



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 18, 2018 – 07:40 am GMT

PDB ID : 5A0Q  
EMDB ID: : EMD-2981  
Title : Cryo-EM reveals the conformation of a substrate analogue in the human 20S proteasome core  
Authors : daFonseca, P.C.A.; Morris, E.P.  
Deposited on : 2015-04-22  
Resolution : 3.50 Å(reported)  
Based on PDB ID : 3UNE

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

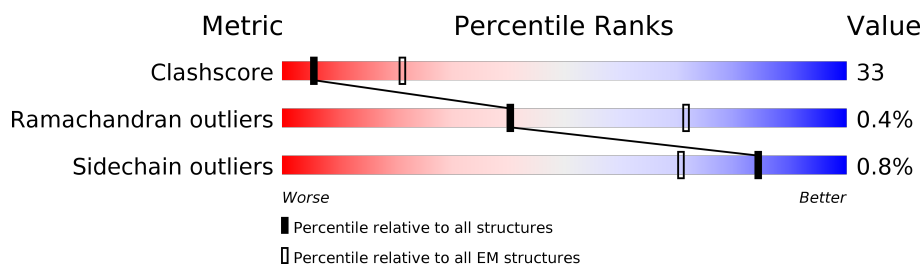
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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

















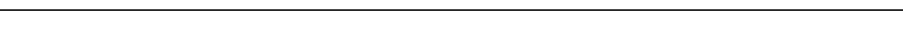




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	246	66% 13% 21%
1	O	246	67% 12% 21%
2	B	234	59% 29% • 9%
2	P	234	60% 27% • 9%
3	C	261	67% 23% • 9%
3	Q	261	66% 23% • 9%
4	D	248	68% 17% • 14%
4	R	248	68% 17% • 14%
5	E	241	67% 20% • 11%

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Mol	Chain	Length	Quality of chain
5	S	241	
6	F	263	
6	T	263	
7	G	255	
7	U	255	
8	H	205	
8	V	205	
9	I	234	
9	W	234	
10	J	204	
10	X	204	
11	K	201	
11	Y	201	
12	L	204	
12	Z	204	
13	M	213	
13	a	213	
14	N	219	
14	b	219	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	KNM	H	300	-	-	X	-
15	KNM	I	300	-	-	X	-
15	KNM	L	300	-	-	X	-
15	KNM	V	300	-	-	X	-
15	KNM	W	300	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	KNM	Z	300	-	-	X	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 43448 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	195	Total	C	N	O	S	0	0
			1514	963	254	284	13		
1	O	195	Total	C	N	O	S	0	0
			1514	963	254	284	13		

- Molecule 2 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	214	Total	C	N	O	S	0	0
			1671	1072	285	309	5		
2	P	214	Total	C	N	O	S	0	0
			1671	1072	285	309	5		

- Molecule 3 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	237	Total	C	N	O	S	0	0
			1860	1175	321	354	10		
3	Q	237	Total	C	N	O	S	0	0
			1860	1175	321	354	10		

- Molecule 4 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	214	Total	C	N	O	S	0	0
			1674	1056	300	313	5		
4	R	214	Total	C	N	O	S	0	0
			1674	1056	300	313	5		

- Molecule 5 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1643	1036	272	325	10		
5	S	215	Total	C	N	O	S	0	0
			1643	1036	272	325	10		

- Molecule 6 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	195	Total	C	N	O	S	0	0
			1535	969	278	278	10		
6	T	195	Total	C	N	O	S	0	0
			1535	969	278	278	10		

- Molecule 7 is a protein called PROTEASOME SUBUNIT ALPHA TYPE-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	209	Total	C	N	O	S	0	0
			1626	1032	279	304	11		
7	U	209	Total	C	N	O	S	0	0
			1626	1032	279	304	11		

- Molecule 8 is a protein called PROTEASOME SUBUNIT BETA TYPE-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	183	Total	C	N	O	S	0	0
			1372	858	236	266	12		
8	V	183	Total	C	N	O	S	0	0
			1372	858	236	266	12		

- Molecule 9 is a protein called PROTEASOME SUBUNIT BETA TYPE-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	198	Total	C	N	O	S	0	0
			1490	939	251	288	12		
9	W	198	Total	C	N	O	S	0	0
			1490	939	251	288	12		

- Molecule 10 is a protein called PROTEASOME SUBUNIT BETA TYPE-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	176	Total	C	N	O	S	0	0
			1374	882	227	251	14		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	176	Total	C	N	O	S	0	0
			1374	882	227	251	14		

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	189	Total	C	N	O	S	0	0
			1512	970	259	275	8		
11	Y	189	Total	C	N	O	S	0	0
			1512	970	259	275	8		

- Molecule 12 is a protein called PROTEASOME SUBUNIT BETA TYPE-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	192	Total	C	N	O	S	0	0
			1480	933	258	280	9		
12	Z	192	Total	C	N	O	S	0	0
			1480	933	258	280	9		

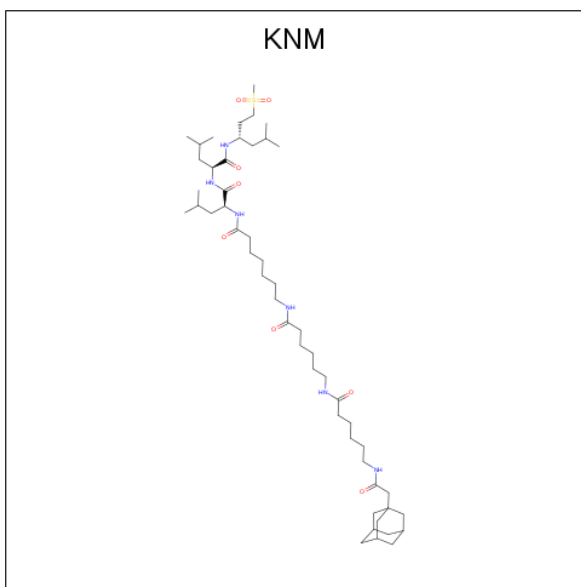
- Molecule 13 is a protein called PROTEASOME SUBUNIT BETA TYPE-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	190	Total	C	N	O	S	0	0
			1453	919	250	275	9		
13	a	190	Total	C	N	O	S	0	0
			1453	919	250	275	9		

- Molecule 14 is a protein called PROTEASOME SUBUNIT BETA TYPE-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	184	Total	C	N	O	S	0	0
			1428	905	245	267	11		
14	b	184	Total	C	N	O	S	0	0
			1428	905	245	267	11		

- Molecule 15 is ADA-(AHX)3-(LEU)3-VINYL SULFONE (three-letter code: KNM) (formula: C<sub>51</sub>H<sub>92</sub>N<sub>6</sub>O<sub>8</sub>S).



