



Full wwPDB EM Validation Report ⓘ

Jul 8, 2025 – 02:47 PM JST

PDB ID : 8IYD / pdb_00008iyd
EMDB ID : EMD-35818
Title : Tail cap of phage lambda tail
Authors : Wang, J.W.; Wang, C.
Deposited on : 2023-04-04
Resolution : 3.10 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 : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

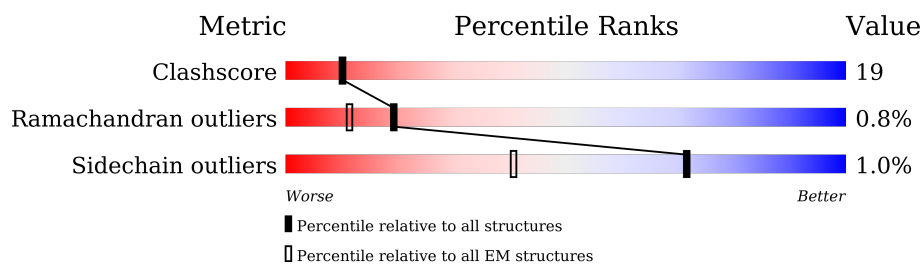
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.

















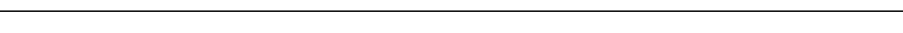
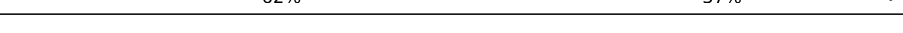





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	246	57% 41% .
1	B	246	62% 36% .
1	C	246	58% 40% ..
1	D	246	60% 38% ..
1	E	246	64% 35% .
1	F	246	67% 32% .
1	H	246	59% 40% .
1	I	246	59% 40% .
1	J	246	63% 35% ..

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Mol	Chain	Length	Quality of chain
1	L	246	 61%38%.
1	M	246	 63%37%.
1	N	246	 57%41%..
1	O	246	 63%36%..
1	P	246	 61%37%.
1	R	246	 58%40%..
1	S	246	 58%41%..
1	T	246	 66%32%..
1	V	246	 64%35%.
1	X	246	 61%37%.
1	Y	246	 61%39%.
1	a	246	 61%39%.
1	b	246	 61%36%..
1	c	246	 67%31%.
1	v	246	 62%37%.
2	G	131	 68%32%
2	K	131	 66%31%...
2	Q	131	 60%35%..
2	U	131	 63%35%.
2	W	131	 67%30%...
2	u	131	 63%32%...

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 49344 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 Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	B	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	C	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	a	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	b	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	c	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	V	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	v	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	D	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	E	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	F	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	H	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	I	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	J	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	L	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	M	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	N	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	P	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	R	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	S	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	T	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	X	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	Y	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		

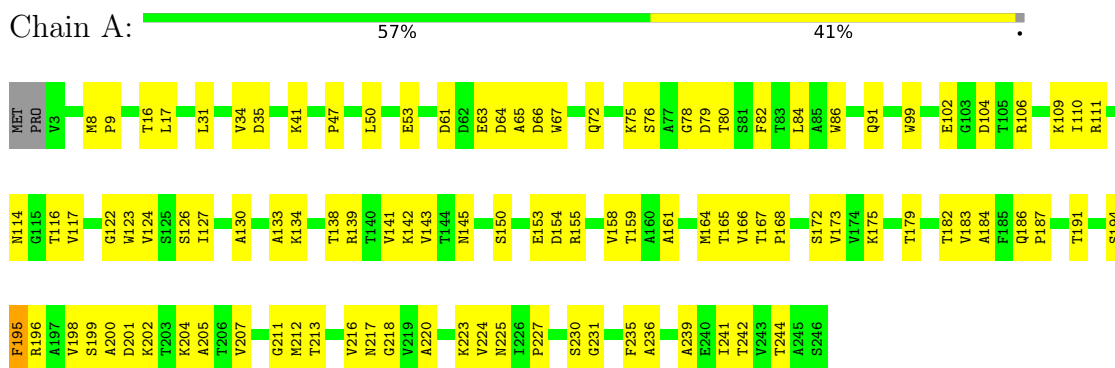
- Molecule 2 is a protein called Tail tube terminator protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	131	Total	C	N	O	S	0	0
			1032	655	159	213	5		
2	u	130	Total	C	N	O	S	0	0
			1024	650	158	212	4		
2	G	131	Total	C	N	O	S	0	0
			1032	655	159	213	5		
2	K	130	Total	C	N	O	S	0	0
			1024	650	158	212	4		
2	Q	131	Total	C	N	O	S	0	0
			1032	655	159	213	5		
2	W	130	Total	C	N	O	S	0	0
			1024	650	158	212	4		

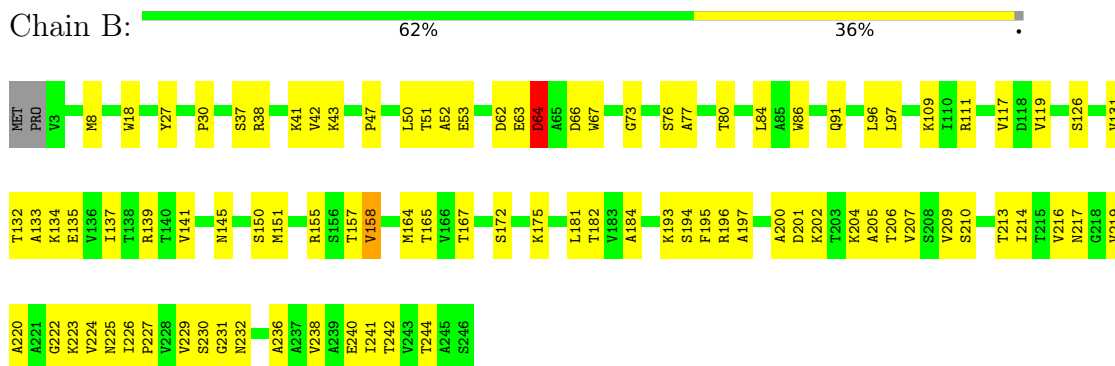
3 Residue-property plots [i](#)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tail tube protein



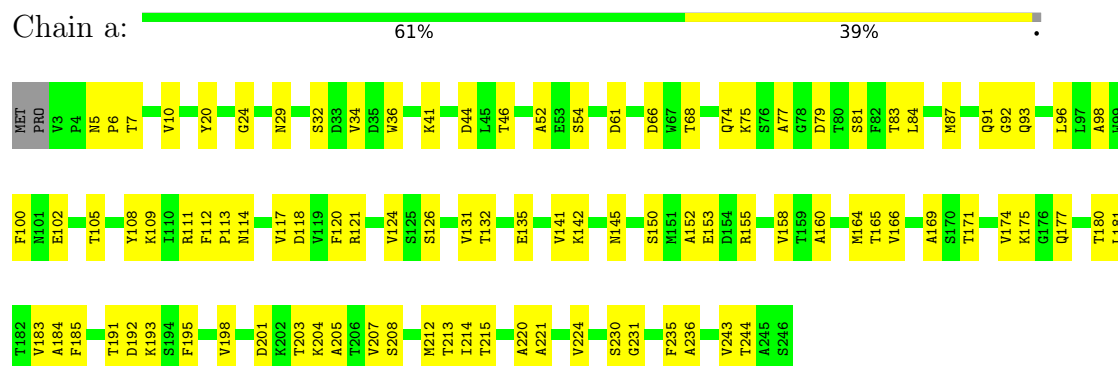
• Molecule 1: Tail tube protein



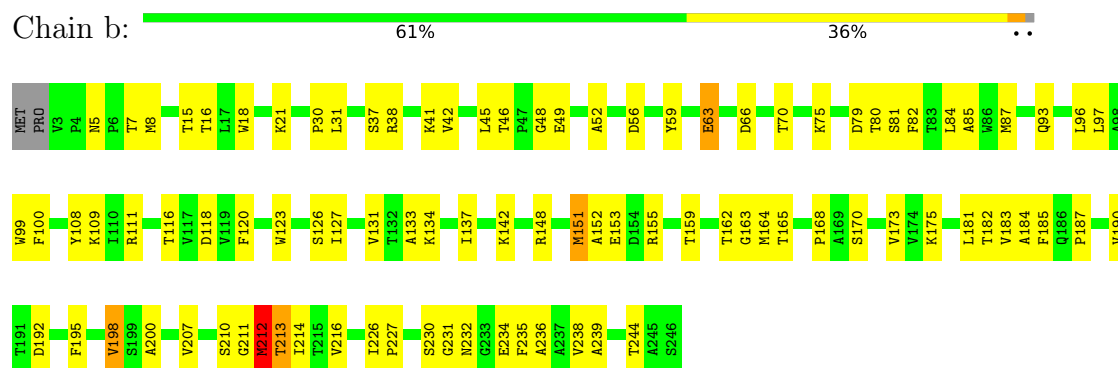
• Molecule 1: Tail tube protein



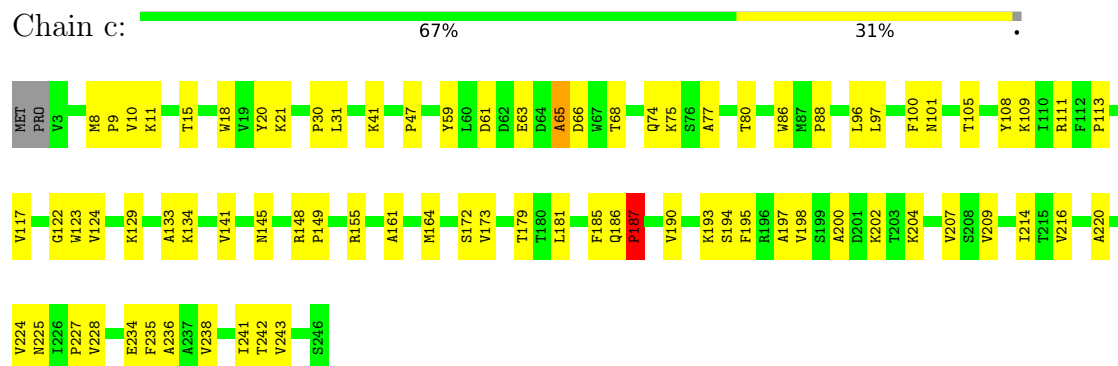
- Molecule 1: Tail tube protein



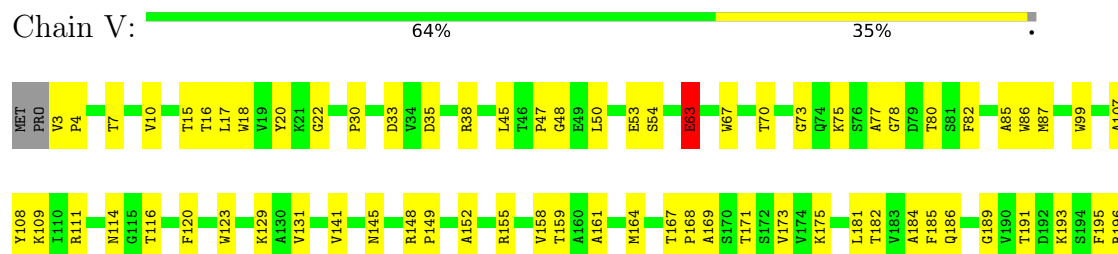
- Molecule 1: Tail tube protein



- Molecule 1: Tail tube protein



- Molecule 1: Tail tube protein





• Molecule 1: Tail tube protein

Chain v: 62% 37%



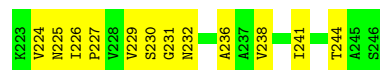
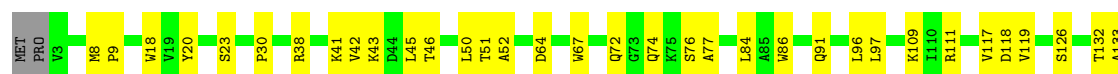
• Molecule 1: Tail tube protein

Chain D: 60% 38%



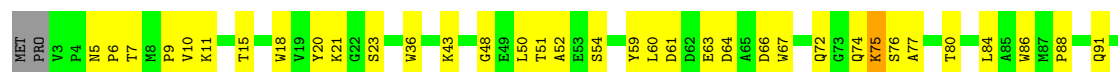
• Molecule 1: Tail tube protein

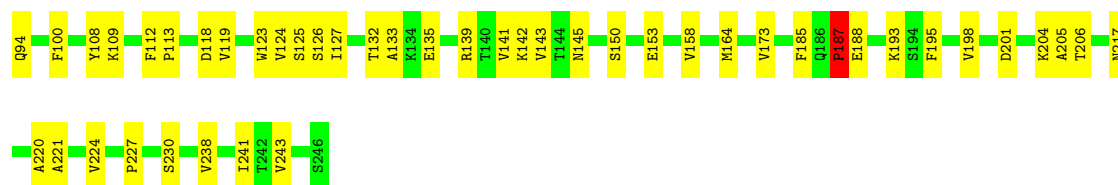
Chain E: 64% 35%



• Molecule 1: Tail tube protein

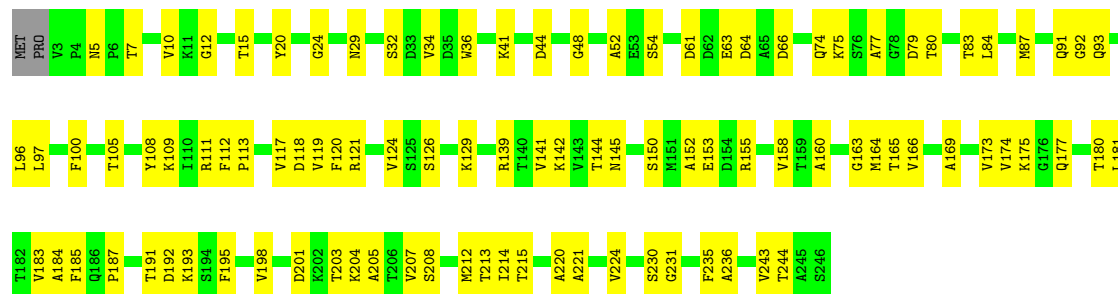
Chain F: 67% 32%





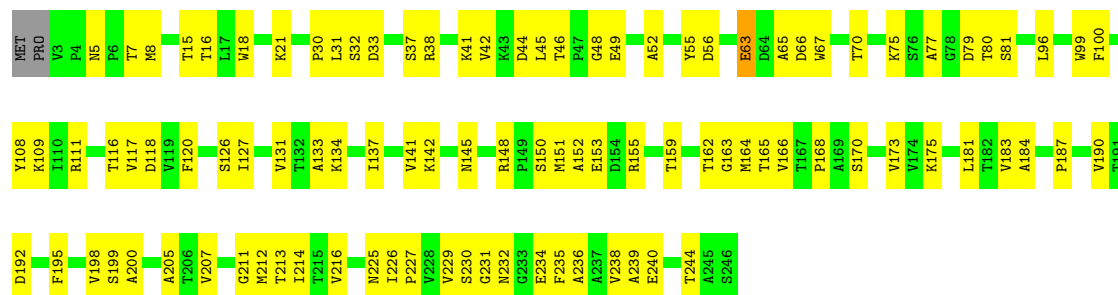
• Molecule 1: Tail tube protein

Chain H: 59% 40%



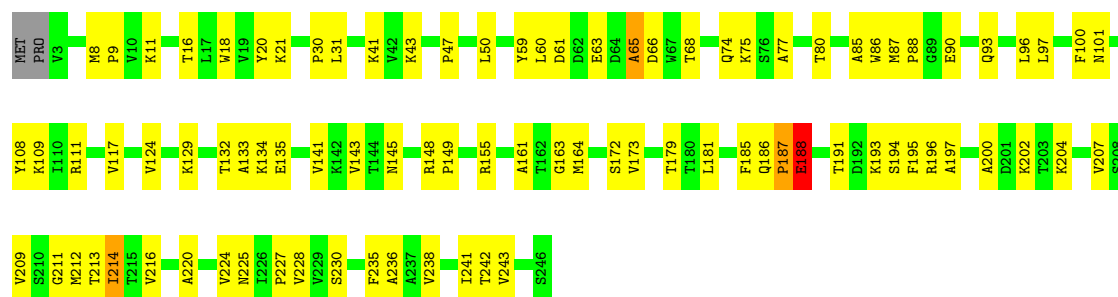
• Molecule 1: Tail tube protein

Chain I: 59% 40%



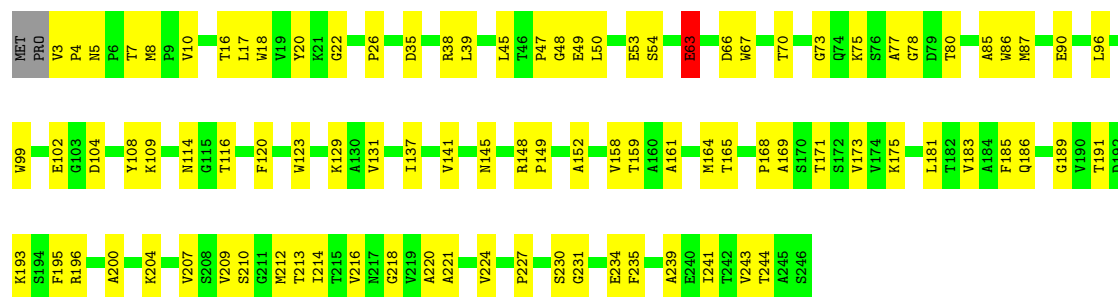
• Molecule 1: Tail tube protein

Chain J: 63% 35%



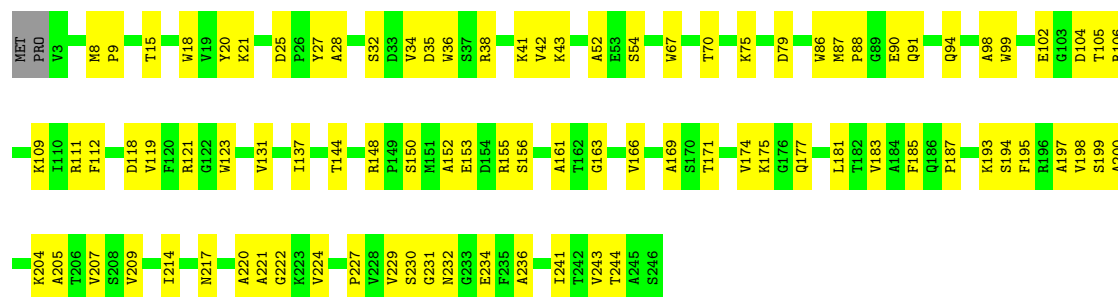
• Molecule 1: Tail tube protein

Chain L: 61% 38%



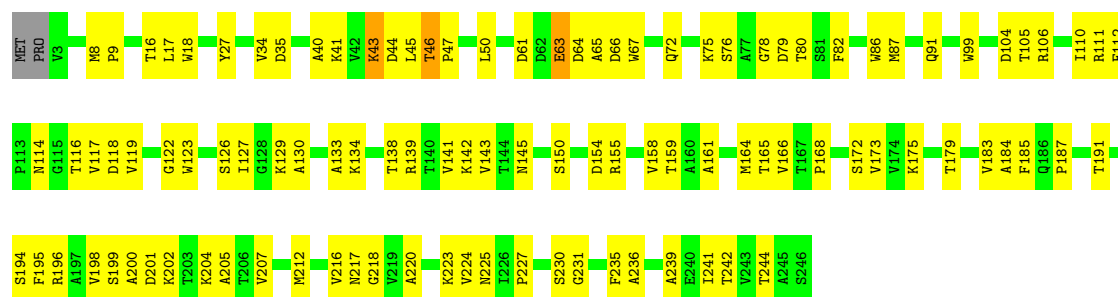
- Molecule 1: Tail tube protein

Chain M: 63% 37%



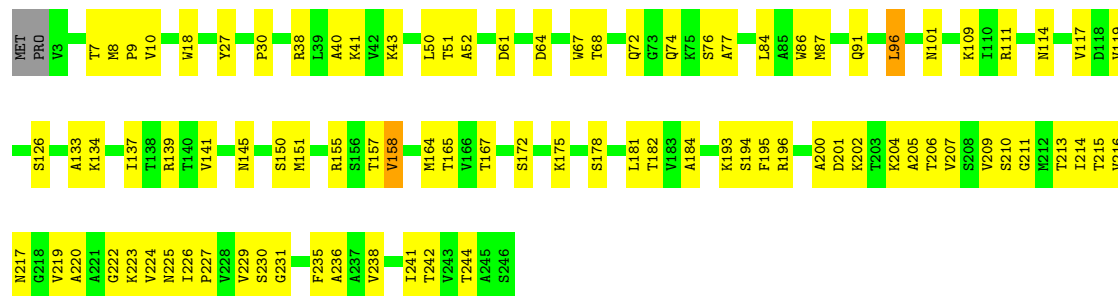
- Molecule 1: Tail tube protein

Chain N: 57% 41%



- Molecule 1: Tail tube protein

Chain O: 63% 36%



- Molecule 1: Tail tube protein

Chain P:  61% 37% .



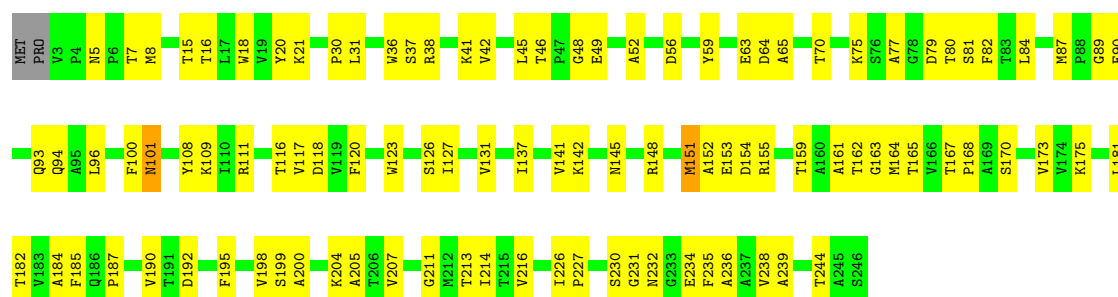
• Molecule 1: Tail tube protein

Chain R:  58% 40% ..



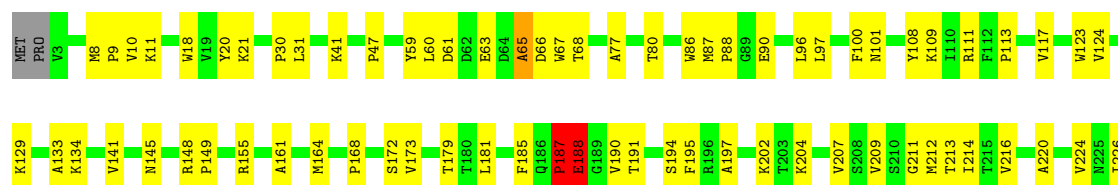
• Molecule 1: Tail tube protein

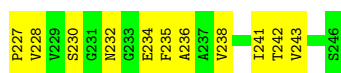
Chain S:  58% 41% ..



• Molecule 1: Tail tube protein

Chain T:  66% 32% ..





