LYS:HZ3	2:J:137:GLU:HG3	1.57	0.69
3:Q:332:ARG:HH11	3:Q:493:THR:HB	1.57	0.69
1:A:485:ARG:O	1:A:485:ARG:NH1	2.25	0.69
2:K:20:ALA:HA	2:K:119:GLU:HG2	1.75	0.69
2:l:45:ASN:ND2	2:l:50:LEU:O	2.26	0.68
2:n:58:ASP:O	2:n:221:ALA:N	2.26	0.68
2:L:16:ARG:NH1	2:L:114:GLN:O	2.27	0.68
2:N:56:LEU:HG	2:N:62:PHE:HB2	1.75	0.68
3:U:416:SER:O	3:U:419:ARG:NH1	2.25	0.68
1:A:299:LYS:HG2	1:A:437:ILE:HD13	1.75	0.68
2:K:110:ILE:HG12	2:K:118:TYR:HE2	1.58	0.68
2:L:46:PRO:HA	2:L:207:SER:HA	1.75	0.68
3:Q:384:ALA:HB1	3:Q:388:ARG:HH21	1.57	0.68
3:X:321:THR:HG22	3:X:326:ILE:HA	1.75	0.68
2:O:107:LEU:HD23	2:O:110:ILE:HD11	1.74	0.68
2:o:56:LEU:HG	2:o:62:PHE:HB2	1.75	0.68
2:H:181:LEU:HD23	2:H:233:LEU:HD22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:46:PRO:HA	2:K:207:SER:HA	1.74	0.68
3:W:382:ARG:HD3	2:O:89:TYR:CD1	2.27	0.68
2:O:72:ASP:OD1	2:O:75:ARG:NH1	2.27	0.68
1:D:249:VAL:HG21	1:D:301:LEU:HD22	1.75	0.68
2:N:11:GLN:OE1	2:N:14:ARG:NH1	2.27	0.68
3:S:347:GLY:HA3	3:S:400:ALA:HA	1.76	0.68
1:B:494:ARG:NH1	1:B:496:LEU:O	2.25	0.68
1:E:453:LEU:HD13	1:E:478:MET:HE3	1.76	0.68
2:k:73:ASN:O	2:k:76:ARG:HG3	1.94	0.68
2:K:70:GLU:HG2	2:K:118:TYR:CD1	2.28	0.68
3:W:391:LEU:HD12	3:W:395:MET:HE3	1.73	0.68
1:D:339:ASN:HB3	1:D:344:GLU:HB3	1.75	0.68
2:o:53:ILE:O	2:o:224:ARG:NH2	2.26	0.68
2:k:45:ASN:O	2:k:48:ARG:NH2	2.27	0.67
2:k:53:ILE:O	2:k:224:ARG:NH2	2.23	0.67
2:n:53:ILE:O	2:n:224:ARG:NH2	2.23	0.67
2:o:43:ALA:HB3	2:o:209:GLU:HB2	1.76	0.67
2:G:135:ARG:NH1	2:G:136:PRO:O	2.27	0.67
2:m:27:ALA:HA	4:j:174:LEU:HA	1.76	0.67
2:K:45:ASN:O	2:K:48:ARG:NH2	2.27	0.67
3:U:332:ARG:HH11	3:U:493:THR:HB	1.59	0.67
1:A:101:TYR:H	1:B:120:ARG:HH12	1.42	0.67
2:G:135:ARG:NH2	2:G:151:PRO:O	2.27	0.67
2:K:110:ILE:HG12	2:K:118:TYR:CE2	2.30	0.67
3:P:332:ARG:HH11	3:P:493:THR:HB	1.58	0.67
3:P:339:ASP:O	3:P:502:ALA:N	2.28	0.67
3:W:384:ALA:HB1	3:W:388:ARG:HH21	1.58	0.67
3:a:339:ASP:O	3:a:502:ALA:N	2.27	0.67
3:b:321:THR:HG22	3:b:326:ILE:HA	1.76	0.67
2:k:163:ILE:HD12	2:k:188:LEU:HA	1.76	0.67
2:o:135:ARG:NH2	2:o:151:PRO:O	2.26	0.67
3:V:505:VAL:HG13	3:V:509:ARG:HH21	1.59	0.67
3:Z:319:ARG:HH22	3:Z:485:ASP:HB2	1.58	0.67
1:F:333:LYS:HB2	1:F:336:GLU:HG3	1.76	0.67
3:c:436:TYR:HB2	3:c:450:MET:SD	2.35	0.67
1:B:374:ASP:OD2	1:E:380:ARG:NH1	2.26	0.67
2:k:46:PRO:HA	2:k:207:SER:HA	1.77	0.67
2:M:135:ARG:NH2	2:M:151:PRO:O	2.27	0.67
3:a:416:SER:O	3:a:419:ARG:NH1	2.27	0.67
1:E:247:PRO:HG2	1:E:304:LYS:HB2	1.77	0.67
2:G:56:LEU:HG	2:G:62:PHE:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:56:LEU:HG	2:H:62:PHE:HB2	1.77	0.66
3:c:365:HIS:ND1	2:O:83:ASP:OD2	2.25	0.66
2:l:24:ILE:HD13	2:l:121:GLU:HG2	1.76	0.66
2:m:46:PRO:HA	2:m:207:SER:HA	1.77	0.66
1:E:570:TRP:HB3	1:E:581:ILE:HD12	1.78	0.66
1:D:439:ARG:HG3	1:D:440:PRO:HD3	1.78	0.66
3:X:307:LYS:HE2	3:X:435:GLY:HA2	1.75	0.66
2:G:124:VAL:HB	2:G:139:TYR:HB2	1.76	0.66
3:R:416:SER:O	3:R:419:ARG:NH1	2.28	0.66
1:D:294:PRO:HG2	1:D:439:ARG:HG2	1.76	0.66
3:W:448:SER:HA	3:W:451:LYS:HE3	1.78	0.66
1:D:498:VAL:HG13	1:D:584:ILE:HG12	1.77	0.66
1:E:310:LEU:HG	1:E:314:MET:HE1	1.77	0.66
3:Y:339:ASP:O	3:Y:502:ALA:N	2.28	0.66
3:b:416:SER:O	3:b:419:ARG:NH1	2.24	0.66
2:I:124:VAL:HB	2:I:139:TYR:HB2	1.76	0.66
1:F:464:LEU:HB3	1:F:469:GLY:HA2	1.78	0.66
2:m:16:ARG:HE	2:m:117:PRO:HD3	1.60	0.66
2:n:140:ARG:NH2	2:n:155:VAL:H	1.94	0.66
3:Q:339:ASP:O	3:Q:502:ALA:N	2.26	0.66
3:R:438:ALA:HB3	3:R:447:LYS:HG3	1.76	0.66
3:X:485:ASP:HB2	3:X:490:ILE:HB	1.76	0.66
3:T:473:ASP:OD1	3:T:521:ARG:NH2	2.26	0.65
2:l:121:GLU:HB3	2:l:156:MET:HE2	1.78	0.65
2:J:16:ARG:NH1	2:J:114:GLN:O	2.21	0.65
2:O:214:ASP:HB3	2:O:217:ARG:HG2	1.76	0.65
2:k:83:ASP:OD2	3:W:365:HIS:ND1	2.23	0.65
2:H:73:ASN:HD21	2:H:76:ARG:HH21	1.44	0.65
3:Y:403:LEU:HD13	3:Y:439:VAL:HG13	1.78	0.65
1:A:239:GLU:HB3	1:A:355:ARG:HG2	1.78	0.65
1:A:563:ASN:HD22	1:B:426:LEU:HB3	1.61	0.65
2:M:20:ALA:HA	2:M:119:GLU:HG2	1.77	0.65
2:M:135:ARG:NH1	2:M:136:PRO:O	2.29	0.65
3:S:325:MET:HE1	3:Z:477:ASP:HB3	1.78	0.65
2:O:140:ARG:HH11	2:O:154:VAL:HG13	1.61	0.65
1:C:499:THR:HG23	1:C:585:ARG:HH12	1.61	0.65
1:F:161:ILE:HB	1:F:219:SER:HB3	1.79	0.65
1:F:335:PRO:HA	1:F:338:LEU:HD13	1.79	0.65
3:U:339:ASP:O	3:U:502:ALA:N	2.29	0.65
3:b:391:LEU:HD12	3:b:395:MET:HE3	1.79	0.65
2:m:67:LYS:HZ2	2:m:69:ASN:HD21	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:45:ASN:O	2:L:48:ARG:NH2	2.30	0.65
2:N:135:ARG:NH1	2:N:136:PRO:O	2.29	0.65
1:C:232:ARG:NH1	1:C:233:ILE:O	2.30	0.65
1:C:294:PRO:O	1:C:299:LYS:NZ	2.29	0.65
2:I:57:TYR:HB3	2:I:60:VAL:HB	1.77	0.65
3:Q:436:TYR:HD1	3:Q:450:MET:HE3	1.62	0.65
3:V:339:ASP:O	3:V:502:ALA:N	2.30	0.65
3:Z:408:ASP:HB3	3:Z:411:ALA:HB2	1.79	0.65
2:M:182:ARG:HE	2:M:234:LEU:HD12	1.62	0.65
3:P:322:GLN:OE1	3:P:322:GLN:N	2.30	0.64
3:S:452:LYS:HG3	3:a:452:LYS:HG3	1.78	0.64
2:G:20:ALA:HA	2:G:119:GLU:HG2	1.79	0.64
3:S:307:LYS:HE2	3:S:435:GLY:HA2	1.79	0.64
3:c:319:ARG:NH1	3:c:479:SER:O	2.30	0.64
1:E:165:ARG:HB2	1:E:177:VAL:HG23	1.78	0.64
2:L:124:VAL:HB	2:L:139:TYR:HB2	1.80	0.64
3:T:339:ASP:O	3:T:502:ALA:N	2.29	0.64
3:R:314:MET:HE1	3:R:334:VAL:HG13	1.79	0.64
3:T:416:SER:O	3:T:419:ARG:NH1	2.29	0.64
3:U:436:TYR:HD1	3:U:450:MET:HE3	1.61	0.64
3:b:376:PHE:HD1	3:b:379:LYS:HZ3	1.43	0.64
1:A:112:THR:HG22	1:A:125:THR:HG22	1.80	0.64
1:C:136:LYS:HZ2	1:C:155:PHE:HZ	1.46	0.64
2:l:16:ARG:HG3	2:l:117:PRO:HG3	1.79	0.64
2:n:67:LYS:HE2	2:n:69:ASN:HD21	1.62	0.64
2:M:150:GLU:HG3	2:M:154:VAL:HG22	1.77	0.64
3:V:487:VAL:HG13	3:W:522:SER:HA	1.78	0.64
3:Y:319:ARG:HH22	3:Y:490:ILE:HB	1.62	0.64
2:J:53:ILE:O	2:J:224:ARG:NH2	2.26	0.64
2:L:178:THR:HA	2:L:233:LEU:HD21	1.80	0.64
3:X:420:ILE:HB	3:X:432:GLU:HB2	1.80	0.64
2:N:135:ARG:NH2	2:N:151:PRO:O	2.30	0.64
3:b:332:ARG:HH11	3:b:493:THR:HB	1.63	0.64
1:A:290:LEU:HD22	1:A:426:LEU:HD11	1.80	0.64
1:A:558:ASN:OD1	1:B:434:LYS:NZ	2.31	0.63
3:S:436:TYR:HD2	3:S:450:MET:HE3	1.62	0.63
3:c:485:ASP:HB3	3:c:490:ILE:HB	1.79	0.63
1:B:192:LEU:HB3	1:B:214:LEU:HD11	1.80	0.63
1:D:251:TYR:HE2	1:D:309:SER:HB2	1.63	0.63
2:o:229:ALA:O	2:o:233:LEU:HB2	1.98	0.63
1:B:139:GLN:NE2	1:B:153:GLY:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:57:TYR:OH	2:N:92:ARG:NH2	2.32	0.63
1:C:440:PRO:HD2	1:C:515:SER:HA	1.81	0.63
3:X:339:ASP:O	3:X:502:ALA:N	2.32	0.63
3:b:485:ASP:HB3	3:b:490:ILE:HB	1.80	0.63
1:C:350:ARG:NH2	1:F:335:PRO:O	2.31	0.63
2:o:147:ILE:O	4:f:172:GLN:NE2	2.31	0.63
1:E:314:MET:HE3	1:E:328:TYR:HB2	1.80	0.63
2:k:44:GLU:HA	2:k:208:LEU:HD23	1.81	0.63
3:P:318:ARG:NH2	3:P:330:ASP:O	2.32	0.63
3:b:303:ILE:HG22	3:b:403:LEU:HD23	1.80	0.63
3:b:320:SER:HB3	3:b:331:VAL:HG21	1.81	0.63
1:B:514:ASN:HD21	1:B:519:ILE:HD11	1.63	0.63
2:m:20:ALA:HA	2:m:119:GLU:HG3	1.80	0.63
2:O:110:ILE:HA	2:O:114:GLN:OE1	1.98	0.63
1:C:275:LYS:NZ	1:C:285:PRO:HB3	2.14	0.62
2:N:31:VAL:HG12	2:N:155:VAL:HG22	1.81	0.62
3:R:339:ASP:O	3:R:502:ALA:N	2.31	0.62
3:b:413:ASP:OD2	3:b:415:GLN:NE2	2.30	0.62
3:c:322:GLN:OE1	3:c:322:GLN:N	2.32	0.62
2:I:16:ARG:HG3	2:I:117:PRO:HG3	1.80	0.62
2:I:30:VAL:HB	2:I:156:MET:HB2	1.81	0.62
3:S:322:GLN:OE1	3:S:322:GLN:N	2.32	0.62
2:O:48:ARG:O	2:O:51:GLN:NE2	2.32	0.62
2:H:217:ARG:HD3	2:H:223:ARG:HH21	1.64	0.62
2:I:44:GLU:HA	2:I:208:LEU:HA	1.82	0.62
1:C:389:GLU:HA	1:C:392:VAL:HG12	1.82	0.62
3:T:302:THR:HA	3:T:440:GLY:HA3	1.81	0.62
2:I:41:PHE:HB3	2:I:53:ILE:HD13	1.81	0.62
1:D:263:GLN:HE22	1:D:435:ILE:HD13	1.65	0.62
2:m:219:ARG:HE	2:m:220:ARG:HG3	1.65	0.62
2:o:91:ARG:NH1	2:o:91:ARG:O	2.32	0.62
3:c:303:ILE:HG22	3:c:403:LEU:HD23	1.81	0.62
2:O:150:GLU:HG3	2:O:154:VAL:HG22	1.81	0.62
1:E:521:ASN:ND2	1:E:554:GLU:OE2	2.32	0.62
1:E:531:ILE:HD11	1:F:277:LEU:HB3	1.81	0.62
2:k:20:ALA:HA	2:k:119:GLU:HG2	1.82	0.62
2:o:45:ASN:ND2	2:o:50:LEU:O	2.32	0.62
3:S:485:ASP:HB3	3:S:490:ILE:HB	1.81	0.62
3:W:339:ASP:O	3:W:502:ALA:N	2.31	0.62
3:c:339:ASP:O	3:c:502:ALA:N	2.32	0.62
1:C:175:LEU:HB2	1:F:235:LYS:HZ1	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:26:ARG:HE	4:j:173:TYR:HD2	1.48	0.62
2:n:16:ARG:HE	2:n:117:PRO:HD3	1.65	0.62
3:Q:318:ARG:NH2	3:Q:330:ASP:O	2.32	0.62
3:U:322:GLN:N	3:U:322:GLN:OE1	2.33	0.62
1:B:157:ALA:O	1:E:173:ARG:NH1	2.33	0.62
1:E:162:SER:O	1:E:220:LEU:N	2.28	0.62
2:o:46:PRO:HA	2:o:207:SER:HA	1.81	0.62
3:Y:438:ALA:HB2	3:Y:447:LYS:HE3	1.82	0.62
1:A:237:GLU:HB2	1:B:165:ARG:HH22	1.65	0.61
2:l:30:VAL:HG13	2:l:43:ALA:HB2	1.81	0.61
2:J:107:LEU:HA	2:J:110:ILE:HG22	1.81	0.61
3:Q:314:MET:HE1	3:Q:334:VAL:HG13	1.81	0.61
3:b:339:ASP:O	3:b:502:ALA:N	2.33	0.61
2:L:167:LEU:O	2:L:171:TYR:N	2.33	0.61
3:P:303:ILE:HG22	3:P:403:LEU:HD23	1.81	0.61
3:T:303:ILE:HG22	3:T:403:LEU:HD23	1.81	0.61
1:C:254:ILE:HD11	1:C:301:LEU:HB3	1.83	0.61
1:C:457:LEU:O	1:C:471:ARG:NH2	2.34	0.61
2:o:67:LYS:HE2	4:e:171:GLY:HA2	1.80	0.61
3:P:488:ARG:NH2	3:c:476:ASP:OD2	2.28	0.61
3:a:473:ASP:OD1	3:a:521:ARG:NH2	2.34	0.61
1:A:271:PRO:HB3	1:A:285:PRO:HB3	1.82	0.61
2:K:167:LEU:O	2:K:171:TYR:N	2.33	0.61
1:A:246:VAL:HG11	1:B:403:VAL:HG22	1.82	0.61
2:M:14:ARG:O	2:M:18:GLU:HG2	2.01	0.61
3:V:322:GLN:OE1	3:V:322:GLN:N	2.33	0.61
3:Z:319:ARG:NH2	3:Z:485:ASP:HB2	2.16	0.61
2:O:11:GLN:OE1	2:O:14:ARG:NH2	2.32	0.61
1:A:453:LEU:HD12	1:A:479:ILE:HG12	1.81	0.61
2:o:124:VAL:HB	2:o:139:TYR:HB2	1.82	0.61
3:X:447:LYS:HE2	3:X:447:LYS:HA	1.82	0.61
2:O:53:ILE:O	2:O:224:ARG:NH2	2.23	0.61
1:D:272:PHE:HA	1:D:275:LYS:HD3	1.81	0.61
2:H:109:THR:O	2:H:113:GLU:HG3	1.99	0.61
3:Q:506:PRO:HD2	3:Q:509:ARG:HH21	1.65	0.61
3:c:319:ARG:O	3:c:333:LYS:NZ	2.32	0.61
3:c:392:ALA:HA	3:c:395:MET:HE1	1.81	0.61
1:F:361:SER:H	1:F:364:THR:HB	1.66	0.61
3:P:319:ARG:O	3:P:333:LYS:NZ	2.34	0.61
3:a:303:ILE:HG22	3:a:403:LEU:HD23	1.82	0.61
1:A:367:ILE:HG12	1:A:410:ILE:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:41:PHE:HE2	2:l:213:LEU:HG	1.66	0.61
2:M:59:ARG:NH2	2:M:215:ALA:O	2.34	0.61
1:A:585:ARG:HD2	1:B:575:GLY:HA2	1.83	0.61
2:I:54:SER:O	2:I:62:PHE:N	2.34	0.61
2:M:161:GLU:O	2:M:165:ASN:ND2	2.34	0.61
1:A:377:PHE:HA	1:A:393:VAL:HG22	1.83	0.60
2:n:140:ARG:O	2:n:148:ALA:N	2.32	0.60
3:S:318:ARG:NH2	3:S:330:ASP:O	2.33	0.60
3:V:359:TYR:HD1	3:V:386:MET:HE1	1.66	0.60
3:b:469:GLU:OE1	3:b:521:ARG:NH2	2.32	0.60
1:A:380:ARG:HH12	1:A:394:PRO:HG3	1.66	0.60
1:C:497:GLU:HB2	1:C:587:LEU:HD11	1.83	0.60
2:m:59:ARG:NH2	2:m:215:ALA:O	2.35	0.60
2:I:118:TYR:HB3	2:I:120:VAL:HG22	1.84	0.60
3:P:452:LYS:HG3	3:W:452:LYS:HG3	1.83	0.60
2:m:91:ARG:NH1	2:m:91:ARG:O	2.34	0.60
2:m:163:ILE:HD13	2:m:188:LEU:HD12	1.82	0.60
3:P:458:THR:H	3:P:462:SER:HB2	1.66	0.60
1:C:521:ASN:ND2	1:C:559:GLU:OE1	2.35	0.60
2:m:55:GLU:OE1	2:m:220:ARG:NH2	2.23	0.60
2:J:80:GLN:HG3	3:X:365:HIS:CE1	2.36	0.60
2:M:87:TYR:HD1	3:a:361:VAL:HG21	1.66	0.60
3:c:301:THR:O	3:c:441:SER:N	2.35	0.60
3:c:446:ALA:O	3:c:450:MET:HG2	2.02	0.60
2:o:135:ARG:NH1	2:o:136:PRO:O	2.34	0.60
3:R:325:MET:HA	3:R:325:MET:HE3	1.82	0.60
2:O:31:VAL:HG12	2:O:155:VAL:HG22	1.84	0.60
2:O:45:ASN:O	2:O:48:ARG:NH2	2.29	0.60
2:J:59:ARG:NH2	2:J:215:ALA:O	2.33	0.60
3:T:319:ARG:HD3	3:T:482:GLY:HA3	1.84	0.60
1:D:330:LEU:O	1:D:369:PHE:N	2.33	0.60
1:E:107:THR:HG22	1:E:113:VAL:HG12	1.84	0.60
2:k:59:ARG:HG2	2:k:91:ARG:HH22	1.66	0.60
2:K:89:TYR:CD1	3:Z:382:ARG:HD3	2.36	0.60
2:M:178:THR:HA	2:M:233:LEU:HD21	1.83	0.60
3:Q:307:LYS:HE2	3:Q:435:GLY:HA2	1.83	0.60
2:l:89:TYR:CD1	3:R:382:ARG:HD3	2.37	0.60
2:L:48:ARG:HH12	2:L:207:SER:H	1.49	0.60
1:F:212:ARG:NH2	1:F:358:GLU:O	2.35	0.60
3:Q:420:ILE:HB	3:Q:432:GLU:HB2	1.82	0.60
3:V:416:SER:O	3:V:419:ARG:NH1	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:507:GLU:HA	3:b:510:ILE:HD12	1.84	0.60
1:D:349:ILE:HG22	1:D:399:GLU:HG3	1.83	0.59
2:H:147:ILE:HG22	4:h:172:GLN:HE22	1.65	0.59
2:K:72:ASP:OD2	2:K:76:ARG:NH2	2.35	0.59
2:M:56:LEU:HG	2:M:62:PHE:HB2	1.84	0.59
3:R:388:ARG:HA	3:R:391:LEU:HD23	1.84	0.59
1:B:175:LEU:HD11	1:B:183:GLU:HB3	1.84	0.59
2:k:135:ARG:NH1	2:k:136:PRO:O	2.35	0.59
2:L:56:LEU:HG	2:L:62:PHE:HB2	1.84	0.59
2:G:83:ASP:OD2	3:U:365:HIS:ND1	2.32	0.59
2:H:79:ILE:HD13	3:V:368:LYS:HB3	1.84	0.59
2:H:182:ARG:NH2	2:H:233:LEU:O	2.35	0.59
3:c:350:ALA:O	3:c:354:GLU:HG2	2.02	0.59
2:H:135:ARG:NH1	2:H:136:PRO:O	2.36	0.59
2:I:30:VAL:HG13	2:I:43:ALA:HB2	1.83	0.59
2:N:163:ILE:HD13	2:N:188:LEU:HD12	1.84	0.59
3:X:322:GLN:N	3:X:322:GLN:OE1	2.35	0.59
2:l:66:GLY:HA3	2:l:120:VAL:HA	1.84	0.59
2:L:54:SER:O	2:L:62:PHE:N	2.35	0.59
3:T:485:ASP:N	3:T:490:ILE:O	2.36	0.59
3:a:392:ALA:O	3:a:396:GLN:NE2	2.35	0.59
1:D:122:MET:HE1	1:D:124:LEU:HB2	1.83	0.59
2:H:92:ARG:HH21	3:P:377:ALA:H	1.50	0.59
2:J:83:ASP:OD2	3:X:365:HIS:ND1	2.28	0.59
3:T:452:LYS:HG3	3:Z:452:LYS:HG3	1.84	0.59
3:X:416:SER:O	3:X:419:ARG:NH1	2.33	0.59
3:c:458:THR:H	3:c:462:SER:HG	1.50	0.59
1:D:242:VAL:HG13	1:D:243:LEU:H	1.68	0.59
2:o:89:TYR:CD1	3:U:382:ARG:HD3	2.37	0.59
2:K:163:ILE:HG12	2:K:188:LEU:HD12	1.85	0.59
2:L:101:ASN:O	2:L:105:GLN:HG2	2.01	0.59
3:X:310:GLY:HA2	3:X:415:GLN:HA	1.83	0.59
3:a:421:VAL:HG22	3:a:431:ILE:HG12	1.85	0.59
2:G:54:SER:O	2:G:62:PHE:N	2.34	0.59
2:L:59:ARG:HG2	2:L:91:ARG:HH22	1.67	0.59
1:A:333:LYS:HB2	1:A:336:GLU:HG3	1.84	0.59
2:n:147:ILE:O	4:e:172:GLN:NE2	2.36	0.59
2:H:20:ALA:HA	2:H:119:GLU:HG3	1.84	0.59
2:I:58:ASP:O	2:I:221:ALA:N	2.34	0.59
3:Y:319:ARG:HD3	3:Y:482:GLY:HA3	1.85	0.59
2:O:16:ARG:NH1	2:O:111:PHE:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:167:LEU:O	2:H:171:TYR:N	2.36	0.59
2:K:214:ASP:HB3	2:K:217:ARG:HG2	1.84	0.59
2:M:140:ARG:HE	2:M:154:VAL:HG13	1.67	0.59
3:U:438:ALA:HB3	3:U:447:LYS:HG3	1.84	0.59
3:X:307:LYS:NZ	3:X:432:GLU:O	2.32	0.59
3:R:318:ARG:NH2	3:R:330:ASP:O	2.36	0.58
3:c:473:ASP:OD1	3:c:521:ARG:NH2	2.36	0.58
2:O:52:LYS:HG2	2:O:71:PHE:CZ	2.38	0.58
1:A:264:ILE:HD13	1:A:289:VAL:HG11	1.85	0.58
1:C:440:PRO:O	1:C:487:TYR:OH	2.21	0.58
1:D:495:PHE:HD2	1:D:508:MET:HE1	1.67	0.58
2:H:53:ILE:O	2:H:224:ARG:NH2	2.32	0.58
2:K:135:ARG:NH1	2:K:136:PRO:O	2.36	0.58
3:V:448:SER:HA	3:V:451:LYS:HZ3	1.68	0.58
3:X:485:ASP:HB3	3:X:488:ARG:HB2	1.84	0.58
1:D:175:LEU:HD11	1:D:183:GLU:HB2	1.85	0.58
2:o:16:ARG:HD2	2:o:117:PRO:HD3	1.85	0.58
2:K:22:LYS:HB3	2:K:26:ARG:HH22	1.68	0.58
2:N:89:TYR:CD1	3:c:382:ARG:HD3	2.38	0.58
3:Q:438:ALA:HB3	3:Q:447:LYS:HG3	1.85	0.58
3:a:318:ARG:NH2	3:a:330:ASP:O	2.36	0.58
1:A:287:LYS:HD2	1:A:404:GLU:HG3	1.85	0.58
1:F:457:LEU:HD11	1:F:527:LYS:HE2	1.85	0.58
2:m:121:GLU:HG2	2:m:156:MET:HE1	1.85	0.58
2:o:189:ARG:O	2:o:189:ARG:NH1	2.33	0.58
2:G:53:ILE:O	2:G:224:ARG:NH2	2.26	0.58
1:B:269:GLU:O	1:B:273:LEU:N	2.34	0.58
2:o:63:ALA:HB3	2:o:123:CYS:HB3	1.85	0.58
2:n:54:SER:O	2:n:62:PHE:N	2.35	0.58
3:V:322:GLN:HG2	3:V:325:MET:HB3	1.86	0.58
3:V:452:LYS:HG3	3:X:452:LYS:HG3	1.85	0.58
3:W:337:THR:HG1	3:W:341:THR:HG1	1.50	0.58
3:c:318:ARG:NH2	3:c:330:ASP:O	2.37	0.58
1:B:288:GLY:HA3	1:B:431:LEU:HA	1.86	0.58
1:F:247:PRO:O	1:F:308:ASN:ND2	2.36	0.58
1:B:299:LYS:HG2	1:B:437:ILE:HD13	1.86	0.58
1:D:300:THR:HG22	1:D:304:LYS:HE2	1.85	0.58
1:F:177:VAL:HG12	1:F:183:GLU:HG3	1.86	0.58
1:F:497:GLU:HB3	1:F:587:LEU:HD21	1.85	0.58
2:J:63:ALA:HB3	2:J:123:CYS:HB3	1.86	0.58
2:L:41:PHE:HB3	2:L:53:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:73:ASN:HD21	2:N:76:ARG:HH21	1.52	0.58
3:S:339:ASP:O	3:S:502:ALA:N	2.36	0.58
3:V:355:PHE:HE1	3:V:386:MET:HB3	1.69	0.58
1:A:497:GLU:HB2	1:A:587:LEU:HD11	1.86	0.58
2:G:16:ARG:NH1	2:G:111:PHE:O	2.37	0.58
2:I:83:ASP:OD2	3:P:365:HIS:ND1	2.34	0.58
2:L:71:PHE:HA	2:L:74:LEU:HD12	1.86	0.58
2:N:18:GLU:HA	2:N:21:ARG:HE	1.68	0.58
3:W:337:THR:OG1	3:W:341:THR:OG1	2.20	0.58
3:X:318:ARG:NH2	3:X:330:ASP:O	2.36	0.58
1:D:333:LYS:HE2	1:D:336:GLU:HG2	1.86	0.58
2:L:24:ILE:HG12	2:L:121:GLU:HG3	1.85	0.58
3:T:322:GLN:OE1	3:T:322:GLN:N	2.36	0.58
3:V:485:ASP:HB3	3:V:490:ILE:HB	1.86	0.58
1:A:310:LEU:HG	1:A:314:MET:HE3	1.85	0.57
2:l:53:ILE:O	2:l:224:ARG:NH2	2.24	0.57
2:l:83:ASP:OD2	3:Q:365:HIS:ND1	2.29	0.57
3:R:301:THR:N	3:R:480:ALA:O	2.37	0.57
3:T:319:ARG:NH2	3:T:485:ASP:HB2	2.17	0.57
3:X:393:ALA:HB1	3:X:398:LEU:HD22	1.84	0.57
1:D:310:LEU:O	1:D:314:MET:HG2	2.05	0.57
2:l:19:LEU:HD22	2:l:117:PRO:HG2	1.86	0.57
3:Q:447:LYS:HA	3:Q:450:MET:HE2	1.86	0.57
3:R:406:GLY:O	3:R:419:ARG:N	2.37	0.57
1:B:260:GLN:HG2	1:B:437:ILE:HG13	1.87	0.57
2:m:109:THR:O	2:m:113:GLU:HG3	2.03	0.57
2:n:17:SER:OG	2:n:143:TYR:OH	2.22	0.57
2:n:118:TYR:HB3	2:n:120:VAL:HG22	1.86	0.57
2:I:46:PRO:HA	2:I:207:SER:HA	1.86	0.57
3:R:332:ARG:NH1	3:R:493:THR:OG1	2.37	0.57
3:S:423:PHE:HA	3:S:429:TRP:HA	1.86	0.57
3:a:509:ARG:HE	3:a:513:LEU:HG	1.70	0.57
1:A:455:GLU:OE2	1:A:471:ARG:HB3	2.04	0.57
2:l:18:GLU:HA	2:l:21:ARG:HG3	1.86	0.57
2:l:92:ARG:HE	3:R:375:THR:HG21	1.69	0.57
2:H:205:VAL:HG11	2:H:231:GLN:HB3	1.85	0.57
1:B:107:THR:HA	1:B:113:VAL:HG12	1.86	0.57
2:K:83:ASP:OD1	3:Y:368:LYS:NZ	2.31	0.57
2:K:135:ARG:NH2	2:K:151:PRO:O	2.37	0.57
3:R:322:GLN:OE1	3:R:327:SER:HB3	2.04	0.57
3:W:414:PRO:HA	3:W:417:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:332:ARG:NE	3:Y:334:VAL:O	2.36	0.57
3:a:355:PHE:HB3	3:a:359:TYR:CE2	2.40	0.57
1:B:99:SER:OG	1:E:123:ARG:NE	2.37	0.57
3:U:458:THR:H	3:U:462:SER:HG	1.51	0.57
3:V:448:SER:HA	3:V:451:LYS:NZ	2.20	0.57
2:l:140:ARG:HG3	2:l:156:MET:HE3	1.86	0.57
3:P:420:ILE:HB	3:P:432:GLU:HB3	1.87	0.57
3:U:345:ILE:HA	3:U:402:PRO:HA	1.85	0.57
3:Y:458:THR:N	3:Y:462:SER:OG	2.33	0.57
3:a:332:ARG:NE	3:a:334:VAL:O	2.37	0.57
2:m:28:LYS:HB2	2:m:52:LYS:HZ2	1.70	0.57
2:o:83:ASP:OD2	3:T:365:HIS:ND1	2.33	0.57
3:S:403:LEU:HD13	3:S:437:GLN:OE1	2.05	0.57
3:W:458:THR:H	3:W:462:SER:HB2	1.69	0.57
1:B:486:MET:HE1	1:B:519:ILE:HG12	1.87	0.57
2:m:58:ASP:HB3	2:m:219:ARG:O	2.04	0.57
2:G:140:ARG:HH11	2:G:154:VAL:HG13	1.70	0.57
3:c:393:ALA:HA	3:c:396:GLN:HE22	1.70	0.57
1:D:332:ILE:HG12	1:D:352:ILE:HD13	1.87	0.57
1:D:419:ASP:OD1	1:D:420:MET:N	2.38	0.57
1:D:498:VAL:HG22	1:D:584:ILE:HG23	1.87	0.57
2:k:135:ARG:NH2	2:k:151:PRO:O	2.38	0.57
2:n:140:ARG:HB3	2:n:148:ALA:HB3	1.87	0.57
3:W:380:ILE:HG23	3:W:423:PHE:CZ	2.39	0.57
1:D:542:LEU:HD21	1:D:547:LEU:HD21	1.86	0.56
1:F:534:VAL:HG22	1:F:540:PRO:HA	1.87	0.56
2:m:16:ARG:HB3	2:m:111:PHE:HE1	1.70	0.56
1:E:421:ILE:HB	1:E:426:LEU:HD11	1.86	0.56
2:G:52:LYS:HE3	2:G:71:PHE:HZ	1.70	0.56
2:K:44:GLU:HA	2:K:208:LEU:HD23	1.86	0.56
2:L:128:ALA:HB2	2:L:134:LYS:HB3	1.86	0.56
1:C:121:LYS:HG2	1:F:101:TYR:HD2	1.71	0.56
1:D:367:ILE:HD13	1:D:412:ILE:HD12	1.88	0.56
1:F:300:THR:HG22	1:F:304:LYS:HE3	1.87	0.56
2:n:30:VAL:HB	2:n:156:MET:HB2	1.85	0.56
3:b:420:ILE:HB	3:b:432:GLU:HB2	1.86	0.56
2:O:138:LEU:HB2	2:O:150:GLU:HB2	1.88	0.56
1:C:499:THR:HG22	1:C:505:LYS:HD3	1.88	0.56
2:m:9:PRO:HB2	2:m:13:MET:HE1	1.88	0.56
2:G:121:GLU:HG3	2:G:156:MET:HB2	1.87	0.56
2:M:82:ALA:HB2	2:M:99:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:351:VAL:HG12	3:Z:355:PHE:CE2	2.41	0.56
1:A:260:GLN:HG2	1:A:437:ILE:HG13	1.86	0.56
1:B:500:TYR:HB2	1:B:503:GLY:HA3	1.88	0.56
2:K:118:TYR:HB3	2:K:120:VAL:HG22	1.86	0.56
2:K:150:GLU:HG3	2:K:154:VAL:HG22	1.87	0.56
1:C:581:ILE:HD13	1:C:584:ILE:HD11	1.86	0.56
2:l:135:ARG:NH2	2:l:151:PRO:O	2.38	0.56
2:n:89:TYR:CD1	3:T:382:ARG:HD3	2.40	0.56
2:L:45:ASN:ND2	2:L:50:LEU:O	2.30	0.56
3:T:515:ARG:O	3:T:519:GLU:HG2	2.05	0.56
3:W:321:THR:HG22	3:W:326:ILE:HA	1.87	0.56
2:G:43:ALA:O	2:G:209:GLU:N	2.36	0.56
2:L:139:TYR:HB3	2:L:147:ILE:HD11	1.88	0.56
3:R:317:ASP:HA	3:R:492:PRO:HB3	1.86	0.56
3:V:303:ILE:HG22	3:V:403:LEU:HD23	1.88	0.56
2:O:178:THR:HG22	2:O:182:ARG:HE	1.71	0.56
1:C:403:VAL:HG21	1:F:331:ASN:HD21	1.71	0.56
1:E:377:PHE:HZ	1:E:396:LEU:HD13	1.70	0.56
2:N:69:ASN:OD1	2:N:70:GLU:N	2.39	0.56
3:S:476:ASP:OD2	3:Z:488:ARG:NH2	2.29	0.56
3:U:485:ASP:HB3	3:U:490:ILE:HB	1.86	0.56
2:O:113:GLU:HG3	2:O:114:GLN:NE2	2.20	0.56
1:C:275:LYS:O	1:C:279:ARG:HG2	2.06	0.56
2:k:45:ASN:ND2	2:k:50:LEU:O	2.25	0.56
3:U:347:GLY:HA3	3:U:400:ALA:HA	1.88	0.56
3:a:346:ALA:O	3:a:401:LEU:N	2.36	0.56
2:n:16:ARG:HB3	2:n:117:PRO:HG3	1.87	0.56
2:n:83:ASP:OD2	3:S:365:HIS:ND1	2.34	0.56
3:Y:459:ASP:H	3:Y:462:SER:HG	1.53	0.56
1:A:192:LEU:HB3	1:A:214:LEU:HD11	1.88	0.55
1:D:247:PRO:HB2	1:D:304:LYS:HB3	1.88	0.55
2:G:22:LYS:O	2:G:26:ARG:HG2	2.05	0.55
2:I:154:VAL:HG12	2:I:156:MET:SD	2.45	0.55
3:W:406:GLY:O	3:W:419:ARG:N	2.36	0.55
2:k:166:ALA:O	2:k:170:SER:OG	2.21	0.55
2:m:54:SER:O	2:m:62:PHE:N	2.37	0.55
2:n:30:VAL:HG13	2:n:43:ALA:HB2	1.88	0.55
2:o:140:ARG:HD3	2:o:154:VAL:HG13	1.88	0.55
2:I:56:LEU:HG	2:I:62:PHE:HB2	1.87	0.55
3:Q:303:ILE:HG22	3:Q:403:LEU:HD23	1.87	0.55
3:b:307:LYS:NZ	3:b:432:GLU:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:44:GLU:HA	2:O:208:LEU:HD23	1.87	0.55
1:F:107:THR:HA	1:F:113:VAL:HG12	1.87	0.55
2:l:140:ARG:O	2:l:148:ALA:N	2.32	0.55
3:V:508:SER:O	3:V:512:GLU:HG3	2.06	0.55
3:Y:508:SER:O	3:Y:512:GLU:HG3	2.06	0.55
1:A:297:CYS:HB3	1:A:437:ILE:HG22	1.89	0.55
1:B:447:ASP:OD1	1:B:451:LYS:NZ	2.40	0.55
1:F:494:ARG:HB3	1:F:587:LEU:HD13	1.88	0.55
2:k:92:ARG:HG3	3:X:375:THR:HG21	1.88	0.55
2:N:167:LEU:O	2:N:171:TYR:N	2.39	0.55
3:Q:452:LYS:HG3	3:c:452:LYS:HG3	1.89	0.55
3:a:459:ASP:H	3:a:462:SER:HG	1.54	0.55
1:D:275:LYS:HZ1	1:D:407:GLU:HB3	1.71	0.55
1:D:515:SER:H	1:D:518:MET:HG3	1.71	0.55
2:n:44:GLU:HA	2:n:208:LEU:HD23	1.88	0.55
2:K:83:ASP:OD2	3:Y:365:HIS:ND1	2.28	0.55
3:U:421:VAL:HG22	3:U:431:ILE:HG12	1.88	0.55
3:Z:485:ASP:N	3:Z:490:ILE:O	2.40	0.55
1:C:264:ILE:HD12	1:C:267:ALA:HB3	1.89	0.55