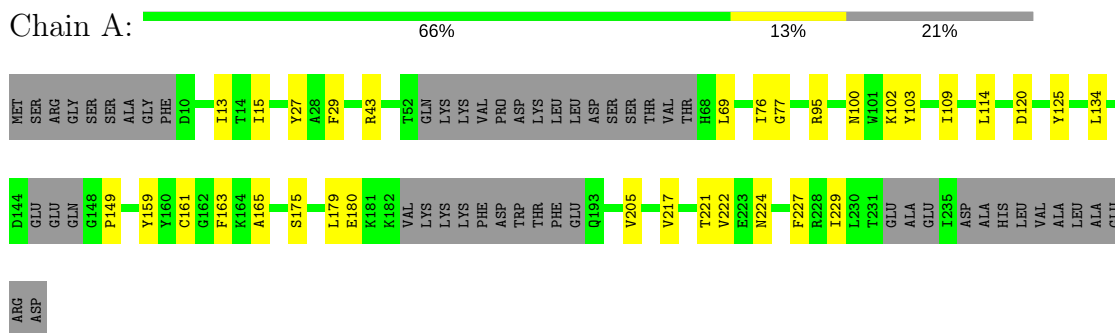
Mol	Chain	Residues	Atoms					AltConf
15	H	1	Total 31	C 22	N 3	O 5	S 1	0
15	I	1	Total 30	C 22	N 3	O 4	S 1	0
15	L	1	Total 31	C 22	N 3	O 5	S 1	0
15	V	1	Total 31	C 22	N 3	O 5	S 1	0
15	W	1	Total 30	C 22	N 3	O 4	S 1	0
15	Z	1	Total 31	C 22	N 3	O 5	S 1	0



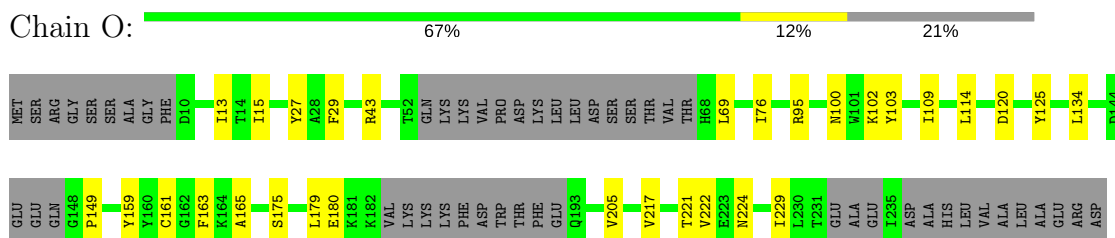
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

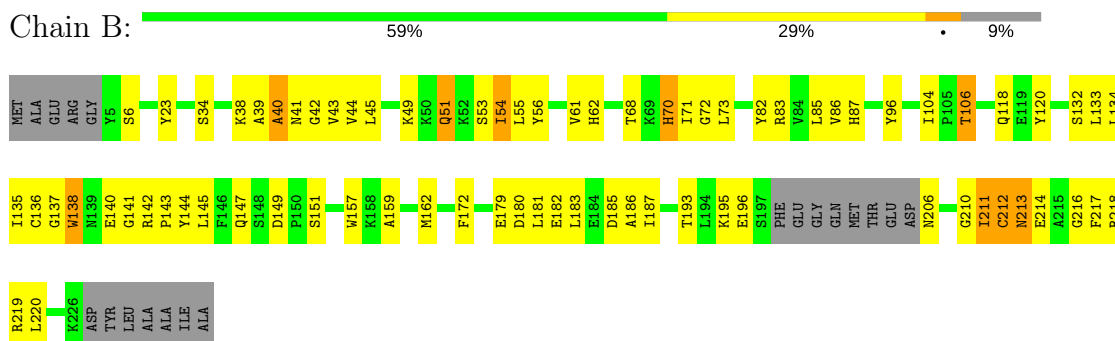
#### • Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-6



#### • Molecule 1: PROTEASOME SUBUNIT ALPHA TYPE-6

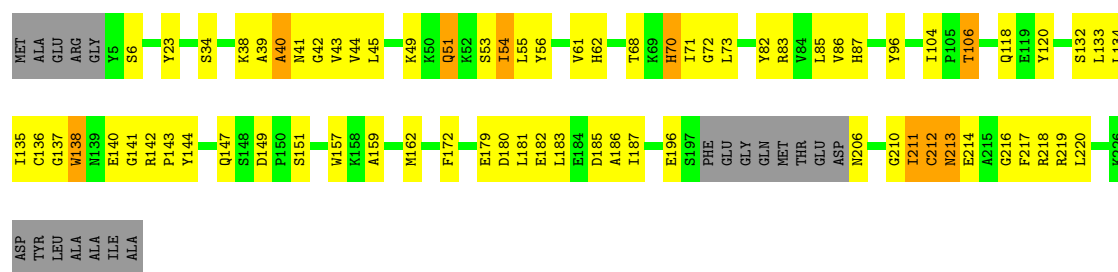


#### • Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-2



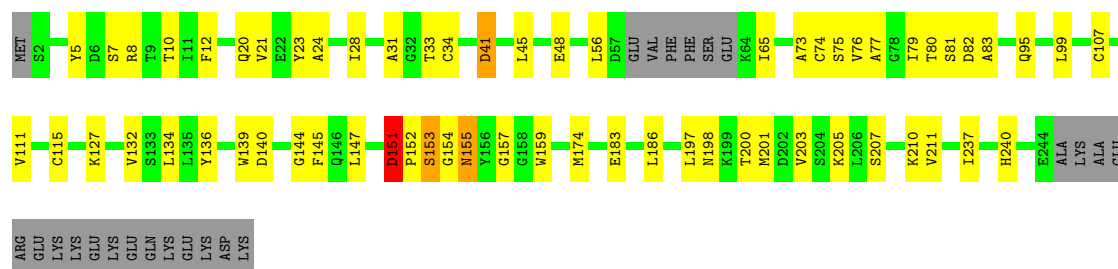
#### • Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE-2





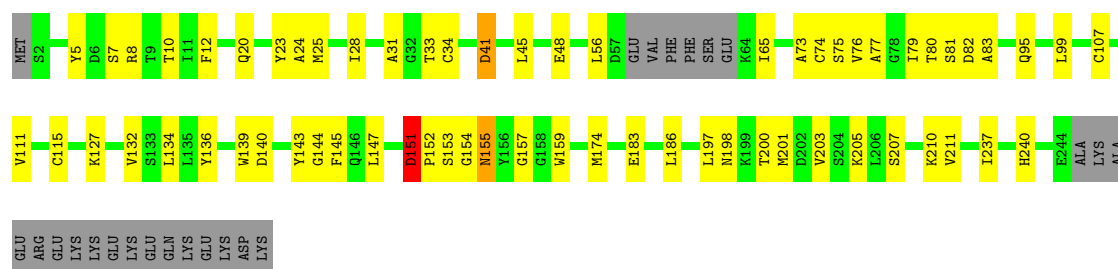
• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4

Chain C: 67% 23% 9%



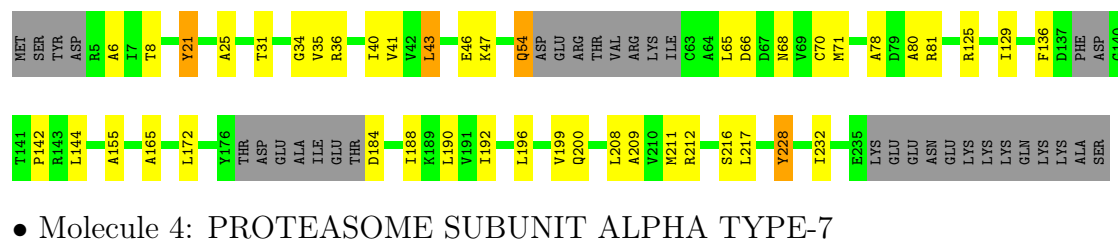
• Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE-4

Chain Q: 66% 23% 9%



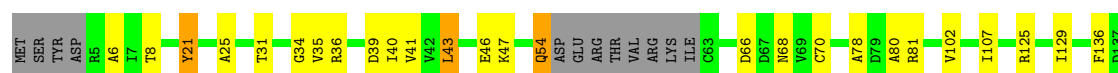
• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-7

