Full wwPDB EM Validation Report

May 18, 2025 – 10:28 AM EDT

PDB ID	:	8D6Y / pdb_00008d6y
EMDB ID	:	EMD-27226
Title	:	Structure of the Mycobacterium tuberculosis 20S proteasome bound to the ADP-bound Mpa ATPase
Authors	:	Xiao, X.; Li, H.
Deposited on	:	2022-06-06
Resolution	:	10.00 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:

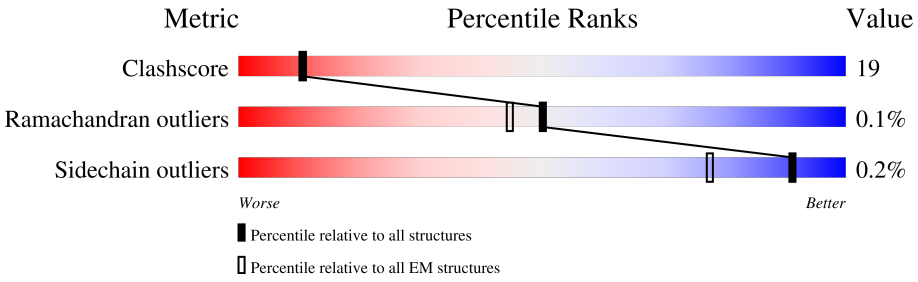
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 10.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 <=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	13% 53% 26% 21%
1	B	609	11% 49% 29% 22%
1	C	609	8% 56% 21% 22%
1	D	609	10% 49% 26% 24%
1	E	609	13% 47% 28% 24%
1	F	609	16% 47% 29% 24%
2	G	248	45% 42% 13%
2	H	248	51% 35% • 13%

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Mol	Chain	Length	Quality of chain
2	I	248	45% 42% 13%
2	J	248	46% 40% 13%
2	K	248	52% 35% 13%
2	L	248	46% 40% 13%
2	M	248	49% 37% 13%
2	N	248	47% 40% 13%
2	O	248	55% 32% 13%
2	k	248	48% 39% 13%
2	l	248	52% 34% 13%
2	m	248	53% 33% 13%
2	n	248	53% 34% 13%
2	o	248	47% 40% 13%
3	P	291	51% 26% 24%
3	Q	291	51% 25% 24%
3	R	291	46% 30% 24%
3	S	291	44% 32% 24%
3	T	291	45% 31% 24%
3	U	291	46% 31% 24%
3	V	291	53% 23% 24%
3	W	291	49% 27% 24%
3	X	291	46% 30% 24%
3	Y	291	47% 29% 24%
3	Z	291	48% 28% 24%
3	a	291	45% 32% 24%
3	b	291	56% 20% 24%

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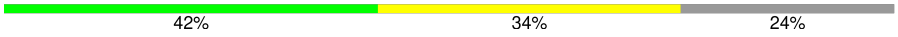
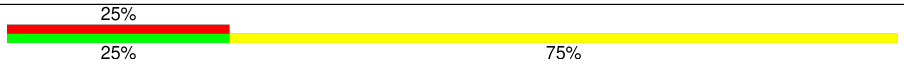
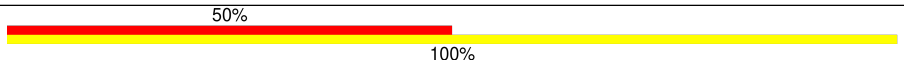
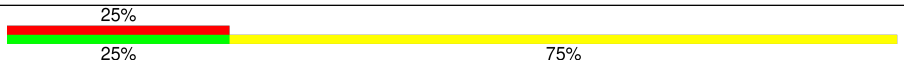
Mol	Chain	Length	Quality of chain
3	c	291	
4	d	4	
4	e	4	
4	f	4	
4	g	4	
4	h	4	
4	i	4	
4	j	4	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 68262 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	480	Total	C	N	O	S	0	0
			3747	2360	647	729	11		
1	B	475	Total	C	N	O	S	0	0
			3707	2337	637	722	11		
1	C	472	Total	C	N	O	S	0	0
			3649	2300	632	706	11		
1	D	460	Total	C	N	O	S	0	0
			3593	2266	621	695	11		
1	E	461	Total	C	N	O	S	0	0
			3597	2268	622	696	11		
1	F	460	Total	C	N	O	S	0	0
			3589	2267	615	696	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.

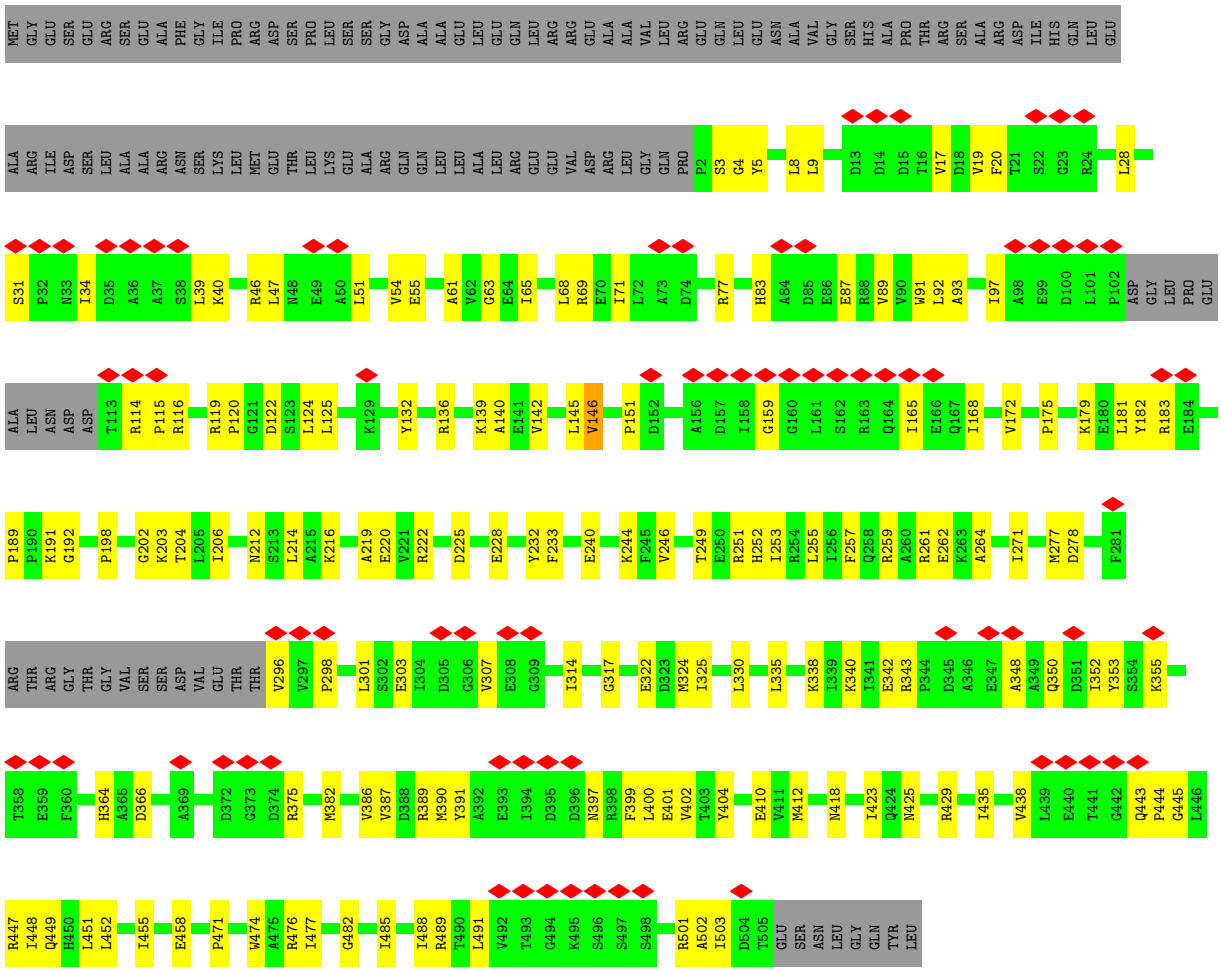
Mol	Chain	Residues	Atoms				AltConf	Trace
4	d	4	Total	C	N	O	0	0
			34	22	5	7		
4	e	4	Total	C	N	O	0	0
			34	22	5	7		
4	f	4	Total	C	N	O	0	0
			34	22	5	7		
4	g	4	Total	C	N	O	0	0
			34	22	5	7		
4	h	4	Total	C	N	O	0	0
			34	22	5	7		
4	i	4	Total	C	N	O	0	0
			34	22	5	7		
4	j	4	Total	C	N	O	0	0
			34	22	5	7		

3 Residue-property plots (i)

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.

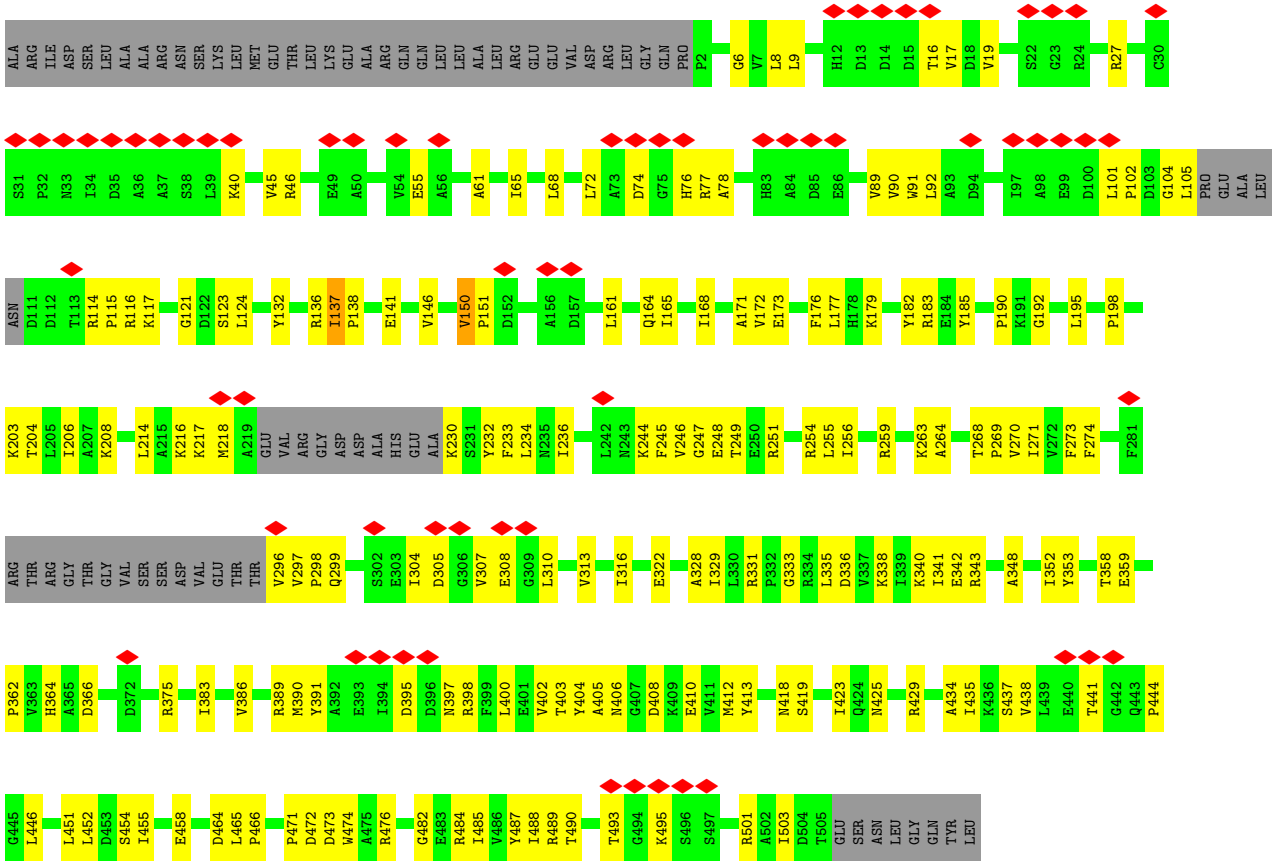
• Molecule 1: AAA ATPase forming ring-shaped complexes

Chain A:



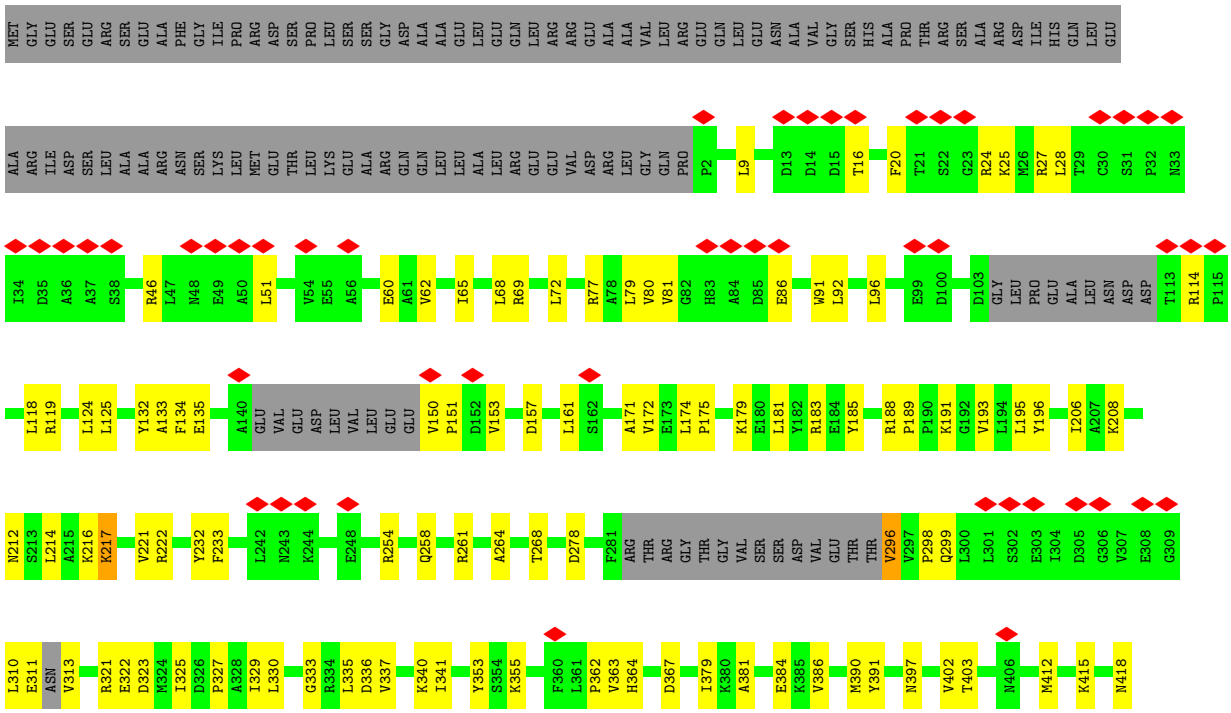
• Molecule 1: AAA ATPase forming ring-shaped complexes

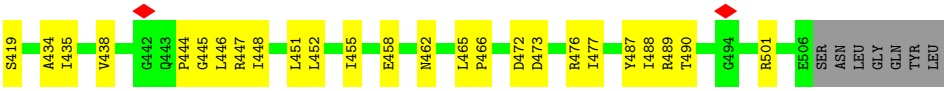
Chain B:



• Molecule 1: AAA ATPase forming ring-shaped complexes

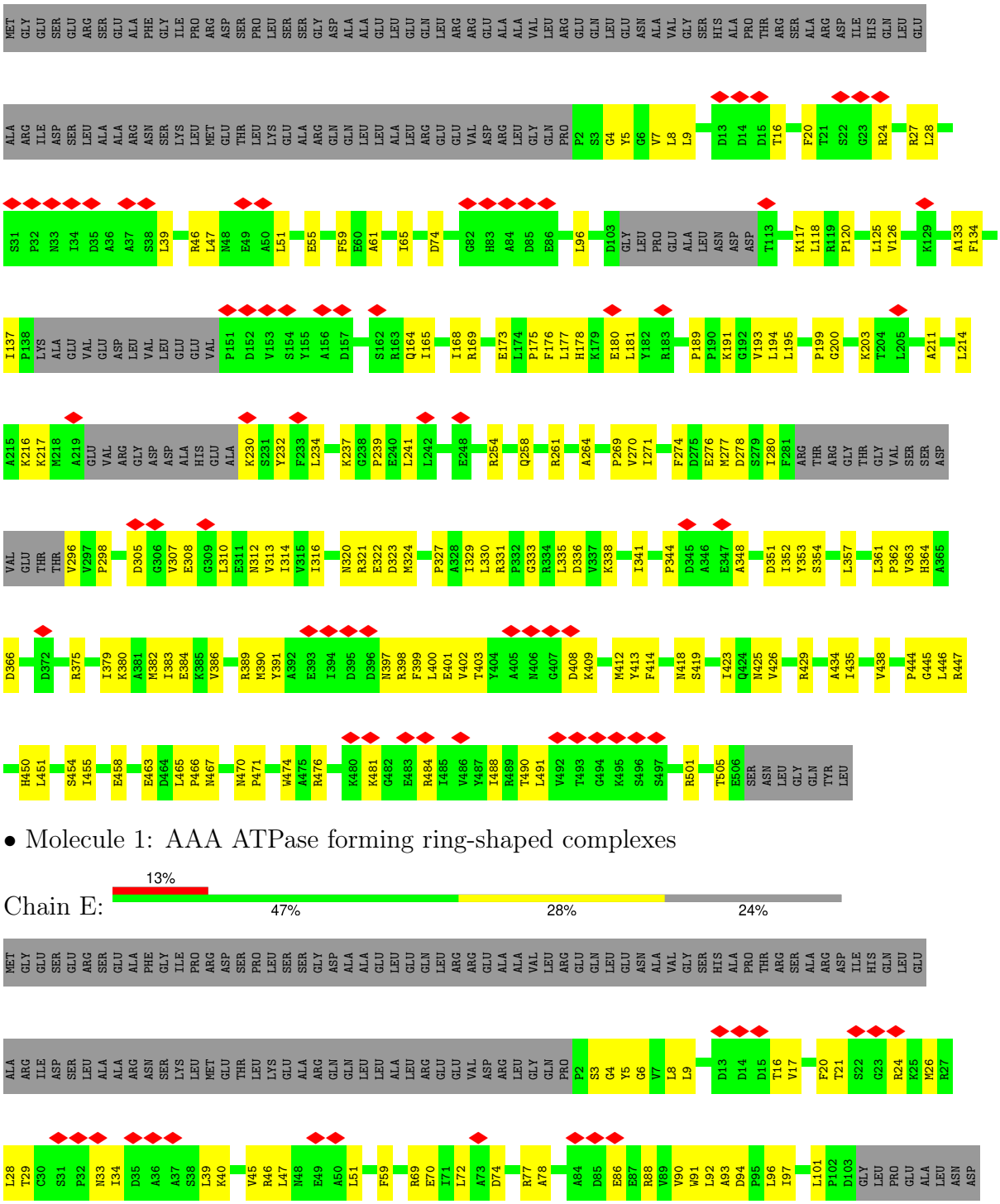
Chain C:





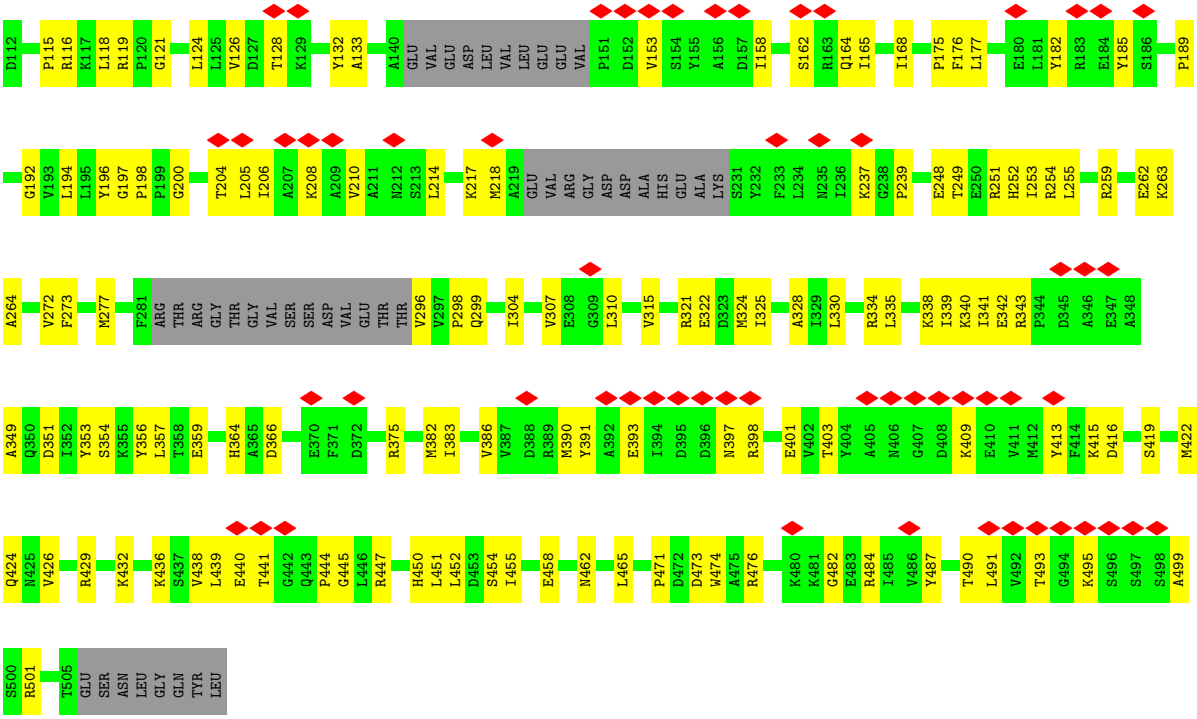
• Molecule 1: AAA ATPase forming ring-shaped complexes

Chain D:



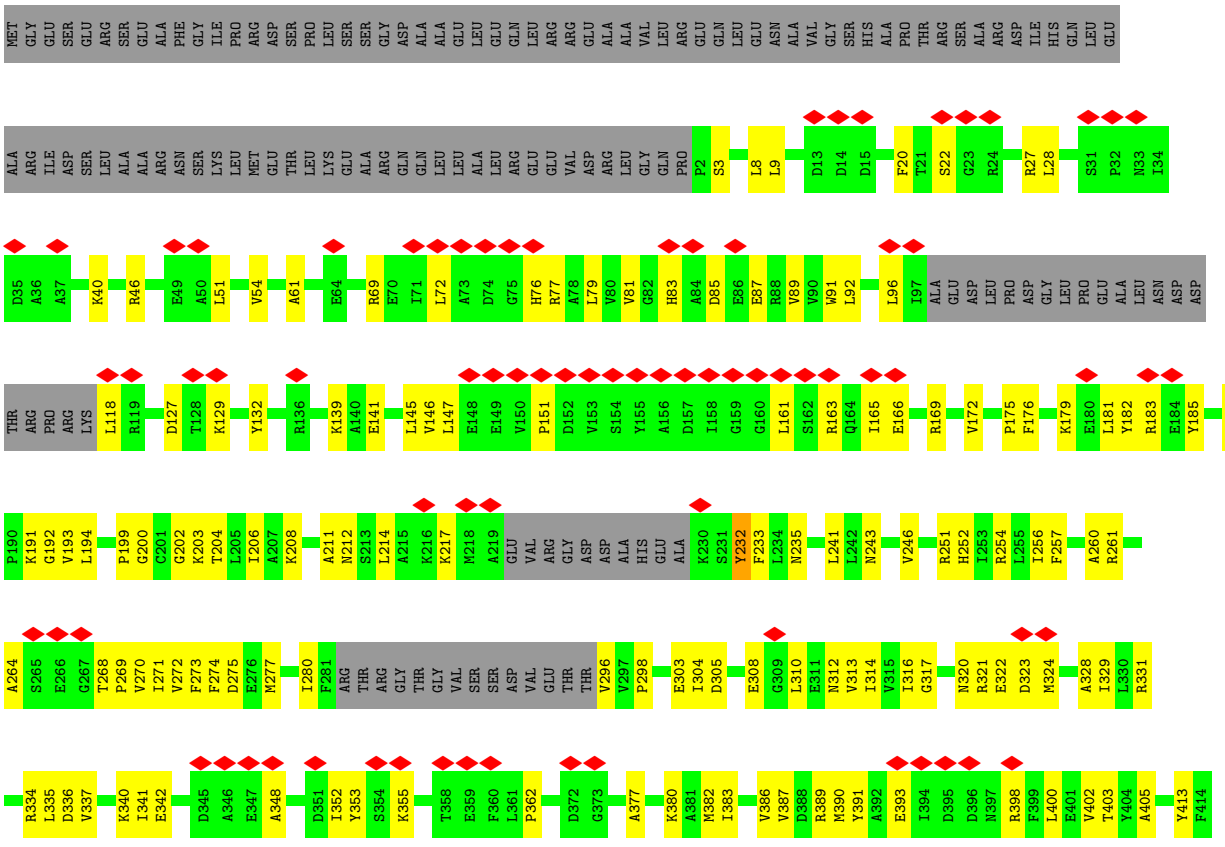
• Molecule 1: AAA ATPase forming ring-shaped complexes

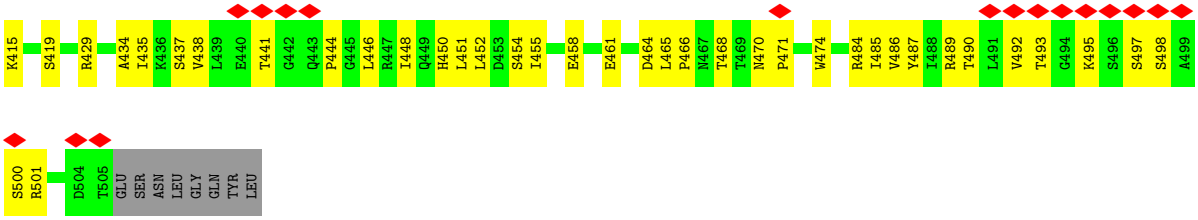
Chain E:



• Molecule 1: AAA ATPase forming ring-shaped complexes

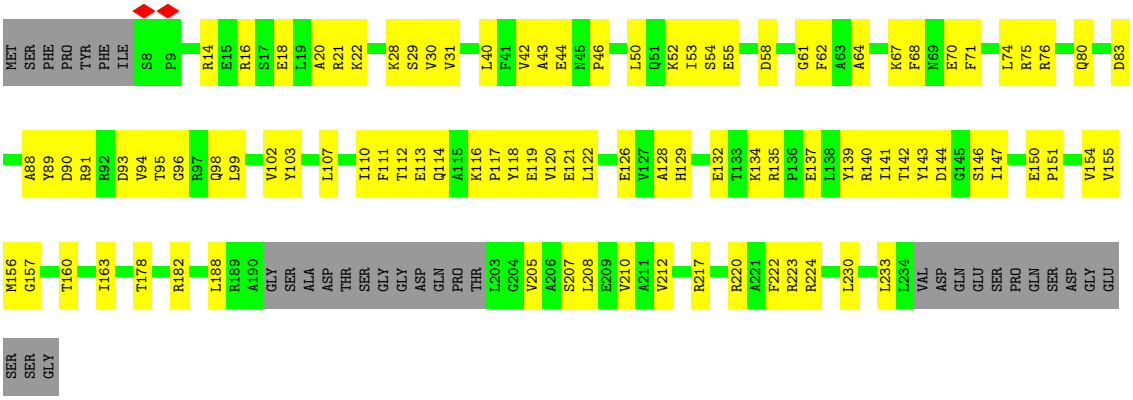
Chain F:





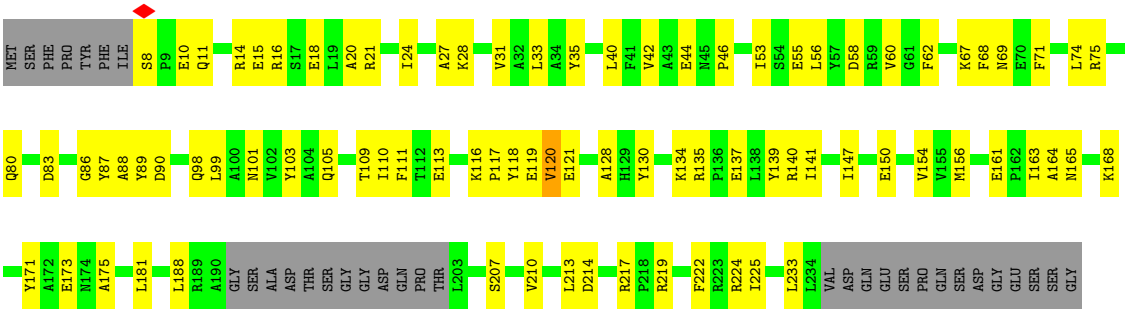
• Molecule 2: Proteasome subunit alpha

Chain k:



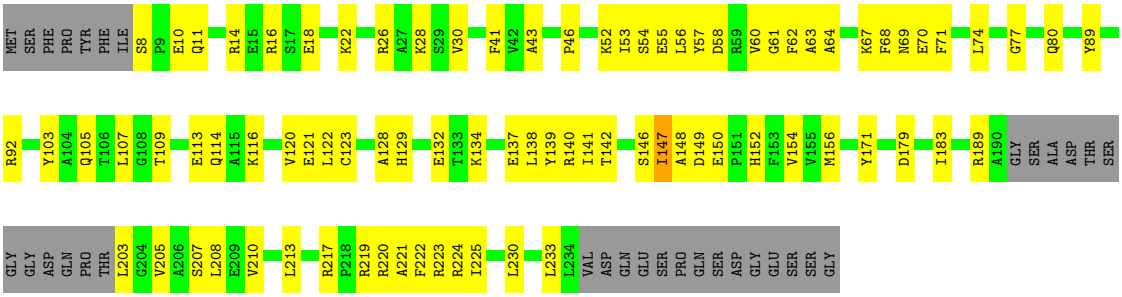
• Molecule 2: Proteasome subunit alpha

Chain l:



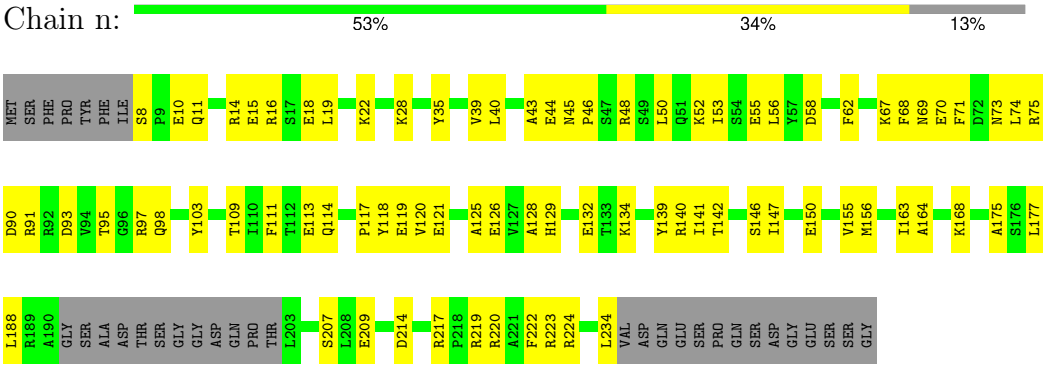
• Molecule 2: Proteasome subunit alpha

Chain m:



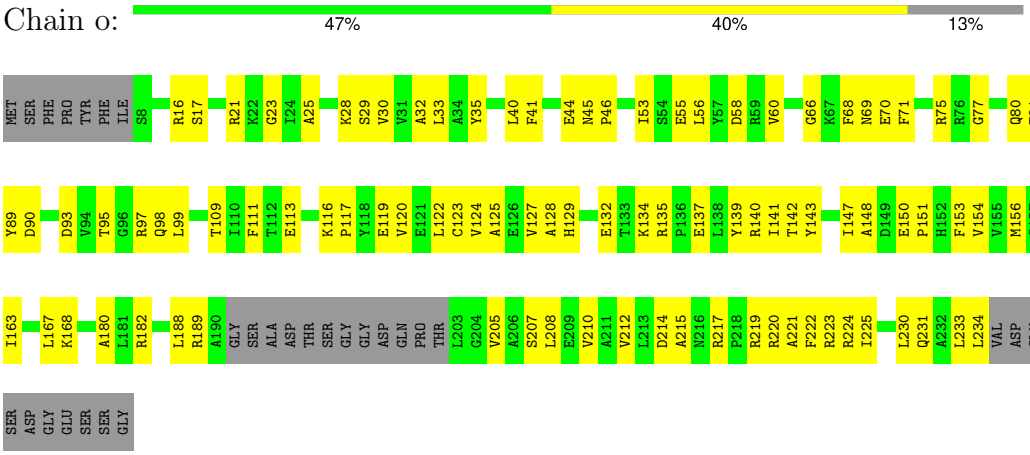
• Molecule 2: Proteasome subunit alpha

Chain n:



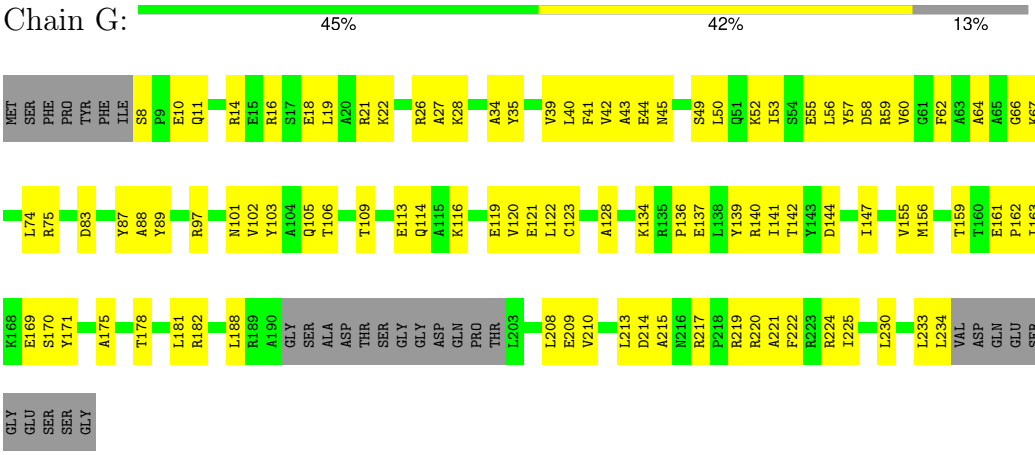
• Molecule 2: Proteasome subunit alpha

Chain o:



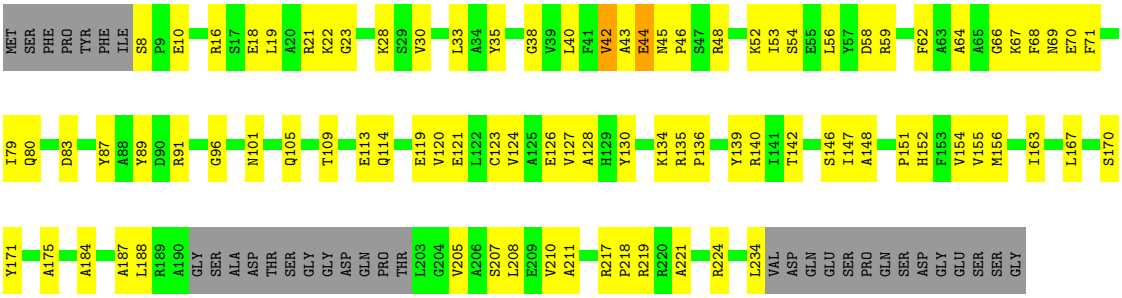
• Molecule 2: Proteasome subunit alpha

Chain G:



• Molecule 2: Proteasome subunit alpha

Chain H:

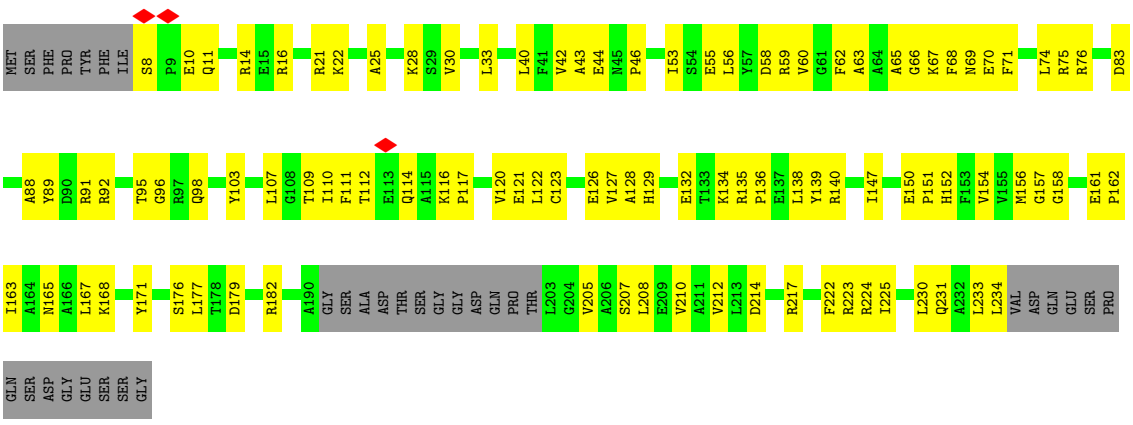


• Molecule 2: Proteasome subunit alpha

Chain I:

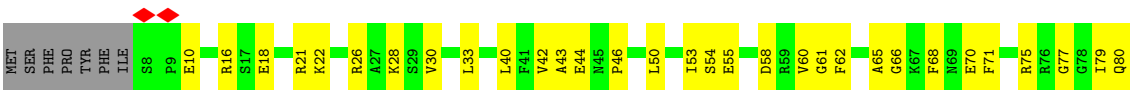
• Molecule 2: Proteasome subunit alpha

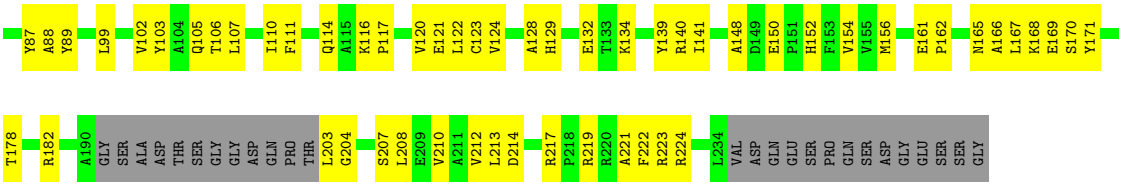
Chain J:



• Molecule 2: Proteasome subunit alpha

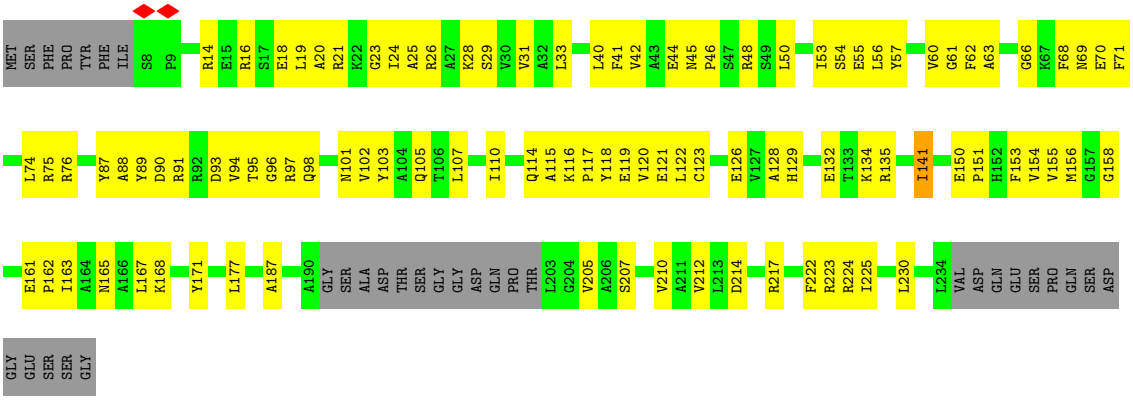
Chain K:





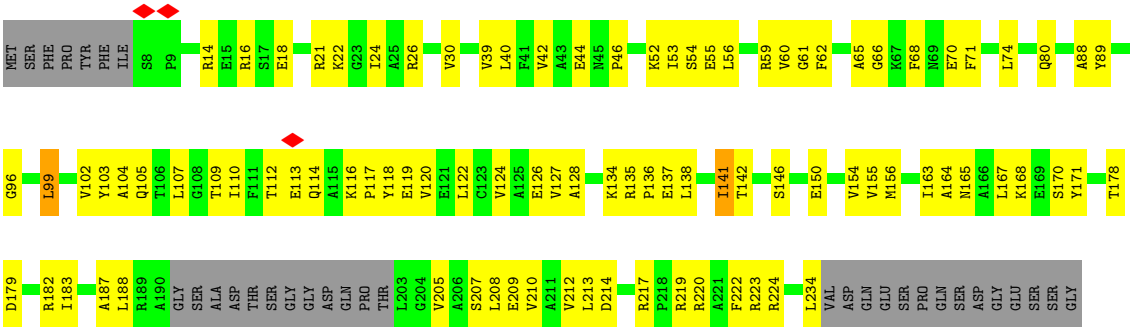
• Molecule 2: Proteasome subunit alpha

Chain L:



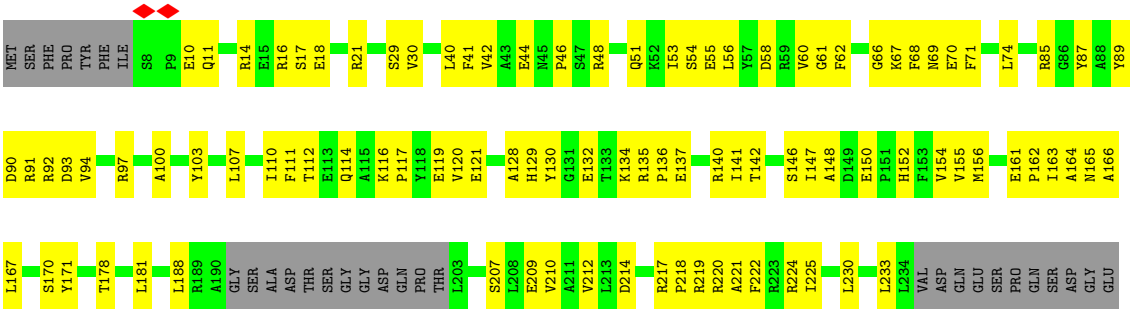
• Molecule 2: Proteasome subunit alpha

Chain M:



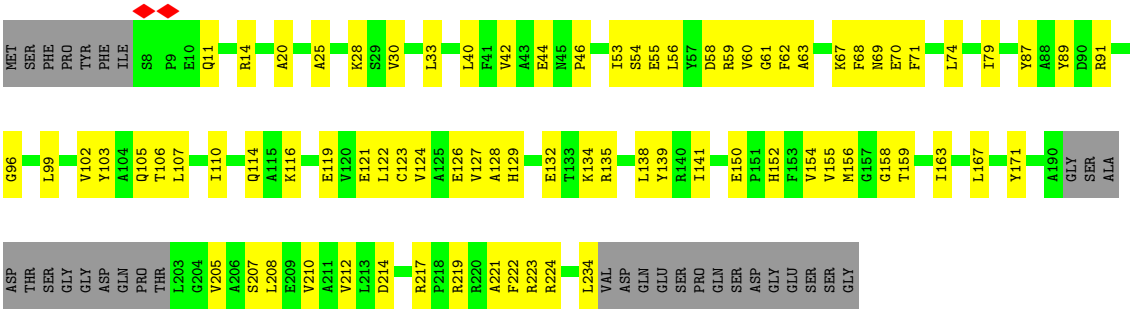
• Molecule 2: Proteasome subunit alpha

Chain N:



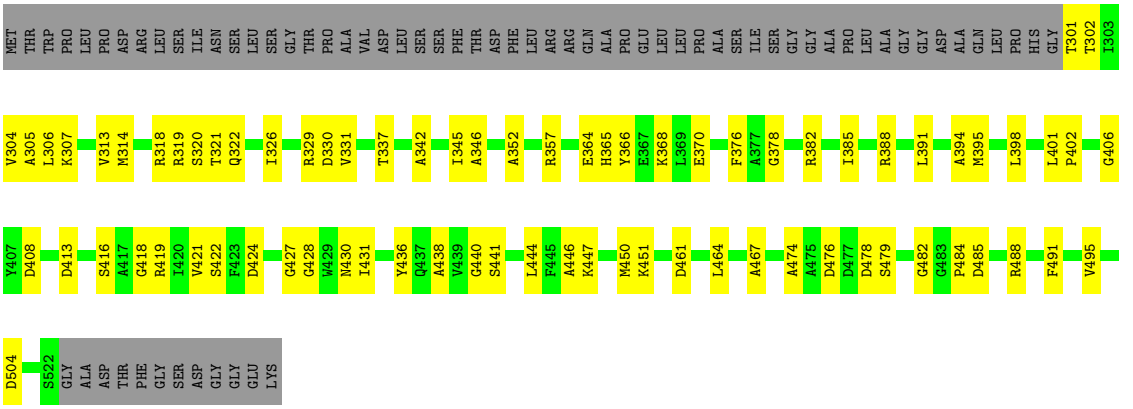
• Molecule 2: Proteasome subunit alpha

Chain O:



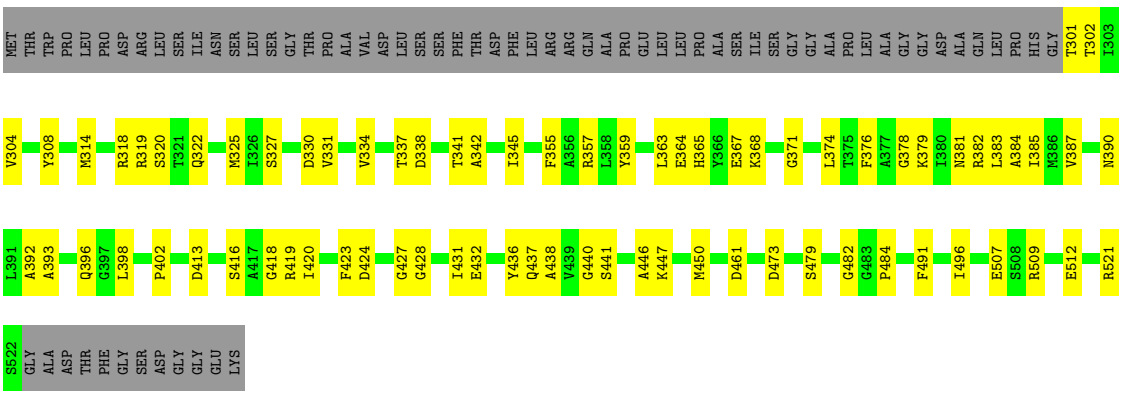
• Molecule 3: Proteasome subunit beta

Chain P:



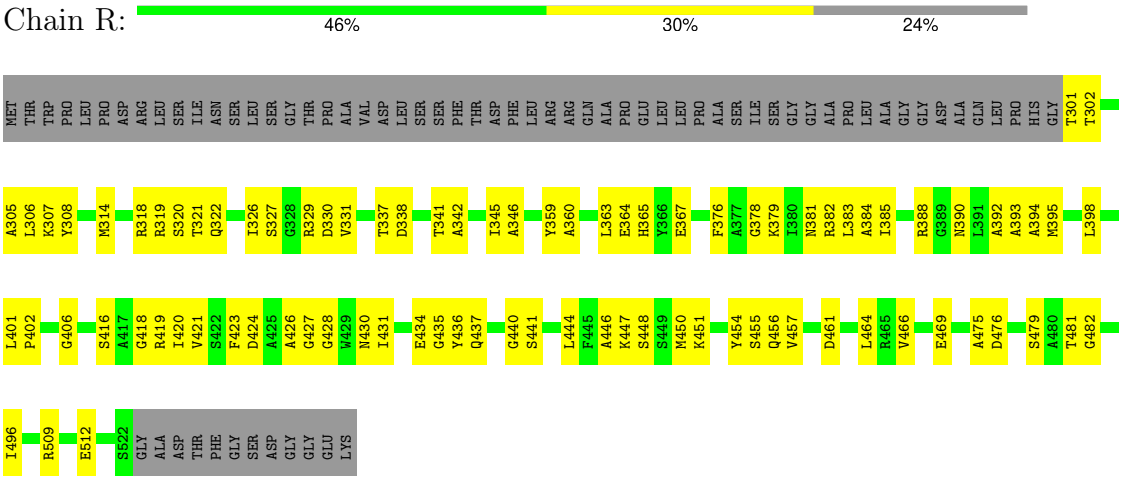
• Molecule 3: Proteasome subunit beta

Chain Q:



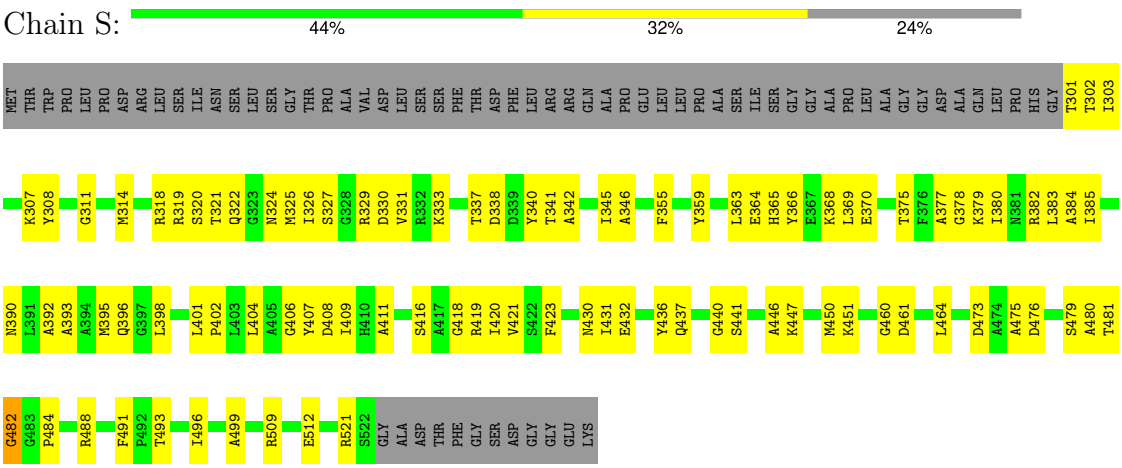
• Molecule 3: Proteasome subunit beta

Chain R:



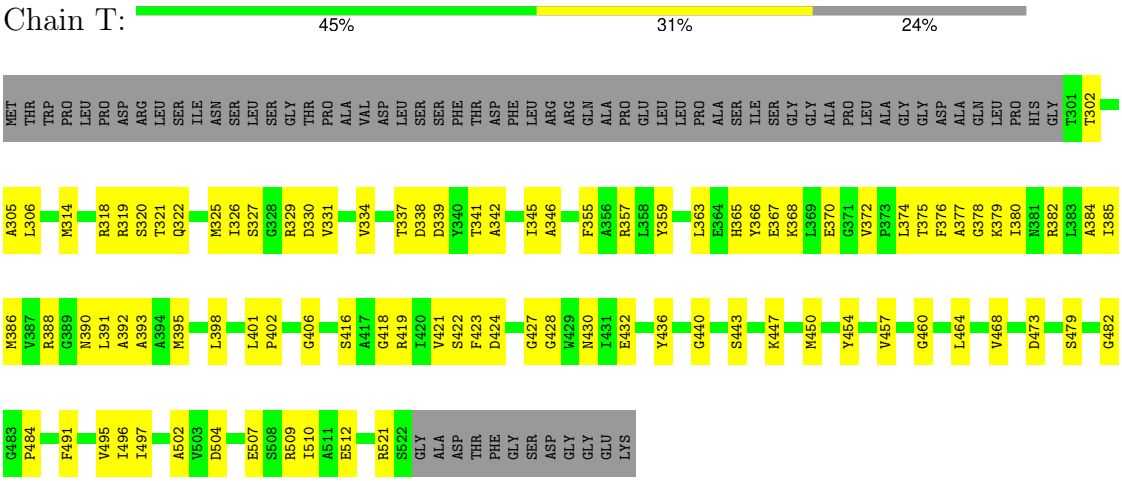
• Molecule 3: Proteasome subunit beta

Chain S:



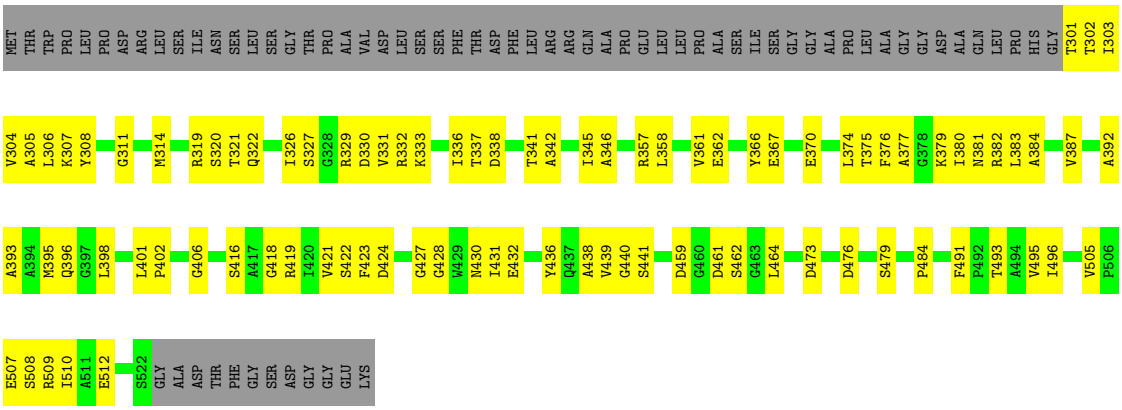
• Molecule 3: Proteasome subunit beta

Chain T:



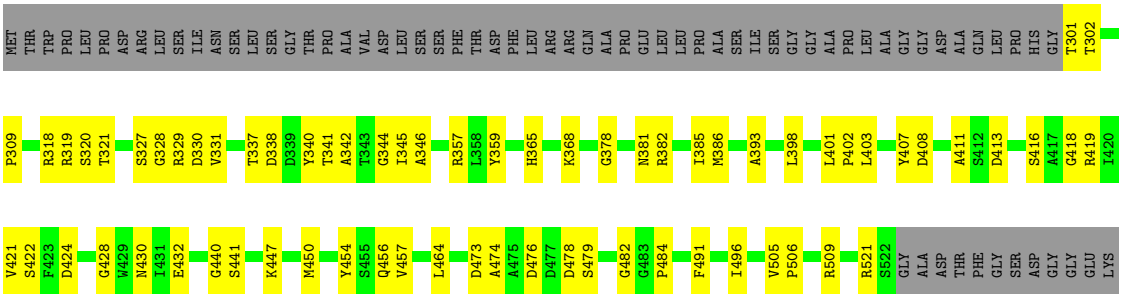
• Molecule 3: Proteasome subunit beta

Chain U:



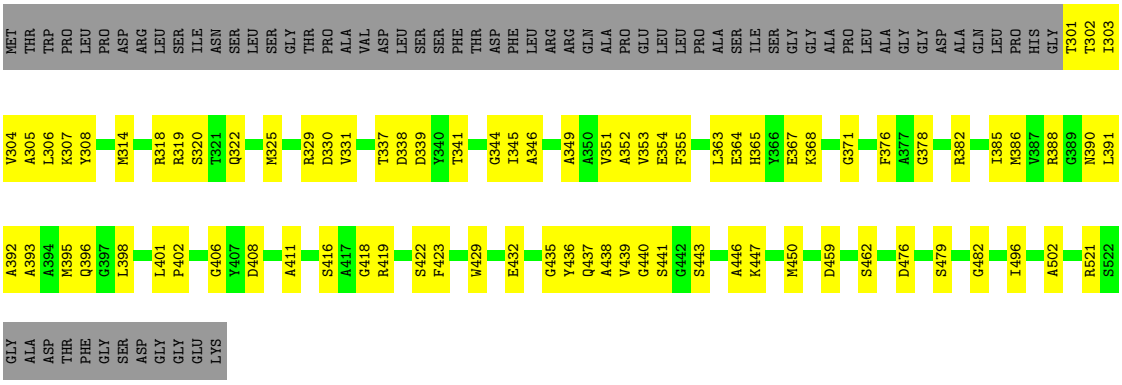
• Molecule 3: Proteasome subunit beta

Chain V:



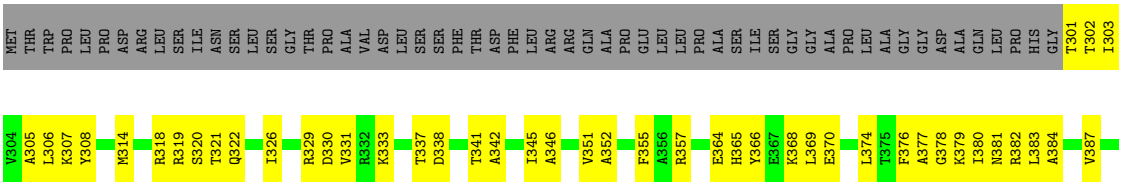
• Molecule 3: Proteasome subunit beta

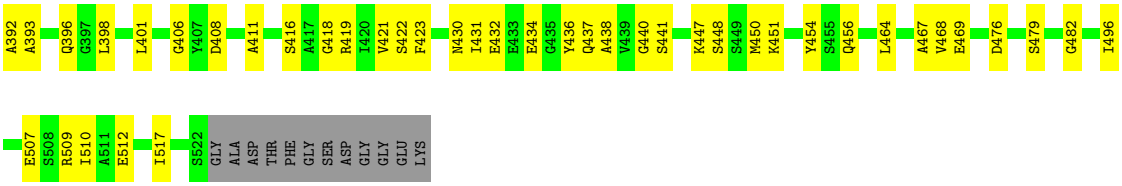
Chain W:



• Molecule 3: Proteasome subunit beta

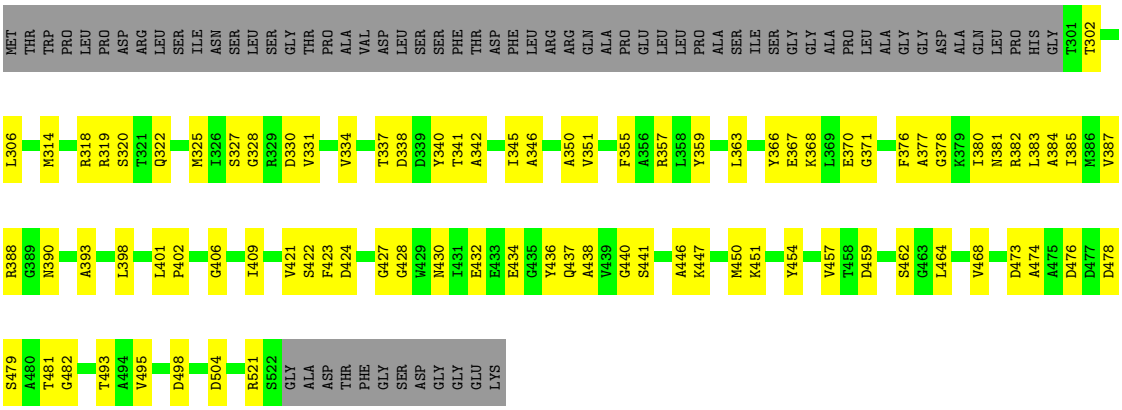
Chain X:





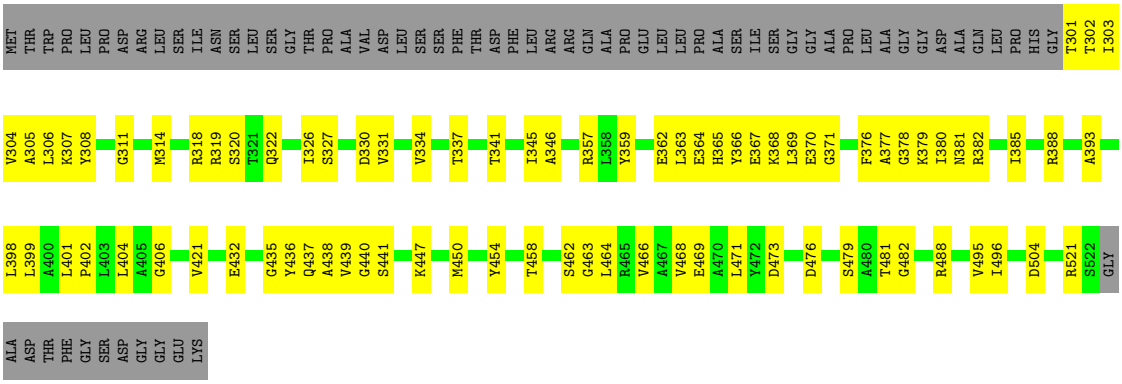
• Molecule 3: Proteasome subunit beta

Chain Y:



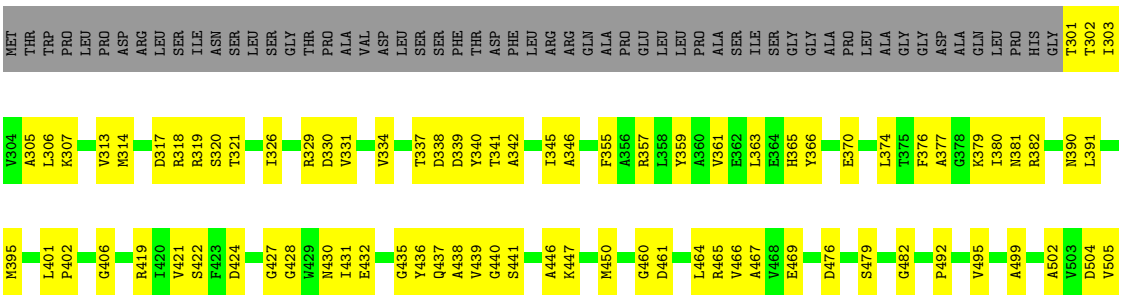
• Molecule 3: Proteasome subunit beta

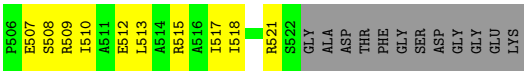
Chain Z:



• Molecule 3: Proteasome subunit beta

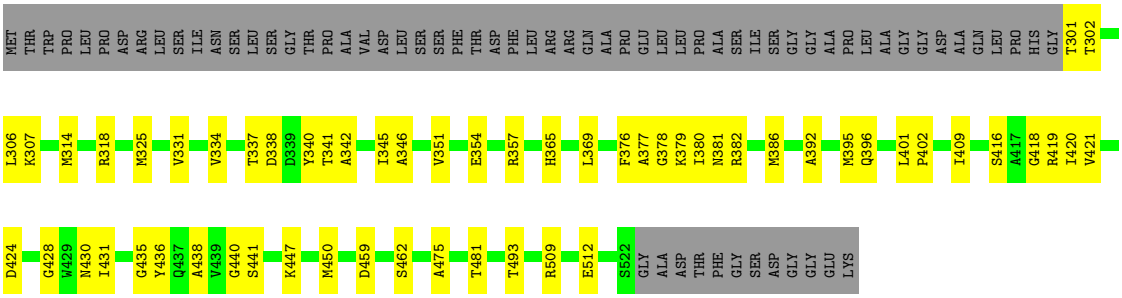
Chain a:





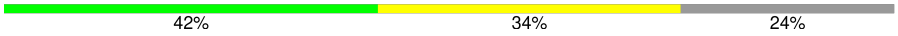
• Molecule 3: Proteasome subunit beta

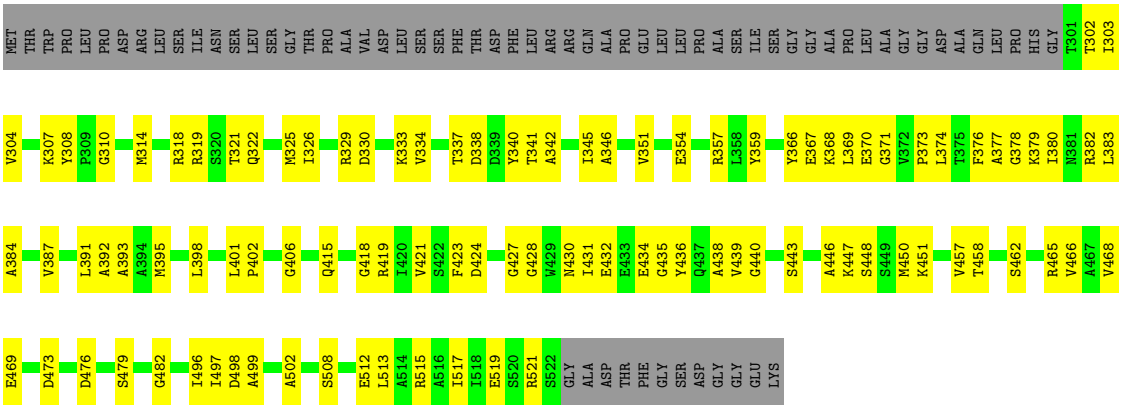
Chain b:



• Molecule 3: Proteasome subunit beta

Chain c:





• Molecule 4: Proteasome-associated ATPase

Chain d:

• Molecule 4: Proteasome-associated ATPase

Chain e:

• Molecule 4: Proteasome-associated ATPase

Chain f:

• Molecule 4: Proteasome-associated ATPase

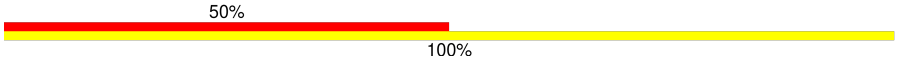
Chain g:

• Molecule 4: Proteasome-associated ATPase

Chain h:

• Molecule 4: Proteasome-associated ATPase

Chain i:



• Molecule 4: Proteasome-associated ATPase

Chain j:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	508000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.32	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.140	Depositor
Minimum map value	-1.162	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.193	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	423.936, 423.936, 423.936	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.312, 3.312, 3.312	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.28	0/3808	0.46	0/5150
1	B	0.21	0/3766	0.44	0/5092
1	C	0.22	0/3706	0.44	2/5011 (0.0%)
1	D	0.20	0/3651	0.45	0/4933
1	E	0.21	0/3655	0.45	0/4939
1	F	0.22	0/3646	0.46	0/4929
2	G	0.27	0/1683	0.43	0/2274
2	H	0.30	0/1683	0.47	0/2274
2	I	0.32	0/1683	0.51	0/2274
2	J	0.32	0/1683	0.47	0/2274
2	K	0.38	0/1683	0.52	0/2274
2	L	0.33	0/1683	0.50	0/2274
2	M	0.38	0/1683	0.53	0/2274
2	N	0.24	0/1683	0.38	0/2274
2	O	0.37	0/1683	0.53	0/2274
2	k	0.30	0/1683	0.45	0/2274
2	l	0.39	0/1683	0.54	0/2274
2	m	0.45	0/1683	0.59	0/2274
2	n	0.25	0/1683	0.41	0/2274
2	o	0.34	0/1683	0.48	0/2274
3	P	0.45	0/1662	0.55	0/2254
3	Q	0.20	0/1662	0.35	0/2254
3	R	0.24	0/1662	0.44	0/2254
3	S	0.27	0/1662	0.45	1/2254 (0.0%)
3	T	0.20	0/1660	0.35	0/2251
3	U	0.21	0/1662	0.38	0/2254
3	V	0.34	0/1662	0.45	0/2254
3	W	0.38	0/1662	0.53	0/2254
3	X	0.20	0/1662	0.39	0/2254
3	Y	0.27	0/1662	0.44	0/2254
3	Z	0.40	0/1662	0.49	0/2254
3	a	0.34	0/1662	0.48	0/2254
3	b	0.31	0/1662	0.45	0/2254
3	c	0.32	0/1662	0.46	0/2254

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
4	d	0.08	0/34	0.15	0/43
4	e	0.12	0/34	0.29	0/43
4	f	0.12	0/34	0.31	0/43
4	g	0.14	0/34	0.48	0/43
4	h	0.12	0/34	0.35	0/43
4	i	0.10	0/34	0.33	0/43
4	j	0.10	0/34	0.34	0/43
All	All	0.29	0/69298	0.46	3/93744 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	S	480	ALA	N-CA-C	-6.31	106.55	114.56
1	C	296	VAL	CA-C-N	5.42	123.65	120.24
1	C	296	VAL	C-N-CA	5.42	123.65	120.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3747	0	3755	125	0
1	B	3707	0	3718	143	0
1	C	3649	0	3644	92	0
1	D	3593	0	3607	123	0
1	E	3597	0	3610	139	0
1	F	3589	0	3606	142	0
2	G	1658	0	1659	90	0
2	H	1658	0	1659	71	0
2	I	1658	0	1659	75	0
2	J	1658	0	1659	83	0
2	K	1658	0	1659	77	0
2	L	1658	0	1659	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	1658	0	1659	82	0
2	N	1658	0	1659	74	0
2	O	1658	0	1659	65	0
2	k	1658	0	1659	82	0
2	l	1658	0	1659	69	0
2	m	1658	0	1659	70	0
2	n	1658	0	1659	74	0
2	o	1658	0	1659	67	0
3	P	1638	0	1630	51	0
3	Q	1638	0	1630	59	0
3	R	1638	0	1630	68	0
3	S	1638	0	1630	81	0
3	T	1636	0	1625	70	0
3	U	1638	0	1630	69	0
3	V	1638	0	1630	47	0
3	W	1638	0	1630	68	0
3	X	1638	0	1630	66	0
3	Y	1638	0	1630	66	0
3	Z	1638	0	1630	65	0
3	a	1638	0	1630	62	0
3	b	1638	0	1630	41	0
3	c	1638	0	1630	72	0
4	d	34	0	30	4	0
4	e	34	0	30	3	0
4	f	34	0	30	3	0
4	g	34	0	30	5	0
4	h	34	0	30	5	0
4	i	34	0	30	7	0
4	j	34	0	30	4	0
All	All	68262	0	68191	2527	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 19.