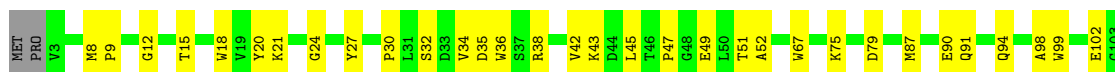
• Molecule 1: Tail tube protein

Chain X: 61% 37%



• Molecule 1: Tail tube protein

Chain Y: 61% 39%



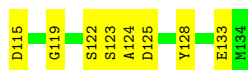
• Molecule 2: Tail tube terminator protein

Chain U: 63% 35%

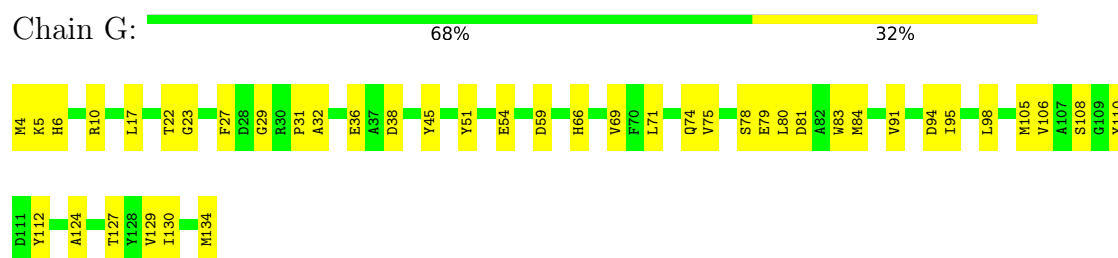


• Molecule 2: Tail tube terminator protein

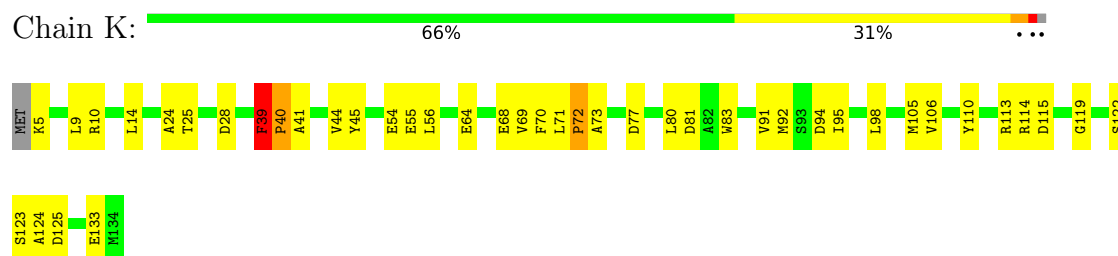
Chain u: 63% 32%



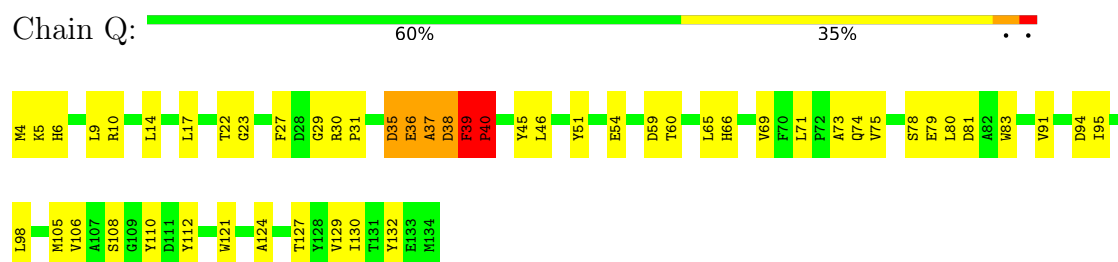
- Molecule 2: Tail tube terminator protein



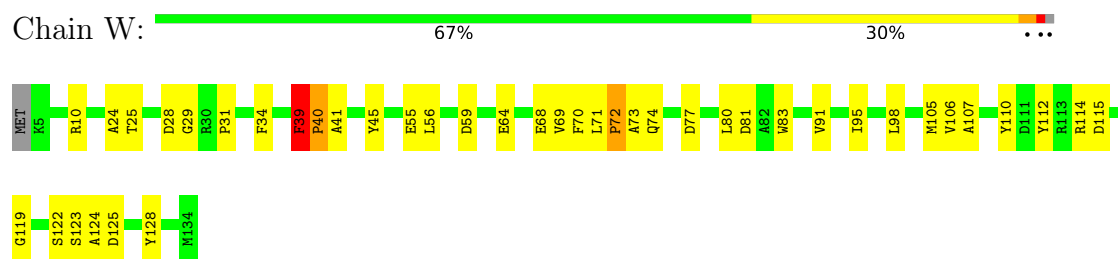
- Molecule 2: Tail tube terminator protein



- Molecule 2: Tail tube terminator protein



- Molecule 2: Tail tube terminator protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15959	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.21	0/1834	0.46	0/2505
1	B	0.19	0/1834	0.49	2/2505 (0.1%)
1	C	0.20	0/1834	0.47	0/2505
1	D	0.23	0/1834	0.45	0/2505
1	E	0.17	0/1834	0.45	0/2505
1	F	0.24	0/1834	0.51	1/2505 (0.0%)
1	H	0.20	0/1834	0.43	0/2505
1	I	0.23	0/1834	0.50	0/2505
1	J	0.23	0/1834	0.48	1/2505 (0.0%)
1	L	0.19	0/1834	0.41	0/2505
1	M	0.15	0/1834	0.37	0/2505
1	N	0.23	0/1834	0.51	0/2505
1	O	0.24	0/1834	0.48	0/2505
1	P	0.25	1/1834 (0.1%)	0.46	0/2505
1	R	0.21	0/1834	0.42	0/2505
1	S	0.23	0/1834	0.50	0/2505
1	T	0.24	0/1834	0.47	1/2505 (0.0%)
1	V	0.19	0/1834	0.41	0/2505
1	X	0.22	0/1834	0.44	0/2505
1	Y	0.18	0/1834	0.41	0/2505
1	a	0.20	0/1834	0.40	0/2505
1	b	0.26	0/1834	0.51	0/2505
1	c	0.24	0/1834	0.50	1/2505 (0.0%)
1	v	0.15	0/1834	0.37	0/2505
2	G	0.21	0/1058	0.48	0/1444
2	K	0.22	0/1050	0.49	0/1434
2	Q	0.29	0/1058	0.65	5/1444 (0.3%)
2	U	0.20	0/1058	0.48	0/1444
2	W	0.22	0/1050	0.49	0/1434
2	u	0.26	0/1050	0.51	0/1434
All	All	0.22	1/50340 (0.0%)	0.46	11/68754 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	1
2	U	0	1
2	W	0	1
2	u	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	222	GLY	C-O	-7.31	1.20	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	37	ALA	N-CA-C	-7.18	103.61	112.38
1	c	187	PRO	N-CA-C	-7.00	98.05	112.47
1	F	187	PRO	N-CA-C	-6.11	99.88	112.47
2	Q	73	ALA	CB-CA-C	-5.90	109.78	116.63
2	Q	39	PHE	CB-CA-C	5.82	121.63	110.17
1	B	64	ASP	CA-C-N	-5.78	111.98	122.50
1	B	64	ASP	C-N-CA	-5.78	111.98	122.50
1	J	187	PRO	N-CA-C	-5.46	101.23	112.47
1	T	187	PRO	N-CA-C	-5.20	101.76	112.47
2	Q	39	PHE	CA-CB-CG	-5.07	108.73	113.80
2	Q	39	PHE	CA-C-O	-5.02	113.28	120.16