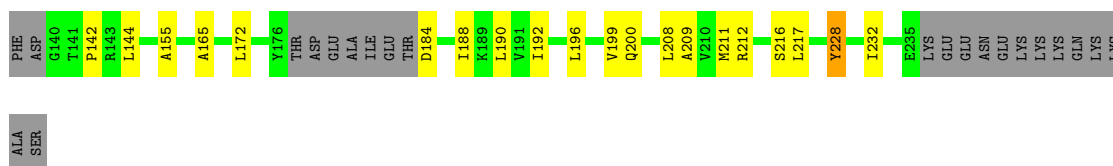
Chain D: 68% 17% 14%



• Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE-7

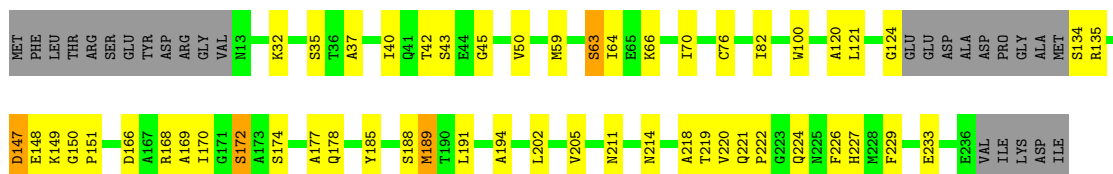
Chain R: 68% 17% 14%





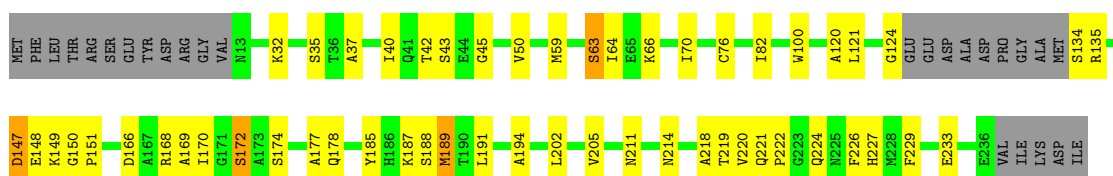
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-5

Chain E: 67% 20% 11%



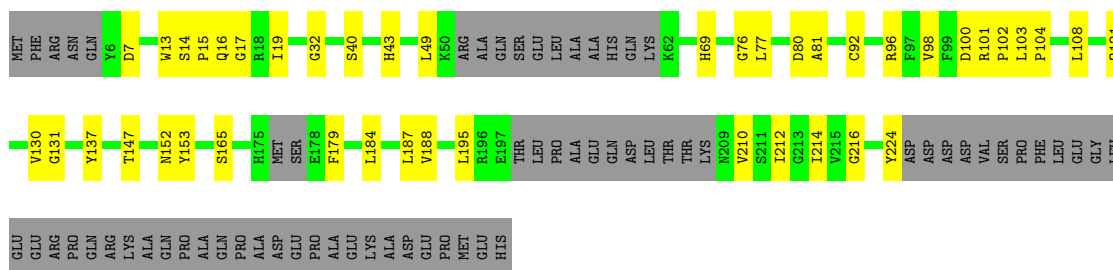
• Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE-5

Chain S: 67% 21% 11%



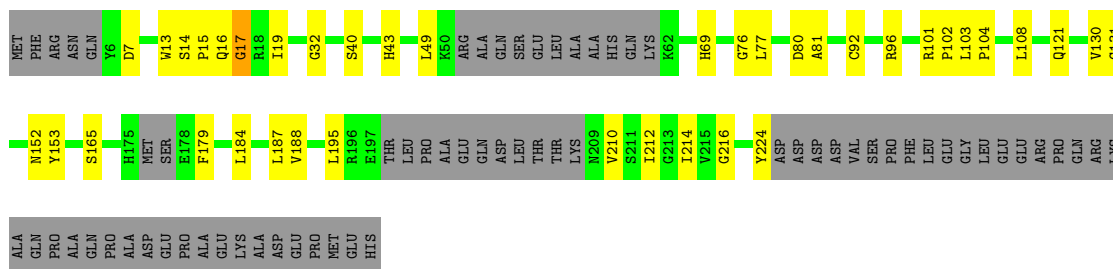
• Molecule 6: PROTEASOME SUBUNIT ALPHA TYPE-1

Chain F: 58% 16% 26%

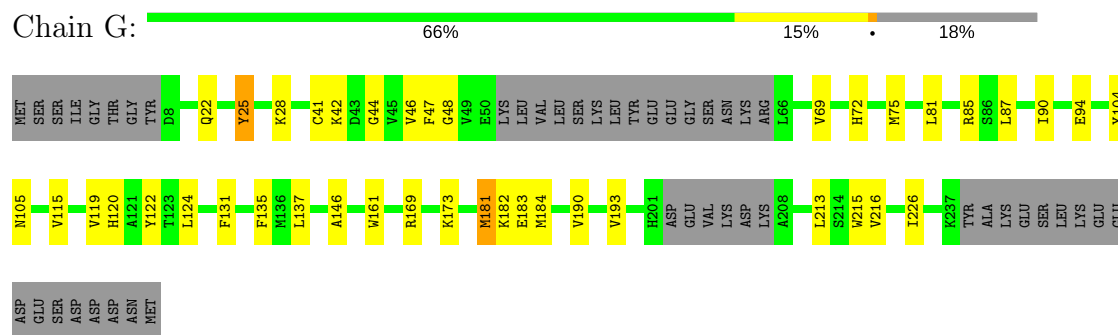


• Molecule 6: PROTEASOME SUBUNIT ALPHA TYPE-1

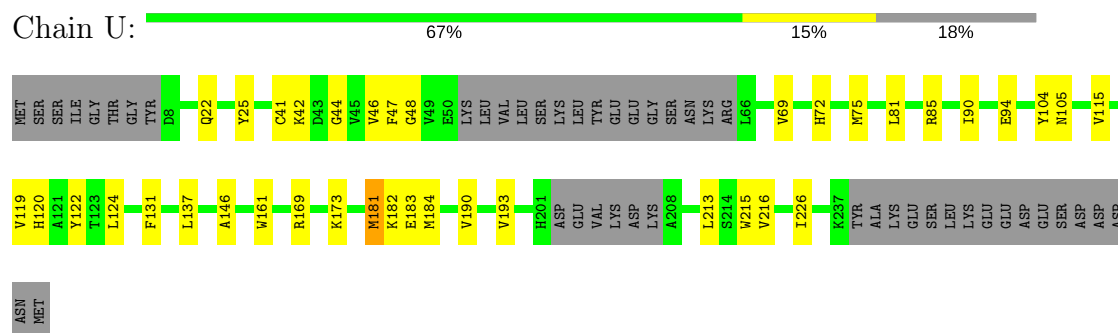
Chain T: 59% 14% 26%



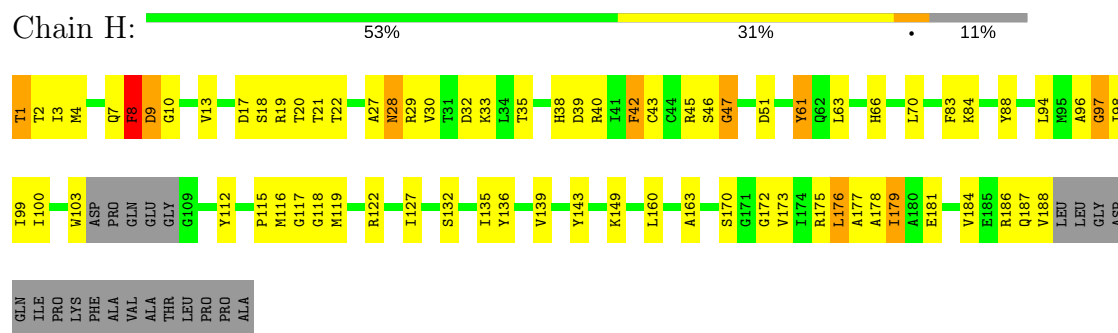
• Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-3