All (2527) 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)
2:N:46:PRO:HA	2:N:207:SER:HA	1.30	1.11
2:O:46:PRO:HA	2:O:207:SER:HA	1.42	1.01
3:P:436:TYR:HB2	3:P:450:MET:HE2	1.43	1.01
2:J:46:PRO:HA	2:J:207:SER:HA	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:436:TYR:HB2	3:S:450:MET:HE2	1.49	0.95
2:m:46:PRO:HA	2:m:207:SER:HA	1.48	0.94
1:A:216:LYS:HB3	1:A:228:GLU:HB3	1.52	0.91
2:n:139:TYR:HB3	2:n:147:ILE:HD11	1.53	0.91
1:B:104:GLY:HA2	1:B:114:ARG:HH12	1.36	0.90
1:E:390:MET:HE2	1:E:455:ILE:HG12	1.51	0.90
3:R:392:ALA:HA	3:R:395:MET:HE3	1.59	0.85
1:B:296:VAL:HG12	1:B:297:VAL:H	1.39	0.85
1:E:321:ARG:HE	1:E:324:MET:HE1	1.42	0.84
2:H:124:VAL:HB	2:H:139:TYR:HB2	1.59	0.84
1:C:327:PRO:HB3	1:D:467:ASN:HB3	1.59	0.84
2:H:56:LEU:HG	2:H:62:PHE:HB2	1.59	0.83
1:F:145:LEU:HD21	1:F:256:ILE:HG22	1.59	0.83
3:S:396:GLN:HE22	3:S:398:LEU:HD13	1.44	0.83
1:F:270:VAL:HB	1:F:313:VAL:HG22	1.60	0.82
2:G:139:TYR:HB3	2:G:147:ILE:HD11	1.62	0.81
1:A:401:GLU:HB2	1:A:491:LEU:HD11	1.61	0.81
1:F:386:VAL:HG13	1:F:455:ILE:HD11	1.63	0.81
2:k:107:LEU:HD13	2:k:110:ILE:HD11	1.64	0.79
2:k:110:ILE:HD12	2:k:118:TYR:HB2	1.63	0.79
2:K:46:PRO:HA	2:K:207:SER:HA	1.62	0.79
3:V:359:TYR:HB2	3:V:386:MET:HE1	1.62	0.79
2:G:56:LEU:HG	2:G:62:PHE:HB2	1.65	0.78
3:X:418:GLY:O	3:X:419:ARG:NH1	2.16	0.78
3:Q:320:SER:HB3	3:Q:331:VAL:HG21	1.66	0.78
3:U:302:THR:HA	3:U:440:GLY:HA3	1.65	0.78
1:E:237:LYS:HG2	1:E:239:PRO:HD2	1.65	0.77
1:E:101:LEU:HD22	1:E:115:PRO:HB2	1.64	0.77
3:T:345:ILE:HG12	3:T:402:PRO:HB3	1.67	0.77
2:O:122:LEU:HD11	2:O:141:ILE:HD12	1.66	0.77
2:M:104:ALA:HA	2:M:141:ILE:HD13	1.67	0.76
2:I:139:TYR:HB3	2:I:147:ILE:HD11	1.68	0.76
1:F:321:ARG:HG3	1:F:324:MET:HE1	1.67	0.76
1:A:382:MET:HE2	1:A:451:LEU:HD12	1.68	0.76
3:U:345:ILE:HG12	3:U:402:PRO:HB3	1.68	0.76
2:l:140:ARG:NH1	2:l:156:MET:SD	2.59	0.76
2:H:28:LYS:HZ2	2:H:46:PRO:HD2	1.49	0.76
2:O:128:ALA:HB2	2:O:134:LYS:HB3	1.68	0.75
1:A:116:ARG:HH21	1:A:262:GLU:HG2	1.49	0.75
2:o:32:ALA:HB3	2:o:154:VAL:HB	1.69	0.75
2:H:46:PRO:HA	2:H:207:SER:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:LYS:HB3	1:F:183:ARG:HH12	1.51	0.75
1:B:452:LEU:HA	1:B:455:ILE:HD12	1.67	0.75
2:n:121:GLU:HG2	2:n:156:MET:HE2	1.67	0.75
3:b:392:ALA:O	3:b:396:GLN:NE2	2.20	0.75
2:K:107:LEU:HD13	2:K:110:ILE:HD11	1.69	0.75
3:P:476:ASP:O	3:c:329:ARG:NH2	2.20	0.74
2:m:56:LEU:HG	2:m:62:PHE:HB2	1.69	0.74
2:m:64:ALA:HA	2:m:122:LEU:HA	1.69	0.74
2:K:121:GLU:HG2	2:K:156:MET:HE2	1.70	0.74
3:R:461:ASP:OD1	3:R:509:ARG:NH2	2.21	0.74
3:V:329:ARG:NH2	3:W:476:ASP:O	2.20	0.74
3:V:506:PRO:HD2	3:V:509:ARG:HH21	1.50	0.74
1:D:164:GLN:HG2	1:D:341:ILE:HD13	1.68	0.74
3:X:346:ALA:HB3	3:X:401:LEU:HB2	1.70	0.74
2:I:43:ALA:HB3	2:I:209:GLU:HB3	1.70	0.74
1:F:191:LYS:HZ3	1:F:308:GLU:HB2	1.51	0.74
1:F:175:PRO:HB3	1:F:189:PRO:HB3	1.70	0.73
3:Z:307:LYS:NZ	3:Z:308:TYR:O	2.21	0.73
2:M:138:LEU:HB2	2:M:150:GLU:HB2	1.69	0.73
3:Q:337:THR:H	3:Q:342:ALA:HA	1.53	0.73
3:R:321:THR:HG22	3:R:326:ILE:HA	1.70	0.73
2:K:53:ILE:O	2:K:224:ARG:NH2	2.20	0.73
2:k:46:PRO:HA	2:k:207:SER:HA	1.68	0.73
2:m:53:ILE:O	2:m:224:ARG:NH2	2.21	0.73
2:G:28:LYS:HD2	2:G:44:GLU:HG3	1.70	0.73
3:V:319:ARG:NH1	3:V:479:SER:O	2.21	0.73
3:X:302:THR:HA	3:X:440:GLY:HA3	1.70	0.73
2:N:92:ARG:NH2	2:N:132:GLU:OE2	2.22	0.73
3:R:307:LYS:HE2	3:R:435:GLY:HA2	1.70	0.73
3:W:392:ALA:O	3:W:396:GLN:NE2	2.21	0.73
2:G:16:ARG:NH2	2:G:114:GLN:O	2.22	0.73
2:N:217:ARG:NE	2:N:220:ARG:O	2.21	0.73
3:Z:302:THR:HA	3:Z:440:GLY:HA3	1.71	0.73
2:N:107:LEU:HD13	2:N:110:ILE:HD11	1.71	0.72
3:Q:319:ARG:NH1	3:Q:479:SER:O	2.22	0.72
1:F:192:GLY:HA3	1:F:335:LEU:HA	1.69	0.72
2:L:45:ASN:O	2:L:48:ARG:NH2	2.22	0.72
2:l:214:ASP:HB3	2:l:217:ARG:HG2	1.70	0.72
3:S:320:SER:HB3	3:S:331:VAL:HG21	1.70	0.72
3:W:418:GLY:O	3:W:419:ARG:NH1	2.23	0.72
2:M:105:GLN:HG3	2:N:69:ASN:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:n:67:LYS:HE2	4:d:171:GLY:HA3	1.71	0.72
3:Q:302:THR:HA	3:Q:440:GLY:HA3	1.71	0.72
1:C:402:VAL:HG22	1:C:488:ILE:HG12	1.72	0.72
2:M:107:LEU:HD13	2:M:110:ILE:HD11	1.71	0.72
1:A:3:SER:HB3	1:A:46:ARG:HD3	1.70	0.71
1:A:402:VAL:HG22	1:A:488:ILE:HG12	1.71	0.71
3:T:329:ARG:NH2	3:Y:476:ASP:O	2.23	0.71
3:S:345:ILE:HA	3:S:402:PRO:HA	1.71	0.71
2:l:56:LEU:HG	2:l:62:PHE:HB2	1.71	0.71
2:H:139:TYR:HB3	2:H:147:ILE:HD11	1.72	0.71
2:K:88:ALA:O	3:Z:381:ASN:ND2	2.22	0.71
1:C:189:PRO:O	1:C:191:LYS:NZ	2.24	0.71
2:L:70:GLU:OE2	2:L:116:LYS:NZ	2.24	0.71
1:F:179:LYS:HB3	1:F:183:ARG:NH1	2.05	0.71
2:l:140:ARG:NH2	2:l:150:GLU:OE1	2.20	0.71
3:Q:392:ALA:O	3:Q:396:GLN:NE2	2.23	0.71
3:U:345:ILE:HA	3:U:402:PRO:HA	1.70	0.71
1:A:203:LYS:H	1:A:206:ILE:HD13	1.55	0.71
3:a:302:THR:HA	3:a:440:GLY:HA3	1.72	0.71
3:c:424:ASP:OD1	3:c:428:GLY:N	2.23	0.71
3:T:424:ASP:OD1	3:T:428:GLY:N	2.24	0.71
1:B:77:ARG:NH1	1:C:135:GLU:OE2	2.23	0.71
1:B:438:VAL:HG22	1:B:444:PRO:HA	1.70	0.71
2:J:110:ILE:HB	2:J:114:GLN:HE22	1.54	0.71
3:b:418:GLY:O	3:b:419:ARG:NH1	2.24	0.71
1:B:402:VAL:HG22	1:B:488:ILE:HG12	1.73	0.70
3:V:418:GLY:O	3:V:419:ARG:NH1	2.24	0.70
3:X:421:VAL:HG22	3:X:431:ILE:HG12	1.73	0.70
3:c:319:ARG:NH1	3:c:479:SER:O	2.24	0.70
1:B:464:ASP:O	1:B:501:ARG:NH1	2.24	0.70
2:l:139:TYR:HB3	2:l:147:ILE:HD11	1.72	0.70
2:K:22:LYS:HB3	2:K:26:ARG:HH22	1.55	0.70
3:U:505:VAL:HG13	3:U:509:ARG:HH21	1.56	0.70
1:B:353:TYR:CE1	1:B:423:ILE:HG23	2.26	0.70
2:l:87:TYR:O	3:Q:357:ARG:NH2	2.23	0.70
2:G:44:GLU:HA	2:G:208:LEU:HD23	1.72	0.70
2:n:45:ASN:O	2:n:48:ARG:NH2	2.24	0.70
2:H:53:ILE:O	2:H:224:ARG:NH2	2.25	0.70
3:U:329:ARG:NH2	3:X:476:ASP:O	2.25	0.70
2:H:16:ARG:NH1	2:H:114:GLN:O	2.24	0.70
2:L:24:ILE:HD13	2:L:121:GLU:HG3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:314:MET:HE1	3:T:334:VAL:HG13	1.73	0.70
2:n:53:ILE:O	2:n:224:ARG:NH2	2.22	0.69
2:o:70:GLU:OE2	2:o:116:LYS:NZ	2.25	0.69
2:G:66:GLY:HA3	2:G:120:VAL:HG12	1.73	0.69
2:I:19:LEU:HD21	2:I:116:LYS:HE2	1.74	0.69
3:U:338:ASP:OD1	3:U:341:THR:N	2.25	0.69
3:a:424:ASP:OD1	3:a:428:GLY:N	2.24	0.69
1:A:382:MET:HE1	1:A:448:ILE:HA	1.72	0.69
1:D:305:ASP:HA	1:D:308:GLU:HG2	1.75	0.69
3:W:446:ALA:O	3:W:450:MET:HG2	1.92	0.69
3:c:321:THR:HG22	3:c:326:ILE:HA	1.74	0.69
2:K:128:ALA:HB2	2:K:134:LYS:HB3	1.74	0.69
3:R:329:ARG:NH2	3:a:476:ASP:O	2.24	0.69
3:Y:424:ASP:OD1	3:Y:428:GLY:N	2.25	0.69
1:F:208:LYS:HG2	1:F:233:PHE:HZ	1.56	0.69
2:o:88:ALA:O	3:U:381:ASN:ND2	2.26	0.69
2:L:161:GLU:O	2:L:165:ASN:ND2	2.26	0.69
3:S:345:ILE:HG12	3:S:402:PRO:HB3	1.75	0.69
3:X:416:SER:O	3:X:419:ARG:NH1	2.23	0.69
2:N:17:SER:OG	2:N:21:ARG:NH2	2.25	0.69
3:S:307:LYS:NZ	3:S:308:TYR:O	2.24	0.69
3:W:416:SER:O	3:W:419:ARG:NH1	2.22	0.69
3:X:376:PHE:HA	3:X:379:LYS:HE2	1.75	0.69
2:J:63:ALA:HB3	2:J:123:CYS:HB3	1.75	0.68
2:K:60:VAL:HG11	2:K:99:LEU:HD21	1.75	0.68
3:P:418:GLY:O	3:P:419:ARG:NH1	2.25	0.68
3:Y:319:ARG:NH1	3:Y:479:SER:O	2.25	0.68
2:M:46:PRO:HA	2:M:207:SER:HA	1.75	0.68
2:M:114:GLN:HE21	2:M:117:PRO:HA	1.57	0.68
2:N:212:VAL:HG22	2:N:225:ILE:HD11	1.75	0.68
3:V:345:ILE:HA	3:V:402:PRO:HA	1.75	0.68
1:C:296:VAL:HG12	1:C:298:PRO:HD3	1.75	0.68
2:M:21:ARG:HE	2:M:22:LYS:HZ2	1.40	0.68
3:R:302:THR:HA	3:R:440:GLY:HA3	1.74	0.68
3:S:364:GLU:O	3:S:368:LYS:HG3	1.93	0.68
3:T:473:ASP:OD1	3:T:521:ARG:NH1	2.25	0.68
3:W:302:THR:HA	3:W:440:GLY:HA3	1.73	0.68
2:L:28:LYS:HB3	2:L:44:GLU:HG3	1.75	0.68
2:m:70:GLU:OE2	2:m:116:LYS:NZ	2.26	0.68
2:N:135:ARG:HH22	2:N:152:HIS:HA	1.58	0.68
3:R:418:GLY:O	3:R:419:ARG:NH1	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:LYS:HE2	1:F:342:GLU:HB2	1.76	0.68
1:F:387:VAL:HA	1:F:390:MET:HG2	1.74	0.68
3:R:424:ASP:OD1	3:R:428:GLY:N	2.27	0.68
3:X:306:LEU:HA	3:X:436:TYR:HA	1.74	0.68
2:o:210:VAL:HG11	2:o:230:LEU:HD13	1.76	0.68
2:J:107:LEU:HD13	2:J:110:ILE:HD11	1.75	0.68
3:a:307:LYS:HE3	3:a:435:GLY:HA2	1.74	0.68
1:D:96:LEU:HD22	1:D:118:LEU:HD11	1.76	0.68
3:R:319:ARG:NH1	3:R:479:SER:O	2.25	0.68
3:Z:393:ALA:HB1	3:Z:398:LEU:HB2	1.76	0.68
3:R:416:SER:O	3:R:419:ARG:NH1	2.23	0.68
3:T:319:ARG:NH1	3:T:479:SER:O	2.27	0.67
1:A:77:ARG:NH1	1:B:61:ALA:O	2.26	0.67
1:C:172:VAL:HG12	1:C:214:LEU:HD21	1.74	0.67
2:m:128:ALA:HB2	2:m:134:LYS:HB3	1.76	0.67
3:W:436:TYR:HB2	3:W:450:MET:HE2	1.76	0.67
3:Z:345:ILE:HA	3:Z:402:PRO:HA	1.75	0.67
1:B:173:GLU:HA	1:B:214:LEU:HD13	1.77	0.67
1:D:9:LEU:HD21	1:D:20:PHE:HB2	1.76	0.67
3:T:418:GLY:O	3:T:419:ARG:NH1	2.27	0.67
3:T:337:THR:H	3:T:342:ALA:HA	1.59	0.67
3:a:319:ARG:NH1	3:a:479:SER:O	2.27	0.67
1:B:72:LEU:HD23	1:B:74:ASP:H	1.59	0.67
2:o:135:ARG:NH2	2:o:151:PRO:O	2.27	0.67
2:H:66:GLY:HA3	2:H:120:VAL:HG22	1.76	0.67
2:M:128:ALA:HB2	2:M:134:LYS:HG3	1.75	0.67
2:K:217:ARG:NH1	2:K:222:PHE:O	2.27	0.67
3:P:451:LYS:HE2	3:W:521:ARG:HH12	1.60	0.67
3:S:322:GLN:OE1	3:S:322:GLN:N	2.28	0.67
3:S:329:ARG:NH2	3:Z:476:ASP:O	2.28	0.67
3:Z:341:THR:HG23	3:Z:404:LEU:HD11	1.76	0.67
3:b:302:THR:HA	3:b:440:GLY:HA3	1.77	0.67
2:o:30:VAL:HB	2:o:156:MET:HB2	1.76	0.67
3:c:374:LEU:O	3:c:379:LYS:NZ	2.28	0.67
1:E:72:LEU:HD12	1:E:74:ASP:H	1.58	0.67
3:Q:418:GLY:O	3:Q:419:ARG:NH1	2.28	0.67
3:Z:473:ASP:OD1	3:Z:521:ARG:NH1	2.25	0.66
2:H:128:ALA:HB2	2:H:134:LYS:HB3	1.76	0.66
2:J:66:GLY:HA3	2:J:120:VAL:HG12	1.77	0.66
3:Z:319:ARG:NH1	3:Z:479:SER:O	2.28	0.66
3:b:338:ASP:OD1	3:b:341:THR:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:479:SER:HB3	3:Z:326:ILE:HD11	1.76	0.66
2:G:88:ALA:O	3:V:381:ASN:ND2	2.27	0.66
2:J:112:THR:HG22	2:K:116:LYS:HD2	1.75	0.66
2:L:45:ASN:ND2	2:L:50:LEU:O	2.23	0.66
2:o:128:ALA:HB2	2:o:134:LYS:HB3	1.76	0.66
3:X:392:ALA:O	3:X:396:GLN:NE2	2.28	0.66
1:A:165:ILE:HA	1:A:168:ILE:HD12	1.78	0.66
1:E:438:VAL:HG22	1:E:444:PRO:HA	1.77	0.66
2:n:128:ALA:HB1	2:n:132:GLU:HG3	1.78	0.66
2:n:146:SER:HA	4:e:172:GLN:HB2	1.78	0.66
2:H:71:PHE:HB3	2:H:120:VAL:HG11	1.77	0.66
1:F:200:GLY:HA3	1:F:419:SER:HB2	1.77	0.66
3:P:322:GLN:OE1	3:P:322:GLN:N	2.29	0.66
3:X:374:LEU:O	3:X:379:LYS:NZ	2.29	0.66
1:D:24:ARG:NH1	1:E:21:THR:OG1	2.29	0.66
1:E:403:THR:HB	1:E:487:TYR:HB3	1.77	0.66
2:k:70:GLU:HB3	2:k:118:TYR:HD2	1.61	0.66
2:M:53:ILE:O	2:M:224:ARG:NH2	2.21	0.66
3:W:303:ILE:HG21	3:W:344:GLY:HA3	1.78	0.66
2:k:68:PHE:HA	2:k:71:PHE:CZ	2.31	0.66
2:k:80:GLN:OE1	3:W:365:HIS:NE2	2.27	0.66
2:J:205:VAL:HG13	2:J:230:LEU:HD22	1.78	0.66
3:c:376:PHE:HA	3:c:379:LYS:HE2	1.78	0.66
2:O:121:GLU:HG3	2:O:156:MET:HE2	1.76	0.66
2:k:20:ALA:HA	2:k:119:GLU:HG3	1.78	0.66
2:I:128:ALA:HB2	2:I:134:LYS:HB3	1.77	0.66
3:Q:322:GLN:OE1	3:Q:322:GLN:N	2.29	0.66
1:B:176:PHE:HE2	1:B:269:PRO:HB3	1.62	0.65
1:F:382:MET:HE2	1:F:451:LEU:HD12	1.76	0.65
3:Z:318:ARG:NH2	3:Z:330:ASP:O	2.29	0.65
1:C:458:GLU:O	1:C:462:ASN:ND2	2.29	0.65
2:K:30:VAL:HG13	2:K:43:ALA:HB2	1.78	0.65
1:E:252:HIS:HA	1:E:255:LEU:HD23	1.79	0.65
3:X:301:THR:O	3:X:441:SER:N	2.29	0.65
1:A:501:ARG:NH2	1:F:323:ASP:OD1	2.29	0.65
2:m:63:ALA:HB3	2:m:123:CYS:HB3	1.77	0.65
2:M:116:LYS:NZ	2:M:117:PRO:O	2.26	0.65
2:N:121:GLU:HG2	2:N:156:MET:HE2	1.78	0.65
3:P:345:ILE:HA	3:P:402:PRO:HA	1.78	0.65
2:o:210:VAL:HG13	2:o:225:ILE:HB	1.79	0.65
2:J:83:ASP:OD2	3:X:365:HIS:ND1	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:48:ARG:HH12	2:L:207:SER:H	1.44	0.65
3:S:302:THR:HA	3:S:440:GLY:HA3	1.78	0.65
3:V:302:THR:HA	3:V:440:GLY:HA3	1.78	0.65
3:c:447:LYS:HD2	3:c:450:MET:HE2	1.79	0.65
2:L:135:ARG:NH2	2:L:151:PRO:O	2.30	0.65
2:m:205:VAL:HG13	2:m:230:LEU:HG	1.79	0.65
2:I:56:LEU:HG	2:I:62:PHE:HB2	1.78	0.65
3:b:307:LYS:HE2	3:b:435:GLY:HA2	1.78	0.65
2:O:135:ARG:HH22	2:O:152:HIS:CE1	2.14	0.65
1:C:72:LEU:HD23	1:C:79:LEU:HB2	1.78	0.65
3:Q:432:GLU:HG3	3:Q:437:GLN:HB2	1.79	0.65
1:D:363:VAL:HB	1:D:375:ARG:HH11	1.62	0.65
2:m:11:GLN:OE1	2:m:14:ARG:NH2	2.29	0.65
2:m:217:ARG:HH12	2:m:223:ARG:HB2	1.63	0.64
2:n:46:PRO:HA	2:n:207:SER:HA	1.80	0.64
2:o:41:PHE:HB3	2:o:53:ILE:HD13	1.79	0.64
2:I:71:PHE:HB3	2:I:120:VAL:HG21	1.80	0.64
3:Q:345:ILE:HA	3:Q:402:PRO:HA	1.77	0.64
3:Y:447:LYS:HA	3:Y:450:MET:SD	2.37	0.64
3:S:418:GLY:O	3:S:419:ARG:NH1	2.29	0.64
3:X:319:ARG:NH1	3:X:479:SER:O	2.29	0.64
3:T:507:GLU:HA	3:T:510:ILE:HD12	1.79	0.64
1:D:362:PRO:O	1:D:446:LEU:N	2.29	0.64
3:U:402:PRO:HG2	3:U:423:PHE:HD2	1.61	0.64
3:V:338:ASP:OD1	3:V:341:THR:N	2.30	0.64
2:J:182:ARG:HH12	2:J:234:LEU:HA	1.62	0.64
2:M:134:LYS:NZ	2:M:137:GLU:OE1	2.31	0.64
3:c:391:LEU:HG	3:c:395:MET:HE2	1.78	0.64
1:F:296:VAL:HG13	1:F:298:PRO:HD2	1.79	0.64
1:F:452:LEU:HA	1:F:455:ILE:HD12	1.79	0.64
1:D:323:ASP:OD1	1:E:501:ARG:NH2	2.31	0.64
1:E:296:VAL:HG12	1:E:298:PRO:HD3	1.80	0.64
1:F:438:VAL:HG22	1:F:444:PRO:HA	1.79	0.64
2:G:10:GLU:OE1	2:G:14:ARG:NH1	2.31	0.64
2:G:128:ALA:HB2	2:G:134:LYS:HB3	1.78	0.64
2:H:68:PHE:HA	2:H:71:PHE:CZ	2.31	0.64
2:m:16:ARG:NH2	2:m:114:GLN:O	2.31	0.64
2:n:140:ARG:NH1	2:n:155:VAL:O	2.30	0.64
1:E:9:LEU:HD21	1:E:20:PHE:HB2	1.80	0.64
3:c:302:THR:HA	3:c:440:GLY:HA3	1.78	0.64
2:I:59:ARG:NH2	2:I:215:ALA:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:217:ARG:HH12	2:L:223:ARG:HB2	1.62	0.63
3:c:377:ALA:HA	3:c:380:ILE:HD12	1.80	0.63
1:C:9:LEU:HD21	1:C:20:PHE:HB2	1.79	0.63
1:C:333:GLY:N	1:C:336:ASP:OD2	2.28	0.63
2:m:142:THR:HB	2:m:146:SER:HB3	1.80	0.63
2:o:140:ARG:O	2:o:148:ALA:N	2.31	0.63
3:W:301:THR:N	3:W:441:SER:HG	1.96	0.63
3:X:377:ALA:HA	3:X:380:ILE:HD12	1.80	0.63
3:U:307:LYS:NZ	3:U:308:TYR:O	2.23	0.63
1:A:438:VAL:HG22	1:A:444:PRO:HA	1.78	0.63
3:R:434:GLU:OE2	3:R:447:LYS:NZ	2.31	0.63
1:F:257:PHE:HE1	1:F:272:VAL:HG11	1.61	0.63
2:l:161:GLU:O	2:l:165:ASN:ND2	2.31	0.63
2:n:68:PHE:N	4:d:172:GLN:O	2.25	0.63
1:E:88:ARG:HH12	1:E:126:VAL:HG21	1.64	0.63
2:k:128:ALA:HB2	2:k:134:LYS:HB3	1.79	0.63
2:o:139:TYR:HB3	2:o:147:ILE:HD11	1.79	0.63
2:L:150:GLU:HG3	2:L:154:VAL:HG22	1.79	0.63
3:U:322:GLN:N	3:U:322:GLN:OE1	2.32	0.63
3:Y:320:SER:HB2	3:Y:331:VAL:HG21	1.80	0.63
3:Z:438:ALA:HB3	3:Z:447:LYS:HG2	1.81	0.63
3:a:377:ALA:HA	3:a:380:ILE:HD12	1.80	0.63
1:B:27:ARG:HD3	1:C:46:ARG:HD2	1.80	0.63
2:n:56:LEU:HG	2:n:62:PHE:HB2	1.80	0.63
2:G:144:ASP:OD2	4:g:171:GLY:N	2.31	0.63
2:L:56:LEU:HB2	2:L:60:VAL:HG12	1.81	0.63
3:b:337:THR:H	3:b:342:ALA:HA	1.63	0.63
1:D:175:PRO:HB3	1:D:189:PRO:HB3	1.80	0.62
1:E:69:ARG:HA	1:E:251:ARG:HH22	1.64	0.62
2:k:83:ASP:OD2	3:W:365:HIS:ND1	2.32	0.62
2:K:68:PHE:HA	2:K:71:PHE:CZ	2.34	0.62
2:N:163:ILE:HD13	2:N:188:LEU:HD12	1.81	0.62
3:P:424:ASP:OD1	3:P:428:GLY:N	2.31	0.62
3:W:322:GLN:OE1	3:W:322:GLN:N	2.32	0.62
3:Y:377:ALA:HA	3:Y:380:ILE:HD12	1.82	0.62
2:o:97:ARG:HD2	2:G:49:SER:HB2	1.80	0.62
2:o:140:ARG:HD3	2:o:154:VAL:HG13	1.80	0.62
3:V:424:ASP:OD1	3:V:428:GLY:N	2.31	0.62
1:E:88:ARG:HH21	1:E:128:THR:HA	1.64	0.62
2:o:68:PHE:HA	2:o:71:PHE:CZ	2.35	0.62
2:G:56:LEU:HB2	2:G:60:VAL:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:42:VAL:HG22	2:M:210:VAL:HG22	1.80	0.62
2:M:155:VAL:HG21	2:M:164:ALA:HA	1.81	0.62
3:V:464:LEU:HD21	3:V:496:ILE:HD11	1.81	0.62
1:A:277:MET:HE2	1:A:317:GLY:HA3	1.82	0.62
1:B:322:GLU:OE2	1:C:501:ARG:NH2	2.32	0.62
3:S:301:THR:N	3:S:441:SER:HG	1.97	0.62
3:Z:376:PHE:HA	3:Z:379:LYS:HE2	1.81	0.62
1:D:24:ARG:NH1	1:E:5:TYR:O	2.20	0.62
2:K:165:ASN:HA	2:K:168:LYS:HE3	1.82	0.62
3:T:374:LEU:O	3:T:379:LYS:NZ	2.32	0.62
3:a:338:ASP:OD1	3:a:341:THR:N	2.30	0.62
2:O:42:VAL:HG22	2:O:210:VAL:HG22	1.80	0.62
2:O:107:LEU:HA	2:O:110:ILE:HG22	1.81	0.62
2:k:55:GLU:OE1	3:W:368:LYS:NZ	2.29	0.62
2:l:18:GLU:HA	2:l:21:ARG:HG2	1.82	0.62
3:S:359:TYR:CE1	3:S:383:LEU:HB3	2.35	0.62
3:W:355:PHE:HZ	3:W:390:ASN:HB2	1.65	0.62
3:Y:473:ASP:OD1	3:Y:521:ARG:NH1	2.24	0.62
1:B:338:LYS:HD3	1:C:465:LEU:HD23	1.80	0.62
1:E:390:MET:HE1	1:E:426:VAL:HG21	1.80	0.62
3:Y:302:THR:HA	3:Y:440:GLY:HA3	1.80	0.62
1:A:87:GLU:HB2	1:B:65:ILE:HB	1.80	0.62
1:A:298:PRO:HA	1:A:301:LEU:HD13	1.82	0.62
1:D:476:ARG:HE	1:E:499:ALA:HB3	1.64	0.62
2:l:56:LEU:HB2	2:l:60:VAL:HG12	1.81	0.62
2:L:88:ALA:O	3:a:381:ASN:ND2	2.33	0.62
2:N:97:ARG:NH1	2:N:137:GLU:OE2	2.33	0.62
3:a:346:ALA:O	3:a:401:LEU:N	2.23	0.62
3:U:484:PRO:HB3	3:U:491:PHE:HD1	1.65	0.62
3:X:346:ALA:O	3:X:401:LEU:N	2.30	0.62
3:a:446:ALA:O	3:a:450:MET:HG3	1.99	0.62
1:D:408:ASP:OD2	1:D:481:LYS:NZ	2.31	0.61
2:m:109:THR:O	2:m:113:GLU:HG3	2.00	0.61
2:H:146:SER:HA	4:h:172:GLN:HB2	1.81	0.61
2:J:121:GLU:OE2	2:J:140:ARG:NH1	2.29	0.61
3:S:446:ALA:O	3:S:450:MET:HG3	1.99	0.61
3:S:451:LYS:HE2	3:a:521:ARG:HH12	1.64	0.61
3:a:321:THR:HG22	3:a:326:ILE:HA	1.81	0.61
1:C:329:ILE:HG12	1:C:335:LEU:HD13	1.83	0.61
2:n:16:ARG:NH1	2:n:111:PHE:O	2.33	0.61
2:J:33:LEU:HD21	2:J:40:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:99:LEU:HA	2:M:102:VAL:HG12	1.81	0.61
3:a:438:ALA:H	3:a:447:LYS:HD3	1.63	0.61
3:b:301:THR:O	3:b:441:SER:N	2.34	0.61
3:c:304:VAL:HG23	3:c:438:ALA:HB2	1.81	0.61
1:A:61:ALA:O	1:F:77:ARG:NH1	2.29	0.61
1:C:151:PRO:HG2	1:C:212:ASN:HB2	1.81	0.61
2:l:24:ILE:HG21	2:l:121:GLU:HG2	1.82	0.61
2:J:150:GLU:HG3	2:J:154:VAL:HG22	1.82	0.61
2:M:56:LEU:HD21	2:M:62:PHE:HD2	1.66	0.61
2:I:167:LEU:O	2:I:171:TYR:N	2.33	0.61
2:I:217:ARG:HH12	2:I:223:ARG:HB2	1.66	0.61
2:J:68:PHE:HA	2:J:71:PHE:CZ	2.35	0.61
3:Z:345:ILE:HG12	3:Z:402:PRO:HB3	1.82	0.61
1:F:386:VAL:HG21	1:F:451:LEU:HD13	1.82	0.61
2:M:167:LEU:O	2:M:171:TYR:N	2.33	0.61
3:S:406:GLY:O	3:S:419:ARG:N	2.33	0.61
1:D:271:ILE:HG12	1:D:314:ILE:HB	1.81	0.61
1:F:191:LYS:NZ	1:F:304:ILE:O	2.32	0.61
2:k:122:LEU:HD23	2:k:141:ILE:HD13	1.82	0.61
3:S:377:ALA:HA	3:S:380:ILE:HD12	1.82	0.61
3:X:322:GLN:N	3:X:322:GLN:OE1	2.33	0.61
2:L:53:ILE:O	2:L:224:ARG:NH2	2.23	0.61
3:P:302:THR:HA	3:P:440:GLY:HA3	1.82	0.61
1:C:386:VAL:HB	1:C:455:ILE:HD11	1.83	0.61
1:E:484:ARG:NH2	1:F:486:VAL:O	2.31	0.61
3:b:377:ALA:HA	3:b:380:ILE:HD12	1.81	0.61
3:c:338:ASP:OD1	3:c:341:THR:N	2.33	0.61
1:A:252:HIS:HB3	1:A:255:LEU:HB2	1.82	0.61
1:A:330:LEU:HD11	1:A:338:LYS:HG2	1.83	0.61
1:E:340:LYS:NZ	1:F:497:SER:O	2.31	0.61
2:k:116:LYS:NZ	2:k:117:PRO:O	2.34	0.61
2:o:77:GLY:O	2:o:80:GLN:NE2	2.34	0.61
2:H:123:CYS:HB2	2:H:154:VAL:HG11	1.83	0.61
3:R:301:THR:O	3:R:441:SER:N	2.34	0.61
2:o:17:SER:OG	2:o:21:ARG:NH1	2.34	0.61
2:M:68:PHE:HA	2:M:71:PHE:CE2	2.36	0.61
2:O:129:HIS:HB2	2:O:132:GLU:CD	2.26	0.61
1:A:364:HIS:HE1	1:A:443:GLN:HB3	1.65	0.60
1:C:161:LEU:HD13	1:C:206:ILE:HD11	1.83	0.60
1:B:89:VAL:HG12	1:C:62:VAL:HG12	1.81	0.60
2:J:10:GLU:OE1	2:J:11:GLN:NE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:165:ASN:HA	2:L:168:LYS:HG2	1.83	0.60
2:N:167:LEU:O	2:N:171:TYR:N	2.34	0.60
1:D:296:VAL:HG12	1:D:298:PRO:HD3	1.83	0.60
2:l:128:ALA:HB2	2:l:134:LYS:HB3	1.84	0.60
2:G:122:LEU:HB3	2:G:141:ILE:HB	1.83	0.60
2:H:109:THR:O	2:H:113:GLU:HG3	2.00	0.60
2:M:205:VAL:HG22	2:M:234:LEU:HD23	1.82	0.60
3:R:345:ILE:HG12	3:R:402:PRO:HB3	1.83	0.60
3:U:319:ARG:NH1	3:U:479:SER:O	2.33	0.60
3:W:319:ARG:NH1	3:W:479:SER:O	2.34	0.60
3:Z:322:GLN:N	3:Z:322:GLN:OE1	2.33	0.60
2:O:54:SER:O	2:O:62:PHE:N	2.33	0.60
2:J:182:ARG:NH1	2:J:233:LEU:O	2.34	0.60
2:L:162:PRO:HA	2:L:165:ASN:HD21	1.66	0.60
3:V:320:SER:HB3	3:V:328:GLY:HA3	1.83	0.60
3:W:304:VAL:HG23	3:W:438:ALA:HB2	1.83	0.60
3:a:495:VAL:HG22	3:a:504:ASP:HA	1.83	0.60
3:b:416:SER:O	3:b:419:ARG:NH1	2.26	0.60
1:B:406:ASN:ND2	1:B:408:ASP:OD2	2.35	0.60
2:k:46:PRO:CA	2:k:207:SER:HA	2.30	0.60
2:m:77:GLY:O	2:m:80:GLN:NE2	2.34	0.60
2:m:210:VAL:HG13	2:m:225:ILE:HB	1.83	0.60
3:R:390:ASN:O	3:R:394:ALA:N	2.32	0.60
3:S:338:ASP:OD1	3:S:341:THR:N	2.34	0.60
3:b:318:ARG:HD3	3:b:493:THR:HG23	1.83	0.60
3:c:436:TYR:HD1	3:c:450:MET:HE3	1.66	0.60
2:J:88:ALA:O	3:Y:381:ASN:ND2	2.34	0.60
2:L:68:PHE:HA	2:L:71:PHE:CZ	2.36	0.60
2:M:60:VAL:HG22	2:M:126:GLU:HG3	1.84	0.60
1:A:114:ARG:HB3	1:A:115:PRO:HD2	1.83	0.60
1:B:177:LEU:HD21	1:B:217:LYS:HE2	1.84	0.60
1:F:246:VAL:HG13	1:F:251:ARG:HH21	1.66	0.60
2:l:10:GLU:OE2	2:l:11:GLN:NE2	2.34	0.60
2:l:53:ILE:O	2:l:224:ARG:NH2	2.22	0.60
3:U:320:SER:HB3	3:U:331:VAL:HG21	1.83	0.60
3:Z:377:ALA:HA	3:Z:380:ILE:HD12	1.82	0.60
1:A:68:LEU:HD21	1:A:71:ILE:HD11	1.84	0.60
1:B:362:PRO:O	1:B:446:LEU:N	2.33	0.60
1:F:310:LEU:HG	1:F:312:ASN:H	1.66	0.60
3:P:385:ILE:HD13	3:P:388:ARG:HH22	1.67	0.60
1:B:391:TYR:OH	1:B:418:ASN:ND2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:46:PRO:HA	2:l:207:SER:HA	1.83	0.60
2:l:68:PHE:HA	2:l:71:PHE:CZ	2.37	0.60
2:n:16:ARG:HG3	2:n:117:PRO:HG3	1.83	0.60
2:I:45:ASN:ND2	2:I:50:LEU:O	2.34	0.60
2:M:54:SER:O	2:M:62:PHE:N	2.34	0.60
2:N:128:ALA:HB2	2:N:134:LYS:HB3	1.83	0.60
3:S:337:THR:H	3:S:342:ALA:HA	1.67	0.60
3:T:345:ILE:HA	3:T:402:PRO:HA	1.83	0.60
3:X:318:ARG:NH2	3:X:330:ASP:O	2.34	0.60
1:A:412:MET:HE1	1:A:477:ILE:HG21	1.82	0.60
1:F:471:PRO:HA	1:F:474:TRP:CD1	2.36	0.60
2:K:61:GLY:N	2:K:213:LEU:HD11	2.17	0.60
3:P:345:ILE:HG12	3:P:402:PRO:HB3	1.84	0.60
3:U:424:ASP:OD1	3:U:428:GLY:N	2.35	0.60
3:X:321:THR:HG22	3:X:326:ILE:HA	1.84	0.60
1:C:390:MET:O	1:C:397:ASN:ND2	2.35	0.59
1:D:386:VAL:HB	1:D:455:ILE:HD11	1.82	0.59
2:G:53:ILE:HG13	2:G:224:ARG:HH12	1.67	0.59
3:X:434:GLU:OE2	3:X:447:LYS:NZ	2.35	0.59
1:A:435:ILE:HG23	1:F:181:LEU:HD23	1.84	0.59
1:E:272:VAL:HB	1:E:315:VAL:HG12	1.84	0.59
1:F:199:PRO:HA	1:F:320:ASN:OD1	2.01	0.59
2:k:14:ARG:NH1	2:k:18:GLU:OE2	2.31	0.59
2:M:18:GLU:O	2:M:22:LYS:HG2	2.03	0.59
2:N:42:VAL:HG22	2:N:210:VAL:HG22	1.85	0.59
3:P:364:GLU:OE2	3:P:368:LYS:NZ	2.21	0.59
3:Y:495:VAL:HG22	3:Y:504:ASP:HA	1.84	0.59
2:k:96:GLY:H	2:k:126:GLU:CD	2.09	0.59
2:l:67:LYS:HZ3	4:i:172:GLN:HG2	1.66	0.59
3:V:318:ARG:NH2	3:V:330:ASP:O	2.34	0.59
3:Y:318:ARG:NH2	3:Y:330:ASP:O	2.34	0.59
2:k:150:GLU:HG3	2:k:154:VAL:HG22	1.84	0.59
2:n:164:ALA:C	2:n:168:LYS:HZ3	2.11	0.59
2:J:212:VAL:HG22	2:J:225:ILE:HD11	1.84	0.59
2:L:217:ARG:NH1	2:L:223:ARG:HB2	2.18	0.59
3:b:345:ILE:HA	3:b:402:PRO:HA	1.83	0.59
1:C:322:GLU:HB3	1:D:501:ARG:HH12	1.67	0.59
3:Y:337:THR:H	3:Y:342:ALA:HA	1.67	0.59
3:Z:306:LEU:HA	3:Z:436:TYR:HA	1.83	0.59
3:c:376:PHE:HE1	3:c:406:GLY:HA3	1.67	0.59
1:E:321:ARG:HH22	1:E:471:PRO:HB2	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:492:VAL:HG22	1:F:500:SER:HB3	1.83	0.59
2:m:22:LYS:HB3	2:m:26:ARG:HH12	1.66	0.59
2:H:152:HIS:HD2	2:H:171:TYR:HE2	1.51	0.59
2:N:146:SER:HA	2:O:67:LYS:HE2	1.85	0.59
3:Y:320:SER:HB3	3:Y:328:GLY:H	1.68	0.59
3:b:301:THR:N	3:b:441:SER:HG	2.00	0.59
1:F:193:VAL:HB	1:F:316:ILE:HG12	1.84	0.59
2:L:60:VAL:HG22	2:L:126:GLU:HG3	1.85	0.59
2:N:11:GLN:OE1	2:N:14:ARG:NH2	2.29	0.59
1:F:241:LEU:HD11	1:F:280:ILE:HG12	1.83	0.59
2:G:134:LYS:NZ	2:G:137:GLU:OE1	2.33	0.59
2:J:167:LEU:O	2:J:171:TYR:N	2.36	0.59
2:O:44:GLU:HA	2:O:208:LEU:HD23	1.85	0.59
1:A:435:ILE:HD13	1:F:182:TYR:CD1	2.38	0.59
1:B:115:PRO:HB3	1:B:136:ARG:HH21	1.67	0.59