2:L:163:ILE:HD13	2:L:188:LEU:HD12	1.87	0.55
2:M:70:GLU:OE1	2:M:119:GLU:N	2.40	0.55
3:S:416:SER:O	3:S:419:ARG:NH1	2.33	0.55
3:U:317:ASP:HA	3:U:492:PRO:HB3	1.89	0.55
3:W:347:GLY:HA3	3:W:400:ALA:HA	1.88	0.55
3:Y:317:ASP:HA	3:Y:492:PRO:HB3	1.89	0.55
2:O:45:ASN:ND2	2:O:47:SER:O	2.40	0.55
1:B:144:ASN:ND2	1:B:148:THR:O	2.40	0.55
2:l:21:ARG:HD2	2:l:22:LYS:N	2.21	0.55
2:m:118:TYR:HB3	2:m:120:VAL:HG22	1.89	0.55
2:n:11:GLN:CD	2:n:14:ARG:HH21	2.14	0.55
2:N:82:ALA:HB2	2:N:99:LEU:HD21	1.88	0.55
3:T:408:ASP:HB3	3:T:411:ALA:HB2	1.89	0.55
3:U:447:LYS:HA	3:U:450:MET:HE2	1.89	0.55
3:X:436:TYR:O	3:X:437:GLN:NE2	2.39	0.55
3:Y:436:TYR:HB2	3:Y:447:LYS:HZ3	1.71	0.55
1:F:482:VAL:HG23	1:F:551:ILE:HD11	1.88	0.55
3:S:355:PHE:HE2	3:S:400:ALA:HB3	1.71	0.55
3:S:484:PRO:HB3	3:S:491:PHE:CD2	2.42	0.55
3:Z:319:ARG:O	3:Z:333:LYS:NZ	2.40	0.55
2:O:167:LEU:O	2:O:171:TYR:N	2.40	0.55
1:A:448:ILE:HA	1:A:451:LYS:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:SER:OG	1:B:539:GLN:NE2	2.38	0.55
1:D:485:ARG:HG2	1:D:548:LEU:HD22	1.89	0.55
2:L:59:ARG:NH2	2:L:215:ALA:O	2.39	0.55
3:W:301:THR:N	3:W:441:SER:HG	2.05	0.55
3:Z:318:ARG:NH2	3:Z:330:ASP:O	2.39	0.55
3:a:301:THR:O	3:a:441:SER:N	2.40	0.55
1:C:478:MET:HG2	1:C:544:ILE:HG13	1.89	0.54
1:E:526:ALA:HB1	1:E:542:LEU:HD11	1.89	0.54
2:G:88:ALA:O	3:V:382:ARG:NH1	2.40	0.54
3:V:480:ALA:N	3:W:324:ASN:OD1	2.40	0.54
1:B:457:LEU:HD21	1:B:542:LEU:HD13	1.88	0.54
1:D:168:LEU:HD21	1:D:185:VAL:HG22	1.88	0.54
1:D:251:TYR:CE2	1:D:309:SER:HB2	2.41	0.54
2:k:89:TYR:CD1	3:X:382:ARG:HD3	2.41	0.54
2:o:92:ARG:HB2	3:U:375:THR:HG21	1.88	0.54
2:o:211:ALA:HA	2:o:224:ARG:HA	1.89	0.54
2:H:28:LYS:HB3	2:H:44:GLU:HG3	1.89	0.54
3:U:318:ARG:NH2	3:U:330:ASP:O	2.40	0.54
3:a:364:GLU:HG2	3:a:368:LYS:HE2	1.89	0.54
2:k:107:LEU:HD22	2:k:143:TYR:HA	1.90	0.54
2:n:8:SER:HB3	2:n:11:GLN:HG2	1.89	0.54
2:n:214:ASP:HB3	2:n:217:ARG:HG2	1.88	0.54
2:I:139:TYR:HB3	2:I:147:ILE:HD11	1.89	0.54
3:U:396:GLN:HE22	3:U:398:LEU:HD23	1.73	0.54
3:Z:445:PHE:CE2	3:Z:473:ASP:HB3	2.43	0.54
3:b:346:ALA:HB3	3:b:401:LEU:HB3	1.89	0.54
1:A:448:ILE:HD13	1:A:516:GLY:HA2	1.89	0.54
2:k:10:GLU:OE1	2:k:14:ARG:NH2	2.41	0.54
2:J:114:GLN:OE1	2:J:114:GLN:N	2.40	0.54
2:M:105:GLN:NE2	2:N:72:ASP:OD2	2.41	0.54
1:F:284:ARG:HE	1:F:285:PRO:HD2	1.72	0.54
2:J:128:ALA:HB2	2:J:134:LYS:HB3	1.90	0.54
2:J:182:ARG:HE	2:J:234:LEU:HD12	1.72	0.54
3:Y:406:GLY:O	3:Y:419:ARG:N	2.39	0.54
2:m:11:GLN:HA	2:m:14:ARG:CD	2.38	0.54
2:m:53:ILE:O	2:m:224:ARG:NH2	2.24	0.54
2:o:127:VAL:HG12	2:o:136:PRO:HB3	1.90	0.54
2:o:146:SER:HG	4:f:171:GLY:N	2.06	0.54
2:G:91:ARG:NH1	2:G:91:ARG:O	2.41	0.54
2:I:58:ASP:HB3	2:I:219:ARG:O	2.07	0.54
2:N:154:VAL:HG12	2:N:156:MET:SD	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:346:ALA:O	3:c:401:LEU:N	2.30	0.54
2:l:16:ARG:NH1	2:l:111:PHE:O	2.41	0.54
2:l:140:ARG:HH11	2:l:154:VAL:HG13	1.72	0.54
2:m:211:ALA:HA	2:m:224:ARG:HA	1.89	0.54
2:M:165:ASN:O	2:M:169:GLU:HG2	2.08	0.54
2:N:91:ARG:NH2	3:b:361:VAL:HG22	2.22	0.54
3:V:479:SER:OG	3:W:324:ASN:O	2.25	0.54
1:A:500:TYR:OH	1:A:506:GLU:OE1	2.24	0.54
1:B:499:THR:HB	1:B:583:TYR:HB3	1.89	0.54
1:D:360:ALA:HA	1:D:408:ASN:HD21	1.72	0.54
2:H:54:SER:O	2:H:62:PHE:N	2.37	0.54
2:N:214:ASP:HB3	2:N:217:ARG:HG2	1.90	0.54
3:S:303:ILE:HD11	3:S:333:LYS:HB3	1.90	0.54
3:Y:354:GLU:OE2	3:Z:388:ARG:NH1	2.41	0.54
3:c:485:ASP:O	3:c:490:ILE:N	2.40	0.54
1:E:541:GLY:H	1:F:281:TYR:HH	1.51	0.54
2:k:165:ASN:O	2:k:169:GLU:HG2	2.07	0.54
2:l:67:LYS:HE2	4:i:171:GLY:HA2	1.89	0.54
2:M:44:GLU:HA	2:M:208:LEU:HD23	1.90	0.54
3:P:515:ARG:O	3:P:519:GLU:HG2	2.08	0.54
3:Q:322:GLN:OE1	3:Q:322:GLN:N	2.41	0.54
3:Q:346:ALA:O	3:Q:401:LEU:N	2.32	0.54
1:F:105:LEU:HD21	1:F:116:PHE:CD2	2.43	0.54
2:k:176:SER:OG	2:k:179:ASP:OD2	2.25	0.54
2:n:33:LEU:HD11	2:n:180:ALA:HB1	1.89	0.54
2:I:214:ASP:HB3	2:I:217:ARG:HG2	1.89	0.54
3:X:430:ASN:ND2	3:X:431:ILE:O	2.41	0.54
3:c:509:ARG:HE	3:c:513:LEU:HG	1.73	0.54
2:l:74:LEU:HD13	2:l:122:LEU:HD11	1.89	0.53
2:m:28:LYS:HB3	2:m:44:GLU:HG3	1.90	0.53
2:o:80:GLN:HG3	3:T:365:HIS:CE1	2.43	0.53
2:H:87:TYR:HD1	3:V:361:VAL:HG21	1.72	0.53
2:H:121:GLU:OE2	2:H:140:ARG:NH1	2.41	0.53
2:J:30:VAL:HG13	2:J:43:ALA:HB2	1.89	0.53
2:J:161:GLU:OE2	2:J:165:ASN:ND2	2.34	0.53
3:R:305:ALA:HB2	3:R:403:LEU:HD21	1.91	0.53
2:O:161:GLU:HG3	2:O:162:PRO:HD3	1.90	0.53
1:E:377:PHE:CZ	1:E:396:LEU:HD13	2.43	0.53
1:F:142:ARG:HE	1:F:151:GLU:HB3	1.72	0.53
2:k:70:GLU:HG2	2:k:118:TYR:CD1	2.43	0.53
2:l:16:ARG:HG2	2:l:111:PHE:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:54:SER:O	2:l:62:PHE:N	2.36	0.53
3:c:307:LYS:HE3	3:c:435:GLY:HA2	1.89	0.53
1:C:123:ARG:NH2	1:F:101:TYR:OH	2.40	0.53
1:E:335:PRO:HG3	1:E:375:SER:HB2	1.89	0.53
2:M:14:ARG:NH2	2:M:15:GLU:OE2	2.41	0.53
2:N:45:ASN:ND2	2:N:209:GLU:OE1	2.38	0.53
2:O:179:ASP:OD1	2:O:182:ARG:NH2	2.42	0.53
1:A:314:MET:SD	1:A:328:TYR:HD2	2.31	0.53
2:k:124:VAL:HB	2:k:139:TYR:HB2	1.90	0.53
2:o:205:VAL:HG22	2:o:234:LEU:HD23	1.89	0.53
2:I:28:LYS:HB3	2:I:52:LYS:NZ	2.23	0.53
2:L:140:ARG:HG2	2:L:148:ALA:HB3	1.89	0.53
3:R:332:ARG:HH12	3:R:334:VAL:HB	1.72	0.53
3:U:307:LYS:HE3	3:U:435:GLY:HA2	1.90	0.53
3:W:319:ARG:NH2	3:W:485:ASP:HB2	2.22	0.53
2:k:22:LYS:HB3	2:k:26:ARG:NH2	2.23	0.53
2:m:89:TYR:CD1	3:S:382:ARG:HD3	2.43	0.53
2:H:73:ASN:ND2	2:H:76:ARG:HH21	2.05	0.53
2:J:44:GLU:HA	2:J:208:LEU:HD23	1.90	0.53
3:V:318:ARG:NH2	3:V:330:ASP:O	2.40	0.53
3:Y:507:GLU:HA	3:Y:510:ILE:HD12	1.90	0.53
1:B:104:LEU:HD22	1:B:135:LEU:HD12	1.90	0.53
2:k:217:ARG:HH12	2:k:223:ARG:HB2	1.74	0.53
2:m:30:VAL:O	2:m:156:MET:HB3	2.09	0.53
2:m:56:LEU:HG	2:m:62:PHE:HB2	1.89	0.53
2:o:18:GLU:HG3	2:o:22:LYS:HE3	1.91	0.53
2:I:28:LYS:HB3	2:I:52:LYS:HZ2	1.72	0.53
2:M:110:ILE:HA	2:M:114:GLN:OE1	2.09	0.53
3:P:480:ALA:N	3:c:324:ASN:OD1	2.42	0.53
1:B:372:GLU:HB3	1:E:394:PRO:HB3	1.90	0.53
1:E:377:PHE:HD1	1:E:393:VAL:HG22	1.72	0.53
1:E:574:SER:HB2	1:E:580:ARG:HA	1.91	0.53
3:W:355:PHE:HZ	3:W:390:ASN:HB2	1.74	0.53
3:a:366:TYR:CD1	3:a:374:LEU:HG	2.43	0.53
1:B:164:LEU:HA	1:B:176:VAL:HG12	1.89	0.53
2:m:205:VAL:HG21	2:m:231:GLN:HA	1.91	0.53
2:G:140:ARG:NH2	2:G:150:GLU:OE2	2.41	0.53
2:H:209:GLU:OE2	2:H:224:ARG:NH1	2.42	0.53
3:S:307:LYS:NZ	3:S:432:GLU:O	2.41	0.53
3:S:324:ASN:O	3:Z:479:SER:OG	2.21	0.53
3:T:485:ASP:HB3	3:T:490:ILE:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:363:LEU:HD22	3:X:374:LEU:HD12	1.91	0.53
3:a:329:ARG:O	3:a:490:ILE:HG21	2.09	0.53
1:C:249:VAL:O	1:C:308:ASN:ND2	2.41	0.53
1:D:562:PRO:O	1:D:565:THR:OG1	2.26	0.53
1:E:243:LEU:HD13	1:E:329:PHE:HD2	1.74	0.53
1:E:290:LEU:HB2	1:E:431:LEU:HD23	1.91	0.53
1:F:144:ASN:ND2	1:F:148:THR:O	2.42	0.53
1:F:313:LYS:O	1:F:317:VAL:HB	2.09	0.53
2:K:217:ARG:NH1	2:K:223:ARG:HB2	2.23	0.53
2:N:88:ALA:O	3:c:381:ASN:ND2	2.42	0.53
3:U:393:ALA:O	3:U:396:GLN:NE2	2.41	0.53
1:D:493:ASN:HB3	1:D:510:PHE:H	1.74	0.53
2:k:76:ARG:HD2	2:k:77:GLY:N	2.24	0.53
2:k:150:GLU:HG3	2:k:154:VAL:HG22	1.91	0.53
2:G:58:ASP:HB2	2:G:91:ARG:HH21	1.74	0.53
2:I:167:LEU:O	2:I:171:TYR:N	2.42	0.53
2:K:22:LYS:HB3	2:K:26:ARG:NH2	2.24	0.53
3:S:338:ASP:OD1	3:S:341:THR:OG1	2.26	0.53
3:b:318:ARG:NH2	3:b:330:ASP:O	2.41	0.53
3:c:515:ARG:O	3:c:519:GLU:HG2	2.09	0.53
1:B:333:LYS:HB2	1:B:336:GLU:HB2	1.90	0.52
1:B:500:TYR:CZ	1:B:577:LYS:HD2	2.43	0.52
2:k:128:ALA:HB2	2:k:134:LYS:HB3	1.91	0.52
2:n:65:ALA:HB2	2:n:156:MET:HB3	1.89	0.52
2:M:22:LYS:O	2:M:26:ARG:HG2	2.09	0.52
2:m:12:ALA:O	2:m:15:GLU:HG2	2.09	0.52
2:K:16:ARG:NH1	2:K:111:PHE:O	2.41	0.52
2:M:55:GLU:HB2	2:M:222:PHE:CG	2.44	0.52
2:M:167:LEU:O	2:M:171:TYR:N	2.42	0.52
3:Q:319:ARG:NH1	3:Q:479:SER:O	2.42	0.52
3:X:485:ASP:O	3:X:489:GLY:N	2.43	0.52
1:C:501:ALA:HB3	1:C:579:GLU:HG3	1.91	0.52
2:m:16:ARG:NH2	2:m:114:GLN:O	2.42	0.52
2:H:45:ASN:ND2	2:H:50:LEU:O	2.24	0.52
2:N:142:THR:OG1	2:N:144:ASP:OD1	2.23	0.52
2:N:150:GLU:HG3	2:N:154:VAL:HG22	1.90	0.52
3:P:515:ARG:HA	3:P:518:ILE:HG12	1.92	0.52
3:U:407:TYR:CZ	3:U:417:ALA:HB3	2.45	0.52
3:W:318:ARG:HB2	3:W:319:ARG:HH11	1.74	0.52
3:Z:351:VAL:HG12	3:Z:355:PHE:HE2	1.73	0.52
1:C:341:PHE:HB3	1:F:340:LYS:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:VAL:HA	1:C:486:MET:HG2	1.92	0.52
2:L:40:LEU:HD13	2:L:177:LEU:HD11	1.91	0.52
3:R:346:ALA:O	3:R:401:LEU:N	2.25	0.52
3:X:319:ARG:O	3:X:333:LYS:NZ	2.42	0.52
1:C:512:ASP:O	1:C:572:ARG:NH2	2.42	0.52
2:J:73:ASN:HD21	2:J:76:ARG:HH21	1.56	0.52
2:J:178:THR:HA	2:J:233:LEU:HD21	1.92	0.52
2:L:44:GLU:HA	2:L:208:LEU:HD23	1.92	0.52
3:R:310:GLY:HA2	3:R:415:GLN:HA	1.90	0.52
3:U:346:ALA:O	3:U:401:LEU:N	2.41	0.52
3:V:406:GLY:O	3:V:419:ARG:N	2.40	0.52
3:W:329:ARG:O	3:W:490:ILE:HG21	2.09	0.52
3:a:314:MET:HE1	3:a:334:VAL:HG13	1.91	0.52
1:D:498:VAL:HG11	1:D:581:ILE:HD13	1.91	0.52
1:E:187:TRP:N	1:E:227:GLY:O	2.43	0.52
2:n:211:ALA:HA	2:n:224:ARG:HA	1.90	0.52
2:o:166:ALA:O	2:o:170:SER:OG	2.23	0.52
3:S:422:SER:O	3:S:430:ASN:N	2.42	0.52
3:X:458:THR:H	3:X:462:SER:HB2	1.73	0.52
1:B:187:TRP:HB2	1:B:228:TYR:CE1	2.45	0.52
1:D:264:ILE:HG12	1:D:306:VAL:HG11	1.91	0.52
1:F:373:MET:HE1	1:F:377:PHE:HD2	1.73	0.52
2:l:170:SER:HB3	2:l:183:ILE:HG23	1.91	0.52
2:m:80:GLN:HG3	3:R:365:HIS:CE1	2.44	0.52
2:m:217:ARG:HH12	2:m:223:ARG:HB2	1.75	0.52
2:L:181:LEU:HD12	2:L:233:LEU:HD22	1.91	0.52
1:A:547:LEU:O	1:A:551:ILE:HG12	2.09	0.52
1:C:310:LEU:HD21	1:C:365:PRO:HB2	1.91	0.52
1:D:467:PHE:HB3	1:D:470:ASP:OD1	2.09	0.52
1:F:460:HIS:ND1	1:F:540:PRO:O	2.43	0.52
2:l:76:ARG:HG3	3:Q:369:LEU:HD22	1.92	0.52
2:m:220:ARG:NH1	3:R:364:GLU:OE2	2.43	0.52
2:o:176:SER:OG	2:o:179:ASP:OD2	2.22	0.52
3:S:420:ILE:HB	3:S:432:GLU:HB2	1.92	0.52
2:O:54:SER:O	2:O:62:PHE:N	2.39	0.52
1:A:521:ASN:HD21	1:A:525:ARG:HH22	1.58	0.52
1:C:513:PHE:HB3	1:C:561:LEU:HD13	1.92	0.52
1:D:512:ASP:HB3	1:D:572:ARG:HH12	1.74	0.52
2:n:67:LYS:HA	4:d:172:GLN:O	2.08	0.52
2:G:127:VAL:HG12	2:G:136:PRO:HB3	1.92	0.52
2:L:58:ASP:HB3	2:L:219:ARG:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:347:GLY:HA3	3:Q:400:ALA:HA	1.92	0.52
3:T:329:ARG:O	3:T:490:ILE:HG21	2.10	0.52
3:V:446:ALA:O	3:V:450:MET:HG3	2.10	0.52
1:A:453:LEU:HD11	1:A:547:LEU:HD11	1.91	0.52
1:A:467:PHE:HB3	1:A:470:ASP:OD1	2.10	0.52
1:D:257:LEU:O	1:D:261:ILE:HG12	2.10	0.52
2:L:48:ARG:O	2:L:51:GLN:NE2	2.42	0.52
2:N:114:GLN:HE21	2:N:117:PRO:HA	1.74	0.52
3:R:473:ASP:CG	3:R:521:ARG:HH22	2.17	0.52
3:T:346:ALA:O	3:T:401:LEU:N	2.37	0.52
3:U:307:LYS:NZ	3:U:432:GLU:O	2.39	0.52
3:W:303:ILE:HG22	3:W:403:LEU:HD23	1.92	0.52
3:Y:414:PRO:HA	3:Y:417:ALA:HB2	1.91	0.52
3:b:355:PHE:HZ	3:b:390:ASN:HB2	1.75	0.52
3:c:420:ILE:O	3:c:432:GLU:N	2.33	0.52
2:O:15:GLU:O	2:O:18:GLU:HG2	2.10	0.52
1:A:355:ARG:O	1:A:359:LYS:HG2	2.10	0.51
2:l:211:ALA:HA	2:l:224:ARG:HA	1.91	0.51
2:I:43:ALA:O	2:I:209:GLU:N	2.43	0.51
3:S:321:THR:HG22	3:S:326:ILE:HA	1.92	0.51
2:O:142:THR:OG1	2:O:144:ASP:OD1	2.27	0.51
1:C:355:ARG:HD2	1:C:359:LYS:HE2	1.92	0.51
1:F:453:LEU:HD12	1:F:479:ILE:HG12	1.92	0.51
2:n:13:MET:HE1	2:n:16:ARG:HH11	1.74	0.51
2:J:99:LEU:O	2:J:103:TYR:HD1	1.93	0.51
3:S:318:ARG:HB3	3:S:330:ASP:HA	1.92	0.51
3:Z:307:LYS:HG3	3:Z:420:ILE:HG13	1.92	0.51
3:Z:438:ALA:HB3	3:Z:447:LYS:HG3	1.91	0.51
3:b:318:ARG:HA	3:b:331:VAL:O	2.11	0.51
1:D:455:GLU:O	1:D:471:ARG:NH2	2.43	0.51
1:F:475:ILE:HA	1:F:478:MET:HG3	1.93	0.51
2:l:107:LEU:HD11	2:l:122:LEU:HD12	1.91	0.51
2:o:87:TYR:HD1	3:T:361:VAL:HG21	1.76	0.51
3:Q:506:PRO:HD2	3:Q:509:ARG:NH2	2.26	0.51
3:R:515:ARG:O	3:R:519:GLU:HG2	2.10	0.51
3:T:306:LEU:HA	3:T:436:TYR:HA	1.93	0.51
3:T:318:ARG:NH2	3:T:330:ASP:O	2.44	0.51
3:U:424:ASP:OD1	3:U:428:GLY:N	2.43	0.51
3:W:384:ALA:HB2	3:W:429:TRP:HE3	1.75	0.51
3:Z:365:HIS:NE2	3:Z:369:LEU:HD11	2.26	0.51
3:a:407:TYR:CZ	3:a:417:ALA:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:151:PRO:HG2	2:I:152:HIS:CD2	2.45	0.51
2:I:217:ARG:HB2	2:I:221:ALA:HA	1.93	0.51
2:J:150:GLU:HG3	2:J:154:VAL:HG22	1.91	0.51
3:R:324:ASN:OD1	3:a:479:SER:OG	2.24	0.51
3:U:345:ILE:HG12	3:U:402:PRO:HB3	1.92	0.51
3:c:314:MET:HE1	3:c:334:VAL:HG13	1.92	0.51
1:C:264:ILE:HD13	1:C:289:VAL:HG11	1.92	0.51
1:E:406:LEU:HB3	1:E:409:VAL:HB	1.92	0.51
1:F:378:ARG:HG2	1:F:420:MET:SD	2.51	0.51
2:l:58:ASP:O	2:l:221:ALA:N	2.37	0.51
2:M:106:THR:O	2:M:110:ILE:HG12	2.09	0.51
2:N:78:GLY:HA3	2:N:103:TYR:OH	2.10	0.51
3:Q:383:LEU:HD23	3:Q:423:PHE:CE1	2.45	0.51
3:Q:484:PRO:HB3	3:Q:491:PHE:CD2	2.45	0.51
3:R:329:ARG:O	3:R:490:ILE:HG21	2.10	0.51
3:S:436:TYR:HB2	3:S:450:MET:SD	2.51	0.51
3:S:437:GLN:HE22	3:S:439:VAL:HG13	1.76	0.51
3:V:320:SER:HB2	3:V:331:VAL:HG21	1.91	0.51
3:W:402:PRO:HG2	3:W:423:PHE:HB2	1.91	0.51
1:A:485:ARG:HG3	1:A:551:ILE:HG21	1.93	0.51
1:C:548:LEU:HA	1:C:551:ILE:HD12	1.92	0.51
1:D:249:VAL:HB	1:D:304:LYS:HB2	1.92	0.51
1:D:423:PRO:HA	1:D:426:LEU:HB2	1.92	0.51
2:K:89:TYR:O	3:Z:378:GLY:HA2	2.11	0.51
2:N:30:VAL:HB	2:N:156:MET:HE2	1.92	0.51
3:P:392:ALA:HA	3:P:395:MET:CE	2.41	0.51
3:S:317:ASP:HA	3:S:492:PRO:HB3	1.93	0.51
3:T:450:MET:HA	3:T:453:LEU:HB2	1.93	0.51
1:A:310:LEU:HD11	1:A:365:PRO:HB2	1.92	0.51
1:D:439:ARG:HB2	1:D:514:ASN:O	2.11	0.51
1:E:105:LEU:HD21	1:E:116:PHE:HB2	1.91	0.51
1:E:453:LEU:HD12	1:E:479:ILE:HG12	1.91	0.51
2:l:124:VAL:HB	2:l:139:TYR:HB2	1.92	0.51
2:l:167:LEU:O	2:l:171:TYR:N	2.44	0.51
2:n:58:ASP:HB2	2:n:91:ARG:NH2	2.25	0.51
2:M:68:PHE:HA	2:M:71:PHE:CE2	2.46	0.51
2:M:89:TYR:O	3:b:378:GLY:HA2	2.10	0.51
3:Y:318:ARG:NH2	3:Y:330:ASP:O	2.43	0.51
2:O:85:ARG:HG3	2:O:94:VAL:HG22	1.93	0.51
1:E:105:LEU:HD11	1:E:116:PHE:HB2	1.93	0.51
1:E:449:TYR:O	1:E:453:LEU:N	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:58:ASP:HB2	2:m:91:ARG:HH21	1.75	0.51
2:n:217:ARG:NH1	2:n:223:ARG:HB2	2.26	0.51
3:P:355:PHE:HZ	3:P:390:ASN:HB2	1.76	0.51
3:S:301:THR:N	3:S:441:SER:HG	2.08	0.51
3:S:437:GLN:C	3:S:450:MET:HE1	2.35	0.51
3:T:319:ARG:O	3:T:333:LYS:NZ	2.44	0.51
3:U:507:GLU:HA	3:U:510:ILE:HD12	1.91	0.51
3:V:359:TYR:OH	3:V:379:LYS:O	2.27	0.51
3:W:473:ASP:OD1	3:W:521:ARG:NH2	2.42	0.51
3:X:401:LEU:HD12	3:X:402:PRO:HD2	1.93	0.51
3:c:310:GLY:HA2	3:c:415:GLN:HA	1.92	0.51
1:B:100:GLY:HA3	1:E:120:ARG:HH21	1.75	0.51
2:m:16:ARG:NE	2:m:117:PRO:HD3	2.25	0.51
2:K:155:VAL:HG12	2:K:160:THR:HG22	1.93	0.51
2:L:107:LEU:HD23	2:L:110:ILE:HD11	1.92	0.51
3:R:432:GLU:HG3	3:R:437:GLN:HB2	1.93	0.51
3:U:324:ASN:OD1	3:X:480:ALA:N	2.42	0.51
3:X:450:MET:HA	3:X:453:LEU:HB2	1.93	0.51
3:c:345:ILE:HA	3:c:402:PRO:HA	1.93	0.51
1:D:251:TYR:CD1	1:D:261:ILE:HD12	2.46	0.51
1:D:279:ARG:CZ	1:D:285:PRO:HG3	2.41	0.51
1:D:369:PHE:HA	1:D:412:ILE:O	2.11	0.51
1:E:482:VAL:HG22	1:E:551:ILE:HD11	1.92	0.51
1:E:485:ARG:HG3	1:E:548:LEU:HD22	1.93	0.51
2:m:58:ASP:HB2	2:m:91:ARG:NH2	2.26	0.51
2:o:59:ARG:NH2	2:o:215:ALA:O	2.44	0.51
3:Q:317:ASP:HA	3:Q:492:PRO:HB3	1.93	0.51
3:R:446:ALA:O	3:R:450:MET:HG3	2.11	0.51
3:Y:391:LEU:O	3:Y:395:MET:HG2	2.11	0.51
3:Y:436:TYR:HB2	3:Y:447:LYS:NZ	2.25	0.51
1:C:105:LEU:O	1:C:137:LYS:NZ	2.31	0.50
1:F:338:LEU:HD11	1:F:376:ILE:HD13	1.92	0.50
2:G:53:ILE:HG22	2:G:222:PHE:HZ	1.75	0.50
2:J:78:GLY:HA3	2:J:103:TYR:OH	2.11	0.50
2:N:53:ILE:O	2:N:224:ARG:NH2	2.28	0.50
3:S:329:ARG:O	3:S:490:ILE:HG21	2.11	0.50
3:b:391:LEU:O	3:b:395:MET:HG2	2.11	0.50
1:A:238:VAL:H	1:A:355:ARG:HH12	1.58	0.50
1:A:497:GLU:HB3	1:A:585:ARG:HB3	1.93	0.50
1:C:283:LEU:HD13	1:F:527:LYS:HB2	1.93	0.50
1:D:302:ILE:O	1:D:306:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:LEU:HD11	1:E:183:GLU:HB2	1.94	0.50
1:E:318:ARG:NH2	1:E:364:THR:OG1	2.44	0.50
1:E:337:LEU:HD13	1:E:349:ILE:HG12	1.93	0.50
2:k:88:ALA:O	3:X:381:ASN:ND2	2.44	0.50
2:l:73:ASN:OD1	2:l:76:ARG:NH2	2.45	0.50
2:l:137:GLU:OE1	2:l:139:TYR:OH	2.25	0.50
2:n:89:TYR:O	3:T:378:GLY:HA2	2.11	0.50
2:L:63:ALA:HB3	2:L:123:CYS:HB3	1.94	0.50
2:L:150:GLU:HG3	2:L:154:VAL:HG22	1.92	0.50
2:M:54:SER:O	2:M:62:PHE:N	2.42	0.50
3:S:438:ALA:HB3	3:S:447:LYS:HG3	1.93	0.50
3:Z:407:TYR:CZ	3:Z:417:ALA:HB3	2.45	0.50
3:Z:416:SER:O	3:Z:419:ARG:NH1	2.40	0.50
1:A:375:SER:HB3	1:B:394:PRO:HB2	1.92	0.50
2:m:205:VAL:HG13	2:m:230:LEU:HG	1.93	0.50
2:H:166:ALA:O	2:H:170:SER:OG	2.24	0.50
2:J:65:ALA:HB3	2:J:156:MET:HB3	1.93	0.50
2:L:53:ILE:O	2:L:224:ARG:NH2	2.35	0.50
2:N:161:GLU:HG3	2:N:162:PRO:HD3	1.93	0.50
3:R:484:PRO:HB3	3:R:491:PHE:CD2	2.46	0.50
3:S:346:ALA:O	3:S:401:LEU:N	2.38	0.50
3:X:346:ALA:O	3:X:401:LEU:N	2.28	0.50
3:X:484:PRO:HB3	3:X:491:PHE:CD2	2.46	0.50
3:Y:310:GLY:HA2	3:Y:415:GLN:HA	1.94	0.50
3:a:307:LYS:HG3	3:a:420:ILE:HG13	1.92	0.50
2:l:165:ASN:O	2:l:169:GLU:OE1	2.29	0.50
2:o:54:SER:O	2:o:62:PHE:N	2.43	0.50
2:o:88:ALA:O	3:U:381:ASN:ND2	2.45	0.50
2:G:58:ASP:HB2	2:G:91:ARG:NH2	2.27	0.50
2:J:217:ARG:NH1	2:J:223:ARG:HB2	2.26	0.50
2:K:16:ARG:NH1	2:K:114:GLN:O	2.45	0.50
2:K:23:GLY:HA3	2:K:119:GLU:CD	2.36	0.50
2:K:45:ASN:ND2	2:K:50:LEU:O	2.41	0.50
2:K:58:ASP:HB3	2:K:219:ARG:O	2.12	0.50
2:L:121:GLU:HB3	2:L:156:MET:SD	2.52	0.50
3:Q:473:ASP:OD1	3:Q:521:ARG:NH2	2.44	0.50
3:S:458:THR:N	3:S:462:SER:OG	2.33	0.50
3:Z:378:GLY:O	3:Z:382:ARG:HG2	2.12	0.50
1:E:272:PHE:HE2	1:E:408:ASN:HD21	1.59	0.50
2:k:211:ALA:HA	2:k:224:ARG:HA	1.93	0.50
2:m:44:GLU:HA	2:m:208:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:8:SER:O	2:G:11:GLN:HG3	2.12	0.50
2:G:205:VAL:HG21	2:G:231:GLN:HA	1.92	0.50
2:J:171:TYR:HE2	2:J:173:GLU:HG3	1.76	0.50
3:Q:505:VAL:HG13	3:Q:509:ARG:NH2	2.27	0.50
3:S:485:ASP:N	3:S:490:ILE:O	2.44	0.50
3:Z:515:ARG:O	3:Z:519:GLU:HG2	2.11	0.50
2:O:45:ASN:ND2	2:O:50:LEU:O	2.42	0.50
2:O:217:ARG:HB2	2:O:221:ALA:HA	1.93	0.50
1:A:534:VAL:HG12	1:A:539:GLN:O	2.11	0.50
1:D:275:LYS:O	1:D:279:ARG:HD3	2.11	0.50
1:E:533:SER:O	1:E:537:THR:OG1	2.27	0.50
1:F:104:LEU:HA	1:F:115:VAL:HG22	1.93	0.50
2:k:73:ASN:OD1	2:k:76:ARG:NE	2.44	0.50
2:G:89:TYR:CD1	3:V:382:ARG:HD3	2.47	0.50
2:I:89:TYR:O	3:Q:378:GLY:HA2	2.11	0.50
3:P:484:PRO:HB3	3:P:491:PHE:CD2	2.46	0.50
2:O:58:ASP:HB2	2:O:91:ARG:NH2	2.27	0.50
2:O:217:ARG:NH1	2:O:223:ARG:HB2	2.27	0.50
1:A:328:TYR:O	1:A:366:VAL:HG23	2.12	0.50
1:B:497:GLU:OE2	1:B:499:THR:OG1	2.28	0.50
1:E:419:ASP:OD1	1:E:419:ASP:N	2.45	0.50
2:m:68:PHE:O	2:m:72:ASP:HB2	2.12	0.50
2:o:89:TYR:O	3:U:378:GLY:HA2	2.11	0.50
2:L:140:ARG:HB2	2:L:156:MET:HE1	1.92	0.50
3:Z:414:PRO:HA	3:Z:417:ALA:HB2	1.93	0.50
1:C:310:LEU:O	1:C:314:MET:HG2	2.12	0.50
1:D:460:HIS:CD2	1:D:543:ARG:HE	2.29	0.50
1:D:478:MET:SD	1:D:547:LEU:HD11	2.52	0.50
1:E:333:LYS:NZ	1:F:398:SER:O	2.45	0.50
1:F:327:SER:OG	1:F:359:LYS:NZ	2.40	0.50
2:l:18:GLU:HA	2:l:21:ARG:CG	2.41	0.50
2:l:92:ARG:NE	3:R:375:THR:HG21	2.27	0.50
2:l:109:THR:O	2:l:113:GLU:HG3	2.11	0.50
2:n:31:VAL:HG23	2:n:42:VAL:HB	1.94	0.50
2:N:55:GLU:HB2	2:N:222:PHE:CG	2.47	0.50
3:Q:310:GLY:HA2	3:Q:415:GLN:HA	1.94	0.50
3:R:402:PRO:HG2	3:R:423:PHE:HB2	1.93	0.50
3:Y:319:ARG:O	3:Y:333:LYS:NZ	2.34	0.50
2:O:41:PHE:HB3	2:O:53:ILE:HD13	1.94	0.50
1:E:494:ARG:HE	1:E:507:VAL:HG11	1.77	0.50
2:n:67:LYS:HE2	2:n:69:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:31:VAL:HB	2:J:42:VAL:HB	1.94	0.50
3:Q:305:ALA:O	3:Q:437:GLN:N	2.43	0.50
3:S:473:ASP:OD1	3:S:521:ARG:NH2	2.35	0.50
1:B:509:TYR:HB2	1:B:511:LYS:HG2	1.94	0.49
1:C:464:LEU:HG	1:C:469:GLY:HA2	1.94	0.49
1:D:187:TRP:HB2	1:D:228:TYR:CE1	2.47	0.49
2:m:101:ASN:O	2:m:105:GLN:HG2	2.11	0.49
2:n:144:ASP:OD2	4:e:171:GLY:N	2.44	0.49
2:G:43:ALA:HB3	2:G:209:GLU:HB3	1.92	0.49
3:W:355:PHE:HD1	3:W:386:MET:HE2	1.77	0.49
3:W:484:PRO:HB3	3:W:491:PHE:CD2	2.47	0.49
3:Y:402:PRO:HG2	3:Y:423:PHE:HB2	1.92	0.49
3:b:407:TYR:CZ	3:b:417:ALA:HB3	2.47	0.49
2:O:107:LEU:HA	2:O:110:ILE:HG12	1.94	0.49
1:C:223:ASP:HB2	1:C:230:PHE:HE2	1.76	0.49
1:D:164:LEU:HA	1:D:176:VAL:HG12	1.94	0.49
1:E:164:LEU:HB2	1:E:220:LEU:HG	1.94	0.49
1:E:284:ARG:HE	1:E:285:PRO:HD2	1.78	0.49
1:F:192:LEU:HB3	1:F:214:LEU:HD11	1.93	0.49
2:J:130:TYR:CD2	2:J:218:PRO:HA	2.47	0.49
2:N:31:VAL:HG23	2:N:42:VAL:HB	1.94	0.49
3:Q:485:ASP:HB3	3:Q:490:ILE:HB	1.93	0.49
1:C:457:LEU:HD13	1:C:542:LEU:HD23	1.95	0.49
1:C:479:ILE:O	1:C:482:VAL:HG12	2.11	0.49
1:D:494:ARG:HH12	1:D:559:GLU:CD	2.19	0.49
1:D:525:ARG:HB3	1:D:550:SER:HB2	1.95	0.49
2:n:28:LYS:HB3	2:n:44:GLU:HG3	1.94	0.49
3:Q:402:PRO:HG2	3:Q:423:PHE:HB2	1.94	0.49
3:R:332:ARG:NH1	3:R:334:VAL:HB	2.27	0.49
3:U:476:ASP:CG	3:X:488:ARG:HH22	2.20	0.49
3:Y:321:THR:HG22	3:Y:326:ILE:HA	1.95	0.49
1:A:523:VAL:HG12	1:A:527:LYS:HE2	1.93	0.49
1:B:436:LYS:HE2	1:B:438:GLU:HG2	1.95	0.49
1:D:155:PHE:HE2	1:D:191:PRO:HD3	1.77	0.49
2:N:57:TYR:HB3	2:N:60:VAL:HB	1.92	0.49
3:P:321:THR:HG22	3:P:326:ILE:HA	1.94	0.49
3:U:302:THR:HA	3:U:440:GLY:HA3	1.94	0.49
1:C:105:LEU:HD11	1:C:116:PHE:HB2	1.95	0.49
1:D:279:ARG:NH2	1:D:285:PRO:HG3	2.28	0.49
1:E:417:ARG:HG3	1:E:420:MET:HE2	1.93	0.49
2:k:58:ASP:O	2:k:221:ALA:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:67:LYS:HA	4:j:172:GLN:O	2.13	0.49
2:I:65:ALA:HB2	2:I:156:MET:HB3	1.94	0.49
2:J:76:ARG:HD2	2:J:77:GLY:N	2.28	0.49
3:P:406:GLY:O	3:P:419:ARG:N	2.44	0.49
3:T:383:LEU:HD23	3:T:423:PHE:CE1	2.47	0.49
3:U:394:ALA:HB1	3:U:399:LEU:HD23	1.93	0.49
3:W:408:ASP:N	3:W:417:ALA:O	2.42	0.49
3:a:311:GLY:HA2	3:a:407:TYR:CE1	2.47	0.49
1:A:182:GLU:OE1	1:A:184:ARG:NH1	2.46	0.49
1:B:457:LEU:HD13	1:B:527:LYS:HE2	1.94	0.49
1:C:496:LEU:HD21	1:C:562:PRO:HB3	1.93	0.49
1:C:569:ASP:O	1:C:572:ARG:HG2	2.13	0.49
1:D:155:PHE:CE2	1:D:191:PRO:HD3	2.48	0.49
1:E:327:SER:O	1:E:359:LYS:NZ	2.33	0.49
1:F:192:LEU:HD22	1:F:214:LEU:HD21	1.94	0.49