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	39	PHE	Peptide
2	U	39	PHE	Peptide
2	W	39	PHE	Peptide
2	u	39	PHE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1799	0	1768	81	0
1	B	1799	0	1768	80	0
1	C	1799	0	1768	78	0
1	D	1799	0	1768	81	0
1	E	1799	0	1768	73	0
1	F	1799	0	1768	66	0
1	H	1799	0	1768	80	0
1	I	1799	0	1768	81	0
1	J	1799	0	1768	88	0
1	L	1799	0	1768	75	0
1	M	1799	0	1768	71	0
1	N	1799	0	1768	86	0
1	O	1799	0	1768	75	0
1	P	1799	0	1768	72	0
1	R	1799	0	1768	80	0
1	S	1799	0	1768	83	0
1	T	1799	0	1768	82	0
1	V	1799	0	1768	59	0
1	X	1799	0	1768	79	0
1	Y	1799	0	1768	87	0
1	a	1799	0	1768	70	0
1	b	1799	0	1768	82	0
1	c	1799	0	1768	78	0
1	v	1799	0	1768	76	0
2	G	1032	0	956	35	0
2	K	1024	0	947	36	0
2	Q	1032	0	956	44	0
2	U	1032	0	956	40	0
2	W	1024	0	947	36	0
2	u	1024	0	947	37	0
All	All	49344	0	48141	1843	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 (1843) 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:U:6:HIS:HE2	2:U:132:TYR:HH	1.10	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:35:ASP:HB3	2:Q:38:ASP:HB2	1.48	0.92
2:Q:6:HIS:HE2	2:Q:132:TYR:HH	1.07	0.92
1:E:8:MET:HE3	1:E:9:PRO:HD2	1.49	0.92
1:J:161:ALA:HB3	1:J:187:PRO:HB2	1.52	0.91
1:T:161:ALA:HB3	1:T:187:PRO:HB2	1.54	0.89
1:F:11:LYS:HE3	2:W:106:VAL:HG12	1.55	0.86
1:L:77:ALA:H	1:M:67:TRP:HZ3	1.25	0.84
1:c:161:ALA:HB3	1:c:187:PRO:CB	2.08	0.83
1:a:150:SER:OG	1:a:155:ARG:NH2	2.12	0.82
1:C:96:LEU:HD21	1:C:141:VAL:HG11	1.59	0.82
1:S:200:ALA:HB2	1:S:227:PRO:HD3	1.63	0.81
1:I:200:ALA:HB2	1:I:227:PRO:HD3	1.64	0.80
1:T:187:PRO:HG3	1:T:191:THR:HB	1.61	0.80
1:c:161:ALA:HB3	1:c:187:PRO:HB2	1.64	0.80
1:D:79:ASP:HA	1:D:143:VAL:O	1.80	0.80
2:U:92:MET:HA	2:U:95:ILE:HD11	1.63	0.80
1:O:50:LEU:HD13	1:O:77:ALA:HB2	1.64	0.79
2:G:106:VAL:HG12	1:J:11:LYS:HD3	1.64	0.79
2:Q:39:PHE:O	2:Q:40:PRO:C	2.25	0.78
1:X:94:GLN:NE2	1:Y:156:SER:OG	2.15	0.78
1:Y:164:MET:HE3	1:Y:164:MET:H	1.48	0.77
1:R:150:SER:OG	1:R:155:ARG:NH2	2.17	0.77
1:E:50:LEU:HD13	1:E:77:ALA:HB2	1.65	0.77
1:E:195:PHE:HA	1:E:230:SER:HA	1.64	0.77
1:I:225:ASN:ND2	1:I:240:GLU:OE1	2.18	0.77
1:I:151:MET:HE3	1:I:152:ALA:H	1.50	0.77
1:O:195:PHE:HA	1:O:230:SER:HA	1.66	0.77
1:S:195:PHE:HB2	1:S:230:SER:HA	1.67	0.77
2:G:75:VAL:HB	2:G:79:GLU:HG3	1.67	0.76
2:Q:106:VAL:HG12	1:T:11:LYS:HD3	1.66	0.76
1:B:30:PRO:O	1:B:109:LYS:NZ	2.19	0.76
1:Y:87:MET:HE2	1:Y:90:GLU:HG2	1.67	0.76
1:X:159:THR:HG23	1:X:161:ALA:H	1.51	0.76
1:V:159:THR:HG23	1:V:161:ALA:H	1.51	0.76
1:J:187:PRO:HG3	1:J:191:THR:HB	1.68	0.76
1:a:158:VAL:HG13	1:a:192:ASP:HB2	1.69	0.75
1:L:159:THR:HG23	1:L:161:ALA:H	1.50	0.75
1:E:30:PRO:O	1:E:109:LYS:NZ	2.18	0.75
1:X:175:LYS:HZ1	1:X:221:ALA:HB2	1.51	0.75
1:H:158:VAL:HG13	1:H:192:ASP:HB2	1.69	0.75
1:O:10:VAL:HG11	1:O:114:ASN:HB3	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:30:PRO:O	1:O:109:LYS:NZ	2.19	0.74
1:B:195:PHE:HA	1:B:230:SER:HA	1.67	0.74
1:v:183:VAL:HB	1:v:212:MET:HE1	1.70	0.74
1:I:175:LYS:NZ	1:I:244:THR:O	2.20	0.74
1:T:148:ARG:HH11	1:T:148:ARG:HA	1.51	0.74
2:U:4:MET:HG2	2:U:6:HIS:H	1.51	0.74
1:b:30:PRO:O	1:b:109:LYS:NZ	2.18	0.74
1:b:175:LYS:NZ	1:b:244:THR:O	2.21	0.74
1:P:119:VAL:HG23	1:P:150:SER:HB3	1.69	0.74
1:S:175:LYS:NZ	1:S:244:THR:O	2.21	0.74
1:a:77:ALA:O	1:a:145:ASN:ND2	2.19	0.74
1:c:148:ARG:HA	1:c:148:ARG:HH11	1.52	0.74
1:N:212:MET:HE2	1:N:212:MET:HA	1.70	0.74
1:R:158:VAL:HG13	1:R:192:ASP:HB2	1.69	0.73
1:H:96:LEU:HD21	1:H:141:VAL:HG21	1.70	0.73
1:B:50:LEU:HD13	1:B:77:ALA:HB2	1.70	0.73
1:b:211:GLY:C	1:b:213:THR:H	1.95	0.73
1:F:119:VAL:HG23	1:F:150:SER:HB3	1.70	0.73
1:I:16:THR:OG1	1:I:18:TRP:NE1	2.21	0.73
1:F:51:THR:HG22	1:F:52:ALA:H	1.53	0.73
1:A:79:ASP:HA	1:A:143:VAL:O	1.89	0.73
1:R:169:ALA:H	1:R:181:LEU:HG	1.54	0.73
1:H:77:ALA:O	1:H:145:ASN:ND2	2.21	0.73
1:b:16:THR:OG1	1:b:18:TRP:NE1	2.21	0.73
1:E:139:ARG:NH2	1:I:153:GLU:OE2	2.22	0.73
1:H:126:SER:HB3	1:H:142:LYS:HB3	1.70	0.73
1:C:119:VAL:HG23	1:C:150:SER:HB3	1.70	0.72
1:b:159:THR:HG21	1:b:190:VAL:HB	1.71	0.72
1:b:200:ALA:HB2	1:b:227:PRO:HD3	1.71	0.72
1:N:86:TRP:NE1	1:R:153:GLU:OE2	2.20	0.72
1:c:77:ALA:O	1:c:145:ASN:ND2	2.18	0.72
1:C:11:LYS:HE3	2:K:106:VAL:HG12	1.71	0.72
1:A:195:PHE:HB3	1:A:230:SER:HA	1.70	0.72
1:I:159:THR:HG21	1:I:190:VAL:HB	1.70	0.72
1:R:96:LEU:HD21	1:R:141:VAL:HG21	1.70	0.72
1:S:159:THR:HG21	1:S:190:VAL:HB	1.70	0.72
1:I:21:LYS:HZ3	1:I:37:SER:HB3	1.53	0.72
2:Q:29:GLY:HA2	2:Q:45:TYR:HB3	1.71	0.72
1:A:186:GLN:N	1:A:186:GLN:OE1	2.22	0.72
1:E:175:LYS:NZ	1:E:244:THR:O	2.23	0.72
1:P:198:VAL:HG13	1:P:227:PRO:HG2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:16:THR:OG1	1:S:18:TRP:NE1	2.23	0.72
1:T:185:PHE:HZ	1:T:195:PHE:HB3	1.54	0.72
1:Y:90:GLU:N	1:Y:90:GLU:OE2	2.22	0.72
1:N:150:SER:OG	1:N:155:ARG:NH2	2.23	0.72
1:T:117:VAL:O	1:T:155:ARG:NH1	2.23	0.71
1:c:96:LEU:HD21	1:c:141:VAL:HG21	1.72	0.71
1:H:169:ALA:H	1:H:181:LEU:HG	1.56	0.71
1:N:45:LEU:HD21	1:N:110:ILE:HD13	1.71	0.71
1:O:41:LYS:HD3	1:T:59:TYR:CE2	2.25	0.71
1:F:198:VAL:HG13	1:F:227:PRO:HG2	1.72	0.71
1:J:148:ARG:HH11	1:J:148:ARG:HA	1.53	0.71
1:L:67:TRP:HZ3	1:Y:148:ARG:HD2	1.56	0.71
1:R:191:THR:OG1	1:R:193:LYS:NZ	2.22	0.71
1:E:38:ARG:NH2	1:J:61:ASP:OD2	2.24	0.71
2:G:29:GLY:HA2	2:G:45:TYR:HB3	1.72	0.71
1:X:164:MET:HE3	1:X:165:THR:H	1.55	0.71
2:u:39:PHE:CE2	2:u:72:PRO:HA	2.26	0.71
1:E:196:ARG:NH1	1:I:232:ASN:O	2.24	0.71
1:N:79:ASP:HA	1:N:143:VAL:O	1.90	0.71
1:V:78:GLY:HA2	1:V:145:ASN:HB2	1.73	0.70
1:O:175:LYS:NZ	1:O:244:THR:O	2.24	0.70
1:A:102:GLU:HG2	1:A:104:ASP:H	1.53	0.70
1:B:196:ARG:NH1	1:b:232:ASN:O	2.25	0.70
1:V:54:SER:HG	1:V:70:THR:HG1	1.34	0.70
1:V:175:LYS:HZ1	1:V:221:ALA:HB2	1.57	0.70
2:U:29:GLY:HA2	2:U:45:TYR:HB3	1.73	0.70
1:J:31:LEU:HD12	1:J:111:ARG:HH22	1.57	0.70
1:I:21:LYS:NZ	1:I:37:SER:HB3	2.07	0.70
1:N:205:ALA:HB3	1:N:224:VAL:HG21	1.74	0.70
1:B:97:LEU:HD21	1:b:151:MET:HG2	1.74	0.69
1:a:96:LEU:HD21	1:a:141:VAL:HG21	1.71	0.69
1:c:148:ARG:HH11	1:c:149:PRO:HD2	1.57	0.69
1:v:131:VAL:HG22	1:v:137:ILE:HD12	1.73	0.69
1:N:8:MET:HG2	1:N:9:PRO:HD2	1.74	0.69
1:A:164:MET:HA	1:A:184:ALA:O	1.92	0.69
1:v:126:SER:OG	1:X:49:GLU:OE1	2.09	0.69
1:F:126:SER:HB3	1:F:142:LYS:HB3	1.74	0.69
1:L:49:GLU:OE1	1:Y:126:SER:OG	2.10	0.69
1:L:175:LYS:HZ1	1:L:221:ALA:HB2	1.58	0.69
1:C:61:ASP:OD2	1:I:42:VAL:N	2.24	0.69
1:V:10:VAL:HG11	1:V:114:ASN:HB3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:THR:HB	1:E:182:THR:HB	1.75	0.69
1:B:175:LYS:NZ	1:B:244:THR:O	2.26	0.69
1:c:117:VAL:O	1:c:155:ARG:NH1	2.25	0.69
1:T:181:LEU:HB2	1:T:214:ILE:HG13	1.75	0.69
1:B:167:THR:HB	1:B:182:THR:HB	1.74	0.69
1:Y:131:VAL:HG22	1:Y:137:ILE:HD12	1.74	0.69
1:v:169:ALA:HB3	1:v:241:ILE:HD11	1.75	0.69
1:D:65:ALA:O	1:R:74:GLN:NE2	2.25	0.69
2:K:41:ALA:HB3	2:K:70:PHE:HB2	1.75	0.69
1:P:202:LYS:NZ	1:T:234:GLU:O	2.25	0.69
1:v:161:ALA:HB3	1:v:187:PRO:HB2	1.75	0.69
1:P:102:GLU:HG3	1:P:104:ASP:HB2	1.75	0.69
1:J:117:VAL:O	1:J:155:ARG:NH1	2.26	0.69
1:L:67:TRP:CZ3	1:Y:148:ARG:HD2	2.28	0.69
1:Y:20:TYR:OH	1:Y:24:GLY:N	2.26	0.68
1:B:131:VAL:HG23	1:B:137:ILE:HG12	1.75	0.68
1:a:41:LYS:HG3	1:a:87:MET:HE1	1.75	0.68
1:I:30:PRO:O	1:I:109:LYS:NZ	2.20	0.68
1:L:185:PHE:O	1:L:191:THR:OG1	2.09	0.68
1:C:126:SER:HB3	1:C:142:LYS:HB3	1.75	0.68
1:M:131:VAL:HG22	1:M:137:ILE:HD12	1.76	0.68
1:N:139:ARG:NH2	1:R:153:GLU:OE2	2.26	0.68
1:T:96:LEU:HD21	1:T:141:VAL:HG21	1.75	0.68
1:v:90:GLU:N	1:v:90:GLU:OE2	2.27	0.68
1:X:210:SER:O	1:X:213:THR:OG1	2.11	0.68
1:C:198:VAL:HG13	1:C:227:PRO:HG2	1.75	0.68
1:M:8:MET:HE3	1:M:9:PRO:HD2	1.75	0.68
1:H:41:LYS:HG3	1:H:87:MET:HE1	1.76	0.68
1:J:148:ARG:HH11	1:J:149:PRO:HD2	1.59	0.68
1:O:167:THR:HB	1:O:182:THR:HB	1.76	0.68
1:S:77:ALA:O	1:S:145:ASN:ND2	2.24	0.68
1:A:35:ASP:H	1:A:196:ARG:HH22	1.42	0.68
2:K:95:ILE:HG22	2:K:98:LEU:H	1.58	0.68
1:H:118:ASP:OD1	1:H:152:ALA:N	2.27	0.67
1:B:205:ALA:HB3	1:B:224:VAL:HG11	1.76	0.67
1:b:165:THR:HB	1:b:184:ALA:HB3	1.77	0.67
1:O:139:ARG:NH2	1:S:153:GLU:OE2	2.27	0.67
1:T:148:ARG:HH11	1:T:149:PRO:HD2	1.60	0.67
1:D:61:ASP:HB2	1:Y:42:VAL:HG12	1.77	0.67
1:F:48:GLY:N	1:F:80:THR:OG1	2.27	0.67
1:F:61:ASP:OD2	1:S:42:VAL:N	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:80:LEU:HD23	2:K:124:ALA:HB2	1.74	0.67
1:E:97:LEU:HD21	1:I:151:MET:HG3	1.77	0.67
1:I:165:THR:HB	1:I:184:ALA:HB3	1.76	0.67
1:O:205:ALA:HB3	1:O:224:VAL:HG11	1.76	0.67
2:Q:78:SER:OG	2:W:28:ASP:OD2	2.10	0.67
1:T:31:LEU:HD12	1:T:111:ARG:HH12	1.59	0.67
1:A:205:ALA:HB3	1:A:224:VAL:HG21	1.76	0.67
1:c:124:VAL:O	1:P:72:GLN:NE2	2.26	0.67
1:v:150:SER:OG	1:v:155:ARG:NH2	2.27	0.67
2:G:4:MET:HG2	2:G:6:HIS:H	1.60	0.67
1:J:181:LEU:HB2	1:J:214:ILE:HG13	1.75	0.67
1:N:45:LEU:HG	1:N:46:THR:H	1.59	0.67
1:A:72:GLN:NE2	1:H:124:VAL:O	2.28	0.67
1:T:77:ALA:HB2	1:T:148:ARG:HH12	1.59	0.67
1:Y:198:VAL:HA	1:Y:207:VAL:HG21	1.76	0.67
1:I:166:VAL:HG22	1:I:183:VAL:HG22	1.77	0.67
1:M:161:ALA:HB3	1:M:187:PRO:HB2	1.77	0.67
1:a:169:ALA:H	1:a:181:LEU:HG	1.60	0.66
1:D:150:SER:C	1:D:155:ARG:HH22	2.03	0.66
1:X:10:VAL:HG11	1:X:114:ASN:HB3	1.77	0.66
1:Y:150:SER:OG	1:Y:155:ARG:NH2	2.28	0.66
1:E:151:MET:O	1:E:155:ARG:NH2	2.27	0.66
1:C:48:GLY:N	1:C:80:THR:OG1	2.27	0.66
1:b:85:ALA:HB3	1:b:87:MET:HE2	1.76	0.66
1:V:185:PHE:O	1:V:191:THR:OG1	2.12	0.66
1:v:204:LYS:HD2	1:v:222:GLY:HA3	1.78	0.66
1:Y:169:ALA:HB3	1:Y:241:ILE:HD11	1.77	0.66
1:X:53:GLU:OE1	1:X:53:GLU:N	2.26	0.66
1:X:193:LYS:NZ	1:X:230:SER:O	2.25	0.66
1:D:223:LYS:HE3	1:D:242:THR:HG22	1.78	0.66
1:O:200:ALA:HB3	1:O:225:ASN:HB2	1.78	0.66
2:W:41:ALA:HB3	2:W:70:PHE:HB2	1.76	0.66
1:P:96:LEU:HD21	1:P:141:VAL:HG11	1.76	0.66
1:J:224:VAL:HG23	1:J:241:ILE:HB	1.78	0.66
1:L:210:SER:O	1:L:213:THR:OG1	2.12	0.66
1:a:52:ALA:HA	1:a:75:LYS:HA	1.77	0.66
1:V:196:ARG:HH21	1:v:229:VAL:HG11	1.60	0.66
1:D:35:ASP:H	1:D:196:ARG:HH22	1.44	0.66
1:D:205:ALA:HB3	1:D:224:VAL:HG21	1.77	0.66
2:W:80:LEU:HD23	2:W:124:ALA:HB2	1.76	0.66
1:L:78:GLY:HA2	1:L:145:ASN:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:79:ASP:OD2	1:R:142:LYS:NZ	2.29	0.65
1:D:151:MET:O	1:D:155:ARG:NH2	2.28	0.65
1:N:35:ASP:H	1:N:196:ARG:HH22	1.44	0.65
1:S:30:PRO:O	1:S:109:LYS:NZ	2.19	0.65
1:S:30:PRO:HG2	1:S:155:ARG:HH12	1.60	0.65
1:T:87:MET:HB3	1:T:90:GLU:HG2	1.79	0.65
1:b:195:PHE:HB2	1:b:230:SER:HA	1.78	0.65
1:D:111:ARG:HG2	1:D:117:VAL:HG22	1.78	0.65
1:R:175:LYS:NZ	1:R:244:THR:O	2.30	0.65
1:A:65:ALA:O	1:H:74:GLN:NE2	2.28	0.65
1:a:174:VAL:HG22	1:a:177:GLN:HE22	1.61	0.65
1:L:148:ARG:HG3	1:M:67:TRP:CD1	2.32	0.65
1:B:151:MET:O	1:B:155:ARG:NH2	2.30	0.65
1:b:118:ASP:OD1	1:b:152:ALA:N	2.29	0.65
1:c:164:MET:HG2	1:c:235:PHE:CE2	2.32	0.65
1:X:94:GLN:NE2	1:Y:153:GLU:OE1	2.30	0.65
1:E:205:ALA:HB3	1:E:224:VAL:HG11	1.77	0.65
1:O:193:LYS:HZ2	1:O:231:GLY:HA3	1.62	0.65
1:X:7:THR:OG1	1:X:8:MET:SD	2.54	0.65
1:a:175:LYS:NZ	1:a:244:THR:O	2.31	0.65
1:E:193:LYS:NZ	1:E:232:ASN:OD1	2.29	0.65
1:J:185:PHE:HZ	1:J:195:PHE:HB3	1.60	0.65
1:S:163:GLY:H	1:S:187:PRO:HG3	1.61	0.65
1:O:151:MET:O	1:O:155:ARG:NH2	2.30	0.64
1:Y:161:ALA:HB3	1:Y:187:PRO:HB2	1.77	0.64
1:A:139:ARG:NH2	1:a:153:GLU:OE2	2.30	0.64
1:X:196:ARG:HH21	1:Y:229:VAL:HG11	1.61	0.64
1:B:216:VAL:HG11	1:B:241:ILE:HG13	1.79	0.64
1:c:74:GLN:HE21	1:P:68:THR:HG22	1.63	0.64
1:E:41:LYS:HD3	1:J:59:TYR:HE2	1.61	0.64
1:S:118:ASP:OD1	1:S:152:ALA:N	2.30	0.64
1:E:41:LYS:HD3	1:J:59:TYR:CE2	2.32	0.64
1:T:179:THR:HG22	1:T:216:VAL:HB	1.79	0.64
1:A:175:LYS:NZ	1:A:244:THR:O	2.31	0.64
1:C:202:LYS:NZ	1:c:234:GLU:O	2.30	0.64
1:D:139:ARG:NH2	1:H:153:GLU:OE2	2.31	0.64
1:L:196:ARG:HH21	1:M:229:VAL:HG11	1.62	0.64
1:D:112:PHE:HE2	1:D:118:ASP:OD1	1.80	0.64
1:E:216:VAL:HG11	1:E:241:ILE:HG13	1.78	0.64
1:H:175:LYS:NZ	1:H:244:THR:O	2.30	0.64
1:I:30:PRO:HG2	1:I:155:ARG:HH12	1.60	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:96:LEU:HD21	1:J:141:VAL:HG21	1.80	0.64
1:a:118:ASP:OD1	1:a:152:ALA:N	2.30	0.64
1:v:90:GLU:OE1	1:X:7:THR:HA	1.98	0.64
1:I:207:VAL:HG12	1:I:216:VAL:HG22	1.80	0.64
1:M:169:ALA:HB3	1:M:241:ILE:HD11	1.79	0.64
1:P:126:SER:HB3	1:P:142:LYS:HB3	1.79	0.64
1:A:111:ARG:HG2	1:A:117:VAL:HG22	1.80	0.64
1:F:9:PRO:HD3	1:T:87:MET:HE1	1.80	0.64
2:K:39:PHE:CE2	2:K:72:PRO:HA	2.33	0.64
1:X:185:PHE:O	1:X:191:THR:OG1	2.12	0.64
1:B:200:ALA:HB3	1:B:225:ASN:HB2	1.80	0.64
1:v:174:VAL:HG22	1:v:177:GLN:HE21	1.64	0.64
1:E:200:ALA:HB3	1:E:225:ASN:HB2	1.80	0.64
1:L:10:VAL:HG11	1:L:114:ASN:HB3	1.80	0.64
1:M:174:VAL:HG22	1:M:177:GLN:HE21	1.63	0.64
1:S:199:SER:OG	1:S:205:ALA:O	2.16	0.64
1:T:224:VAL:HG23	1:T:241:ILE:HB	1.78	0.64
1:D:168:PRO:HG3	1:D:239:ALA:HB1	1.78	0.63
1:C:164:MET:HE1	1:C:235:PHE:CG	2.33	0.63
1:N:223:LYS:HE3	1:N:242:THR:HG22	1.79	0.63
2:u:80:LEU:HD23	2:u:124:ALA:HB2	1.79	0.63
1:v:198:VAL:HA	1:v:207:VAL:HG21	1.79	0.63
1:L:66:ASP:O	1:Y:75:LYS:N	2.31	0.63
1:R:118:ASP:OD1	1:R:152:ALA:N	2.30	0.63
1:c:224:VAL:HG23	1:c:241:ILE:HB	1.80	0.63
1:M:18:TRP:HB2	1:M:109:LYS:HG2	1.81	0.63
1:X:129:LYS:HB3	1:Y:47:PRO:HG2	1.80	0.63
1:B:41:LYS:HD3	1:c:59:TYR:CE1	2.32	0.63
1:F:72:GLN:NE2	1:T:124:VAL:O	2.32	0.63
1:M:198:VAL:HA	1:M:207:VAL:HG21	1.80	0.63
1:L:193:LYS:NZ	1:L:230:SER:O	2.25	0.63
1:C:18:TRP:CD1	1:C:109:LYS:HZ2	2.15	0.63
1:S:111:ARG:HG2	1:S:117:VAL:HG23	1.81	0.63
1:F:164:MET:N	1:F:164:MET:SD	2.72	0.63
1:P:206:THR:OG1	1:P:217:ASN:OD1	2.09	0.63
1:c:207:VAL:HG12	1:c:216:VAL:HG22	1.80	0.63
1:J:207:VAL:HG12	1:J:216:VAL:HG22	1.81	0.63
1:R:126:SER:HB3	1:R:142:LYS:HB3	1.81	0.63
1:Y:18:TRP:HB2	1:Y:109:LYS:HG2	1.80	0.62
2:u:64:GLU:OE1	2:u:64:GLU:N	2.33	0.62
1:P:50:LEU:HG	1:P:77:ALA:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:52:ALA:HA	1:S:75:LYS:HA	1.81	0.62
1:B:38:ARG:NH2	1:c:61:ASP:OD2	2.31	0.62
2:G:108:SER:HB2	2:G:129:VAL:HG23	1.81	0.62
1:H:195:PHE:HA	1:H:231:GLY:H	1.64	0.62
1:N:111:ARG:HG2	1:N:117:VAL:HG22	1.81	0.62
1:C:60:LEU:HD21	1:I:15:THR:HB	1.81	0.62
1:V:193:LYS:NZ	1:V:230:SER:O	2.25	0.62
1:v:18:TRP:HB2	1:v:109:LYS:HG2	1.80	0.62
1:O:216:VAL:HG11	1:O:241:ILE:HG13	1.81	0.62
1:S:21:LYS:NZ	1:S:37:SER:HB3	2.15	0.62
1:X:100:PHE:O	1:Y:75:LYS:NZ	2.32	0.62
1:V:210:SER:O	1:V:213:THR:OG1	2.12	0.62
1:v:42:VAL:N	1:N:61:ASP:OD2	2.20	0.62
1:I:181:LEU:HB2	1:I:214:ILE:HB	1.82	0.62
1:Y:8:MET:HE3	1:Y:9:PRO:HD2	1.81	0.62
1:b:207:VAL:HG12	1:b:216:VAL:HG22	1.81	0.62
1:c:77:ALA:HB2	1:c:148:ARG:HH12	1.63	0.62
1:b:148:ARG:HG3	1:O:67:TRP:NE1	2.14	0.62
1:D:104:ASP:OD2	1:D:106:ARG:NE	2.26	0.62
1:I:16:THR:HB	1:I:38:ARG:HH21	1.65	0.62
1:I:195:PHE:HB2	1:I:230:SER:HA	1.80	0.62
1:A:223:LYS:HE3	1:A:242:THR:HG22	1.81	0.62
1:O:51:THR:HG22	1:O:52:ALA:H	1.63	0.62
1:S:89:GLY:O	1:S:94:GLN:NE2	2.32	0.62
1:T:148:ARG:HD3	1:T:149:PRO:HD2	1.82	0.62
1:Y:118:ASP:OD1	1:Y:152:ALA:N	2.33	0.62
1:c:181:LEU:HB2	1:c:214:ILE:HG13	1.82	0.62
1:a:74:GLN:NE2	1:N:65:ALA:O	2.28	0.61
1:c:161:ALA:HB3	1:c:187:PRO:HB3	1.80	0.61
1:J:108:TYR:OH	1:J:145:ASN:OD1	2.13	0.61
1:N:175:LYS:NZ	1:N:244:THR:O	2.32	0.61
1:V:22:GLY:HA3	1:V:35:ASP:HB3	1.81	0.61
1:v:175:LYS:NZ	1:v:244:THR:O	2.33	0.61
1:P:51:THR:HG22	1:P:52:ALA:H	1.65	0.61
1:R:198:VAL:HA	1:R:207:VAL:HG11	1.81	0.61
1:S:207:VAL:HG12	1:S:216:VAL:HG22	1.81	0.61
1:D:16:THR:OG1	1:D:111:ARG:HB2	2.00	0.61
1:L:120:PHE:HB3	1:L:145:ASN:HD21	1.65	0.61
1:P:153:GLU:N	1:P:153:GLU:OE1	2.33	0.61
1:P:21:LYS:HG3	1:P:21:LYS:O	1.99	0.61
1:A:168:PRO:HG3	1:A:239:ALA:HB1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:15:THR:HG23	1:v:112:PHE:HA	1.82	0.61
2:K:68:GLU:HG3	2:K:125:ASP:HB3	1.83	0.61
1:Y:132:THR:HG23	1:Y:135:GLU:HB3	1.82	0.61
1:A:150:SER:O	1:A:155:ARG:NH2	2.34	0.61
1:O:196:ARG:NH1	1:S:232:ASN:O	2.32	0.61
1:H:108:TYR:CZ	1:H:120:PHE:HB2	2.35	0.61
2:K:64:GLU:OE1	2:K:64:GLU:N	2.33	0.61
1:N:195:PHE:CZ	1:N:212:MET:HE1	2.36	0.61
1:A:164:MET:HG3	1:A:235:PHE:CE1	2.36	0.61
2:K:81:ASP:OD1	2:K:110:TYR:OH	2.18	0.61
1:N:168:PRO:HG3	1:N:239:ALA:HB1	1.83	0.61
1:Y:174:VAL:HG22	1:Y:177:GLN:HE21	1.64	0.61
1:D:198:VAL:HG23	1:D:227:PRO:HG2	1.81	0.61
1:A:50:LEU:HD23	1:H:100:PHE:CE2	2.36	0.60
1:A:212:MET:HE2	1:A:212:MET:HA	1.83	0.60
1:A:61:ASP:OD2	1:M:42:VAL:N	2.31	0.60
2:u:81:ASP:OD1	2:u:110:TYR:OH	2.18	0.60
1:E:210:SER:O	1:E:213:THR:OG1	2.18	0.60
2:G:81:ASP:OD1	2:G:110:TYR:OH	2.18	0.60
1:R:108:TYR:CZ	1:R:120:PHE:HB2	2.36	0.60
1:Y:15:THR:HG23	1:Y:112:PHE:HA	1.82	0.60
1:H:166:VAL:HG22	1:H:183:VAL:HG22	1.82	0.60
1:H:221:ALA:HA	1:H:243:VAL:HG13	1.83	0.60
1:O:210:SER:O	1:O:213:THR:OG1	2.16	0.60
2:Q:39:PHE:HB3	2:Q:40:PRO:CD	2.32	0.60
2:W:95:ILE:HG22	2:W:98:LEU:H	1.67	0.60
1:H:198:VAL:HA	1:H:207:VAL:HG11	1.83	0.60
1:X:167:THR:HB	1:X:182:THR:HG23	1.83	0.60
1:F:50:LEU:HG	1:F:77:ALA:HB2	1.82	0.60
1:L:164:MET:HE3	1:L:165:THR:H	1.67	0.60
1:M:204:LYS:HD2	1:M:222:GLY:HA3	1.82	0.60
1:E:126:SER:OG	1:I:49:GLU:OE2	2.20	0.60
1:M:119:VAL:HG23	1:M:150:SER:HB3	1.83	0.60
1:X:195:PHE:HE1	1:X:212:MET:HG3	1.67	0.60
1:a:126:SER:HB3	1:a:142:LYS:HB3	1.84	0.60
1:Y:204:LYS:HD2	1:Y:222:GLY:HA3	1.82	0.60
1:J:77:ALA:HB2	1:J:148:ARG:NH1	2.16	0.60
1:T:228:VAL:O	1:T:236:ALA:HA	2.02	0.60
1:a:124:VAL:O	1:N:72:GLN:NE2	2.35	0.60
1:P:18:TRP:CD1	1:P:109:LYS:HZ2	2.19	0.60
2:u:68:GLU:HG3	2:u:125:ASP:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:GLY:O	1:H:15:THR:OG1	2.17	0.60
1:P:209:VAL:HG23	1:P:214:ILE:HG12	1.83	0.60
1:S:31:LEU:O	1:S:111:ARG:NH1	2.35	0.60
1:T:209:VAL:HG22	1:T:214:ILE:HG22	1.82	0.60
2:G:59:ASP:OD1	2:G:59:ASP:N	2.35	0.59
2:Q:95:ILE:HG22	2:Q:98:LEU:H	1.65	0.59
1:S:181:LEU:HB2	1:S:214:ILE:HB	1.82	0.59
1:c:148:ARG:HD3	1:c:149:PRO:HD2	1.82	0.59
1:X:120:PHE:HB3	1:X:145:ASN:HD21	1.65	0.59
1:C:206:THR:OG1	1:C:217:ASN:OD1	2.09	0.59
1:b:148:ARG:HG3	1:O:67:TRP:CE2	2.38	0.59
1:v:109:LYS:HB2	1:v:119:VAL:HG12	1.84	0.59
2:Q:108:SER:HB2	2:Q:129:VAL:HG23	1.84	0.59
1:R:208:SER:HB2	1:R:215:THR:HB	1.85	0.59
1:A:16:THR:OG1	1:A:111:ARG:HB2	2.02	0.59
1:J:148:ARG:HD3	1:J:149:PRO:HD2	1.83	0.59
1:J:197:ALA:HB2	1:J:228:VAL:HG13	1.84	0.59
2:K:73:ALA:O	2:K:114:ARG:NH2	2.35	0.59
1:T:77:ALA:HB2	1:T:148:ARG:NH1	2.16	0.59
1:C:153:GLU:OE1	1:C:153:GLU:N	2.34	0.59
1:c:209:VAL:HG22	1:c:214:ILE:HG22	1.84	0.59
1:F:60:LEU:HD21	1:S:15:THR:HB	1.83	0.59
1:N:195:PHE:HB3	1:N:230:SER:HA	1.84	0.59
2:W:68:GLU:HG3	2:W:125:ASP:HB3	1.84	0.59
1:a:198:VAL:HA	1:a:207:VAL:HG11	1.83	0.59
1:E:51:THR:HG22	1:E:52:ALA:H	1.66	0.59
1:J:187:PRO:O	1:J:188:GLU:HB2	2.03	0.59
1:T:108:TYR:OH	1:T:145:ASN:OD1	2.11	0.59
1:A:66:ASP:O	1:H:75:LYS:N	2.36	0.59
1:c:111:ARG:HA	1:c:117:VAL:HG12	1.85	0.59
1:D:50:LEU:HD23	1:R:100:PHE:CE2	2.37	0.59
1:P:75:LYS:N	1:T:66:ASP:O	2.27	0.59
1:C:63:GLU:OE1	1:C:63:GLU:N	2.36	0.59
1:b:100:PHE:HE2	1:O:50:LEU:HD12	1.68	0.59
1:v:199:SER:OG	1:v:200:ALA:N	2.36	0.59
1:D:66:ASP:O	1:R:75:LYS:N	2.36	0.59
1:E:50:LEU:HB2	1:S:127:ILE:HB	1.85	0.59
1:H:212:MET:O	1:H:212:MET:HG3	2.03	0.59
1:M:175:LYS:NZ	1:M:244:THR:O	2.35	0.59
1:X:164:MET:HE3	1:X:165:THR:N	2.17	0.58
1:B:51:THR:HG22	1:B:52:ALA:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:SER:OG	1:b:49:GLU:OE2	2.19	0.58
2:W:74:GLN:OE1	2:W:114:ARG:NH2	2.36	0.58
1:X:50:LEU:HD23	1:Y:67:TRP:HH2	1.67	0.58
1:Y:91:GLN:HA	1:Y:94:GLN:HE22	1.67	0.58
1:F:66:ASP:N	1:F:66:ASP:OD1	2.36	0.58
1:F:204:LYS:HA	1:F:220:ALA:HB3	1.85	0.58
1:N:104:ASP:OD2	1:N:106:ARG:NE	2.25	0.58
2:U:36:GLU:C	2:U:38:ASP:H	2.10	0.58
1:H:208:SER:HB2	1:H:215:THR:HB	1.84	0.58
1:J:77:ALA:HB2	1:J:148:ARG:HH12	1.68	0.58
1:O:91:GLN:NE2	1:S:192:ASP:OD1	2.36	0.58
1:V:53:GLU:HG2	1:V:73:GLY:HA3	1.85	0.58
1:I:31:LEU:O	1:I:111:ARG:NH1	2.37	0.58
1:B:67:TRP:CE2	1:I:148:ARG:HG3	2.39	0.58
1:c:77:ALA:HB2	1:c:148:ARG:NH1	2.18	0.58
2:u:95:ILE:O	2:u:96:PRO:C	2.46	0.58
1:V:47:PRO:HA	1:V:80:THR:HG23	1.86	0.58
1:N:16:THR:OG1	1:N:111:ARG:HB2	2.03	0.58
1:N:164:MET:HA	1:N:184:ALA:O	2.04	0.58
1:b:16:THR:HB	1:b:38:ARG:HH21	1.69	0.58
1:v:87:MET:HE2	1:v:90:GLU:HG2	1.86	0.58
1:R:212:MET:HG3	1:R:212:MET:O	2.03	0.58
1:S:168:PRO:HG2	1:S:170:SER:HB3	1.84	0.58
1:T:187:PRO:O	1:T:188:GLU:HB2	2.04	0.58
2:W:39:PHE:CE2	2:W:72:PRO:HA	2.38	0.58
1:v:52:ALA:HA	1:v:75:LYS:HA	1.84	0.58
1:D:72:GLN:NE2	1:R:124:VAL:O	2.37	0.58
1:O:194:SER:O	1:O:231:GLY:N	2.37	0.58
1:P:36:TRP:HZ3	1:P:108:TYR:HA	1.69	0.58
1:B:91:GLN:NE2	1:b:192:ASP:OD1	2.37	0.58
1:c:164:MET:SD	1:c:193:LYS:NZ	2.69	0.58
1:R:108:TYR:OH	1:R:145:ASN:OD1	2.14	0.58
1:B:86:TRP:HE1	1:B:139:ARG:HH21	1.52	0.57
1:C:75:LYS:N	1:c:66:ASP:O	2.32	0.57
1:a:208:SER:HB2	1:a:215:THR:HB	1.86	0.57
1:D:75:LYS:HG3	1:H:66:ASP:O	2.04	0.57
1:J:164:MET:HG3	1:J:185:PHE:HD1	1.69	0.57
1:b:52:ALA:HA	1:b:75:LYS:HA	1.86	0.57
1:E:194:SER:O	1:E:231:GLY:N	2.37	0.57
1:F:153:GLU:OE1	1:F:153:GLU:N	2.35	0.57