1:D:438:VAL:HG22	1:D:444:PRO:HA	1.83	0.59
1:E:86:GLU:OE1	1:F:83:HIS:ND1	2.30	0.59
2:o:23:GLY:HA3	2:o:119:GLU:HG3	1.85	0.59
2:H:8:SER:OG	2:H:10:GLU:OE1	2.21	0.59
3:T:320:SER:HB3	3:T:331:VAL:HG21	1.84	0.59
1:A:296:VAL:HG22	1:A:298:PRO:HD3	1.85	0.59
1:D:241:LEU:HD22	1:D:280:ILE:HG12	1.85	0.59
1:F:329:ILE:HG12	1:F:335:LEU:HD13	1.83	0.59
2:n:68:PHE:HA	2:n:71:PHE:CZ	2.38	0.59
2:H:83:ASP:OD2	3:V:365:HIS:ND1	2.21	0.59
2:I:152:HIS:HB3	2:I:171:TYR:CE2	2.37	0.59
2:L:118:TYR:HB3	2:L:120:VAL:HG22	1.84	0.59
3:Z:346:ALA:O	3:Z:401:LEU:N	2.24	0.59
2:O:124:VAL:HB	2:O:139:TYR:HB2	1.84	0.59
2:I:77:GLY:O	2:I:80:GLN:NE2	2.36	0.58
2:J:165:ASN:HA	2:J:168:LYS:HZ2	1.68	0.58
3:b:345:ILE:HG12	3:b:402:PRO:HB3	1.85	0.58
1:D:28:LEU:HD22	1:D:51:LEU:HB3	1.84	0.58
1:D:351:ASP:O	1:D:354:SER:OG	2.21	0.58
2:l:68:PHE:H	4:i:172:GLN:HG3	1.68	0.58
2:m:71:PHE:HB3	2:m:120:VAL:HG21	1.85	0.58
2:H:140:ARG:O	2:H:148:ALA:N	2.33	0.58
3:W:318:ARG:NH2	3:W:330:ASP:O	2.35	0.58
3:W:346:ALA:O	3:W:401:LEU:N	2.28	0.58
3:b:351:VAL:O	3:b:354:GLU:HG2	2.02	0.58
1:B:65:ILE:HD12	1:B:137:ILE:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:52:LYS:HD2	4:f:174:LEU:HA	1.84	0.58
2:L:71:PHE:HA	2:L:74:LEU:HD12	1.85	0.58
3:Q:446:ALA:O	3:Q:450:MET:HG2	2.03	0.58
3:W:355:PHE:HE1	3:W:386:MET:HB3	1.68	0.58
1:F:257:PHE:CD2	1:F:303:GLU:HB3	2.38	0.58
2:l:16:ARG:NH1	2:l:111:PHE:O	2.30	0.58
2:L:55:GLU:HA	2:L:61:GLY:HA2	1.84	0.58
3:X:337:THR:H	3:X:342:ALA:HA	1.68	0.58
3:a:436:TYR:HB2	3:a:450:MET:HE2	1.85	0.58
2:k:110:ILE:HA	2:k:114:GLN:OE1	2.03	0.58
2:l:110:ILE:HD12	2:l:118:TYR:HB2	1.85	0.58
2:J:28:LYS:HD2	2:J:44:GLU:HG3	1.84	0.58
3:Q:374:LEU:O	3:Q:379:LYS:NZ	2.36	0.58
3:Z:364:GLU:O	3:Z:368:LYS:HG3	2.03	0.58
3:a:374:LEU:O	3:a:379:LYS:NZ	2.37	0.58
1:C:185:TYR:OH	1:D:445:GLY:N	2.31	0.58
1:F:429:ARG:NH2	1:F:461:GLU:OE1	2.32	0.58
2:o:53:ILE:O	2:o:224:ARG:NH2	2.33	0.58
2:K:44:GLU:HA	2:K:208:LEU:HD23	1.86	0.58
2:L:167:LEU:O	2:L:171:TYR:N	2.36	0.58
3:X:364:GLU:O	3:X:368:LYS:HG3	2.03	0.58
1:E:386:VAL:HB	1:E:455:ILE:HD11	1.86	0.58
2:m:68:PHE:HA	2:m:71:PHE:CZ	2.39	0.58
3:b:424:ASP:OD1	3:b:428:GLY:N	2.36	0.58
1:A:429:ARG:NH2	1:A:458:GLU:OE1	2.35	0.58
2:k:135:ARG:NH2	2:k:151:PRO:O	2.37	0.58
2:G:14:ARG:O	2:G:18:GLU:HG2	2.03	0.58
3:P:484:PRO:HB3	3:P:491:PHE:HD1	1.69	0.58
1:B:173:GLU:HG2	1:B:214:LEU:HB2	1.86	0.58
1:C:119:ARG:HH12	1:C:261:ARG:NH2	2.02	0.58
2:I:126:GLU:OE1	2:I:134:LYS:NZ	2.37	0.58
1:E:168:ILE:HG22	1:E:210:VAL:HG21	1.86	0.57
2:l:89:TYR:CD2	3:R:382:ARG:HD3	2.39	0.57
2:m:68:PHE:HB3	4:j:172:GLN:HG3	1.85	0.57
2:L:54:SER:O	2:L:62:PHE:N	2.34	0.57
3:R:436:TYR:HD1	3:R:450:MET:HE3	1.67	0.57
2:k:89:TYR:CD2	3:X:382:ARG:HD3	2.39	0.57
2:J:214:ASP:HB3	2:J:217:ARG:HG2	1.86	0.57
2:L:46:PRO:HA	2:L:207:SER:HA	1.85	0.57
1:A:83:HIS:ND1	1:F:85:ASP:O	2.37	0.57
1:B:244:LYS:C	1:B:246:VAL:H	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:GLN:HA	1:D:261:ARG:HG3	1.85	0.57
2:n:43:ALA:O	2:n:209:GLU:N	2.26	0.57
2:o:86:GLY:O	3:T:357:ARG:NH2	2.37	0.57
2:K:99:LEU:O	2:K:102:VAL:HG12	2.05	0.57
2:N:40:LEU:HA	2:N:212:VAL:HG12	1.86	0.57
3:R:447:LYS:HD2	3:R:450:MET:HE2	1.86	0.57
1:F:203:LYS:HG2	1:F:341:ILE:HG13	1.85	0.57
2:k:163:ILE:HD12	2:k:188:LEU:HA	1.84	0.57
2:K:99:LEU:HA	2:K:102:VAL:HG12	1.86	0.57
3:P:306:LEU:HD13	3:P:467:ALA:HB2	1.87	0.57
3:Y:338:ASP:OD1	3:Y:341:THR:N	2.35	0.57
3:Z:359:TYR:OH	3:Z:379:LYS:O	2.23	0.57
2:O:56:LEU:HG	2:O:62:PHE:HB2	1.86	0.57
1:D:322:GLU:OE2	1:E:501:ARG:NH1	2.37	0.57
2:k:129:HIS:HB2	2:k:132:GLU:CD	2.29	0.57
2:J:55:GLU:HB2	2:J:222:PHE:CG	2.39	0.57
2:M:14:ARG:O	2:M:18:GLU:HG2	2.04	0.57
3:Q:437:GLN:HA	3:Q:447:LYS:HE2	1.85	0.57
1:B:161:LEU:HB3	1:B:164:GLN:HB2	1.87	0.57
1:C:353:TYR:CE2	1:C:390:MET:HE1	2.39	0.57
1:F:176:PHE:HB3	1:F:217:LYS:HE3	1.86	0.57
2:L:89:TYR:CD1	3:a:382:ARG:HD3	2.40	0.57
3:P:319:ARG:NH1	3:P:479:SER:O	2.37	0.57
3:S:484:PRO:HB3	3:S:491:PHE:HD1	1.69	0.57
3:V:337:THR:H	3:V:342:ALA:HA	1.69	0.57
1:F:274:PHE:HB2	1:F:277:MET:HE2	1.85	0.57
2:o:109:THR:O	2:o:113:GLU:HG3	2.05	0.57
3:P:421:VAL:HG22	3:P:431:ILE:HG12	1.87	0.57
3:T:376:PHE:HA	3:T:379:LYS:HE2	1.87	0.57
3:U:416:SER:O	3:U:419:ARG:NH1	2.31	0.57
3:Y:345:ILE:HG12	3:Y:402:PRO:HB3	1.86	0.57
3:b:376:PHE:HA	3:b:379:LYS:NZ	2.19	0.57
1:B:466:PRO:HD2	1:B:501:ARG:HH22	1.69	0.57
1:D:471:PRO:HA	1:D:474:TRP:CD1	2.39	0.57
2:N:41:PHE:HB3	2:N:53:ILE:HD13	1.86	0.57
3:R:437:GLN:OE1	3:R:447:LYS:NZ	2.36	0.57
2:O:68:PHE:HA	2:O:71:PHE:CE2	2.40	0.57
1:C:183:ARG:HH22	1:C:189:PRO:HD3	1.70	0.57
1:E:447:ARG:HG2	1:E:450:HIS:CE1	2.40	0.57
3:Q:314:MET:HE1	3:Q:334:VAL:HG13	1.87	0.57
3:Z:308:TYR:CE1	3:Z:496:ILE:HD11	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LYS:HG2	1:B:341:ILE:HG13	1.87	0.57
1:B:437:SER:O	1:B:441:THR:HG22	2.04	0.57
1:F:271:ILE:HA	1:F:314:ILE:O	2.04	0.57
2:o:45:ASN:N	2:o:207:SER:O	2.38	0.57
2:G:22:LYS:HG3	2:G:26:ARG:HH12	1.70	0.57
2:M:165:ASN:HA	2:M:168:LYS:HZ2	1.69	0.57
3:U:346:ALA:O	3:U:401:LEU:N	2.25	0.57
3:W:338:ASP:OD1	3:W:341:THR:N	2.38	0.57
2:O:30:VAL:N	2:O:156:MET:O	2.24	0.57
1:A:404:TYR:OH	1:A:410:GLU:OE1	2.21	0.56
1:A:452:LEU:HA	1:A:455:ILE:HD12	1.86	0.56
2:k:111:PHE:O	2:J:116:LYS:NZ	2.37	0.56
2:n:147:ILE:O	4:e:172:GLN:NE2	2.38	0.56
2:G:163:ILE:HD13	2:G:188:LEU:HD12	1.87	0.56
2:M:80:GLN:HA	3:a:365:HIS:HE1	1.69	0.56
2:N:56:LEU:HD21	2:N:62:PHE:HD2	1.70	0.56
2:N:119:GLU:N	2:N:119:GLU:OE2	2.38	0.56
3:U:464:LEU:HD21	3:U:496:ILE:HD11	1.87	0.56
1:A:214:LEU:HD13	1:A:271:ILE:HD11	1.87	0.56
1:B:232:TYR:OH	1:B:268:THR:O	2.20	0.56
1:D:274:PHE:HB2	1:D:277:MET:HE3	1.88	0.56
1:F:191:LYS:HD3	1:F:308:GLU:HA	1.87	0.56
2:l:20:ALA:HA	2:l:119:GLU:HG2	1.87	0.56
2:n:83:ASP:OD2	3:S:365:HIS:ND1	2.34	0.56
2:G:109:THR:O	2:G:113:GLU:HG3	2.04	0.56
2:J:111:PHE:O	2:K:116:LYS:NZ	2.38	0.56
3:c:368:LYS:HD2	2:O:79:ILE:HG23	1.85	0.56
1:F:389:ARG:HD3	1:F:452:LEU:HD22	1.86	0.56
2:l:46:PRO:HG2	4:i:174:LEU:HD13	1.87	0.56
2:l:55:GLU:HG2	3:Q:368:LYS:HZ1	1.70	0.56
2:K:40:LEU:HA	2:K:212:VAL:HG12	1.87	0.56
3:S:301:THR:O	3:S:441:SER:N	2.37	0.56
1:D:264:ALA:HB1	1:D:310:LEU:HD21	1.87	0.56
3:b:376:PHE:HA	3:b:379:LYS:HZ2	1.70	0.56
1:B:364:HIS:CE1	1:B:366:ASP:OD2	2.58	0.56
1:C:438:VAL:HG22	1:C:444:PRO:HA	1.86	0.56
2:m:156:MET:HA	2:m:156:MET:HE3	1.87	0.56
3:T:495:VAL:HG22	3:T:504:ASP:HA	1.88	0.56
3:Z:466:VAL:HA	3:Z:469:GLU:OE1	2.06	0.56
3:a:313:VAL:HG21	3:a:464:LEU:HD23	1.87	0.56
2:O:53:ILE:O	2:O:224:ARG:NH2	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:THR:OG1	1:D:27:ARG:NH2	2.27	0.56
2:l:141:ILE:HG13	2:l:147:ILE:HD13	1.88	0.56
2:H:44:GLU:HA	2:H:208:LEU:HD23	1.88	0.56
3:P:321:THR:HG22	3:P:326:ILE:HA	1.88	0.56
3:U:304:VAL:HG23	3:U:438:ALA:HB2	1.87	0.56
2:G:155:VAL:O	2:G:156:MET:HE2	2.06	0.56
2:I:55:GLU:HB2	2:I:222:PHE:CG	2.41	0.56
2:J:128:ALA:HB2	2:J:134:LYS:HG3	1.87	0.56
2:L:122:LEU:C	2:L:156:MET:HE1	2.31	0.56
2:O:96:GLY:H	2:O:126:GLU:CD	2.14	0.56
1:E:340:LYS:HE3	1:E:342:GLU:HB2	1.86	0.56
2:G:11:GLN:OE1	2:G:14:ARG:NH2	2.37	0.56
3:U:301:THR:O	3:U:441:SER:N	2.38	0.56
1:C:151:PRO:HB3	1:C:208:LYS:HB3	1.85	0.56
1:D:425:ASN:ND2	1:D:458:GLU:OE1	2.39	0.56
1:E:351:ASP:O	1:E:354:SER:OG	2.20	0.56
2:J:42:VAL:HG22	2:J:210:VAL:HG22	1.88	0.56
2:L:129:HIS:HB2	2:L:132:GLU:CD	2.31	0.56
3:W:382:ARG:HD3	2:O:89:TYR:CD2	2.40	0.56
1:B:270:VAL:HG12	1:B:313:VAL:HG22	1.88	0.56
1:D:390:MET:O	1:D:397:ASN:ND2	2.39	0.56
1:D:471:PRO:HA	1:D:474:TRP:HD1	1.71	0.56
1:E:164:GLN:O	1:E:168:ILE:HG13	2.06	0.56
1:E:248:GLU:CD	1:E:249:THR:H	2.14	0.56
1:E:357:LEU:HD13	1:E:382:MET:HE3	1.88	0.56
2:G:233:LEU:HD12	2:G:234:LEU:HB2	1.88	0.56
3:T:402:PRO:HG2	3:T:423:PHE:HD2	1.71	0.56
1:A:31:SER:HB2	1:A:54:VAL:HG12	1.87	0.55
1:B:403:THR:HB	1:B:487:TYR:HB3	1.87	0.55
1:B:471:PRO:HA	1:B:474:TRP:CD1	2.42	0.55
1:C:24:ARG:HH21	1:D:7:VAL:HG23	1.71	0.55
2:H:67:LYS:HD3	4:g:171:GLY:HA3	1.87	0.55
2:I:88:ALA:O	3:Q:381:ASN:ND2	2.38	0.55
2:N:111:PHE:O	2:O:116:LYS:NZ	2.36	0.55
3:Q:337:THR:HB	3:Q:341:THR:HG23	1.88	0.55
2:l:27:ALA:HA	4:i:173:TYR:HB3	1.88	0.55
2:H:30:VAL:HG23	2:H:43:ALA:HB2	1.88	0.55
3:P:301:THR:O	3:P:441:SER:N	2.39	0.55
1:B:105:LEU:HA	1:B:259:ARG:HH12	1.71	0.55
1:B:359:GLU:O	1:B:375:ARG:NH1	2.39	0.55
1:D:490:THR:OG1	1:D:501:ARG:N	2.29	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:LEU:HD11	1:F:79:LEU:HB2	1.88	0.55
2:I:121:GLU:HG2	2:I:156:MET:HE1	1.88	0.55
2:J:134:LYS:NZ	2:J:136:PRO:HA	2.22	0.55
3:R:466:VAL:HA	3:R:469:GLU:OE1	2.07	0.55
1:A:17:VAL:HG12	1:A:19:VAL:HG23	1.89	0.55
1:F:166:GLU:HA	1:F:169:ARG:HG2	1.89	0.55
2:k:62:PHE:CZ	2:k:75:ARG:HB2	2.41	0.55
3:Q:364:GLU:O	3:Q:368:LYS:HG3	2.06	0.55
3:R:345:ILE:HA	3:R:402:PRO:HA	1.88	0.55
3:T:385:ILE:HD13	3:T:388:ARG:HH21	1.71	0.55
3:T:393:ALA:HB1	3:T:398:LEU:HB2	1.88	0.55
3:W:376:PHE:HE1	3:W:406:GLY:HA3	1.71	0.55
1:B:429:ARG:HD2	1:B:454:SER:HA	1.88	0.55
1:F:260:ALA:HB1	1:F:270:VAL:HG11	1.89	0.55
2:n:16:ARG:NH2	2:n:114:GLN:O	2.39	0.55
2:o:150:GLU:HG2	2:o:153:PHE:O	2.06	0.55
2:o:182:ARG:NH1	2:o:233:LEU:O	2.31	0.55
2:M:30:VAL:N	2:M:156:MET:O	2.24	0.55
3:W:318:ARG:HB3	3:W:330:ASP:HA	1.89	0.55
2:O:110:ILE:HA	2:O:114:GLN:OE1	2.06	0.55
1:D:484:ARG:HH21	1:E:487:TYR:HE1	1.52	0.55
2:n:109:THR:O	2:n:113:GLU:HG3	2.06	0.55
2:n:142:THR:HG22	2:n:146:SER:HB3	1.89	0.55
2:L:91:ARG:O	2:L:94:VAL:HG22	2.06	0.55
3:Q:355:PHE:HZ	3:Q:390:ASN:HB2	1.71	0.55
3:V:345:ILE:HG12	3:V:402:PRO:HB3	1.89	0.55
3:a:376:PHE:HE1	3:a:406:GLY:HA3	1.71	0.55
3:c:376:PHE:CE2	3:c:419:ARG:HB2	2.42	0.55
1:A:445:GLY:N	1:F:185:TYR:OH	2.36	0.55
1:E:3:SER:OG	1:E:46:ARG:NH1	2.35	0.55
2:k:30:VAL:HG13	2:k:43:ALA:HB2	1.88	0.55
2:k:40:LEU:HA	2:k:212:VAL:HG12	1.88	0.55
2:G:19:LEU:HA	2:G:22:LYS:HG2	1.89	0.55
3:T:302:THR:HA	3:T:440:GLY:HA3	1.88	0.55
1:E:77:ARG:HA	1:E:91:TRP:HA	1.88	0.55
1:E:357:LEU:HD12	1:E:383:ILE:HG12	1.88	0.55
2:k:53:ILE:O	2:k:224:ARG:NH2	2.24	0.55
3:a:339:ASP:O	3:a:502:ALA:N	2.38	0.55
1:D:168:ILE:HD11	1:D:195:LEU:HD21	1.88	0.55
2:J:161:GLU:CD	2:J:165:ASN:HD21	2.15	0.55
3:Q:301:THR:O	3:Q:441:SER:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:429:ARG:NH2	1:F:458:GLU:OE1	2.35	0.55
2:o:140:ARG:HB3	2:o:148:ALA:HB3	1.88	0.55
2:G:121:GLU:HG2	2:G:156:MET:SD	2.47	0.55
2:J:89:TYR:CD2	3:Y:382:ARG:HD3	2.42	0.55
2:N:129:HIS:HB2	2:N:132:GLU:CD	2.32	0.55
3:R:338:ASP:OD1	3:R:341:THR:N	2.36	0.55
3:S:318:ARG:NH2	3:S:330:ASP:O	2.38	0.55
1:D:232:TYR:OH	1:D:271:ILE:O	2.23	0.54
1:D:353:TYR:CE2	1:D:390:MET:HE1	2.41	0.54
2:G:230:LEU:HD12	2:G:233:LEU:HD11	1.89	0.54
2:M:219:ARG:HE	2:M:220:ARG:HG3	1.72	0.54
3:X:406:GLY:O	3:X:419:ARG:N	2.40	0.54
3:c:346:ALA:O	3:c:401:LEU:N	2.24	0.54
2:o:58:ASP:O	2:o:221:ALA:N	2.31	0.54
2:G:18:GLU:OE1	2:G:21:ARG:NE	2.40	0.54
2:H:28:LYS:HE2	4:g:174:LEU:HB2	1.89	0.54
3:b:392:ALA:HA	3:b:395:MET:HE3	1.88	0.54
1:A:46:ARG:HE	1:A:54:VAL:HG23	1.72	0.54
1:D:203:LYS:HZ1	1:D:320:ASN:HA	1.73	0.54
2:k:139:TYR:HB3	2:k:147:ILE:HD11	1.89	0.54
2:l:88:ALA:O	3:R:381:ASN:ND2	2.40	0.54
2:H:121:GLU:OE2	2:H:140:ARG:NH1	2.40	0.54
2:K:22:LYS:HB3	2:K:26:ARG:NH2	2.22	0.54
2:K:55:GLU:HB2	2:K:222:PHE:CG	2.42	0.54
3:Q:318:ARG:NH2	3:Q:330:ASP:O	2.39	0.54
3:W:364:GLU:O	3:W:368:LYS:HG2	2.07	0.54
2:O:62:PHE:HE1	2:O:122:LEU:HB2	1.72	0.54
1:C:446:LEU:HD21	1:C:451:LEU:HG	1.88	0.54
1:F:91:TRP:HB2	1:F:132:TYR:CE1	2.42	0.54
1:F:254:ARG:HH11	1:F:303:GLU:HG2	1.73	0.54
2:k:31:VAL:HG22	2:k:155:VAL:HG22	1.89	0.54
2:H:217:ARG:HB2	2:H:221:ALA:HA	1.89	0.54
2:J:21:ARG:HH21	2:J:22:LYS:HZ2	1.54	0.54
1:A:9:LEU:HD21	1:A:20:PHE:HB2	1.90	0.54
1:F:199:PRO:HD3	1:F:470:ASN:ND2	2.22	0.54
2:H:19:LEU:HA	2:H:22:LYS:HG2	1.89	0.54
2:M:74:LEU:HB3	2:M:103:TYR:HE1	1.73	0.54
2:N:55:GLU:HB2	2:N:222:PHE:CG	2.42	0.54
3:P:461:ASP:HA	3:P:464:LEU:HD12	1.90	0.54
3:T:318:ARG:NH2	3:T:330:ASP:O	2.40	0.54
3:W:345:ILE:HA	3:W:402:PRO:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:345:ILE:HA	3:a:402:PRO:HA	1.90	0.54
2:l:67:LYS:HD2	4:i:171:GLY:HA2	1.89	0.54
2:o:58:ASP:HB3	2:o:219:ARG:O	2.08	0.54
2:M:134:LYS:NZ	2:M:136:PRO:HA	2.22	0.54
3:U:337:THR:H	3:U:342:ALA:HA	1.72	0.54
3:Y:422:SER:OG	3:Y:432:GLU:OE2	2.23	0.54
3:a:376:PHE:HA	3:a:379:LYS:HE2	1.90	0.54
3:a:460:GLY:O	3:a:464:LEU:HG	2.07	0.54
2:O:63:ALA:HB3	2:O:123:CYS:HB3	1.87	0.54
1:B:305:ASP:HA	1:B:308:GLU:HG2	1.89	0.54
1:C:92:LEU:HD23	1:C:133:ALA:HB3	1.89	0.54
1:E:26:MET:HE1	1:E:28:LEU:HD21	1.89	0.54
2:K:89:TYR:CD1	3:Z:382:ARG:HD3	2.41	0.54
2:L:20:ALA:HA	2:L:119:GLU:HG2	1.89	0.54
3:W:301:THR:O	3:W:441:SER:N	2.38	0.54
3:W:308:TYR:CE1	3:W:496:ILE:HD11	2.42	0.54
1:A:489:ARG:HA	1:A:502:ALA:HA	1.90	0.54
1:B:116:ARG:HG2	1:B:117:LYS:H	1.72	0.54
1:B:472:ASP:OD2	1:B:476:ARG:NH1	2.41	0.54
2:G:21:ARG:NH1	2:G:22:LYS:HB3	2.23	0.54
2:I:18:GLU:HA	2:I:21:ARG:HG2	1.90	0.54
2:J:16:ARG:NH1	2:J:114:GLN:O	2.38	0.54
3:V:393:ALA:HB1	3:V:398:LEU:HB2	1.89	0.54
1:A:142:VAL:HG12	1:A:252:HIS:NE2	2.23	0.54
1:C:476:ARG:HE	1:D:501:ARG:HD2	1.71	0.54
1:D:333:GLY:N	1:D:336:ASP:OD1	2.33	0.54
3:U:476:ASP:O	3:X:329:ARG:NH2	2.33	0.54
3:Y:322:GLN:HG2	3:Y:325:MET:HB3	1.89	0.54
3:Y:376:PHE:HE1	3:Y:406:GLY:HA3	1.72	0.54
3:a:319:ARG:CZ	3:a:482:GLY:HA2	2.38	0.54
1:B:105:LEU:O	1:B:259:ARG:NH2	2.41	0.54
1:E:92:LEU:HD23	1:E:133:ALA:HB3	1.90	0.54
2:k:16:ARG:NH1	2:k:114:GLN:O	2.34	0.54
2:m:8:SER:OG	2:m:10:GLU:OE1	2.26	0.54
2:m:210:VAL:HG11	2:m:230:LEU:HD13	1.90	0.54
2:G:57:TYR:HB3	2:G:60:VAL:HB	1.89	0.54
2:K:167:LEU:O	2:K:171:TYR:N	2.39	0.54
3:S:308:TYR:CE2	3:S:496:ILE:HD11	2.43	0.54
3:X:320:SER:HB2	3:X:331:VAL:HG21	1.90	0.54
1:A:443:GLN:OE1	1:A:447:ARG:NH2	2.40	0.53
1:B:101:LEU:HB3	1:B:115:PRO:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:VAL:HG11	1:B:451:LEU:HD13	1.89	0.53
1:D:126:VAL:HG12	1:D:133:ALA:HB2	1.90	0.53
1:E:262:GLU:HG3	1:E:263:LYS:HD3	1.89	0.53
2:J:138:LEU:HB2	2:J:150:GLU:HB2	1.90	0.53
2:K:110:ILE:O	2:K:114:GLN:HG2	2.07	0.53
3:T:484:PRO:HB3	3:T:491:PHE:HD1	1.73	0.53
3:U:358:LEU:O	3:U:361:VAL:HB	2.08	0.53
1:D:194:LEU:HB2	1:D:335:LEU:HD23	1.89	0.53
1:E:264:ALA:HB1	1:E:310:LEU:HD21	1.88	0.53
2:G:8:SER:HB3	2:G:11:GLN:HG2	1.90	0.53
2:H:28:LYS:NZ	2:H:45:ASN:HA	2.23	0.53
2:K:16:ARG:NH1	2:K:114:GLN:O	2.37	0.53
2:N:54:SER:O	2:N:62:PHE:N	2.38	0.53
3:Y:424:ASP:OD1	3:Y:427:GLY:N	2.41	0.53
1:A:255:LEU:O	1:A:259:ARG:HG2	2.09	0.53
2:k:18:GLU:OE1	2:k:21:ARG:NH2	2.27	0.53
2:o:69:ASN:OD1	2:o:70:GLU:N	2.41	0.53
2:G:102:VAL:O	2:G:105:GLN:HG3	2.08	0.53
2:N:141:ILE:HG12	2:N:147:ILE:HG13	1.89	0.53
3:Q:473:ASP:OD1	3:Q:521:ARG:NH1	2.32	0.53
3:Y:322:GLN:OE1	3:Y:322:GLN:N	2.41	0.53
2:O:122:LEU:C	2:O:156:MET:HE1	2.33	0.53
1:C:403:THR:HB	1:C:487:TYR:HB3	1.90	0.53
2:o:35:TYR:CD1	2:o:40:LEU:HG	2.43	0.53
2:K:150:GLU:HG3	2:K:154:VAL:HG22	1.89	0.53
2:N:100:ALA:HB1	2:N:147:ILE:HD11	1.91	0.53
3:Y:367:GLU:O	3:Y:371:GLY:N	2.41	0.53
3:a:303:ILE:N	3:a:439:VAL:O	2.34	0.53
2:J:30:VAL:HG13	2:J:43:ALA:HB2	1.90	0.53
2:J:139:TYR:HB3	2:J:147:ILE:HD11	1.89	0.53
2:M:214:ASP:HB3	2:M:217:ARG:HG2	1.90	0.53
3:Q:461:ASP:HA	3:Q:509:ARG:HH21	1.74	0.53
3:T:355:PHE:HZ	3:T:390:ASN:HB2	1.73	0.53
3:V:476:ASP:O	3:W:329:ARG:NH2	2.41	0.53
3:a:320:SER:HB3	3:a:331:VAL:HG21	1.90	0.53
3:c:337:THR:H	3:c:342:ALA:HA	1.72	0.53
1:B:198:PRO:HG2	1:B:343:ARG:HG3	1.90	0.53
1:C:72:LEU:HD22	1:D:137:ILE:HD12	1.90	0.53
1:E:158:ILE:HD13	1:E:206:ILE:HG13	1.91	0.53
1:F:194:LEU:HB2	1:F:335:LEU:HD23	1.90	0.53
2:n:70:GLU:HB3	2:n:118:TYR:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:150:GLU:OE1	2:I:153:PHE:N	2.36	0.53
3:c:314:MET:HE1	3:c:334:VAL:HG13	1.89	0.53
1:B:482:GLY:HA2	1:C:489:ARG:HD3	1.91	0.53
2:m:67:LYS:HE2	4:j:171:GLY:HA3	1.89	0.53
2:n:58:ASP:OD2	2:n:91:ARG:NH2	2.35	0.53
2:N:53:ILE:O	2:N:224:ARG:NH2	2.33	0.53
3:b:306:LEU:HA	3:b:436:TYR:HA	1.91	0.53
1:A:203:LYS:H	1:A:206:ILE:CD1	2.20	0.53
1:A:278:ASP:HB2	1:A:324:MET:HE3	1.90	0.53
1:B:493:THR:HG23	1:B:495:LYS:H	1.73	0.53
1:D:391:TYR:OH	1:D:418:ASN:ND2	2.32	0.53
2:n:45:ASN:ND2	2:n:50:LEU:O	2.41	0.53
2:G:58:ASP:O	2:G:221:ALA:N	2.38	0.53
2:I:67:LYS:HZ2	4:h:172:GLN:HB3	1.74	0.53
2:I:140:ARG:O	2:I:148:ALA:N	2.33	0.53
2:N:135:ARG:HD2	2:N:136:PRO:HD2	1.89	0.53
3:R:376:PHE:HE1	3:R:406:GLY:HA3	1.73	0.53
3:U:376:PHE:CZ	3:U:419:ARG:HB2	2.44	0.53
3:W:322:GLN:HG2	3:W:325:MET:HB2	1.91	0.53
3:a:432:GLU:HG3	3:a:437:GLN:HB2	1.91	0.53
1:B:165:ILE:HA	1:B:168:ILE:HD12	1.91	0.53
1:C:466:PRO:HG3	1:C:490:THR:HG21	1.90	0.53
1:D:398:ARG:NH1	1:D:491:LEU:O	2.42	0.53
2:k:91:ARG:O	2:k:94:VAL:HG22	2.08	0.53
2:l:163:ILE:HD13	2:l:188:LEU:HA	1.90	0.53
2:K:103:TYR:HB2	2:K:141:ILE:HD13	1.91	0.53
3:P:376:PHE:HE1	3:P:406:GLY:HA3	1.74	0.53
3:T:346:ALA:O	3:T:401:LEU:N	2.28	0.53
1:A:159:GLY:H	1:A:355:LYS:HZ1	1.57	0.53
1:C:96:LEU:HD22	1:C:118:LEU:HD21	1.91	0.53
1:C:254:ARG:HH12	1:C:299:GLN:HB2	1.73	0.53
2:J:177:LEU:HG	2:J:233:LEU:HD21	1.91	0.53
2:L:14:ARG:O	2:L:18:GLU:HG2	2.09	0.53
2:M:110:ILE:O	2:M:114:GLN:HG2	2.08	0.53
3:S:475:ALA:HB2	3:S:481:THR:O	2.09	0.53
3:X:438:ALA:H	3:X:447:LYS:HD3	1.72	0.53
1:A:175:PRO:HB3	1:A:189:PRO:HB3	1.92	0.52
1:A:181:LEU:HG	1:B:435:ILE:HG12	1.91	0.52
1:A:476:ARG:NH2	1:B:464:ASP:OD1	2.41	0.52
1:C:9:LEU:HA	1:C:132:TYR:OH	2.09	0.52
1:C:96:LEU:HB3	1:C:118:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:TYR:CE1	1:E:423:ILE:HG23	2.44	0.52
1:F:400:LEU:HD23	1:F:490:THR:HA	1.91	0.52
2:n:75:ARG:NH1	3:S:368:LYS:O	2.41	0.52
2:K:214:ASP:HB3	2:K:217:ARG:HG2	1.90	0.52
3:V:320:SER:HB2	3:V:331:VAL:HG21	1.90	0.52
1:A:168:ILE:HD13	1:A:206:ILE:HG23	1.91	0.52
2:k:112:THR:HG22	2:J:116:LYS:HD2	1.90	0.52
2:o:217:ARG:HB2	2:o:221:ALA:HA	1.91	0.52
3:P:346:ALA:O	3:P:401:LEU:N	2.26	0.52
3:P:436:TYR:HB2	3:P:450:MET:CE	2.28	0.52
3:R:320:SER:HB3	3:R:331:VAL:HG21	1.91	0.52
1:D:5:TYR:HA	1:D:46:ARG:HA	1.92	0.52
2:G:89:TYR:CD2	3:V:382:ARG:HD3	2.45	0.52
2:M:55:GLU:HB2	2:M:222:PHE:CG	2.45	0.52
3:V:346:ALA:O	3:V:401:LEU:N	2.26	0.52
2:m:55:GLU:HB2	2:m:222:PHE:CG	2.44	0.52
2:L:128:ALA:HB2	2:L:134:LYS:HB3	1.91	0.52
3:P:329:ARG:NH2	3:c:476:ASP:O	2.40	0.52
3:X:436:TYR:HD1	3:X:450:MET:HE3	1.74	0.52
3:Y:345:ILE:HA	3:Y:402:PRO:HA	1.91	0.52
3:Z:376:PHE:HE1	3:Z:406:GLY:HA3	1.75	0.52
3:c:497:ILE:HG23	3:c:502:ALA:HB2	1.90	0.52
1:D:398:ARG:HD3	1:D:491:LEU:HD12	1.92	0.52
1:D:403:THR:HG23	1:D:409:LYS:HG2	1.91	0.52
1:E:198:PRO:HG3	1:E:476:ARG:HH22	1.74	0.52
2:m:54:SER:O	2:m:62:PHE:N	2.40	0.52
2:o:16:ARG:HG3	2:o:117:PRO:HG3	1.91	0.52
2:J:129:HIS:HB2	2:J:132:GLU:CD	2.34	0.52
2:K:54:SER:O	2:K:62:PHE:N	2.42	0.52
3:Q:304:VAL:HA	3:Q:438:ALA:HA	1.91	0.52
3:W:303:ILE:N	3:W:439:VAL:O	2.36	0.52
3:X:468:VAL:HG13	3:X:517:ILE:HD11	1.92	0.52
3:Y:319:ARG:CZ	3:Y:482:GLY:HA2	2.40	0.52
1:A:476:ARG:HG2	1:B:501:ARG:HG3	1.90	0.52
1:B:172:VAL:HG12	1:B:214:LEU:HD22	1.90	0.52
1:C:216:LYS:O	1:C:217:LYS:C	2.53	0.52
1:E:70:GLU:OE2	1:F:139:LYS:HB3	2.10	0.52
2:m:137:GLU:OE1	2:m:139:TYR:OH	2.22	0.52
2:G:210:VAL:HG23	2:G:225:ILE:HB	1.91	0.52
3:b:346:ALA:O	3:b:401:LEU:N	2.26	0.52
1:E:307:VAL:HG23	1:E:310:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:80:GLN:HA	3:R:365:HIS:HE1	1.74	0.52
2:m:121:GLU:HG2	2:m:156:MET:HE2	1.92	0.52
2:o:66:GLY:HA3	2:o:120:VAL:HG12	1.91	0.52
2:K:66:GLY:HA3	2:K:120:VAL:HG12	1.92	0.52
3:a:422:SER:HB3	3:a:437:GLN:HG2	1.92	0.52
3:c:367:GLU:O	3:c:371:GLY:N	2.41	0.52
2:O:30:VAL:HB	2:O:156:MET:HB3	1.90	0.52
1:F:448:ILE:O	1:F:452:LEU:HG	2.10	0.52
2:l:109:THR:O	2:l:113:GLU:HG3	2.09	0.52
2:H:18:GLU:HG3	2:H:22:LYS:NZ	2.25	0.52
2:I:16:ARG:HD3	2:I:117:PRO:HG3	1.92	0.52
2:K:178:THR:O	2:K:182:ARG:HG2	2.09	0.52
3:T:376:PHE:HE1	3:T:406:GLY:HA3	1.75	0.52
3:W:459:ASP:H	3:W:462:SER:HG	1.56	0.52
2:O:138:LEU:HB2	2:O:150:GLU:HB2	1.92	0.52
1:A:296:VAL:HG13	1:A:298:PRO:HD2	1.92	0.52
2:l:134:LYS:NZ	2:l:137:GLU:OE1	2.31	0.52
2:G:43:ALA:HB3	2:G:209:GLU:CG	2.40	0.52
2:L:29:SER:N	2:L:44:GLU:OE2	2.41	0.52
2:N:18:GLU:HA	2:N:21:ARG:HE	1.75	0.52
3:X:408:ASP:HB3	3:X:411:ALA:HB2	1.92	0.52
3:Y:355:PHE:HZ	3:Y:390:ASN:HB2	1.75	0.52
1:E:78:ALA:N	1:E:90:VAL:O	2.30	0.52
1:F:362:PRO:O	1:F:446:LEU:N	2.35	0.52
2:I:217:ARG:NH1	2:I:223:ARG:HB2	2.24	0.52
2:J:40:LEU:HA	2:J:212:VAL:HG12	1.92	0.52
2:J:53:ILE:O	2:J:224:ARG:NH2	2.21	0.52
2:J:65:ALA:HB3	2:J:156:MET:HG2	1.92	0.52
2:K:217:ARG:NH1	2:K:223:ARG:HB2	2.25	0.52
2:N:130:TYR:CD2	2:N:218:PRO:HA	2.45	0.52
3:S:436:TYR:HB2	3:S:450:MET:CE	2.29	0.52
3:U:377:ALA:HA	3:U:380:ILE:HD12	1.92	0.52
3:c:303:ILE:N	3:c:439:VAL:O	2.36	0.52
1:C:381:ALA:HA	1:C:384:GLU:HG2	1.91	0.51
1:C:391:TYR:HA	1:C:415:LYS:HB3	1.92	0.51
1:D:214:LEU:HA	1:D:217:LYS:HD3	1.91	0.51
1:D:389:ARG:NH1	1:D:397:ASN:OD1	2.42	0.51
1:D:447:ARG:HG2	1:D:450:HIS:CE1	2.45	0.51
2:k:54:SER:OG	2:k:55:GLU:N	2.44	0.51
2:G:181:LEU:HD22	2:G:233:LEU:HD13	1.92	0.51
2:H:155:VAL:O	2:H:156:MET:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:162:PRO:HA	2:J:165:ASN:ND2	2.26	0.51
2:N:150:GLU:HG3	2:N:154:VAL:HG22	1.91	0.51
3:b:314:MET:HE1	3:b:334:VAL:HG13	1.92	0.51
2:O:214:ASP:HB3	2:O:217:ARG:HG2	1.92	0.51
1:E:353:TYR:CZ	1:E:423:ILE:HG12	2.45	0.51
1:E:452:LEU:HA	1:E:455:ILE:HD12	1.92	0.51
3:b:365:HIS:NE2	3:b:369:LEU:HD11	2.26	0.51
1:A:151:PRO:HG2	1:A:212:ASN:HB2	1.91	0.51
1:C:367:ASP:OD2	1:C:447:ARG:HA	2.09	0.51
1:E:16:THR:HG22	1:E:29:THR:HG22	1.91	0.51
1:E:182:TYR:CD1	1:F:435:ILE:HD13	2.45	0.51
2:H:28:LYS:HZ2	2:H:45:ASN:HA	1.74	0.51
3:Q:436:TYR:HD1	3:Q:450:MET:SD	2.33	0.51
3:W:307:LYS:HE2	3:W:435:GLY:HA2	1.91	0.51
3:Y:383:LEU:HD23	3:Y:423:PHE:CZ	2.45	0.51
1:B:121:GLY:HA3	1:B:251:ARG:HE	1.74	0.51
2:J:30:VAL:N	2:J:156:MET:O	2.25	0.51
2:M:150:GLU:HG3	2:M:154:VAL:HG22	1.92	0.51
3:P:376:PHE:CE1	3:P:406:GLY:HA3	2.45	0.51
3:V:506:PRO:HD2	3:V:509:ARG:NH2	2.21	0.51
3:X:437:GLN:HA	3:X:447:LYS:HZ3	1.74	0.51
1:C:353:TYR:HE2	1:C:390:MET:HE1	1.76	0.51
1:E:119:ARG:HE	1:E:259:ARG:NH2	2.08	0.51
1:E:121:GLY:HA3	1:E:255:LEU:HD11	1.92	0.51
1:E:471:PRO:HA	1:E:474:TRP:CD1	2.46	0.51
1:E:482:GLY:HA2	1:F:489:ARG:HD3	1.92	0.51
2:l:181:LEU:HD23	2:l:233:LEU:HB3	1.91	0.51
3:Q:413:ASP:OD2	3:Q:416:SER:N	2.43	0.51
3:T:402:PRO:HG2	3:T:423:PHE:CD2	2.46	0.51
3:U:424:ASP:OD1	3:U:427:GLY:N	2.44	0.51
3:V:413:ASP:OD1	3:V:416:SER:N	2.35	0.51
3:b:382:ARG:HB3	3:b:386:MET:HE1	1.91	0.51
3:c:318:ARG:NH2	3:c:330:ASP:O	2.43	0.51
3:c:387:VAL:HG11	3:c:402:PRO:HG3	1.93	0.51
1:A:482:GLY:HA2	1:B:489:ARG:HD3	1.92	0.51
1:C:363:VAL:HG21	1:C:379:ILE:HG12	1.91	0.51
2:G:87:TYR:O	3:U:357:ARG:NH2	2.37	0.51
3:Q:424:ASP:OD1	3:Q:428:GLY:N	2.44	0.51
3:U:402:PRO:HG2	3:U:423:PHE:CD2	2.43	0.51