2:k:154:VAL:HG12	2:k:156:MET:HE2	1.95	0.49
2:G:217:ARG:HB2	2:G:221:ALA:HA	1.94	0.49
2:L:89:TYR:CD1	3:a:382:ARG:HD3	2.48	0.49
2:N:58:ASP:O	2:N:221:ALA:N	2.41	0.49
3:Q:437:GLN:C	3:Q:450:MET:HE1	2.38	0.49
3:X:303:ILE:HG22	3:X:403:LEU:HD23	1.94	0.49
3:c:315:ALA:HA	3:c:494:ALA:HA	1.94	0.49
2:m:217:ARG:NH1	2:m:223:ARG:HB2	2.28	0.49
2:n:68:PHE:H	4:d:172:GLN:HG2	1.76	0.49
3:U:515:ARG:O	3:U:519:GLU:HG2	2.12	0.49
3:V:351:VAL:HG21	3:V:398:LEU:HB3	1.94	0.49
3:a:322:GLN:HB2	3:a:325:MET:HE3	1.93	0.49
3:a:429:TRP:CZ3	3:a:431:ILE:HG13	2.48	0.49
3:b:513:LEU:O	3:b:517:ILE:HG13	2.12	0.49
3:c:406:GLY:O	3:c:419:ARG:N	2.39	0.49
1:B:309:SER:O	1:B:312:LYS:HG3	2.13	0.49
1:C:394:PRO:HB3	1:F:372:GLU:HG2	1.95	0.49
1:E:453:LEU:HD11	1:E:547:LEU:HD21	1.93	0.49
2:n:54:SER:HB3	2:n:75:ARG:HD2	1.95	0.49
2:n:91:ARG:NH2	2:n:219:ARG:HH21	2.10	0.49
2:G:205:VAL:HG13	2:G:230:LEU:HG	1.95	0.49
3:b:307:LYS:HE2	3:b:435:GLY:HA2	1.94	0.49
1:D:460:HIS:NE2	1:D:462:ASP:OD2	2.46	0.49
1:E:483:VAL:HA	1:E:486:MET:HG2	1.94	0.49
2:n:59:ARG:CG	2:n:91:ARG:HH22	2.23	0.49
2:H:30:VAL:HG13	2:H:43:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:ASP:HB3	2:J:219:ARG:O	2.12	0.49
3:W:380:ILE:HG23	3:W:423:PHE:HZ	1.77	0.49
3:W:391:LEU:O	3:W:395:MET:HG2	2.13	0.49
3:X:407:TYR:CZ	3:X:417:ALA:HB3	2.48	0.49
2:O:52:LYS:HG2	2:O:71:PHE:HZ	1.75	0.49
2:O:58:ASP:HB3	2:O:219:ARG:O	2.13	0.49
1:C:561:LEU:O	1:C:565:THR:HG23	2.13	0.49
1:E:486:MET:HG3	1:E:487:TYR:HD1	1.77	0.49
1:E:573:ILE:HA	1:E:576:LYS:HE2	1.95	0.49
2:m:10:GLU:HA	2:m:13:MET:HE2	1.95	0.49
2:n:28:LYS:HB2	2:n:52:LYS:NZ	2.28	0.49
2:G:165:ASN:O	2:G:169:GLU:HG2	2.13	0.49
3:V:324:ASN:O	3:W:479:SER:OG	2.26	0.49
3:c:329:ARG:O	3:c:490:ILE:HG21	2.13	0.49
1:B:496:LEU:HB3	1:B:508:MET:HE3	1.95	0.48
1:C:332:ILE:HD13	1:C:370:PHE:HE1	1.78	0.48
1:C:446:GLN:HG3	1:C:479:ILE:HG22	1.95	0.48
1:C:482:VAL:O	1:C:486:MET:HG2	2.12	0.48
1:D:357:ARG:NH1	1:D:357:ARG:O	2.43	0.48
2:o:87:TYR:CE1	3:T:357:ARG:HG2	2.48	0.48
2:H:55:GLU:HB2	2:H:222:PHE:CD2	2.48	0.48
2:M:30:VAL:HG13	2:M:43:ALA:HB2	1.95	0.48
3:S:522:SER:HA	3:Z:487:VAL:HG13	1.95	0.48
3:T:366:TYR:CD1	3:T:374:LEU:HG	2.48	0.48
3:T:484:PRO:HB3	3:T:491:PHE:CD2	2.48	0.48
3:V:484:PRO:HB3	3:V:491:PHE:CD1	2.48	0.48
3:X:366:TYR:CD2	3:X:374:LEU:HG	2.47	0.48
3:Z:321:THR:HG22	3:Z:326:ILE:HA	1.95	0.48
3:b:310:GLY:HA2	3:b:415:GLN:HA	1.94	0.48
3:c:312:VAL:HG12	3:c:497:ILE:HB	1.95	0.48
2:O:22:LYS:O	2:O:26:ARG:HG2	2.12	0.48
1:A:486:MET:HE1	1:A:519:ILE:HG12	1.94	0.48
1:B:494:ARG:HG2	1:B:587:LEU:HD22	1.95	0.48
1:C:164:LEU:HD22	1:C:220:LEU:HD11	1.94	0.48
2:m:8:SER:O	2:m:11:GLN:HG3	2.13	0.48
2:n:146:SER:OG	4:e:171:GLY:O	2.30	0.48
2:K:55:GLU:HB2	2:K:222:PHE:CG	2.47	0.48
2:k:107:LEU:HA	2:k:110:ILE:HG12	1.95	0.48
2:k:121:GLU:HG3	2:k:156:MET:HG2	1.94	0.48
2:o:217:ARG:HB2	2:o:221:ALA:HA	1.95	0.48
3:Y:307:LYS:N	3:Y:420:ILE:HD11	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:344:GLY:O	3:c:403:LEU:N	2.37	0.48
3:c:416:SER:O	3:c:419:ARG:NH1	2.46	0.48
1:B:381:GLY:N	1:B:389:GLU:OE2	2.46	0.48
1:C:122:MET:HE1	1:C:147:LEU:HD11	1.94	0.48
1:D:493:ASN:O	1:D:509:TYR:HA	2.14	0.48
1:D:496:LEU:HB2	1:D:508:MET:HE3	1.95	0.48
2:n:122:LEU:HD22	2:n:141:ILE:HD12	1.95	0.48
1:A:400:ILE:HA	1:A:403:VAL:HG12	1.95	0.48
1:F:276:GLU:HG2	1:F:277:LEU:HD22	1.96	0.48
2:H:23:GLY:HA3	2:H:119:GLU:HG2	1.94	0.48
2:I:210:VAL:HB	2:I:225:ILE:O	2.14	0.48
2:J:73:ASN:ND2	2:J:76:ARG:HH21	2.11	0.48
2:M:91:ARG:HH11	2:M:92:ARG:HA	1.79	0.48
3:P:407:TYR:CZ	3:P:417:ALA:HB3	2.48	0.48
3:W:422:SER:HA	3:W:437:GLN:HE22	1.79	0.48
1:B:324:GLU:OE2	1:B:359:LYS:NZ	2.44	0.48
2:k:164:ALA:C	2:k:168:LYS:HZ2	2.21	0.48
2:o:69:ASN:OD1	2:o:70:GLU:N	2.47	0.48
2:G:167:LEU:O	2:G:171:TYR:N	2.46	0.48
2:M:58:ASP:HB3	2:M:219:ARG:O	2.14	0.48
3:Q:338:ASP:OD1	3:Q:341:THR:OG1	2.25	0.48
3:V:359:TYR:HD1	3:V:386:MET:CE	2.27	0.48
3:Y:346:ALA:HB3	3:Y:401:LEU:HB2	1.96	0.48
3:a:321:THR:HG22	3:a:326:ILE:HA	1.96	0.48
3:a:345:ILE:HA	3:a:402:PRO:HA	1.95	0.48
2:O:59:ARG:HD3	2:O:219:ARG:HH21	1.78	0.48
1:A:105:LEU:HD21	1:A:116:PHE:HB2	1.96	0.48
1:A:349:ILE:HD12	1:A:395:GLN:NE2	2.29	0.48
1:C:379:THR:HG22	1:C:381:GLY:H	1.78	0.48
1:C:560:ASP:O	1:C:564:THR:OG1	2.22	0.48
1:D:459:VAL:HG22	1:D:475:ILE:HD11	1.96	0.48
1:F:144:ASN:HD21	1:F:148:THR:HB	1.77	0.48
2:o:165:ASN:HA	2:o:168:LYS:HE3	1.96	0.48
3:P:392:ALA:HA	3:P:395:MET:HE2	1.95	0.48
3:R:320:SER:HB3	3:R:331:VAL:HG21	1.96	0.48
3:S:515:ARG:O	3:S:519:GLU:HG2	2.14	0.48
1:D:452:TYR:CE2	1:D:520:GLN:HG2	2.49	0.48
1:D:525:ARG:HE	1:D:554:GLU:HB3	1.78	0.48
2:k:78:GLY:HA3	2:k:103:TYR:OH	2.13	0.48
2:G:58:ASP:O	2:G:221:ALA:N	2.43	0.48
2:L:73:ASN:O	2:L:76:ARG:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:53:ILE:O	2:M:224:ARG:NH2	2.27	0.48
3:S:307:LYS:HG3	3:S:420:ILE:HG13	1.96	0.48
3:T:317:ASP:HA	3:T:492:PRO:HB3	1.95	0.48
3:Z:322:GLN:OE1	3:Z:322:GLN:N	2.45	0.48
3:b:457:VAL:HG22	3:b:463:GLY:HA2	1.94	0.48
3:c:407:TYR:CZ	3:c:417:ALA:HB3	2.49	0.48
1:B:328:TYR:CZ	1:B:359:LYS:HE3	2.49	0.48
1:B:498:VAL:HG22	1:B:584:ILE:HG22	1.95	0.48
1:C:449:TYR:HE2	1:C:486:MET:SD	2.37	0.48
1:F:314:MET:HE1	1:F:364:THR:HG23	1.96	0.48
2:m:11:GLN:HA	2:m:14:ARG:NE	2.29	0.48
2:o:28:LYS:HD2	2:o:44:GLU:HB3	1.96	0.48
2:J:68:PHE:HA	2:J:71:PHE:CE2	2.48	0.48
2:K:73:ASN:HA	2:K:76:ARG:HG2	1.95	0.48
2:M:11:GLN:OE1	2:M:14:ARG:NH2	2.42	0.48
2:M:58:ASP:HB2	2:M:91:ARG:HH21	1.78	0.48
2:M:161:GLU:OE2	2:M:165:ASN:ND2	2.47	0.48
3:Q:515:ARG:O	3:Q:519:GLU:HG2	2.14	0.48
3:V:424:ASP:OD1	3:V:428:GLY:N	2.47	0.48
3:W:407:TYR:CZ	3:W:417:ALA:HB3	2.49	0.48
3:Z:329:ARG:O	3:Z:490:ILE:HG21	2.14	0.48
3:b:515:ARG:O	3:b:519:GLU:HG2	2.14	0.48
2:O:59:ARG:HG2	2:O:91:ARG:NH2	2.29	0.48
2:O:107:LEU:HD22	2:O:143:TYR:HA	1.96	0.48
1:D:165:ARG:HG3	1:D:177:VAL:HG13	1.96	0.48
2:l:214:ASP:HB3	2:l:217:ARG:HG2	1.95	0.48
2:n:142:THR:OG1	2:n:144:ASP:OD1	2.28	0.48
2:o:59:ARG:HG2	2:o:91:ARG:NH2	2.29	0.48
2:G:59:ARG:NH2	2:G:215:ALA:O	2.46	0.48
2:J:151:PRO:HG2	2:J:152:HIS:CD2	2.49	0.48
2:M:58:ASP:O	2:M:221:ALA:N	2.41	0.48
2:N:141:ILE:HG12	2:N:147:ILE:HG13	1.96	0.48
3:W:394:ALA:HB1	3:W:399:LEU:HD13	1.96	0.48
3:X:473:ASP:OD1	3:X:521:ARG:NH2	2.47	0.48
3:a:347:GLY:HA3	3:a:400:ALA:HA	1.96	0.48
1:C:415:SER:OG	1:C:417:ARG:O	2.26	0.47
2:o:205:VAL:HG13	2:o:230:LEU:HG	1.95	0.47
2:L:23:GLY:HA3	2:L:119:GLU:HB3	1.94	0.47
2:N:54:SER:O	2:N:62:PHE:N	2.43	0.47
3:X:350:ALA:HB1	3:Y:388:ARG:HH21	1.79	0.47
3:Z:384:ALA:HB2	3:Z:429:TRP:HE3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:507:GLU:HA	3:c:510:ILE:HD12	1.95	0.47
1:F:275:LYS:O	1:F:279:ARG:HD3	2.14	0.47
1:F:290:LEU:HD22	1:F:426:LEU:HD22	1.96	0.47
2:l:22:LYS:HG3	2:l:26:ARG:HH22	1.79	0.47
2:o:45:ASN:HB3	2:o:209:GLU:HG2	1.96	0.47
2:o:83:ASP:OD1	3:T:368:LYS:NZ	2.39	0.47
2:H:106:THR:HA	2:H:109:THR:HG22	1.95	0.47
2:L:55:GLU:HB2	2:L:222:PHE:CD2	2.49	0.47
2:N:73:ASN:ND2	2:N:76:ARG:HH21	2.11	0.47
3:U:311:GLY:HA2	3:U:407:TYR:CE1	2.49	0.47
3:Y:380:ILE:HG23	3:Y:423:PHE:CZ	2.49	0.47
3:a:382:ARG:HB3	3:a:386:MET:HE1	1.96	0.47
1:E:265:ARG:HH22	1:E:306:VAL:HG23	1.78	0.47
1:E:360:ALA:HB1	1:E:408:ASN:HB3	1.96	0.47
1:F:337:LEU:HD13	1:F:349:ILE:HD11	1.96	0.47
2:k:40:LEU:HA	2:k:212:VAL:HG12	1.96	0.47
2:l:205:VAL:HG13	2:l:230:LEU:HG	1.94	0.47
2:m:91:ARG:HH11	2:m:91:ARG:C	2.21	0.47
2:M:110:ILE:HG21	2:M:118:TYR:CD2	2.50	0.47
3:R:485:ASP:N	3:R:490:ILE:O	2.48	0.47
3:U:314:MET:O	3:U:495:VAL:N	2.35	0.47
3:V:507:GLU:HA	3:V:510:ILE:HD12	1.96	0.47
3:c:424:ASP:OD1	3:c:428:GLY:N	2.47	0.47
3:c:485:ASP:N	3:c:490:ILE:O	2.47	0.47
1:A:281:TYR:OH	1:D:534:VAL:HG21	2.14	0.47
1:B:335:PRO:HG2	1:E:395:GLN:HB2	1.97	0.47
1:C:328:TYR:CD2	1:C:359:LYS:HD2	2.49	0.47
1:D:219:SER:HB2	1:D:235:LYS:HZ2	1.80	0.47
1:D:260:GLN:O	1:D:263:GLN:HG3	2.14	0.47
1:F:290:LEU:HB2	1:F:431:LEU:HD13	1.95	0.47
1:F:379:THR:O	1:F:382:THR:OG1	2.25	0.47
2:k:178:THR:HG22	2:k:182:ARG:HE	1.79	0.47
2:l:58:ASP:HB3	2:l:219:ARG:O	2.13	0.47
2:G:91:ARG:HH11	2:G:91:ARG:C	2.21	0.47
2:N:87:TYR:HE1	3:b:357:ARG:HG3	1.79	0.47
3:Q:485:ASP:N	3:Q:490:ILE:O	2.48	0.47
3:S:407:TYR:CZ	3:S:417:ALA:HB3	2.49	0.47
3:U:304:VAL:HA	3:U:438:ALA:HA	1.96	0.47
3:a:378:GLY:O	3:a:382:ARG:HG2	2.15	0.47
3:b:366:TYR:CZ	3:b:370:GLU:HG3	2.50	0.47
1:B:379:THR:HG22	1:B:423:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:TYR:N	1:C:512:ASP:OD2	2.44	0.47
1:E:300:THR:HG22	1:E:304:LYS:HE3	1.97	0.47
2:k:70:GLU:OE1	2:k:119:GLU:N	2.48	0.47
2:k:87:TYR:CE1	3:W:357:ARG:HG2	2.50	0.47
2:J:58:ASP:O	2:J:221:ALA:N	2.42	0.47
2:K:89:TYR:CE1	3:Z:382:ARG:HD3	2.49	0.47
2:K:128:ALA:HB2	2:K:134:LYS:HB3	1.95	0.47
2:L:70:GLU:OE1	2:L:119:GLU:N	2.48	0.47
2:L:89:TYR:CE1	3:a:382:ARG:HD3	2.50	0.47
2:N:217:ARG:HB2	2:N:221:ALA:HA	1.96	0.47
3:Q:406:GLY:O	3:Q:419:ARG:N	2.41	0.47
3:U:315:ALA:HA	3:U:494:ALA:HA	1.96	0.47
3:a:302:THR:OG1	3:a:481:THR:OG1	2.32	0.47
4:j:172:GLN:OE1	4:j:172:GLN:N	2.47	0.47
1:A:499:THR:HG23	1:A:505:LYS:HG2	1.97	0.47
1:B:266:ASP:HA	1:B:270:LEU:HD13	1.95	0.47
1:B:367:ILE:HD13	1:B:410:ILE:HB	1.96	0.47
1:C:384:VAL:HB	1:C:387:ASP:HB2	1.95	0.47
1:E:158:VAL:HG12	1:F:185:VAL:HG12	1.96	0.47
2:k:22:LYS:HB3	2:k:26:ARG:HH22	1.79	0.47
2:m:205:VAL:HG11	2:m:231:GLN:HB2	1.96	0.47
2:n:217:ARG:HB2	2:n:221:ALA:HA	1.96	0.47
2:J:28:LYS:NZ	2:J:46:PRO:HD3	2.29	0.47
2:K:69:ASN:OD1	2:K:70:GLU:N	2.48	0.47
2:L:68:PHE:HA	2:L:71:PHE:CE2	2.50	0.47
3:T:484:PRO:HB3	3:T:491:PHE:HD2	1.80	0.47
3:W:338:ASP:OD1	3:W:341:THR:OG1	2.31	0.47
3:X:507:GLU:HA	3:X:510:ILE:HD12	1.97	0.47
1:A:374:ASP:OD1	1:A:415:SER:OG	2.23	0.47
1:C:215:ARG:NH2	1:C:216:PRO:O	2.45	0.47
1:C:449:TYR:O	1:C:453:LEU:N	2.36	0.47
1:C:531:ILE:HG12	1:D:281:TYR:CD2	2.50	0.47
1:D:489:GLU:HA	1:D:509:TYR:CD2	2.50	0.47
1:E:506:GLU:HG3	1:E:577:LYS:HE2	1.97	0.47
2:l:89:TYR:O	3:R:378:GLY:HA2	2.15	0.47
2:l:140:ARG:NH2	2:l:150:GLU:OE2	2.38	0.47
2:m:55:GLU:HB2	2:m:222:PHE:CG	2.50	0.47
2:H:33:LEU:HD11	2:H:180:ALA:HB1	1.97	0.47
2:H:68:PHE:HA	2:H:71:PHE:CE2	2.50	0.47
2:H:78:GLY:HA3	2:H:103:TYR:OH	2.14	0.47
2:I:67:LYS:HG2	2:I:69:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:20:ALA:HA	2:L:119:GLU:HG2	1.97	0.47
2:L:88:ALA:O	3:a:381:ASN:ND2	2.48	0.47
3:T:392:ALA:HA	3:T:395:MET:HE3	1.96	0.47
3:V:384:ALA:HB2	3:V:429:TRP:HE3	1.79	0.47
3:Y:515:ARG:O	3:Y:519:GLU:HG2	2.14	0.47
3:a:317:ASP:HA	3:a:492:PRO:HB3	1.97	0.47
3:a:438:ALA:HB3	3:a:447:LYS:HG2	1.96	0.47
1:C:278:TYR:CE1	1:F:531:ILE:HG21	2.50	0.47
1:C:496:LEU:HD11	1:C:562:PRO:HA	1.96	0.47
2:m:167:LEU:O	2:m:171:TYR:N	2.48	0.47
2:n:29:SER:HA	2:n:156:MET:O	2.15	0.47
2:G:211:ALA:HB2	2:G:224:ARG:HG2	1.96	0.47
2:I:165:ASN:O	2:I:169:GLU:HG2	2.14	0.47
2:J:18:GLU:OE1	2:J:21:ARG:NH1	2.45	0.47
2:K:140:ARG:NH2	2:K:155:VAL:H	2.13	0.47
2:M:41:PHE:HB3	2:M:53:ILE:HD13	1.96	0.47
2:M:73:ASN:HA	2:M:76:ARG:HG3	1.95	0.47
3:Q:302:THR:HA	3:Q:440:GLY:HA3	1.96	0.47
3:Q:407:TYR:CZ	3:Q:417:ALA:HB3	2.50	0.47
3:Q:414:PRO:HA	3:Q:417:ALA:HB2	1.97	0.47
3:S:322:GLN:HG2	3:S:325:MET:HB3	1.97	0.47
3:Z:484:PRO:HB3	3:Z:491:PHE:CD2	2.50	0.47
1:A:272:PHE:CE1	1:A:408:ASN:HA	2.50	0.47
1:B:495:PHE:CZ	1:B:562:PRO:HD3	2.50	0.47
1:D:330:LEU:N	1:D:367:ILE:O	2.45	0.47
1:F:373:MET:HE3	1:F:373:MET:O	2.15	0.47
1:F:425:ILE:HD12	1:F:430:ARG:HD3	1.97	0.47
2:G:58:ASP:HB3	2:G:219:ARG:O	2.15	0.47
2:J:217:ARG:HH12	2:J:223:ARG:HB2	1.80	0.47
2:K:87:TYR:HD1	3:Y:361:VAL:HG21	1.80	0.47
3:Q:423:PHE:CD2	3:Q:429:TRP:HB3	2.50	0.47
3:V:480:ALA:HB2	3:W:324:ASN:ND2	2.29	0.47
3:X:305:ALA:HB2	3:X:314:MET:HG2	1.97	0.47
3:b:378:GLY:O	3:b:382:ARG:HG2	2.14	0.47
1:B:393:VAL:O	1:B:397:LEU:HG	2.15	0.47
1:C:439:ARG:HH22	1:C:561:LEU:HD22	1.80	0.47
1:D:243:LEU:CD1	1:D:355:ARG:HB3	2.45	0.47
1:E:528:LYS:O	1:E:531:ILE:HG22	2.15	0.47
2:k:110:ILE:HA	2:k:114:GLN:OE1	2.14	0.47
2:l:19:LEU:HA	2:l:22:LYS:NZ	2.30	0.47
2:l:68:PHE:HA	2:l:71:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:22:LYS:HG3	2:m:26:ARG:HH22	1.79	0.47
2:o:44:GLU:HA	2:o:208:LEU:HD23	1.97	0.47
2:o:68:PHE:HA	2:o:71:PHE:CE2	2.50	0.47
2:G:52:LYS:HG3	2:G:71:PHE:CZ	2.50	0.47
2:J:83:ASP:OD1	3:X:368:LYS:NZ	2.31	0.47
2:N:30:VAL:HG13	2:N:43:ALA:HB2	1.97	0.47
3:Q:366:TYR:CE2	3:Q:374:LEU:HG	2.50	0.47
3:U:332:ARG:NH1	3:U:493:THR:HB	2.26	0.47
3:U:378:GLY:O	3:U:382:ARG:HG2	2.14	0.47
3:X:469:GLU:OE2	3:X:521:ARG:NH2	2.48	0.47
3:Z:458:THR:H	3:Z:462:SER:HG	1.60	0.47
3:a:422:SER:O	3:a:430:ASN:N	2.46	0.47
1:A:104:LEU:HD22	1:A:135:LEU:HD12	1.96	0.46
1:D:254:ILE:HD11	1:D:261:ILE:HD11	1.97	0.46
1:F:528:LYS:HD3	1:F:532:LYS:HE3	1.97	0.46
2:G:219:ARG:HB3	2:G:220:ARG:HD3	1.97	0.46
2:I:124:VAL:N	2:I:139:TYR:O	2.38	0.46
2:K:70:GLU:CG	2:K:118:TYR:HD1	2.25	0.46
2:M:217:ARG:NH1	2:M:223:ARG:HB2	2.30	0.46
3:T:497:ILE:HA	3:T:502:ALA:HA	1.97	0.46
3:V:324:ASN:ND2	3:W:478:ASP:OD1	2.47	0.46
3:V:432:GLU:HG3	3:V:437:GLN:HB2	1.97	0.46
3:W:358:LEU:HD23	3:W:386:MET:HE3	1.97	0.46
3:Z:319:ARG:HD3	3:Z:482:GLY:HA3	1.96	0.46
1:D:446:GLN:HA	1:D:483:VAL:HG21	1.95	0.46
2:m:182:ARG:NH2	2:m:233:LEU:O	2.48	0.46
2:o:82:ALA:HB2	2:o:99:LEU:HD11	1.97	0.46
2:G:54:SER:OG	2:G:75:ARG:HD2	2.15	0.46
2:G:59:ARG:HG2	2:G:91:ARG:NH2	2.30	0.46
2:I:34:ALA:HB1	2:I:136:PRO:HG2	1.97	0.46
2:J:79:ILE:HG22	3:X:365:HIS:CE1	2.51	0.46
2:J:137:GLU:OE1	2:J:139:TYR:OH	2.22	0.46
2:K:45:ASN:ND2	2:K:47:SER:O	2.48	0.46
2:K:104:ALA:HA	2:K:141:ILE:HG21	1.97	0.46
2:M:96:GLY:H	2:M:126:GLU:CD	2.23	0.46
2:M:154:VAL:HG12	2:M:156:MET:SD	2.56	0.46
3:Q:318:ARG:HA	3:Q:331:VAL:O	2.15	0.46
3:S:345:ILE:HB	3:S:352:ALA:HB1	1.96	0.46
3:W:383:LEU:HD23	3:W:423:PHE:CE1	2.50	0.46
3:Y:437:GLN:HA	3:Y:447:LYS:HD2	1.97	0.46
3:a:407:TYR:HB2	3:a:497:ILE:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:THR:HG21	1:F:97:PRO:HD2	1.96	0.46
1:D:254:ILE:HB	1:D:257:LEU:HD12	1.98	0.46
2:l:217:ARG:HB2	2:l:221:ALA:HA	1.98	0.46
2:m:28:LYS:HB2	2:m:52:LYS:NZ	2.30	0.46
2:H:105:GLN:NE2	2:I:72:ASP:OD2	2.48	0.46
2:J:142:THR:OG1	2:J:144:ASP:OD1	2.29	0.46
2:K:130:TYR:CD2	2:K:218:PRO:HA	2.51	0.46
2:L:40:LEU:HD21	2:L:181:LEU:HD23	1.96	0.46
3:P:329:ARG:O	3:P:490:ILE:HG21	2.15	0.46
3:P:475:ALA:HA	3:P:481:THR:HB	1.96	0.46
3:P:485:ASP:HB3	3:P:490:ILE:HB	1.97	0.46
3:R:378:GLY:O	3:R:382:ARG:HG2	2.16	0.46
3:T:340:TYR:OH	3:T:499:ALA:O	2.28	0.46
3:Y:464:LEU:HD21	3:Y:505:VAL:HG11	1.97	0.46
1:A:495:PHE:HB3	1:A:508:MET:SD	2.56	0.46
1:D:452:TYR:HB3	1:D:523:VAL:HG21	1.97	0.46
1:E:496:LEU:HB2	1:E:508:MET:HE2	1.97	0.46
1:E:525:ARG:HB3	1:E:550:SER:OG	2.16	0.46
2:k:87:TYR:HE1	3:W:357:ARG:HG2	1.81	0.46
2:k:140:ARG:HH22	2:k:155:VAL:H	1.62	0.46
2:l:33:LEU:HD11	2:l:180:ALA:HB1	1.97	0.46
2:m:53:ILE:HG21	2:m:211:ALA:HB3	1.97	0.46
2:m:88:ALA:O	3:S:382:ARG:NH1	2.46	0.46
2:o:96:GLY:H	2:o:126:GLU:CD	2.23	0.46
2:G:182:ARG:HH12	2:G:234:LEU:HA	1.80	0.46
2:I:80:GLN:HG3	3:P:365:HIS:CE1	2.51	0.46
2:L:58:ASP:O	2:L:221:ALA:N	2.44	0.46
3:T:469:GLU:HG3	3:T:521:ARG:HH21	1.79	0.46
3:W:315:ALA:HA	3:W:494:ALA:HA	1.96	0.46
3:Y:407:TYR:CZ	3:Y:417:ALA:HB3	2.51	0.46
3:Y:485:ASP:N	3:Y:490:ILE:O	2.46	0.46
3:a:332:ARG:HD3	3:a:493:THR:HG21	1.97	0.46
1:B:142:ARG:HD3	1:B:151:GLU:HB3	1.98	0.46
1:B:417:ARG:HB3	1:B:420:MET:HE1	1.97	0.46
1:B:486:MET:HG3	1:B:555:PHE:HZ	1.80	0.46
1:C:136:LYS:NZ	1:C:190:ASP:HB2	2.31	0.46
2:m:67:LYS:NZ	2:m:69:ASN:HD21	2.10	0.46
2:o:58:ASP:HB3	2:o:219:ARG:O	2.14	0.46
2:I:89:TYR:CD1	3:Q:382:ARG:HD3	2.51	0.46
2:I:91:ARG:HH21	2:I:94:VAL:HG21	1.79	0.46
2:K:78:GLY:HA3	2:K:103:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:140:ARG:HE	2:K:154:VAL:HG13	1.80	0.46
2:N:90:ASP:HB3	2:N:93:ASP:CG	2.40	0.46
3:R:319:ARG:HD3	3:R:482:GLY:HA3	1.97	0.46
3:T:437:GLN:HA	3:T:447:LYS:NZ	2.30	0.46
3:W:511:ALA:HB1	3:W:515:ARG:HH21	1.80	0.46
3:Y:383:LEU:HD22	3:Y:423:PHE:CZ	2.51	0.46
3:Y:416:SER:O	3:Y:419:ARG:NH1	2.39	0.46
3:b:346:ALA:O	3:b:401:LEU:N	2.33	0.46
3:c:332:ARG:NH1	3:c:493:THR:HB	2.31	0.46
1:B:115:VAL:HG11	1:B:143:LEU:HD11	1.96	0.46
2:l:22:LYS:O	2:l:26:ARG:HG2	2.16	0.46
2:G:128:ALA:HB2	2:G:134:LYS:HB3	1.97	0.46
2:I:217:ARG:NH1	2:I:223:ARG:HB2	2.30	0.46
2:K:58:ASP:O	2:K:221:ALA:N	2.41	0.46
2:K:173:GLU:OE1	2:K:173:GLU:N	2.47	0.46
2:M:45:ASN:ND2	2:M:50:LEU:O	2.44	0.46
3:T:457:VAL:HG22	3:T:463:GLY:HA2	1.98	0.46
3:X:393:ALA:O	3:X:398:LEU:HB3	2.15	0.46
1:B:427:ARG:HD2	1:B:428:PRO:O	2.16	0.46
1:C:157:ALA:HB1	1:D:173:ARG:HH11	1.80	0.46
1:D:219:SER:H	1:D:235:LYS:NZ	2.13	0.46
2:k:122:LEU:HD23	2:k:141:ILE:HD13	1.98	0.46
2:o:89:TYR:CE1	3:U:382:ARG:HD3	2.50	0.46
2:H:8:SER:O	2:H:12:ALA:N	2.37	0.46
2:I:8:SER:O	2:I:11:GLN:HG3	2.16	0.46
3:U:322:GLN:HG2	3:U:325:MET:HB3	1.97	0.46
3:V:318:ARG:HB3	3:V:330:ASP:HA	1.97	0.46
3:X:320:SER:HB3	3:X:328:GLY:HA3	1.97	0.46
3:Y:441:SER:OG	3:Y:478:ASP:OD2	2.28	0.46
3:c:317:ASP:HA	3:c:492:PRO:HB3	1.98	0.46
1:B:144:ASN:HD21	1:B:148:THR:HB	1.79	0.46
1:C:498:VAL:HG22	1:C:584:ILE:HG12	1.98	0.46
2:G:205:VAL:HG22	2:G:234:LEU:HD23	1.98	0.46
2:I:152:HIS:HB3	2:I:171:TYR:CE2	2.51	0.46
2:L:8:SER:HB2	2:L:11:GLN:HG2	1.97	0.46
2:M:54:SER:OG	2:M:75:ARG:HD2	2.16	0.46
3:Q:301:THR:O	3:Q:441:SER:N	2.47	0.46
3:T:346:ALA:N	3:T:401:LEU:O	2.48	0.46
3:V:329:ARG:O	3:V:490:ILE:HG21	2.15	0.46
3:W:418:GLY:O	3:W:419:ARG:NH1	2.43	0.46
1:A:272:PHE:CE2	1:A:365:PRO:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:PHE:HB3	1:A:357:ARG:NH1	2.31	0.46
1:A:463:ASP:HB3	1:A:474:CYS:SG	2.56	0.46
1:A:545:GLN:HA	1:A:548:LEU:HB2	1.97	0.46
1:D:377:PHE:HE1	1:D:421:ILE:HG23	1.81	0.46
1:D:565:THR:HG22	1:D:566:ASN:H	1.81	0.46
1:F:486:MET:HG2	1:F:555:PHE:CZ	2.50	0.46
2:k:182:ARG:NH2	2:k:233:LEU:O	2.49	0.46
2:K:223:ARG:HH12	2:K:225:ILE:HG12	1.81	0.46
2:M:47:SER:OG	2:M:50:LEU:HB2	2.16	0.46
2:M:87:TYR:CD1	3:a:361:VAL:HG21	2.47	0.46
2:M:214:ASP:N	2:M:221:ALA:O	2.38	0.46
2:N:14:ARG:O	2:N:18:GLU:HG2	2.16	0.46
3:W:317:ASP:HA	3:W:492:PRO:HB3	1.98	0.46
3:Z:447:LYS:HA	3:Z:450:MET:HG2	1.97	0.46
1:A:310:LEU:HD22	1:A:367:ILE:HD12	1.98	0.46
1:E:374:ASP:HB3	1:E:420:MET:HE3	1.98	0.46
2:k:11:GLN:OE1	2:k:14:ARG:NH1	2.47	0.46
2:k:57:TYR:HB3	2:k:60:VAL:HB	1.98	0.46
2:n:91:ARG:CZ	2:n:219:ARG:NH2	2.79	0.46
2:I:116:LYS:NZ	2:I:119:GLU:OE2	2.49	0.46
3:R:304:VAL:O	3:R:314:MET:HG2	2.16	0.46
3:S:301:THR:O	3:S:441:SER:N	2.48	0.46
3:T:338:ASP:OD1	3:T:341:THR:HG22	2.16	0.46
3:V:338:ASP:OD1	3:V:341:THR:OG1	2.30	0.46
3:c:354:GLU:OE1	3:c:357:ARG:NE	2.46	0.46
2:O:58:ASP:HB2	2:O:91:ARG:HH21	1.80	0.46
1:A:478:MET:HG2	1:A:544:ILE:HD13	1.98	0.45
2:l:18:GLU:O	2:l:21:ARG:HG3	2.15	0.45
2:o:182:ARG:HA	2:o:185:VAL:HG12	1.98	0.45
2:L:61:GLY:H	2:L:213:LEU:HD11	1.80	0.45
2:L:166:ALA:O	2:L:170:SER:OG	2.30	0.45
2:N:76:ARG:HD2	2:N:77:GLY:N	2.30	0.45
2:N:217:ARG:NH1	2:N:223:ARG:HB2	2.30	0.45
3:Q:307:LYS:NZ	3:Q:432:GLU:O	2.35	0.45
3:S:378:GLY:O	3:S:382:ARG:HG2	2.16	0.45
3:T:401:LEU:HD22	3:T:439:VAL:HB	1.97	0.45
3:U:436:TYR:HB2	3:U:450:MET:SD	2.56	0.45
3:V:318:ARG:HA	3:V:331:VAL:O	2.16	0.45
3:W:366:TYR:CD1	3:W:374:LEU:HG	2.51	0.45
3:Z:345:ILE:HB	3:Z:352:ALA:HB1	1.98	0.45
3:b:385:ILE:O	3:b:388:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:357:ARG:HG3	2:O:87:TYR:CE1	2.52	0.45
1:A:267:ALA:HA	1:A:286:PRO:HG2	1.97	0.45
1:A:425:ILE:HD11	1:A:431:LEU:HD23	1.98	0.45
1:A:510:PHE:CE2	1:A:555:PHE:HB3	2.51	0.45
1:C:328:TYR:HD2	1:C:359:LYS:HB3	1.81	0.45
1:D:391:THR:HG23	1:D:393:VAL:H	1.81	0.45
1:E:531:ILE:HD11	1:F:277:LEU:HD12	1.97	0.45
2:I:57:TYR:OH	2:I:91:ARG:O	2.31	0.45
2:G:78:GLY:HA3	2:G:103:TYR:OH	2.16	0.45
2:M:156:MET:SD	2:M:156:MET:N	2.89	0.45
2:N:45:ASN:HB3	2:N:209:GLU:HB2	1.98	0.45
2:N:87:TYR:CD1	3:b:361:VAL:HG21	2.52	0.45
2:N:177:LEU:HD12	2:N:233:LEU:HD21	1.97	0.45
3:Q:436:TYR:HB2	3:Q:450:MET:SD	2.56	0.45
3:R:407:TYR:CZ	3:R:417:ALA:HB3	2.50	0.45
3:U:329:ARG:O	3:U:490:ILE:HG21	2.17	0.45
3:W:378:GLY:O	3:W:382:ARG:HG2	2.16	0.45
3:W:450:MET:HB2	3:W:470:ALA:HB2	1.98	0.45
1:B:161:ILE:HB	1:E:183:GLU:HG2	1.98	0.45
1:D:142:ARG:NE	1:D:151:GLU:OE2	2.49	0.45
1:D:269:GLU:O	1:D:273:LEU:N	2.48	0.45
1:E:486:MET:HG3	1:E:487:TYR:CD1	2.52	0.45
2:k:105:GLN:O	2:k:109:THR:HG23	2.16	0.45
2:n:59:ARG:NH2	2:n:215:ALA:O	2.44	0.45
2:I:79:ILE:HG22	3:P:365:HIS:CE1	2.52	0.45
2:J:134:LYS:NZ	2:J:137:GLU:HG3	2.28	0.45
3:P:310:GLY:HA2	3:P:415:GLN:HA	1.97	0.45
3:X:485:ASP:N	3:X:490:ILE:O	2.46	0.45
3:Y:378:GLY:O	3:Y:382:ARG:HG2	2.16	0.45
3:a:346:ALA:N	3:a:401:LEU:O	2.48	0.45
3:b:450:MET:O	3:b:454:TYR:HB2	2.17	0.45
1:B:310:LEU:HG	1:B:314:MET:HE2	1.99	0.45
2:n:17:SER:HG	2:n:143:TYR:HH	1.61	0.45
2:n:110:ILE:HD13	2:n:118:TYR:CE2	2.52	0.45
2:o:91:ARG:HH11	2:o:91:ARG:C	2.24	0.45
2:H:76:ARG:HD2	2:H:77:GLY:N	2.32	0.45
2:H:137:GLU:OE1	2:H:139:TYR:OH	2.26	0.45
2:J:110:ILE:HG12	2:J:118:TYR:CE2	2.51	0.45
2:K:61:GLY:N	2:K:213:LEU:HD11	2.31	0.45
3:P:497:ILE:HA	3:P:502:ALA:HA	1.98	0.45
3:Q:432:GLU:HG3	3:Q:437:GLN:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:301:THR:O	3:R:441:SER:N	2.43	0.45
3:T:393:ALA:HA	3:T:396:GLN:HE21	1.81	0.45
3:W:346:ALA:O	3:W:401:LEU:HD23	2.16	0.45
3:W:381:ASN:ND2	2:O:88:ALA:O	2.50	0.45
3:Z:306:LEU:HA	3:Z:436:TYR:HA	1.98	0.45
3:c:321:THR:HG22	3:c:326:ILE:HA	1.98	0.45
3:c:359:TYR:OH	3:c:379:LYS:HB3	2.17	0.45
2:O:58:ASP:O	2:O:221:ALA:N	2.43	0.45
1:A:427:ARG:HD3	1:A:428:PRO:HD2	1.98	0.45
1:C:187:TRP:HB2	1:C:228:TYR:CE1	2.52	0.45
1:F:213:LYS:O	1:F:215:ARG:NH1	2.50	0.45
2:o:128:ALA:HB2	2:o:134:LYS:HB3	1.97	0.45