1:H:183:VAL:HB	1:H:212:MET:HE1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:228:VAL:O	1:J:236:ALA:HA	2.04	0.57
2:Q:94:ASP:O	2:Q:95:ILE:HD13	2.04	0.57
2:u:5:LYS:NZ	2:u:133:GLU:O	2.37	0.57
1:D:60:LEU:HD23	1:X:133:ALA:HB2	1.84	0.57
1:F:21:LYS:O	1:F:21:LYS:HG3	2.05	0.57
1:I:168:PRO:HG2	1:I:170:SER:HB3	1.85	0.57
1:a:117:VAL:O	1:a:155:ARG:NH1	2.37	0.57
1:B:210:SER:O	1:B:213:THR:OG1	2.23	0.57
1:E:86:TRP:HE1	1:E:139:ARG:HH21	1.50	0.57
1:J:185:PHE:HE1	1:J:235:PHE:HZ	1.52	0.57
1:M:15:THR:HG23	1:M:112:PHE:HA	1.85	0.57
1:T:109:LYS:HD2	1:T:117:VAL:HG21	1.87	0.57
1:Y:199:SER:OG	1:Y:200:ALA:N	2.37	0.57
1:I:229:VAL:HG23	1:I:236:ALA:HB2	1.85	0.57
1:L:22:GLY:HA3	1:L:35:ASP:HB3	1.86	0.57
1:L:67:TRP:CZ3	1:Y:148:ARG:HA	2.39	0.57
1:M:104:ASP:OD1	1:M:106:ARG:NH2	2.38	0.57
1:v:27:TYR:OH	1:v:148:ARG:O	2.17	0.57
1:D:173:VAL:HG21	1:D:179:THR:HB	1.87	0.57
1:E:50:LEU:HD12	1:S:100:PHE:HE2	1.70	0.57
1:O:204:LYS:HA	1:O:220:ALA:HB3	1.87	0.57
1:R:52:ALA:HA	1:R:75:LYS:HA	1.86	0.57
1:C:204:LYS:HA	1:C:220:ALA:HB3	1.87	0.57
1:c:228:VAL:O	1:c:236:ALA:HA	2.05	0.57
1:H:191:THR:HG1	1:H:193:LYS:HZ3	1.51	0.57
1:O:86:TRP:HE1	1:O:139:ARG:HH21	1.53	0.57
1:T:187:PRO:HG3	1:T:191:THR:CB	2.33	0.57
1:X:22:GLY:HA3	1:X:35:ASP:OD1	2.04	0.57
1:H:52:ALA:HA	1:H:75:LYS:HA	1.86	0.57
1:J:30:PRO:HG2	1:J:155:ARG:NH2	2.20	0.57
1:L:77:ALA:N	1:M:67:TRP:HZ3	2.00	0.57
1:P:227:PRO:HB3	1:T:227:PRO:HB3	1.86	0.57
1:b:213:THR:HG23	1:b:214:ILE:H	1.69	0.57
1:H:174:VAL:O	1:H:177:GLN:NE2	2.38	0.57
1:A:161:ALA:HA	1:A:187:PRO:HG3	1.87	0.56
1:A:198:VAL:HG23	1:A:227:PRO:HG2	1.86	0.56
1:B:194:SER:O	1:B:231:GLY:N	2.38	0.56
1:C:66:ASP:N	1:C:66:ASP:OD1	2.35	0.56
1:v:102:GLU:OE1	1:v:106:ARG:NH2	2.38	0.56
1:D:175:LYS:NZ	1:D:244:THR:O	2.38	0.56
1:F:195:PHE:HA	1:F:230:SER:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:52:ALA:HA	1:M:75:LYS:HA	1.86	0.56
2:Q:35:ASP:CB	2:Q:38:ASP:HB2	2.29	0.56
2:Q:36:GLU:C	2:Q:38:ASP:N	2.62	0.56
1:T:164:MET:HG2	1:T:235:PHE:CE2	2.39	0.56
1:X:78:GLY:HA2	1:X:145:ASN:HB2	1.86	0.56
1:v:150:SER:O	1:v:155:ARG:NH2	2.39	0.56
1:H:44:ASP:OD1	1:H:83:THR:HB	2.05	0.56
2:K:5:LYS:NZ	2:K:133:GLU:O	2.38	0.56
1:Y:175:LYS:NZ	1:Y:244:THR:O	2.38	0.56
1:C:51:THR:HG22	1:C:52:ALA:H	1.70	0.56
1:v:139:ARG:NH2	1:X:153:GLU:OE2	2.34	0.56
2:K:91:VAL:HG12	2:K:95:ILE:HD11	1.86	0.56
1:L:20:TYR:HD2	1:L:26:PRO:HB3	1.69	0.56
1:R:166:VAL:HG22	1:R:183:VAL:HG22	1.87	0.56
2:W:59:ASP:N	2:W:59:ASP:OD1	2.39	0.56
1:b:108:TYR:CZ	1:b:120:PHE:HB2	2.40	0.56
1:O:126:SER:OG	1:S:49:GLU:OE2	2.24	0.56
1:T:30:PRO:HG2	1:T:155:ARG:NH2	2.21	0.56
1:E:181:LEU:HB3	1:E:214:ILE:HB	1.88	0.56
1:Y:104:ASP:OD1	1:Y:106:ARG:NH2	2.29	0.56
1:C:132:THR:HG23	1:C:135:GLU:HB3	1.88	0.56
1:E:91:GLN:NE2	1:I:192:ASP:OD1	2.37	0.56
1:F:67:TRP:CZ2	1:T:148:ARG:HG2	2.40	0.56
1:H:174:VAL:H	1:H:177:GLN:HE22	1.52	0.56
1:I:199:SER:OG	1:I:205:ALA:O	2.23	0.56
1:J:124:VAL:HA	1:J:143:VAL:HA	1.87	0.56
1:M:199:SER:OG	1:M:200:ALA:N	2.37	0.56
1:O:38:ARG:NH2	1:T:61:ASP:OD2	2.39	0.56
1:a:195:PHE:HA	1:a:231:GLY:H	1.71	0.56
1:b:127:ILE:HB	1:O:50:LEU:HB2	1.88	0.56
1:b:173:VAL:O	1:b:244:THR:N	2.38	0.56
1:N:205:ALA:HA	1:N:217:ASN:O	2.06	0.56
1:A:173:VAL:HG21	1:A:179:THR:HB	1.88	0.56
1:a:108:TYR:CZ	1:a:120:PHE:HB2	2.41	0.56
1:M:166:VAL:HG22	1:M:183:VAL:HG22	1.88	0.56
1:P:5:ASN:OD1	1:P:7:THR:OG1	2.16	0.56
1:S:16:THR:HB	1:S:38:ARG:HH21	1.71	0.56
1:T:168:PRO:HA	1:T:181:LEU:HD23	1.87	0.56
1:X:20:TYR:HD2	1:X:26:PRO:HB3	1.69	0.56
1:X:101:ASN:OD1	1:Y:148:ARG:NH2	2.39	0.56
1:I:108:TYR:CZ	1:I:120:PHE:HB2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:108:TYR:CZ	1:S:120:PHE:HB2	2.41	0.56
1:c:31:LEU:HD12	1:c:111:ARG:HH22	1.70	0.56
1:M:150:SER:O	1:M:155:ARG:NH2	2.38	0.56
1:P:124:VAL:HG12	1:P:143:VAL:HG12	1.88	0.56
1:B:150:SER:OG	1:B:155:ARG:NH1	2.39	0.55
2:U:78:SER:OG	2:u:28:ASP:OD2	2.12	0.55
1:a:195:PHE:HB2	1:a:230:SER:HA	1.88	0.55
1:L:53:GLU:HG2	1:L:73:GLY:HA3	1.87	0.55
1:O:229:VAL:HG13	1:O:236:ALA:HB2	1.87	0.55
1:Y:52:ALA:HA	1:Y:75:LYS:HA	1.87	0.55
1:B:139:ARG:NH2	1:b:153:GLU:OE2	2.39	0.55
1:C:5:ASN:OD1	1:C:7:THR:OG1	2.18	0.55
1:b:168:PRO:HG2	1:b:170:SER:HB3	1.86	0.55
2:G:78:SER:OG	2:K:28:ASP:OD2	2.12	0.55
1:S:226:ILE:HG22	1:S:239:ALA:HB3	1.89	0.55
1:Y:183:VAL:HB	1:Y:212:MET:HE1	1.88	0.55
1:B:41:LYS:HD3	1:c:59:TYR:HE1	1.72	0.55
1:H:160:ALA:HA	1:H:193:LYS:HZ2	1.72	0.55
1:S:63:GLU:H	1:S:63:GLU:CD	2.15	0.55
1:A:114:ASN:OD1	1:A:116:THR:OG1	2.22	0.55
1:B:181:LEU:HB3	1:B:214:ILE:HB	1.88	0.55
1:a:44:ASP:OD1	1:a:83:THR:HB	2.05	0.55
1:C:195:PHE:HA	1:C:230:SER:HA	1.88	0.55
1:b:211:GLY:C	1:b:213:THR:N	2.62	0.55
1:E:194:SER:OG	1:E:195:PHE:N	2.38	0.55
1:I:52:ALA:HA	1:I:75:LYS:HA	1.89	0.55
1:T:133:ALA:O	1:T:134:LYS:HG2	2.07	0.55
1:B:66:ASP:OD1	1:B:66:ASP:N	2.39	0.55
1:B:194:SER:OG	1:B:195:PHE:N	2.39	0.55
1:b:85:ALA:HB2	1:P:59:TYR:OH	2.06	0.55
1:c:20:TYR:HD1	1:c:21:LYS:H	1.54	0.55
1:c:30:PRO:HG2	1:c:155:ARG:NH2	2.22	0.55
1:D:150:SER:OG	1:D:155:ARG:NH2	2.39	0.55
1:J:97:LEU:HD23	1:J:101:ASN:HD22	1.72	0.55
1:R:183:VAL:HB	1:R:212:MET:HE1	1.89	0.55
1:b:21:LYS:NZ	1:b:37:SER:HB3	2.22	0.55
1:c:197:ALA:HB2	1:c:228:VAL:HG13	1.88	0.55
1:D:117:VAL:O	1:D:155:ARG:NH1	2.40	0.55
1:E:18:TRP:CH2	1:E:38:ARG:HG3	2.42	0.55
1:F:76:SER:O	1:F:76:SER:OG	2.25	0.55
1:I:56:ASP:HA	1:I:70:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:173:VAL:HG21	1:N:179:THR:HB	1.89	0.55
1:v:104:ASP:OD1	1:v:106:ARG:NH2	2.39	0.55
1:J:164:MET:HG2	1:J:235:PHE:CE2	2.41	0.55
1:L:47:PRO:HA	1:L:80:THR:HG23	1.89	0.55
1:b:31:LEU:O	1:b:111:ARG:NH1	2.40	0.54
1:b:41:LYS:HG3	1:b:87:MET:HE1	1.88	0.54
1:b:116:THR:HG22	1:b:152:ALA:HB1	1.89	0.54
1:C:127:ILE:HD13	1:C:141:VAL:HG12	1.88	0.54
1:v:91:GLN:HA	1:v:94:GLN:HE22	1.73	0.54
1:F:18:TRP:CD1	1:F:109:LYS:HZ2	2.25	0.54
1:I:153:GLU:OE1	1:I:153:GLU:N	2.39	0.54
1:N:45:LEU:HG	1:N:46:THR:N	2.21	0.54
1:P:204:LYS:HA	1:P:220:ALA:HB3	1.88	0.54
2:Q:39:PHE:HB3	2:Q:40:PRO:HD2	1.89	0.54
1:A:104:ASP:OD2	1:A:106:ARG:NE	2.24	0.54
1:a:75:LYS:N	1:N:66:ASP:O	2.40	0.54
1:v:20:TYR:HE1	1:v:35:ASP:HB3	1.71	0.54
1:D:9:PRO:HD3	1:R:87:MET:HE2	1.90	0.54
1:M:194:SER:O	1:M:231:GLY:N	2.36	0.54
1:C:59:TYR:CE2	1:I:41:LYS:HD2	2.42	0.54
1:H:48:GLY:N	1:H:80:THR:HG22	2.23	0.54
1:H:181:LEU:HB2	1:H:214:ILE:HB	1.88	0.54
1:M:118:ASP:OD1	1:M:152:ALA:N	2.40	0.54
2:W:39:PHE:CZ	2:W:72:PRO:HA	2.42	0.54
1:Y:150:SER:O	1:Y:155:ARG:NH2	2.40	0.54
1:B:67:TRP:NE1	1:I:148:ARG:HG3	2.22	0.54
1:C:40:ALA:HB3	1:C:87:MET:HE1	1.90	0.54
1:c:74:GLN:NE2	1:P:68:THR:HG22	2.21	0.54
1:D:17:LEU:HD13	1:D:110:ILE:HG12	1.89	0.54
2:W:91:VAL:HG12	2:W:95:ILE:HD11	1.89	0.54
1:P:74:GLN:NE2	1:T:65:ALA:O	2.41	0.54
1:P:127:ILE:HD13	1:P:141:VAL:HG12	1.88	0.54
1:P:195:PHE:HA	1:P:230:SER:HA	1.89	0.54
1:R:48:GLY:N	1:R:80:THR:HG22	2.22	0.54
1:T:10:VAL:HG21	1:T:113:PRO:HG2	1.89	0.54
1:a:100:PHE:CE2	1:N:50:LEU:HD23	2.42	0.54
1:c:133:ALA:O	1:c:134:LYS:HG2	2.07	0.54
1:I:173:VAL:O	1:I:244:THR:N	2.39	0.54
1:J:31:LEU:HD12	1:J:111:ARG:NH2	2.21	0.54
2:W:64:GLU:OE1	2:W:64:GLU:N	2.41	0.54
1:X:85:ALA:HB1	1:Y:9:PRO:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:TYR:OH	1:H:24:GLY:N	2.41	0.54
1:P:221:ALA:HA	1:P:243:VAL:HB	1.90	0.54
2:W:25:THR:OG1	2:W:39:PHE:O	2.24	0.54
2:W:81:ASP:OD1	2:W:110:TYR:OH	2.26	0.54
1:F:5:ASN:OD1	1:F:7:THR:OG1	2.19	0.54
2:K:39:PHE:O	2:K:40:PRO:C	2.51	0.54
2:K:54:GLU:HG2	2:K:55:GLU:N	2.22	0.54
1:P:41:LYS:HD2	1:P:87:MET:HE1	1.90	0.54
1:C:20:TYR:OH	1:C:23:SER:O	2.21	0.53
1:c:10:VAL:HG21	1:c:113:PRO:HG2	1.90	0.53
1:c:148:ARG:HG2	1:P:67:TRP:CZ2	2.43	0.53
2:u:69:VAL:O	2:u:123:SER:HA	2.09	0.53
1:V:207:VAL:HG23	1:V:216:VAL:HG22	1.91	0.53
1:D:47:PRO:HA	1:D:80:THR:HG23	1.89	0.53
1:T:204:LYS:HB3	1:T:220:ALA:HB3	1.90	0.53
1:a:20:TYR:OH	1:a:24:GLY:N	2.41	0.53
1:v:75:LYS:HG3	1:X:67:TRP:CD1	2.43	0.53
1:M:153:GLU:OE2	1:M:156:SER:OG	2.20	0.53
1:M:205:ALA:HB3	1:M:224:VAL:HG21	1.89	0.53
1:X:209:VAL:HG22	1:X:214:ILE:HG12	1.90	0.53
2:U:40:PRO:HA	2:U:70:PHE:O	2.09	0.53
1:b:226:ILE:HG22	1:b:239:ALA:HB3	1.91	0.53
1:v:118:ASP:OD1	1:v:152:ALA:N	2.41	0.53
1:E:204:LYS:HA	1:E:220:ALA:HB3	1.89	0.53
1:J:164:MET:N	1:J:164:MET:SD	2.81	0.53
1:Y:205:ALA:HB3	1:Y:224:VAL:HG21	1.89	0.53
1:B:193:LYS:HZ2	1:B:231:GLY:HA3	1.73	0.53
1:b:63:GLU:CD	1:b:63:GLU:H	2.16	0.53
1:v:181:LEU:HB2	1:v:214:ILE:HB	1.89	0.53
1:L:5:ASN:ND2	1:L:8:MET:HG3	2.23	0.53
1:T:207:VAL:HG12	1:T:216:VAL:HG22	1.89	0.53
1:Y:20:TYR:HH	1:Y:24:GLY:N	2.06	0.53
1:a:150:SER:HG	1:a:155:ARG:NH2	2.06	0.53
1:E:76:SER:O	1:E:76:SER:OG	2.26	0.53
1:F:153:GLU:HB2	1:T:97:LEU:HD13	1.90	0.53
1:H:204:LYS:HA	1:H:220:ALA:HB3	1.89	0.53
1:Y:204:LYS:HA	1:Y:220:ALA:HB3	1.91	0.53
1:C:67:TRP:CZ2	1:J:148:ARG:HG2	2.44	0.53
1:b:133:ALA:O	1:b:134:LYS:HG2	2.08	0.53
1:H:174:VAL:H	1:H:177:GLN:NE2	2.07	0.53
1:I:133:ALA:O	1:I:134:LYS:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:91:GLN:HA	1:M:94:GLN:HE22	1.73	0.53
1:O:18:TRP:CH2	1:O:38:ARG:HG3	2.43	0.53
1:X:99:TRP:HE1	1:X:123:TRP:HA	1.74	0.53
1:X:164:MET:HE1	1:X:183:VAL:HG23	1.90	0.53
1:A:75:LYS:HG3	1:a:66:ASP:O	2.09	0.53
1:B:193:LYS:NZ	1:B:232:ASN:OD1	2.30	0.53
1:v:194:SER:O	1:v:231:GLY:N	2.37	0.53
1:I:63:GLU:CD	1:I:63:GLU:H	2.16	0.53
1:T:148:ARG:HD3	1:T:149:PRO:CD	2.38	0.53
2:W:81:ASP:CG	2:W:112:TYR:HH	2.17	0.53
1:X:207:VAL:HG23	1:X:216:VAL:HG22	1.90	0.53
2:U:81:ASP:OD2	2:u:10:ARG:NH2	2.42	0.53
1:v:205:ALA:HB3	1:v:224:VAL:HG21	1.90	0.53
1:F:91:GLN:HA	1:F:94:GLN:HG3	1.91	0.53
1:J:20:TYR:HD1	1:J:21:LYS:H	1.56	0.53
1:D:164:MET:HB3	1:D:235:PHE:CD2	2.43	0.53
1:O:150:SER:OG	1:O:155:ARG:NH1	2.42	0.53
1:O:201:ASP:O	1:O:202:LYS:HG2	2.09	0.53
1:R:181:LEU:HB2	1:R:214:ILE:HB	1.91	0.53
1:B:50:LEU:HD12	1:I:100:PHE:HE2	1.72	0.52
1:V:77:ALA:H	1:v:67:TRP:HZ3	1.57	0.52
2:G:17:LEU:HD12	2:G:91:VAL:HG11	1.91	0.52
1:J:133:ALA:O	1:J:134:LYS:HG2	2.08	0.52
1:P:48:GLY:N	1:P:80:THR:OG1	2.41	0.52
1:R:195:PHE:HB2	1:R:230:SER:HA	1.91	0.52
1:S:41:LYS:HG3	1:S:87:MET:HE1	1.91	0.52
1:S:84:LEU:HD11	1:S:93:GLN:NE2	2.24	0.52
1:X:120:PHE:HB3	1:X:145:ASN:ND2	2.24	0.52
1:D:168:PRO:HB2	1:D:241:ILE:HD11	1.91	0.52
1:H:79:ASP:N	1:H:79:ASP:OD1	2.39	0.52
2:W:69:VAL:O	2:W:123:SER:HA	2.10	0.52
1:C:50:LEU:HG	1:C:77:ALA:HB2	1.91	0.52
1:D:62:ASP:O	1:D:63:GLU:C	2.51	0.52
1:N:199:SER:H	1:N:202:LYS:NZ	2.07	0.52
1:C:68:THR:HG22	1:J:74:GLN:NE2	2.24	0.52
1:C:227:PRO:HB3	1:c:227:PRO:HB3	1.90	0.52
1:c:148:ARG:NH1	1:c:149:PRO:HD2	2.24	0.52
2:u:41:ALA:HB3	2:u:70:PHE:HB2	1.92	0.52
1:V:50:LEU:HD23	1:v:67:TRP:HH2	1.74	0.52
1:D:205:ALA:HA	1:D:217:ASN:O	2.10	0.52
1:S:173:VAL:O	1:S:244:THR:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:87:MET:HE2	1:N:9:PRO:HD3	1.91	0.52
1:E:119:VAL:HG13	1:E:150:SER:HB3	1.92	0.52
2:G:36:GLU:OE1	2:G:36:GLU:N	2.41	0.52
1:H:195:PHE:HB2	1:H:230:SER:HA	1.92	0.52
1:J:187:PRO:HG3	1:J:191:THR:CB	2.36	0.52
1:N:47:PRO:HA	1:N:80:THR:HG23	1.90	0.52
1:N:114:ASN:OD1	1:N:116:THR:OG1	2.25	0.52
1:P:52:ALA:HA	1:P:75:LYS:HA	1.90	0.52
1:P:132:THR:HG23	1:P:135:GLU:HB3	1.90	0.52
1:S:230:SER:HB2	1:S:235:PHE:HD2	1.75	0.52
1:B:205:ALA:HA	1:B:219:VAL:H	1.74	0.52
1:b:46:THR:OG1	1:b:81:SER:O	2.24	0.52
1:v:98:ALA:O	1:v:102:GLU:HG3	2.10	0.52
1:F:127:ILE:HD13	1:F:141:VAL:HG12	1.91	0.52
1:R:20:TYR:OH	1:R:24:GLY:N	2.40	0.52
1:T:97:LEU:HD23	1:T:101:ASN:HD22	1.74	0.52
1:C:74:GLN:NE2	1:c:65:ALA:O	2.43	0.52
1:C:181:LEU:HD11	1:C:241:ILE:HD11	1.92	0.52
1:N:75:LYS:HG3	1:R:66:ASP:O	2.09	0.52
1:O:18:TRP:NE1	1:O:111:ARG:HG3	2.24	0.52
1:R:195:PHE:HA	1:R:231:GLY:H	1.74	0.52
1:X:96:LEU:HD21	1:X:141:VAL:HG21	1.92	0.52
2:U:105:MET:HB2	2:U:130:ILE:HG22	1.92	0.52
1:J:148:ARG:HD3	1:J:149:PRO:CD	2.40	0.52
2:Q:110:TYR:HE1	2:Q:112:TYR:CZ	2.27	0.52
1:C:52:ALA:HA	1:C:75:LYS:HA	1.92	0.52
1:C:124:VAL:HG12	1:C:143:VAL:HG12	1.92	0.52
1:c:97:LEU:HD23	1:c:101:ASN:HD22	1.75	0.52
1:S:116:THR:HG22	1:S:152:ALA:HB1	1.91	0.52
1:T:20:TYR:HD1	1:T:21:LYS:H	1.57	0.52
1:A:153:GLU:CD	1:H:97:LEU:HD12	2.35	0.52
2:G:10:ARG:NH2	2:W:81:ASP:OD2	2.40	0.52
2:G:31:PRO:HA	2:W:114:ARG:HH12	1.75	0.52
1:D:172:SER:HA	1:D:242:THR:O	2.10	0.51
1:E:206:THR:OG1	1:E:217:ASN:OD1	2.20	0.51
1:F:139:ARG:HH11	1:F:139:ARG:HG3	1.75	0.51
1:F:206:THR:OG1	1:F:217:ASN:OD1	2.13	0.51
1:F:221:ALA:HA	1:F:243:VAL:HB	1.92	0.51
1:L:75:LYS:HB2	1:M:67:TRP:CE3	2.45	0.51
1:O:194:SER:OG	1:O:195:PHE:N	2.38	0.51
2:W:39:PHE:O	2:W:40:PRO:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:74:GLN:OE1	2:U:74:GLN:O	2.28	0.51
1:b:56:ASP:HA	1:b:70:THR:HG22	1.92	0.51
1:v:105:THR:HG22	1:v:121:ARG:HG2	1.92	0.51
1:L:75:LYS:HB2	1:M:67:TRP:CD2	2.45	0.51
1:L:200:ALA:HA	1:M:236:ALA:HB3	1.93	0.51
1:L:207:VAL:HG23	1:L:216:VAL:HG22	1.92	0.51
1:B:18:TRP:NE1	1:B:111:ARG:HG3	2.25	0.51
1:C:221:ALA:HA	1:C:243:VAL:HB	1.91	0.51
1:b:5:ASN:OD1	1:b:7:THR:OG1	2.18	0.51
2:u:81:ASP:OD2	2:Q:10:ARG:NH2	2.40	0.51
1:V:86:TRP:NE1	1:V:129:LYS:HZ3	2.09	0.51
1:D:34:VAL:HA	1:D:196:ARG:NH2	2.26	0.51
1:F:173:VAL:HB	1:F:243:VAL:HG22	1.93	0.51
2:G:32:ALA:H	2:W:74:GLN:HE22	1.57	0.51
1:N:172:SER:HA	1:N:242:THR:O	2.10	0.51
1:O:18:TRP:HE1	1:O:111:ARG:HG3	1.75	0.51
1:R:204:LYS:HA	1:R:220:ALA:HB3	1.92	0.51
1:A:205:ALA:HA	1:A:217:ASN:O	2.10	0.51
1:E:201:ASP:O	1:E:202:LYS:HG2	2.10	0.51
1:N:164:MET:SD	1:N:165:THR:N	2.83	0.51
2:U:27:PHE:CD1	2:U:31:PRO:HG3	2.45	0.51
1:D:150:SER:O	1:D:155:ARG:NH2	2.39	0.51
1:R:201:ASP:OD2	1:R:203:THR:OG1	2.28	0.51
1:S:108:TYR:CE1	1:S:120:PHE:HB2	2.46	0.51
1:V:70:THR:HG23	1:M:123:TRP:HE1	1.76	0.51
2:K:92:MET:HE1	2:K:105:MET:HE1	1.91	0.51
1:O:51:THR:HG22	1:O:52:ALA:N	2.26	0.51
1:O:181:LEU:HB3	1:O:214:ILE:HB	1.93	0.51
1:O:206:THR:OG1	1:O:217:ASN:OD1	2.19	0.51
1:P:76:SER:O	1:P:76:SER:OG	2.23	0.51
1:D:118:ASP:OD1	1:D:118:ASP:N	2.44	0.51
1:F:227:PRO:HB3	1:J:227:PRO:HB3	1.92	0.51
1:B:62:ASP:O	1:B:63:GLU:C	2.52	0.51
1:C:36:TRP:HZ3	1:C:108:TYR:HA	1.75	0.51
1:a:166:VAL:HG22	1:a:183:VAL:HG22	1.92	0.51
2:u:81:ASP:CG	2:Q:10:ARG:HH22	2.18	0.51
1:E:205:ALA:HA	1:E:219:VAL:H	1.75	0.51
1:M:205:ALA:HA	1:M:217:ASN:O	2.10	0.51
1:N:205:ALA:HB2	1:N:218:GLY:HA2	1.93	0.51
1:X:200:ALA:HA	1:Y:236:ALA:HB3	1.92	0.51
1:V:148:ARG:HG3	1:v:67:TRP:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:PHE:HB3	1:D:230:SER:HA	1.92	0.51
1:E:18:TRP:NE1	1:E:111:ARG:HG3	2.26	0.51
1:E:229:VAL:HG13	1:E:236:ALA:HB2	1.93	0.51
1:I:46:THR:OG1	1:I:81:SER:OG	2.20	0.51
1:J:148:ARG:NH1	1:J:149:PRO:HD2	2.25	0.51
2:K:68:GLU:HG2	2:K:123:SER:OG	2.11	0.51
2:Q:4:MET:HG2	2:Q:6:HIS:H	1.76	0.51
1:R:150:SER:HG	1:R:155:ARG:NH2	2.09	0.51
2:U:10:ARG:NH2	2:K:81:ASP:OD2	2.41	0.51
1:c:148:ARG:HD3	1:c:149:PRO:CD	2.40	0.51
1:O:41:LYS:HD3	1:T:59:TYR:HE2	1.76	0.51
1:X:78:GLY:CA	1:X:145:ASN:HB2	2.41	0.51
1:Y:194:SER:O	1:Y:231:GLY:N	2.36	0.51
1:B:8:MET:HA	1:B:8:MET:HE2	1.94	0.50
2:U:38:ASP:O	2:U:41:ALA:HB2	2.11	0.50
1:c:194:SER:OG	1:c:195:PHE:N	2.44	0.50
2:u:68:GLU:HG2	2:u:123:SER:OG	2.11	0.50
1:V:200:ALA:HA	1:v:236:ALA:HB3	1.93	0.50
1:H:108:TYR:OH	1:H:145:ASN:OD1	2.25	0.50
1:I:126:SER:HB3	1:I:142:LYS:HB3	1.92	0.50
2:Q:46:LEU:HD23	2:Q:65:LEU:HA	1.94	0.50
1:C:18:TRP:HB2	1:C:109:LYS:HG2	1.93	0.50
1:C:173:VAL:HB	1:C:243:VAL:HG22	1.93	0.50
1:H:36:TRP:CD1	1:H:109:LYS:HZ3	2.29	0.50
1:H:165:THR:HB	1:H:184:ALA:HB3	1.93	0.50
1:J:230:SER:HB3	1:J:235:PHE:CE2	2.46	0.50
1:M:204:LYS:HA	1:M:220:ALA:HB3	1.92	0.50
2:Q:75:VAL:HB	2:Q:79:GLU:HG3	1.93	0.50
1:T:172:SER:HA	1:T:242:THR:O	2.10	0.50
1:T:197:ALA:HB2	1:T:228:VAL:HG13	1.91	0.50
1:a:165:THR:HB	1:a:184:ALA:HB3	1.92	0.50
1:b:181:LEU:HB2	1:b:214:ILE:HB	1.93	0.50
1:D:86:TRP:NE1	1:H:153:GLU:OE2	2.24	0.50
1:I:162:THR:N	1:I:187:PRO:HB3	2.26	0.50
1:P:224:VAL:HG13	1:P:241:ILE:HB	1.93	0.50
1:T:194:SER:OG	1:T:195:PHE:N	2.44	0.50
1:A:124:VAL:HG22	1:A:143:VAL:HG22	1.93	0.50
2:U:106:VAL:HG12	1:c:11:LYS:HD3	1.94	0.50
1:b:42:VAL:N	1:P:61:ASP:OD2	2.42	0.50
1:b:162:THR:N	1:b:187:PRO:HB3	2.27	0.50
1:c:47:PRO:HA	1:c:80:THR:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:185:PHE:HE1	1:v:193:LYS:HG3	1.76	0.50
1:D:153:GLU:CD	1:R:97:LEU:HD12	2.36	0.50
1:J:194:SER:OG	1:J:195:PHE:N	2.44	0.50
1:O:205:ALA:HA	1:O:219:VAL:H	1.76	0.50
1:D:59:TYR:O	1:D:60:LEU:C	2.54	0.50
1:N:195:PHE:HZ	1:N:212:MET:HE1	1.73	0.50
1:P:66:ASP:N	1:P:66:ASP:OD1	2.42	0.50
1:P:91:GLN:HA	1:P:94:GLN:HG3	1.94	0.50
1:J:43:LYS:HD3	2:K:55:GLU:HG3	1.92	0.50
2:u:96:PRO:O	2:u:97:ALA:C	2.55	0.50
1:V:227:PRO:HB3	1:v:227:PRO:HB3	1.94	0.50
1:H:117:VAL:O	1:H:155:ARG:NH1	2.44	0.50
1:T:148:ARG:NH1	1:T:149:PRO:HD2	2.25	0.50
1:a:204:LYS:HA	1:a:220:ALA:HB3	1.94	0.50
1:b:30:PRO:HG3	1:b:155:ARG:HH22	1.77	0.50
1:V:167:THR:HB	1:V:182:THR:HG23	1.92	0.50
1:V:186:GLN:HB3	1:V:189:GLY:HA2	1.92	0.50
1:v:204:LYS:HA	1:v:220:ALA:HB3	1.94	0.50
1:J:164:MET:SD	1:J:193:LYS:NZ	2.78	0.50
1:L:209:VAL:HG22	1:L:214:ILE:HG12	1.92	0.50
1:N:129:LYS:NZ	1:R:118:ASP:OD2	2.45	0.50
1:A:172:SER:HA	1:A:242:THR:O	2.11	0.50
1:c:86:TRP:CD1	1:c:129:LYS:HZ1	2.30	0.50
1:F:201:ASP:OD2	1:F:204:LYS:HE2	2.12	0.50
1:I:118:ASP:OD1	1:I:152:ALA:N	2.45	0.50
1:I:163:GLY:HA3	1:I:187:PRO:HA	1.94	0.50
2:u:77:ASP:OD2	2:Q:29:GLY:HA3	2.12	0.49
1:V:209:VAL:HG22	1:V:214:ILE:HG12	1.94	0.49
1:E:150:SER:OG	1:E:155:ARG:NH1	2.45	0.49
1:L:131:VAL:HG12	1:L:137:ILE:HG23	1.94	0.49
1:O:43:LYS:NZ	1:T:59:TYR:HE1	2.10	0.49
1:P:109:LYS:HA	1:P:118:ASP:O	2.12	0.49
1:X:3:VAL:HB	1:X:4:PRO:HD3	1.93	0.49
1:A:205:ALA:HB2	1:A:218:GLY:HA2	1.93	0.49
1:C:210:SER:O	1:C:213:THR:HG22	2.12	0.49
1:P:173:VAL:HB	1:P:243:VAL:HG22	1.94	0.49
1:C:102:GLU:HG3	1:C:104:ASP:HB2	1.94	0.49
1:F:75:LYS:N	1:J:66:ASP:O	2.33	0.49
2:K:94:ASP:O	2:K:95:ILE:HD13	2.12	0.49
1:S:153:GLU:OE1	1:S:153:GLU:N	2.44	0.49
1:B:204:LYS:HA	1:B:220:ALA:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:66:HIS:CD2	2:U:127:THR:HG22	2.48	0.49
1:N:34:VAL:HA	1:N:196:ARG:NH2	2.27	0.49
1:B:201:ASP:O	1:B:202:LYS:HG2	2.11	0.49
1:C:91:GLN:HA	1:C:94:GLN:HG3	1.95	0.49
1:a:191:THR:HG1	1:a:193:LYS:HZ3	1.54	0.49
2:G:69:VAL:HG11	2:G:83:TRP:CD1	2.48	0.49
1:R:44:ASP:OD1	1:R:83:THR:HB	2.12	0.49
1:R:221:ALA:HA	1:R:243:VAL:HG13	1.95	0.49
1:X:164:MET:HB3	1:X:235:PHE:HD2	1.78	0.49
1:X:168:PRO:HB3	1:X:239:ALA:HB1	1.93	0.49
1:C:6:PRO:O	1:J:88:PRO:HD2	2.13	0.49
1:C:100:PHE:HA	1:C:124:VAL:HG21	1.94	0.49
1:I:30:PRO:HG2	1:I:155:ARG:NH1	2.27	0.49
1:O:238:VAL:HG11	1:S:238:VAL:HG11	1.95	0.49
2:Q:9:LEU:HD22	2:Q:130:ILE:HD12	1.95	0.49
1:T:181:LEU:O	1:T:213:THR:OG1	2.27	0.49
1:T:211:GLY:O	1:T:212:MET:HE3	2.11	0.49
1:X:227:PRO:HB3	1:Y:227:PRO:HB3	1.94	0.49
1:Y:116:THR:HB	1:Y:152:ALA:HB1	1.94	0.49
1:C:164:MET:HB2	1:C:184:ALA:O	2.12	0.49
1:b:230:SER:HB2	1:b:235:PHE:HD2	1.77	0.49
2:u:24:ALA:HB1	2:u:40:PRO:O	2.13	0.49
1:V:116:THR:HB	1:V:152:ALA:HB1	1.94	0.49
1:v:30:PRO:HB3	1:v:119:VAL:HG11	1.95	0.49
1:D:205:ALA:HB2	1:D:218:GLY:HA2	1.94	0.49
2:G:27:PHE:CD1	2:G:31:PRO:HG3	2.48	0.49
2:G:51:TYR:HE1	2:G:59:ASP:HA	1.78	0.49
2:G:98:LEU:HD23	2:G:105:MET:HE1	1.93	0.49
1:N:183:VAL:HG11	1:N:195:PHE:CE1	2.48	0.49
2:Q:17:LEU:HD23	2:Q:91:VAL:HG11	1.93	0.49
1:Y:109:LYS:HB2	1:Y:119:VAL:HG12	1.95	0.49
1:A:183:VAL:HG11	1:A:195:PHE:CZ	2.47	0.49
1:B:43:LYS:H	1:B:84:LEU:HA	1.78	0.49
1:v:18:TRP:CE2	1:v:38:ARG:HG3	2.48	0.49
1:D:79:ASP:CA	1:D:143:VAL:O	2.58	0.49
2:G:29:GLY:HA3	2:W:77:ASP:OD2	2.13	0.49
1:N:45:LEU:HD12	1:N:82:PHE:HB3	1.93	0.49
1:R:164:MET:HG2	1:R:235:PHE:HB3	1.94	0.49
1:T:10:VAL:CG2	1:T:113:PRO:HG2	2.41	0.49
1:T:66:ASP:OD1	1:T:66:ASP:N	2.40	0.49
1:X:16:THR:OG1	1:X:18:TRP:NE1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:90:GLU:O	1:Y:94:GLN:NE2	2.46	0.49
1:A:235:PHE:CD1	1:A:236:ALA:N	2.81	0.49
1:D:124:VAL:HG22	1:D:143:VAL:HG22	1.95	0.49
1:D:183:VAL:HB	1:D:212:MET:SD	2.53	0.49
1:N:185:PHE:O	1:N:187:PRO:HD3	2.12	0.49
1:S:161:ALA:C	1:S:187:PRO:HB3	2.38	0.49
1:T:187:PRO:CG	1:T:191:THR:HB	2.39	0.49
1:X:75:LYS:HB2	1:Y:67:TRP:CE3	2.48	0.49
1:Y:99:TRP:CE2	1:Y:106:ARG:HG2	2.48	0.49
1:a:181:LEU:HB2	1:a:214:ILE:HB	1.94	0.49
1:c:18:TRP:HB2	1:c:109:LYS:HG2	1.95	0.49
1:J:75:LYS:HB3	1:J:148:ARG:NH2	2.28	0.49
1:J:111:ARG:HA	1:J:117:VAL:HG12	1.95	0.49
1:P:238:VAL:HG11	1:T:238:VAL:HG11	1.95	0.49
1:X:63:GLU:H	1:X:63:GLU:CD	2.21	0.49
1:B:76:SER:O	1:B:76:SER:OG	2.24	0.48
2:u:73:ALA:O	2:u:74:GLN:NE2	2.46	0.48
1:F:36:TRP:HZ3	1:F:108:TYR:HA	1.78	0.48
1:J:179:THR:HG22	1:J:216:VAL:HB	1.95	0.48
1:O:18:TRP:CZ3	1:O:38:ARG:HG3	2.47	0.48
1:P:47:PRO:HA	1:P:80:THR:HG23	1.95	0.48
1:S:30:PRO:HB2	1:S:117:VAL:HG11	1.95	0.48
1:B:43:LYS:NZ	1:c:59:TYR:HE2	2.10	0.48
1:B:50:LEU:HB2	1:I:127:ILE:HB	1.95	0.48
1:a:201:ASP:OD2	1:a:203:THR:OG1	2.30	0.48