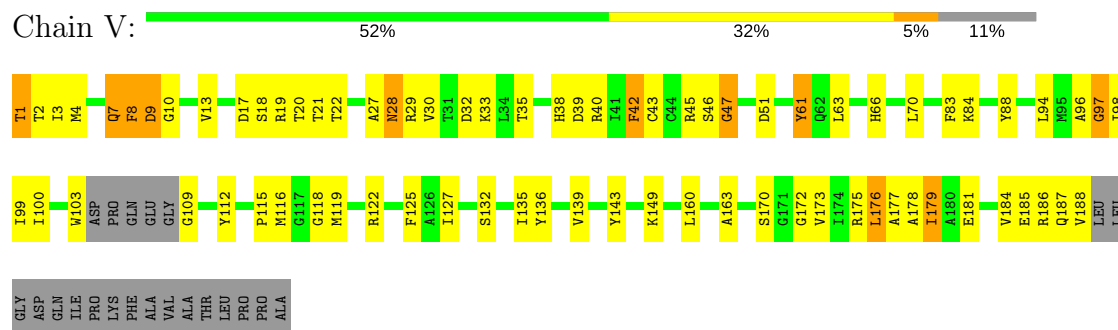
• Molecule 7: PROTEASOME SUBUNIT ALPHA TYPE-3



• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-6

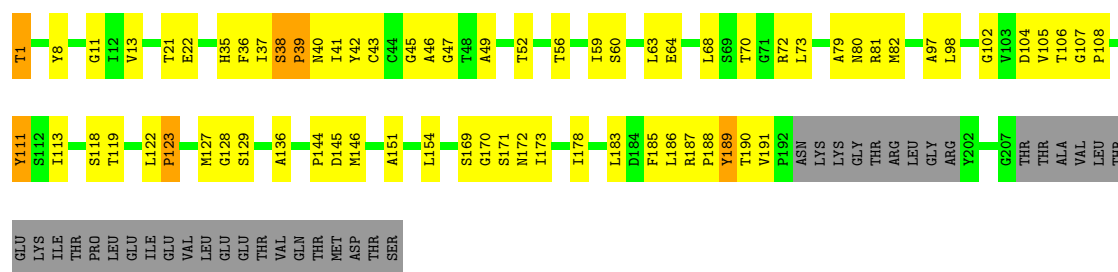


• Molecule 8: PROTEASOME SUBUNIT BETA TYPE-6



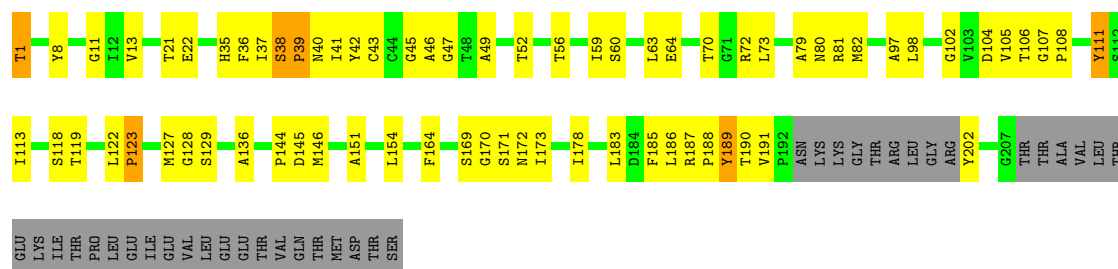
• Molecule 9: PROTEASOME SUBUNIT BETA TYPE-7





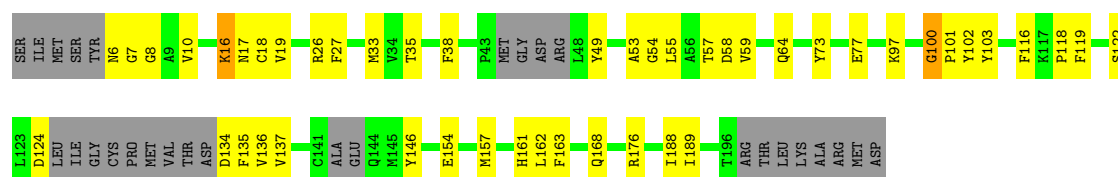
• Molecule 9: PROTEASOME SUBUNIT BETA TYPE-7

Chain W: 54% 28% 15%



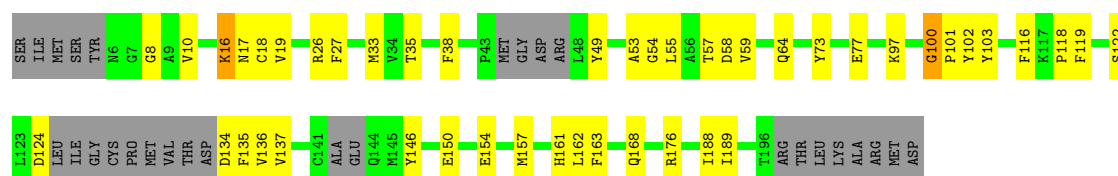
• Molecule 10: PROTEASOME SUBUNIT BETA TYPE-3

Chain J: 63% 22% 14%



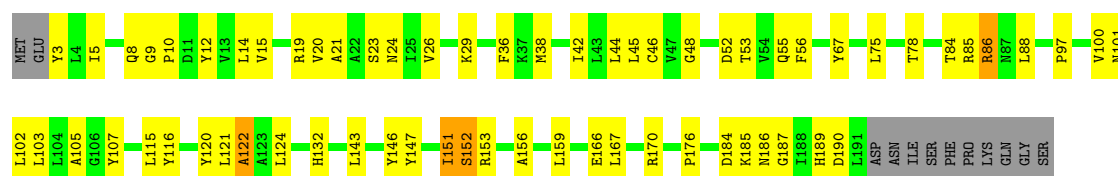
• Molecule 10: PROTEASOME SUBUNIT BETA TYPE-3

Chain X: 64% 22% 14%



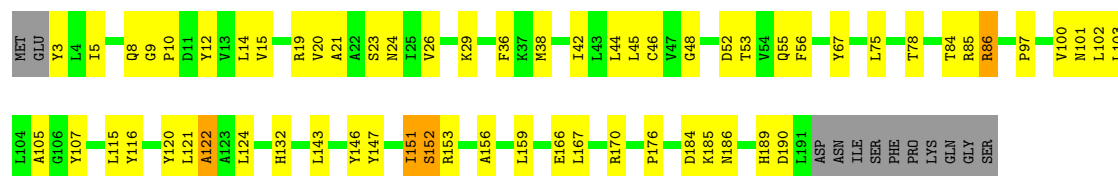
• Molecule 11: PROTEASOME SUBUNIT BETA TYPE-2