2:H:87:TYR:CD1	3:V:361:VAL:HG21	2.51	0.45
2:I:33:LEU:HD11	2:I:180:ALA:HB1	1.97	0.45
2:J:96:GLY:H	2:J:126:GLU:CD	2.25	0.45
2:J:118:TYR:HB3	2:J:120:VAL:HG22	1.98	0.45
3:Q:469:GLU:HG3	3:Q:521:ARG:HH21	1.80	0.45
3:T:320:SER:HB3	3:T:331:VAL:HG21	1.99	0.45
3:U:321:THR:HG22	3:U:326:ILE:HA	1.98	0.45
3:c:393:ALA:HA	3:c:396:GLN:NE2	2.30	0.45
1:A:388:VAL:HG12	1:A:390:THR:H	1.82	0.45
2:n:67:LYS:HB3	2:n:70:GLU:HG3	1.99	0.45
2:n:107:LEU:O	2:n:111:PHE:HD1	1.98	0.45
2:G:68:PHE:HA	2:G:71:PHE:CE2	2.52	0.45
2:L:11:GLN:CD	2:L:14:ARG:HH12	2.25	0.45
2:L:73:ASN:HA	2:L:76:ARG:CD	2.47	0.45
3:P:307:LYS:HG3	3:P:420:ILE:HG13	1.98	0.45
3:P:416:SER:O	3:P:419:ARG:NH1	2.36	0.45
3:R:317:ASP:O	3:R:333:LYS:HG3	2.17	0.45
3:R:359:TYR:OH	3:R:379:LYS:HB3	2.16	0.45
3:U:432:GLU:HG3	3:U:437:GLN:HB2	1.98	0.45
3:V:303:ILE:HD11	3:V:333:LYS:HB3	1.98	0.45
1:A:296:GLY:HA3	1:B:427:ARG:HD3	1.99	0.45
1:A:328:TYR:CE1	1:A:359:LYS:HD2	2.51	0.45
1:B:446:GLN:HA	1:B:483:VAL:HG21	1.98	0.45
1:B:523:VAL:HG12	1:B:527:LYS:HE3	1.97	0.45
1:C:264:ILE:O	1:C:268:VAL:HG22	2.16	0.45
1:C:275:LYS:HZ1	1:C:285:PRO:HB3	1.82	0.45
1:C:508:MET:HE3	1:C:512:ASP:HB3	1.98	0.45
1:C:509:TYR:HB2	1:C:511:LYS:HG2	1.99	0.45
1:C:530:ALA:O	1:C:534:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:TYR:CZ	1:D:520:GLN:HG2	2.52	0.45
1:E:457:LEU:O	1:E:471:ARG:NH2	2.50	0.45
2:k:89:TYR:O	3:X:378:GLY:HA2	2.16	0.45
2:m:68:PHE:HA	2:m:71:PHE:CE2	2.51	0.45
2:H:56:LEU:HD23	2:H:56:LEU:HA	1.87	0.45
2:J:103:TYR:HA	2:J:106:THR:HG22	1.99	0.45
2:J:154:VAL:HG12	2:J:156:MET:SD	2.57	0.45
2:K:142:THR:HG22	2:K:146:SER:HB3	1.98	0.45
2:N:73:ASN:O	2:N:76:ARG:HG3	2.16	0.45
2:N:89:TYR:CE1	3:c:382:ARG:HD3	2.52	0.45
3:R:414:PRO:HA	3:R:417:ALA:HB2	1.98	0.45
3:U:423:PHE:CE2	3:U:429:TRP:HB3	2.52	0.45
3:X:319:ARG:NH1	3:X:479:SER:O	2.38	0.45
3:Y:319:ARG:NH2	3:Y:485:ASP:HB2	2.31	0.45
3:a:362:GLU:OE2	3:a:382:ARG:NE	2.50	0.45
2:O:30:VAL:HG13	2:O:43:ALA:HB2	1.97	0.45
2:O:78:GLY:HA3	2:O:103:TYR:OH	2.16	0.45
1:C:137:LYS:HE3	1:C:172:HIS:HE1	1.81	0.45
1:C:485:ARG:O	1:C:493:ASN:ND2	2.46	0.45
1:D:105:LEU:HD21	1:D:116:PHE:CD2	2.52	0.45
1:D:353:PHE:CG	1:D:399:GLU:HB3	2.51	0.45
1:E:314:MET:HE3	1:E:328:TYR:CD2	2.51	0.45
2:k:217:ARG:NH1	2:k:223:ARG:HB2	2.32	0.45
2:n:119:GLU:OE1	2:n:119:GLU:N	2.47	0.45
2:n:128:ALA:HA	2:n:134:LYS:HE3	1.98	0.45
2:G:166:ALA:O	2:G:170:SER:OG	2.28	0.45
2:K:31:VAL:HG12	2:K:155:VAL:HG22	1.98	0.45
2:N:57:TYR:CG	2:N:58:ASP:N	2.85	0.45
3:S:414:PRO:HA	3:S:417:ALA:HB2	1.97	0.45
3:V:517:ILE:O	3:V:521:ARG:HG2	2.17	0.45
3:W:318:ARG:NH2	3:W:330:ASP:O	2.48	0.45
3:Y:346:ALA:O	3:Y:401:LEU:N	2.36	0.45
1:C:397:LEU:HD11	1:C:424:ALA:HB1	1.99	0.45
1:F:570:TRP:CD1	1:F:580:ARG:HH22	2.35	0.45
2:k:28:LYS:HB3	2:k:52:LYS:NZ	2.31	0.45
2:l:155:VAL:HG12	2:l:160:THR:HG22	1.99	0.45
2:o:110:ILE:O	2:o:114:GLN:HB3	2.16	0.45
2:o:111:PHE:HA	2:o:117:PRO:HB3	1.99	0.45
2:G:53:ILE:HG21	2:G:211:ALA:HB3	1.99	0.45
2:G:55:GLU:HA	2:G:61:GLY:HA2	1.99	0.45
2:J:171:TYR:CE2	2:J:173:GLU:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:393:ALA:O	3:T:396:GLN:NE2	2.50	0.45
3:X:341:THR:HG22	3:X:406:GLY:HA3	1.97	0.45
3:b:385:ILE:O	3:b:388:ARG:HD3	2.16	0.45
3:c:484:PRO:HB3	3:c:491:PHE:CD2	2.51	0.45
1:A:365:PRO:HA	1:A:408:ASN:HB3	1.99	0.45
1:A:533:SER:HB2	1:A:539:GLN:HE21	1.81	0.45
1:B:192:LEU:HD11	1:B:231:GLU:HA	1.99	0.45
1:E:460:HIS:HE2	1:E:539:GLN:HB2	1.82	0.45
2:G:109:THR:O	2:G:113:GLU:HG3	2.17	0.45
2:J:73:ASN:O	2:J:76:ARG:HG3	2.16	0.45
2:N:85:ARG:HG3	2:N:94:VAL:HG22	1.98	0.45
3:P:359:TYR:HD1	3:P:386:MET:HE1	1.82	0.45
3:T:508:SER:OG	3:T:509:ARG:NH1	2.49	0.45
3:U:508:SER:O	3:U:512:GLU:HG2	2.17	0.45
3:W:320:SER:HB3	3:W:331:VAL:HG21	1.99	0.45
3:X:450:MET:O	3:X:454:TYR:HB2	2.17	0.45
3:Y:301:THR:N	3:Y:480:ALA:O	2.50	0.45
3:c:307:LYS:HG3	3:c:420:ILE:HG13	1.98	0.45
3:c:422:SER:O	3:c:430:ASN:N	2.37	0.45
1:A:123:ARG:NH2	1:D:101:TYR:OH	2.49	0.44
1:B:500:TYR:HE1	1:B:506:GLU:HB2	1.81	0.44
1:C:162:SER:OG	1:C:176:VAL:HB	2.17	0.44
1:D:298:GLY:C	1:D:300:THR:H	2.25	0.44
2:k:142:THR:OG1	2:k:144:ASP:OD1	2.28	0.44
2:M:76:ARG:HD2	2:M:77:GLY:N	2.32	0.44
3:Q:491:PHE:HB2	3:Q:507:GLU:OE2	2.17	0.44
3:c:420:ILE:O	3:c:431:ILE:HD12	2.17	0.44
1:A:165:ARG:HG3	1:A:177:VAL:HG23	1.98	0.44
1:D:104:LEU:HA	1:D:115:VAL:HG22	1.99	0.44
1:D:351:LEU:O	1:D:355:ARG:HG2	2.16	0.44
2:l:59:ARG:NH2	2:l:215:ALA:O	2.50	0.44
2:o:22:LYS:O	2:o:26:ARG:HG2	2.18	0.44
2:K:87:TYR:CE1	3:Y:357:ARG:HG2	2.53	0.44
2:L:43:ALA:O	2:L:209:GLU:N	2.39	0.44
3:P:338:ASP:OD1	3:P:341:THR:HG22	2.17	0.44
3:P:485:ASP:N	3:P:490:ILE:O	2.50	0.44
3:U:351:VAL:HG21	3:U:398:LEU:HD12	1.99	0.44
3:V:414:PRO:HA	3:V:417:ALA:HB2	2.00	0.44
3:Y:388:ARG:HD2	3:Y:427:GLY:HA3	1.97	0.44
3:c:414:PRO:HA	3:c:417:ALA:HB2	1.98	0.44
1:A:349:ILE:HD12	1:A:395:GLN:HE21	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:SER:OG	1:D:123:ARG:HB3	2.18	0.44
1:C:533:SER:O	1:C:537:THR:HG22	2.17	0.44
1:E:531:ILE:HA	1:E:534:VAL:HG12	1.98	0.44
2:H:122:LEU:C	2:H:156:MET:HE1	2.42	0.44
2:I:57:TYR:CG	2:I:58:ASP:N	2.84	0.44
2:K:68:PHE:HA	2:K:71:PHE:CE2	2.53	0.44
2:M:217:ARG:HB2	2:M:221:ALA:HA	1.99	0.44
2:N:28:LYS:HB2	2:N:52:LYS:NZ	2.33	0.44
3:P:355:PHE:CZ	3:P:390:ASN:HB2	2.51	0.44
3:P:408:ASP:N	3:P:417:ALA:O	2.41	0.44
3:P:469:GLU:HG2	3:P:521:ARG:HH21	1.82	0.44
3:R:338:ASP:OD1	3:R:341:THR:OG1	2.29	0.44
3:S:303:ILE:HG22	3:S:403:LEU:HD23	1.99	0.44
3:S:318:ARG:O	3:S:331:VAL:HG22	2.18	0.44
3:Y:484:PRO:HB3	3:Y:491:PHE:CD2	2.52	0.44
3:Z:307:LYS:HE3	3:Z:435:GLY:HA2	1.97	0.44
3:a:469:GLU:OE2	3:a:521:ARG:NE	2.45	0.44
3:b:364:GLU:HG2	3:b:368:LYS:HE2	1.98	0.44
1:B:297:CYS:HB3	1:B:437:ILE:HG22	2.00	0.44
1:B:473:ALA:HA	1:B:476:LYS:HE2	2.00	0.44
1:E:140:THR:O	1:E:153:GLY:N	2.50	0.44
1:F:446:GLN:HG2	1:F:479:ILE:HG22	1.99	0.44
2:k:98:GLN:NE2	3:X:370:GLU:OE1	2.50	0.44
2:l:90:ASP:HB3	2:l:93:ASP:CG	2.42	0.44
2:I:68:PHE:HA	2:I:71:PHE:CZ	2.53	0.44
2:I:182:ARG:HA	2:I:185:VAL:HG12	1.99	0.44
2:M:78:GLY:HA3	2:M:103:TYR:OH	2.17	0.44
2:N:68:PHE:HA	2:N:71:PHE:CE2	2.53	0.44
2:N:110:ILE:O	2:N:114:GLN:HG2	2.17	0.44
3:P:362:GLU:OE2	3:P:382:ARG:NE	2.46	0.44
3:P:388:ARG:HG3	3:P:427:GLY:HA3	1.98	0.44
3:W:318:ARG:HD3	3:W:493:THR:HG23	1.99	0.44
3:a:319:ARG:NH1	3:a:479:SER:O	2.48	0.44
4:j:172:GLN:O	4:j:172:GLN:HG2	2.17	0.44
1:C:416:ASN:HB2	1:C:566:ASN:ND2	2.32	0.44
1:D:291:LEU:HD13	1:D:302:ILE:HB	1.98	0.44
1:F:244:GLU:HG2	1:F:331:ASN:HB2	2.00	0.44
1:F:332:ILE:HD11	1:F:370:PHE:CE2	2.53	0.44
1:F:375:SER:O	1:F:378:ARG:NH1	2.51	0.44
1:F:500:TYR:HB3	1:F:579:GLU:OE1	2.17	0.44
1:F:523:VAL:HG12	1:F:527:LYS:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:33:LEU:HD21	2:l:40:LEU:HD23	2.00	0.44
2:m:41:PHE:HE2	2:m:213:LEU:HG	1.82	0.44
2:n:87:TYR:CE1	3:S:357:ARG:HG2	2.53	0.44
2:o:78:GLY:HA3	2:o:103:TYR:OH	2.17	0.44
2:L:20:ALA:O	2:L:24:ILE:HD12	2.18	0.44
3:Q:423:PHE:HA	3:Q:429:TRP:HA	1.99	0.44
3:S:332:ARG:HA	3:S:332:ARG:HD2	1.68	0.44
3:U:450:MET:HA	3:U:453:LEU:HB2	2.00	0.44
3:X:324:ASN:OD1	3:X:325:MET:N	2.51	0.44
3:X:351:VAL:HG21	3:X:398:LEU:HG	2.00	0.44
3:b:317:ASP:HA	3:b:492:PRO:HB3	2.00	0.44
3:c:420:ILE:HB	3:c:432:GLU:HB2	1.98	0.44
1:B:296:GLY:HA3	1:E:427:ARG:HD2	1.99	0.44
1:D:277:LEU:HA	1:D:280:GLU:HG3	2.00	0.44
1:E:192:LEU:HD22	1:E:214:LEU:HD21	2.00	0.44
1:E:500:TYR:CE2	1:E:577:LYS:HG2	2.52	0.44
1:F:373:MET:HB2	1:F:415:SER:HB2	1.98	0.44
2:k:49:SER:HB3	2:O:97:ARG:HD2	1.99	0.44
2:k:59:ARG:NH2	2:k:215:ALA:O	2.42	0.44
2:l:41:PHE:HB3	2:l:53:ILE:HD13	1.99	0.44
2:o:45:ASN:HB2	2:o:52:LYS:HE3	2.00	0.44
2:H:76:ARG:HD3	2:H:80:GLN:HE22	1.82	0.44
2:J:61:GLY:N	2:J:213:LEU:HD11	2.33	0.44
2:J:161:GLU:HB3	2:J:162:PRO:HD3	2.00	0.44
2:L:140:ARG:NE	2:L:150:GLU:OE2	2.31	0.44
3:Q:321:THR:HG22	3:Q:326:ILE:HA	1.99	0.44
3:T:378:GLY:O	3:T:382:ARG:HG2	2.18	0.44
3:T:422:SER:O	3:T:430:ASN:N	2.50	0.44
3:c:378:GLY:O	3:c:382:ARG:HG2	2.17	0.44
1:C:136:LYS:NZ	1:C:155:PHE:HZ	2.13	0.44
1:C:235:LYS:HG2	1:C:237:GLU:H	1.83	0.44
1:D:275:LYS:NZ	1:D:407:GLU:HB3	2.32	0.44
1:E:496:LEU:HD23	1:E:586:THR:HA	2.00	0.44
1:F:482:VAL:CG2	1:F:551:ILE:HD11	2.48	0.44
2:k:92:ARG:HH21	3:X:377:ALA:H	1.64	0.44
2:n:138:LEU:HD13	2:n:154:VAL:HG23	1.99	0.44
2:H:60:VAL:HA	2:H:125:ALA:O	2.18	0.44
3:R:458:THR:H	3:R:462:SER:HB2	1.82	0.44
3:S:423:PHE:CD2	3:S:429:TRP:HB3	2.53	0.44
3:U:498:ASP:OD1	3:U:498:ASP:N	2.51	0.44
1:A:328:TYR:CD1	1:A:359:LYS:HB3	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:MET:HE1	1:D:124:LEU:HD13	1.99	0.44
2:m:128:ALA:HB2	2:m:134:LYS:HB3	2.00	0.44
2:o:14:ARG:HH22	2:o:21:ARG:NH1	2.15	0.44
2:L:142:THR:OG1	2:L:144:ASP:OD1	2.30	0.44
3:P:378:GLY:O	3:P:382:ARG:HG2	2.18	0.44
3:R:450:MET:HA	3:R:453:LEU:HB2	1.99	0.44
3:T:414:PRO:HA	3:T:417:ALA:HB2	2.00	0.44
3:U:346:ALA:O	3:U:401:LEU:HD23	2.18	0.44
3:V:317:ASP:HA	3:V:492:PRO:HB3	1.99	0.44
3:W:438:ALA:HB3	3:W:447:LYS:HG3	1.99	0.44
3:a:420:ILE:HG21	3:a:437:GLN:HB2	1.98	0.44
3:b:485:ASP:N	3:b:490:ILE:O	2.50	0.44
1:B:105:LEU:HD12	1:B:114:ASP:HB3	2.00	0.44
1:C:292:TYR:HA	1:C:415:SER:O	2.18	0.44
1:E:190:ASP:HA	1:E:193:ILE:HG22	2.00	0.44
1:E:479:ILE:HA	1:E:482:VAL:HG12	2.00	0.44
2:k:55:GLU:HB2	2:k:222:PHE:CD2	2.52	0.44
2:m:89:TYR:O	3:S:378:GLY:HA2	2.18	0.44
2:G:69:ASN:OD1	2:G:70:GLU:N	2.51	0.44
2:K:217:ARG:HH12	2:K:223:ARG:HB2	1.82	0.44
3:P:318:ARG:HA	3:P:331:VAL:O	2.17	0.44
3:P:438:ALA:N	3:P:447:LYS:HD3	2.33	0.44
3:S:420:ILE:O	3:S:432:GLU:N	2.43	0.44
3:V:475:ALA:HA	3:V:481:THR:HB	1.99	0.44
3:W:340:TYR:OH	3:W:499:ALA:O	2.33	0.44
3:b:376:PHE:CE2	3:b:380:ILE:HD11	2.53	0.44
1:B:440:PRO:HD2	1:B:514:ASN:O	2.18	0.43
1:C:479:ILE:HA	1:C:482:VAL:HG12	2.00	0.43
1:E:221:LEU:O	1:E:230:PHE:N	2.45	0.43
1:F:222:VAL:HG23	1:F:228:TYR:C	2.43	0.43
2:k:167:LEU:O	2:k:171:TYR:N	2.51	0.43
2:o:69:ASN:OD1	2:o:70:GLU:HG3	2.18	0.43
2:o:229:ALA:O	2:o:233:LEU:CB	2.66	0.43
2:H:67:LYS:NZ	2:H:69:ASN:HD21	2.15	0.43
2:H:68:PHE:N	4:g:172:GLN:O	2.49	0.43
2:H:89:TYR:CD1	3:P:382:ARG:HD3	2.53	0.43
2:I:69:ASN:OD1	2:I:70:GLU:N	2.51	0.43
2:J:87:TYR:CE1	3:X:357:ARG:HG3	2.52	0.43
3:Q:378:GLY:O	3:Q:382:ARG:HG2	2.18	0.43
3:V:450:MET:HA	3:V:453:LEU:HB2	2.00	0.43
3:b:329:ARG:O	3:b:490:ILE:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:358:LEU:HB2	2:O:87:TYR:OH	2.18	0.43
2:O:55:GLU:HB2	2:O:222:PHE:CG	2.53	0.43
2:O:66:GLY:HA3	2:O:120:VAL:HA	2.00	0.43
1:A:419:ASP:N	1:A:419:ASP:OD1	2.50	0.43
1:B:463:ASP:HB3	1:B:474:CYS:SG	2.58	0.43
1:C:294:PRO:HA	1:C:295:PRO:HD3	1.91	0.43
2:k:16:ARG:NH2	2:k:114:GLN:O	2.51	0.43
2:k:55:GLU:HB2	2:k:222:PHE:CG	2.53	0.43
2:k:107:LEU:HD13	2:k:142:THR:O	2.18	0.43
2:K:105:GLN:NE2	2:L:73:ASN:OD1	2.49	0.43
2:L:31:VAL:HG12	2:L:155:VAL:HG13	2.00	0.43
3:Q:408:ASP:N	3:Q:417:ALA:O	2.48	0.43
3:S:446:ALA:O	3:S:450:MET:HG2	2.18	0.43
3:U:487:VAL:HG13	3:X:522:SER:HA	2.00	0.43
3:W:518:ILE:O	3:W:522:SER:N	2.51	0.43
3:X:329:ARG:O	3:X:490:ILE:HG21	2.17	0.43
3:Y:350:ALA:O	3:Y:353:VAL:N	2.51	0.43
3:Y:421:VAL:HG13	3:Y:431:ILE:HD13	1.99	0.43
3:a:429:TRP:HZ3	3:a:431:ILE:HG13	1.82	0.43
2:O:31:VAL:HG23	2:O:42:VAL:HB	2.00	0.43
2:O:163:ILE:HG12	2:O:188:LEU:HD12	1.99	0.43
1:A:478:MET:HE1	1:A:547:LEU:HD12	1.99	0.43
1:B:161:ILE:HD13	1:B:221:LEU:HA	2.00	0.43
1:B:527:LYS:HD3	1:E:281:TYR:O	2.18	0.43
1:C:157:ALA:HB3	1:D:187:TRP:HZ2	1.82	0.43
1:C:534:VAL:HG21	1:D:281:TYR:CE2	2.53	0.43
1:D:247:PRO:HD3	1:D:329:PHE:HB3	1.99	0.43
1:F:479:ILE:HA	1:F:482:VAL:HG12	2.00	0.43
1:F:583:TYR:CE2	1:F:585:ARG:HB2	2.53	0.43
2:k:140:ARG:NE	2:k:150:GLU:OE2	2.47	0.43
2:l:82:ALA:HB2	2:l:99:LEU:HD21	2.00	0.43
2:m:99:LEU:O	2:m:102:VAL:HG12	2.18	0.43
2:o:28:LYS:NZ	2:o:44:GLU:HG3	2.34	0.43
2:K:79:ILE:HD13	3:Y:368:LYS:HB3	1.99	0.43
2:M:124:VAL:HG23	2:M:141:ILE:HD11	2.00	0.43
3:Q:322:GLN:HG2	3:Q:325:MET:HB2	2.00	0.43
3:R:430:ASN:ND2	3:R:431:ILE:O	2.51	0.43
3:R:469:GLU:HG3	3:R:521:ARG:HH21	1.83	0.43
3:T:438:ALA:HB3	3:T:447:LYS:HG2	2.00	0.43
3:U:444:LEU:HD22	3:Y:445:PHE:CZ	2.53	0.43
3:W:301:THR:O	3:W:441:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:319:ARG:HD3	3:W:482:GLY:HA3	2.00	0.43
3:X:348:THR:HB	3:X:351:VAL:HB	2.00	0.43
3:Y:447:LYS:HE2	3:Y:447:LYS:HA	2.00	0.43
3:Z:305:ALA:O	3:Z:437:GLN:N	2.50	0.43
1:A:503:GLY:H	1:A:579:GLU:CD	2.26	0.43
1:E:243:LEU:HD23	1:E:243:LEU:H	1.83	0.43
1:E:314:MET:HE3	1:E:328:TYR:HD2	1.83	0.43
1:E:457:LEU:HD21	1:E:527:LYS:HE2	2.00	0.43
1:E:507:VAL:HG12	1:E:509:TYR:HE1	1.83	0.43
2:k:58:ASP:HB3	2:k:219:ARG:O	2.17	0.43
2:N:45:ASN:ND2	2:N:51:GLN:HA	2.33	0.43
2:N:89:TYR:O	3:c:378:GLY:HA2	2.18	0.43
3:Q:306:LEU:HA	3:Q:436:TYR:HA	1.99	0.43
3:S:486:LEU:HD22	3:S:515:ARG:NH1	2.33	0.43
3:T:448:SER:OG	3:Z:445:PHE:HD1	2.02	0.43
3:U:340:TYR:HD1	3:U:407:TYR:HB3	1.83	0.43
3:X:312:VAL:HG12	3:X:497:ILE:HB	2.01	0.43
3:Y:380:ILE:HG23	3:Y:423:PHE:HZ	1.83	0.43
3:Z:310:GLY:N	3:Z:415:GLN:OE1	2.51	0.43
3:b:383:LEU:HD22	3:b:423:PHE:CZ	2.53	0.43
3:b:383:LEU:HD22	3:b:423:PHE:CE1	2.54	0.43
1:D:264:ILE:HD13	1:D:435:ILE:CD1	2.49	0.43
1:E:487:TYR:CD2	1:E:511:LYS:HE2	2.53	0.43
2:k:124:VAL:N	2:k:139:TYR:O	2.45	0.43
2:l:160:THR:O	2:l:164:ALA:CB	2.67	0.43
2:H:130:TYR:CG	2:H:218:PRO:HA	2.53	0.43
2:H:217:ARG:HB2	2:H:221:ALA:HA	2.00	0.43
2:J:41:PHE:HB3	2:J:53:ILE:HD13	2.00	0.43
2:N:96:GLY:H	2:N:126:GLU:CD	2.26	0.43
2:N:110:ILE:HD12	2:N:118:TYR:CD2	2.54	0.43
3:U:446:ALA:O	3:U:450:MET:HG2	2.19	0.43
3:W:394:ALA:HB3	3:W:395:MET:HE2	2.00	0.43
3:a:312:VAL:HG12	3:a:497:ILE:HB	2.00	0.43
2:O:155:VAL:HG12	2:O:160:THR:HG22	2.00	0.43
1:A:239:GLU:HB2	1:A:330:LEU:HD21	2.00	0.43
1:D:116:PHE:CE1	1:D:121:LYS:HB2	2.54	0.43
1:D:172:HIS:CE1	1:D:187:TRP:HB3	2.53	0.43
1:D:565:THR:HG22	1:D:566:ASN:N	2.33	0.43
1:E:453:LEU:CD1	1:E:547:LEU:HD21	2.49	0.43
2:k:54:SER:O	2:k:62:PHE:N	2.44	0.43
2:m:45:ASN:ND2	2:m:47:SER:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:114:GLN:HG2	2:n:116:LYS:H	1.82	0.43
2:H:16:ARG:HG3	2:H:117:PRO:HD3	2.00	0.43
2:L:109:THR:O	2:L:112:THR:N	2.52	0.43
2:L:164:ALA:O	2:L:168:LYS:HG2	2.19	0.43
3:P:384:ALA:HB2	3:P:429:TRP:HE3	1.84	0.43
3:U:305:ALA:N	3:U:437:GLN:O	2.43	0.43
3:V:450:MET:O	3:V:454:TYR:HB2	2.19	0.43
3:Y:306:LEU:HD21	3:Y:467:ALA:HB2	2.00	0.43
3:c:384:ALA:O	3:c:388:ARG:HG3	2.18	0.43
1:A:183:GLU:HG2	1:D:179:HIS:NE2	2.33	0.43
1:B:261:ILE:HG13	1:B:262:GLU:N	2.33	0.43
1:C:164:LEU:O	1:C:217:GLY:N	2.39	0.43
1:C:495:PHE:HZ	1:C:561:LEU:HB2	1.82	0.43
1:D:292:TYR:CZ	1:D:436:LYS:HB2	2.53	0.43
1:E:237:GLU:HG3	1:E:355:ARG:HH22	1.82	0.43
2:J:28:LYS:NZ	2:J:44:GLU:HB3	2.33	0.43
2:K:178:THR:O	2:K:182:ARG:HG3	2.19	0.43
3:Q:404:LEU:HD23	3:Q:421:VAL:HB	2.00	0.43
3:S:437:GLN:HE22	3:S:439:VAL:CG1	2.31	0.43
3:T:446:ALA:O	3:T:450:MET:HG3	2.18	0.43
3:W:318:ARG:HB3	3:W:330:ASP:HA	2.01	0.43
3:Z:335:TYR:O	3:Z:343:THR:N	2.32	0.43
2:O:140:ARG:O	2:O:148:ALA:N	2.44	0.43
1:B:168:LEU:HD12	1:B:173:ARG:HB2	2.00	0.43
1:B:500:TYR:OH	1:B:506:GLU:HG3	2.18	0.43
1:E:486:MET:HE2	1:E:487:TYR:CE1	2.54	0.43
1:E:544:ILE:O	1:E:548:LEU:HG	2.18	0.43
2:k:163:ILE:HD12	2:k:188:LEU:HD12	2.00	0.43
2:l:122:LEU:O	2:l:156:MET:HE1	2.18	0.43
2:n:61:GLY:N	2:n:213:LEU:HD11	2.34	0.43
2:H:73:ASN:O	2:H:76:ARG:HG3	2.18	0.43
2:M:155:VAL:HG12	2:M:160:THR:HG22	2.01	0.43
3:S:310:GLY:HA2	3:S:415:GLN:HA	2.00	0.43
3:V:378:GLY:O	3:V:382:ARG:HG2	2.18	0.43
3:V:380:ILE:HG22	3:V:429:TRP:CD2	2.54	0.43
3:W:507:GLU:HA	3:W:510:ILE:HD12	1.99	0.43
3:X:315:ALA:HA	3:X:494:ALA:HA	2.00	0.43
3:Y:355:PHE:HZ	3:Y:390:ASN:ND2	2.17	0.43
3:Y:366:TYR:CE1	3:Y:370:GLU:HG3	2.54	0.43
3:c:366:TYR:CD1	3:c:374:LEU:HG	2.53	0.43
1:A:426:LEU:HD12	1:A:434:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:ASN:OD1	1:B:564:THR:N	2.47	0.43
1:C:275:LYS:HZ2	1:C:285:PRO:HB3	1.82	0.43
1:D:140:THR:O	1:D:153:GLY:N	2.44	0.43
1:D:493:ASN:HB2	1:D:509:TYR:CD2	2.53	0.43
1:D:533:SER:HA	1:D:536:GLU:HG2	2.01	0.43
1:F:377:PHE:HE1	1:F:392:VAL:HB	1.82	0.43
2:m:134:LYS:HE3	2:m:135:ARG:O	2.18	0.43
2:o:210:VAL:HB	2:o:225:ILE:O	2.19	0.43
2:H:44:GLU:HA	2:H:208:LEU:HD23	2.01	0.43
2:N:58:ASP:HB3	2:N:219:ARG:O	2.19	0.43
2:N:118:TYR:HB3	2:N:120:VAL:HG22	2.01	0.43
2:N:176:SER:HB3	2:N:179:ASP:OD2	2.19	0.43
3:W:393:ALA:O	3:W:398:LEU:HB2	2.19	0.43
3:Y:332:ARG:HD3	3:Y:493:THR:HG21	2.00	0.43
3:a:307:LYS:HE3	3:a:435:GLY:HA2	2.01	0.43
3:b:318:ARG:HB3	3:b:330:ASP:HA	1.99	0.43
2:O:48:ARG:HH22	2:O:207:SER:N	2.17	0.43
1:A:513:PHE:CE1	1:A:565:THR:HA	2.54	0.43
1:B:495:PHE:CD2	1:B:508:MET:HE1	2.54	0.43
1:F:269:GLU:HG2	1:F:273:LEU:HG	2.01	0.43
1:F:310:LEU:HD22	1:F:367:ILE:HD13	2.01	0.43
2:m:67:LYS:HZ2	2:m:69:ASN:ND2	2.14	0.43
2:H:59:ARG:HD3	2:H:219:ARG:O	2.18	0.43
2:I:76:ARG:O	2:I:80:GLN:OE1	2.37	0.43
2:J:167:LEU:O	2:J:171:TYR:N	2.52	0.43
2:M:88:ALA:O	3:b:381:ASN:ND2	2.52	0.43
3:V:307:LYS:HG3	3:V:420:ILE:HG13	2.01	0.43
3:Y:312:VAL:HG12	3:Y:497:ILE:HB	2.01	0.43
3:a:366:TYR:CE2	3:a:370:GLU:HG3	2.53	0.43
3:b:307:LYS:HG3	3:b:420:ILE:HG13	2.01	0.43
3:b:394:ALA:HB3	3:b:395:MET:HE2	2.01	0.43
1:A:566:ASN:OD1	1:A:567:PRO:HD2	2.19	0.42
1:B:453:LEU:HD11	1:B:547:LEU:HD11	2.00	0.42
1:D:288:GLY:HA3	1:D:431:LEU:HA	2.00	0.42
1:D:457:LEU:O	1:D:471:ARG:NH2	2.52	0.42
2:m:29:SER:O	2:m:44:GLU:HG2	2.19	0.42
2:m:78:GLY:HA3	2:m:103:TYR:OH	2.18	0.42
2:H:21:ARG:CZ	2:H:21:ARG:HB3	2.49	0.42
2:H:53:ILE:HG21	2:H:211:ALA:HB3	2.00	0.42
2:K:110:ILE:HG21	2:K:118:TYR:CD2	2.54	0.42
2:L:41:PHE:HE2	2:L:213:LEU:HG	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:66:GLY:HA3	2:N:120:VAL:HG12	2.00	0.42
3:R:408:ASP:HB3	3:R:411:ALA:HB2	2.00	0.42
3:U:325:MET:HE1	3:X:477:ASP:HB3	2.00	0.42
3:U:473:ASP:OD1	3:U:521:ARG:NH2	2.43	0.42
3:Y:383:LEU:O	3:Y:387:VAL:HG23	2.19	0.42
3:Z:318:ARG:HA	3:Z:331:VAL:O	2.18	0.42
3:a:423:PHE:HA	3:a:429:TRP:HA	2.01	0.42
1:D:449:TYR:CE2	1:D:482:VAL:HG11	2.54	0.42
1:F:294:PRO:O	1:F:299:LYS:NZ	2.46	0.42
2:k:90:ASP:OD2	2:k:92:ARG:HG2	2.19	0.42
2:l:217:ARG:HD3	2:l:223:ARG:NH1	2.34	0.42
2:n:35:TYR:HB2	2:n:175:ALA:O	2.18	0.42
2:o:107:LEU:HD23	2:o:107:LEU:HA	1.92	0.42
2:o:161:GLU:HB2	2:o:162:PRO:HD3	2.01	0.42
2:K:140:ARG:O	2:K:148:ALA:N	2.38	0.42
3:P:346:ALA:O	3:P:401:LEU:HD23	2.19	0.42
3:Q:320:SER:HB3	3:Q:331:VAL:HG21	2.01	0.42
3:R:438:ALA:O	3:R:443:SER:HB2	2.19	0.42
3:S:401:LEU:HD12	3:S:402:PRO:HD2	2.01	0.42
3:V:515:ARG:O	3:V:518:ILE:N	2.52	0.42
3:W:346:ALA:O	3:W:401:LEU:N	2.51	0.42
3:W:380:ILE:HG22	3:W:429:TRP:CD2	2.54	0.42
3:a:406:GLY:O	3:a:419:ARG:N	2.48	0.42
3:a:414:PRO:HA	3:a:417:ALA:HB2	2.00	0.42
2:O:73:ASN:O	2:O:76:ARG:HG2	2.19	0.42
1:B:117:THR:HG21	1:B:143:LEU:HD22	2.01	0.42
1:C:289:VAL:HG22	1:C:433:VAL:HB	2.00	0.42
1:D:245:GLU:HB2	1:D:329:PHE:O	2.19	0.42
1:D:303:ALA:HA	1:D:306:VAL:HG22	2.02	0.42
1:D:460:HIS:CG	1:D:543:ARG:HE	2.36	0.42
1:F:391:THR:C	1:F:394:PRO:HD2	2.44	0.42
1:F:397:LEU:HD22	1:F:430:ARG:NH1	2.33	0.42
1:F:475:ILE:HA	1:F:478:MET:CG	2.49	0.42
2:m:18:GLU:HG3	2:m:22:LYS:NZ	2.35	0.42
2:o:167:LEU:HD23	2:o:167:LEU:HA	1.86	0.42
2:G:35:TYR:HB2	2:G:175:ALA:O	2.19	0.42
2:H:211:ALA:HA	2:H:224:ARG:HA	2.02	0.42
2:I:82:ALA:HB2	2:I:99:LEU:HD21	2.01	0.42
2:I:150:GLU:HB2	2:I:154:VAL:HG22	2.01	0.42
2:J:110:ILE:HD12	2:J:114:GLN:CD	2.44	0.42
2:M:25:ALA:O	2:M:158:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:507:GLU:HA	3:P:510:ILE:HD12	2.01	0.42
3:Q:453:LEU:O	3:Q:456:GLN:HG2	2.20	0.42
3:U:423:PHE:CD2	3:U:429:TRP:HB3	2.53	0.42
3:U:437:GLN:C	3:U:450:MET:HE1	2.44	0.42
3:W:515:ARG:O	3:W:519:GLU:HG2	2.18	0.42
3:Y:484:PRO:HB3	3:Y:491:PHE:HD2	1.85	0.42
3:c:498:ASP:N	3:c:498:ASP:OD1	2.52	0.42
3:c:509:ARG:NE	3:c:513:LEU:HG	2.32	0.42
4:i:172:GLN:N	4:i:172:GLN:OE1	2.52	0.42
1:A:177:VAL:HG13	1:A:181:ASP:HA	2.02	0.42
1:A:244:GLU:HB2	1:A:331:ASN:HB3	2.01	0.42
1:A:531:ILE:HG23	1:B:277:LEU:HD23	2.01	0.42
1:C:294:PRO:HD2	1:C:438:GLU:HA	2.01	0.42
1:F:187:TRP:HB2	1:F:228:TYR:CE1	2.54	0.42
1:F:312:LYS:O	1:F:316:GLU:HG3	2.20	0.42
1:F:328:TYR:HD1	1:F:366:VAL:HG22	1.83	0.42
2:m:54:SER:OG	2:m:75:ARG:HD2	2.19	0.42
2:G:89:TYR:O	3:V:378:GLY:HA2	2.18	0.42
2:I:68:PHE:HA	2:I:71:PHE:CE2	2.53	0.42
2:I:142:THR:HG22	2:I:146:SER:HB3	2.01	0.42
2:K:167:LEU:HD23	2:K:167:LEU:HA	1.92	0.42
2:N:156:MET:SD	2:N:156:MET:N	2.92	0.42
3:Q:486:LEU:HD11	3:Q:518:ILE:HD13	2.01	0.42
3:Q:509:ARG:HA	3:Q:512:GLU:HG2	2.02	0.42
3:S:314:MET:SD	3:S:495:VAL:HB	2.59	0.42
3:X:338:ASP:OD1	3:X:341:THR:OG1	2.25	0.42
3:c:316:GLY:N	3:c:493:THR:O	2.42	0.42
3:c:354:GLU:HA	3:c:357:ARG:HE	1.84	0.42
1:A:249:VAL:O	1:A:308:ASN:ND2	2.32	0.42
1:A:498:VAL:HB	1:A:506:GLU:HB3	2.01	0.42
1:C:525:ARG:NH2	1:C:557:GLU:HB3	2.34	0.42
1:E:337:LEU:HD11	1:E:370:PHE:HE2	1.85	0.42
1:F:530:ALA:HA	1:F:546:HIS:CE1	2.54	0.42
2:k:85:ARG:HG3	2:k:94:VAL:HG22	2.02	0.42
2:k:96:GLY:H	2:k:126:GLU:CD	2.27	0.42
2:m:96:GLY:H	2:m:126:GLU:CD	2.28	0.42
2:o:67:LYS:HA	4:e:172:GLN:O	2.18	0.42
2:o:211:ALA:HB2	2:o:224:ARG:HG2	2.02	0.42
2:H:55:GLU:HB2	2:H:222:PHE:CG	2.54	0.42
2:K:124:VAL:N	2:K:139:TYR:O	2.40	0.42
2:L:96:GLY:H	2:L:126:GLU:CD	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:105:GLN:OE1	2:M:69:ASN:HB2	2.19	0.42
2:M:58:ASP:HB2	2:M:91:ARG:NH2	2.34	0.42
3:T:304:VAL:HA	3:T:438:ALA:HA	2.02	0.42
3:X:332:ARG:NE	3:X:334:VAL:O	2.51	0.42
3:X:406:GLY:O	3:X:419:ARG:N	2.47	0.42
3:Z:345:ILE:HA	3:Z:402:PRO:HA	2.00	0.42
3:a:464:LEU:O	3:a:468:VAL:HG23	2.20	0.42
2:O:141:ILE:HG13	2:O:147:ILE:HG13	2.01	0.42