2:G:10:ARG:HH22	2:W:81:ASP:CG	2.21	0.48
1:H:109:LYS:HB3	1:H:119:VAL:HG22	1.95	0.48
2:Q:98:LEU:HD23	2:Q:105:MET:HE1	1.95	0.48
1:R:164:MET:SD	1:R:165:THR:N	2.86	0.48
2:W:68:GLU:HG2	2:W:123:SER:OG	2.14	0.48
1:A:78:GLY:HA2	1:A:145:ASN:ND2	2.28	0.48
1:A:167:THR:O	1:A:182:THR:OG1	2.27	0.48
1:c:10:VAL:CG2	1:c:113:PRO:HG2	2.43	0.48
2:Q:6:HIS:NE2	2:Q:132:TYR:OH	2.20	0.48
2:Q:74:GLN:OE1	2:Q:74:GLN:O	2.32	0.48
1:R:12:GLY:O	1:R:15:THR:OG1	2.23	0.48
1:R:117:VAL:O	1:R:155:ARG:NH1	2.47	0.48
1:S:195:PHE:CB	1:S:230:SER:HA	2.42	0.48
1:C:72:GLN:NE2	1:J:124:VAL:O	2.47	0.48
1:a:79:ASP:N	1:a:79:ASP:OD1	2.46	0.48
1:b:153:GLU:OE1	1:b:153:GLU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:213:THR:HG23	1:b:214:ILE:N	2.28	0.48
1:F:52:ALA:HA	1:F:75:LYS:HA	1.95	0.48
1:J:85:ALA:HB3	1:J:87:MET:HE2	1.95	0.48
1:J:204:LYS:HB3	1:J:220:ALA:HB3	1.95	0.48
1:R:48:GLY:H	1:R:80:THR:HG22	1.77	0.48
2:U:10:ARG:HH22	2:K:81:ASP:CG	2.21	0.48
1:c:204:LYS:HB3	1:c:220:ALA:HB3	1.95	0.48
1:v:92:GLY:O	1:v:96:LEU:N	2.40	0.48
1:D:164:MET:HB3	1:D:235:PHE:CE2	2.47	0.48
1:D:164:MET:HE1	1:D:183:VAL:HG13	1.96	0.48
1:F:132:THR:HG23	1:F:135:GLU:HB3	1.95	0.48
1:F:238:VAL:HG11	1:J:238:VAL:HG11	1.94	0.48
2:G:105:MET:HB2	2:G:130:ILE:HG22	1.96	0.48
1:H:164:MET:SD	1:H:165:THR:N	2.87	0.48
1:M:185:PHE:HE1	1:M:193:LYS:HG3	1.79	0.48
1:A:8:MET:HG2	1:A:9:PRO:HD2	1.94	0.48
1:B:229:VAL:HG13	1:B:236:ALA:HB2	1.96	0.48
2:U:39:PHE:HB3	2:U:72:PRO:HG3	1.95	0.48
1:a:164:MET:SD	1:a:165:THR:N	2.86	0.48
1:b:213:THR:C	1:b:214:ILE:HG13	2.39	0.48
1:v:79:ASP:N	1:v:79:ASP:OD1	2.47	0.48
2:K:69:VAL:O	2:K:123:SER:HA	2.13	0.48
1:N:161:ALA:HA	1:N:187:PRO:HG2	1.96	0.48
1:P:185:PHE:CZ	1:P:193:LYS:HB3	2.48	0.48
1:R:61:ASP:OD1	1:X:38:ARG:NH2	2.45	0.48
1:T:41:LYS:HE2	1:T:41:LYS:HB2	1.75	0.48
1:Y:98:ALA:O	1:Y:102:GLU:HG3	2.12	0.48
1:a:185:PHE:HD2	1:a:191:THR:HG21	1.79	0.48
1:c:179:THR:HG22	1:c:216:VAL:HB	1.96	0.48
1:V:18:TRP:HB2	1:V:109:LYS:HG2	1.96	0.48
1:E:42:VAL:HG12	1:J:61:ASP:HB3	1.96	0.48
1:L:63:GLU:CD	1:L:63:GLU:H	2.22	0.48
1:O:96:LEU:HD11	1:O:141:VAL:HG21	1.96	0.48
1:O:117:VAL:O	1:O:155:ARG:NH2	2.47	0.48
2:Q:51:TYR:HE1	2:Q:59:ASP:HA	1.78	0.48
1:T:18:TRP:HB2	1:T:109:LYS:HG2	1.95	0.48
1:B:204:LYS:O	1:B:220:ALA:N	2.23	0.48
2:U:98:LEU:HD23	2:U:105:MET:HE1	1.94	0.48
1:V:120:PHE:HD1	1:V:149:PRO:HB3	1.79	0.48
1:E:72:GLN:HB2	1:S:123:TRP:CE3	2.49	0.48
1:E:175:LYS:HA	1:E:175:LYS:HD3	1.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:18:TRP:CE2	1:M:38:ARG:HG3	2.49	0.48
1:X:168:PRO:HA	1:X:181:LEU:HG	1.95	0.48
1:Y:21:LYS:NZ	1:Y:35:ASP:HA	2.28	0.48
1:A:9:PRO:HD3	1:H:87:MET:HE2	1.95	0.48
2:U:29:GLY:HA3	2:K:77:ASP:OD2	2.14	0.48
2:U:46:LEU:HD23	2:U:65:LEU:HA	1.96	0.48
1:a:164:MET:HE1	1:a:183:VAL:CG1	2.44	0.48
1:E:43:LYS:NZ	1:J:59:TYR:HE1	2.12	0.48
1:F:187:PRO:O	1:F:188:GLU:HB2	2.14	0.48
1:J:97:LEU:HD23	1:J:101:ASN:ND2	2.29	0.48
1:J:173:VAL:O	1:J:243:VAL:HG13	2.14	0.48
1:J:187:PRO:CG	1:J:191:THR:HB	2.42	0.48
1:N:198:VAL:HG23	1:N:202:LYS:HZ1	1.78	0.48
1:R:36:TRP:CD1	1:R:109:LYS:HZ3	2.32	0.48
1:b:182:THR:HA	1:b:213:THR:OG1	2.14	0.48
1:c:172:SER:HA	1:c:242:THR:O	2.13	0.48
1:V:48:GLY:HA3	1:V:78:GLY:O	2.14	0.48
1:E:200:ALA:HB2	1:E:227:PRO:HD3	1.96	0.48
1:F:63:GLU:N	1:F:63:GLU:OE2	2.46	0.48
1:N:78:GLY:HA2	1:N:145:ASN:ND2	2.29	0.48
2:U:108:SER:HB2	2:U:129:VAL:HG23	1.96	0.47
1:a:183:VAL:O	1:a:212:MET:HE2	2.14	0.47
1:V:7:THR:HA	1:M:90:GLU:OE1	2.14	0.47
1:V:63:GLU:H	1:V:63:GLU:CD	2.21	0.47
1:F:224:VAL:HG13	1:F:241:ILE:HB	1.96	0.47
1:J:93:GLN:N	1:J:93:GLN:OE1	2.47	0.47
1:P:201:ASP:OD2	1:P:204:LYS:HE2	2.14	0.47
2:u:71:LEU:O	2:u:122:SER:OG	2.30	0.47
1:E:96:LEU:HD11	1:E:141:VAL:HG21	1.95	0.47
1:S:198:VAL:O	1:S:227:PRO:HD2	2.13	0.47
2:U:6:HIS:NE2	2:U:132:TYR:OH	2.22	0.47
1:b:42:VAL:H	1:P:61:ASP:CG	2.21	0.47
1:v:205:ALA:HA	1:v:217:ASN:O	2.15	0.47
1:D:194:SER:O	1:D:231:GLY:N	2.47	0.47
1:F:173:VAL:H	1:F:243:VAL:HA	1.79	0.47
1:H:79:ASP:HB3	1:H:144:THR:HA	1.96	0.47
1:L:67:TRP:CD1	1:Y:75:LYS:HB2	2.49	0.47
1:L:67:TRP:NE1	1:Y:75:LYS:HB2	2.29	0.47
1:M:32:SER:OG	1:M:34:VAL:HG22	2.14	0.47
1:O:40:ALA:HB3	1:O:87:MET:HE1	1.96	0.47
1:A:34:VAL:HA	1:A:196:ARG:NH2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:HG23	1:A:183:VAL:HG22	1.96	0.47
1:C:209:VAL:HG23	1:C:214:ILE:HG12	1.95	0.47
1:C:224:VAL:HG13	1:C:241:ILE:HB	1.97	0.47
1:C:238:VAL:HG11	1:c:238:VAL:HG11	1.96	0.47
1:v:75:LYS:N	1:X:66:ASP:O	2.48	0.47
1:D:99:TRP:NE1	1:D:104:ASP:O	2.48	0.47
1:F:77:ALA:O	1:F:145:ASN:HB2	2.15	0.47
1:I:183:VAL:HB	1:I:212:MET:SD	2.54	0.47
1:J:209:VAL:HG22	1:J:214:ILE:HG22	1.96	0.47
1:P:181:LEU:HD11	1:P:241:ILE:HD11	1.96	0.47
1:T:47:PRO:HA	1:T:80:THR:HG23	1.96	0.47
1:X:18:TRP:HB2	1:X:109:LYS:HG2	1.97	0.47
1:X:186:GLN:HB3	1:X:189:GLY:HA2	1.96	0.47
1:A:154:ASP:N	1:A:154:ASP:OD1	2.48	0.47
1:C:201:ASP:OD2	1:C:204:LYS:HE2	2.14	0.47
1:b:164:MET:HG3	1:b:235:PHE:CG	2.49	0.47
1:v:32:SER:OG	1:v:34:VAL:HG22	2.14	0.47
1:v:195:PHE:HA	1:v:230:SER:HA	1.96	0.47
1:E:91:GLN:HE22	1:I:192:ASP:CG	2.21	0.47
1:H:5:ASN:OD1	1:H:7:THR:HG22	2.15	0.47
1:L:48:GLY:HA3	1:L:78:GLY:O	2.15	0.47
1:L:175:LYS:NZ	1:L:244:THR:O	2.47	0.47
1:N:168:PRO:HB2	1:N:241:ILE:HD11	1.96	0.47
1:S:148:ARG:NH2	1:S:154:ASP:OD1	2.47	0.47
1:Y:185:PHE:HE1	1:Y:193:LYS:HG3	1.79	0.47
1:a:105:THR:HG22	1:a:121:ARG:HG2	1.97	0.47
1:b:163:GLY:HA3	1:b:187:PRO:HA	1.95	0.47
1:D:8:MET:HG2	1:D:9:PRO:HD2	1.94	0.47
1:E:45:LEU:HD12	1:E:46:THR:N	2.30	0.47
1:N:166:VAL:HG23	1:N:183:VAL:HG22	1.95	0.47
1:N:201:ASP:OD1	1:N:202:LYS:N	2.48	0.47
2:Q:5:LYS:HG2	2:Q:9:LEU:HD11	1.96	0.47
1:R:50:LEU:CD2	1:R:149:PRO:HG3	2.45	0.47
1:R:129:LYS:HZ3	1:R:139:ARG:HH21	1.63	0.47
1:A:41:LYS:HB3	1:b:59:TYR:CE1	2.49	0.47
1:A:200:ALA:HB3	1:A:225:ASN:HB2	1.96	0.47
1:B:175:LYS:HA	1:B:175:LYS:HD3	1.71	0.47
1:a:5:ASN:OD1	1:a:7:THR:HG22	2.15	0.47
1:a:91:GLN:OE1	1:a:92:GLY:N	2.48	0.47
1:b:211:GLY:O	1:b:213:THR:N	2.47	0.47
1:c:20:TYR:HD1	1:c:21:LYS:N	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:THR:HG22	1:F:52:ALA:N	2.26	0.47
2:G:74:GLN:OE1	2:G:74:GLN:O	2.33	0.47
1:H:111:ARG:HE	1:H:111:ARG:HB3	1.49	0.47
1:H:204:LYS:HE2	1:H:204:LYS:HB2	1.69	0.47
2:K:115:ASP:CG	2:K:119:GLY:H	2.23	0.47
1:L:67:TRP:HE1	1:Y:75:LYS:HB2	1.78	0.47
1:M:79:ASP:OD1	1:M:79:ASP:N	2.45	0.47
1:O:76:SER:O	1:O:76:SER:OG	2.24	0.47
1:O:175:LYS:HD3	1:O:175:LYS:HA	1.71	0.47
2:Q:69:VAL:HG11	2:Q:83:TRP:CD1	2.49	0.47
1:S:46:THR:OG1	1:S:81:SER:O	2.26	0.47
1:S:126:SER:HB3	1:S:142:LYS:HB3	1.97	0.47
1:B:133:ALA:O	1:B:134:LYS:HG2	2.15	0.47
1:C:43:LYS:H	1:C:84:LEU:HA	1.79	0.47
1:E:204:LYS:O	1:E:220:ALA:N	2.23	0.47
1:M:105:THR:HG22	1:M:121:ARG:HG2	1.96	0.47
1:N:105:THR:O	1:N:105:THR:OG1	2.29	0.47
1:X:33:ASP:OD1	1:X:111:ARG:NH2	2.46	0.47
1:A:204:LYS:HA	1:A:220:ALA:HB3	1.97	0.47
1:b:108:TYR:CE1	1:b:120:PHE:HB2	2.50	0.47
2:u:40:PRO:HA	2:u:71:LEU:HD23	1.97	0.47
1:V:164:MET:HE2	1:V:164:MET:HA	1.97	0.47
1:D:78:GLY:HA2	1:D:145:ASN:ND2	2.29	0.47
1:M:99:TRP:HB2	1:M:106:ARG:HH12	1.78	0.47
1:N:16:THR:OG1	1:N:18:TRP:NE1	2.42	0.47
1:N:43:LYS:O	1:N:44:ASP:HB2	2.15	0.47
1:X:87:MET:HB2	1:X:90:GLU:HG2	1.97	0.47
2:U:30:ARG:HH22	2:U:121:TRP:HH2	1.63	0.47
1:D:105:THR:O	1:D:105:THR:OG1	2.30	0.47
1:I:118:ASP:OD1	1:I:151:MET:HE3	2.15	0.47
1:J:18:TRP:HB2	1:J:109:LYS:HG2	1.97	0.47
1:S:165:THR:HB	1:S:184:ALA:HB3	1.96	0.47
1:X:18:TRP:CZ3	1:X:38:ARG:HB2	2.50	0.47
1:A:47:PRO:HA	1:A:80:THR:HG23	1.96	0.46
1:b:131:VAL:HG12	1:T:60:LEU:HD11	1.97	0.46
1:c:173:VAL:O	1:c:243:VAL:HG13	2.15	0.46
1:c:185:PHE:HZ	1:c:195:PHE:HB3	1.80	0.46
1:v:148:ARG:HA	1:X:67:TRP:CZ3	2.50	0.46
2:G:94:ASP:C	2:G:95:ILE:HD13	2.39	0.46
1:I:108:TYR:CE1	1:I:120:PHE:HB2	2.50	0.46
1:P:77:ALA:O	1:P:145:ASN:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:100:PHE:HB2	1:R:124:VAL:HG11	1.97	0.46
1:R:112:PHE:HE2	1:R:118:ASP:HB2	1.80	0.46
1:A:201:ASP:OD1	1:A:202:LYS:N	2.48	0.46
1:B:96:LEU:HD11	1:B:141:VAL:HG21	1.96	0.46
1:D:111:ARG:HE	1:D:111:ARG:HB3	1.41	0.46
1:D:201:ASP:OD1	1:D:202:LYS:N	2.48	0.46
1:E:207:VAL:HG11	1:E:226:ILE:HG21	1.97	0.46
1:L:7:THR:HA	1:Y:90:GLU:OE1	2.15	0.46
1:S:5:ASN:OD1	1:S:7:THR:OG1	2.19	0.46
1:C:133:ALA:HB2	2:u:56:LEU:HD12	1.97	0.46
1:a:221:ALA:HA	1:a:243:VAL:HG13	1.97	0.46
1:V:18:TRP:CZ3	1:V:38:ARG:HB2	2.51	0.46
1:V:168:PRO:HA	1:V:181:LEU:HG	1.97	0.46
1:H:164:MET:HG2	1:H:235:PHE:HB3	1.96	0.46
1:J:86:TRP:CD1	1:J:129:LYS:HZ1	2.33	0.46
1:L:96:LEU:HD21	1:L:141:VAL:HG21	1.96	0.46
1:O:164:MET:SD	1:O:165:THR:N	2.88	0.46
1:Y:18:TRP:CE2	1:Y:38:ARG:HG3	2.50	0.46
1:Y:32:SER:OG	1:Y:34:VAL:HG22	2.15	0.46
1:C:45:LEU:HD12	1:C:82:PHE:HB3	1.97	0.46
1:C:76:SER:HB2	1:c:68:THR:OG1	2.16	0.46
1:v:99:TRP:HB2	1:v:106:ARG:HH12	1.80	0.46
1:E:18:TRP:CZ3	1:E:38:ARG:HG3	2.50	0.46
2:G:81:ASP:OD1	2:G:112:TYR:OH	2.32	0.46
1:H:91:GLN:OE1	1:H:92:GLY:N	2.49	0.46
1:B:204:LYS:HD2	1:B:222:GLY:HA3	1.98	0.46
1:C:76:SER:O	1:C:76:SER:OG	2.24	0.46
2:U:51:TYR:HE1	2:U:59:ASP:HA	1.79	0.46
1:V:212:MET:N	1:V:212:MET:SD	2.89	0.46
1:D:127:ILE:HD13	1:D:141:VAL:HG22	1.98	0.46
2:K:10:ARG:HD3	2:K:45:TYR:HA	1.97	0.46
1:L:18:TRP:HB2	1:L:109:LYS:HG2	1.97	0.46
1:L:18:TRP:CZ3	1:L:38:ARG:HB2	2.50	0.46
1:N:41:LYS:HB3	1:S:59:TYR:CE1	2.50	0.46
1:S:199:SER:HA	1:S:226:ILE:HD11	1.98	0.46
2:U:69:VAL:HG11	2:U:83:TRP:CD1	2.51	0.46
1:V:3:VAL:HB	1:V:4:PRO:HD3	1.95	0.46
1:v:21:LYS:NZ	1:v:35:ASP:HA	2.31	0.46
1:L:17:LEU:HD12	1:L:109:LYS:O	2.16	0.46
1:N:40:ALA:HB3	1:N:87:MET:HE1	1.98	0.46
2:Q:81:ASP:OD2	2:W:10:ARG:NH2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:17:LEU:HD21	1:R:39:LEU:HD12	1.97	0.46
1:Y:30:PRO:HB3	1:Y:119:VAL:HG11	1.98	0.46
1:Y:165:THR:HB	1:Y:184:ALA:HB3	1.97	0.46
1:C:100:PHE:HA	1:C:124:VAL:CG2	2.46	0.46
1:a:84:LEU:HD11	1:a:93:GLN:HE21	1.81	0.46
1:J:16:THR:HG23	1:J:111:ARG:HB3	1.98	0.46
1:M:54:SER:HB2	1:M:70:THR:HG21	1.96	0.46
1:X:195:PHE:HA	1:X:231:GLY:H	1.80	0.46
1:a:180:THR:HG23	1:a:213:THR:HG23	1.96	0.46
1:c:75:LYS:HB3	1:c:148:ARG:NH2	2.31	0.46
2:K:40:PRO:HA	2:K:71:LEU:HD23	1.98	0.46
1:M:195:PHE:HA	1:M:230:SER:HA	1.97	0.46
1:R:79:ASP:OD1	1:R:79:ASP:N	2.47	0.46
1:Y:79:ASP:N	1:Y:79:ASP:OD1	2.48	0.46
1:B:77:ALA:O	1:B:145:ASN:HB2	2.16	0.46
1:B:206:THR:OG1	1:B:217:ASN:OD1	2.19	0.46
1:b:100:PHE:CE2	1:O:50:LEU:HD12	2.50	0.46
1:c:31:LEU:HD12	1:c:111:ARG:NH2	2.31	0.46
1:v:25:ASP:HB3	1:v:28:ALA:HB2	1.98	0.46
1:E:206:THR:HG23	1:E:219:VAL:HG21	1.98	0.46
1:F:185:PHE:CZ	1:F:193:LYS:HB3	2.50	0.46
1:I:211:GLY:C	1:I:213:THR:H	2.24	0.46
1:M:102:GLU:OE2	1:M:104:ASP:HB3	2.16	0.46
1:O:223:LYS:HG2	1:O:242:THR:HG22	1.98	0.46
1:P:194:SER:O	1:P:230:SER:OG	2.32	0.46
2:Q:30:ARG:HH22	2:Q:121:TRP:HH2	1.64	0.46
1:R:165:THR:HB	1:R:184:ALA:HB3	1.98	0.46
1:X:47:PRO:HA	1:X:80:THR:HG23	1.98	0.46
1:A:159:THR:HG21	1:A:191:THR:HA	1.98	0.46
1:C:50:LEU:HB3	1:J:100:PHE:CE2	2.50	0.46
1:C:173:VAL:H	1:C:243:VAL:HA	1.81	0.46
1:a:112:PHE:HE2	1:a:118:ASP:HB2	1.81	0.46
1:E:86:TRP:NE1	1:E:139:ARG:HH21	2.13	0.46
1:J:211:GLY:O	1:J:212:MET:HE3	2.15	0.46
2:K:39:PHE:CZ	2:K:72:PRO:HA	2.51	0.46
1:M:75:LYS:HB3	1:M:75:LYS:HE2	1.72	0.46
1:S:185:PHE:C	1:S:187:PRO:HD3	2.41	0.46
1:T:230:SER:HB3	1:T:235:PHE:CE2	2.51	0.46
1:c:108:TYR:OH	1:c:145:ASN:OD1	2.25	0.45
1:D:199:SER:O	1:H:236:ALA:HB3	2.16	0.45
1:F:100:PHE:HA	1:F:124:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:54:GLU:HA	2:G:54:GLU:OE1	2.14	0.45
1:a:185:PHE:CD2	1:a:191:THR:HG21	2.51	0.45
2:u:71:LEU:HD12	2:u:80:LEU:HD12	1.99	0.45
1:L:99:TRP:HE1	1:L:123:TRP:HA	1.81	0.45
1:L:227:PRO:HB3	1:M:227:PRO:HB3	1.97	0.45
1:M:79:ASP:HB3	1:M:144:THR:HA	1.98	0.45
1:O:204:LYS:O	1:O:220:ALA:N	2.23	0.45
2:W:115:ASP:CG	2:W:119:GLY:H	2.24	0.45
1:Y:205:ALA:HA	1:Y:217:ASN:O	2.17	0.45
1:A:164:MET:O	1:A:165:THR:OG1	2.31	0.45
1:A:195:PHE:HB3	1:A:230:SER:CA	2.44	0.45
1:A:199:SER:O	1:a:236:ALA:HB3	2.17	0.45
1:C:159:THR:HG21	1:C:190:VAL:HG12	1.99	0.45
1:E:178:SER:HB2	1:E:215:THR:HG22	1.98	0.45
1:F:76:SER:HB2	1:J:68:THR:OG1	2.16	0.45
1:F:173:VAL:HB	1:F:243:VAL:HG13	1.98	0.45
1:I:48:GLY:HA2	1:I:79:ASP:O	2.17	0.45
1:J:60:LEU:HD11	1:S:131:VAL:HG12	1.99	0.45
1:L:120:PHE:HD1	1:L:149:PRO:HB3	1.81	0.45
1:O:77:ALA:O	1:O:145:ASN:HB2	2.16	0.45
1:Y:163:GLY:N	1:Y:187:PRO:HB3	2.31	0.45
1:C:131:VAL:HG21	1:c:15:THR:HG21	1.98	0.45
1:v:163:GLY:N	1:v:187:PRO:HB3	2.32	0.45
1:D:159:THR:HG21	1:D:191:THR:HA	1.98	0.45
1:J:132:THR:OG1	1:J:135:GLU:OE1	2.24	0.45
1:R:10:VAL:HG21	1:R:113:PRO:O	2.16	0.45
1:R:91:GLN:OE1	1:R:92:GLY:N	2.49	0.45
1:S:48:GLY:HA2	1:S:79:ASP:O	2.17	0.45
1:S:118:ASP:OD1	1:S:151:MET:HE3	2.16	0.45
1:X:97:LEU:HA	1:X:97:LEU:HD23	1.62	0.45
1:A:109:LYS:HE3	1:A:111:ARG:HG3	1.98	0.45
1:A:164:MET:SD	1:A:165:THR:N	2.90	0.45
1:A:194:SER:O	1:A:231:GLY:N	2.49	0.45
1:C:90:GLU:HG2	1:C:91:GLN:O	2.16	0.45
1:a:61:ASP:OD1	1:V:38:ARG:NH2	2.50	0.45
1:H:10:VAL:HG21	1:H:113:PRO:O	2.16	0.45
1:J:163:GLY:HA3	1:J:186:GLN:O	2.17	0.45
1:J:172:SER:HA	1:J:242:THR:O	2.15	0.45
1:J:196:ARG:NE	1:J:196:ARG:HA	2.32	0.45
1:L:16:THR:OG1	1:L:18:TRP:NE1	2.46	0.45
1:L:102:GLU:HG2	1:L:104:ASP:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:164:MET:HB3	1:L:235:PHE:HD2	1.80	0.45
1:M:152:ALA:HA	1:M:155:ARG:HH12	1.82	0.45
2:U:59:ASP:OD1	2:U:59:ASP:N	2.42	0.45
1:L:3:VAL:HB	1:L:4:PRO:HD3	1.98	0.45
1:N:154:ASP:OD1	1:N:154:ASP:N	2.48	0.45
1:R:63:GLU:HG3	1:R:64:ASP:N	2.31	0.45
1:R:191:THR:HG1	1:R:193:LYS:HZ3	1.57	0.45
1:A:82:PHE:HD1	1:A:84:LEU:HD22	1.82	0.45
1:B:50:LEU:HD12	1:I:100:PHE:CE2	2.52	0.45
1:b:212:MET:SD	1:b:212:MET:C	2.99	0.45
2:u:5:LYS:HE2	2:u:9:LEU:HD21	1.98	0.45
1:V:85:ALA:HB1	1:v:9:PRO:HB3	1.99	0.45
1:V:86:TRP:CD1	1:V:129:LYS:HZ3	2.35	0.45
1:P:210:SER:O	1:P:213:THR:HG22	2.17	0.45
1:X:120:PHE:HD1	1:X:149:PRO:HB3	1.82	0.45
1:a:164:MET:HG2	1:a:235:PHE:HB3	1.99	0.45
1:c:123:TRP:HH2	1:P:54:SER:HB2	1.81	0.45
1:E:164:MET:SD	1:E:165:THR:N	2.90	0.45
2:G:94:ASP:O	2:G:95:ILE:HD13	2.17	0.45
1:I:164:MET:HG3	1:I:235:PHE:CG	2.52	0.45
1:P:173:VAL:H	1:P:243:VAL:HA	1.81	0.45
1:S:56:ASP:HA	1:S:70:THR:HG22	1.98	0.45
1:T:41:LYS:HG3	2:W:55:GLU:OE2	2.17	0.45
1:D:43:LYS:HA	1:D:43:LYS:HD2	1.77	0.45
1:D:154:ASP:N	1:D:154:ASP:OD1	2.50	0.45
1:D:200:ALA:HB3	1:D:225:ASN:HB2	1.98	0.45
1:L:87:MET:HB3	1:L:90:GLU:HG2	1.98	0.45
2:Q:39:PHE:CB	2:Q:40:PRO:HD2	2.47	0.45
1:R:185:PHE:HD2	1:R:191:THR:HG21	1.82	0.45
1:X:169:ALA:HB1	1:X:171:THR:HG22	1.98	0.45
1:Y:20:TYR:CD1	1:Y:20:TYR:C	2.95	0.45
1:Y:79:ASP:HB3	1:Y:144:THR:HA	1.98	0.45
2:U:22:THR:OG1	2:U:23:GLY:N	2.50	0.45
1:c:97:LEU:HD23	1:c:101:ASN:ND2	2.31	0.45
1:D:136:VAL:HG23	1:I:55:TYR:OH	2.17	0.45
1:D:204:LYS:HG2	1:D:220:ALA:HB3	1.99	0.45
1:H:150:SER:HB3	1:H:155:ARG:HH22	1.81	0.45
1:L:169:ALA:HB1	1:L:171:THR:HG22	1.98	0.45
1:N:130:ALA:HB3	1:N:138:THR:OG1	2.17	0.45
2:Q:36:GLU:C	2:Q:38:ASP:H	2.23	0.45
2:Q:71:LEU:HD23	2:Q:71:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:109:LYS:HB3	1:R:119:VAL:HG22	1.99	0.45
2:W:105:MET:HE3	2:W:128:TYR:CG	2.52	0.45
1:B:200:ALA:HB2	1:B:227:PRO:HD3	1.98	0.44
1:C:205:ALA:HB3	1:C:224:VAL:HG21	1.99	0.44
1:E:50:LEU:HD12	1:S:100:PHE:CE2	2.50	0.44
1:H:173:VAL:HG23	1:H:177:GLN:HE21	1.82	0.44
1:N:76:SER:O	1:N:76:SER:OG	2.34	0.44
1:N:198:VAL:HG13	1:N:227:PRO:HG2	1.98	0.44
1:O:207:VAL:HG11	1:O:226:ILE:HG21	1.98	0.44
1:R:36:TRP:CG	1:R:109:LYS:HZ3	2.35	0.44
1:R:185:PHE:CD2	1:R:191:THR:HG21	2.53	0.44
1:S:231:GLY:HA3	1:S:234:GLU:OE2	2.18	0.44
1:T:97:LEU:HD23	1:T:101:ASN:ND2	2.32	0.44
1:X:84:LEU:HD23	1:X:139:ARG:O	2.17	0.44
1:Y:91:GLN:HA	1:Y:94:GLN:NE2	2.32	0.44
1:b:5:ASN:HD21	1:b:8:MET:HB2	1.82	0.44
1:c:88:PRO:HD2	1:P:6:PRO:O	2.17	0.44
1:c:187:PRO:HG2	1:c:190:VAL:O	2.17	0.44
1:V:33:ASP:OD1	1:V:111:ARG:NH2	2.47	0.44
1:F:59:TYR:CE1	1:S:41:LYS:HD2	2.52	0.44
1:I:32:SER:O	1:I:109:LYS:NZ	2.50	0.44
1:I:230:SER:HB2	1:I:235:PHE:HD2	1.82	0.44
1:M:181:LEU:HB2	1:M:214:ILE:HB	1.99	0.44
1:T:31:LEU:HD12	1:T:111:ARG:HH22	1.82	0.44
1:Y:195:PHE:HA	1:Y:230:SER:HA	1.99	0.44
1:A:211:GLY:C	1:A:213:THR:H	2.25	0.44
1:C:173:VAL:HB	1:C:243:VAL:HG13	1.99	0.44
1:v:12:GLY:O	1:v:15:THR:OG1	2.34	0.44
1:E:74:GLN:HG2	1:I:65:ALA:O	2.18	0.44
1:E:165:THR:OG1	1:E:184:ALA:HB3	2.16	0.44
1:H:61:ASP:OD1	1:L:38:ARG:NH2	2.48	0.44
1:I:131:VAL:HG22	1:I:137:ILE:HD13	2.00	0.44
1:M:41:LYS:HE3	1:M:41:LYS:HB2	1.89	0.44
1:O:204:LYS:HD2	1:O:222:GLY:HA3	1.97	0.44
1:R:107:ALA:HB2	1:R:121:ARG:HD3	1.99	0.44
1:Y:162:THR:HB	1:Y:164:MET:HE1	1.98	0.44
1:c:200:ALA:HB3	1:c:225:ASN:HB2	2.00	0.44
1:H:36:TRP:CG	1:H:109:LYS:HZ3	2.35	0.44
1:J:47:PRO:HA	1:J:80:THR:HG23	1.99	0.44
1:R:205:ALA:HB3	1:R:224:VAL:HG21	2.00	0.44
1:S:111:ARG:HE	1:S:111:ARG:HB3	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:105:THR:HG22	1:Y:121:ARG:HG2	1.98	0.44
1:B:47:PRO:HA	1:B:80:THR:HG23	2.00	0.44
1:a:183:VAL:HB	1:a:212:MET:HE1	1.99	0.44
1:v:104:ASP:CG	1:v:106:ARG:HH21	2.25	0.44
1:D:167:THR:O	1:D:182:THR:OG1	2.26	0.44
1:E:77:ALA:O	1:E:145:ASN:HB2	2.18	0.44
1:F:6:PRO:O	1:T:88:PRO:HD2	2.18	0.44
2:G:81:ASP:OD2	2:K:10:ARG:NH2	2.51	0.44
1:H:105:THR:HG22	1:H:121:ARG:HG2	1.99	0.44
1:L:85:ALA:HB1	1:M:9:PRO:HB3	1.99	0.44
1:M:91:GLN:HA	1:M:94:GLN:NE2	2.31	0.44
1:M:98:ALA:O	1:M:102:GLU:HG3	2.17	0.44
1:A:127:ILE:HD13	1:A:141:VAL:HG22	1.99	0.44
1:a:36:TRP:CG	1:a:109:LYS:HZ3	2.36	0.44
2:u:115:ASP:CG	2:u:119:GLY:H	2.26	0.44
1:V:17:LEU:HD12	1:V:109:LYS:O	2.17	0.44
1:D:183:VAL:HG11	1:D:195:PHE:CZ	2.52	0.44
1:J:202:LYS:HD3	1:J:202:LYS:HA	1.74	0.44
1:N:46:THR:O	1:N:46:THR:HG22	2.18	0.44
1:N:112:PHE:HE2	1:N:118:ASP:OD1	2.00	0.44
1:O:200:ALA:HB2	1:O:227:PRO:HD3	1.98	0.44
1:T:181:LEU:HB2	1:T:214:ILE:CG1	2.46	0.44
1:Y:99:TRP:CD2	1:Y:106:ARG:HD2	2.52	0.44
1:C:109:LYS:HA	1:C:118:ASP:O	2.18	0.44
1:V:87:MET:HE3	1:V:87:MET:HB2	1.76	0.44
1:H:97:LEU:HA	1:H:97:LEU:HD23	1.61	0.44
1:L:173:VAL:O	1:L:243:VAL:HG13	2.18	0.44
1:M:21:LYS:NZ	1:M:35:ASP:HA	2.33	0.44
1:S:163:GLY:HA3	1:S:187:PRO:HA	1.99	0.44
1:B:197:ALA:H	1:B:209:VAL:HG21	1.82	0.44
1:b:131:VAL:HG22	1:b:137:ILE:HD13	1.99	0.44
2:u:67:ILE:HD11	2:u:92:MET:HE2	1.99	0.44
1:V:173:VAL:O	1:V:243:VAL:HG13	2.18	0.44
1:F:109:LYS:HA	1:F:118:ASP:O	2.18	0.44
1:I:80:THR:O	1:I:142:LYS:HA	2.17	0.44
1:L:70:THR:HG23	1:Y:123:TRP:HE1	1.82	0.44
1:L:195:PHE:HA	1:L:231:GLY:H	1.82	0.44
1:R:105:THR:HG22	1:R:121:ARG:HG2	1.99	0.44
1:S:30:PRO:HG2	1:S:155:ARG:NH1	2.30	0.44
1:S:79:ASP:OD2	1:S:142:LYS:NZ	2.46	0.44
2:u:69:VAL:HG21	2:u:84:MET:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:16:THR:OG1	1:V:18:TRP:NE1	2.47	0.44
1:V:218:GLY:HA3	1:V:243:VAL:HG21	2.00	0.44
1:D:199:SER:OG	1:D:201:ASP:OD1	2.35	0.44
2:G:36:GLU:HG2	2:G:38:ASP:OD1	2.18	0.44
1:H:185:PHE:HE2	1:H:193:LYS:HG3	1.83	0.44
1:I:44:ASP:OD1	1:I:45:LEU:N	2.49	0.44
1:I:111:ARG:HG2	1:I:117:VAL:HG23	1.98	0.44
1:N:200:ALA:HB3	1:N:225:ASN:HB2	2.00	0.44
1:R:204:LYS:HE2	1:R:204:LYS:HB2	1.67	0.44
1:B:206:THR:HG23	1:B:219:VAL:HG21	2.00	0.43
1:c:202:LYS:HD3	1:c:202:LYS:HA	1.75	0.43
1:E:20:TYR:OH	1:E:23:SER:O	2.22	0.43
1:L:86:TRP:CD1	1:L:129:LYS:HE2	2.52	0.43
1:N:111:ARG:HE	1:N:111:ARG:HB3	1.43	0.43
2:Q:59:ASP:N	2:Q:59:ASP:OD1	2.40	0.43
1:X:85:ALA:HB3	1:X:87:MET:HE2	1.99	0.43
1:A:130:ALA:HB3	1:A:138:THR:OG1	2.18	0.43
1:A:153:GLU:OE1	1:A:153:GLU:N	2.51	0.43
1:B:27:TYR:CE1	1:B:119:VAL:HG22	2.53	0.43
2:U:80:LEU:HD13	2:U:124:ALA:HB2	2.00	0.43
1:a:32:SER:OG	1:a:34:VAL:HG23	2.17	0.43
1:b:126:SER:HB3	1:b:142:LYS:HB3	2.00	0.43
1:b:198:VAL:O	1:b:227:PRO:HD2	2.19	0.43
1:E:67:TRP:CD1	1:S:148:ARG:HB2	2.52	0.43
1:H:129:LYS:HZ3	1:H:139:ARG:HH21	1.66	0.43
1:H:180:THR:HG23	1:H:213:THR:HG23	2.00	0.43
1:I:231:GLY:HA3	1:I:234:GLU:OE2	2.18	0.43
1:M:20:TYR:HE1	1:M:35:ASP:HB3	1.83	0.43
1:P:76:SER:HB2	1:T:68:THR:OG1	2.18	0.43
2:Q:105:MET:HB2	2:Q:130:ILE:HG22	1.99	0.43
1:T:161:ALA:HB3	1:T:187:PRO:CB	2.38	0.43
1:X:17:LEU:HD12	1:X:109:LYS:O	2.18	0.43
1:B:164:MET:SD	1:B:165:THR:N	2.91	0.43
1:b:48:GLY:HA2	1:b:79:ASP:O	2.18	0.43
1:V:30:PRO:HG2	1:V:155:ARG:NH2	2.34	0.43
1:D:126:SER:HB3	1:D:142:LYS:HB3	2.00	0.43
1:H:29:ASN:CG	1:H:32:SER:HB3	2.43	0.43
1:M:18:TRP:HB3	1:M:36:TRP:HB3	2.00	0.43
1:M:25:ASP:HB3	1:M:28:ALA:HB2	2.00	0.43
1:N:91:GLN:O	1:N:91:GLN:HG3	2.17	0.43
1:N:199:SER:O	1:R:236:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:205:ALA:HB3	1:P:224:VAL:HG21	2.00	0.43
1:S:80:THR:O	1:S:142:LYS:HA	2.18	0.43
1:X:22:GLY:HA3	1:X:35:ASP:CG	2.43	0.43
1:Y:152:ALA:HA	1:Y:155:ARG:HH12	1.84	0.43
1:a:204:LYS:HE2	1:a:204:LYS:HB2	1.68	0.43
1:a:205:ALA:HB3	1:a:224:VAL:HG21	2.00	0.43
1:E:43:LYS:H	1:E:84:LEU:HA	1.83	0.43
1:H:173:VAL:O	1:H:243:VAL:HA	2.18	0.43
1:L:204:LYS:HA	1:L:220:ALA:HB3	2.00	0.43