Chain K: 62% 30% 6%



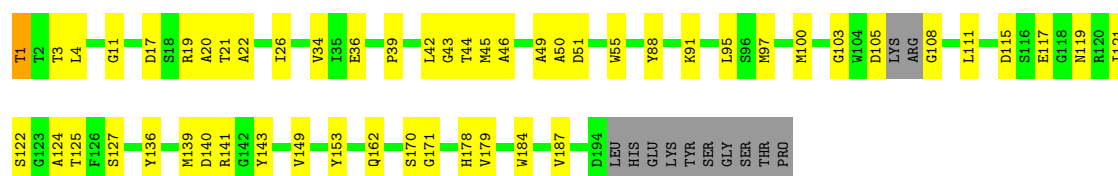
• Molecule 11: PROTEASOME SUBUNIT BETA TYPE-2

Chain Y: 



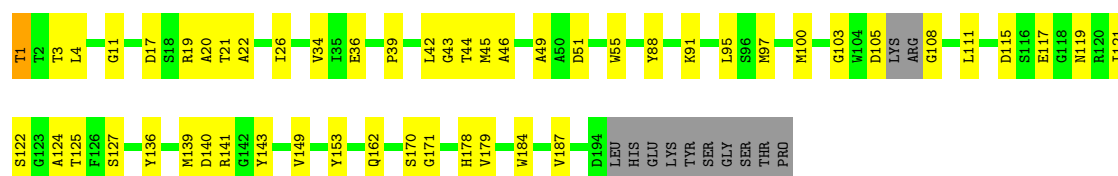
• Molecule 12: PROTEASOME SUBUNIT BETA TYPE-5

Chain L: 



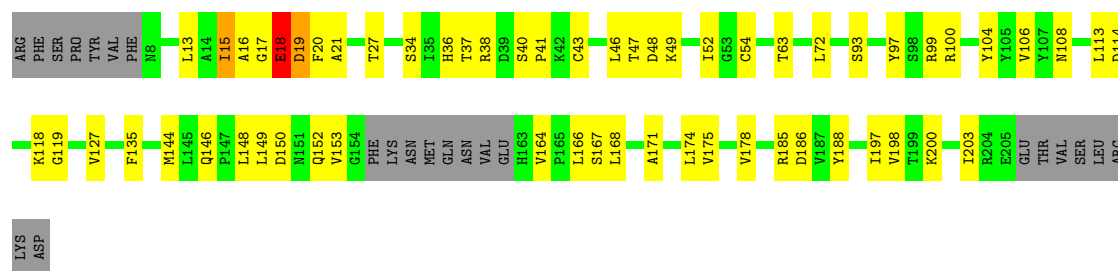
• Molecule 12: PROTEASOME SUBUNIT BETA TYPE-5

Chain Z: 




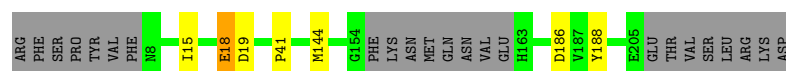
• Molecule 13: PROTEASOME SUBUNIT BETA TYPE-1

Chain M: 



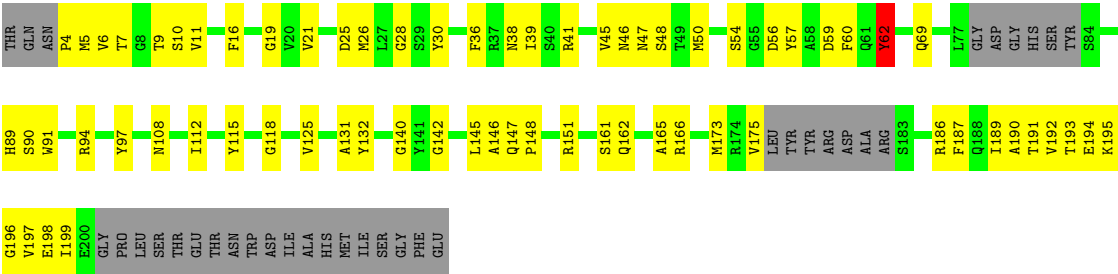
• Molecule 13: PROTEASOME SUBUNIT BETA TYPE-1

Chain a: 

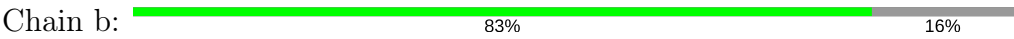


• Molecule 14: PROTEASOME SUBUNIT BETA TYPE-4

Chain N: 



● Molecule 14: PROTEASOME SUBUNIT BETA TYPE-4



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	76500	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	FULL RECORDED IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	4.8	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	134461	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: KNM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.95	0/1537	1.10	5/2073 (0.2%)
1	O	0.95	0/1537	1.10	5/2073 (0.2%)
10	J	0.92	1/1398 (0.1%)	1.07	3/1884 (0.2%)
10	X	0.92	1/1398 (0.1%)	1.07	3/1884 (0.2%)
11	K	0.87	0/1543	1.06	4/2088 (0.2%)
11	Y	0.87	0/1543	1.06	4/2088 (0.2%)
12	L	1.06	2/1508 (0.1%)	1.13	3/2038 (0.1%)
12	Z	1.06	2/1508 (0.1%)	1.13	3/2038 (0.1%)
13	M	0.91	0/1477	1.11	3/1990 (0.2%)
13	a	0.91	0/1477	1.11	3/1990 (0.2%)
14	N	0.91	1/1451 (0.1%)	1.08	2/1957 (0.1%)
14	b	0.91	1/1451 (0.1%)	1.08	2/1957 (0.1%)
2	B	0.90	0/1707	1.05	5/2312 (0.2%)
2	P	0.90	0/1707	1.05	5/2312 (0.2%)
3	C	0.94	3/1887 (0.2%)	1.07	7/2542 (0.3%)
3	Q	0.94	3/1887 (0.2%)	1.07	7/2542 (0.3%)
4	D	1.00	1/1695 (0.1%)	1.09	2/2283 (0.1%)
4	R	1.00	1/1695 (0.1%)	1.09	2/2283 (0.1%)
5	E	0.82	0/1668	1.02	4/2252 (0.2%)
5	S	0.82	0/1668	1.02	4/2252 (0.2%)
6	F	0.99	0/1562	1.12	6/2105 (0.3%)
6	T	1.00	0/1562	1.19	7/2105 (0.3%)
7	G	0.97	0/1656	1.12	2/2232 (0.1%)
7	U	0.97	0/1656	1.12	2/2232 (0.1%)
8	H	1.05	1/1394 (0.1%)	1.16	7/1884 (0.4%)
8	V	1.04	1/1394 (0.1%)	1.16	7/1884 (0.4%)
9	I	0.96	2/1515 (0.1%)	1.14	4/2050 (0.2%)
9	W	0.96	2/1515 (0.1%)	1.14	4/2050 (0.2%)
All	All	0.95	22/43996 (0.1%)	1.10	115/59380 (0.2%)

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
1	A	0	1
1	O	0	1
10	J	0	1
10	X	0	1
11	K	0	1
11	Y	0	1
13	M	0	2
13	a	0	2
5	E	0	1
5	S	0	1
7	G	0	1
7	U	0	1
9	I	0	2
9	W	0	2
All	All	0	18