1:A:337:LEU:HG	1:A:348:HIS:ND1	2.35	0.42
1:B:187:TRP:HB2	1:B:228:TYR:CD1	2.55	0.42
1:B:240:ASP:OD1	1:B:241:LEU:N	2.53	0.42
1:D:247:PRO:HG3	1:D:307:ALA:HB3	2.02	0.42
1:F:569:ASP:OD1	1:F:570:TRP:N	2.52	0.42
2:G:79:ILE:HG22	3:U:365:HIS:CE1	2.55	0.42
2:I:14:ARG:CZ	2:I:14:ARG:HA	2.50	0.42
2:I:55:GLU:HB2	2:I:222:PHE:CG	2.54	0.42
2:K:57:TYR:HB3	2:K:60:VAL:HB	2.02	0.42
2:M:91:ARG:NH1	2:M:92:ARG:HA	2.35	0.42
3:P:433:GLU:OE1	3:P:433:GLU:N	2.49	0.42
3:W:375:THR:OG1	2:O:93:ASP:OD1	2.31	0.42
3:c:316:GLY:O	3:c:493:THR:N	2.52	0.42
1:A:299:LYS:HE2	1:A:299:LYS:HB2	1.92	0.42
1:A:455:GLU:CD	1:A:475:ILE:HD12	2.45	0.42
1:B:545:GLN:NE2	1:B:549:ASP:OD1	2.52	0.42
1:C:337:LEU:HD22	1:C:348:HIS:HB3	2.01	0.42
1:C:495:PHE:CZ	1:C:561:LEU:HB2	2.54	0.42
2:k:68:PHE:HA	2:k:71:PHE:CE2	2.54	0.42
2:l:28:LYS:HB2	2:l:52:LYS:NZ	2.34	0.42
2:l:88:ALA:O	3:R:381:ASN:ND2	2.53	0.42
2:L:138:LEU:HB2	2:L:150:GLU:HB2	2.00	0.42
3:Q:304:VAL:HA	3:Q:438:ALA:HA	2.01	0.42
3:U:376:PHE:O	3:U:379:LYS:HG2	2.20	0.42
3:W:304:VAL:HA	3:W:438:ALA:HA	2.01	0.42
3:Z:303:ILE:HG22	3:Z:403:LEU:HD23	2.00	0.42
3:c:354:GLU:O	3:c:357:ARG:HG2	2.20	0.42
1:D:242:VAL:HG13	1:D:243:LEU:N	2.33	0.42
2:k:48:ARG:NH2	2:k:208:LEU:O	2.53	0.42
2:m:29:SER:N	2:m:44:GLU:OE2	2.41	0.42
2:n:58:ASP:HB3	2:n:220:ARG:HA	2.01	0.42
2:J:85:ARG:NH2	2:J:94:VAL:HG13	2.34	0.42
2:K:112:THR:HG23	2:L:116:LYS:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:20:ALA:O	2:M:24:ILE:HG12	2.19	0.42
3:P:315:ALA:HA	3:P:494:ALA:HA	2.02	0.42
3:W:485:ASP:N	3:W:490:ILE:O	2.52	0.42
3:b:332:ARG:NH1	3:b:493:THR:HB	2.33	0.42
3:c:401:LEU:HD11	3:c:423:PHE:O	2.20	0.42
1:B:174:ALA:HB2	1:B:188:LEU:HD21	2.01	0.42
1:B:269:GLU:HB3	1:B:273:LEU:HG	2.02	0.42
1:C:379:THR:HG23	1:C:423:PRO:HD2	2.01	0.42
1:C:478:MET:SD	1:C:547:LEU:HG	2.60	0.42
1:D:289:VAL:HB	1:D:412:ILE:HG12	2.02	0.42
1:D:373:MET:HE1	1:D:413:GLY:HA3	2.02	0.42
1:D:460:HIS:CE1	1:D:539:GLN:HB2	2.55	0.42
1:D:532:LYS:O	1:D:536:GLU:HG2	2.19	0.42
1:E:101:TYR:HE2	1:F:123:ARG:HB2	1.84	0.42
1:E:265:ARG:NH1	1:E:269:GLU:HB2	2.35	0.42
1:E:334:GLY:HA3	1:E:335:PRO:HD3	1.81	0.42
2:k:61:GLY:N	2:k:213:LEU:HD11	2.34	0.42
2:k:140:ARG:CZ	2:k:154:VAL:HG13	2.50	0.42
2:G:214:ASP:HB3	2:G:217:ARG:HG2	2.02	0.42
2:J:55:GLU:HB2	2:J:222:PHE:CG	2.55	0.42
2:L:48:ARG:NH2	2:L:208:LEU:O	2.53	0.42
3:Q:505:VAL:HB	3:Q:510:ILE:HD11	2.01	0.42
3:T:383:LEU:O	3:T:387:VAL:HG23	2.20	0.42
3:U:485:ASP:N	3:U:490:ILE:O	2.52	0.42
3:X:378:GLY:O	3:X:382:ARG:HG2	2.19	0.42
3:X:408:ASP:N	3:X:417:ALA:O	2.46	0.42
3:a:305:ALA:HB2	3:a:403:LEU:HD21	2.02	0.42
3:a:351:VAL:O	3:a:354:GLU:HG2	2.20	0.42
3:a:475:ALA:HA	3:a:481:THR:HB	2.01	0.42
3:b:511:ALA:HB1	3:b:515:ARG:HH21	1.85	0.42
2:O:59:ARG:HA	2:O:221:ALA:HB3	2.02	0.42
1:B:184:ARG:NH2	1:B:224:THR:O	2.53	0.42
1:C:432:ASP:OD1	1:C:432:ASP:N	2.51	0.42
1:D:245:GLU:O	1:D:329:PHE:HB3	2.20	0.42
1:D:311:ALA:HB2	1:D:327:SER:HB2	2.00	0.42
1:E:448:ILE:HD13	1:E:516:GLY:HA2	2.01	0.42
1:F:188:LEU:HD12	1:F:192:LEU:HB3	2.02	0.42
2:l:11:GLN:HA	2:l:14:ARG:NH1	2.33	0.42
2:l:18:GLU:O	2:l:22:LYS:HG2	2.19	0.42
2:m:71:PHE:HA	2:m:74:LEU:HD12	2.02	0.42
2:n:68:PHE:HA	2:n:71:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:56:LEU:HB2	2:G:60:VAL:HG12	2.01	0.42
2:M:31:VAL:HG12	2:M:155:VAL:HG13	2.02	0.42
2:N:107:LEU:HA	2:N:110:ILE:HG12	2.02	0.42
3:Q:337:THR:OG1	3:Q:341:THR:OG1	2.37	0.42
3:S:458:THR:H	3:S:462:SER:HG	1.60	0.42
3:Z:319:ARG:CD	3:Z:482:GLY:HA3	2.50	0.42
1:A:493:ASN:HA	1:A:510:PHE:CD2	2.55	0.41
1:C:259:ARG:HA	1:C:262:GLU:HG2	2.02	0.41
1:D:166:GLU:HG2	1:D:175:LEU:HB3	2.02	0.41
1:D:566:ASN:N	1:D:567:PRO:HD2	2.35	0.41
1:E:472:SER:O	1:E:476:LYS:HG2	2.20	0.41
1:F:419:ASP:N	1:F:419:ASP:OD1	2.53	0.41
2:l:10:GLU:HG3	2:m:19:LEU:HD12	2.02	0.41
2:l:129:HIS:HB2	2:l:132:GLU:OE1	2.20	0.41
2:n:61:GLY:H	2:n:213:LEU:HD11	1.85	0.41
2:o:159:THR:O	2:o:162:PRO:HD2	2.20	0.41
2:K:68:PHE:HA	2:K:71:PHE:CZ	2.55	0.41
2:L:217:ARG:NH1	2:L:223:ARG:HB2	2.35	0.41
3:P:480:ALA:HB2	3:c:324:ASN:ND2	2.35	0.41
3:Q:484:PRO:HB3	3:Q:491:PHE:HD2	1.84	0.41
3:S:315:ALA:HA	3:S:494:ALA:HA	2.02	0.41
3:T:459:ASP:OD1	3:T:459:ASP:N	2.51	0.41
3:U:449:SER:O	3:U:453:LEU:HG	2.19	0.41
3:Y:381:ASN:HA	3:Y:429:TRP:CZ3	2.55	0.41
3:a:423:PHE:CD2	3:a:429:TRP:HB3	2.55	0.41
2:O:129:HIS:HB2	2:O:132:GLU:OE1	2.20	0.41
1:A:164:LEU:HA	1:A:176:VAL:HG12	2.00	0.41
1:E:479:ILE:O	1:E:482:VAL:HG12	2.20	0.41
1:F:418:GLU:H	1:F:418:GLU:CD	2.28	0.41
1:F:544:ILE:O	1:F:548:LEU:HG	2.20	0.41
2:m:129:HIS:HB2	2:m:132:GLU:OE1	2.20	0.41
2:n:161:GLU:HB2	2:n:162:PRO:HD3	2.03	0.41
2:G:44:GLU:HA	2:G:208:LEU:HD23	2.02	0.41
2:G:211:ALA:HA	2:G:224:ARG:HA	2.02	0.41
2:H:54:SER:HB3	2:H:75:ARG:HD2	2.02	0.41
2:H:110:ILE:HD13	2:H:118:TYR:CE2	2.55	0.41
2:I:110:ILE:HD13	2:I:110:ILE:HA	1.91	0.41
2:I:110:ILE:O	2:I:114:GLN:HB3	2.20	0.41
2:J:40:LEU:HA	2:J:212:VAL:HG12	2.02	0.41
2:N:106:THR:O	2:N:110:ILE:HG12	2.20	0.41
3:R:319:ARG:NH1	3:R:329:ARG:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:469:GLU:HB2	3:R:517:ILE:HD13	2.02	0.41
3:U:351:VAL:CG2	3:U:398:LEU:HD12	2.50	0.41
3:W:378:GLY:HA2	2:O:89:TYR:O	2.19	0.41
3:Z:351:VAL:HA	3:Z:354:GLU:OE1	2.20	0.41
3:b:311:GLY:HA2	3:b:407:TYR:CE1	2.55	0.41
3:b:350:ALA:HB1	3:c:388:ARG:CZ	2.50	0.41
1:A:353:PHE:HB3	1:A:357:ARG:HH12	1.84	0.41
1:C:192:LEU:HD23	1:C:214:LEU:HD11	2.01	0.41
1:C:487:TYR:HA	1:C:511:LYS:HB3	2.02	0.41
1:C:534:VAL:HG21	1:D:281:TYR:HE2	1.86	0.41
1:C:543:ARG:HD2	1:C:546:HIS:NE2	2.36	0.41
1:D:508:MET:SD	1:D:512:ASP:HB2	2.60	0.41
1:D:539:GLN:HG3	1:D:543:ARG:NH2	2.35	0.41
1:E:238:VAL:O	1:E:242:VAL:HG23	2.20	0.41
1:E:561:LEU:N	1:E:562:PRO:HD2	2.35	0.41
1:F:449:TYR:O	1:F:453:LEU:N	2.34	0.41
2:n:19:LEU:HD22	2:n:117:PRO:HG2	2.02	0.41
2:o:43:ALA:HB1	2:o:52:LYS:HD2	2.02	0.41
2:o:87:TYR:CD1	3:T:361:VAL:HG21	2.55	0.41
2:G:130:TYR:HB2	2:G:217:ARG:O	2.20	0.41
2:H:28:LYS:HB2	2:H:52:LYS:NZ	2.35	0.41
2:K:123:CYS:HB2	2:K:156:MET:HE1	2.02	0.41
2:N:91:ARG:HB3	2:N:92:ARG:HH21	1.85	0.41
3:T:509:ARG:HA	3:T:512:GLU:HG2	2.02	0.41
3:V:472:TYR:CE2	3:V:521:ARG:HG3	2.55	0.41
3:b:484:PRO:HB3	3:b:491:PHE:CD2	2.55	0.41
1:A:251:TYR:CD1	1:A:261:ILE:HD12	2.56	0.41
1:C:419:ASP:OD1	1:C:419:ASP:N	2.53	0.41
1:C:482:VAL:HA	1:C:551:ILE:HD11	2.02	0.41
1:E:464:LEU:O	1:E:469:GLY:N	2.50	0.41
2:l:28:LYS:HB2	2:l:52:LYS:HZ3	1.84	0.41
2:m:97:ARG:NH2	2:m:98:GLN:HG2	2.35	0.41
2:m:231:GLN:NE2	2:m:231:GLN:O	2.54	0.41
2:n:69:ASN:OD1	2:n:70:GLU:N	2.54	0.41
2:o:217:ARG:NH1	2:o:223:ARG:HD3	2.36	0.41
2:G:87:TYR:CE1	3:U:357:ARG:HG2	2.55	0.41
2:G:176:SER:HB3	2:G:179:ASP:OD2	2.20	0.41
2:I:41:PHE:HE2	2:I:213:LEU:HG	1.84	0.41
2:J:159:THR:HG23	2:J:159:THR:O	2.21	0.41
2:L:87:TYR:HD1	3:Z:361:VAL:HG21	1.86	0.41
2:M:161:GLU:HB3	2:M:162:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:408:ASP:HB3	3:P:411:ALA:HB2	2.03	0.41
3:P:414:PRO:HA	3:P:417:ALA:HB2	2.01	0.41
3:V:336:ILE:HG12	3:V:495:VAL:HG11	2.02	0.41
3:X:366:TYR:CE1	3:X:370:GLU:HG3	2.56	0.41
3:X:511:ALA:HB1	3:X:515:ARG:HH21	1.86	0.41
3:a:422:SER:OG	3:a:432:GLU:OE2	2.28	0.41
1:A:292:TYR:CZ	1:A:436:LYS:HB2	2.55	0.41
1:C:179:HIS:CG	1:D:182:GLU:HB3	2.56	0.41
1:D:251:TYR:CE1	1:D:261:ILE:HD12	2.56	0.41
1:D:272:PHE:CD2	1:D:314:MET:HE1	2.55	0.41
1:F:340:LYS:HE2	1:F:340:LYS:HB3	1.79	0.41
2:k:63:ALA:HB3	2:k:123:CYS:HB3	2.03	0.41
2:m:67:LYS:HG3	4:j:173:TYR:CD1	2.55	0.41
2:m:111:PHE:CD1	2:m:117:PRO:HB3	2.55	0.41
2:H:33:LEU:HD21	2:H:40:LEU:HD23	2.01	0.41
2:J:54:SER:O	2:J:62:PHE:N	2.49	0.41
2:N:53:ILE:HG21	2:N:211:ALA:HB3	2.02	0.41
3:Q:311:GLY:HA2	3:Q:407:TYR:CE1	2.56	0.41
3:T:345:ILE:HB	3:T:352:ALA:HB1	2.01	0.41
3:X:318:ARG:HA	3:X:331:VAL:O	2.21	0.41
3:Z:445:PHE:HE2	3:Z:473:ASP:HB3	1.85	0.41
3:a:315:ALA:HA	3:a:494:ALA:HA	2.02	0.41
3:c:432:GLU:HG3	3:c:437:GLN:HB2	2.02	0.41
1:B:510:PHE:O	1:B:514:ASN:N	2.54	0.41
1:B:574:SER:O	1:B:578:GLY:N	2.52	0.41
1:F:168:LEU:HD12	1:F:173:ARG:HB2	2.02	0.41
1:F:486:MET:HG2	1:F:555:PHE:HZ	1.86	0.41
2:o:41:PHE:HE2	2:o:213:LEU:HG	1.84	0.41
2:G:16:ARG:HB3	2:G:111:PHE:HE1	1.85	0.41
2:G:55:GLU:HB2	2:G:222:PHE:CG	2.56	0.41
2:G:59:ARG:HA	2:G:221:ALA:HB3	2.03	0.41
2:H:87:TYR:CE1	3:V:357:ARG:HG2	2.55	0.41
2:H:110:ILE:HG21	2:H:118:TYR:CE2	2.56	0.41
2:I:116:LYS:HD2	2:I:117:PRO:HD2	2.02	0.41
3:T:347:GLY:HA3	3:T:400:ALA:HA	2.01	0.41
3:T:383:LEU:HA	3:T:386:MET:HE3	2.03	0.41
3:V:485:ASP:O	3:V:490:ILE:N	2.51	0.41
3:Y:341:THR:HG22	3:Y:376:PHE:HE1	1.85	0.41
3:Z:318:ARG:HB3	3:Z:330:ASP:HA	2.02	0.41
3:Z:380:ILE:HG22	3:Z:429:TRP:CD2	2.55	0.41
3:b:511:ALA:HB1	3:b:515:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:443:SER:O	3:c:447:LYS:HG3	2.20	0.41
2:O:223:ARG:HH12	2:O:225:ILE:HD11	1.85	0.41
1:E:237:GLU:O	1:E:241:LEU:HG	2.21	0.41
1:E:487:TYR:OH	1:E:514:ASN:ND2	2.39	0.41
1:E:514:ASN:OD1	1:E:518:MET:HE3	2.20	0.41
1:F:493:ASN:HA	1:F:510:PHE:HD2	1.86	0.41
2:n:128:ALA:HB2	2:n:134:LYS:HB3	2.01	0.41
2:I:44:GLU:HA	2:I:208:LEU:HD23	2.02	0.41
2:I:62:PHE:CD2	2:I:75:ARG:HD3	2.55	0.41
2:I:161:GLU:HB2	2:I:162:PRO:HD3	2.02	0.41
2:M:45:ASN:ND2	2:M:47:SER:O	2.53	0.41
2:M:130:TYR:CG	2:M:218:PRO:HA	2.55	0.41
3:Q:329:ARG:O	3:Q:490:ILE:HG21	2.20	0.41
3:Q:335:TYR:OH	3:Q:353:VAL:HG22	2.19	0.41
3:Q:385:ILE:O	3:Q:388:ARG:HG2	2.20	0.41
3:S:303:ILE:HB	3:S:439:VAL:HG23	2.02	0.41
3:V:304:VAL:O	3:V:314:MET:HG2	2.21	0.41
3:V:395:MET:SD	3:V:396:GLN:N	2.94	0.41
3:X:363:LEU:O	3:X:367:GLU:OE1	2.38	0.41
3:Z:318:ARG:HB2	3:Z:319:ARG:HH11	1.85	0.41
3:Z:337:THR:HG21	3:Z:359:TYR:CD2	2.55	0.41
3:c:508:SER:O	3:c:512:GLU:HG3	2.20	0.41
1:A:126:CYS:HA	1:A:149:VAL:HB	2.02	0.41
1:A:219:SER:HB2	1:A:233:ILE:O	2.20	0.41
1:A:301:LEU:HD12	1:A:304:LYS:HD2	2.02	0.41
1:B:101:TYR:HE2	1:E:121:LYS:HE2	1.85	0.41
1:B:295:PRO:HG3	1:B:416:ASN:HD22	1.84	0.41
1:B:385:SER:HB2	1:E:387:ASP:H	1.86	0.41
2:l:71:PHE:HA	2:l:74:LEU:HD12	2.02	0.41
2:n:10:GLU:HB3	2:n:14:ARG:NH1	2.35	0.41
2:n:11:GLN:OE1	2:n:14:ARG:NH2	2.53	0.41
2:n:101:ASN:O	2:n:105:GLN:HG2	2.20	0.41
2:o:59:ARG:HG2	2:o:91:ARG:HH21	1.85	0.41
2:H:68:PHE:HB2	4:g:172:GLN:HG2	2.03	0.41
2:J:163:ILE:HD13	2:J:188:LEU:HD12	2.00	0.41
2:L:43:ALA:HB3	2:L:209:GLU:HB3	2.02	0.41
2:M:59:ARG:HG2	2:M:91:ARG:NH2	2.35	0.41
2:N:103:TYR:HA	2:N:106:THR:HG22	2.02	0.41
3:S:517:ILE:O	3:S:521:ARG:HG2	2.21	0.41
3:Y:314:MET:HE1	3:Y:334:VAL:HG13	2.02	0.41
3:Y:518:ILE:O	3:Y:522:SER:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:359:TYR:OH	3:b:379:LYS:O	2.33	0.41
1:A:286:PRO:HB3	1:A:433:VAL:HG21	2.02	0.41
1:B:349:ILE:HD12	1:B:396:LEU:HD21	2.03	0.41
1:B:565:THR:HG23	1:B:567:PRO:HD3	2.02	0.41
1:C:190:ASP:N	1:C:191:PRO:HD2	2.35	0.41
1:C:219:SER:H	1:C:232:ARG:NH1	2.19	0.41
1:C:329:PHE:CE2	1:C:331:ASN:HB2	2.56	0.41
1:C:495:PHE:CZ	1:C:562:PRO:HD3	2.56	0.41
1:D:166:GLU:HG2	1:D:175:LEU:HD23	2.02	0.41
1:F:496:LEU:HB2	1:F:508:MET:HB3	2.03	0.41
2:k:20:ALA:O	2:k:24:ILE:HG12	2.20	0.41
2:m:57:TYR:HE2	2:m:91:ARG:HG2	1.86	0.41
2:m:87:TYR:CE1	3:R:357:ARG:HG2	2.55	0.41
2:m:130:TYR:CG	2:m:218:PRO:HA	2.56	0.41
2:m:214:ASP:HB3	2:m:217:ARG:HG2	2.03	0.41
2:n:160:THR:O	2:n:164:ALA:CB	2.69	0.41
2:G:214:ASP:N	2:G:221:ALA:O	2.34	0.41
2:H:64:ALA:HA	2:H:121:GLU:O	2.21	0.41
2:I:81:PHE:O	2:I:85:ARG:HG2	2.21	0.41
2:N:23:GLY:HA3	2:N:119:GLU:HB2	2.02	0.41
3:P:332:ARG:NE	3:P:334:VAL:O	2.54	0.41
3:P:366:TYR:CE1	3:P:370:GLU:HG3	2.56	0.41
3:P:479:SER:OG	3:c:324:ASN:O	2.37	0.41
3:Q:366:TYR:CD2	3:Q:374:LEU:HG	2.56	0.41
3:S:351:VAL:HG12	3:S:355:PHE:CE2	2.56	0.41
3:U:329:ARG:NH2	3:X:476:ASP:O	2.50	0.41
3:U:344:GLY:O	3:U:403:LEU:N	2.49	0.41
3:c:437:GLN:C	3:c:450:MET:HE1	2.46	0.41
1:A:563:ASN:O	1:B:423:PRO:HB3	2.20	0.41
1:B:374:ASP:OD1	1:B:415:SER:HB2	2.21	0.41
1:C:167:ILE:HA	1:C:174:ALA:HA	2.03	0.41
1:C:187:TRP:HB2	1:C:228:TYR:CD1	2.56	0.41
1:C:447:ASP:O	1:C:451:LYS:HG2	2.20	0.41
1:E:239:GLU:HG2	1:E:332:ILE:HD13	2.03	0.41
2:k:79:ILE:HD13	3:W:368:LYS:HB3	2.03	0.41
2:n:33:LEU:HD21	2:n:40:LEU:HD23	2.03	0.41
2:n:119:GLU:HG3	4:d:173:TYR:OH	2.21	0.41
2:G:12:ALA:O	2:G:15:GLU:HG3	2.21	0.41
2:H:127:VAL:HG12	2:H:136:PRO:HB3	2.02	0.41
2:K:96:GLY:H	2:K:126:GLU:CD	2.29	0.41
2:K:130:TYR:CG	2:K:218:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:217:ARG:HB2	2:K:221:ALA:HA	2.03	0.41
2:N:140:ARG:NH2	2:N:154:VAL:HA	2.36	0.41
3:P:361:VAL:HA	3:P:364:GLU:HG2	2.03	0.41
3:R:452:LYS:HE2	3:b:449:SER:HA	2.02	0.41
3:V:347:GLY:HA3	3:V:400:ALA:HA	2.03	0.41
3:V:380:ILE:HG22	3:V:429:TRP:CE3	2.56	0.41
3:Y:380:ILE:HG22	3:Y:429:TRP:CE3	2.56	0.41
3:c:332:ARG:HH11	3:c:493:THR:HB	1.86	0.41
1:A:168:LEU:HD23	1:A:173:ARG:HD2	2.03	0.40
1:A:253:ASP:O	1:A:451:LYS:HD2	2.21	0.40
1:A:255:GLY:HA3	1:A:451:LYS:HD3	2.02	0.40
1:C:393:VAL:O	1:C:397:LEU:HG	2.21	0.40
1:D:339:ASN:HB2	1:D:345:THR:N	2.35	0.40
2:k:223:ARG:HH12	2:k:225:ILE:HG12	1.85	0.40
2:L:141:ILE:HA	2:L:146:SER:O	2.20	0.40
2:N:211:ALA:HB2	2:N:224:ARG:HG2	2.03	0.40
3:R:304:VAL:HA	3:R:438:ALA:HA	2.01	0.40
3:R:497:ILE:HA	3:R:502:ALA:HA	2.04	0.40
3:T:315:ALA:HA	3:T:494:ALA:HA	2.03	0.40
3:Y:355:PHE:HZ	3:Y:390:ASN:CG	2.29	0.40
3:Y:393:ALA:HA	3:Y:396:GLN:CD	2.46	0.40
3:c:302:THR:HA	3:c:440:GLY:HA3	2.02	0.40
3:c:422:SER:HB3	3:c:437:GLN:HG3	2.03	0.40
1:B:427:ARG:HG2	1:B:428:PRO:HD2	2.03	0.40
1:B:448:ILE:HD13	1:B:516:GLY:HA2	2.02	0.40
1:C:299:LYS:HG2	1:C:437:ILE:HD13	2.03	0.40
1:C:416:ASN:HB2	1:C:566:ASN:HD22	1.85	0.40
1:D:249:VAL:HG13	1:D:253:ASP:HB2	2.02	0.40
1:D:279:ARG:NH2	1:D:407:GLU:HG2	2.37	0.40
1:D:515:SER:O	1:D:519:ILE:HG13	2.22	0.40
1:E:161:ILE:HA	1:E:221:LEU:HA	2.03	0.40
1:F:272:PHE:CE2	1:F:365:PRO:HB3	2.56	0.40
2:k:48:ARG:HH12	2:k:207:SER:N	2.13	0.40
2:k:161:GLU:HB3	2:k:162:PRO:HD3	2.04	0.40
2:l:55:GLU:HB2	2:l:222:PHE:CG	2.56	0.40
2:n:176:SER:OG	2:n:179:ASP:OD2	2.27	0.40
2:H:10:GLU:OE2	2:I:19:LEU:HD12	2.20	0.40
2:I:57:TYR:HE1	2:I:91:ARG:NE	2.19	0.40
2:K:60:VAL:HG22	2:K:126:GLU:HG3	2.03	0.40
2:K:208:LEU:HD23	2:K:208:LEU:HA	1.92	0.40
2:L:107:LEU:HD12	2:L:141:ILE:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:214:ASP:HB3	2:M:217:ARG:HG2	2.02	0.40
2:N:25:ALA:O	2:N:158:GLY:HA2	2.21	0.40
2:N:128:ALA:HB2	2:N:134:LYS:HB3	2.02	0.40
3:P:347:GLY:HA3	3:P:400:ALA:HA	2.03	0.40
3:V:407:TYR:CZ	3:V:417:ALA:HB3	2.56	0.40
2:O:72:ASP:HA	2:O:75:ARG:NH1	2.36	0.40
1:A:453:LEU:HD11	1:A:547:LEU:CD1	2.52	0.40
1:A:482:VAL:HG21	1:A:547:LEU:HB3	2.04	0.40
1:C:275:LYS:HA	1:C:275:LYS:HD3	1.80	0.40
1:D:300:THR:O	1:D:304:LYS:HG2	2.21	0.40
1:E:353:PHE:CE2	1:E:396:LEU:HG	2.56	0.40
1:F:115:VAL:HG12	1:F:117:THR:HG23	2.03	0.40
2:m:35:TYR:HB2	2:m:175:ALA:O	2.22	0.40
2:m:141:ILE:HA	2:m:147:ILE:HA	2.03	0.40
2:m:219:ARG:NE	2:m:220:ARG:HG3	2.33	0.40
2:n:155:VAL:O	2:n:156:MET:HE2	2.21	0.40
3:T:359:TYR:CE2	3:T:363:LEU:HD11	2.56	0.40
3:W:319:ARG:HH21	3:W:485:ASP:HB2	1.87	0.40
3:X:342:ALA:HB3	3:X:497:ILE:HD11	2.03	0.40
3:X:345:ILE:HB	3:X:352:ALA:HB1	2.03	0.40
3:X:432:GLU:HG3	3:X:437:GLN:CG	2.41	0.40
3:Z:380:ILE:HG23	3:Z:423:PHE:CZ	2.57	0.40
3:Z:424:ASP:OD1	3:Z:428:GLY:N	2.55	0.40
3:c:449:SER:OG	3:c:469:GLU:OE1	2.39	0.40
2:O:25:ALA:O	2:O:158:GLY:HA2	2.22	0.40
1:C:500:TYR:HB3	1:C:579:GLU:OE2	2.21	0.40
1:E:407:GLU:HG2	1:E:408:ASN:N	2.36	0.40
1:E:531:ILE:HA	1:E:531:ILE:HD12	1.89	0.40
1:F:440:PRO:HD2	1:F:514:ASN:O	2.21	0.40
1:F:486:MET:O	1:F:511:LYS:HB3	2.22	0.40
2:k:68:PHE:HA	2:k:71:PHE:CZ	2.57	0.40
2:n:68:PHE:HB3	4:d:172:GLN:HG3	2.02	0.40
2:n:93:ASP:OD1	3:T:375:THR:OG1	2.29	0.40
2:n:109:THR:HG22	2:n:113:GLU:OE2	2.21	0.40
2:o:14:ARG:HH22	2:o:21:ARG:HH12	1.69	0.40
2:o:178:THR:O	2:o:181:LEU:HG	2.21	0.40
2:G:111:PHE:CD1	2:G:117:PRO:HB3	2.56	0.40
2:I:12:ALA:O	2:I:15:GLU:HG3	2.22	0.40
2:N:129:HIS:HB2	2:N:132:GLU:CD	2.47	0.40
3:S:375:THR:O	3:S:379:LYS:HG3	2.21	0.40
3:V:476:ASP:OD2	3:W:488:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:305:ALA:HB2	3:W:403:LEU:HD21	2.03	0.40
3:W:311:GLY:HA2	3:W:407:TYR:CD1	2.56	0.40
3:W:375:THR:O	3:W:379:LYS:HG3	2.22	0.40
3:X:438:ALA:CB	3:X:447:LYS:HE3	2.51	0.40
3:c:444:LEU:HD23	3:c:447:LYS:HZ1	1.86	0.40
2:O:101:ASN:O	2:O:105:GLN:HG2	2.22	0.40
1:A:561:LEU:HD13	1:B:426:LEU:HD23	2.02	0.40
1:C:161:ILE:HD12	1:D:175:LEU:HD13	2.04	0.40
1:D:164:LEU:HD21	1:D:167:ILE:HD11	2.03	0.40
1:D:346:GLU:HA	1:D:395:GLN:HG2	2.04	0.40
1:F:525:ARG:HD2	1:F:550:SER:HA	2.02	0.40
2:k:41:PHE:HB3	2:k:53:ILE:HD13	2.04	0.40
2:m:59:ARG:NH1	2:m:217:ARG:O	2.47	0.40
2:n:113:GLU:HG2	2:n:114:GLN:N	2.35	0.40
2:H:155:VAL:HG12	2:H:160:THR:HG22	2.04	0.40
2:K:30:VAL:HG13	2:K:43:ALA:HB2	2.03	0.40
3:Q:388:ARG:HA	3:Q:391:LEU:HG	2.03	0.40
3:R:457:VAL:HG22	3:R:463:GLY:HA2	2.03	0.40
3:U:313:VAL:HG23	3:U:496:ILE:HG12	2.04	0.40
3:X:447:LYS:HE2	3:X:447:LYS:CA	2.51	0.40
3:Y:319:ARG:N	3:Y:319:ARG:HD2	2.36	0.40
3:a:337:THR:OG1	3:a:341:THR:OG1	2.39	0.40
3:b:385:ILE:HA	3:b:388:ARG:CD	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/609 (75%)	446 (97%)	12 (3%)	0	100	100
1	B	472/609 (78%)	459 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	458/609 (75%)	444 (97%)	14 (3%)	0	100	100
1	D	444/609 (73%)	427 (96%)	17 (4%)	0	100	100
1	E	472/609 (78%)	453 (96%)	19 (4%)	0	100	100
1	F	473/609 (78%)	463 (98%)	10 (2%)	0	100	100
2	G	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
2	H	211/248 (85%)	204 (97%)	6 (3%)	1 (0%)	24	59
2	I	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
2	J	211/248 (85%)	202 (96%)	9 (4%)	0	100	100
2	K	211/248 (85%)	203 (96%)	8 (4%)	0	100	100
2	L	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
2	M	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
2	N	211/248 (85%)	208 (99%)	3 (1%)	0	100	100
2	O	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
2	k	211/248 (85%)	207 (98%)	4 (2%)	0	100	100
2	l	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
2	m	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
2	n	211/248 (85%)	200 (95%)	11 (5%)	0	100	100
2	o	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
3	P	220/291 (76%)	215 (98%)	5 (2%)	0	100	100
3	Q	220/291 (76%)	214 (97%)	6 (3%)	0	100	100
3	R	220/291 (76%)	216 (98%)	4 (2%)	0	100	100
3	S	220/291 (76%)	215 (98%)	5 (2%)	0	100	100
3	T	220/291 (76%)	217 (99%)	3 (1%)	0	100	100
3	U	220/291 (76%)	216 (98%)	4 (2%)	0	100	100
3	V	220/291 (76%)	216 (98%)	4 (2%)	0	100	100
3	W	220/291 (76%)	213 (97%)	7 (3%)	0	100	100
3	X	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	Y	220/291 (76%)	217 (99%)	3 (1%)	0	100	100
3	Z	220/291 (76%)	216 (98%)	4 (2%)	0	100	100
3	a	220/291 (76%)	216 (98%)	4 (2%)	0	100	100
3	b	220/291 (76%)	215 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	220/291 (76%)	217 (99%)	3 (1%)	0	100	100
4	d	2/4 (50%)	2 (100%)	0	0	100	100
4	e	2/4 (50%)	2 (100%)	0	0	100	100
4	f	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	g	2/4 (50%)	2 (100%)	0	0	100	100
4	h	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
4	i	2/4 (50%)	2 (100%)	0	0	100	100
4	j	2/4 (50%)	2 (100%)	0	0	100	100
All	All	8825/11228 (79%)	8594 (97%)	230 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	58	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/511 (78%)	396 (100%)	0	100	100
1	B	403/511 (79%)	403 (100%)	0	100	100
1	C	394/511 (77%)	394 (100%)	0	100	100
1	D	384/511 (75%)	383 (100%)	1 (0%)	86	88
1	E	403/511 (79%)	403 (100%)	0	100	100
1	F	403/511 (79%)	403 (100%)	0	100	100
2	G	165/192 (86%)	165 (100%)	0	100	100
2	H	165/192 (86%)	164 (99%)	1 (1%)	78	84
2	I	165/192 (86%)	165 (100%)	0	100	100
2	J	165/192 (86%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	165/192 (86%)	165 (100%)	0	100	100
2	L	165/192 (86%)	165 (100%)	0	100	100
2	M	165/192 (86%)	164 (99%)	1 (1%)	78	84
2	N	165/192 (86%)	165 (100%)	0	100	100
2	O	165/192 (86%)	165 (100%)	0	100	100
2	k	165/192 (86%)	165 (100%)	0	100	100
2	l	165/192 (86%)	165 (100%)	0	100	100
2	m	165/192 (86%)	165 (100%)	0	100	100
2	n	165/192 (86%)	165 (100%)	0	100	100
2	o	165/192 (86%)	165 (100%)	0	100	100
3	P	165/217 (76%)	165 (100%)	0	100	100
3	Q	165/217 (76%)	165 (100%)	0	100	100
3	R	165/217 (76%)	165 (100%)	0	100	100
3	S	165/217 (76%)	165 (100%)	0	100	100
3	T	164/217 (76%)	164 (100%)	0	100	100
3	U	165/217 (76%)	165 (100%)	0	100	100
3	V	165/217 (76%)	165 (100%)	0	100	100
3	W	165/217 (76%)	165 (100%)	0	100	100
3	X	165/217 (76%)	165 (100%)	0	100	100
3	Y	165/217 (76%)	165 (100%)	0	100	100
3	Z	165/217 (76%)	165 (100%)	0	100	100
3	a	165/217 (76%)	165 (100%)	0	100	100
3	b	165/217 (76%)	164 (99%)	1 (1%)	78	84
3	c	165/217 (76%)	165 (100%)	0	100	100
4	d	3/3 (100%)	3 (100%)	0	100	100
4	e	3/3 (100%)	3 (100%)	0	100	100
4	f	3/3 (100%)	3 (100%)	0	100	100
4	g	3/3 (100%)	3 (100%)	0	100	100
4	h	3/3 (100%)	3 (100%)	0	100	100
4	i	3/3 (100%)	3 (100%)	0	100	100
4	j	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7023/8813 (80%)	7019 (100%)	4 (0%)	87 91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	364	THR
2	H	147	ILE
2	M	141	ILE
3	b	322	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	446	GLN
1	A	521	ASN
1	A	529	ASN
1	A	563	ASN
1	B	395	GLN
1	B	502	ASN
1	C	274	HIS
1	C	339	ASN
1	C	348	HIS
1	C	529	ASN
1	D	263	GLN
1	D	521	ASN
1	D	529	ASN
1	E	529	ASN
1	E	566	ASN
1	F	331	ASN
1	F	395	GLN
1	F	521	ASN
2	k	129	HIS
2	l	114	GLN
2	l	152	HIS
2	m	45	ASN
2	m	129	HIS
2	m	174	ASN
2	n	165	ASN
2	o	51	GLN
2	G	45	ASN
2	G	114	GLN