1:M:109:LYS:HE3	1:M:111:ARG:HD2	2.00	0.43
1:N:99:TRP:NE1	1:N:104:ASP:O	2.49	0.43
1:N:204:LYS:HG2	1:N:220:ALA:HB3	2.00	0.43
1:P:133:ALA:HB2	2:W:56:LEU:HD12	1.99	0.43
1:T:202:LYS:HD3	1:T:202:LYS:HA	1.76	0.43
2:W:29:GLY:HA2	2:W:45:TYR:HB3	2.00	0.43
1:v:123:TRP:HE1	1:X:70:THR:HG23	1.83	0.43
1:D:27:TYR:CE1	1:D:119:VAL:HG13	2.53	0.43
1:E:238:VAL:HG11	1:I:238:VAL:HG11	2.00	0.43
1:L:195:PHE:HE1	1:L:212:MET:HG3	1.83	0.43
1:L:224:VAL:HG12	1:L:241:ILE:HB	2.01	0.43
2:Q:54:GLU:HA	2:Q:54:GLU:OE2	2.19	0.43
1:S:79:ASP:HB3	1:S:142:LYS:HZ3	1.83	0.43
1:S:162:THR:N	1:S:187:PRO:HB3	2.34	0.43
1:T:8:MET:SD	1:T:9:PRO:HD2	2.59	0.43
1:T:173:VAL:O	1:T:243:VAL:HG13	2.19	0.43
2:W:107:ALA:HA	2:W:128:TYR:CD1	2.52	0.43
1:b:231:GLY:HA3	1:b:234:GLU:OE2	2.18	0.43
1:v:166:VAL:HG22	1:v:183:VAL:HG22	2.01	0.43
1:F:18:TRP:CG	1:F:109:LYS:HE3	2.54	0.43
1:F:126:SER:HA	1:J:50:LEU:O	2.19	0.43
1:L:164:MET:HB3	1:L:235:PHE:CD2	2.54	0.43
1:N:17:LEU:HD13	1:N:110:ILE:HG12	2.00	0.43
2:Q:14:LEU:HD23	2:Q:14:LEU:HA	1.77	0.43
1:A:47:PRO:HG3	1:H:129:LYS:HD2	2.01	0.43
1:a:29:ASN:CG	1:a:32:SER:HB3	2.44	0.43
1:c:41:LYS:HE2	1:c:41:LYS:HB2	1.77	0.43
1:v:148:ARG:HD2	1:X:67:TRP:CH2	2.53	0.43
1:D:150:SER:C	1:D:155:ARG:NH2	2.72	0.43
1:D:195:PHE:HZ	1:D:212:MET:HE1	1.84	0.43
1:E:200:ALA:HA	1:I:236:ALA:O	2.19	0.43
1:F:74:GLN:NE2	1:J:65:ALA:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:ASN:N	1:F:145:ASN:OD1	2.51	0.43
1:I:77:ALA:O	1:I:145:ASN:ND2	2.51	0.43
1:I:79:ASP:HB3	1:I:142:LYS:HZ3	1.84	0.43
1:L:218:GLY:HA3	1:L:243:VAL:HG21	2.00	0.43
1:O:86:TRP:HB3	1:O:137:ILE:HG22	2.00	0.43
2:U:39:PHE:HD1	2:U:39:PHE:HA	1.75	0.43
1:D:130:ALA:HB3	1:D:138:THR:OG1	2.19	0.43
1:E:117:VAL:O	1:E:155:ARG:NH2	2.51	0.43
1:E:209:VAL:HG13	1:E:214:ILE:HG12	2.00	0.43
1:F:205:ALA:HB3	1:F:224:VAL:HG21	2.00	0.43
1:H:32:SER:OG	1:H:34:VAL:HG23	2.19	0.43
1:M:86:TRP:CH2	1:M:88:PRO:HG3	2.53	0.43
1:O:165:THR:OG1	1:O:184:ALA:HB3	2.18	0.43
1:P:159:THR:HG23	1:P:161:ALA:H	1.83	0.43
2:Q:22:THR:OG1	2:Q:23:GLY:N	2.49	0.43
1:X:131:VAL:HG21	1:Y:45:LEU:HD23	1.99	0.43
1:Y:12:GLY:O	1:Y:15:THR:OG1	2.34	0.43
1:A:126:SER:HB3	1:A:142:LYS:HB3	1.99	0.43
1:a:10:VAL:HG21	1:a:113:PRO:O	2.18	0.43
1:b:80:THR:O	1:b:142:LYS:HA	2.19	0.43
1:b:183:VAL:HG11	1:b:185:PHE:CZ	2.54	0.43
1:L:20:TYR:CD1	1:L:20:TYR:C	2.97	0.43
1:M:150:SER:OG	1:M:155:ARG:NH2	2.52	0.43
1:P:38:ARG:NH1	1:P:39:LEU:O	2.51	0.43
1:S:64:ASP:N	1:S:64:ASP:OD1	2.51	0.43
1:Y:109:LYS:CB	1:Y:119:VAL:HG12	2.49	0.43
1:A:202:LYS:HD3	1:A:202:LYS:HA	1.83	0.43
1:B:209:VAL:HG13	1:B:214:ILE:HG12	2.00	0.43
1:B:238:VAL:HG11	1:b:238:VAL:HG11	2.00	0.43
2:U:17:LEU:HD12	2:U:91:VAL:HG11	2.00	0.43
2:U:81:ASP:OD1	2:U:110:TYR:OH	2.36	0.43
1:a:36:TRP:CD1	1:a:109:LYS:HZ3	2.36	0.43
1:v:163:GLY:H	1:v:187:PRO:HB3	1.84	0.43
1:v:198:VAL:HG13	1:v:199:SER:O	2.18	0.43
1:F:15:THR:OG1	1:F:113:PRO:HD3	2.19	0.43
1:O:206:THR:HG23	1:O:219:VAL:HG21	2.00	0.43
1:R:183:VAL:H	1:R:212:MET:CE	2.32	0.43
1:T:31:LEU:CD1	1:T:111:ARG:HH22	2.32	0.43
1:T:86:TRP:NE1	1:T:129:LYS:HZ1	2.17	0.43
2:W:73:ALA:O	2:W:114:ARG:NH2	2.52	0.43
1:X:129:LYS:HD2	1:X:129:LYS:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:129:LYS:HZ1	1:X:137:ILE:HG22	1.84	0.43
1:A:207:VAL:HG22	1:A:216:VAL:HG22	2.00	0.42
1:a:132:THR:HG23	1:a:135:GLU:HB2	2.01	0.42
1:D:98:ALA:HA	1:D:101:ASN:HB2	2.01	0.42
1:H:153:GLU:N	1:H:153:GLU:OE1	2.52	0.42
1:I:111:ARG:HE	1:I:111:ARG:HB3	1.69	0.42
2:K:14:LEU:HD21	2:K:44:VAL:HB	2.01	0.42
1:L:186:GLN:HB3	1:L:189:GLY:HA2	1.99	0.42
1:N:65:ALA:C	1:N:67:TRP:N	2.77	0.42
1:P:159:THR:HG21	1:P:190:VAL:HG12	2.00	0.42
1:P:168:PRO:HA	1:P:181:LEU:HG	2.01	0.42
1:T:20:TYR:HD1	1:T:21:LYS:N	2.17	0.42
1:T:187:PRO:HG2	1:T:190:VAL:O	2.18	0.42
1:Y:181:LEU:HB2	1:Y:214:ILE:HB	2.01	0.42
1:b:96:LEU:O	1:b:99:TRP:HB3	2.19	0.42
1:V:67:TRP:HH2	1:M:148:ARG:NE	2.16	0.42
1:v:36:TRP:CD1	1:v:109:LYS:HZ3	2.37	0.42
1:v:79:ASP:HB3	1:v:144:THR:HA	2.01	0.42
1:D:52:ALA:HB1	1:D:72:GLN:HG3	2.01	0.42
1:H:201:ASP:OD2	1:H:203:THR:OG1	2.32	0.42
1:I:96:LEU:HD11	1:I:141:VAL:HG21	2.02	0.42
1:J:86:TRP:NE1	1:J:129:LYS:HZ1	2.17	0.42
1:N:235:PHE:HD1	1:N:236:ALA:N	2.17	0.42
1:P:145:ASN:OD1	1:P:145:ASN:N	2.52	0.42
2:Q:27:PHE:CD1	2:Q:31:PRO:HG3	2.53	0.42
2:Q:66:HIS:CD2	2:Q:127:THR:HG22	2.54	0.42
1:S:96:LEU:HD11	1:S:141:VAL:HG21	2.01	0.42
1:Y:198:VAL:HG13	1:Y:199:SER:O	2.18	0.42
1:A:8:MET:HE2	1:A:8:MET:HB3	1.91	0.42
1:B:43:LYS:HD3	1:B:43:LYS:HA	1.88	0.42
1:E:133:ALA:O	1:E:134:LYS:HG2	2.19	0.42
1:F:50:LEU:HB3	1:T:100:PHE:CE2	2.54	0.42
1:H:183:VAL:H	1:H:212:MET:CE	2.31	0.42
1:H:183:VAL:H	1:H:212:MET:HE2	1.84	0.42
1:I:96:LEU:O	1:I:99:TRP:HB3	2.20	0.42
1:M:87:MET:HE2	1:M:87:MET:HB3	1.92	0.42
1:N:127:ILE:HD13	1:N:141:VAL:HG22	2.00	0.42
1:Y:204:LYS:HB2	1:Y:204:LYS:HE2	1.87	0.42
1:A:199:SER:H	1:A:202:LYS:NZ	2.17	0.42
1:B:172:SER:HA	1:B:242:THR:O	2.19	0.42
1:C:67:TRP:CD2	1:J:148:ARG:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:230:SER:HB2	1:b:235:PHE:CD2	2.53	0.42
1:D:8:MET:HE2	1:D:8:MET:HB3	1.92	0.42
1:E:18:TRP:HE1	1:E:111:ARG:HG3	1.84	0.42
2:G:5:LYS:H	2:G:134:MET:HE1	1.83	0.42
2:G:106:VAL:CG1	1:J:11:LYS:HD3	2.43	0.42
1:H:108:TYR:CE1	1:H:120:PHE:HB2	2.53	0.42
2:K:113:ARG:NE	2:K:125:ASP:OD1	2.53	0.42
1:N:63:GLU:H	1:N:63:GLU:HG3	1.40	0.42
1:N:65:ALA:O	1:N:67:TRP:N	2.52	0.42
1:O:86:TRP:NE1	1:O:139:ARG:HH21	2.13	0.42
1:O:133:ALA:O	1:O:134:LYS:HG2	2.18	0.42
1:a:169:ALA:HB1	1:a:171:THR:HG22	2.01	0.42
1:c:186:GLN:HA	1:c:187:PRO:HD3	1.87	0.42
1:v:91:GLN:HA	1:v:94:GLN:NE2	2.33	0.42
1:v:232:ASN:N	1:v:234:GLU:OE1	2.53	0.42
1:D:202:LYS:HD3	1:D:202:LYS:HA	1.82	0.42
1:D:204:LYS:HA	1:D:220:ALA:HB3	2.02	0.42
1:F:20:TYR:OH	1:F:23:SER:O	2.21	0.42
1:I:116:THR:HG22	1:I:152:ALA:HB1	2.01	0.42
1:I:198:VAL:O	1:I:227:PRO:HD2	2.19	0.42
1:I:226:ILE:HG22	1:I:239:ALA:HB3	2.02	0.42
1:J:172:SER:O	1:J:172:SER:OG	2.35	0.42
1:J:181:LEU:O	1:J:213:THR:OG1	2.29	0.42
2:K:5:LYS:HE2	2:K:9:LEU:HD21	2.00	0.42
2:K:24:ALA:HB2	2:K:83:TRP:CZ2	2.55	0.42
1:L:20:TYR:CD2	1:L:26:PRO:HB3	2.53	0.42
1:L:120:PHE:HB3	1:L:145:ASN:ND2	2.32	0.42
1:L:168:PRO:HA	1:L:181:LEU:HG	2.02	0.42
1:A:168:PRO:HB2	1:A:241:ILE:HD11	2.02	0.42
1:B:165:THR:OG1	1:B:184:ALA:HB3	2.19	0.42
1:B:223:LYS:HG2	1:B:242:THR:HG22	2.00	0.42
1:C:185:PHE:CZ	1:C:193:LYS:HB3	2.54	0.42
1:c:148:ARG:HB2	1:P:67:TRP:CD2	2.54	0.42
2:u:107:ALA:HA	2:u:128:TYR:CD1	2.54	0.42
1:v:75:LYS:H	1:v:75:LYS:HG2	1.59	0.42
1:v:109:LYS:HE3	1:v:111:ARG:HD2	1.99	0.42
1:D:47:PRO:HG3	1:R:129:LYS:HD2	2.02	0.42
1:D:153:GLU:OE1	1:D:153:GLU:N	2.53	0.42
1:F:100:PHE:HA	1:F:124:VAL:CG2	2.50	0.42
1:J:8:MET:SD	1:J:9:PRO:HD2	2.60	0.42
1:T:187:PRO:HG3	1:T:191:THR:CA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:71:LEU:O	2:W:122:SER:OG	2.30	0.42
1:V:164:MET:HA	1:V:184:ALA:O	2.19	0.42
1:V:224:VAL:HG12	1:V:241:ILE:HB	2.02	0.42
1:F:67:TRP:CD2	1:T:148:ARG:HB2	2.55	0.42
1:F:133:ALA:HB2	2:K:56:LEU:HD12	2.01	0.42
2:K:71:LEU:O	2:K:122:SER:OG	2.28	0.42
1:M:27:TYR:OH	1:M:148:ARG:O	2.13	0.42
1:O:27:TYR:CE1	1:O:119:VAL:HG22	2.55	0.42
1:S:118:ASP:CG	1:S:151:MET:HE3	2.45	0.42
1:S:164:MET:HG3	1:S:235:PHE:CG	2.54	0.42
1:T:185:PHE:HE1	1:T:235:PHE:HZ	1.68	0.42
1:X:218:GLY:HA3	1:X:243:VAL:HG21	2.02	0.42
1:X:224:VAL:HG12	1:X:241:ILE:HB	2.01	0.42
1:B:157:THR:O	1:B:158:VAL:HG12	2.20	0.42
1:C:233:GLY:O	1:c:198:VAL:HG21	2.19	0.42
2:U:110:TYR:HE1	2:U:112:TYR:CZ	2.38	0.42
2:u:14:LEU:HD21	2:u:44:VAL:HB	2.01	0.42
1:v:18:TRP:HB3	1:v:36:TRP:HB3	2.00	0.42
1:D:161:ALA:HA	1:D:187:PRO:HG3	2.02	0.42
1:E:157:THR:O	1:E:158:VAL:HG12	2.19	0.42
1:L:116:THR:HB	1:L:152:ALA:HB1	2.02	0.42
1:M:171:THR:H	1:M:241:ILE:HD13	1.83	0.42
1:O:151:MET:HE3	1:O:151:MET:HB3	1.75	0.42
2:Q:37:ALA:C	2:Q:39:PHE:H	2.27	0.42
1:R:169:ALA:HB1	1:R:171:THR:HG22	2.01	0.42
1:R:180:THR:HG23	1:R:213:THR:HG23	2.02	0.42
1:X:173:VAL:O	1:X:243:VAL:HG13	2.20	0.42
1:A:133:ALA:O	1:A:134:LYS:HG2	2.20	0.42
1:C:59:TYR:HB2	1:C:62:ASP:OD1	2.20	0.42
1:b:84:LEU:HD11	1:b:93:GLN:HE21	1.85	0.42
1:b:97:LEU:HD23	1:b:97:LEU:HA	1.73	0.42
1:b:195:PHE:CB	1:b:230:SER:HA	2.48	0.42
1:b:213:THR:CG2	1:b:214:ILE:N	2.83	0.42
1:c:181:LEU:HB2	1:c:214:ILE:CG1	2.48	0.42
2:u:27:PHE:CD2	2:u:31:PRO:HG3	2.55	0.42
1:E:43:LYS:HA	1:E:43:LYS:HD3	1.88	0.42
2:G:66:HIS:CD2	2:G:127:THR:HG22	2.55	0.42
1:H:129:LYS:NZ	1:H:139:ARG:HH21	2.17	0.42
1:I:150:SER:OG	1:I:155:ARG:NH2	2.53	0.42
1:M:232:ASN:N	1:M:234:GLU:OE1	2.53	0.42
1:O:164:MET:HB3	1:O:235:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:131:VAL:HG22	1:S:137:ILE:HD13	2.01	0.42
1:X:183:VAL:HG21	1:X:195:PHE:CE2	2.55	0.42
1:X:212:MET:SD	1:X:212:MET:N	2.93	0.42
1:A:204:LYS:HG2	1:A:220:ALA:HB3	2.01	0.42
1:B:67:TRP:CZ2	1:I:75:LYS:HE2	2.55	0.42
1:B:224:VAL:O	1:B:240:GLU:HG2	2.20	0.42
1:V:75:LYS:HB2	1:v:67:TRP:CE3	2.55	0.42
1:v:153:GLU:OE2	1:v:156:SER:OG	2.34	0.42
1:v:171:THR:H	1:v:241:ILE:HD13	1.84	0.42
1:E:197:ALA:H	1:E:209:VAL:HG21	1.84	0.42
1:E:204:LYS:HD2	1:E:222:GLY:HA3	2.01	0.42
2:G:22:THR:OG1	2:G:23:GLY:N	2.50	0.42
1:H:163:GLY:H	1:H:187:PRO:HG3	1.85	0.42
1:J:187:PRO:HG3	1:J:191:THR:CA	2.50	0.42
1:L:183:VAL:HG21	1:L:195:PHE:CE2	2.55	0.42
2:W:25:THR:O	2:W:41:ALA:HA	2.19	0.42
1:X:50:LEU:H	1:X:50:LEU:HD12	1.85	0.42
1:B:18:TRP:HA	1:B:37:SER:O	2.20	0.41
1:B:117:VAL:O	1:B:155:ARG:NH2	2.53	0.41
1:C:38:ARG:NH1	2:U:57:ASP:OD2	2.51	0.41
1:C:77:ALA:O	1:C:145:ASN:HB2	2.20	0.41
1:C:123:TRP:CZ3	1:C:125:SER:HB3	2.55	0.41
1:c:8:MET:SD	1:c:9:PRO:HD2	2.60	0.41
1:V:120:PHE:HB3	1:V:145:ASN:HD21	1.85	0.41
1:M:163:GLY:N	1:M:187:PRO:HB3	2.35	0.41
1:P:15:THR:OG1	1:P:113:PRO:HD3	2.20	0.41
1:P:35:ASP:OD2	1:T:232:ASN:ND2	2.50	0.41
1:R:29:ASN:CG	1:R:32:SER:HB3	2.44	0.41
1:A:76:SER:HA	1:a:68:THR:OG1	2.20	0.41
1:B:43:LYS:HZ3	1:c:59:TYR:HE2	1.67	0.41
1:B:119:VAL:HG13	1:B:150:SER:HB3	2.00	0.41
1:C:15:THR:OG1	1:C:113:PRO:HD3	2.21	0.41
2:U:14:LEU:HD12	2:U:28:ASP:OD1	2.20	0.41
1:c:86:TRP:NE1	1:c:129:LYS:HZ1	2.17	0.41
1:c:204:LYS:HE2	1:c:204:LYS:HB2	1.80	0.41
2:u:46:LEU:HD23	2:u:65:LEU:HD13	2.02	0.41
1:D:175:LYS:HA	1:D:175:LYS:HD3	1.81	0.41
1:J:200:ALA:HB3	1:J:225:ASN:HB2	2.02	0.41
1:P:18:TRP:CD2	1:P:38:ARG:HB2	2.55	0.41
1:P:20:TYR:OH	1:P:23:SER:O	2.19	0.41
1:P:195:PHE:CZ	1:P:212:MET:HA	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:O	1:A:91:GLN:HG3	2.19	0.41
1:B:42:VAL:HG12	1:c:61:ASP:HB3	2.01	0.41
2:U:36:GLU:C	2:U:38:ASP:N	2.76	0.41
2:U:95:ILE:HD12	2:U:95:ILE:N	2.35	0.41
1:a:160:ALA:HA	1:a:193:LYS:HZ2	1.85	0.41
1:b:123:TRP:CE3	1:O:72:GLN:HB2	2.56	0.41
1:I:63:GLU:CD	1:I:63:GLU:N	2.77	0.41
1:J:191:THR:OG1	1:J:193:LYS:HE3	2.20	0.41
2:K:25:THR:O	2:K:41:ALA:HA	2.20	0.41
1:N:112:PHE:HE2	1:N:118:ASP:CG	2.28	0.41
1:O:201:ASP:CG	1:O:224:VAL:HG13	2.45	0.41
1:P:183:VAL:HG12	1:P:184:ALA:N	2.36	0.41
1:R:173:VAL:O	1:R:243:VAL:HA	2.19	0.41
2:W:10:ARG:HD3	2:W:45:TYR:HA	2.01	0.41
1:B:64:ASP:OD2	1:B:64:ASP:N	2.53	0.41
1:C:21:LYS:HG3	1:C:21:LYS:O	2.19	0.41
1:V:195:PHE:HA	1:V:231:GLY:H	1.86	0.41
1:E:211:GLY:C	1:E:213:THR:H	2.28	0.41
1:H:79:ASP:OD2	1:H:142:LYS:HE2	2.20	0.41
1:H:185:PHE:HB3	1:H:191:THR:HG21	2.01	0.41
2:K:25:THR:OG1	2:K:39:PHE:O	2.38	0.41
1:N:27:TYR:CE1	1:N:119:VAL:HG13	2.55	0.41
1:N:123:TRP:HH2	1:R:54:SER:OG	2.03	0.41
1:O:43:LYS:H	1:O:84:LEU:HA	1.84	0.41
1:Y:43:LYS:HA	1:Y:43:LYS:HD2	1.86	0.41
1:Y:164:MET:H	1:Y:164:MET:CE	2.25	0.41
1:A:99:TRP:NE1	1:A:104:ASP:O	2.51	0.41
1:C:187:PRO:O	1:C:188:GLU:HB2	2.20	0.41
1:a:61:ASP:HA	1:V:15:THR:O	2.21	0.41
1:b:45:LEU:HA	1:b:82:PHE:HB3	2.01	0.41
2:u:24:ALA:HB3	2:u:26:PHE:CE1	2.56	0.41
1:V:20:TYR:HB3	1:V:107:ALA:HB3	2.03	0.41
1:H:84:LEU:HD11	1:H:93:GLN:HE21	1.86	0.41
1:I:5:ASN:HD21	1:I:8:MET:HB2	1.85	0.41
1:I:67:TRP:HZ2	1:S:101:ASN:ND2	2.19	0.41
1:N:199:SER:OG	1:N:201:ASP:OD1	2.38	0.41
1:O:91:GLN:HE22	1:S:192:ASP:CG	2.28	0.41
2:W:31:PRO:HG2	2:W:34:PHE:CE2	2.56	0.41
1:A:201:ASP:OD1	1:A:224:VAL:HG23	2.21	0.41
1:B:200:ALA:HA	1:b:236:ALA:O	2.21	0.41
1:C:104:ASP:OD1	1:C:105:THR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LYS:HD3	1:C:175:LYS:HA	1.89	0.41
1:b:21:LYS:HZ3	1:b:37:SER:HB3	1.84	0.41
1:b:159:THR:N	1:b:192:ASP:OD2	2.43	0.41
1:V:169:ALA:HB1	1:V:171:THR:HG22	2.02	0.41
1:D:39:LEU:HD13	1:D:39:LEU:HA	1.88	0.41
1:E:132:THR:HG23	1:E:135:GLU:HG2	2.02	0.41
1:F:54:SER:HB2	1:T:123:TRP:HH2	1.85	0.41
1:I:5:ASN:OD1	1:I:7:THR:OG1	2.18	0.41
1:J:41:LYS:HE2	1:J:41:LYS:HB2	1.75	0.41
1:J:90:GLU:OE2	1:J:93:GLN:NE2	2.54	0.41
1:M:43:LYS:HD2	1:M:43:LYS:HA	1.90	0.41
1:N:227:PRO:HB3	1:R:227:PRO:HB3	2.03	0.41
1:X:78:GLY:O	1:X:79:ASP:HB3	2.20	0.41
1:Y:18:TRP:HB3	1:Y:36:TRP:HB3	2.02	0.41
1:B:53:GLU:OE1	1:B:73:GLY:HA3	2.21	0.41
1:C:133:ALA:HB2	2:u:56:LEU:CD1	2.50	0.41
1:a:98:ALA:O	1:a:102:GLU:HG3	2.21	0.41
1:b:15:THR:HB	1:P:60:LEU:HD21	2.01	0.41
1:b:66:ASP:OD1	1:b:66:ASP:N	2.53	0.41
1:b:75:LYS:O	1:O:68:THR:HG23	2.21	0.41
1:V:99:TRP:HE1	1:V:123:TRP:HA	1.85	0.41
1:D:123:TRP:HH2	1:H:54:SER:OG	2.04	0.41
1:F:43:LYS:H	1:F:84:LEU:HA	1.85	0.41
2:G:71:LEU:HD23	2:G:71:LEU:HA	1.82	0.41
1:H:112:PHE:HE2	1:H:118:ASP:HB2	1.86	0.41
1:H:205:ALA:HB3	1:H:224:VAL:HG21	2.03	0.41
1:L:50:LEU:H	1:L:50:LEU:HD12	1.86	0.41
1:M:20:TYR:CE1	1:M:35:ASP:HB3	2.55	0.41
1:M:197:ALA:H	1:M:209:VAL:HG21	1.86	0.41
1:M:204:LYS:HB2	1:M:204:LYS:HE2	1.89	0.41
1:N:122:GLY:HA3	1:N:145:ASN:HA	2.03	0.41
1:N:133:ALA:O	1:N:134:LYS:HG2	2.20	0.41
1:N:159:THR:HG21	1:N:191:THR:HA	2.03	0.41
1:N:194:SER:O	1:N:231:GLY:N	2.53	0.41
1:X:175:LYS:NZ	1:X:244:THR:O	2.53	0.41
1:A:150:SER:HG	1:A:155:ARG:HH12	1.62	0.41
1:c:100:PHE:CE2	1:P:50:LEU:HB3	2.56	0.41
1:V:120:PHE:CB	1:V:145:ASN:HD21	2.33	0.41
1:O:209:VAL:HG13	1:O:214:ILE:HG12	2.02	0.41
2:Q:60:THR:O	2:Q:60:THR:OG1	2.35	0.41
1:R:32:SER:OG	1:R:34:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:24:ALA:HB2	2:W:83:TRP:CZ2	2.56	0.41
1:Y:20:TYR:HB2	1:Y:36:TRP:CZ3	2.55	0.41
1:A:41:LYS:HB3	1:b:59:TYR:HE1	1.85	0.41
1:A:65:ALA:C	1:A:67:TRP:N	2.79	0.41
1:A:86:TRP:NE1	1:a:153:GLU:OE2	2.26	0.41
1:A:122:GLY:HA3	1:A:145:ASN:HA	2.02	0.41
1:A:123:TRP:HH2	1:a:54:SER:OG	2.04	0.41
1:A:199:SER:OG	1:A:201:ASP:OD1	2.39	0.41
1:B:18:TRP:HE1	1:B:111:ARG:HG3	1.84	0.41
1:B:18:TRP:CD1	1:B:111:ARG:HG3	2.56	0.41
1:B:207:VAL:HG11	1:B:226:ILE:HG21	2.02	0.41
1:C:168:PRO:HA	1:C:181:LEU:HG	2.01	0.41
2:U:13:VAL:HG21	2:U:65:LEU:HD21	2.03	0.41
2:U:51:TYR:O	2:U:51:TYR:CG	2.74	0.41
1:a:6:PRO:HA	1:a:114:ASN:ND2	2.36	0.41
1:b:118:ASP:OD1	1:b:151:MET:HE3	2.20	0.41
1:c:105:THR:HA	1:c:122:GLY:O	2.21	0.41
1:c:173:VAL:HB	1:c:243:VAL:HG22	2.03	0.41
2:u:39:PHE:O	2:u:40:PRO:C	2.64	0.41
1:V:82:PHE:CE1	1:V:141:VAL:HB	2.56	0.41
1:V:204:LYS:HA	1:V:220:ALA:HB3	2.02	0.41
1:F:124:VAL:HG12	1:F:143:VAL:HG12	2.02	0.41
2:G:84:MET:HE3	2:G:84:MET:HB3	1.88	0.41
2:G:95:ILE:HG22	2:G:98:LEU:H	1.85	0.41
1:H:183:VAL:HG23	1:H:214:ILE:HD11	2.01	0.41
1:J:20:TYR:HD1	1:J:21:LYS:N	2.18	0.41
1:L:108:TYR:CE1	1:L:120:PHE:HB2	2.55	0.41
1:L:193:LYS:HZ1	1:L:234:GLU:H	1.68	0.41
1:M:221:ALA:HA	1:M:243:VAL:HB	2.03	0.41
1:N:118:ASP:OD1	1:N:118:ASP:N	2.54	0.41
1:N:126:SER:HB3	1:N:142:LYS:HB3	2.02	0.41
1:N:204:LYS:HA	1:N:220:ALA:HB3	2.02	0.41
1:O:178:SER:HB2	1:O:215:THR:HG22	2.01	0.41
1:O:211:GLY:C	1:O:213:THR:H	2.28	0.41
1:P:148:ARG:HB2	1:T:67:TRP:NE1	2.36	0.41
1:P:173:VAL:HB	1:P:243:VAL:HG13	2.03	0.41
2:Q:80:LEU:HD13	2:Q:124:ALA:HB2	2.03	0.41
1:R:84:LEU:HD11	1:R:93:GLN:HE21	1.86	0.41
1:R:111:ARG:HE	1:R:111:ARG:HB3	1.48	0.41
1:R:132:THR:HG23	1:R:135:GLU:HB2	2.02	0.41
1:R:153:GLU:OE1	1:R:153:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:173:VAL:HB	1:T:243:VAL:HG22	2.03	0.41
1:X:38:ARG:HD3	1:X:39:LEU:C	2.46	0.41
1:X:164:MET:HB3	1:X:235:PHE:CD2	2.54	0.41
1:X:164:MET:HA	1:X:184:ALA:O	2.21	0.41
1:Y:27:TYR:OH	1:Y:148:ARG:O	2.12	0.41
1:v:86:TRP:CH2	1:v:88:PRO:HG3	2.56	0.41
1:E:109:LYS:HA	1:E:118:ASP:O	2.21	0.41
1:J:66:ASP:OD1	1:J:66:ASP:N	2.41	0.41
1:L:54:SER:OG	1:L:70:THR:OG1	2.18	0.41
1:N:183:VAL:HG11	1:N:195:PHE:CZ	2.56	0.41
1:O:74:GLN:NE2	1:S:65:ALA:O	2.54	0.41
2:Q:5:LYS:O	2:Q:9:LEU:HD12	2.21	0.41
1:Y:221:ALA:HA	1:Y:243:VAL:HB	2.03	0.41
1:A:17:LEU:HD13	1:A:110:ILE:HG12	2.02	0.40
1:B:91:GLN:HE22	1:b:192:ASP:CG	2.28	0.40
1:B:132:THR:HG23	1:B:135:GLU:HG2	2.02	0.40
1:B:201:ASP:CG	1:B:224:VAL:HG13	2.46	0.40
1:c:185:PHE:CZ	1:c:195:PHE:HB3	2.55	0.40
2:u:29:GLY:HA2	2:u:45:TYR:HB3	2.02	0.40
1:V:131:VAL:HG21	1:v:45:LEU:HD23	2.03	0.40
1:v:109:LYS:CB	1:v:119:VAL:HG12	2.49	0.40
1:D:35:ASP:H	1:D:196:ARG:NH2	2.14	0.40
1:I:66:ASP:OD1	1:I:66:ASP:N	2.53	0.40
1:N:207:VAL:HG22	1:N:216:VAL:HG22	2.02	0.40
1:O:200:ALA:HA	1:S:236:ALA:O	2.20	0.40
1:R:223:LYS:HB2	1:R:223:LYS:HE2	1.75	0.40
1:S:167:THR:HB	1:S:182:THR:HG23	2.02	0.40
1:S:211:GLY:C	1:S:213:THR:H	2.27	0.40
1:Y:8:MET:CE	1:Y:9:PRO:HD2	2.48	0.40
2:U:30:ARG:HB2	2:U:45:TYR:CD1	2.55	0.40
1:F:10:VAL:HG11	1:F:113:PRO:HG2	2.03	0.40
1:F:86:TRP:CZ2	1:F:88:PRO:HG3	2.57	0.40
1:F:123:TRP:CZ3	1:F:125:SER:HB3	2.55	0.40
1:J:87:MET:CB	1:J:90:GLU:HG2	2.51	0.40
2:K:92:MET:HE1	2:K:105:MET:CE	2.51	0.40
1:M:99:TRP:HA	1:M:106:ARG:HH22	1.86	0.40
1:S:20:TYR:HD1	1:S:36:TRP:CE2	2.39	0.40
1:S:90:GLU:O	1:S:94:GLN:NE2	2.54	0.40
1:B:86:TRP:NE1	1:B:139:ARG:HH21	2.17	0.40
1:C:86:TRP:CH2	1:C:88:PRO:HG3	2.57	0.40
1:a:111:ARG:HE	1:a:111:ARG:HB3	1.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:v:221:ALA:HA	1:v:243:VAL:HB	2.03	0.40
1:E:201:ASP:CG	1:E:224:VAL:HG13	2.46	0.40
1:I:32:SER:OG	1:I:33:ASP:N	2.54	0.40
1:L:38:ARG:HD3	1:L:39:LEU:C	2.46	0.40
1:N:195:PHE:CB	1:N:230:SER:HA	2.51	0.40
1:O:61:ASP:OD2	1:O:61:ASP:C	2.64	0.40
1:O:172:SER:HA	1:O:242:THR:O	2.21	0.40
1:R:5:ASN:OD1	1:R:7:THR:HG22	2.20	0.40
1:S:204:LYS:HE2	1:S:204:LYS:HB2	1.89	0.40
1:X:204:LYS:HA	1:X:220:ALA:HB3	2.03	0.40
1:Y:171:THR:H	1:Y:241:ILE:HD13	1.86	0.40
1:A:31:LEU:HD12	1:A:31:LEU:HA	1.78	0.40
1:A:195:PHE:HZ	1:A:212:MET:HE1	1.86	0.40
2:U:4:MET:HG3	2:U:134:MET:HE1	2.03	0.40
1:a:46:THR:HB	1:a:81:SER:O	2.22	0.40
1:a:108:TYR:CE1	1:a:120:PHE:HB2	2.57	0.40
2:u:84:MET:HB3	2:u:84:MET:HE3	1.83	0.40
2:u:102:ILE:CD1	2:u:105:MET:HB2	2.52	0.40
1:V:108:TYR:CE1	1:V:120:PHE:HB2	2.57	0.40
1:F:112:PHE:HE2	1:F:118:ASP:HB2	1.87	0.40
1:L:39:LEU:HA	1:L:39:LEU:HD23	1.86	0.40
1:L:87:MET:HE3	1:L:87:MET:HB2	1.75	0.40
1:L:168:PRO:HB3	1:L:239:ALA:HB1	2.04	0.40
1:M:54:SER:HB2	1:M:70:THR:CG2	2.51	0.40
1:P:45:LEU:HD21	1:P:110:ILE:HD13	2.03	0.40
1:P:148:ARG:HB2	1:T:67:TRP:CE2	2.57	0.40
1:S:5:ASN:HD21	1:S:8:MET:HB2	1.86	0.40
1:S:45:LEU:HA	1:S:82:PHE:HB3	2.02	0.40
1:Y:49:GLU:HG3	1:Y:51:THR:HG23	2.03	0.40
1:Y:197:ALA:H	1:Y:209:VAL:HG21	1.86	0.40
1:C:153:GLU:HB2	1:J:97:LEU:HD13	2.03	0.40
1:a:131:VAL:HG11	1:N:45:LEU:HD23	2.04	0.40
2:u:92:MET:SD	2:u:95:ILE:HG13	2.61	0.40
1:D:133:ALA:O	1:D:134:LYS:HG2	2.22	0.40
2:G:80:LEU:HB3	2:G:124:ALA:HB2	2.03	0.40
1:I:79:ASP:OD2	1:I:142:LYS:NZ	2.49	0.40
1:O:157:THR:O	1:O:158:VAL:HG12	2.21	0.40
1:R:183:VAL:H	1:R:212:MET:HE2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/246 (98%)	209 (86%)	32 (13%)	1 (0%)	30	63
1	B	242/246 (98%)	217 (90%)	24 (10%)	1 (0%)	30	63
1	C	242/246 (98%)	220 (91%)	20 (8%)	2 (1%)	16	48
1	D	242/246 (98%)	210 (87%)	31 (13%)	1 (0%)	30	63
1	E	242/246 (98%)	218 (90%)	22 (9%)	2 (1%)	16	48
1	F	242/246 (98%)	220 (91%)	19 (8%)	3 (1%)	11	38
1	H	242/246 (98%)	216 (89%)	25 (10%)	1 (0%)	30	63
1	I	242/246 (98%)	215 (89%)	27 (11%)	0	100	100
1	J	242/246 (98%)	215 (89%)	25 (10%)	2 (1%)	16	48
1	L	242/246 (98%)	222 (92%)	18 (7%)	2 (1%)	16	48
1	M	242/246 (98%)	226 (93%)	16 (7%)	0	100	100
1	N	242/246 (98%)	208 (86%)	32 (13%)	2 (1%)	16	48
1	O	242/246 (98%)	218 (90%)	21 (9%)	3 (1%)	11	38
1	P	242/246 (98%)	221 (91%)	19 (8%)	2 (1%)	16	48
1	R	242/246 (98%)	223 (92%)	17 (7%)	2 (1%)	16	48
1	S	242/246 (98%)	214 (88%)	28 (12%)	0	100	100
1	T	242/246 (98%)	216 (89%)	23 (10%)	3 (1%)	11	38
1	V	242/246 (98%)	224 (93%)	16 (7%)	2 (1%)	16	48
1	X	242/246 (98%)	219 (90%)	20 (8%)	3 (1%)	11	38
1	Y	242/246 (98%)	224 (93%)	18 (7%)	0	100	100
1	a	242/246 (98%)	224 (93%)	18 (7%)	0	100	100
1	b	242/246 (98%)	213 (88%)	28 (12%)	1 (0%)	30	63
1	c	242/246 (98%)	215 (89%)	25 (10%)	2 (1%)	16	48
1	v	242/246 (98%)	225 (93%)	17 (7%)	0	100	100
2	G	129/131 (98%)	109 (84%)	20 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	128/131 (98%)	120 (94%)	5 (4%)	3 (2%)	5	23
2	Q	129/131 (98%)	108 (84%)	18 (14%)	3 (2%)	5	23
2	U	129/131 (98%)	107 (83%)	21 (16%)	1 (1%)	16	48
2	W	128/131 (98%)	117 (91%)	8 (6%)	3 (2%)	5	23
2	u	128/131 (98%)	113 (88%)	10 (8%)	5 (4%)	2	14
All	All	6579/6690 (98%)	5906 (90%)	623 (10%)	50 (1%)	19	48