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	1	THR	C-N	19.41	1.78	1.34
8	V	1	THR	C-N	19.41	1.78	1.34
9	I	123	PRO	N-CD	-7.63	1.37	1.47
9	W	123	PRO	N-CD	-7.63	1.37	1.47
12	L	1	THR	C-N	6.47	1.49	1.34
12	Z	1	THR	C-N	6.47	1.49	1.34
12	L	162	GLN	CD-OE1	6.09	1.37	1.24
12	Z	162	GLN	CD-OE1	6.09	1.37	1.24
4	D	54	GLN	CD-OE1	5.87	1.36	1.24
4	R	54	GLN	CD-OE1	5.85	1.36	1.24
10	J	168	GLN	CD-OE1	5.83	1.36	1.24
10	X	168	GLN	CD-OE1	5.83	1.36	1.24
3	C	20	GLN	CD-OE1	5.82	1.36	1.24
14	b	69	GLN	CD-OE1	5.82	1.36	1.24
3	Q	20	GLN	CD-OE1	5.80	1.36	1.24
14	N	69	GLN	CD-OE1	5.80	1.36	1.24
3	C	95	GLN	CD-OE1	5.71	1.36	1.24
3	Q	95	GLN	CD-OE1	5.71	1.36	1.24
3	Q	152	PRO	N-CD	5.12	1.55	1.47
3	C	152	PRO	N-CD	5.11	1.55	1.47
9	I	39	PRO	N-CD	5.10	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	39	PRO	N-CD	5.10	1.54	1.47

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	17	GLY	N-CA-C	15.39	151.57	113.10
8	H	47	GLY	N-CA-C	-9.29	89.87	113.10
8	V	47	GLY	N-CA-C	-9.29	89.87	113.10
11	Y	38	MET	CG-SD-CE	-8.17	87.13	100.20
11	K	38	MET	CG-SD-CE	-8.15	87.16	100.20
3	Q	153	SER	N-CA-C	-8.05	89.26	111.00
3	C	153	SER	N-CA-C	-8.04	89.28	111.00
2	B	120	TYR	CB-CG-CD2	-7.78	116.33	121.00
2	P	120	TYR	CB-CG-CD2	-7.78	116.33	121.00
7	G	25	TYR	CB-CG-CD2	-7.67	116.40	121.00
7	U	25	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	A	27	TYR	CB-CG-CD2	-7.65	116.41	121.00
1	O	27	TYR	CB-CG-CD2	-7.59	116.44	121.00
11	K	152	SER	N-CA-CB	7.55	121.83	110.50
11	Y	152	SER	N-CA-CB	7.55	121.83	110.50
1	A	27	TYR	CB-CG-CD1	7.50	125.50	121.00
1	O	27	TYR	CB-CG-CD1	7.50	125.50	121.00
9	I	119	THR	N-CA-C	-7.29	91.32	111.00
9	W	119	THR	N-CA-C	-7.29	91.32	111.00
2	B	120	TYR	CB-CG-CD1	7.24	125.34	121.00
2	P	120	TYR	CB-CG-CD1	7.24	125.34	121.00
12	L	1	THR	O-C-N	-7.23	111.12	122.70
12	Z	1	THR	O-C-N	-7.23	111.12	122.70
8	H	8	PHE	N-CA-C	7.23	130.51	111.00
2	P	23	TYR	CB-CG-CD2	-6.97	116.81	121.00
8	V	179	ILE	N-CA-C	-6.96	92.21	111.00
6	F	224	TYR	CB-CG-CD2	-6.95	116.83	121.00
6	T	224	TYR	CB-CG-CD2	-6.95	116.83	121.00
8	H	179	ILE	N-CA-C	-6.95	92.23	111.00
2	B	23	TYR	CB-CG-CD2	-6.90	116.86	121.00
5	E	59	MET	CG-SD-CE	-6.86	89.23	100.20
5	S	59	MET	CG-SD-CE	-6.86	89.23	100.20
9	I	119	THR	N-CA-CB	6.80	123.22	110.30
9	W	119	THR	N-CA-CB	6.80	123.22	110.30
8	V	7	GLN	CB-CA-C	-6.79	96.81	110.40
14	N	62	TYR	CB-CG-CD2	-6.78	116.93	121.00
14	b	62	TYR	CB-CG-CD2	-6.78	116.93	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	54	GLY	N-CA-C	-6.75	96.22	113.10
10	J	54	GLY	N-CA-C	-6.74	96.24	113.10
6	F	224	TYR	CB-CG-CD1	6.69	125.02	121.00
6	T	224	TYR	CB-CG-CD1	6.69	125.02	121.00
6	T	179	PHE	CB-CG-CD1	6.66	125.46	120.80
8	V	97	GLY	N-CA-C	-6.65	96.47	113.10
8	H	97	GLY	N-CA-C	-6.64	96.51	113.10
6	F	179	PHE	CB-CG-CD1	6.61	125.43	120.80
4	D	21	TYR	CB-CG-CD2	-6.52	117.09	121.00
4	R	21	TYR	CB-CG-CD2	-6.52	117.09	121.00
5	E	124	GLY	N-CA-C	-6.51	96.83	113.10
5	S	124	GLY	N-CA-C	-6.51	96.83	113.10
2	B	23	TYR	CB-CG-CD1	6.39	124.83	121.00
2	P	23	TYR	CB-CG-CD1	6.38	124.83	121.00
12	L	1	THR	C-N-CA	6.16	137.10	121.70
12	Z	1	THR	C-N-CA	6.16	137.10	121.70
8	H	61	TYR	CB-CG-CD2	-6.12	117.33	121.00
8	V	61	TYR	CB-CG-CD2	-6.12	117.33	121.00
14	N	62	TYR	CB-CG-CD1	6.11	124.67	121.00
14	b	62	TYR	CB-CG-CD1	6.11	124.67	121.00
9	W	189	TYR	N-CA-C	6.09	127.43	111.00
9	I	189	TYR	N-CA-C	6.08	127.42	111.00
10	J	100	GLY	C-N-CD	6.02	141.04	128.40
10	X	100	GLY	C-N-CD	5.99	140.97	128.40
12	Z	139	MET	CG-SD-CE	-5.91	90.75	100.20
12	L	139	MET	CG-SD-CE	-5.90	90.77	100.20
3	C	23	TYR	CB-CG-CD1	5.89	124.53	121.00
3	Q	23	TYR	CB-CG-CD1	5.89	124.53	121.00
7	G	25	TYR	CB-CG-CD1	5.86	124.52	121.00
7	U	25	TYR	CB-CG-CD1	5.86	124.52	121.00
9	I	38	SER	C-N-CD	5.79	140.57	128.40
9	W	38	SER	C-N-CD	5.79	140.57	128.40
3	C	151	ASP	C-N-CD	5.72	140.41	128.40
3	Q	151	ASP	C-N-CD	5.71	140.40	128.40
8	H	61	TYR	CB-CG-CD1	5.68	124.41	121.00
8	V	61	TYR	CB-CG-CD1	5.68	124.41	121.00
4	D	21	TYR	CB-CG-CD1	5.63	124.38	121.00
4	R	21	TYR	CB-CG-CD1	5.63	124.38	121.00
11	K	107	TYR	CB-CG-CD2	-5.57	117.66	121.00
11	Y	107	TYR	CB-CG-CD2	-5.54	117.68	121.00
6	T	179	PHE	CB-CG-CD2	-5.51	116.94	120.80
5	E	172	SER	N-CA-C	5.51	125.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	172	SER	N-CA-C	5.49	125.81	111.00
8	V	42	PHE	CB-CG-CD1	5.47	124.63	120.80
6	F	179	PHE	CB-CG-CD2	-5.47	116.97	120.80
8	H	42	PHE	CB-CG-CD1	5.44	124.61	120.80
10	X	8	GLY	N-CA-C	-5.44	99.50	113.10
10	J	8	GLY	N-CA-C	-5.44	99.51	113.10
3	C	201	MET	CG-SD-CE	-5.43	91.50	100.20
3	Q	201	MET	CG-SD-CE	-5.43	91.50	100.20
1	O	29	PHE	CB-CG-CD2	-5.40	117.02	120.80
1	A	29	PHE	CB-CG-CD2	-5.37	117.04	120.80
13	M	186	ASP	N-CA-C	-5.36	96.54	111.00
13	a	186	ASP	N-CA-C	-5.36	96.54	111.00
2	P	142	ARG	C-N-CD	-5.33	108.87	120.60
2	B	142	ARG	C-N-CD	-5.33	108.87	120.60
11	K	107	TYR	CB-CG-CD1	5.33	124.19	121.00
11	Y	107	TYR	CB-CG-CD1	5.33	124.19	121.00
3	C	23	TYR	CB-CG-CD2	-5.32	117.81	121.00
3	Q	23	TYR	CB-CG-CD2	-5.32	117.81	121.00
3	C	174	MET	CG-SD-CE	-5.30	91.72	100.20
3	Q	174	MET	CG-SD-CE	-5.29	91.75	100.20
13	M	19	ASP	CB-CG-OD2	5.22	123.00	118.30
13	a	19	ASP	CB-CG-OD2	5.22	123.00	118.30
6	F	131	GLY	N-CA-C	-5.19	100.13	113.10
6	T	131	GLY	N-CA-C	-5.19	100.13	113.10
3	Q	155	ASN	N-CA-C	-5.18	97.00	111.00
3	C	155	ASN	N-CA-C	-5.18	97.02	111.00
1	A	125	TYR	CB-CG-CD1	5.15	124.09	121.00
1	O	125	TYR	CB-CG-CD1	5.14	124.08	121.00
1	A	125	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	O	125	TYR	CB-CG-CD2	-5.12	117.93	121.00
6	F	165	SER	CB-CA-C	-5.09	100.44	110.10
6	T	165	SER	CB-CA-C	-5.09	100.44	110.10
13	M	144	MET	CG-SD-CE	-5.03	92.15	100.20
13	a	144	MET	CG-SD-CE	-5.03	92.16	100.20
5	E	64	ILE	N-CA-C	-5.00	97.50	111.00
5	S	64	ILE	N-CA-C	-5.00	97.50	111.00