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Mol	Chain	Res	Type
2	G	231	GLN
2	H	73	ASN
2	H	216	ASN
2	I	129	HIS
2	K	105	GLN
2	L	80	GLN
2	N	73	ASN
2	N	114	GLN
2	N	216	ASN
3	P	381	ASN
3	Q	381	ASN
3	Q	410	HIS
3	R	430	ASN
3	S	381	ASN
3	S	437	GLN
3	T	396	GLN
3	W	437	GLN
3	X	410	HIS
3	X	430	ASN
3	Z	396	GLN
3	a	390	ASN
3	a	396	GLN
3	c	456	GLN
4	f	172	GLN
4	g	172	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 oligosaccharides 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.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27225. These allow visual inspection of the internal detail of the map and identification of artifacts.

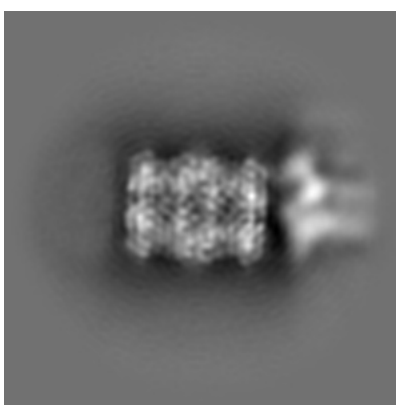
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