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	VAL
1	B	158	VAL
1	C	158	VAL
2	u	39	PHE
2	u	40	PRO
2	u	72	PRO
1	V	63	GLU
1	V	158	VAL
1	D	158	VAL
1	E	64	ASP
1	E	158	VAL
1	F	158	VAL
2	K	39	PHE
2	K	72	PRO
1	L	63	GLU
1	L	158	VAL
1	N	158	VAL
1	O	158	VAL
1	P	158	VAL
2	Q	35	ASP
2	Q	39	PHE
2	Q	40	PRO
2	W	39	PHE
2	W	72	PRO
1	X	63	GLU
1	X	79	ASP
1	X	158	VAL
2	U	40	PRO
1	J	188	GLU
1	O	64	ASP

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Mol	Chain	Res	Type
1	T	188	GLU
1	c	65	ALA
1	J	65	ALA
1	R	63	GLU
1	R	65	ALA
1	T	65	ALA
2	u	97	ALA
1	C	64	ASP
1	b	212	MET
1	F	64	ASP
1	P	64	ASP
1	F	187	PRO
1	H	63	GLU
2	K	40	PRO
2	W	40	PRO
2	u	96	PRO
1	N	46	THR
1	O	9	PRO
1	c	187	PRO
1	T	187	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/196 (99%)	190 (98%)	4 (2%)	48	72
1	B	194/196 (99%)	193 (100%)	1 (0%)	86	92
1	C	194/196 (99%)	190 (98%)	4 (2%)	48	72
1	D	194/196 (99%)	190 (98%)	4 (2%)	48	72
1	E	194/196 (99%)	194 (100%)	0	100	100
1	F	194/196 (99%)	193 (100%)	1 (0%)	86	92
1	H	194/196 (99%)	193 (100%)	1 (0%)	86	92
1	I	194/196 (99%)	193 (100%)	1 (0%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	194/196 (99%)	191 (98%)	3 (2%)	60	80
1	L	194/196 (99%)	192 (99%)	2 (1%)	73	86
1	M	194/196 (99%)	194 (100%)	0	100	100
1	N	194/196 (99%)	191 (98%)	3 (2%)	60	80
1	O	194/196 (99%)	190 (98%)	4 (2%)	48	72
1	P	194/196 (99%)	192 (99%)	2 (1%)	73	86
1	R	194/196 (99%)	193 (100%)	1 (0%)	86	92
1	S	194/196 (99%)	192 (99%)	2 (1%)	73	86
1	T	194/196 (99%)	191 (98%)	3 (2%)	60	80
1	V	194/196 (99%)	192 (99%)	2 (1%)	73	86
1	X	194/196 (99%)	193 (100%)	1 (0%)	86	92
1	Y	194/196 (99%)	194 (100%)	0	100	100
1	a	194/196 (99%)	194 (100%)	0	100	100
1	b	194/196 (99%)	188 (97%)	6 (3%)	35	63
1	c	194/196 (99%)	193 (100%)	1 (0%)	86	92
1	v	194/196 (99%)	194 (100%)	0	100	100
2	G	109/109 (100%)	109 (100%)	0	100	100
2	K	108/109 (99%)	107 (99%)	1 (1%)	75	88
2	Q	109/109 (100%)	106 (97%)	3 (3%)	38	66
2	U	109/109 (100%)	108 (99%)	1 (1%)	75	88
2	W	108/109 (99%)	108 (100%)	0	100	100
2	u	108/109 (99%)	107 (99%)	1 (1%)	75	88
All	All	5307/5358 (99%)	5255 (99%)	52 (1%)	71	86