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	E	147	ASP	Peptide
7	G	181	MET	Peptide
9	I	1	THR	Mainchain
9	I	111	TYR	Sidechain
10	J	16	LYS	Peptide
11	K	153	ARG	Sidechain
13	M	18	GLU	Peptide
13	M	188	TYR	Sidechain
1	O	95	ARG	Sidechain
5	S	147	ASP	Peptide
7	U	181	MET	Peptide
9	W	1	THR	Mainchain
9	W	111	TYR	Sidechain
10	X	16	LYS	Peptide
11	Y	153	ARG	Sidechain
13	a	18	GLU	Peptide
13	a	188	TYR	Sidechain

## 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	1514	0	1527	73	0
1	O	1514	0	1527	74	0
2	B	1671	0	1681	153	0
2	P	1671	0	1681	151	0
3	C	1860	0	1886	84	0
3	Q	1860	0	1886	86	0
4	D	1674	0	1712	67	0
4	R	1674	0	1712	68	0
5	E	1643	0	1636	93	0
5	S	1643	0	1636	94	0
6	F	1535	0	1540	73	0
6	T	1535	0	1540	68	0
7	G	1626	0	1602	96	0
7	U	1626	0	1602	93	0
8	H	1372	0	1338	141	0
8	V	1372	0	1338	118	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1490	0	1490	142	0
9	W	1490	0	1490	164	0
10	J	1374	0	1383	74	0
10	X	1374	0	1383	86	0
11	K	1512	0	1520	121	0
11	Y	1512	0	1520	117	0
12	L	1480	0	1441	106	0
12	Z	1480	0	1441	96	0
13	M	1453	0	1455	163	0
13	a	1453	0	1455	0	0
14	N	1428	0	1432	188	0
14	b	1428	0	1432	0	0
15	H	31	0	39	33	0
15	I	30	0	39	45	0
15	L	31	0	39	30	0
15	V	31	0	39	31	0
15	W	30	0	39	43	0
15	Z	31	0	39	29	0
All	All	43448	0	43520	2537	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 33.