3:a:466:VAL:O	3:a:469:GLU:HG3	2.11	0.51
1:B:273:PHE:HA	1:B:316:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ARG:NE	1:D:324:MET:HE1	2.26	0.51
1:E:299:GLN:HG3	1:F:243:ASN:HB2	1.91	0.51
1:F:429:ARG:HB3	1:F:454:SER:OG	2.11	0.51
2:k:107:LEU:HA	2:k:110:ILE:HG12	1.93	0.51
2:m:67:LYS:NZ	2:m:69:ASN:HD21	2.09	0.51
2:o:189:ARG:O	2:o:189:ARG:NH1	2.39	0.51
2:N:44:GLU:HG3	2:N:188:LEU:HD21	1.93	0.51
2:N:89:TYR:CD2	3:c:382:ARG:HD3	2.45	0.51
2:m:179:ASP:O	2:m:183:ILE:HD12	2.11	0.51
2:I:63:ALA:O	2:I:122:LEU:HD12	2.11	0.51
2:J:69:ASN:OD1	2:J:70:GLU:N	2.44	0.51
2:J:71:PHE:HA	2:J:74:LEU:HD12	1.91	0.51
2:J:121:GLU:HG2	2:J:156:MET:HE2	1.92	0.51
3:S:437:GLN:HA	3:S:447:LYS:NZ	2.25	0.51
3:V:408:ASP:HB3	3:V:411:ALA:HB2	1.93	0.51
3:Z:495:VAL:HG22	3:Z:504:ASP:HA	1.93	0.51
2:O:33:LEU:HD21	2:O:40:LEU:HD23	1.91	0.51
1:B:216:LYS:O	1:B:217:LYS:HD2	2.11	0.51
1:D:270:VAL:HB	1:D:313:VAL:HG22	1.92	0.51
1:F:328:ALA:O	1:F:334:ARG:NH1	2.44	0.51
2:k:18:GLU:HB3	2:k:22:LYS:NZ	2.26	0.51
2:l:171:TYR:HE2	2:l:173:GLU:HG2	1.76	0.51
2:n:8:SER:HB3	2:n:11:GLN:HG2	1.91	0.51
2:G:34:ALA:HB1	2:G:136:PRO:HG2	1.91	0.51
2:G:55:GLU:HB2	2:G:222:PHE:CG	2.45	0.51
2:I:89:TYR:CD2	3:Q:382:ARG:HD3	2.46	0.51
3:T:377:ALA:HA	3:T:380:ILE:HD12	1.91	0.51
3:Z:319:ARG:CZ	3:Z:482:GLY:HA2	2.41	0.51
3:b:438:ALA:H	3:b:447:LYS:HD3	1.76	0.51
3:c:351:VAL:O	3:c:354:GLU:HG2	2.11	0.51
3:c:468:VAL:HG23	3:c:517:ILE:HD11	1.93	0.51
1:E:432:LYS:O	1:E:436:LYS:HG2	2.11	0.51
2:k:142:THR:OG1	2:k:144:ASP:OD1	2.25	0.51
3:Q:484:PRO:HB3	3:Q:491:PHE:HD1	1.75	0.51
3:a:340:TYR:OH	3:a:499:ALA:O	2.20	0.51
1:A:244:LYS:C	1:A:246:VAL:H	2.19	0.50
1:D:239:PRO:HD3	1:D:276:GLU:HB3	1.91	0.50
1:D:270:VAL:O	1:D:314:ILE:N	2.33	0.50
1:D:414:PHE:HZ	1:D:463:GLU:HG3	1.76	0.50
1:F:145:LEU:HG	1:F:146:VAL:H	1.75	0.50
1:F:405:ALA:N	1:F:484:ARG:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:o:41:PHE:HZ	2:o:125:ALA:HB3	1.76	0.50
2:M:89:TYR:CD2	3:b:382:ARG:HD3	2.46	0.50
3:P:446:ALA:O	3:P:450:MET:HG3	2.11	0.50
1:C:321:ARG:NH1	1:C:323:ASP:OD2	2.44	0.50
1:D:364:HIS:CD2	1:D:366:ASP:HB2	2.46	0.50
1:F:91:TRP:CD1	1:F:132:TYR:HE1	2.29	0.50
3:P:444:LEU:HA	3:P:447:LYS:HZ2	1.76	0.50
3:T:416:SER:O	3:T:419:ARG:NH1	2.36	0.50
3:X:303:ILE:HG22	3:X:314:MET:HE3	1.93	0.50
3:X:345:ILE:HB	3:X:352:ALA:HB1	1.92	0.50
3:Z:320:SER:HB3	3:Z:331:VAL:HG21	1.94	0.50
2:k:76:ARG:O	2:k:80:GLN:HG2	2.11	0.50
2:G:119:GLU:OE1	2:G:119:GLU:N	2.44	0.50
2:H:35:TYR:HB2	2:H:175:ALA:O	2.11	0.50
2:I:89:TYR:O	3:Q:378:GLY:HA2	2.11	0.50
2:J:231:GLN:NE2	2:J:231:GLN:O	2.44	0.50
2:M:134:LYS:HZ1	2:M:136:PRO:HA	1.76	0.50
3:S:432:GLU:HG3	3:S:437:GLN:HB2	1.94	0.50
3:W:432:GLU:HG3	3:W:437:GLN:HB2	1.94	0.50
3:Y:459:ASP:H	3:Y:462:SER:HG	1.58	0.50
3:a:305:ALA:HA	3:a:314:MET:HA	1.94	0.50
3:b:376:PHE:CE2	3:b:380:ILE:HD11	2.47	0.50
1:A:322:GLU:HA	1:A:325:ILE:HG13	1.91	0.50
1:C:472:ASP:OD1	1:C:473:ASP:N	2.45	0.50
2:H:163:ILE:HD13	2:H:188:LEU:HD23	1.93	0.50
2:N:68:PHE:HA	2:N:71:PHE:CZ	2.46	0.50
3:R:318:ARG:NH2	3:R:330:ASP:O	2.44	0.50
3:S:340:TYR:CG	3:S:409:ILE:HD11	2.47	0.50
3:U:331:VAL:HB	3:U:333:LYS:HE3	1.92	0.50
3:U:473:ASP:OD1	3:Y:451:LYS:NZ	2.36	0.50
3:a:337:THR:H	3:a:342:ALA:HA	1.77	0.50
1:B:8:LEU:HD23	1:B:40:LYS:O	2.11	0.50
2:m:89:TYR:CD2	3:S:382:ARG:HD3	2.46	0.50
2:n:74:LEU:O	2:n:103:TYR:OH	2.27	0.50
2:N:58:ASP:HB3	2:N:219:ARG:O	2.12	0.50
3:S:416:SER:O	3:S:419:ARG:NH1	2.41	0.50
3:T:305:ALA:C	3:T:306:LEU:HD12	2.36	0.50
3:V:474:ALA:O	3:V:478:ASP:N	2.43	0.50
1:A:189:PRO:O	1:A:191:LYS:NZ	2.44	0.50
1:A:400:LEU:HD21	1:A:503:ILE:HD12	1.94	0.50
1:B:254:ARG:HH12	1:B:299:GLN:HB3	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:MET:O	1:E:397:ASN:ND2	2.44	0.50
2:o:163:ILE:HD12	2:o:188:LEU:HA	1.94	0.50
2:M:163:ILE:H	2:M:163:ILE:HD12	1.77	0.50
3:Q:382:ARG:HA	3:Q:385:ILE:HD12	1.93	0.50
3:T:339:ASP:O	3:T:502:ALA:N	2.45	0.50
3:W:345:ILE:HB	3:W:352:ALA:HB1	1.93	0.50
2:G:220:ARG:HH12	3:U:367:GLU:CD	2.20	0.50
2:N:90:ASP:HB3	2:N:93:ASP:CG	2.37	0.50
3:P:406:GLY:O	3:P:419:ARG:N	2.42	0.50
3:S:324:ASN:OD1	3:Z:479:SER:OG	2.27	0.50
3:T:424:ASP:OD1	3:T:427:GLY:N	2.44	0.50
3:U:484:PRO:HB3	3:U:491:PHE:CD1	2.46	0.50
3:W:436:TYR:HB2	3:W:450:MET:CE	2.40	0.50
1:A:220:GLU:C	1:A:222:ARG:H	2.20	0.50
1:A:350:GLN:HG3	1:A:387:VAL:HG11	1.94	0.50
1:C:195:LEU:HD22	1:C:341:ILE:HD11	1.93	0.50
2:k:30:VAL:O	2:k:156:MET:N	2.45	0.50
2:l:11:GLN:O	2:l:14:ARG:NH1	2.45	0.50
2:l:83:ASP:OD2	3:Q:365:HIS:ND1	2.37	0.50
2:m:189:ARG:HH11	2:m:203:LEU:HA	1.75	0.50
2:m:217:ARG:NH1	2:m:223:ARG:HB2	2.25	0.50
2:n:217:ARG:HH12	2:n:223:ARG:HB2	1.77	0.50
2:H:58:ASP:OD2	2:H:91:ARG:NH2	2.39	0.50
3:W:320:SER:HB3	3:W:331:VAL:HG21	1.93	0.50
3:a:419:ARG:HB3	3:a:431:ILE:HD11	1.94	0.50
1:A:364:HIS:CE1	1:A:443:GLN:HB3	2.47	0.50
1:C:69:ARG:HG3	1:C:81:VAL:HG13	1.93	0.50
1:E:47:LEU:HD13	1:E:51:LEU:HA	1.94	0.50
1:F:151:PRO:HB2	1:F:212:ASN:HB2	1.94	0.50
2:l:69:ASN:H	4:i:172:GLN:HE21	1.60	0.50
2:o:122:LEU:HB3	2:o:141:ILE:HG23	1.94	0.50
2:K:122:LEU:C	2:K:156:MET:HE1	2.37	0.50
1:B:91:TRP:HB2	1:B:132:TYR:CE1	2.46	0.49
1:B:141:GLU:HA	1:B:245:PHE:CE2	2.47	0.49
1:C:386:VAL:HG11	1:C:451:LEU:HD13	1.94	0.49
1:D:199:PRO:HD3	1:D:470:ASN:ND2	2.27	0.49
1:D:429:ARG:HB3	1:D:454:SER:OG	2.12	0.49
1:F:76:HIS:O	1:F:92:LEU:N	2.45	0.49
1:F:305:ASP:CG	1:F:334:ARG:HE	2.20	0.49
2:l:60:VAL:HG11	2:l:99:LEU:HD12	1.94	0.49
3:T:384:ALA:HB1	3:T:388:ARG:HH12	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:TRP:CD1	1:B:132:TYR:HE1	2.30	0.49
1:B:296:VAL:HG12	1:B:297:VAL:N	2.19	0.49
1:E:6:GLY:O	1:E:45:VAL:N	2.42	0.49
1:F:163:ARG:O	1:F:166:GLU:HG3	2.12	0.49
2:G:43:ALA:HB3	2:G:209:GLU:HG2	1.93	0.49
2:J:55:GLU:HG2	3:X:368:LYS:HZ1	1.77	0.49
3:S:322:GLN:HG2	3:S:325:MET:HB2	1.95	0.49
3:c:393:ALA:HB1	3:c:398:LEU:HB2	1.94	0.49
1:F:235:ASN:HB2	1:F:273:PHE:HD2	1.77	0.49
2:n:129:HIS:O	2:n:132:GLU:HG2	2.11	0.49
2:G:22:LYS:O	2:G:26:ARG:HG2	2.12	0.49
2:J:10:GLU:OE1	2:J:14:ARG:NH1	2.45	0.49
2:M:66:GLY:HA3	2:M:120:VAL:HG12	1.95	0.49
3:W:319:ARG:CZ	3:W:482:GLY:HA2	2.42	0.49
3:Z:307:LYS:HD2	3:Z:311:GLY:O	2.13	0.49
3:a:508:SER:O	3:a:512:GLU:HG2	2.11	0.49
2:m:141:ILE:HD13	2:m:147:ILE:HB	1.95	0.49
2:n:11:GLN:O	2:n:15:GLU:HG2	2.12	0.49
2:o:16:ARG:NH1	2:o:111:PHE:O	2.45	0.49
2:G:214:ASP:HB3	2:G:217:ARG:HG2	1.93	0.49
2:I:64:ALA:HB2	2:I:122:LEU:HD13	1.94	0.49
2:J:8:SER:OG	2:J:11:GLN:HG2	2.12	0.49
2:J:134:LYS:HZ2	2:J:136:PRO:HA	1.76	0.49
2:L:55:GLU:HB2	2:L:222:PHE:CG	2.47	0.49
2:L:205:VAL:HG13	2:L:230:LEU:HD23	1.95	0.49
3:R:475:ALA:HA	3:R:481:THR:HB	1.93	0.49
3:T:422:SER:OG	3:T:432:GLU:OE2	2.31	0.49
3:W:391:LEU:O	3:W:395:MET:HG2	2.12	0.49
1:A:179:LYS:O	1:A:183:ARG:HG3	2.12	0.49
1:B:102:PRO:C	1:B:116:ARG:HD2	2.37	0.49
1:B:232:TYR:CZ	1:B:263:LYS:HB3	2.48	0.49
2:k:74:LEU:O	2:k:103:TYR:OH	2.25	0.49
2:H:140:ARG:HB3	2:H:148:ALA:HB3	1.94	0.49
2:J:11:GLN:OE1	2:J:14:ARG:NH2	2.39	0.49
2:L:55:GLU:HG2	3:Z:368:LYS:HZ3	1.76	0.49
2:M:217:ARG:NH1	2:M:223:ARG:HB2	2.28	0.49
3:Z:495:VAL:HA	3:Z:504:ASP:HA	1.95	0.49
3:a:366:TYR:CZ	3:a:370:GLU:HG3	2.48	0.49
2:O:58:ASP:CG	2:O:91:ARG:HH21	2.21	0.49
1:B:353:TYR:HB3	1:B:383:ILE:HG12	1.95	0.49
1:D:321:ARG:HE	1:D:324:MET:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:LEU:HD23	1:E:465:LEU:HD21	1.94	0.49
1:F:257:PHE:CZ	1:F:274:PHE:HZ	2.30	0.49
2:l:101:ASN:O	2:l:105:GLN:HG2	2.13	0.49
2:n:89:TYR:CD1	3:T:382:ARG:HD3	2.47	0.49
2:H:18:GLU:HA	2:H:21:ARG:HG2	1.95	0.49
2:I:53:ILE:O	2:I:224:ARG:NH2	2.37	0.49
2:N:18:GLU:O	2:N:21:ARG:HG2	2.12	0.49
3:Z:393:ALA:O	3:Z:398:LEU:N	2.46	0.49
2:n:35:TYR:CE1	2:n:40:LEU:HG	2.48	0.49
2:H:152:HIS:HD2	2:H:171:TYR:CE2	2.29	0.49
2:M:122:LEU:HB3	2:M:141:ILE:HG23	1.94	0.49
2:N:178:THR:O	2:N:181:LEU:HG	2.13	0.49
1:A:425:ASN:ND2	1:A:458:GLU:OE1	2.46	0.49
1:B:348:ALA:O	1:B:352:ILE:HG13	2.13	0.49
1:D:237:LYS:HB2	1:D:239:PRO:HD2	1.94	0.49
1:D:379:ILE:HA	1:D:382:MET:HG3	1.94	0.49
2:l:8:SER:HB3	2:l:11:GLN:OE1	2.12	0.49
2:H:119:GLU:OE1	2:H:119:GLU:N	2.46	0.49
2:K:55:GLU:H	3:Y:368:LYS:HE2	1.78	0.49
2:L:57:TYR:CD2	2:L:94:VAL:HG21	2.47	0.49
2:L:107:LEU:HA	2:L:110:ILE:HG22	1.95	0.49
3:S:341:THR:HB	3:S:404:LEU:HD11	1.94	0.49
3:Z:301:THR:O	3:Z:441:SER:N	2.46	0.49
3:Z:378:GLY:O	3:Z:382:ARG:HG2	2.13	0.49
1:B:78:ALA:N	1:B:90:VAL:O	2.39	0.49
1:B:329:ILE:HG12	1:B:335:LEU:HD13	1.95	0.49
1:E:33:ASN:OD1	1:E:34:ILE:N	2.46	0.49
1:E:175:PRO:HB3	1:E:189:PRO:HB3	1.94	0.49
1:E:251:ARG:HA	1:E:254:ARG:NH2	2.27	0.49
1:F:46:ARG:HE	1:F:54:VAL:HG23	1.77	0.49
2:k:178:THR:O	2:k:182:ARG:HG2	2.13	0.49
2:o:29:SER:HA	2:o:156:MET:O	2.13	0.49
3:R:364:GLU:O	3:R:367:GLU:HG2	2.13	0.49
3:T:464:LEU:HD11	3:T:496:ILE:HD11	1.94	0.49
3:T:484:PRO:HB3	3:T:491:PHE:CD1	2.47	0.49
3:a:424:ASP:OD1	3:a:427:GLY:N	2.46	0.49
1:E:91:TRP:HB2	1:E:132:TYR:CD1	2.48	0.49
2:l:55:GLU:HB2	2:l:222:PHE:CG	2.47	0.49
2:n:43:ALA:HB3	2:n:209:GLU:HB3	1.94	0.49
2:L:121:GLU:HB3	2:L:156:MET:HE2	1.94	0.49
3:a:437:GLN:HA	3:a:447:LYS:HZ3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:457:VAL:HG22	3:c:466:VAL:HG21	1.95	0.49
3:c:508:SER:O	3:c:512:GLU:HG2	2.13	0.49
1:B:297:VAL:N	1:B:298:PRO:HD3	2.28	0.48
1:F:176:PHE:HE2	1:F:269:PRO:HB3	1.77	0.48
2:o:95:THR:H	2:o:98:GLN:CD	2.21	0.48
2:K:30:VAL:HB	2:K:156:MET:HB3	1.95	0.48
2:N:152:HIS:HB3	2:N:171:TYR:CE2	2.48	0.48
3:R:476:ASP:O	3:a:329:ARG:NH2	2.44	0.48
3:W:376:PHE:CE1	3:W:406:GLY:HA3	2.48	0.48
3:Z:305:ALA:HB2	3:Z:314:MET:HG2	1.94	0.48
1:E:429:ARG:HB3	1:E:454:SER:OG	2.13	0.48
1:F:352:ILE:HA	1:F:355:LYS:HE3	1.94	0.48
2:H:18:GLU:HG3	2:H:22:LYS:HZ1	1.77	0.48
2:L:95:THR:O	2:L:98:GLN:HG2	2.13	0.48
2:N:162:PRO:HA	2:N:165:ASN:HD21	1.78	0.48
3:U:307:LYS:HD2	3:U:311:GLY:O	2.14	0.48
3:c:436:TYR:HB2	3:c:450:MET:SD	2.53	0.48
1:E:322:GLU:HG2	1:F:501:ARG:HH12	1.78	0.48
1:F:493:THR:HG23	1:F:495:LYS:H	1.78	0.48
2:k:70:GLU:HB3	2:k:118:TYR:CD2	2.46	0.48
2:J:21:ARG:HH21	2:J:22:LYS:NZ	2.10	0.48
2:K:75:ARG:O	2:K:79:ILE:HG13	2.14	0.48
3:U:393:ALA:O	3:U:396:GLN:HG2	2.13	0.48
3:U:422:SER:OG	3:U:432:GLU:OE2	2.27	0.48
3:Z:303:ILE:N	3:Z:439:VAL:O	2.38	0.48
3:a:376:PHE:CE1	3:a:406:GLY:HA3	2.47	0.48
2:l:116:LYS:HD2	2:l:117:PRO:HD2	1.95	0.48
2:G:28:LYS:O	2:G:52:LYS:NZ	2.46	0.48
2:G:69:ASN:OD1	2:G:70:GLU:N	2.46	0.48
2:J:162:PRO:HA	2:J:165:ASN:HD22	1.79	0.48
3:R:346:ALA:O	3:R:401:LEU:N	2.30	0.48
3:S:319:ARG:HB3	3:S:482:GLY:H	1.78	0.48
3:S:488:ARG:NH2	3:Z:476:ASP:OD2	2.37	0.48
1:F:127:ASP:OD1	1:F:129:LYS:HG2	2.14	0.48
1:F:393:GLU:OE2	1:F:415:LYS:NZ	2.46	0.48
2:l:35:TYR:HB2	2:l:175:ALA:O	2.13	0.48
2:m:67:LYS:HG2	2:m:69:ASN:OD1	2.13	0.48
2:M:55:GLU:HA	2:M:61:GLY:HA2	1.96	0.48
2:M:71:PHE:HA	2:M:74:LEU:HD12	1.96	0.48
2:N:140:ARG:O	2:N:148:ALA:N	2.46	0.48
3:Q:355:PHE:CZ	3:Q:390:ASN:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:55:GLU:HB2	2:O:222:PHE:CG	2.48	0.48
1:B:236:ILE:HD13	1:B:274:PHE:CE1	2.48	0.48
1:D:451:LEU:O	1:D:455:ILE:HG13	2.14	0.48
1:E:422:MET:SD	1:E:462:ASN:ND2	2.85	0.48
1:F:451:LEU:O	1:F:455:ILE:HG13	2.13	0.48
2:k:217:ARG:NH1	2:k:223:ARG:HB2	2.29	0.48
2:l:87:TYR:HE1	3:Q:357:ARG:HG3	1.79	0.48
2:n:8:SER:OG	2:n:10:GLU:OE1	2.31	0.48
2:o:33:LEU:HD11	2:o:180:ALA:HB1	1.95	0.48
2:G:68:PHE:HA	2:G:71:PHE:CZ	2.49	0.48
2:I:79:ILE:HD13	3:P:368:LYS:HB3	1.96	0.48
3:Q:359:TYR:CE2	3:Q:363:LEU:HD11	2.48	0.48
3:S:421:VAL:HG22	3:S:431:ILE:HA	1.96	0.48
3:T:338:ASP:OD2	3:T:341:THR:HB	2.12	0.48
3:V:340:TYR:HD1	3:V:407:TYR:HB3	1.79	0.48
3:b:346:ALA:N	3:b:401:LEU:O	2.35	0.48
1:B:218:MET:HE3	1:B:230:LYS:HB2	1.94	0.48
1:D:402:VAL:HG12	1:D:488:ILE:HG12	1.95	0.48
1:E:40:LYS:HD2	1:E:59:PHE:HZ	1.78	0.48
1:E:386:VAL:HG11	1:E:451:LEU:HB3	1.96	0.48
2:o:28:LYS:NZ	4:e:174:LEU:HA	2.29	0.48
2:o:128:ALA:HB2	2:o:134:LYS:HE2	1.94	0.48
2:K:58:ASP:HB3	2:K:219:ARG:O	2.14	0.48
2:M:61:GLY:N	2:M:213:LEU:HD11	2.27	0.48
3:U:421:VAL:HG22	3:U:431:ILE:HG12	1.94	0.48
3:a:357:ARG:O	3:a:361:VAL:HG23	2.13	0.48
1:C:91:TRP:HB2	1:C:132:TYR:CD1	2.48	0.48
1:F:9:LEU:HD11	1:F:20:PHE:HB2	1.95	0.48
1:F:377:ALA:O	1:F:380:LYS:HG3	2.14	0.48
2:L:96:GLY:H	2:L:126:GLU:CD	2.20	0.48
3:U:393:ALA:O	3:U:398:LEU:HB2	2.14	0.48
3:c:392:ALA:HA	3:c:395:MET:HE3	1.96	0.48
3:c:419:ARG:O	3:c:421:VAL:HG23	2.13	0.48
2:O:58:ASP:HB3	2:O:219:ARG:O	2.14	0.48
2:O:102:VAL:O	2:O:105:GLN:HG3	2.13	0.48
1:A:8:LEU:HD23	1:A:40:LYS:O	2.13	0.48
1:B:76:HIS:O	1:B:92:LEU:N	2.33	0.48
1:B:151:PRO:HD3	1:B:232:TYR:C	2.39	0.48
1:B:400:LEU:HD12	1:B:490:THR:HA	1.96	0.48
2:k:55:GLU:HB2	2:k:222:PHE:CG	2.49	0.48
2:G:53:ILE:O	2:G:224:ARG:NH2	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:89:TYR:CD2	3:P:382:ARG:HD3	2.48	0.48
2:I:48:ARG:HH12	2:I:207:SER:HA	1.79	0.48
2:M:70:GLU:HG2	2:M:118:TYR:CD1	2.49	0.48
3:S:476:ASP:OD2	3:Z:488:ARG:NH2	2.36	0.48
3:U:459:ASP:H	3:U:462:SER:HG	1.60	0.48
3:a:461:ASP:CG	3:a:509:ARG:HH21	2.22	0.48
3:c:304:VAL:HA	3:c:438:ALA:HA	1.95	0.48
1:B:91:TRP:HB2	1:B:132:TYR:CD1	2.49	0.48
1:F:9:LEU:HD21	1:F:20:PHE:HB2	1.95	0.48
2:k:114:GLN:H	2:k:114:GLN:CD	2.20	0.48
2:o:28:LYS:HE3	2:o:46:PRO:HD2	1.95	0.48
2:o:56:LEU:HB2	2:o:60:VAL:HG12	1.96	0.48
2:o:137:GLU:N	2:o:137:GLU:OE1	2.47	0.48
2:H:151:PRO:HB2	2:H:152:HIS:ND1	2.28	0.48
2:I:65:ALA:N	2:I:121:GLU:O	2.46	0.48
3:X:376:PHE:HE1	3:X:406:GLY:HA3	1.78	0.48
3:c:319:ARG:O	3:c:333:LYS:NZ	2.40	0.48
2:O:69:ASN:OD1	2:O:70:GLU:N	2.46	0.48
1:B:472:ASP:O	1:B:476:ARG:HG3	2.14	0.47
1:E:304:ILE:HA	1:E:307:VAL:HG12	1.96	0.47
2:n:19:LEU:HA	2:n:22:LYS:NZ	2.28	0.47
2:G:178:THR:O	2:G:181:LEU:HG	2.14	0.47
2:K:99:LEU:HD11	2:K:124:VAL:HG21	1.96	0.47
2:L:26:ARG:HG2	2:L:26:ARG:O	2.14	0.47
3:S:393:ALA:O	3:S:398:LEU:N	2.47	0.47
3:V:505:VAL:HG13	3:V:509:ARG:NH2	2.29	0.47
3:Y:421:VAL:HA	3:Y:430:ASN:O	2.14	0.47
3:c:345:ILE:HG12	3:c:402:PRO:HB3	1.96	0.47
1:B:244:LYS:HA	1:B:249:THR:HG23	1.96	0.47
2:n:28:LYS:HB2	2:n:52:LYS:NZ	2.29	0.47
2:H:69:ASN:OD1	2:H:70:GLU:N	2.47	0.47
2:I:161:GLU:O	2:I:165:ASN:ND2	2.46	0.47
2:J:59:ARG:HB3	2:J:127:VAL:HG23	1.95	0.47
2:J:152:HIS:HB3	2:J:171:TYR:CE2	2.49	0.47
2:K:28:LYS:HE2	2:K:46:PRO:HD3	1.96	0.47
2:L:63:ALA:HB3	2:L:123:CYS:HB3	1.97	0.47
2:L:102:VAL:O	2:L:105:GLN:HG3	2.13	0.47
3:R:393:ALA:O	3:R:398:LEU:HB2	2.14	0.47
3:S:307:LYS:HE2	3:S:418:GLY:H	1.78	0.47
3:U:306:LEU:HA	3:U:436:TYR:HA	1.94	0.47
3:V:447:LYS:HA	3:V:450:MET:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:393:ALA:HB1	3:Y:398:LEU:HB2	1.96	0.47
1:A:353:TYR:CZ	1:A:423:ILE:HG23	2.48	0.47
1:B:179:LYS:O	1:B:183:ARG:HD3	2.14	0.47
1:B:255:LEU:O	1:B:259:ARG:HG2	2.13	0.47
1:F:268:THR:O	1:F:312:ASN:ND2	2.46	0.47
2:n:18:GLU:O	2:n:22:LYS:HG2	2.14	0.47
2:n:219:ARG:HE	2:n:220:ARG:HG3	1.79	0.47
2:o:55:GLU:HB2	2:o:222:PHE:CG	2.49	0.47
2:o:159:THR:O	2:o:162:PRO:HD2	2.14	0.47
2:H:58:ASP:HB3	2:H:219:ARG:O	2.14	0.47
2:H:135:ARG:HH11	2:H:136:PRO:HD2	1.78	0.47
2:I:150:GLU:OE1	2:I:152:HIS:N	2.41	0.47
2:M:53:ILE:HD12	2:M:209:GLU:HG2	1.96	0.47
2:O:96:GLY:N	2:O:126:GLU:OE1	2.44	0.47
1:C:418:ASN:OD1	1:C:419:SER:N	2.47	0.47
1:D:398:ARG:HA	1:D:413:TYR:CD1	2.49	0.47
1:E:176:PHE:CD2	1:E:214:LEU:HD21	2.49	0.47
2:m:68:PHE:HA	2:m:71:PHE:CE2	2.49	0.47
2:n:68:PHE:HA	2:n:71:PHE:CE2	2.49	0.47
2:G:19:LEU:HD21	2:G:116:LYS:HE3	1.96	0.47
3:Q:484:PRO:HB3	3:Q:491:PHE:CD1	2.49	0.47
3:U:461:ASP:HA	3:U:464:LEU:HD12	1.96	0.47
1:B:146:VAL:HG13	1:B:256:ILE:HG22	1.97	0.47
1:B:434:ALA:HB2	1:B:446:LEU:HG	1.95	0.47
1:E:118:LEU:HD13	1:E:124:LEU:HD11	1.96	0.47
1:F:204:THR:O	1:F:208:LYS:HG3	2.15	0.47
1:F:246:VAL:HG13	1:F:251:ARG:NH2	2.27	0.47
2:k:14:ARG:O	2:k:18:GLU:HG2	2.14	0.47
2:k:99:LEU:HA	2:k:102:VAL:HG12	1.96	0.47
2:K:102:VAL:O	2:K:105:GLN:HG3	2.14	0.47
3:W:301:THR:N	3:W:441:SER:OG	2.48	0.47
1:C:311:GLU:O	1:C:313:VAL:N	2.48	0.47
1:D:400:LEU:HB2	1:D:412:MET:HE3	1.97	0.47
2:N:116:LYS:NZ	2:N:117:PRO:O	2.47	0.47
3:W:330:ASP:N	3:W:330:ASP:OD1	2.46	0.47
3:X:378:GLY:O	3:X:382:ARG:HG2	2.15	0.47
3:Y:346:ALA:O	3:Y:401:LEU:N	2.25	0.47
3:Z:367:GLU:O	3:Z:371:GLY:N	2.46	0.47
2:O:99:LEU:HA	2:O:102:VAL:HG12	1.97	0.47
1:C:68:LEU:HD22	1:C:124:LEU:HD11	1.97	0.47
1:C:412:MET:HE3	1:C:477:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:ALA:O	1:E:97:ILE:HG12	2.14	0.47
1:E:185:TYR:HB2	1:F:435:ILE:HD11	1.95	0.47
1:F:91:TRP:HB2	1:F:132:TYR:CD1	2.50	0.47
2:k:107:LEU:HD12	2:k:143:TYR:HA	1.95	0.47
2:m:58:ASP:HB3	2:m:219:ARG:O	2.14	0.47
2:o:44:GLU:OE1	2:o:46:PRO:HD3	2.15	0.47
2:o:220:ARG:HH12	3:T:367:GLU:CD	2.22	0.47
2:G:18:GLU:HA	2:G:21:ARG:CD	2.45	0.47
2:G:222:PHE:CE2	2:G:224:ARG:HG3	2.49	0.47
2:H:16:ARG:O	2:H:19:LEU:HG	2.14	0.47
2:H:68:PHE:HB3	4:g:172:GLN:NE2	2.30	0.47
2:M:56:LEU:HG	2:M:62:PHE:HB2	1.96	0.47
2:M:118:TYR:HB3	2:M:120:VAL:HG22	1.97	0.47
3:P:337:THR:H	3:P:342:ALA:HA	1.79	0.47
3:R:337:THR:H	3:R:342:ALA:HA	1.79	0.47
3:S:402:PRO:HG2	3:S:423:PHE:CD2	2.49	0.47
3:U:304:VAL:HA	3:U:438:ALA:HA	1.96	0.47
3:U:305:ALA:HB2	3:U:314:MET:SD	2.54	0.47
3:V:382:ARG:HA	3:V:385:ILE:HD12	1.97	0.47
3:W:406:GLY:O	3:W:419:ARG:N	2.46	0.47
3:Y:366:TYR:O	3:Y:370:GLU:HG2	2.15	0.47
3:Z:365:HIS:NE2	3:Z:369:LEU:HD11	2.30	0.47
3:a:438:ALA:N	3:a:447:LYS:HD3	2.30	0.47
1:E:473:ASP:O	1:E:476:ARG:HG2	2.13	0.47
2:k:30:VAL:HB	2:k:156:MET:HB2	1.96	0.47
2:k:74:LEU:HB3	2:k:103:TYR:HE1	1.80	0.47
2:m:56:LEU:H	2:m:61:GLY:HA2	1.80	0.47
2:L:25:ALA:O	2:L:158:GLY:HA2	2.14	0.47
3:Q:509:ARG:O	3:Q:512:GLU:HG2	2.15	0.47
3:S:319:ARG:CZ	3:S:482:GLY:HA2	2.45	0.47
3:b:459:ASP:H	3:b:462:SER:HG	1.60	0.47
1:B:343:ARG:NH2	1:B:473:ASP:OD2	2.48	0.47
1:E:386:VAL:HG11	1:E:451:LEU:HD13	1.97	0.47
1:F:466:PRO:HD2	1:F:501:ARG:HH21	1.80	0.47
2:l:89:TYR:O	3:R:378:GLY:HA2	2.15	0.47
2:H:96:GLY:H	2:H:126:GLU:CD	2.23	0.47
2:K:103:TYR:O	2:K:107:LEU:HD23	2.15	0.47
2:M:99:LEU:HD11	2:M:124:VAL:HG21	1.96	0.47
2:M:178:THR:HB	2:M:182:ARG:NH1	2.30	0.47
3:P:391:LEU:O	3:P:395:MET:HG2	2.15	0.47
3:T:322:GLN:HB2	3:T:325:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:447:LYS:HA	3:T:450:MET:HE3	1.95	0.47
3:X:422:SER:O	3:X:430:ASN:N	2.43	0.47
3:c:436:TYR:CD1	3:c:450:MET:HE3	2.48	0.47
1:A:181:LEU:HD23	1:B:435:ILE:HG23	1.96	0.47
1:D:353:TYR:CZ	1:D:390:MET:HE1	2.50	0.47
1:F:402:VAL:HG13	1:F:485:ILE:HG23	1.97	0.47
2:l:156:MET:HA	2:l:156:MET:HE3	1.97	0.47
2:m:22:LYS:HB3	2:m:26:ARG:NH1	2.30	0.47
2:o:124:VAL:HB	2:o:139:TYR:HB2	1.97	0.47
2:G:28:LYS:CD	2:G:44:GLU:HG3	2.43	0.47
2:G:67:LYS:HA	4:f:172:GLN:O	2.15	0.47
2:I:14:ARG:NH1	2:I:15:GLU:OE2	2.47	0.47
2:J:58:ASP:CG	2:J:91:ARG:HH21	2.22	0.47
2:M:59:ARG:NH2	2:M:128:ALA:O	2.45	0.47
3:P:306:LEU:O	3:P:313:VAL:HG12	2.15	0.47
3:U:357:ARG:O	3:U:361:VAL:HG23	2.15	0.47
3:V:320:SER:O	3:V:328:GLY:N	2.33	0.47
3:Y:438:ALA:N	3:Y:447:LYS:HD3	2.30	0.47
1:A:140:ALA:C	1:A:142:VAL:H	2.23	0.46
1:A:192:GLY:HA3	1:A:335:LEU:HG	1.97	0.46
1:A:352:ILE:HG23	1:A:355:LYS:HE3	1.96	0.46
1:B:402:VAL:HG23	1:B:412:MET:HE1	1.96	0.46
2:k:58:ASP:CG	2:k:91:ARG:HH21	2.24	0.46
2:l:62:PHE:CZ	2:l:75:ARG:HB2	2.50	0.46
2:m:41:PHE:HE2	2:m:213:LEU:HG	1.80	0.46
2:G:57:TYR:CG	2:G:58:ASP:N	2.83	0.46
2:K:16:ARG:HG2	2:K:117:PRO:HG3	1.96	0.46
2:M:59:ARG:HB3	2:M:127:VAL:HG23	1.97	0.46
2:N:161:GLU:O	2:N:165:ASN:ND2	2.48	0.46
3:S:460:GLY:O	3:S:464:LEU:HG	2.14	0.46
3:W:363:LEU:HD12	3:W:364:GLU:N	2.31	0.46
3:W:401:LEU:O	3:W:401:LEU:HD12	2.15	0.46
3:X:436:TYR:CD1	3:X:450:MET:HE3	2.51	0.46
3:Y:320:SER:O	3:Y:327:SER:N	2.46	0.46
3:c:319:ARG:CZ	3:c:482:GLY:HA2	2.44	0.46
1:A:198:PRO:HG3	1:A:343:ARG:HG3	1.96	0.46
1:B:203:LYS:HA	1:B:206:ILE:HD13	1.97	0.46
1:B:425:ASN:ND2	1:B:458:GLU:OE1	2.47	0.46
1:D:364:HIS:HA	1:D:445:GLY:HA3	1.96	0.46
1:F:172:VAL:C	1:F:175:PRO:HD2	2.40	0.46
2:l:11:GLN:O	2:l:14:ARG:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:129:HIS:HB2	2:m:132:GLU:CD	2.39	0.46
2:m:154:VAL:HG12	2:m:156:MET:SD	2.56	0.46
2:G:141:ILE:HG13	2:G:147:ILE:HD13	1.97	0.46
2:H:35:TYR:N	2:H:38:GLY:O	2.46	0.46
3:Q:345:ILE:HG12	3:Q:402:PRO:HB3	1.97	0.46
3:S:408:ASP:HB3	3:S:411:ALA:HB2	1.97	0.46
3:W:341:THR:HG22	3:W:406:GLY:HA3	1.97	0.46
3:c:458:THR:H	3:c:462:SER:HG	1.62	0.46
1:A:501:ARG:NH1	1:F:322:GLU:OE2	2.44	0.46
1:B:182:TYR:CD1	1:C:435:ILE:HD13	2.51	0.46
1:C:68:LEU:HA	1:C:80:VAL:HG12	1.98	0.46
1:D:386:VAL:O	1:D:390:MET:HG3	2.16	0.46
1:E:343:ARG:HD2	1:E:416:ASP:O	2.15	0.46
1:F:331:ARG:HH21	1:F:334:ARG:NH2	2.13	0.46
2:k:50:LEU:HB3	2:k:68:PHE:CZ	2.50	0.46
2:m:18:GLU:O	2:m:22:LYS:HG3	2.16	0.46
2:n:55:GLU:HB2	2:n:222:PHE:CG	2.50	0.46
2:H:54:SER:O	2:H:62:PHE:N	2.49	0.46
2:H:205:VAL:HG22	2:H:234:LEU:HG	1.97	0.46
2:L:41:PHE:CE2	2:L:63:ALA:HB2	2.50	0.46
3:R:318:ARG:HA	3:R:331:VAL:O	2.15	0.46
3:X:307:LYS:O	3:X:454:TYR:OH	2.29	0.46
3:X:376:PHE:CE1	3:X:406:GLY:HA3	2.50	0.46
3:X:447:LYS:HD2	3:X:450:MET:HE2	1.97	0.46
2:O:28:LYS:HB3	2:O:44:GLU:HG3	1.98	0.46
1:A:93:ALA:O	1:A:97:ILE:HG12	2.15	0.46
1:A:340:LYS:HE3	1:A:342:GLU:HB3	1.97	0.46
1:E:126:VAL:HG12	1:E:133:ALA:HA	1.96	0.46
1:F:69:ARG:HG3	1:F:81:VAL:HG23	1.96	0.46
2:l:58:ASP:HB3	2:l:219:ARG:O	2.15	0.46
2:m:92:ARG:NH2	2:m:132:GLU:OE2	2.39	0.46
2:K:77:GLY:HA2	2:K:80:GLN:CD	2.39	0.46
2:K:140:ARG:HE	2:K:154:VAL:HG13	1.80	0.46
2:N:10:GLU:OE1	2:N:14:ARG:NH1	2.48	0.46
2:N:30:VAL:HB	2:N:156:MET:HB3	1.96	0.46
3:S:393:ALA:HA	3:S:396:GLN:HE21	1.81	0.46
3:a:421:VAL:HA	3:a:430:ASN:O	2.15	0.46
1:A:89:VAL:HG23	1:B:65:ILE:HD11	1.98	0.46
1:B:185:TYR:HB2	1:C:435:ILE:HD11	1.97	0.46
1:B:233:PHE:CD1	1:B:271:ILE:HB	2.51	0.46
1:D:191:LYS:HG2	1:D:308:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ARG:CZ	1:D:491:LEU:HB2	2.46	0.46
1:E:177:LEU:HD21	1:E:217:LYS:HD2	1.98	0.46
1:F:208:LYS:HG2	1:F:233:PHE:CZ	2.44	0.46
2:I:178:THR:O	2:I:181:LEU:HG	2.16	0.46
2:J:217:ARG:NH1	2:J:223:ARG:HB2	2.30	0.46
2:L:31:VAL:HG12	2:L:155:VAL:HG13	1.96	0.46
3:P:366:TYR:CZ	3:P:370:GLU:HG3	2.50	0.46
2:O:103:TYR:HA	2:O:106:THR:HG22	1.97	0.46
1:A:261:ARG:HA	1:A:264:ALA:HB3	1.98	0.46
1:D:176:PHE:HE2	1:D:269:PRO:HB3	1.80	0.46
1:D:211:ALA:HA	1:D:271:ILE:HD12	1.96	0.46
1:E:192:GLY:HA3	1:E:335:LEU:HA	1.98	0.46
1:E:264:ALA:CB	1:E:310:LEU:HD21	2.45	0.46
1:E:398:ARG:HG2	1:E:413:TYR:CE1	2.50	0.46
1:F:232:TYR:HE1	1:F:269:PRO:HB2	1.79	0.46
2:G:137:GLU:HB3	2:G:139:TYR:CE1	2.51	0.46
2:I:58:ASP:HB3	2:I:219:ARG:O	2.15	0.46
2:K:53:ILE:HG23	2:K:62:PHE:O	2.15	0.46
2:L:56:LEU:N	2:L:60:VAL:O	2.43	0.46
3:T:464:LEU:O	3:T:468:VAL:HG22	2.16	0.46
3:W:318:ARG:HA	3:W:331:VAL:O	2.16	0.46
3:Y:384:ALA:HA	3:Y:387:VAL:HG12	1.96	0.46
3:a:314:MET:HE1	3:a:334:VAL:HG13	1.96	0.46
3:b:378:GLY:O	3:b:382:ARG:HG2	2.15	0.46