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	63	GLU
1	A	64	ASP
1	A	195	PHE
1	B	64	ASP
1	C	41	LYS
1	C	51	THR

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Mol	Chain	Res	Type
1	C	75	LYS
1	C	217	ASN
2	U	17	LEU
1	b	63	GLU
1	b	151	MET
1	b	198	VAL
1	b	210	SER
1	b	212	MET
1	b	213	THR
1	c	63	GLU
2	u	96	PRO
1	V	45	LEU
1	V	63	GLU
1	D	60	LEU
1	D	61	ASP
1	D	63	GLU
1	D	64	ASP
1	F	75	LYS
1	H	64	ASP
1	I	63	GLU
1	J	63	GLU
1	J	188	GLU
1	J	214	ILE
2	K	39	PHE
1	L	45	LEU
1	L	63	GLU
1	N	43	LYS
1	N	63	GLU
1	N	64	ASP
1	O	7	THR
1	O	8	MET
1	O	96	LEU
1	O	101	ASN
1	P	57	ASP
1	P	74	GLN
2	Q	36	GLU
2	Q	38	ASP
2	Q	40	PRO
1	R	64	ASP
1	S	101	ASN
1	S	151	MET
1	T	63	GLU

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Mol	Chain	Res	Type
1	T	188	GLU
1	T	226	ILE
1	X	63	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	B	72	GLN
1	C	177	GLN
1	c	74	GLN
1	V	74	GLN
1	V	101	ASN
1	E	5	ASN
1	H	177	GLN
1	I	94	GLN
1	L	91	GLN
1	L	145	ASN
1	N	91	GLN
1	O	72	GLN
1	R	225	ASN
1	S	94	GLN
1	X	5	ASN
1	X	74	GLN
1	X	91	GLN
1	X	94	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.