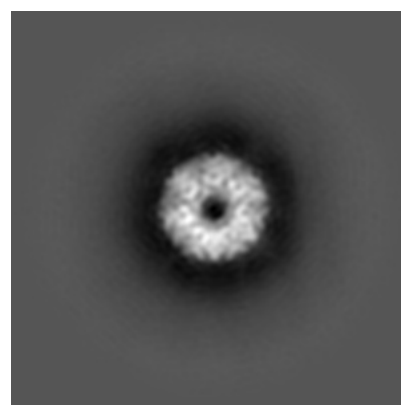
6.1.1 Primary map



X



Y

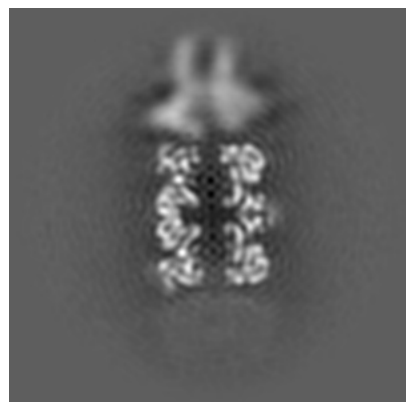


Z

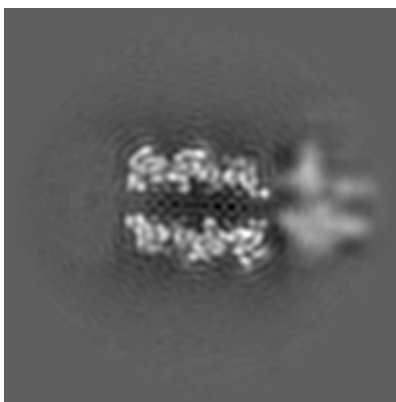
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