1:D:216:LYS:HZ1	1:D:230:LYS:HA	1.80	0.46
2:l:68:PHE:HA	2:l:71:PHE:CE2	2.50	0.46
2:n:75:ARG:NH2	3:S:369:LEU:O	2.42	0.46
2:o:28:LYS:HD2	2:o:44:GLU:OE1	2.16	0.46
2:G:167:LEU:O	2:G:171:TYR:N	2.49	0.46
2:J:107:LEU:HA	2:J:110:ILE:HG12	1.98	0.46
2:M:52:LYS:HE2	2:M:65:ALA:HA	1.98	0.46
3:S:421:VAL:HG13	3:S:430:ASN:C	2.40	0.46
3:X:301:THR:N	3:X:441:SER:HG	2.13	0.46
3:Y:350:ALA:HB1	3:Z:388:ARG:HH21	1.79	0.46
1:A:28:LEU:HD22	1:A:51:LEU:HB3	1.97	0.46
1:A:71:ILE:HD12	1:A:92:LEU:HD11	1.98	0.46
1:A:119:ARG:HH22	1:A:259:ARG:HH11	1.64	0.46
1:A:352:ILE:O	1:A:355:LYS:HG2	2.16	0.46
1:C:278:ASP:OD1	1:C:278:ASP:N	2.49	0.46
2:k:18:GLU:HB3	2:k:22:LYS:HZ3	1.81	0.46
2:K:107:LEU:HA	2:K:110:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:88:ALA:O	3:b:381:ASN:ND2	2.49	0.46
2:N:74:LEU:HB3	2:N:103:TYR:HE1	1.81	0.46
2:N:112:THR:HA	2:O:116:LYS:NZ	2.30	0.46
3:Y:322:GLN:N	3:Y:325:MET:O	2.41	0.46
3:Y:422:SER:HB3	3:Y:437:GLN:HG2	1.98	0.46
1:A:46:ARG:HB3	1:A:55:GLU:HB3	1.98	0.46
1:B:340:LYS:HE2	1:B:342:GLU:HB3	1.97	0.46
1:E:357:LEU:HB2	1:E:383:ILE:HD11	1.97	0.46
1:E:364:HIS:HA	1:E:445:GLY:HA3	1.98	0.46
1:F:204:THR:HG22	1:F:208:LYS:HE3	1.98	0.46
2:o:89:TYR:CD2	3:U:382:ARG:HD3	2.51	0.46
2:o:205:VAL:HG22	2:o:234:LEU:HD11	1.96	0.46
2:G:45:ASN:ND2	2:G:50:LEU:O	2.49	0.46
2:J:176:SER:OG	2:J:179:ASP:OD2	2.25	0.46
3:R:360:ALA:O	3:R:363:LEU:HG	2.16	0.46
3:S:420:ILE:O	3:S:431:ILE:HD12	2.16	0.46
3:Y:306:LEU:HD21	3:Y:450:MET:HG3	1.97	0.46
3:c:308:TYR:OH	3:c:498:ASP:HB3	2.16	0.46
3:c:446:ALA:O	3:c:450:MET:HG2	2.16	0.46
1:B:171:ALA:O	1:B:190:PRO:HG2	2.16	0.46
2:k:42:VAL:HG22	2:k:210:VAL:HG22	1.97	0.46
2:k:142:THR:OG1	2:k:146:SER:HB2	2.16	0.46
2:G:122:LEU:HG	2:G:141:ILE:HD13	1.98	0.46
2:K:87:TYR:O	3:Y:357:ARG:NH2	2.48	0.46
2:N:71:PHE:HA	2:N:74:LEU:HD12	1.97	0.46
3:P:484:PRO:HB3	3:P:491:PHE:CD1	2.49	0.46
3:S:340:TYR:OH	3:S:499:ALA:O	2.30	0.46
3:S:473:ASP:CG	3:S:521:ARG:HH22	2.24	0.46
3:T:392:ALA:HA	3:T:395:MET:HE3	1.98	0.46
3:X:383:LEU:HD23	3:X:423:PHE:CZ	2.51	0.46
3:Z:438:ALA:N	3:Z:447:LYS:HD3	2.31	0.46
1:A:91:TRP:CD1	1:A:132:TYR:HE1	2.34	0.45
1:B:419:SER:O	1:B:423:ILE:HG12	2.16	0.45
1:E:96:LEU:HB3	1:E:118:LEU:HD11	1.98	0.45
2:K:54:SER:H	2:K:62:PHE:HB3	1.79	0.45
2:L:212:VAL:HG22	2:L:225:ILE:HD11	1.98	0.45
2:M:109:THR:O	2:M:112:THR:N	2.48	0.45
2:N:161:GLU:HG3	2:N:162:PRO:HD3	1.99	0.45
3:S:340:TYR:HD1	3:S:407:TYR:HB3	1.81	0.45
3:S:509:ARG:O	3:S:512:GLU:HG2	2.16	0.45
3:V:456:GLN:OE1	3:V:456:GLN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LYS:HG3	1:B:245:PHE:N	2.30	0.45
1:E:194:LEU:HD22	1:E:330:LEU:HD11	1.98	0.45
1:F:464:ASP:HB2	1:F:498:SER:HB2	1.97	0.45
2:l:16:ARG:HG3	2:l:117:PRO:HG3	1.98	0.45
2:n:55:GLU:HG2	3:S:368:LYS:NZ	2.31	0.45
2:n:97:ARG:NH2	3:T:370:GLU:O	2.48	0.45
2:H:45:ASN:O	2:H:48:ARG:NH2	2.49	0.45
2:K:65:ALA:HB3	2:K:156:MET:HG2	1.98	0.45
2:L:107:LEU:HA	2:L:107:LEU:HD23	1.81	0.45
2:M:138:LEU:O	2:M:150:GLU:N	2.25	0.45
2:M:142:THR:HG22	2:M:146:SER:HB3	1.97	0.45
2:N:142:THR:OG1	2:N:146:SER:HB2	2.15	0.45
3:R:306:LEU:HD11	3:R:450:MET:SD	2.57	0.45
3:S:481:THR:O	3:S:482:GLY:C	2.57	0.45
3:T:320:SER:C	3:T:327:SER:HG	2.24	0.45
3:a:317:ASP:HA	3:a:492:PRO:HB3	1.98	0.45
1:A:68:LEU:HD22	1:A:124:LEU:HD11	1.97	0.45
1:A:352:ILE:HA	1:A:355:LYS:HE3	1.97	0.45
1:B:402:VAL:HG13	1:B:485:ILE:HG23	1.97	0.45
1:B:429:ARG:NH2	1:B:458:GLU:OE1	2.48	0.45
1:C:24:ARG:NH1	1:C:25:LYS:HD2	2.31	0.45
1:C:60:GLU:HB2	1:C:134:PHE:CE2	2.52	0.45
1:C:91:TRP:CD1	1:C:132:TYR:HE1	2.34	0.45
1:D:357:LEU:HA	1:D:361:LEU:HD12	1.98	0.45
2:k:80:GLN:HA	3:W:365:HIS:HE1	1.81	0.45
2:l:28:LYS:HD2	2:l:44:GLU:HG3	1.97	0.45
2:n:140:ARG:HH22	2:n:155:VAL:H	1.64	0.45
2:I:17:SER:OG	2:I:21:ARG:NH2	2.49	0.45
2:I:163:ILE:HG22	2:I:190:ALA:HB3	1.98	0.45
2:L:16:ARG:HG3	2:L:117:PRO:HD3	1.99	0.45
2:L:54:SER:OG	2:L:55:GLU:N	2.48	0.45
2:M:16:ARG:NH1	2:M:114:GLN:O	2.49	0.45
2:N:181:LEU:HD21	2:N:233:LEU:HB3	1.98	0.45
3:Z:322:GLN:OE1	3:Z:327:SER:HB3	2.16	0.45
2:O:68:PHE:HA	2:O:71:PHE:CZ	2.51	0.45
1:A:389:ARG:NH1	1:A:397:ASN:OD1	2.48	0.45
1:B:296:VAL:CG1	1:B:297:VAL:H	2.20	0.45
1:D:16:THR:HG1	1:D:27:ARG:HH21	1.59	0.45
1:D:193:VAL:HG22	1:D:316:ILE:HG12	1.99	0.45
1:E:429:ARG:NH2	1:E:458:GLU:OE1	2.37	0.45
1:F:403:THR:HB	1:F:487:TYR:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:164:ALA:O	2:l:168:LYS:HG3	2.17	0.45
2:G:166:ALA:O	2:G:170:SER:OG	2.26	0.45
2:H:87:TYR:O	3:V:357:ARG:NH2	2.48	0.45
2:L:23:GLY:O	2:L:26:ARG:NH1	2.50	0.45
3:R:376:PHE:CE1	3:R:406:GLY:HA3	2.51	0.45
3:W:304:VAL:HA	3:W:438:ALA:HA	1.97	0.45
3:W:382:ARG:O	3:W:386:MET:HG2	2.16	0.45
3:Z:450:MET:HE3	3:Z:454:TYR:HA	1.98	0.45
1:A:139:LYS:NZ	1:A:246:VAL:HG13	2.31	0.45
1:D:65:ILE:HD13	1:D:125:LEU:HA	1.97	0.45
1:D:386:VAL:HG11	1:D:451:LEU:HD13	1.98	0.45
1:D:466:PRO:HG3	1:D:490:THR:HG21	1.98	0.45
1:E:91:TRP:HB2	1:E:132:TYR:CE1	2.51	0.45
1:E:393:GLU:HA	1:E:415:LYS:NZ	2.31	0.45
1:F:96:LEU:HD22	1:F:118:LEU:HD11	1.98	0.45
2:l:74:LEU:HB3	2:l:103:TYR:HE1	1.81	0.45
2:n:93:ASP:OD1	3:T:375:THR:OG1	2.30	0.45
2:L:97:ARG:HD2	2:L:101:ASN:OD1	2.16	0.45
3:R:308:TYR:CE1	3:R:496:ILE:HD11	2.51	0.45
1:E:196:TYR:OH	1:F:464:ASP:OD2	2.23	0.45
1:F:8:LEU:HD23	1:F:40:LYS:O	2.17	0.45
2:m:138:LEU:HD13	2:m:154:VAL:HG23	1.99	0.45
2:n:46:PRO:HD2	4:d:174:LEU:HD22	1.99	0.45
2:o:205:VAL:HG22	2:o:234:LEU:HD21	1.99	0.45
2:K:33:LEU:HD21	2:K:40:LEU:HD23	1.97	0.45
3:P:495:VAL:HG22	3:P:504:ASP:HA	1.98	0.45
3:U:374:LEU:O	3:U:379:LYS:NZ	2.50	0.45
3:Y:320:SER:HB3	3:Y:328:GLY:N	2.31	0.45
3:Y:368:LYS:HD2	3:Y:368:LYS:HA	1.68	0.45
3:Z:304:VAL:HA	3:Z:438:ALA:HA	1.97	0.45
2:O:103:TYR:O	2:O:107:LEU:HD23	2.17	0.45
1:E:321:ARG:NE	1:E:324:MET:HE1	2.21	0.45
1:E:490:THR:OG1	1:E:501:ARG:N	2.42	0.45
1:F:274:PHE:HD2	1:F:277:MET:HE2	1.82	0.45
1:F:348:ALA:O	1:F:352:ILE:HG13	2.15	0.45
2:l:130:TYR:HB2	2:l:217:ARG:O	2.17	0.45
2:H:101:ASN:O	2:H:105:GLN:HG2	2.17	0.45
2:I:48:ARG:NH2	2:I:207:SER:H	2.14	0.45
2:I:181:LEU:HD21	2:I:233:LEU:HD12	1.97	0.45
2:K:152:HIS:HB3	2:K:171:TYR:CE2	2.52	0.45
3:R:447:LYS:HD2	3:R:450:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:508:SER:O	3:U:512:GLU:HG3	2.17	0.45
3:b:509:ARG:O	3:b:512:GLU:HG2	2.16	0.45
2:O:56:LEU:HB2	2:O:60:VAL:HG12	1.99	0.45
2:O:167:LEU:O	2:O:171:TYR:N	2.50	0.45
1:A:65:ILE:HB	1:F:87:GLU:HB2	1.97	0.45
1:A:449:GLN:HA	1:A:452:LEU:HB2	1.98	0.45
1:D:386:VAL:C	1:D:390:MET:HE3	2.42	0.45
1:E:164:GLN:NE2	1:E:206:ILE:HG21	2.30	0.45
2:k:18:GLU:CD	2:k:21:ARG:HH12	2.24	0.45
2:G:40:LEU:HD23	2:G:41:PHE:N	2.32	0.45
2:G:83:ASP:OD1	3:U:361:VAL:HG13	2.17	0.45
2:M:80:GLN:HA	3:a:365:HIS:CE1	2.51	0.45
3:Q:376:PHE:HA	3:Q:379:LYS:HE2	1.99	0.45
3:R:378:GLY:O	3:R:382:ARG:HG2	2.17	0.45
3:R:383:LEU:HD23	3:R:423:PHE:CZ	2.52	0.45
3:R:424:ASP:OD1	3:R:427:GLY:N	2.50	0.45
3:a:301:THR:O	3:a:441:SER:N	2.47	0.45
1:B:264:ALA:HB1	1:B:310:LEU:HD21	1.98	0.45
1:D:357:LEU:HD12	1:D:383:ILE:HG12	1.99	0.45
1:F:202:GLY:O	1:F:206:ILE:HG13	2.17	0.45
2:G:59:ARG:HA	2:G:221:ALA:HB3	1.99	0.45
2:I:60:VAL:HG11	2:I:99:LEU:HD12	1.99	0.45
2:M:56:LEU:HD21	2:M:62:PHE:CD2	2.47	0.45
2:M:116:LYS:NZ	2:M:119:GLU:HG3	2.31	0.45
2:M:217:ARG:HH12	2:M:223:ARG:HB2	1.82	0.45
3:R:359:TYR:OH	3:R:379:LYS:O	2.31	0.45
3:S:382:ARG:HA	3:S:385:ILE:HD12	1.99	0.45
3:S:461:ASP:HA	3:S:464:LEU:HD12	1.98	0.45
3:U:330:ASP:OD1	3:U:330:ASP:N	2.46	0.45
3:U:375:THR:C	3:U:379:LYS:HZ3	2.25	0.45
3:V:301:THR:O	3:V:441:SER:N	2.49	0.45
3:Y:378:GLY:O	3:Y:382:ARG:HG2	2.17	0.45
1:A:4:GLY:N	1:A:47:LEU:O	2.50	0.45
1:A:5:TYR:HE1	1:F:27:ARG:HB2	1.82	0.45
1:C:28:LEU:HD22	1:C:51:LEU:HB3	1.99	0.45
2:G:89:TYR:O	3:V:378:GLY:HA2	2.17	0.45
3:Q:304:VAL:O	3:Q:314:MET:HG2	2.17	0.45
3:S:378:GLY:O	3:S:382:ARG:HG2	2.17	0.45
3:U:507:GLU:HA	3:U:510:ILE:HD12	1.98	0.45
3:W:355:PHE:CE1	3:W:386:MET:HB3	2.51	0.45
3:X:393:ALA:HB1	3:X:398:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:436:TYR:HB2	3:X:450:MET:SD	2.57	0.45
3:Y:318:ARG:HB3	3:Y:330:ASP:HA	1.99	0.45
3:Z:376:PHE:CE1	3:Z:406:GLY:HA3	2.51	0.45
3:b:475:ALA:HA	3:b:481:THR:HB	1.98	0.45
1:A:271:ILE:HG23	1:A:314:ILE:HG13	1.99	0.44
1:D:117:LYS:HD2	1:D:117:LYS:HA	1.68	0.44
1:D:254:ARG:NH1	1:D:258:GLN:OE1	2.50	0.44
1:D:261:ARG:HA	1:D:264:ALA:HB3	1.98	0.44
1:F:257:PHE:HD2	1:F:303:GLU:HB3	1.81	0.44
2:k:121:GLU:OE2	2:k:140:ARG:HG3	2.16	0.44
2:k:178:THR:HG22	2:k:233:LEU:HD12	1.98	0.44
2:k:220:ARG:NH2	3:W:367:GLU:OE1	2.50	0.44
2:G:217:ARG:NH1	2:G:222:PHE:O	2.49	0.44
2:J:109:THR:O	2:J:112:THR:OG1	2.28	0.44
2:K:46:PRO:CA	2:K:207:SER:HA	2.40	0.44
3:P:376:PHE:CE2	3:P:408:ASP:HA	2.52	0.44
3:S:307:LYS:HD2	3:S:311:GLY:O	2.17	0.44
1:B:27:ARG:CD	1:C:46:ARG:HD2	2.47	0.44
1:B:232:TYR:HE1	1:B:270:VAL:HB	1.82	0.44
1:E:91:TRP:CD1	1:E:132:TYR:HE1	2.34	0.44
2:m:107:LEU:HD22	2:m:141:ILE:HG22	1.99	0.44
2:n:28:LYS:HB2	2:n:52:LYS:HZ3	1.81	0.44
2:H:52:LYS:N	2:H:52:LYS:HD2	2.32	0.44
2:I:92:ARG:HG2	2:I:129:HIS:NE2	2.32	0.44
2:I:184:ALA:O	2:I:188:LEU:HD23	2.17	0.44
2:N:58:ASP:O	2:N:221:ALA:N	2.37	0.44
3:R:363:LEU:HD12	3:R:364:GLU:N	2.32	0.44
3:U:418:GLY:O	3:U:419:ARG:NH1	2.47	0.44
1:A:91:TRP:HB2	1:A:132:TYR:CD1	2.52	0.44
1:A:348:ALA:O	1:A:352:ILE:HG13	2.16	0.44
1:B:46:ARG:HB3	1:B:55:GLU:HB3	2.00	0.44
1:B:404:TYR:OH	1:B:410:GLU:OE1	2.27	0.44
1:C:150:VAL:HA	1:C:233:PHE:HB3	1.99	0.44
2:k:29:SER:HA	2:k:157:GLY:HA3	1.99	0.44
2:k:67:LYS:HB3	2:k:70:GLU:OE1	2.17	0.44
2:H:33:LEU:HG	2:H:40:LEU:HB3	2.00	0.44
2:H:79:ILE:HG23	3:V:368:LYS:HD2	1.99	0.44
2:I:28:LYS:NZ	2:I:44:GLU:HB3	2.32	0.44
3:Q:367:GLU:O	3:Q:371:GLY:N	2.50	0.44
3:Q:509:ARG:HA	3:Q:512:GLU:HG2	1.98	0.44
3:R:388:ARG:HG2	3:R:426:ALA:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:392:ALA:O	3:U:395:MET:HG3	2.18	0.44
3:V:484:PRO:HB3	3:V:491:PHE:CD1	2.53	0.44
3:X:432:GLU:HG3	3:X:437:GLN:HB2	1.98	0.44
3:c:359:TYR:CZ	3:c:383:LEU:HB2	2.52	0.44
3:c:383:LEU:HD23	3:c:423:PHE:CZ	2.52	0.44
4:j:172:GLN:OE1	4:j:172:GLN:N	2.46	0.44
1:C:24:ARG:HH11	1:C:25:LYS:HB2	1.82	0.44
1:D:180:GLU:HG2	1:D:181:LEU:N	2.33	0.44
1:D:232:TYR:OH	1:D:234:LEU:HB3	2.17	0.44
1:E:162:SER:HA	1:E:165:ILE:HG12	1.99	0.44
2:K:77:GLY:HA2	2:K:80:GLN:NE2	2.33	0.44
2:M:40:LEU:HA	2:M:212:VAL:HG12	1.98	0.44
2:N:87:TYR:O	3:b:357:ARG:NH2	2.50	0.44
3:Q:420:ILE:O	3:Q:431:ILE:HD12	2.18	0.44
3:R:319:ARG:CZ	3:R:482:GLY:HA2	2.48	0.44
3:R:420:ILE:O	3:R:431:ILE:HD12	2.17	0.44
3:R:464:LEU:HD22	3:R:509:ARG:CZ	2.47	0.44
3:S:302:THR:HB	3:S:481:THR:HG21	1.98	0.44
3:S:303:ILE:HG22	3:S:314:MET:HE3	2.00	0.44
3:X:305:ALA:N	3:X:437:GLN:O	2.45	0.44
3:Y:340:TYR:CE2	3:Y:409:ILE:HG21	2.53	0.44
3:Y:359:TYR:CE2	3:Y:363:LEU:HD11	2.51	0.44
3:Y:385:ILE:HG12	3:Y:388:ARG:HH22	1.82	0.44
3:Y:454:TYR:HA	3:Y:457:VAL:HG23	1.98	0.44
1:A:65:ILE:HD11	1:F:89:VAL:HG23	2.00	0.44
1:B:244:LYS:HG3	1:B:245:PHE:H	1.82	0.44
1:B:244:LYS:HD2	1:B:247:GLY:HA2	1.99	0.44
1:C:330:LEU:HD23	1:D:465:LEU:HD21	1.98	0.44
1:E:77:ARG:NH1	1:F:61:ALA:O	2.47	0.44
1:E:391:TYR:HA	1:E:415:LYS:HG3	2.00	0.44
2:o:123:CYS:SG	2:o:154:VAL:HG11	2.58	0.44
2:I:11:GLN:HA	2:I:14:ARG:HG2	1.99	0.44
2:I:107:LEU:HA	2:I:110:ILE:HG12	1.99	0.44
2:K:50:LEU:HB3	2:K:68:PHE:CE1	2.52	0.44
2:L:74:LEU:HB3	2:L:103:TYR:HE1	1.83	0.44
2:M:167:LEU:HD23	2:M:167:LEU:HA	1.81	0.44
3:R:364:GLU:HA	3:R:367:GLU:HG2	1.99	0.44
3:T:321:THR:HG22	3:T:326:ILE:HA	2.00	0.44
1:A:145:LEU:HD11	1:A:251:ARG:HH21	1.82	0.44
1:A:353:TYR:CZ	1:A:390:MET:HE1	2.52	0.44
1:A:386:VAL:C	1:A:390:MET:HE3	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:PRO:HA	1:A:474:TRP:CD1	2.52	0.44
1:B:248:GLU:O	1:B:249:THR:OG1	2.28	0.44
1:C:434:ALA:O	1:C:438:VAL:HG23	2.17	0.44
1:F:352:ILE:O	1:F:355:LYS:HG2	2.17	0.44
2:l:135:ARG:HH21	2:l:137:GLU:HA	1.83	0.44
2:M:39:VAL:HG22	2:M:213:LEU:HB2	1.99	0.44
2:M:170:SER:OG	2:M:183:ILE:HD12	2.18	0.44
2:N:68:PHE:HA	2:N:71:PHE:CE2	2.53	0.44
3:Q:308:TYR:CE1	3:Q:496:ILE:HD11	2.53	0.44
3:W:314:MET:N	3:W:314:MET:SD	2.91	0.44
3:W:388:ARG:NH2	3:c:354:GLU:OE2	2.50	0.44
3:c:376:PHE:CE1	3:c:406:GLY:HA3	2.49	0.44
1:A:202:GLY:C	1:A:204:THR:H	2.25	0.44
1:A:435:ILE:HD11	1:F:185:TYR:HB2	2.00	0.44
1:D:74:ASP:OD1	1:D:74:ASP:N	2.50	0.44
1:D:200:GLY:HA3	1:D:419:SER:HB2	2.00	0.44
1:E:200:GLY:C	1:E:419:SER:HB2	2.43	0.44
2:l:140:ARG:CZ	2:l:154:VAL:HG13	2.48	0.44
2:o:44:GLU:HG2	2:o:208:LEU:HD23	2.00	0.44
2:o:129:HIS:HB2	2:o:132:GLU:CD	2.42	0.44
2:K:161:GLU:HB3	2:K:162:PRO:HD3	1.99	0.44
2:N:51:GLN:HB3	2:N:209:GLU:OE2	2.18	0.44
3:P:307:LYS:HZ1	3:P:416:SER:HA	1.81	0.44
3:R:322:GLN:OE1	3:R:327:SER:HB3	2.17	0.44
3:S:473:ASP:OD1	3:S:521:ARG:NH2	2.50	0.44
2:O:11:GLN:NE2	2:O:14:ARG:HH22	2.16	0.44
1:B:195:LEU:HD22	1:B:341:ILE:HD11	2.00	0.44
1:D:434:ALA:O	1:D:438:VAL:HG23	2.18	0.44
2:o:81:PHE:HD2	2:o:99:LEU:HD13	1.83	0.44
2:J:231:GLN:NE2	2:J:234:LEU:O	2.51	0.44
2:K:123:CYS:N	2:K:156:MET:HE1	2.33	0.44
2:K:222:PHE:CE2	2:K:224:ARG:HG3	2.53	0.44
3:Q:384:ALA:HA	3:Q:387:VAL:HG22	1.99	0.44
3:T:357:ARG:HH12	3:U:381:ASN:CG	2.25	0.44
3:T:443:SER:O	3:T:447:LYS:HG2	2.17	0.44
3:T:509:ARG:O	3:T:512:GLU:HG2	2.18	0.44
3:V:321:THR:HA	3:V:327:SER:H	1.82	0.44
3:X:366:TYR:O	3:X:370:GLU:HG2	2.17	0.44
3:Z:458:THR:H	3:Z:462:SER:HG	1.65	0.44
3:a:318:ARG:NH2	3:a:330:ASP:O	2.47	0.44
3:a:507:GLU:HA	3:a:510:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:308:TYR:CE1	3:c:496:ILE:HD11	2.53	0.44
2:O:25:ALA:O	2:O:158:GLY:HA2	2.17	0.44
2:O:74:LEU:HB3	2:O:103:TYR:HE1	1.83	0.44
1:A:402:VAL:HG13	1:A:485:ILE:HG23	2.00	0.44
1:B:123:SER:HB2	1:B:137:ILE:CG1	2.48	0.44
1:E:40:LYS:HD3	1:E:94:ASP:HB3	2.00	0.44
2:m:74:LEU:HG	2:m:103:TYR:CE2	2.52	0.44
2:m:146:SER:HA	4:d:172:GLN:HB2	2.00	0.44
2:n:56:LEU:HD23	2:n:56:LEU:HA	1.76	0.44
2:n:126:GLU:OE1	2:n:126:GLU:N	2.51	0.44
2:G:165:ASN:O	2:G:169:GLU:HG2	2.18	0.44
2:I:87:TYR:O	3:P:357:ARG:NH2	2.46	0.44
2:M:44:GLU:HA	2:M:208:LEU:HD23	2.00	0.44
3:R:305:ALA:C	3:R:306:LEU:HD12	2.43	0.44
3:T:319:ARG:CZ	3:T:482:GLY:HA2	2.48	0.44
3:Y:319:ARG:NH1	3:Y:481:THR:O	2.51	0.44
3:Z:337:THR:HB	3:Z:341:THR:HG22	1.99	0.44
3:c:515:ARG:O	3:c:519:GLU:HG2	2.18	0.44
1:A:240:GLU:HB3	1:A:251:ARG:HH22	1.82	0.43
1:A:244:LYS:NZ	1:A:249:THR:HG23	2.34	0.43
1:E:253:ILE:HB	1:E:254:ARG:HH11	1.83	0.43
1:F:211:ALA:O	1:F:214:LEU:HG	2.18	0.43
2:n:69:ASN:OD1	2:n:70:GLU:N	2.51	0.43
2:J:44:GLU:HA	2:J:208:LEU:HD12	1.99	0.43
2:J:123:CYS:SG	2:J:154:VAL:HG21	2.57	0.43
2:L:16:ARG:NH2	2:L:115:ALA:O	2.51	0.43
2:M:163:ILE:HG12	2:M:188:LEU:HA	1.99	0.43
3:Q:338:ASP:OD2	3:Q:341:THR:HG22	2.17	0.43
3:S:375:THR:C	3:S:379:LYS:HZ3	2.26	0.43
3:T:357:ARG:NH1	3:U:381:ASN:OD1	2.51	0.43
3:X:366:TYR:CZ	3:X:370:GLU:HG3	2.53	0.43
3:Z:314:MET:CE	3:Z:334:VAL:HG13	2.48	0.43
3:c:384:ALA:HA	3:c:387:VAL:HG22	1.99	0.43
3:c:421:VAL:HA	3:c:430:ASN:O	2.18	0.43
1:B:398:ARG:HG2	1:B:413:TYR:CE1	2.54	0.43
1:D:194:LEU:HB3	1:D:338:LYS:HG3	2.00	0.43
1:D:278:ASP:N	1:D:278:ASP:OD1	2.46	0.43
1:E:88:ARG:NH2	1:E:128:THR:HA	2.32	0.43
1:F:161:LEU:O	1:F:165:ILE:HG12	2.18	0.43
1:F:252:HIS:O	1:F:256:ILE:HG23	2.17	0.43
1:F:277:MET:HE3	1:F:317:GLY:CA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:52:LYS:HG3	2:m:71:PHE:CZ	2.53	0.43
2:G:140:ARG:O	2:G:147:ILE:HD12	2.18	0.43
2:G:142:THR:OG1	2:G:144:ASP:OD1	2.32	0.43
2:J:62:PHE:CZ	2:J:75:ARG:HB2	2.53	0.43
2:J:95:THR:O	2:J:98:GLN:HG2	2.17	0.43
2:K:106:THR:O	2:K:110:ILE:HG12	2.18	0.43
2:N:66:GLY:HA3	2:N:120:VAL:HG12	2.00	0.43
3:R:446:ALA:O	3:R:450:MET:HG2	2.18	0.43
3:S:319:ARG:O	3:S:333:LYS:NZ	2.51	0.43
3:V:319:ARG:CZ	3:V:482:GLY:HA2	2.48	0.43
3:V:473:ASP:OD1	3:V:521:ARG:NH1	2.44	0.43
3:a:461:ASP:HA	3:a:464:LEU:HD12	1.99	0.43
3:c:378:GLY:O	3:c:382:ARG:HG2	2.17	0.43
1:B:68:LEU:HD22	1:B:124:LEU:HD11	2.01	0.43
1:D:59:PHE:HD2	1:D:134:PHE:HD1	1.67	0.43
1:F:353:TYR:HB3	1:F:383:ILE:HG12	2.00	0.43
2:m:217:ARG:NH1	2:m:222:PHE:O	2.51	0.43
2:n:28:LYS:HB3	2:n:44:GLU:CG	2.48	0.43
2:o:25:ALA:O	2:o:158:GLY:HA2	2.18	0.43
2:K:140:ARG:HB3	2:K:148:ALA:HB3	2.00	0.43
3:P:422:SER:N	3:P:430:ASN:O	2.40	0.43
3:U:376:PHE:HE1	3:U:406:GLY:HA3	1.82	0.43
3:V:344:GLY:O	3:V:403:LEU:N	2.50	0.43
1:A:139:LYS:HZ2	1:A:246:VAL:HG13	1.84	0.43
1:A:386:VAL:O	1:A:390:MET:HE3	2.18	0.43
1:B:204:THR:O	1:B:208:LYS:HG3	2.19	0.43
1:D:4:GLY:N	1:D:47:LEU:O	2.50	0.43
1:E:194:LEU:HD11	1:E:277:MET:HE1	2.01	0.43
1:F:199:PRO:HD3	1:F:470:ASN:HD21	1.83	0.43
1:F:257:PHE:CE1	1:F:272:VAL:HG11	2.48	0.43
2:n:234:LEU:HD23	2:n:234:LEU:HA	1.81	0.43
2:K:166:ALA:O	2:K:170:SER:OG	2.23	0.43
2:M:103:TYR:O	2:M:107:LEU:HD23	2.17	0.43
3:T:391:LEU:HD23	3:T:391:LEU:HA	1.82	0.43
3:U:509:ARG:HA	3:U:512:GLU:OE1	2.18	0.43
3:Y:318:ARG:HA	3:Y:331:VAL:O	2.19	0.43
3:c:406:GLY:O	3:c:418:GLY:HA2	2.18	0.43
2:O:205:VAL:HG22	2:O:234:LEU:HD23	2.00	0.43
1:A:322:GLU:HG3	1:B:465:LEU:HD13	2.01	0.43
1:B:77:ARG:HA	1:B:91:TRP:HA	2.00	0.43
1:C:364:HIS:CD2	1:C:447:ARG:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:TYR:CZ	1:E:424:GLN:HB2	2.54	0.43
2:k:113:GLU:HG2	2:k:114:GLN:N	2.33	0.43
2:l:161:GLU:H	2:l:161:GLU:CD	2.26	0.43
2:m:28:LYS:N	4:j:174:LEU:HD12	2.34	0.43
2:G:18:GLU:O	2:G:21:ARG:HD3	2.19	0.43
2:G:159:THR:O	2:G:162:PRO:HD2	2.19	0.43
2:H:59:ARG:HB3	2:H:127:VAL:HG23	2.00	0.43
2:K:103:TYR:HA	2:K:106:THR:OG1	2.18	0.43
2:L:56:LEU:HG	2:L:62:PHE:HB2	2.00	0.43
2:M:155:VAL:HG22	2:M:167:LEU:HD12	2.00	0.43
3:T:376:PHE:CE1	3:T:406:GLY:HA3	2.53	0.43
3:X:357:ARG:HH12	3:Y:381:ASN:CG	2.27	0.43
3:X:509:ARG:HA	3:X:512:GLU:OE1	2.18	0.43
3:Y:340:TYR:HE2	3:Y:409:ILE:HD13	1.83	0.43
2:O:59:ARG:NH2	2:O:128:ALA:O	2.44	0.43
1:A:382:MET:CE	1:A:448:ILE:HA	2.44	0.43
1:C:232:TYR:CB	1:C:268:THR:HG22	2.49	0.43
1:E:341:ILE:HD12	1:E:341:ILE:HG23	1.83	0.43
2:l:210:VAL:HG23	2:l:225:ILE:HB	2.00	0.43
2:m:22:LYS:O	2:m:26:ARG:HG2	2.18	0.43
2:n:50:LEU:HD22	2:n:68:PHE:CZ	2.53	0.43
2:n:58:ASP:HB3	2:n:219:ARG:O	2.18	0.43
2:n:217:ARG:NH1	2:n:222:PHE:O	2.49	0.43
2:o:80:GLN:HA	3:T:365:HIS:HE1	1.83	0.43
2:G:74:LEU:HD12	2:G:103:TYR:CD1	2.54	0.43
3:P:424:ASP:OD1	3:P:427:GLY:N	2.51	0.43
3:S:321:THR:HG22	3:S:326:ILE:HA	2.01	0.43
3:Z:319:ARG:NH1	3:Z:481:THR:O	2.52	0.43
3:b:421:VAL:HA	3:b:430:ASN:O	2.19	0.43
3:c:359:TYR:OH	3:c:379:LYS:O	2.30	0.43
3:c:369:LEU:HD23	3:c:369:LEU:HA	1.88	0.43
3:c:424:ASP:OD1	3:c:427:GLY:N	2.51	0.43
2:O:55:GLU:HA	2:O:61:GLY:HA2	2.01	0.43
1:B:192:GLY:HA3	1:B:335:LEU:HA	2.00	0.43
1:C:296:VAL:O	1:C:299:GLN:NE2	2.52	0.43
1:E:359:GLU:OE2	1:E:375:ARG:HB3	2.19	0.43
2:m:43:ALA:O	2:m:208:LEU:HD12	2.19	0.43
2:m:220:ARG:NH1	3:R:367:GLU:OE2	2.51	0.43
2:L:163:ILE:HG22	2:L:187:ALA:O	2.19	0.43
2:N:67:LYS:HB3	2:N:70:GLU:HG3	2.00	0.43
3:U:421:VAL:HA	3:U:430:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:338:ASP:OD2	3:X:341:THR:OG1	2.21	0.43
3:Z:305:ALA:N	3:Z:437:GLN:O	2.48	0.43
2:O:163:ILE:HD12	2:O:163:ILE:H	1.84	0.43
1:B:244:LYS:C	1:B:246:VAL:N	2.76	0.43
1:D:175:PRO:CB	1:D:189:PRO:HB3	2.48	0.43
1:E:353:TYR:OH	1:E:423:ILE:HG12	2.18	0.43
2:G:178:THR:O	2:G:182:ARG:HG2	2.19	0.43
2:J:96:GLY:H	2:J:126:GLU:CD	2.25	0.43
2:K:54:SER:HB2	3:Y:368:LYS:CE	2.48	0.43
2:L:87:TYR:O	3:Z:357:ARG:NH2	2.48	0.43
2:N:89:TYR:O	3:c:378:GLY:HA2	2.19	0.43
3:R:436:TYR:CD1	3:R:450:MET:HE3	2.52	0.43
3:S:359:TYR:CE2	3:S:363:LEU:HD11	2.53	0.43
3:X:507:GLU:HA	3:X:510:ILE:HD12	2.01	0.43
3:c:443:SER:O	3:c:447:LYS:HG2	2.19	0.43
1:D:165:ILE:O	1:D:169:ARG:HG2	2.19	0.43
1:D:327:PRO:O	1:D:331:ARG:HG2	2.19	0.43
2:m:152:HIS:HB3	2:m:171:TYR:CE1	2.54	0.43
2:n:119:GLU:OE1	2:n:119:GLU:N	2.52	0.43
2:G:59:ARG:NH2	2:G:215:ALA:O	2.51	0.43
2:I:24:ILE:HD11	2:I:120:VAL:N	2.33	0.43
2:K:10:GLU:HG2	2:L:19:LEU:HD12	2.01	0.43
2:L:76:ARG:NH1	3:Z:369:LEU:HB3	2.34	0.43
2:M:113:GLU:HG2	2:M:114:GLN:N	2.33	0.43
2:N:166:ALA:O	2:N:170:SER:OG	2.26	0.43
2:N:225:ILE:HG22	2:N:230:LEU:HB2	2.01	0.43
3:T:454:TYR:HA	3:T:457:VAL:HG23	2.00	0.43
3:Y:351:VAL:HG21	3:Y:398:LEU:HB3	2.01	0.43
3:a:318:ARG:HA	3:a:331:VAL:O	2.18	0.43
3:c:357:ARG:NH2	2:O:87:TYR:O	2.49	0.43
1:A:447:ARG:HD2	1:A:449:GLN:HE22	1.84	0.43
1:C:153:VAL:HG23	1:C:157:ASP:HB2	2.00	0.43
1:E:321:ARG:HH12	1:E:471:PRO:HB2	1.84	0.43
2:l:74:LEU:O	2:l:103:TYR:OH	2.25	0.43
2:l:135:ARG:NH2	2:l:137:GLU:HA	2.34	0.43
2:n:28:LYS:HB3	2:n:44:GLU:HG3	2.01	0.43
2:n:163:ILE:HG22	2:n:187:ALA:O	2.19	0.43
2:n:214:ASP:OD2	2:n:217:ARG:HG2	2.19	0.43
2:H:130:TYR:CG	2:H:218:PRO:HA	2.54	0.43
2:H:147:ILE:N	4:h:172:GLN:OE1	2.45	0.43
2:I:67:LYS:HA	4:h:172:GLN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:305:ALA:HB2	3:R:314:MET:SD	2.59	0.43
3:R:384:ALA:O	3:R:388:ARG:HG3	2.18	0.43
3:S:383:LEU:HD12	3:S:384:ALA:N	2.34	0.43
3:T:318:ARG:HB3	3:T:330:ASP:HA	2.01	0.43
3:W:443:SER:O	3:W:447:LYS:HG2	2.18	0.43
2:O:217:ARG:NH1	2:O:223:ARG:HB2	2.34	0.43
1:A:159:GLY:H	1:A:355:LYS:NZ	2.16	0.42
1:C:181:LEU:HD23	1:D:435:ILE:HG23	2.00	0.42
1:C:183:ARG:NH2	1:C:188:ARG:HA	2.34	0.42
1:C:264:ALA:HB1	1:C:310:LEU:HD21	2.01	0.42
1:C:448:ILE:O	1:C:452:LEU:HG	2.19	0.42
1:F:199:PRO:HG2	1:F:468:THR:O	2.19	0.42
2:k:14:ARG:HH22	2:k:18:GLU:CD	2.27	0.42
2:k:67:LYS:HB3	2:k:70:GLU:CD	2.44	0.42
2:k:222:PHE:CE2	2:k:224:ARG:HG3	2.54	0.42
2:m:140:ARG:HB3	2:m:148:ALA:HB3	2.01	0.42
2:n:89:TYR:O	3:T:378:GLY:HA2	2.19	0.42
2:n:217:ARG:NH1	2:n:223:ARG:HB2	2.34	0.42
2:I:46:PRO:O	2:I:48:ARG:NH1	2.52	0.42
2:I:234:LEU:HA	2:I:234:LEU:HD23	1.77	0.42
3:U:321:THR:HG22	3:U:326:ILE:HA	2.01	0.42
3:X:384:ALA:HA	3:X:387:VAL:HG12	2.00	0.42
3:Y:498:ASP:N	3:Y:498:ASP:OD1	2.50	0.42
3:b:392:ALA:O	3:b:395:MET:HG2	2.19	0.42
3:c:448:SER:O	3:c:451:LYS:HB3	2.18	0.42
1:B:233:PHE:CG	1:B:234:LEU:N	2.87	0.42
1:B:333:GLY:N	1:B:336:ASP:OD1	2.35	0.42
1:C:65:ILE:HD13	1:C:125:LEU:HA	2.01	0.42
1:E:253:ILE:HB	1:E:254:ARG:NH1	2.34	0.42
1:F:200:GLY:HA3	1:F:419:SER:CB	2.47	0.42
2:m:123:CYS:HA	2:m:139:TYR:O	2.19	0.42
2:o:75:ARG:NH1	3:T:368:LYS:O	2.42	0.42
2:H:211:ALA:HB2	2:H:224:ARG:HG2	2.01	0.42
2:J:46:PRO:HA	2:J:207:SER:CA	2.34	0.42
2:J:70:GLU:OE1	2:J:120:VAL:HG13	2.19	0.42
2:J:76:ARG:HH12	3:X:369:LEU:HB3	1.84	0.42
2:J:122:LEU:C	2:J:156:MET:HE1	2.44	0.42
2:J:163:ILE:HD12	2:J:163:ILE:H	1.83	0.42
2:N:155:VAL:HG21	2:N:164:ALA:HA	2.01	0.42
3:P:485:ASP:CG	3:P:488:ARG:HB2	2.44	0.42
3:U:332:ARG:HD2	3:U:493:THR:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:446:ALA:HB2	3:Y:474:ALA:HB2	2.01	0.42
3:a:339:ASP:OD1	3:a:339:ASP:N	2.52	0.42
3:a:515:ARG:O	3:a:518:ILE:N	2.52	0.42
3:c:310:GLY:H	3:c:415:GLN:HA	1.84	0.42
3:c:340:TYR:OH	3:c:499:ALA:O	2.31	0.42
1:B:304:ILE:HA	1:B:307:VAL:HG12	1.99	0.42
1:B:352:ILE:CG2	1:B:423:ILE:HG21	2.49	0.42
1:B:386:VAL:HB	1:B:390:MET:HE3	2.00	0.42
1:B:395:ASP:HA	1:B:398:ARG:HG3	2.01	0.42
1:D:269:PRO:HA	1:D:312:ASN:OD1	2.19	0.42
1:D:357:LEU:HD13	1:D:382:MET:HE1	2.01	0.42
1:D:474:TRP:NE1	1:D:505:THR:OG1	2.52	0.42
1:E:28:LEU:HD22	1:E:51:LEU:O	2.18	0.42
1:E:196:TYR:O	1:E:341:ILE:N	2.51	0.42
1:E:403:THR:HG23	1:E:409:LYS:HG2	2.02	0.42
2:l:28:LYS:HG2	4:i:174:LEU:HA	2.02	0.42
2:I:106:THR:O	2:I:110:ILE:HG23	2.20	0.42
2:K:168:LYS:HG3	2:K:169:GLU:OE2	2.19	0.42
2:L:214:ASP:OD2	2:L:217:ARG:HG2	2.20	0.42
2:M:60:VAL:HG11	2:M:99:LEU:HD21	2.01	0.42
3:S:401:LEU:HD23	3:S:401:LEU:H	1.84	0.42
3:U:303:ILE:N	3:U:439:VAL:O	2.34	0.42
3:U:366:TYR:CZ	3:U:370:GLU:HG3	2.54	0.42
3:Y:341:THR:HG22	3:Y:406:GLY:HA3	2.01	0.42
3:Z:437:GLN:NE2	3:Z:438:ALA:H	2.16	0.42
1:B:150:VAL:HA	1:B:232:TYR:HA	2.01	0.42
1:D:398:ARG:HD2	1:D:399:PHE:N	2.35	0.42
1:E:349:ALA:O	1:E:353:TYR:CD2	2.72	0.42
2:k:50:LEU:HD22	2:k:68:PHE:CE2	2.55	0.42
2:k:90:ASP:HB3	2:k:93:ASP:OD2	2.20	0.42
2:o:212:VAL:O	2:o:223:ARG:N	2.51	0.42
2:G:27:ALA:HA	4:f:173:TYR:HB3	2.00	0.42
2:I:165:ASN:O	2:I:168:LYS:HB3	2.19	0.42
2:I:165:ASN:O	2:I:169:GLU:OE1	2.37	0.42
2:J:74:LEU:O	2:J:103:TYR:OH	2.31	0.42
2:L:90:ASP:HB3	2:L:93:ASP:OD2	2.18	0.42
2:L:162:PRO:HA	2:L:165:ASN:ND2	2.32	0.42
2:N:140:ARG:N	2:N:148:ALA:O	2.38	0.42
3:R:385:ILE:HA	3:R:388:ARG:NH2	2.35	0.42
3:T:384:ALA:HB1	3:T:388:ARG:NH1	2.34	0.42
3:X:319:ARG:CZ	3:X:482:GLY:HA2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:420:ILE:O	3:b:431:ILE:HD12	2.19	0.42
3:c:366:TYR:O	3:c:370:GLU:HG2	2.19	0.42
1:A:219:ALA:HB2	1:A:225:ASP:HB2	2.02	0.42
1:B:364:HIS:HE1	1:B:366:ASP:OD2	2.02	0.42
1:C:322:GLU:CD	1:C:325:ILE:HD12	2.44	0.42
1:E:197:GLY:HA3	1:E:341:ILE:HB	2.01	0.42
2:k:55:GLU:HA	2:k:61:GLY:HA2	2.01	0.42
2:l:98:GLN:H	2:l:98:GLN:HG3	1.69	0.42
2:n:40:LEU:HD11	2:n:177:LEU:HD12	2.01	0.42
2:n:121:GLU:OE2	2:n:140:ARG:NH1	2.52	0.42
2:G:103:TYR:HA	2:G:106:THR:HG22	2.01	0.42
2:I:205:VAL:HG22	2:I:234:LEU:HD13	2.01	0.42
2:J:16:ARG:HB3	2:J:117:PRO:HG3	2.00	0.42
2:K:18:GLU:OE1	2:K:21:ARG:NH2	2.30	0.42
2:M:128:ALA:N	2:M:134:LYS:HE3	2.34	0.42
2:M:135:ARG:NE	2:M:135:ARG:HA	2.34	0.42
3:S:392:ALA:O	3:S:395:MET:HG3	2.19	0.42
3:W:367:GLU:O	3:W:371:GLY:N	2.52	0.42
3:W:378:GLY:HA2	2:O:89:TYR:O	2.19	0.42
3:Y:441:SER:OG	3:Y:478:ASP:OD2	2.32	0.42
3:c:469:GLU:HG2	3:c:517:ILE:HG12	2.00	0.42
2:O:62:PHE:CE1	2:O:122:LEU:HB2	2.54	0.42
1:A:8:LEU:HD21	1:A:39:LEU:HB3	2.02	0.42
1:A:116:ARG:CZ	1:A:259:ARG:HH12	2.32	0.42
1:B:176:PHE:CE2	1:B:269:PRO:HB3	2.48	0.42
1:B:218:MET:HE3	1:B:230:LYS:HE3	2.02	0.42
1:B:251:ARG:O	1:B:255:LEU:HG	2.19	0.42
1:E:24:ARG:HH22	1:F:22:SER:HB2	1.84	0.42
1:E:192:GLY:HA2	1:E:315:VAL:O	2.20	0.42
1:E:364:HIS:HD2	1:E:366:ASP:HB2	1.85	0.42
1:F:204:THR:OG1	1:F:275:ASP:OD2	2.35	0.42
2:k:28:LYS:O	2:k:157:GLY:HA3	2.19	0.42
2:k:88:ALA:O	3:X:381:ASN:ND2	2.53	0.42
2:k:146:SER:HA	2:J:67:LYS:HE2	2.01	0.42
2:n:90:ASP:HB3	2:n:93:ASP:CG	2.45	0.42
2:I:18:GLU:O	2:I:22:LYS:HG3	2.20	0.42
2:I:103:TYR:HA	2:I:106:THR:HG22	2.00	0.42
2:K:62:PHE:CZ	2:K:75:ARG:HB2	2.54	0.42
2:L:16:ARG:NH1	2:L:114:GLN:O	2.52	0.42
2:M:74:LEU:O	2:M:103:TYR:OH	2.33	0.42
3:P:318:ARG:HB3	3:P:330:ASP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:319:ARG:CZ	3:Q:482:GLY:HA2	2.49	0.42
3:S:380:ILE:O	3:S:383:LEU:HG	2.19	0.42
3:U:303:ILE:HG22	3:U:314:MET:HE3	2.01	0.42
1:B:251:ARG:CZ	1:B:255:LEU:HD11	2.49	0.42
1:C:77:ARG:HD3	1:D:61:ALA:HB1	2.02	0.42
1:C:193:VAL:HG13	1:C:337:VAL:HG23	2.02	0.42
1:D:426:VAL:O	1:D:454:SER:OG	2.35	0.42
1:E:204:THR:O	1:E:208:LYS:HG3	2.20	0.42
1:E:341:ILE:O	1:E:341:ILE:HG22	2.20	0.42
2:l:140:ARG:O	2:l:147:ILE:HD12	2.20	0.42
2:m:56:LEU:HB2	2:m:60:VAL:HG12	2.02	0.42
2:n:119:GLU:CD	2:n:119:GLU:H	2.28	0.42
2:H:30:VAL:HG13	2:H:156:MET:HB2	2.01	0.42
2:H:89:TYR:O	3:P:378:GLY:HA2	2.20	0.42
2:K:213:LEU:HD22	2:K:221:ALA:HB3	2.01	0.42
3:U:320:SER:C	3:U:327:SER:HG	2.28	0.42
3:U:358:LEU:O	3:U:362:GLU:OE1	2.37	0.42
3:c:351:VAL:HG21	3:c:398:LEU:HB3	2.02	0.42
2:O:59:ARG:HB3	2:O:127:VAL:HG23	2.00	0.42
2:O:70:GLU:O	2:O:74:LEU:HG	2.20	0.42
2:O:150:GLU:HG3	2:O:154:VAL:HG22	2.02	0.42
1:A:232:TYR:CG	1:A:233:PHE:N	2.88	0.42
1:C:16:THR:HB	1:C:27:ARG:HE	1.85	0.42
1:C:81:VAL:HA	1:C:86:GLU:O	2.19	0.42
1:C:258:GLN:O	1:C:261:ARG:HG3	2.20	0.42
1:D:120:PRO:O	1:D:254:ARG:NH1	2.41	0.42
1:D:178:HIS:CD2	1:E:439:LEU:HD21	2.55	0.42
1:D:348:ALA:O	1:D:352:ILE:HG13	2.19	0.42
1:D:380:LYS:O	1:D:384:GLU:HG2	2.19	0.42
1:E:6:GLY:N	1:E:45:VAL:O	2.52	0.42
1:E:493:THR:HG23	1:E:495:LYS:H	1.85	0.42
1:F:331:ARG:HH21	1:F:334:ARG:HH22	1.68	0.42
2:k:208:LEU:HD23	2:k:208:LEU:HA	1.79	0.42
2:n:10:GLU:O	2:n:14:ARG:HG2	2.20	0.42
2:n:184:ALA:O	2:n:188:LEU:HD23	2.19	0.42
2:o:214:ASP:HB3	2:o:217:ARG:HG2	2.02	0.42
3:P:320:SER:HB3	3:P:331:VAL:HG21	2.01	0.42
3:R:376:PHE:CZ	3:R:419:ARG:HB2	2.54	0.42
3:S:355:PHE:HZ	3:S:390:ASN:HB2	1.84	0.42
3:Z:464:LEU:O	3:Z:468:VAL:HG23	2.19	0.42
3:a:469:GLU:HB3	3:a:517:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:318:ARG:HA	3:b:331:VAL:O	2.19	0.42
1:C:362:PRO:O	1:C:445:GLY:HA2	2.20	0.42
1:E:168:ILE:HG12	1:E:339:ILE:HD13	2.01	0.42
2:k:64:ALA:HB2	2:k:122:LEU:HD12	2.02	0.42
2:k:137:GLU:OE1	2:k:139:TYR:OH	2.32	0.42
2:m:225:ILE:HG21	2:m:233:LEU:HD12	2.01	0.42
2:G:42:VAL:HG22	2:G:210:VAL:HG12	2.01	0.42
2:G:68:PHE:HA	2:G:71:PHE:CE2	2.55	0.42
2:G:161:GLU:H	2:G:161:GLU:CD	2.26	0.42
2:K:110:ILE:HG13	2:K:111:PHE:N	2.35	0.42
2:K:129:HIS:HB2	2:K:132:GLU:CD	2.45	0.42
2:L:42:VAL:HG22	2:L:210:VAL:HG22	2.02	0.42
3:P:304:VAL:HA	3:P:438:ALA:HA	2.01	0.42
3:Z:471:LEU:HD23	3:Z:471:LEU:HA	1.90	0.42
3:a:465:ARG:HB2	3:a:513:LEU:HD22	2.02	0.42
3:a:504:ASP:OD1	3:a:505:VAL:N	2.52	0.42
3:b:376:PHE:O	3:b:380:ILE:HG13	2.19	0.42
2:O:217:ARG:HG3	2:O:221:ALA:HA	2.02	0.42
1:A:69:ARG:O	1:A:120:PRO:HG3	2.20	0.42
1:A:364:HIS:HD2	1:A:366:ASP:HB2	1.85	0.42
1:E:259:ARG:O	1:E:262:GLU:HG2	2.20	0.42
1:E:322:GLU:O	1:E:325:ILE:HG12	2.20	0.42
1:F:261:ARG:HA	1:F:264:ALA:HB2	2.02	0.42
1:F:271:ILE:HG12	1:F:314:ILE:HB	2.01	0.42
2:n:118:TYR:HB3	2:n:120:VAL:HG22	2.02	0.42
2:I:8:SER:OG	2:I:10:GLU:HG3	2.19	0.42
2:J:135:ARG:NE	2:J:135:ARG:HA	2.35	0.42
2:K:208:LEU:HD23	2:K:208:LEU:HA	1.86	0.42
2:M:178:THR:O	2:M:182:ARG:HD3	2.20	0.42
2:N:30:VAL:O	2:N:156:MET:N	2.52	0.42
3:U:392:ALA:O	3:U:396:GLN:NE2	2.52	0.42
3:W:337:THR:HB	3:W:341:THR:OG1	2.20	0.42
3:W:393:ALA:O	3:W:398:LEU:HB2	2.20	0.42
3:W:408:ASP:HB3	3:W:411:ALA:HB2	2.02	0.42
3:c:367:GLU:OE1	3:c:373:PRO:HA	2.20	0.42
1:B:123:SER:HB2	1:B:137:ILE:HG12	2.02	0.41
1:D:379:ILE:HA	1:D:382:MET:CG	2.50	0.41
1:E:8:LEU:HD11	1:E:17:VAL:HG21	2.02	0.41
2:G:11:GLN:NE2	2:G:14:ARG:HH12	2.18	0.41
2:G:58:ASP:HB3	2:G:219:ARG:O	2.21	0.41
2:H:163:ILE:HG23	2:H:187:ALA:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:141:ILE:HD12	2:L:141:ILE:HA	1.79	0.41
2:M:107:LEU:HA	2:M:110:ILE:HG12	2.02	0.41
2:N:16:ARG:NH1	2:N:114:GLN:O	2.50	0.41
3:Q:320:SER:OG	3:Q:327:SER:OG	2.27	0.41
3:W:349:ALA:O	3:W:353:VAL:HG23	2.20	0.41
3:c:345:ILE:HA	3:c:402:PRO:HA	2.01	0.41
1:B:328:ALA:HA	1:B:331:ARG:HD2	2.02	0.41
1:D:203:LYS:HG2	1:D:341:ILE:HG13	2.01	0.41
1:F:405:ALA:HB2	1:F:484:ARG:HB3	2.01	0.41
2:k:141:ILE:HG13	2:k:147:ILE:HD13	2.02	0.41
2:k:205:VAL:HG23	2:k:230:LEU:HD23	2.01	0.41
2:m:56:LEU:HD23	2:m:56:LEU:HA	1.93	0.41
2:m:80:GLN:HA	3:R:365:HIS:CE1	2.55	0.41
2:m:213:LEU:HD23	2:m:222:PHE:HA	2.02	0.41
2:H:58:ASP:O	2:H:221:ALA:N	2.39	0.41
2:I:123:CYS:SG	2:I:124:VAL:N	2.93	0.41
2:J:225:ILE:O	2:J:230:LEU:HD12	2.20	0.41
2:L:165:ASN:HA	2:L:168:LYS:CG	2.50	0.41
2:N:107:LEU:HA	2:N:110:ILE:HG12	2.03	0.41
3:Q:424:ASP:OD1	3:Q:427:GLY:N	2.53	0.41
3:V:454:TYR:HA	3:V:457:VAL:HG23	2.02	0.41
3:X:464:LEU:O	3:X:468:VAL:HG12	2.20	0.41
3:Y:434:GLU:HG2	3:Y:436:TYR:CE1	2.55	0.41
3:Z:435:GLY:HA3	3:Z:454:TYR:OH	2.20	0.41
2:O:208:LEU:HD23	2:O:208:LEU:HA	1.87	0.41
1:B:9:LEU:HA	1:B:132:TYR:OH	2.20	0.41
1:B:358:THR:O	1:B:375:ARG:NH2	2.54	0.41
1:C:179:LYS:O	1:C:183:ARG:HG2	2.21	0.41
2:k:70:GLU:OE1	2:k:120:VAL:HG13	2.20	0.41
2:l:86:GLY:HA2	2:l:90:ASP:O	2.21	0.41
2:G:213:LEU:HD23	2:G:213:LEU:HA	1.93	0.41
2:K:105:GLN:HA	2:L:69:ASN:HD22	1.85	0.41
2:M:70:GLU:OE1	2:M:120:VAL:HG13	2.20	0.41
2:M:163:ILE:HG23	2:M:187:ALA:C	2.45	0.41
3:T:376:PHE:CZ	3:T:419:ARG:HB2	2.54	0.41
3:U:384:ALA:HA	3:U:387:VAL:HG22	2.01	0.41
3:W:339:ASP:O	3:W:502:ALA:N	2.47	0.41
3:Y:464:LEU:O	3:Y:468:VAL:HG23	2.20	0.41
3:b:447:LYS:HD2	3:b:450:MET:CE	2.50	0.41
3:c:432:GLU:HB3	3:c:434:GLU:OE2	2.20	0.41
2:O:56:LEU:N	2:O:60:VAL:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLY:C	1:A:204:THR:N	2.78	0.41
1:A:253:ILE:HG22	1:A:303:GLU:HG3	2.02	0.41
1:B:471:PRO:HA	1:B:474:TRP:HD1	1.83	0.41
1:C:114:ARG:HA	1:C:114:ARG:HD3	1.74	0.41
1:D:8:LEU:HD11	1:D:39:LEU:HB3	2.02	0.41
1:D:46:ARG:HG2	1:D:55:GLU:HB3	2.01	0.41
1:D:173:GLU:HG2	1:D:214:LEU:HD12	2.01	0.41
1:D:177:LEU:HD21	1:D:217:LYS:HE2	2.02	0.41
1:D:401:GLU:HB2	1:D:491:LEU:HD11	2.02	0.41
1:E:8:LEU:CD2	1:E:39:LEU:HB3	2.51	0.41
1:F:28:LEU:HD22	1:F:51:LEU:HB3	2.03	0.41
2:n:95:THR:OG1	2:n:98:GLN:HG3	2.21	0.41
2:n:140:ARG:HH21	2:n:150:GLU:CD	2.29	0.41
2:o:90:ASP:HB3	2:o:93:ASP:CG	2.45	0.41
2:o:205:VAL:HG21	2:o:231:GLN:OE1	2.19	0.41
2:M:179:ASP:O	2:M:183:ILE:HG12	2.20	0.41
3:X:374:LEU:HD23	3:X:379:LYS:HG2	2.02	0.41
3:Y:432:GLU:HG3	3:Y:437:GLN:HB2	2.02	0.41
1:A:181:LEU:HD21	1:B:438:VAL:HB	2.03	0.41
1:C:355:LYS:HD3	1:C:355:LYS:HA	1.76	0.41
1:D:310:LEU:HD21	1:D:312:ASN:HB3	2.02	0.41
1:E:69:ARG:HE	1:F:141:GLU:HG2	1.85	0.41
1:F:146:VAL:O	1:F:147:LEU:C	2.64	0.41
1:F:175:PRO:HA	1:F:182:TYR:CE2	2.55	0.41
1:F:188:ARG:HH12	1:F:336:ASP:CG	2.28	0.41
2:m:217:ARG:HB2	2:m:221:ALA:HA	2.02	0.41
2:G:121:GLU:HG3	2:G:141:ILE:O	2.21	0.41
2:I:58:ASP:CG	2:I:91:ARG:HH21	2.28	0.41
2:J:56:LEU:HB2	2:J:60:VAL:HG12	2.02	0.41
2:N:214:ASP:HB3	2:N:217:ARG:HG3	2.03	0.41
3:Q:473:ASP:CG	3:Q:521:ARG:HH22	2.28	0.41
3:T:355:PHE:O	3:T:386:MET:HE1	2.21	0.41
3:Y:447:LYS:HA	3:Y:447:LYS:HD2	1.93	0.41
3:a:436:TYR:HB2	3:a:450:MET:CE	2.50	0.41
3:c:322:GLN:HB2	3:c:325:MET:SD	2.59	0.41
1:A:257:PHE:CD1	1:A:307:VAL:HG21	2.56	0.41
1:C:175:PRO:HB3	1:C:189:PRO:HB3	2.02	0.41
1:D:329:ILE:HG12	1:D:335:LEU:HD13	2.03	0.41
2:H:80:GLN:HA	3:V:365:HIS:HE1	1.86	0.41
2:I:40:LEU:HD12	2:I:180:ALA:HB3	2.02	0.41
2:L:110:ILE:HG12	2:L:118:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:56:LEU:HB2	2:N:60:VAL:HG12	2.01	0.41
3:P:305:ALA:HB2	3:P:314:MET:SD	2.61	0.41
3:R:392:ALA:O	3:R:395:MET:HG2	2.20	0.41
3:T:436:TYR:HB2	3:T:450:MET:SD	2.61	0.41
3:V:416:SER:O	3:V:419:ARG:NH1	2.47	0.41
3:c:419:ARG:HH21	3:c:431:ILE:HD13	1.86	0.41
2:O:20:ALA:HA	2:O:119:GLU:HG3	2.02	0.41
1:A:399:PHE:O	1:A:400:LEU:HD12	2.21	0.41
1:B:17:VAL:HG12	1:B:19:VAL:HG23	2.01	0.41
1:B:114:ARG:HD3	1:B:114:ARG:H	1.86	0.41
1:B:115:PRO:HB3	1:B:136:ARG:HE	1.85	0.41
1:F:257:PHE:O	1:F:261:ARG:HG2	2.21	0.41
1:F:437:SER:O	1:F:441:THR:HB	2.21	0.41
2:l:15:GLU:O	2:l:18:GLU:HG3	2.20	0.41
2:m:138:LEU:O	2:m:149:ASP:HA	2.21	0.41
2:H:42:VAL:HG21	2:H:184:ALA:HB1	2.01	0.41
2:H:62:PHE:CZ	2:H:64:ALA:HB2	2.55	0.41
2:J:25:ALA:O	2:J:158:GLY:HA2	2.20	0.41
2:K:42:VAL:HG22	2:K:210:VAL:HG22	2.03	0.41
2:K:55:GLU:HA	2:K:61:GLY:HA2	2.03	0.41
2:L:33:LEU:HA	2:L:153:PHE:HA	2.03	0.41
2:L:75:ARG:NH1	3:Z:368:LYS:O	2.53	0.41
2:M:24:ILE:HD13	2:M:24:ILE:HA	1.95	0.41
3:P:319:ARG:CZ	3:P:482:GLY:HA2	2.51	0.41
3:R:421:VAL:HA	3:R:430:ASN:O	2.20	0.41
3:R:509:ARG:O	3:R:512:GLU:HG2	2.21	0.41
3:S:318:ARG:HA	3:S:331:VAL:O	2.20	0.41
3:T:370:GLU:HB3	3:T:372:VAL:HG12	2.03	0.41
1:A:182:TYR:HA	1:B:435:ILE:HD11	2.03	0.41
1:B:136:ARG:HG2	1:B:138:PRO:HD2	2.03	0.41
1:B:389:ARG:NH1	1:B:397:ASN:OD1	2.53	0.41
1:E:153:VAL:HG21	1:E:205:LEU:HD11	2.02	0.41
1:E:401:GLU:HB2	1:E:491:LEU:HD21	2.02	0.41
2:k:28:LYS:HD2	2:k:44:GLU:HB2	2.01	0.41
2:m:152:HIS:HB3	2:m:171:TYR:CZ	2.56	0.41
2:G:64:ALA:HB2	2:G:122:LEU:CD1	2.51	0.41
2:H:142:THR:HG23	2:H:146:SER:O	2.21	0.41
2:H:167:LEU:HA	2:H:170:SER:OG	2.21	0.41
2:I:34:ALA:HA	2:I:39:VAL:HA	2.03	0.41
2:I:138:LEU:HB2	2:I:150:GLU:O	2.20	0.41
2:J:92:ARG:HG2	2:J:129:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:138:LEU:HB2	2:J:150:GLU:O	2.21	0.41
2:K:70:GLU:OE1	2:K:120:VAL:HG13	2.20	0.41
2:M:137:GLU:OE1	2:M:137:GLU:N	2.54	0.41
2:N:16:ARG:CZ	2:N:117:PRO:HD3	2.50	0.41
3:P:413:ASP:OD1	3:P:413:ASP:N	2.48	0.41
3:R:454:TYR:HA	3:R:457:VAL:HG23	2.02	0.41
3:T:497:ILE:HA	3:T:502:ALA:HA	2.01	0.41
3:T:509:ARG:HA	3:T:512:GLU:HG2	2.03	0.41
3:W:422:SER:HB2	3:W:437:GLN:HG2	2.02	0.41
2:O:159:THR:HG23	2:O:159:THR:O	2.20	0.41
1:A:63:GLY:N	1:A:125:LEU:HD11	2.36	0.41
1:A:391:TYR:OH	1:A:418:ASN:ND2	2.50	0.41
1:A:447:ARG:HD2	1:A:449:GLN:NE2	2.34	0.41
1:C:171:ALA:HB1	1:C:337:VAL:HG21	2.03	0.41
1:D:191:LYS:HE3	1:D:307:VAL:HG13	2.03	0.41
1:E:4:GLY:O	1:E:46:ARG:HG3	2.21	0.41
1:E:204:THR:HG23	1:E:273:PHE:CE2	2.55	0.41
1:E:214:LEU:O	1:E:217:LYS:HG2	2.20	0.41
1:E:328:ALA:O	1:E:334:ARG:NH1	2.53	0.41
1:E:338:LYS:HG2	1:F:465:LEU:HD23	2.02	0.41
1:E:440:GLU:HG3	1:E:441:THR:HG23	2.02	0.41
1:F:3:SER:OG	1:F:46:ARG:HD3	2.21	0.41
1:F:235:ASN:CB	1:F:273:PHE:HB3	2.51	0.41
1:F:398:ARG:HG3	1:F:413:TYR:CE1	2.55	0.41
2:k:95:THR:OG1	2:k:98:GLN:HG3	2.21	0.41
2:k:155:VAL:HG12	2:k:160:THR:HG23	2.01	0.41
2:m:105:GLN:OE1	2:n:73:ASN:ND2	2.45	0.41
2:n:35:TYR:HB2	2:n:175:ALA:O	2.21	0.41
2:G:35:TYR:HB2	2:G:175:ALA:O	2.20	0.41
2:G:62:PHE:CZ	2:G:75:ARG:HB2	2.56	0.41
2:G:122:LEU:HD12	2:G:123:CYS:H	1.86	0.41
2:I:40:LEU:HD23	2:I:40:LEU:HA	1.86	0.41
2:I:56:LEU:HA	2:I:56:LEU:HD23	1.82	0.41
2:K:124:VAL:HG12	2:K:139:TYR:HB2	2.02	0.41
2:L:21:ARG:CZ	2:L:21:ARG:HB3	2.50	0.41
2:L:40:LEU:HG	2:L:42:VAL:HG23	2.03	0.41
2:N:116:LYS:NZ	2:N:119:GLU:OE2	2.52	0.41
3:P:345:ILE:HB	3:P:352:ALA:HB1	2.03	0.41
3:P:394:ALA:HA	3:P:398:LEU:C	2.46	0.41
3:Q:359:TYR:CE1	3:Q:383:LEU:HB2	2.56	0.41
3:Q:402:PRO:HG2	3:Q:423:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:382:ARG:HA	3:R:385:ILE:HD12	2.03	0.41
3:R:448:SER:O	3:R:451:LYS:HB3	2.20	0.41
3:R:455:SER:OG	3:R:456:GLN:OE1	2.35	0.41
3:R:461:ASP:HA	3:R:509:ARG:HH21	1.84	0.41
3:S:320:SER:OG	3:S:327:SER:OG	2.24	0.41
3:S:346:ALA:O	3:S:401:LEU:HD23	2.20	0.41
3:U:336:ILE:HG12	3:U:495:VAL:HG11	2.03	0.41
3:W:385:ILE:HG22	3:W:386:MET:HE2	2.03	0.41
3:X:308:TYR:CE2	3:X:496:ILE:HD11	2.55	0.41
3:X:319:ARG:O	3:X:333:LYS:NZ	2.47	0.41
3:X:351:VAL:HG12	3:X:355:PHE:CE2	2.55	0.41
3:Y:318:ARG:HD3	3:Y:493:THR:HG23	2.03	0.41
3:a:359:TYR:O	3:a:363:LEU:HG	2.20	0.41
2:O:134:LYS:HE3	2:O:135:ARG:O	2.21	0.41
1:B:16:THR:OG1	1:B:27:ARG:NH2	2.44	0.41
1:F:334:ARG:O	1:F:335:LEU:HD12	2.21	0.41
2:l:33:LEU:CD2	2:l:40:LEU:HB2	2.51	0.41
2:n:39:VAL:HG21	2:n:125:ALA:HB1	2.03	0.41
2:H:42:VAL:HG21	2:H:184:ALA:CB	2.51	0.41
2:I:26:ARG:NH2	4:h:173:TYR:OH	2.44	0.41
2:I:64:ALA:HA	2:I:122:LEU:HA	2.02	0.41
2:I:159:THR:O	2:I:162:PRO:HD2	2.21	0.41
3:Q:393:ALA:HB1	3:Q:398:LEU:HD12	2.02	0.41
3:Q:507:GLU:OE1	3:Q:507:GLU:N	2.43	0.41
3:S:330:ASP:OD1	3:S:330:ASP:N	2.52	0.41
3:T:359:TYR:CE2	3:T:363:LEU:HD11	2.56	0.41
3:T:385:ILE:CD1	3:T:388:ARG:HH21	2.33	0.41
3:V:359:TYR:HB2	3:V:386:MET:CE	2.42	0.41
3:V:421:VAL:HA	3:V:430:ASN:O	2.20	0.41
3:X:330:ASP:OD1	3:X:330:ASP:N	2.53	0.41
3:Z:432:GLU:HG3	3:Z:437:GLN:HB2	2.02	0.41
2:O:155:VAL:HG22	2:O:167:LEU:HD12	2.03	0.41
1:B:400:LEU:HD11	1:B:503:ILE:HD12	2.04	0.40
1:B:405:ALA:HB2	1:B:484:ARG:HB2	2.03	0.40
1:E:116:ARG:HD2	1:E:119:ARG:HH22	1.86	0.40
2:k:52:LYS:HB3	2:k:52:LYS:HE3	1.92	0.40
2:m:57:TYR:N	2:m:60:VAL:O	2.36	0.40
2:n:128:ALA:HB2	2:n:134:LYS:HB3	2.03	0.40
2:o:127:VAL:HG21	2:o:215:ALA:HB2	2.03	0.40
2:I:8:SER:O	2:I:12:ALA:N	2.38	0.40
2:I:35:TYR:CD1	2:I:40:LEU:HG	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:42:VAL:HA	2:I:209:GLU:O	2.21	0.40
2:I:83:ASP:OD2	3:P:365:HIS:ND1	2.41	0.40
2:J:151:PRO:HG2	2:J:152:HIS:ND1	2.37	0.40
2:L:66:GLY:HA3	2:L:120:VAL:HG12	2.02	0.40
2:M:165:ASN:HA	2:M:168:LYS:HG2	2.03	0.40
2:N:91:ARG:O	2:N:94:VAL:HG22	2.21	0.40
3:S:318:ARG:HD3	3:S:493:THR:HG23	2.03	0.40
3:S:366:TYR:O	3:S:370:GLU:HG2	2.21	0.40
3:T:421:VAL:HA	3:T:430:ASN:O	2.21	0.40
3:U:341:THR:HG22	3:U:406:GLY:HA3	2.02	0.40
3:U:396:GLN:HG3	3:U:398:LEU:HD23	2.02	0.40
3:W:305:ALA:C	3:W:306:LEU:HD12	2.45	0.40
3:W:447:LYS:HA	3:W:447:LYS:HD2	1.85	0.40
3:X:306:LEU:HD21	3:X:467:ALA:HB2	2.03	0.40
3:X:448:SER:O	3:X:451:LYS:HB3	2.21	0.40
3:Z:359:TYR:CE1	3:Z:363:LEU:HD11	2.56	0.40
3:Z:382:ARG:HA	3:Z:385:ILE:HD12	2.01	0.40
3:Z:399:LEU:HD21	3:Z:401:LEU:HD23	2.02	0.40
3:Z:463:GLY:HA2	3:Z:466:VAL:HG22	2.02	0.40
3:a:355:PHE:HZ	3:a:390:ASN:CG	2.29	0.40
3:a:391:LEU:O	3:a:395:MET:HG2	2.21	0.40
3:c:465:ARG:HA	3:c:513:LEU:HD13	2.02	0.40
2:O:71:PHE:HA	2:O:74:LEU:HD12	2.03	0.40
1:B:383:ILE:HA	1:B:386:VAL:HG22	2.03	0.40
1:C:196:TYR:CZ	1:C:340:LYS:HB2	2.56	0.40
1:F:268:THR:N	1:F:312:ASN:HD21	2.19	0.40
1:F:434:ALA:HA	1:F:450:HIS:CE1	2.56	0.40
2:m:30:VAL:HG21	2:m:53:ILE:HD11	2.04	0.40
2:m:134:LYS:HB3	2:m:134:LYS:HE3	1.91	0.40
2:G:181:LEU:HD21	2:G:233:LEU:HB2	2.02	0.40
2:I:171:TYR:OH	2:I:173:GLU:OE1	2.38	0.40
2:K:129:HIS:HB2	2:K:132:GLU:OE2	2.21	0.40
2:L:40:LEU:HD13	2:L:177:LEU:HD11	2.03	0.40
2:M:26:ARG:O	2:M:26:ARG:HD2	2.21	0.40
2:M:96:GLY:H	2:M:126:GLU:CD	2.28	0.40
3:Q:378:GLY:O	3:Q:382:ARG:HG2	2.20	0.40
3:Q:393:ALA:HB1	3:Q:398:LEU:HB2	2.03	0.40
3:S:368:LYS:HE2	3:S:368:LYS:HB3	1.89	0.40
3:T:460:GLY:O	3:T:464:LEU:HG	2.20	0.40
3:V:422:SER:OG	3:V:432:GLU:OE2	2.22	0.40
3:X:456:GLN:H	3:X:456:GLN:HG2	1.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:359:TYR:CE1	3:Y:383:LEU:HB2	2.56	0.40
3:Z:366:TYR:O	3:Z:370:GLU:HG2	2.21	0.40
3:a:306:LEU:HD13	3:a:467:ALA:HB2	2.02	0.40
1:A:172:VAL:C	1:A:175:PRO:HD2	2.46	0.40
1:A:375:ARG:HE	1:A:375:ARG:HB2	1.78	0.40
1:B:352:ILE:HG22	1:B:423:ILE:HG21	2.02	0.40
1:E:194:LEU:HB3	1:E:338:LYS:HA	2.03	0.40
1:E:353:TYR:HB2	1:E:383:ILE:HG23	2.02	0.40
2:l:213:LEU:HD23	2:l:213:LEU:HA	1.91	0.40
2:H:134:LYS:NZ	2:H:135:ARG:O	2.54	0.40
2:I:31:VAL:HG12	2:I:155:VAL:HG23	2.03	0.40
2:I:140:ARG:N	2:I:148:ALA:O	2.30	0.40
2:J:28:LYS:O	2:J:157:GLY:HA3	2.22	0.40
2:J:182:ARG:NH1	2:J:234:LEU:HA	2.32	0.40
2:K:203:LEU:HB3	2:K:204:GLY:H	1.73	0.40
3:S:359:TYR:OH	3:S:379:LYS:HB3	2.20	0.40
3:T:366:TYR:CD1	3:T:374:LEU:HG	2.57	0.40
3:T:393:ALA:HB1	3:T:398:LEU:HD12	2.04	0.40
3:U:383:LEU:HG	3:U:423:PHE:HE2	1.86	0.40
3:W:351:VAL:HA	3:W:354:GLU:OE1	2.22	0.40
3:b:340:TYR:CD2	3:b:409:ILE:HD11	2.56	0.40
1:A:251:ARG:HG3	1:A:252:HIS:ND1	2.37	0.40
1:C:174:LEU:HB3	1:C:175:PRO:HD3	2.03	0.40
1:D:353:TYR:CZ	1:D:423:ILE:HG23	2.57	0.40
1:F:390:MET:HB2	1:F:391:TYR:CD1	2.56	0.40
2:k:113:GLU:HG2	2:k:114:GLN:CD	2.46	0.40
2:l:31:VAL:CG1	2:l:42:VAL:HB	2.52	0.40
2:l:71:PHE:HB3	2:l:120:VAL:HG21	2.03	0.40
2:m:150:GLU:HB2	2:m:154:VAL:HG22	2.03	0.40
2:o:142:THR:HG22	2:o:143:TYR:H	1.87	0.40
2:o:217:ARG:NH1	2:o:223:ARG:HB2	2.37	0.40
2:G:39:VAL:HB	2:G:213:LEU:HB2	2.03	0.40
2:H:23:GLY:HA3	2:H:119:GLU:HG3	2.02	0.40
2:I:42:VAL:HG22	2:I:210:VAL:HG22	2.03	0.40
2:N:55:GLU:HA	2:N:61:GLY:HA2	2.03	0.40
2:N:85:ARG:HD3	2:N:89:TYR:CD1	2.56	0.40
2:N:103:TYR:O	2:N:107:LEU:HD23	2.21	0.40
3:Q:325:MET:HE1	3:R:444:LEU:HD22	2.02	0.40
3:X:469:GLU:HG2	3:X:517:ILE:HG12	2.03	0.40
3:Y:314:MET:HE1	3:Y:334:VAL:HG13	2.02	0.40
3:Z:359:TYR:O	3:Z:362:GLU:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:325:MET:HE2	3:b:325:MET:HB2	1.88	0.40
1:A:34:ILE:HD13	1:A:34:ILE:HA	1.94	0.40
1:A:122:ASP:CG	1:A:136:ARG:HH21	2.30	0.40
1:A:257:PHE:HD1	1:A:307:VAL:HG21	1.85	0.40
1:B:6:GLY:O	1:B:45:VAL:N	2.50	0.40
1:C:27:ARG:HD3	1:D:46:ARG:HE	1.86	0.40
1:C:96:LEU:HD21	1:C:135:GLU:HA	2.03	0.40
1:D:344:PRO:HD2	1:D:418:ASN:O	2.22	0.40
1:E:198:PRO:HG2	1:E:343:ARG:CG	2.52	0.40
1:F:193:VAL:HA	1:F:337:VAL:HG23	2.02	0.40
2:l:80:GLN:HA	3:Q:365:HIS:CE1	2.57	0.40
2:G:97:ARG:HD2	2:G:101:ASN:OD1	2.22	0.40
2:H:68:PHE:HB3	4:g:172:GLN:HE21	1.85	0.40
2:N:29:SER:HA	2:N:156:MET:O	2.21	0.40
3:P:474:ALA:O	3:P:478:ASP:N	2.51	0.40
3:Q:416:SER:O	3:Q:419:ARG:NH2	2.50	0.40
3:S:366:TYR:CE1	3:S:370:GLU:HG3	2.57	0.40
3:V:338:ASP:OD1	3:V:341:THR:OG1	2.37	0.40
3:W:423:PHE:CE2	3:W:429:TRP:HB3	2.57	0.40
3:c:307:LYS:NZ	3:c:435:GLY:HA2	2.36	0.40
3:c:473:ASP:OD1	3:c:521:ARG:NH1	2.54	0.40
2:O:40:LEU:HA	2:O:212:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	474/609 (78%)	440 (93%)	33 (7%)	1 (0%)	44	78
1	B	467/609 (77%)	436 (93%)	30 (6%)	1 (0%)	44	78
1	C	462/609 (76%)	441 (96%)	18 (4%)	3 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	450/609 (74%)	435 (97%)	15 (3%)	0	100	100
1	E	451/609 (74%)	436 (97%)	15 (3%)	0	100	100
1	F	452/609 (74%)	423 (94%)	28 (6%)	1 (0%)	44	78
2	G	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
2	H	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
2	I	211/248 (85%)	202 (96%)	9 (4%)	0	100	100
2	J	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
2	K	211/248 (85%)	206 (98%)	5 (2%)	0	100	100
2	L	211/248 (85%)	203 (96%)	8 (4%)	0	100	100
2	M	211/248 (85%)	202 (96%)	9 (4%)	0	100	100
2	N	211/248 (85%)	201 (95%)	10 (5%)	0	100	100
2	O	211/248 (85%)	203 (96%)	8 (4%)	0	100	100
2	k	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
2	l	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
2	m	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
2	n	211/248 (85%)	204 (97%)	7 (3%)	0	100	100
2	o	211/248 (85%)	205 (97%)	6 (3%)	0	100	100
3	P	220/291 (76%)	212 (96%)	8 (4%)	0	100	100
3	Q	220/291 (76%)	215 (98%)	5 (2%)	0	100	100
3	R	220/291 (76%)	217 (99%)	3 (1%)	0	100	100
3	S	220/291 (76%)	211 (96%)	8 (4%)	1 (0%)	25	64
3	T	220/291 (76%)	215 (98%)	5 (2%)	0	100	100
3	U	220/291 (76%)	214 (97%)	6 (3%)	0	100	100
3	V	220/291 (76%)	217 (99%)	2 (1%)	1 (0%)	25	64
3	W	220/291 (76%)	211 (96%)	9 (4%)	0	100	100
3	X	220/291 (76%)	212 (96%)	8 (4%)	0	100	100
3	Y	220/291 (76%)	216 (98%)	4 (2%)	0	100	100
3	Z	220/291 (76%)	214 (97%)	6 (3%)	0	100	100
3	a	220/291 (76%)	215 (98%)	5 (2%)	0	100	100
3	b	220/291 (76%)	218 (99%)	2 (1%)	0	100	100
3	c	220/291 (76%)	214 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	2 (100%)	0	0	100	100
4	g	2/4 (50%)	2 (100%)	0	0	100	100
4	h	2/4 (50%)	2 (100%)	0	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	8804/11228 (78%)	8478 (96%)	318 (4%)	8 (0%)	50	83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	VAL
1	C	222	ARG
3	S	482	GLY
1	C	217	LYS
1	B	150	VAL
1	F	232	TYR
3	V	309	PRO
1	C	221	VAL