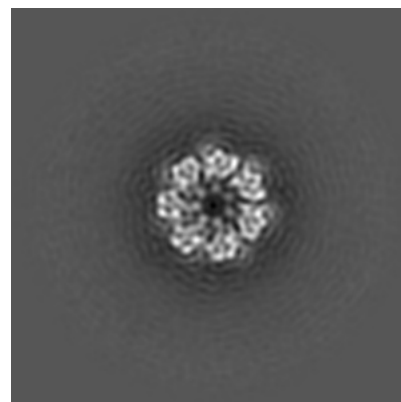
6.2.1 Primary map



X Index: 48



Y Index: 48

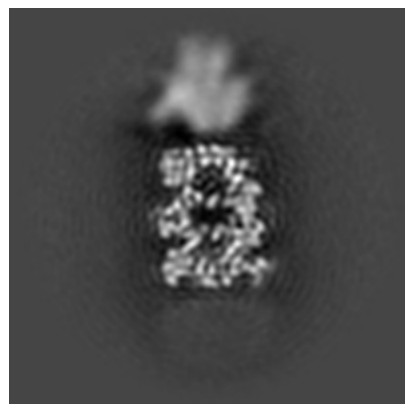


Z Index: 48

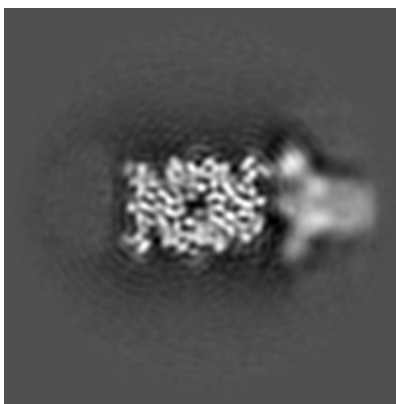
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

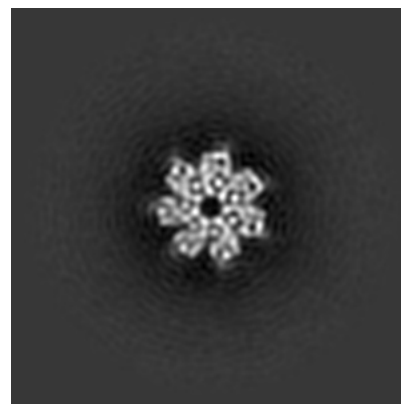
6.3.1 Primary map



X Index: 44



Y Index: 42



Z Index: 59

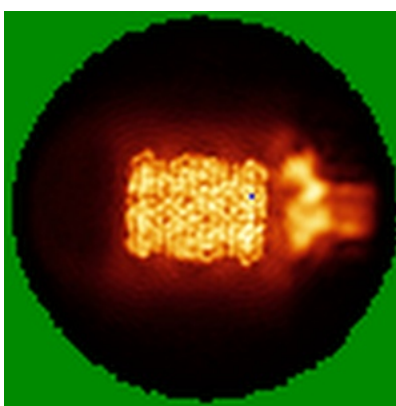
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

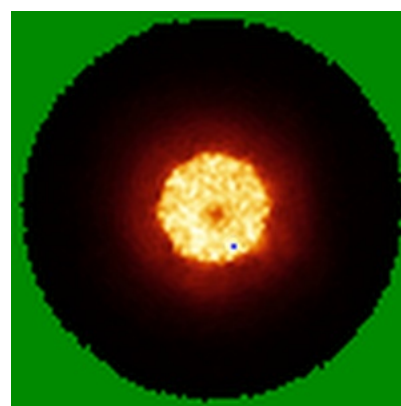
6.4.1 Primary map



X



Y

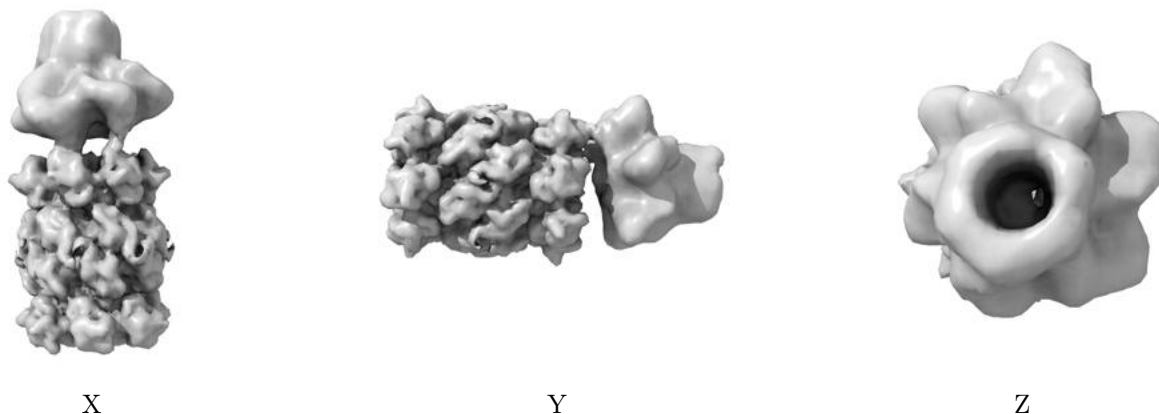


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

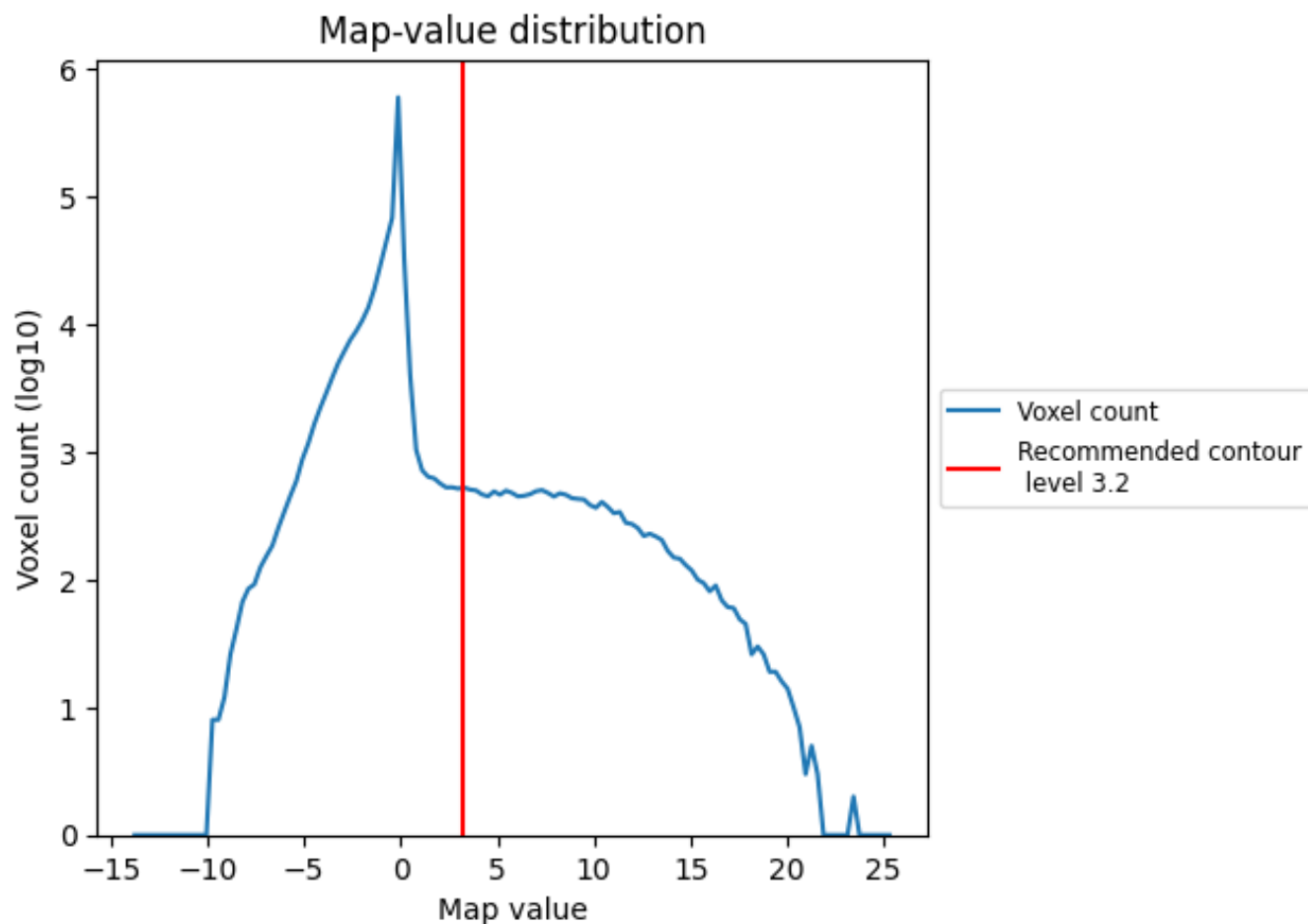
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

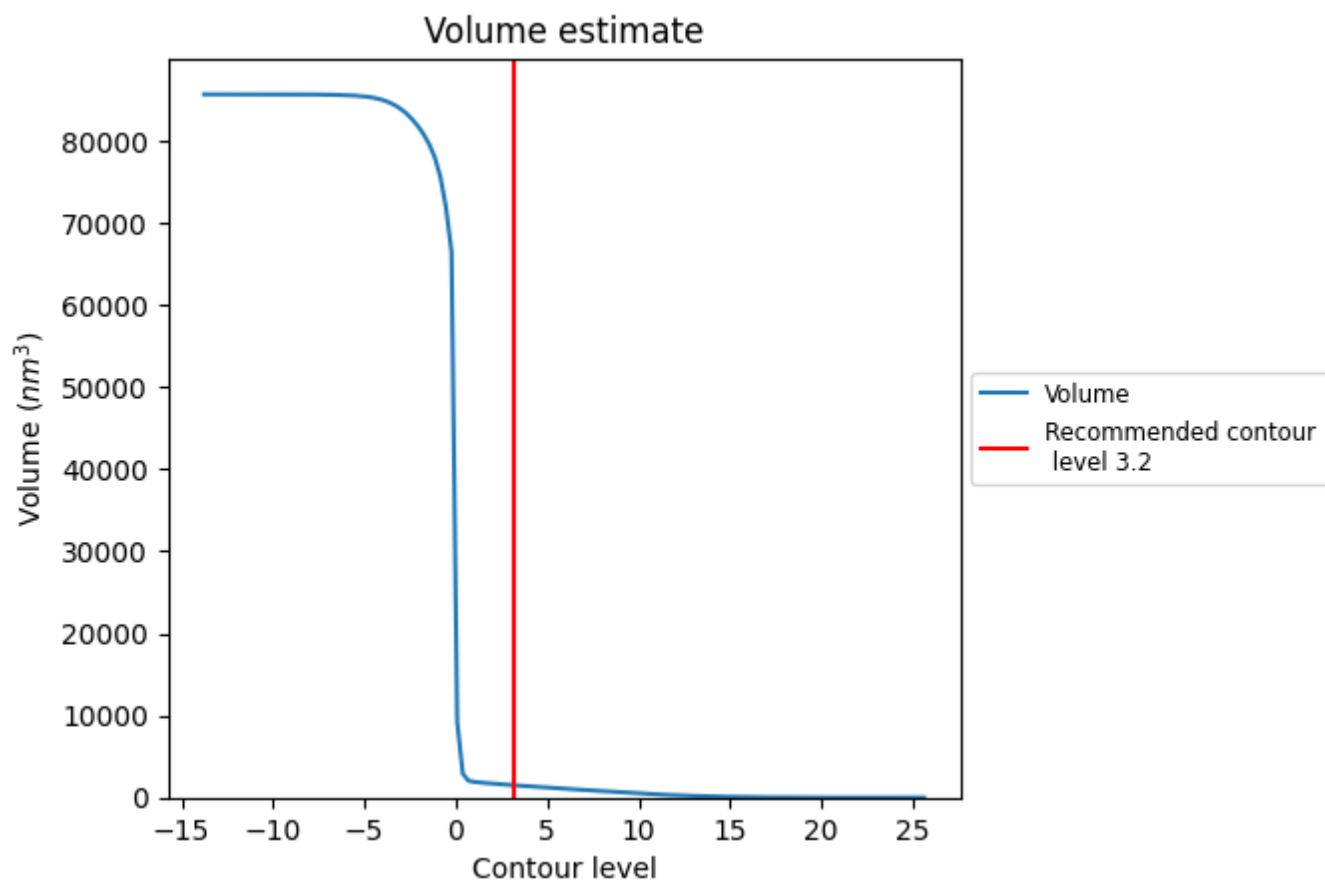
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

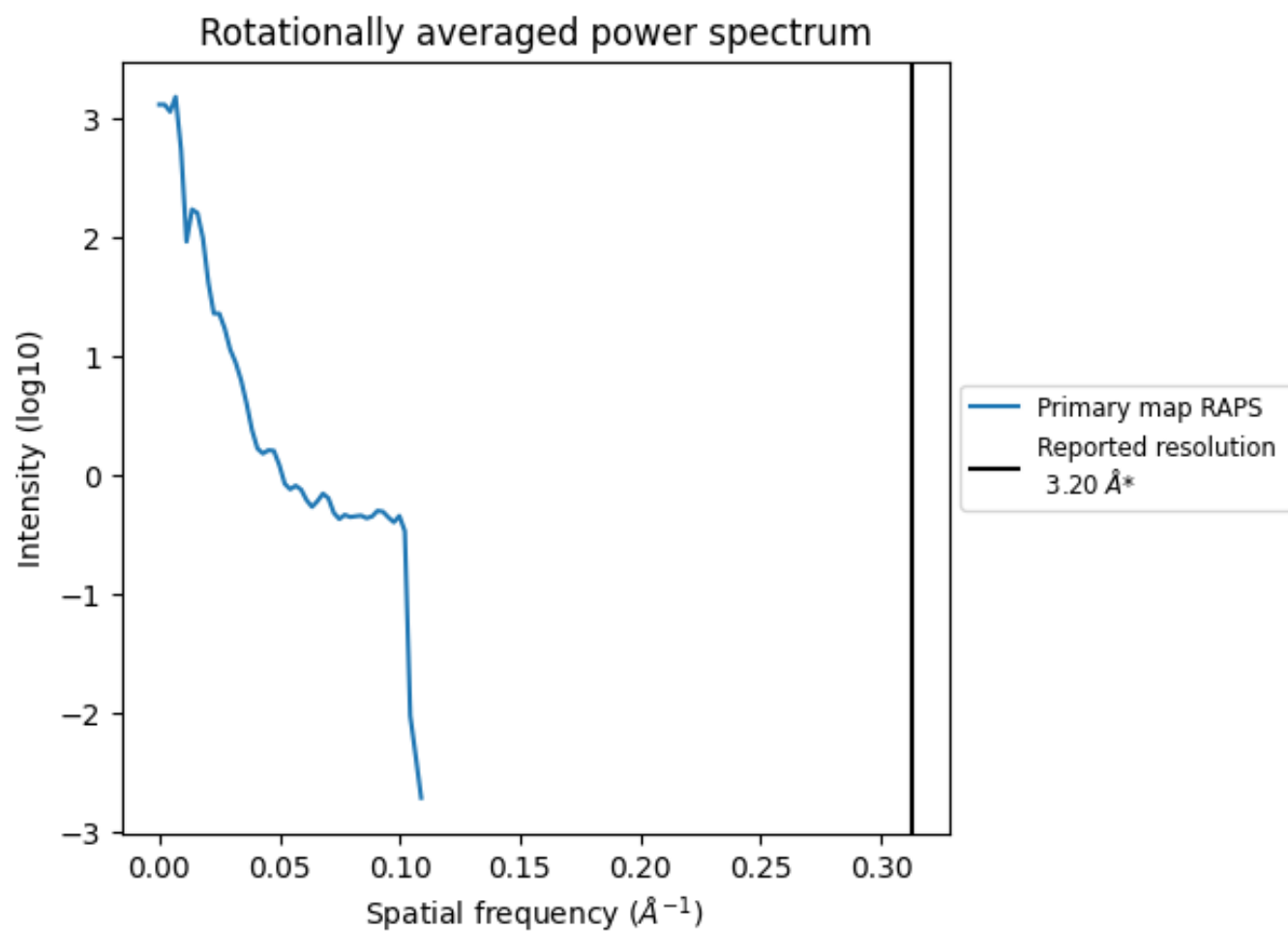
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1496 nm³; this corresponds to an approximate mass of 1352 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

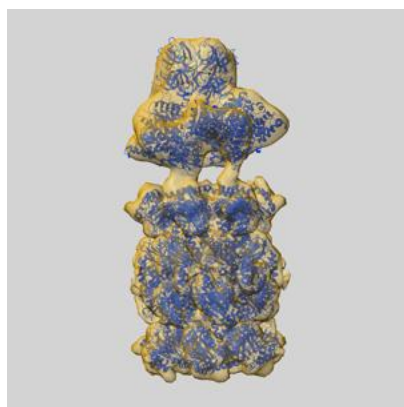
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

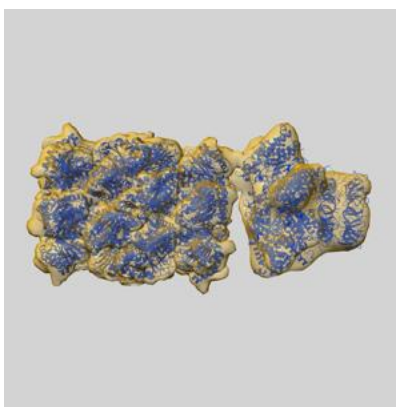
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27225 and PDB model 8D6X. Per-residue inclusion information can be found in section [3](#) on page [8](#).

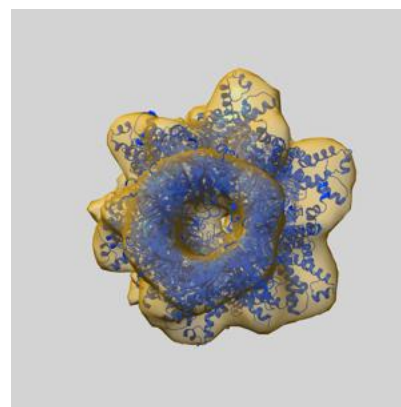
9.1 Map-model overlay [i](#)



X



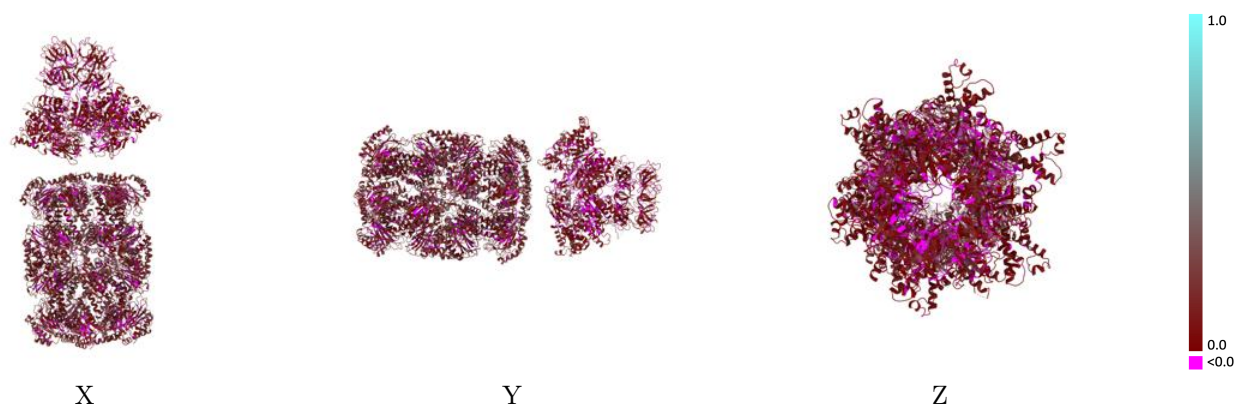
Y



Z

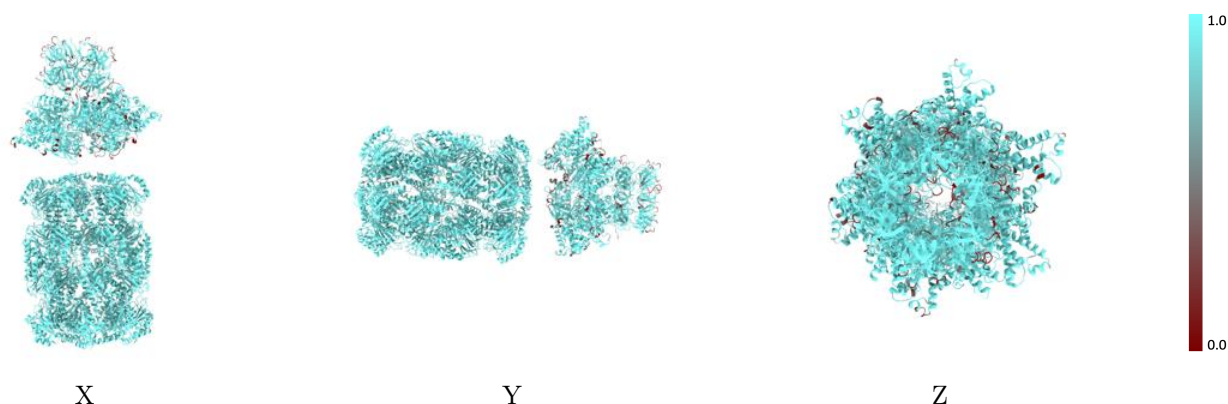
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



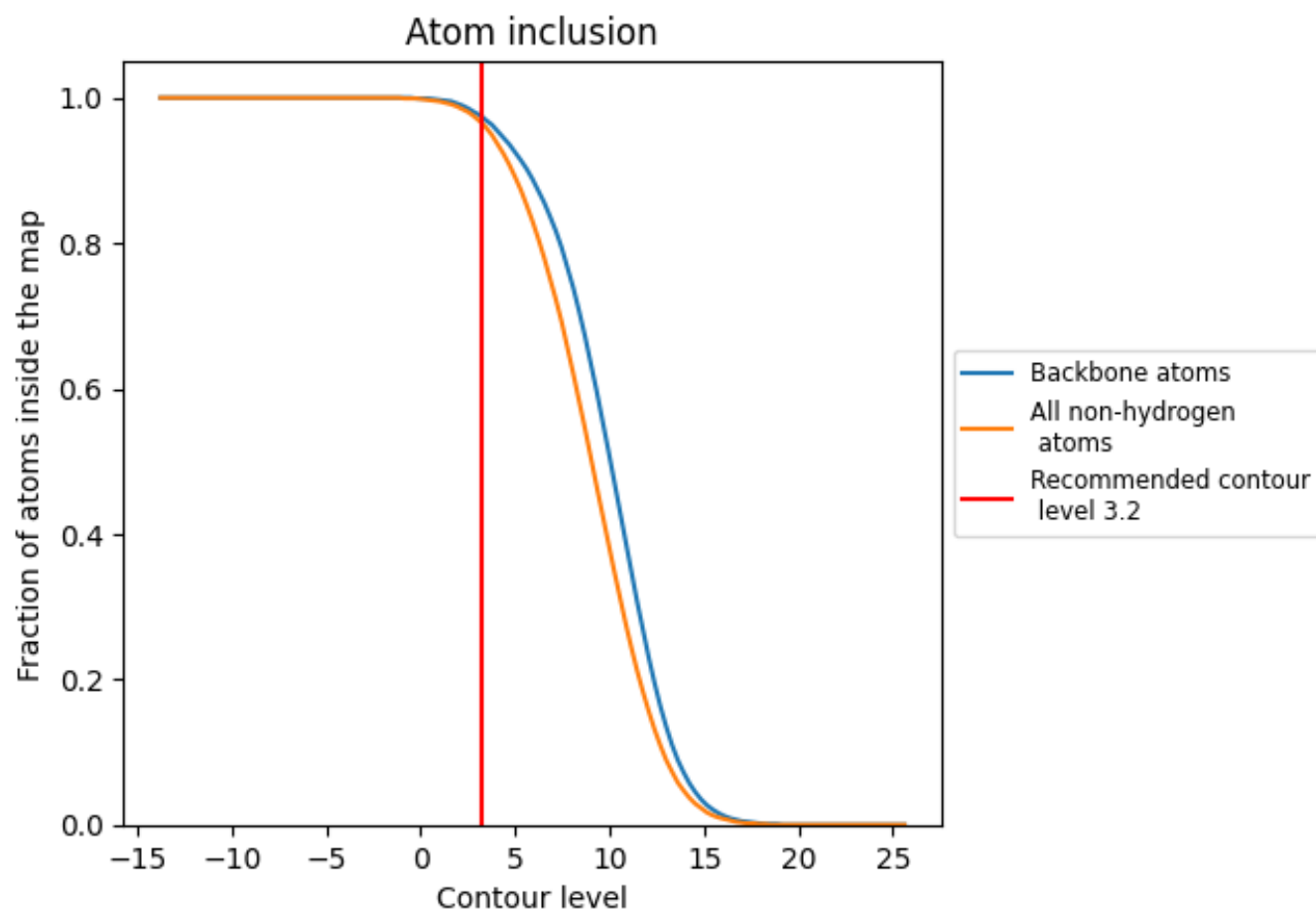
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9660	 0.1130
A	 0.9470	 0.0640
B	 0.9420	 0.0520
C	 0.9050	 0.0630
D	 0.9210	 0.0650
E	 0.9170	 0.0510
F	 0.8950	 0.0490
G	 0.9860	 0.1440
H	 0.9850	 0.1450
I	 0.9910	 0.1470
J	 0.9850	 0.1430
K	 0.9880	 0.1370
L	 0.9810	 0.1380
M	 0.9800	 0.1450
N	 0.9830	 0.1440
O	 0.9810	 0.1390
P	 0.9930	 0.1410
Q	 0.9910	 0.1340
R	 0.9930	 0.1350
S	 0.9910	 0.1350
T	 0.9930	 0.1350
U	 0.9910	 0.1340
V	 0.9910	 0.1380
W	 0.9890	 0.1390
X	 0.9890	 0.1430
Y	 0.9890	 0.1450
Z	 0.9890	 0.1380
a	 0.9930	 0.1440
b	 0.9890	 0.1430
c	 0.9960	 0.1390
d	 0.6970	 -0.1050
e	 0.3940	 -0.0410
f	 0.6060	 -0.0890
g	 0.5150	 -0.0890
h	 0.5150	 -0.0930



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Chain	Atom inclusion	Q-score
i	 0.9090	 -0.0120
j	 0.8790	 -0.0480
k	 0.9800	 0.1430
l	 0.9950	 0.1420
m	 0.9930	 0.1440
n	 0.9950	 0.1460
o	 0.9870	 0.1410