5.3.2 Protein sidechains (i)

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	405/511 (79%)	404 (100%)	1 (0%)	92	94
1	B	402/511 (79%)	401 (100%)	1 (0%)	92	94
1	C	389/511 (76%)	389 (100%)	0	100	100
1	D	389/511 (76%)	389 (100%)	0	100	100
1	E	389/511 (76%)	388 (100%)	1 (0%)	91	92
1	F	389/511 (76%)	389 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	G	165/192 (86%)	165 (100%)	0	100 100
2	H	165/192 (86%)	162 (98%)	3 (2%)	54 71
2	I	165/192 (86%)	164 (99%)	1 (1%)	84 88
2	J	165/192 (86%)	165 (100%)	0	100 100
2	K	165/192 (86%)	165 (100%)	0	100 100
2	L	165/192 (86%)	164 (99%)	1 (1%)	84 88
2	M	165/192 (86%)	163 (99%)	2 (1%)	67 78
2	N	165/192 (86%)	164 (99%)	1 (1%)	84 88
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%)	164 (99%)	1 (1%)	84 88
2	m	165/192 (86%)	164 (99%)	1 (1%)	84 88
2	n	165/192 (86%)	164 (99%)	1 (1%)	84 88
2	o	165/192 (86%)	163 (99%)	2 (1%)	67 78
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%)	164 (99%)	1 (1%)	84 88
3	a	165/217 (76%)	165 (100%)	0	100 100
3	b	165/217 (76%)	165 (100%)	0	100 100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
All	All	7003/8813 (80%)	6986 (100%)	17 (0%)	91	94

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	VAL
1	B	137	ILE
1	E	218	MET
2	l	120	VAL
2	m	147	ILE
2	n	141	ILE
2	o	167	LEU
2	o	168	LYS
2	H	42	VAL
2	H	44	GLU
2	H	210	VAL
2	I	142	THR
2	L	141	ILE
2	M	99	LEU
2	M	141	ILE
2	N	48	ARG
3	Z	421	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	GLN
1	A	433	ASN
1	B	364	HIS
1	C	178	HIS
1	C	462	ASN
1	C	470	ASN
1	D	43	GLN
1	D	178	HIS
1	D	243	ASN
1	D	450	HIS

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Mol	Chain	Res	Type
1	E	164	GLN
1	E	178	HIS
1	E	467	ASN
1	F	178	HIS
1	F	312	ASN
1	F	449	GLN
2	k	165	ASN
2	k	231	GLN
2	l	51	GLN
2	l	231	GLN
2	m	231	GLN
2	G	98	GLN
2	H	98	GLN
2	H	101	ASN
2	H	114	GLN
2	J	98	GLN
2	K	129	HIS
2	K	216	ASN
2	L	129	HIS
2	L	165	ASN
2	M	80	GLN
2	M	114	GLN
2	N	80	GLN
2	N	129	HIS
3	S	381	ASN
3	S	396	GLN
3	T	381	ASN
3	U	456	GLN
3	X	396	GLN
3	X	430	ASN
3	Y	390	ASN
3	Y	430	ASN
3	a	390	ASN
3	a	437	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

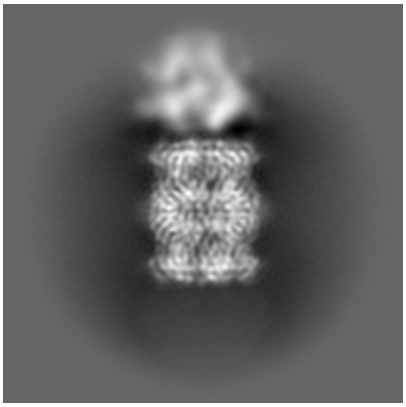
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27226. These allow visual inspection of the internal detail of the map and identification of artifacts.

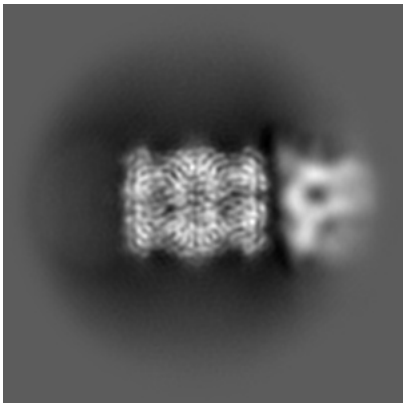
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

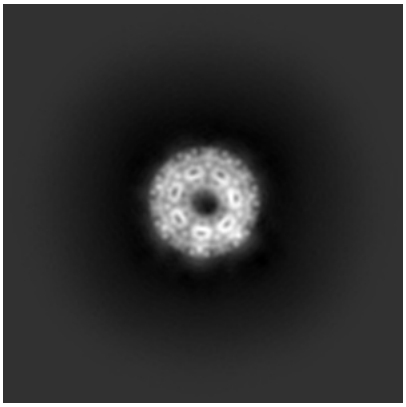
6.1.1 Primary map



X



Y

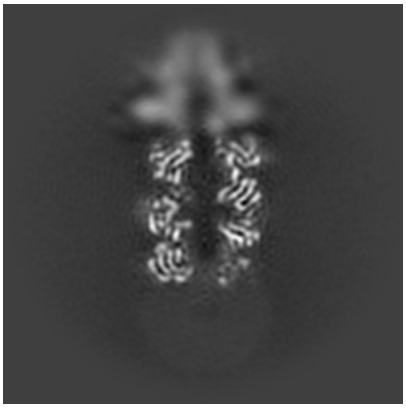


Z

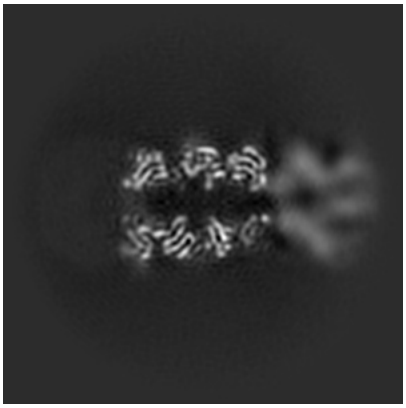
The images above show the map projected in three orthogonal directions.

6.2 Central slices

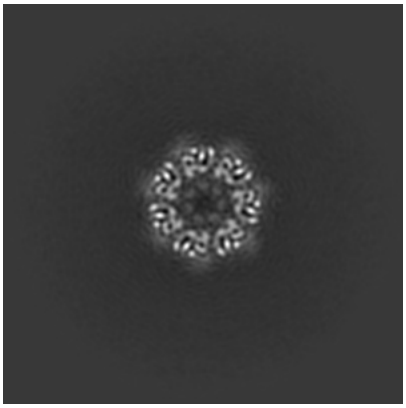
6.2.1 Primary map



X Index: 64



Y Index: 64

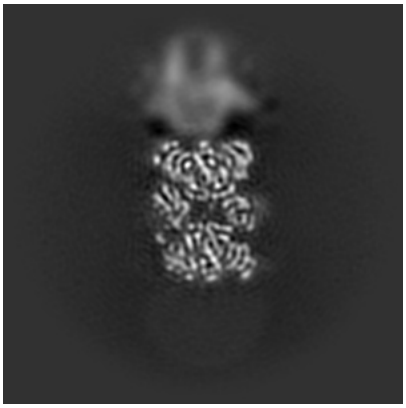


Z Index: 64

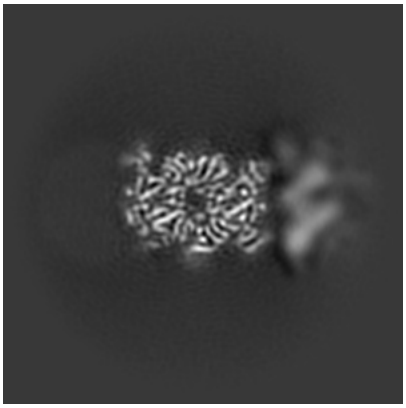
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

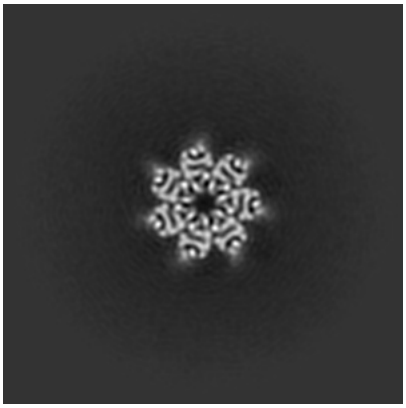
6.3.1 Primary map



X Index: 72



Y Index: 72



Z Index: 79

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

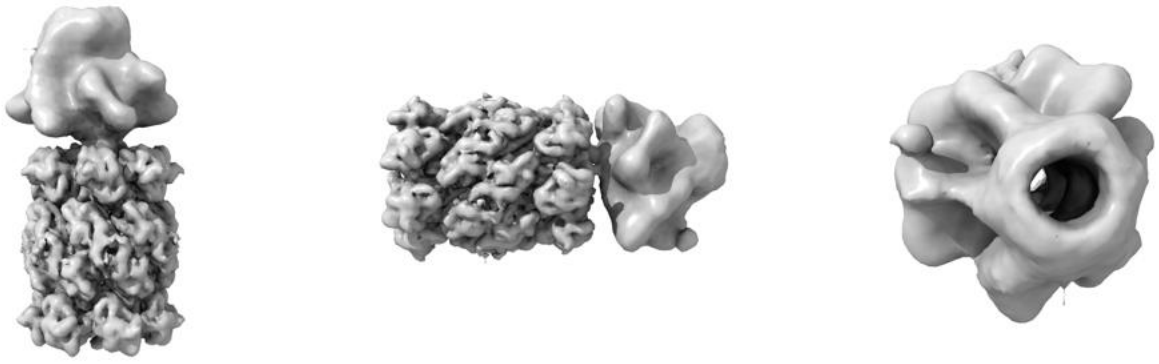
Y

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

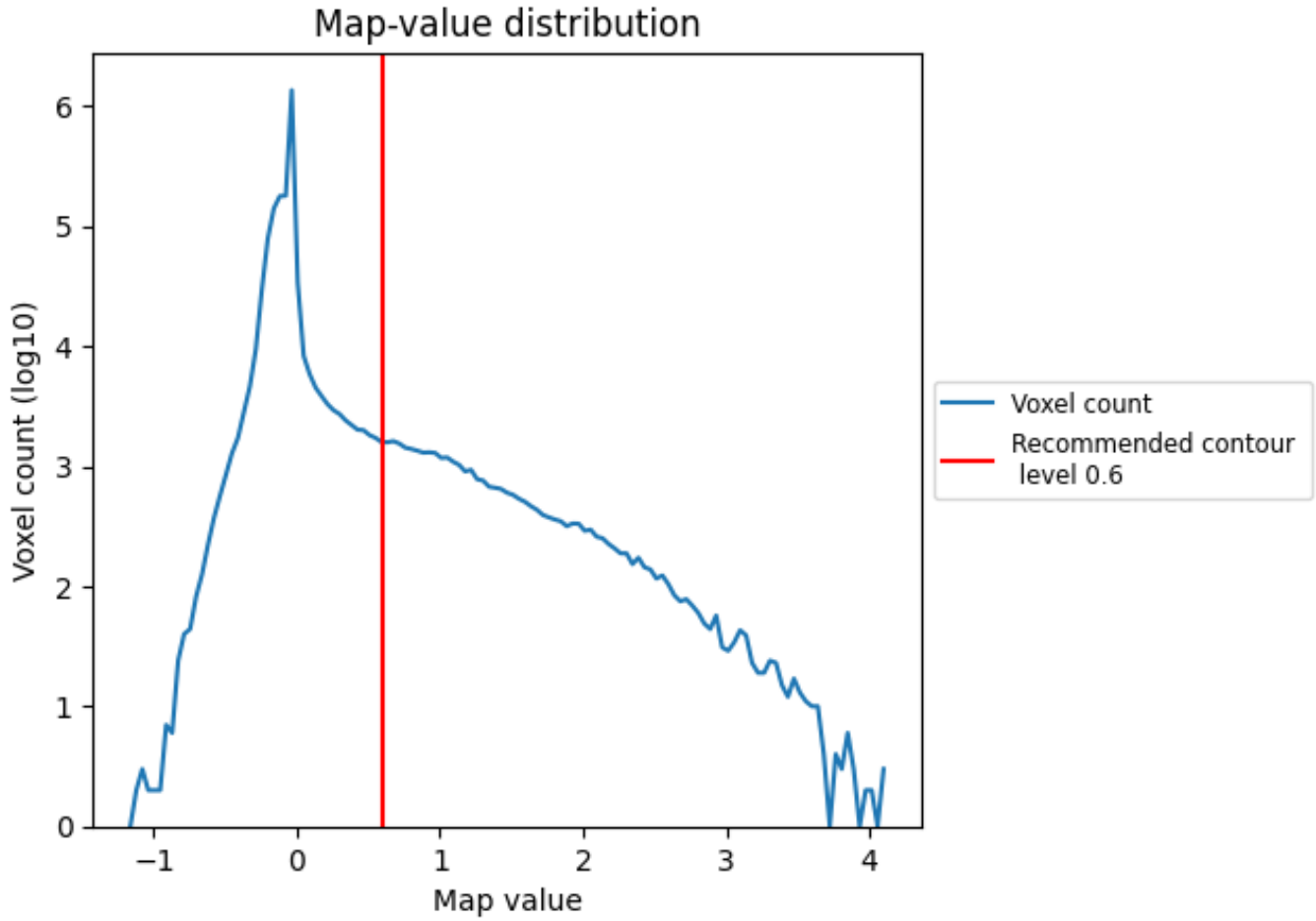
6.6 Mask visualisation (i)

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

7 Map analysis

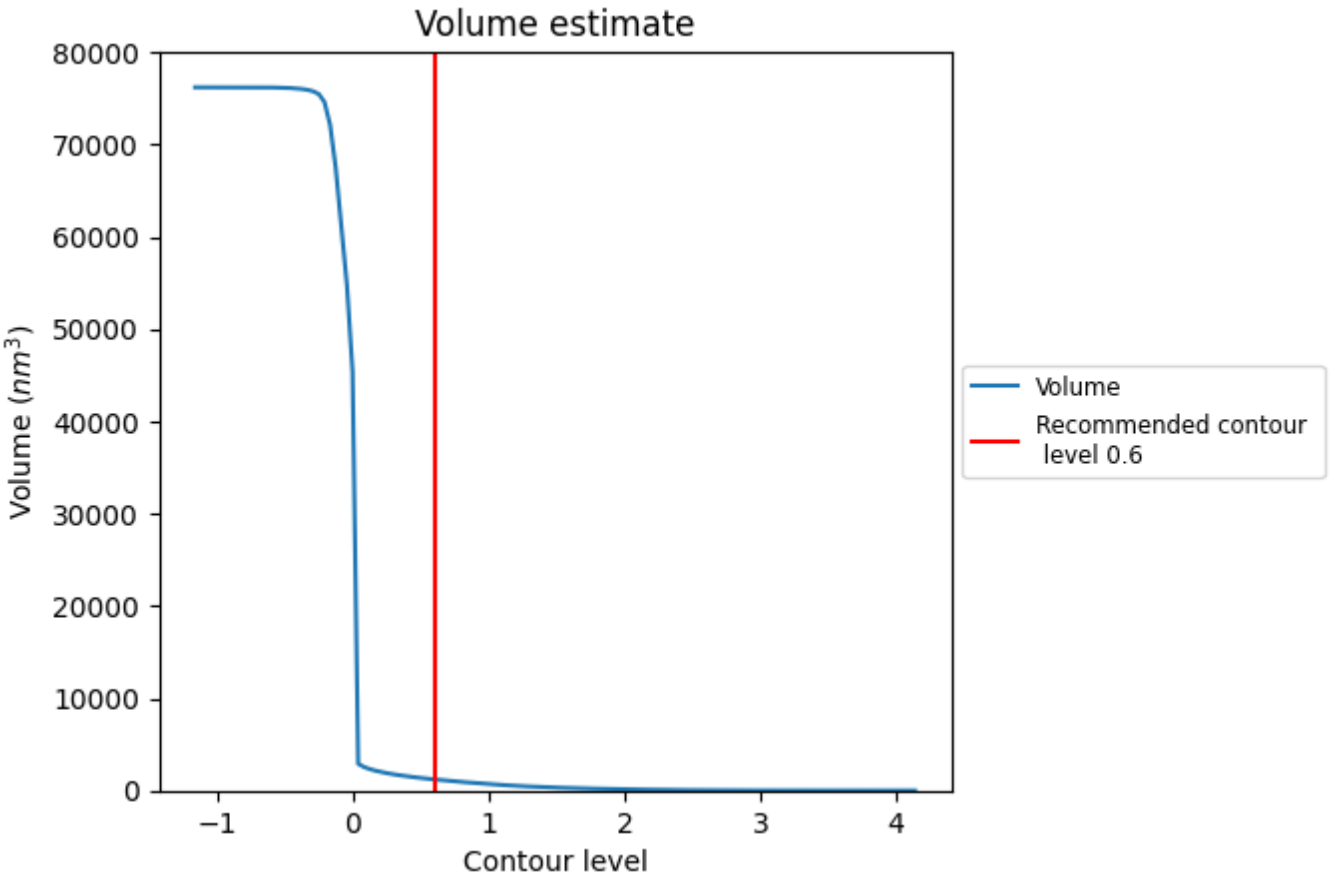
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

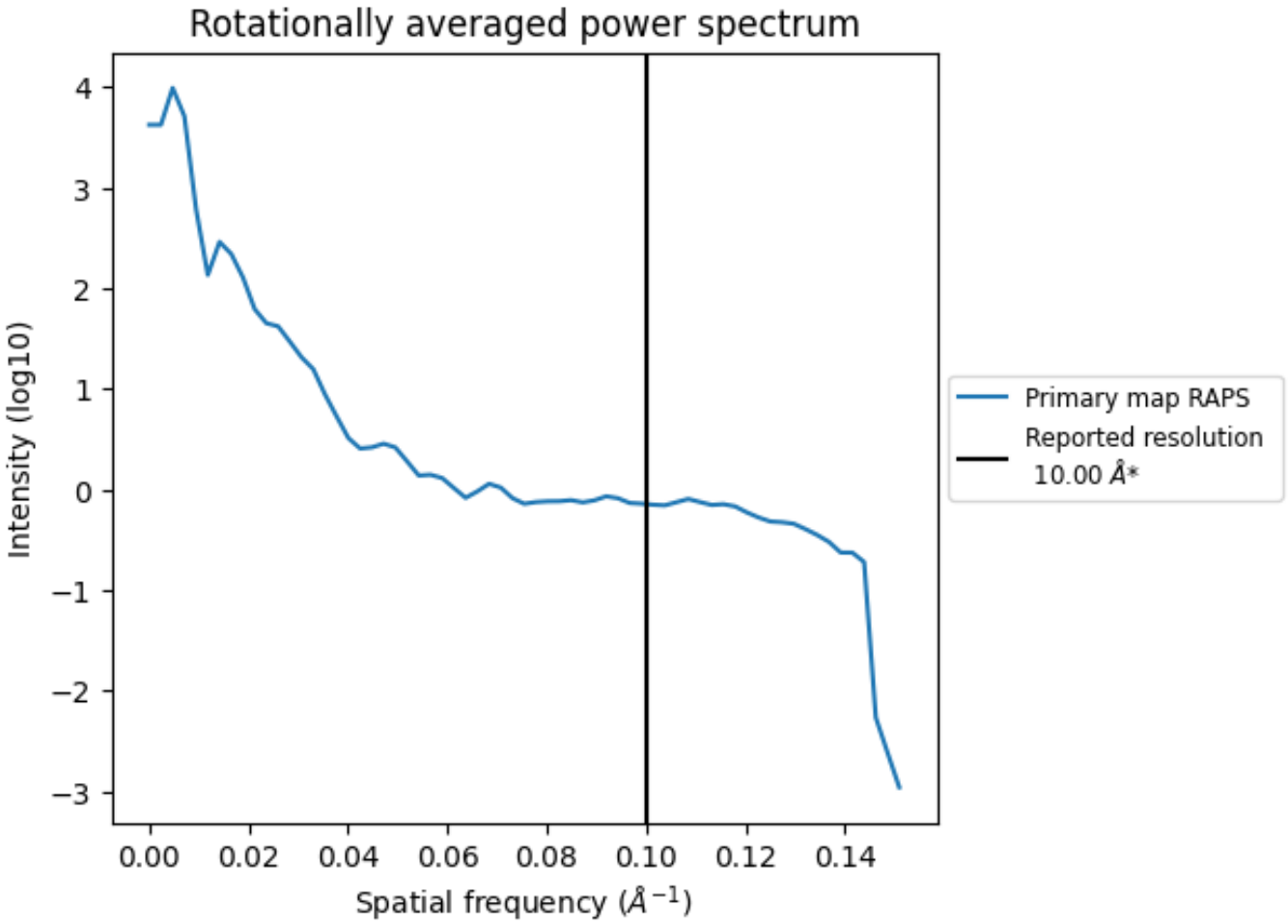
7.2 Volume estimate



The volume at the recommended contour level is 1208 nm^3; this corresponds to an approximate mass of 1092 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 (i)



*Reported resolution corresponds to spatial frequency of 0.100 Å^{-1}

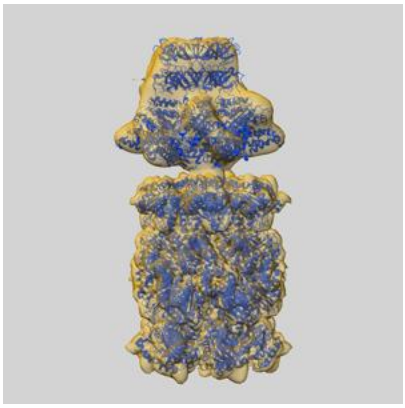
8 Fourier-Shell correlation

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

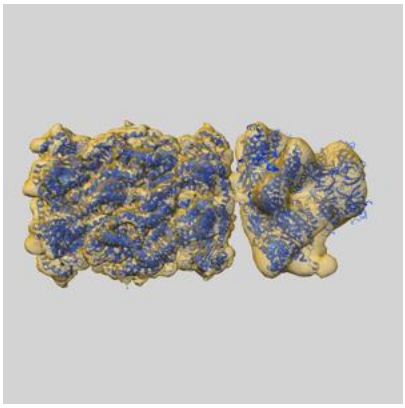
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27226 and PDB model 8D6Y. Per-residue inclusion information can be found in section 3 on page 8.

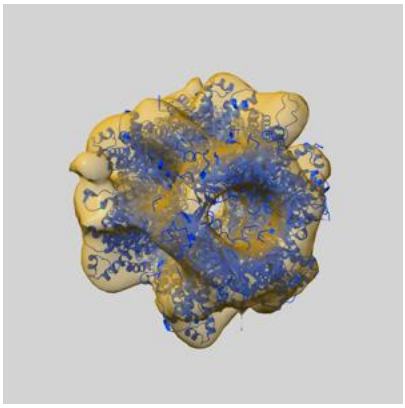
9.1 Map-model overlay



X



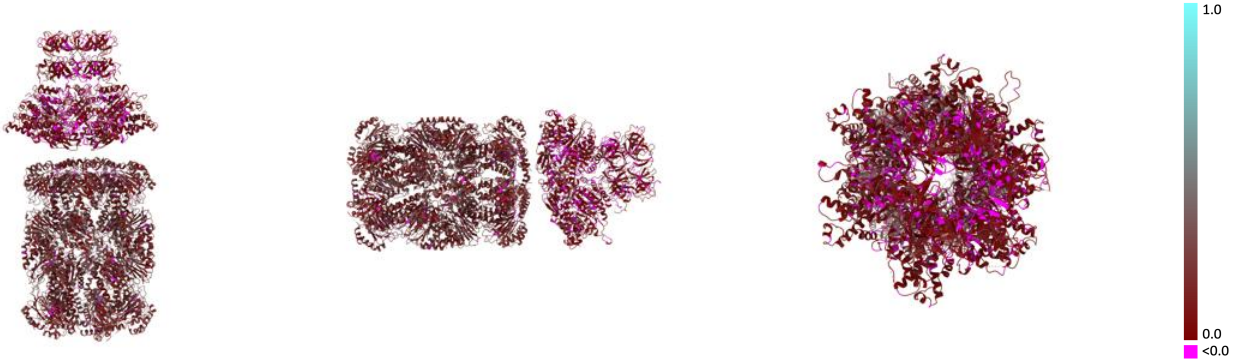
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

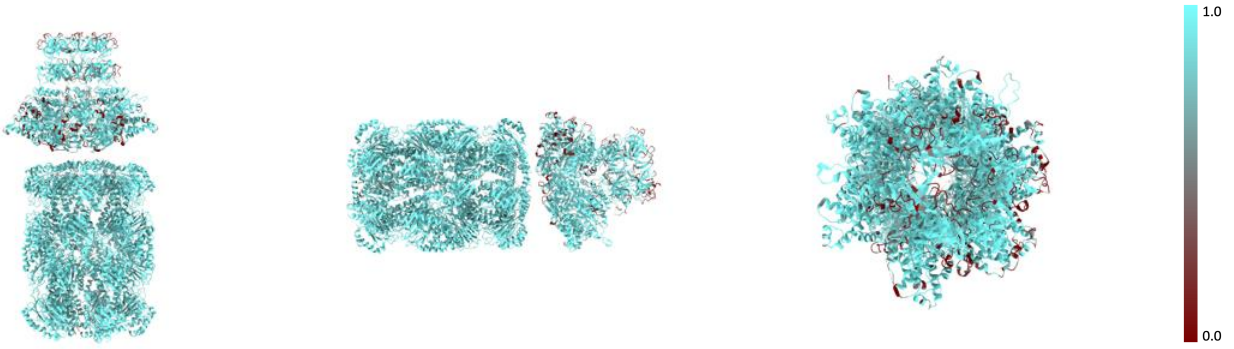
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

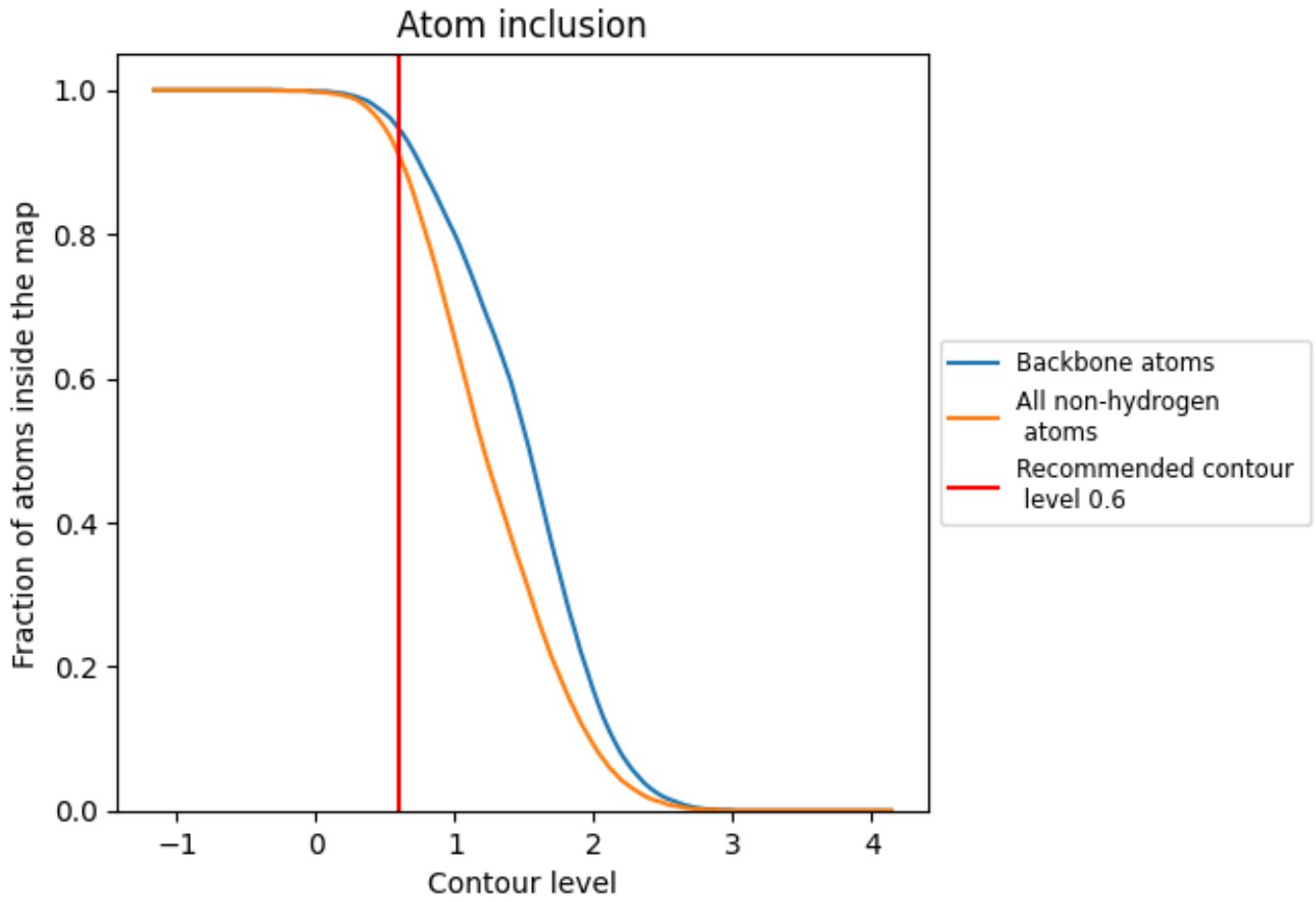
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9090	0.1510
A	0.8200	0.0580
B	0.8410	0.0600
C	0.8690	0.0600
D	0.8450	0.0620
E	0.8050	0.0530
F	0.7740	0.0500
G	0.9610	0.1930
H	0.9650	0.1900
I	0.9630	0.1950
J	0.9330	0.1830
K	0.9400	0.1900
L	0.9230	0.1900
M	0.9250	0.1860
N	0.9340	0.1910
O	0.9250	0.1870
P	0.9630	0.2000
Q	0.9630	0.2090
R	0.9640	0.2050
S	0.9590	0.2070
T	0.9550	0.2060
U	0.9650	0.2100
V	0.9590	0.2010
W	0.9440	0.1990
X	0.9610	0.2100
Y	0.9510	0.1980
Z	0.9570	0.2040
a	0.9530	0.1980
b	0.9510	0.1950
c	0.9500	0.2050
d	0.5150	-0.1190
e	0.3030	-0.1580
f	0.3330	-0.1630
g	0.5450	-0.1860
h	0.3940	-0.1990

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Chain	Atom inclusion	Q-score
i	0.5150	-0.0840
j	0.6970	-0.0030
k	0.9330	0.1950
l	0.9600	0.1930
m	0.9530	0.1920
n	0.9660	0.1910
o	0.9630	0.1920