All (2537) 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)
13:M:152:GLN:HG3	9:W:202:TYR:CD2	1.31	1.63
1:A:109:ILE:CG2	1:A:114:LEU:HD21	1.26	1.62
14:N:26:MET:CE	14:N:186:ARG:HH12	1.10	1.60
1:O:109:ILE:CG2	1:O:114:LEU:HD21	1.26	1.57
14:N:16:PHE:CE1	14:N:166:ARG:N	1.74	1.56
8:H:119:MET:CE	14:N:57:TYR:CD2	1.91	1.52
8:H:119:MET:HE3	14:N:57:TYR:CD2	1.44	1.52
1:O:109:ILE:HG21	1:O:114:LEU:CD2	1.40	1.50
1:A:109:ILE:HG21	1:A:114:LEU:CD2	1.40	1.49
1:O:109:ILE:HD13	1:O:114:LEU:CD2	1.46	1.46
1:A:103:TYR:CA	9:I:81:ARG:NH2	1.78	1.45
13:M:99:ARG:HD3	13:M:104:TYR:CZ	1.51	1.44
14:N:16:PHE:CZ	14:N:166:ARG:N	1.83	1.43
1:O:103:TYR:CA	9:W:81:ARG:NH2	1.78	1.43
1:O:109:ILE:CD1	1:O:114:LEU:HD23	1.47	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HD13	1:A:114:LEU:CD2	1.46	1.42
1:A:109:ILE:CD1	1:A:114:LEU:HD23	1.47	1.41
14:N:26:MET:HE2	14:N:186:ARG:NH1	1.13	1.40
10:J:157:MET:HG2	10:J:161:HIS:CD2	1.58	1.38
13:M:18:GLU:N	13:M:166:LEU:HD13	1.36	1.37
8:H:1:THR:C	8:H:2:THR:N	1.78	1.37
10:X:157:MET:HG2	10:X:161:HIS:CD2	1.58	1.36
12:L:50:ALA:HB1	13:M:97:TYR:OH	1.21	1.36
14:N:16:PHE:CE2	14:N:21:VAL:HB	1.61	1.36
13:M:152:GLN:CG	9:W:202:TYR:CD2	2.05	1.36
1:O:103:TYR:HA	9:W:81:ARG:NH2	1.05	1.36
8:H:20:THR:HG22	15:H:300:KNM:C20	1.56	1.35
10:X:157:MET:CG	10:X:161:HIS:HD2	1.37	1.35
4:R:192:ILE:HG13	4:R:228:TYR:CD1	1.61	1.35
8:V:20:THR:HG22	15:V:300:KNM:C20	1.56	1.35
1:A:103:TYR:HA	9:I:81:ARG:NH2	1.05	1.35
8:H:119:MET:CE	14:N:57:TYR:HB3	1.57	1.35
7:U:75:MET:HB2	7:U:137:LEU:CD2	1.56	1.35
13:M:152:GLN:CG	9:W:202:TYR:HD2	1.39	1.34
4:D:192:ILE:HG13	4:D:228:TYR:CD1	1.61	1.34
10:J:157:MET:CG	10:J:161:HIS:HD2	1.37	1.34
8:V:1:THR:C	8:V:2:THR:N	1.78	1.34
5:E:42:THR:CG2	5:E:194:ALA:CB	2.06	1.33
7:G:75:MET:HB2	7:G:137:LEU:CD2	1.56	1.33
5:S:42:THR:CG2	5:S:194:ALA:CB	2.06	1.33
11:K:23:SER:C	11:K:24:ASN:OD1	1.67	1.32
11:Y:23:SER:C	11:Y:24:ASN:OD1	1.67	1.31
7:G:190:VAL:HG11	7:G:215:TRP:CZ2	1.65	1.31
5:S:229:PHE:CZ	5:S:233:GLU:HG2	1.63	1.31
12:L:140:ASP:OD2	11:Y:170:ARG:HD3	1.26	1.31
5:E:229:PHE:CZ	5:E:233:GLU:HG2	1.63	1.31
7:G:190:VAL:CG1	7:G:215:TRP:HZ2	1.44	1.30
7:U:190:VAL:HG11	7:U:215:TRP:CZ2	1.65	1.30
7:U:190:VAL:CG1	7:U:215:TRP:HZ2	1.44	1.29
14:N:4:PRO:CB	14:N:56:ASP:OD2	1.80	1.29
4:D:184:ASP:O	4:D:188:ILE:HD12	1.29	1.27
4:R:184:ASP:O	4:R:188:ILE:HD12	1.29	1.27
6:T:184:LEU:HD11	6:T:214:ILE:CD1	1.65	1.27
11:K:170:ARG:HD3	12:Z:140:ASP:OD2	1.26	1.26
13:M:99:ARG:HD3	13:M:104:TYR:CE2	1.68	1.26
2:B:138:TRP:NE1	2:B:143:PRO:HD3	1.49	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:17:GLY:HA3	13:M:166:LEU:CD2	1.66	1.26
2:P:138:TRP:NE1	2:P:143:PRO:HD3	1.49	1.25
11:K:23:SER:O	11:K:24:ASN:CG	1.72	1.25
9:W:36:PHE:CE1	9:W:38:SER:C	2.10	1.25
5:E:229:PHE:CE2	5:E:233:GLU:CG	2.19	1.24
5:S:229:PHE:CE2	5:S:233:GLU:CG	2.19	1.24
9:I:36:PHE:CE1	9:I:38:SER:C	2.10	1.24
12:L:50:ALA:CB	13:M:97:TYR:OH	1.84	1.24
6:F:184:LEU:HD11	6:F:214:ILE:CD1	1.65	1.24
6:T:184:LEU:CD1	6:T:214:ILE:HD12	1.68	1.24
11:Y:23:SER:O	11:Y:24:ASN:CG	1.72	1.24
4:R:184:ASP:O	4:R:188:ILE:CD1	1.86	1.23
6:F:184:LEU:CD1	6:F:214:ILE:HD12	1.68	1.22
7:G:190:VAL:HB	7:G:215:TRP:NE1	1.53	1.22
8:H:47:GLY:O	15:H:300:KNM:H24	1.37	1.22
9:I:36:PHE:HE1	9:I:39:PRO:N	1.37	1.22
4:D:184:ASP:O	4:D:188:ILE:CD1	1.86	1.22
14:N:16:PHE:CZ	14:N:165:ALA:C	2.12	1.22
10:X:137:VAL:HG23	10:X:146:TYR:CZ	1.74	1.22
14:N:16:PHE:HE2	14:N:21:VAL:CB	1.53	1.21
1:O:76:ILE:CD1	1:O:114:LEU:HD11	1.71	1.21
10:J:137:VAL:HG23	10:J:146:TYR:CE2	1.75	1.21
5:S:229:PHE:CE2	5:S:233:GLU:HG2	1.75	1.21
12:Z:55:TRP:HZ2	12:Z:95:LEU:CD1	1.53	1.21
10:J:64:GLN:NE2	11:K:85:ARG:HH22	1.38	1.21
8:V:47:GLY:O	15:V:300:KNM:H24	1.37	1.21
10:X:64:GLN:NE2	11:Y:85:ARG:HH22	1.38	1.21
10:X:137:VAL:HG23	10:X:146:TYR:CE2	1.75	1.20
7:U:190:VAL:HB	7:U:215:TRP:NE1	1.53	1.20
9:W:36:PHE:HE1	9:W:39:PRO:N	1.37	1.20
1:A:76:ILE:CD1	1:A:114:LEU:HD11	1.71	1.20
13:M:48:ASP:O	13:M:203:ILE:HG13	1.41	1.20
10:X:64:GLN:NE2	11:Y:85:ARG:NH2	1.88	1.20
7:G:75:MET:CB	7:G:137:LEU:CD2	2.20	1.19
5:E:229:PHE:CE2	5:E:233:GLU:HG2	1.75	1.19
12:L:55:TRP:HZ2	12:L:95:LEU:CD1	1.53	1.19
10:J:137:VAL:HG23	10:J:146:TYR:CZ	1.74	1.19
10:J:64:GLN:NE2	11:K:85:ARG:NH2	1.88	1.19
5:S:166:ASP:CB	5:S:185:TYR:OH	1.91	1.18
9:W:47:GLY:H	15:W:300:KNM:C16	1.56	1.18
13:M:174:LEU:HD13	9:W:202:TYR:CE2	1.78	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:75:MET:CB	7:U:137:LEU:CD2	2.20	1.18
5:E:166:ASP:HB3	5:E:185:TYR:OH	1.02	1.18
8:H:119:MET:CE	14:N:57:TYR:CB	2.22	1.18
5:S:166:ASP:HB3	5:S:185:TYR:OH	1.02	1.17
5:E:166:ASP:CB	5:E:185:TYR:OH	1.91	1.17
11:K:170:ARG:NH2	12:Z:136:TYR:CD1	2.13	1.17
4:R:40:ILE:HG21	4:R:211:MET:O	1.45	1.17
8:H:119:MET:CE	14:N:57:TYR:CG	2.28	1.16
12:L:136:TYR:CD1	11:Y:170:ARG:NH2	2.13	1.16
2:B:41:ASN:HB2	2:B:183:LEU:HB2	1.28	1.16
3:C:207:SER:H	3:C:210:LYS:HD2	1.00	1.16
9:I:47:GLY:H	15:I:300:KNM:C16	1.56	1.16
8:H:88:TYR:OH	14:N:62:TYR:CB	1.93	1.15
12:L:26:ILE:HD12	10:X:176:ARG:O	1.44	1.15
4:R:40:ILE:CG2	4:R:211:MET:O	1.95	1.15
10:X:157:MET:SD	10:X:161:HIS:CD2	2.40	1.15
8:H:88:TYR:CZ	14:N:62:TYR:HB2	1.82	1.15
5:S:224:GLN:NE2	5:S:227:HIS:ND1	1.94	1.14
4:D:40:ILE:CG2	4:D:211:MET:O	1.95	1.14
14:N:50:MET:CE	14:N:192:VAL:HG23	1.77	1.14
5:E:166:ASP:HB3	5:E:185:TYR:CZ	1.82	1.14
10:J:157:MET:SD	10:J:161:HIS:CD2	2.40	1.14
14:N:26:MET:HB2	14:N:186:ARG:NH2	1.63	1.14
8:H:119:MET:HE3	14:N:57:TYR:CG	1.82	1.14
5:S:166:ASP:HB3	5:S:185:TYR:CZ	1.81	1.14
12:Z:55:TRP:HZ2	12:Z:95:LEU:HD13	0.98	1.13
14:N:50:MET:HE2	14:N:192:VAL:HG23	1.22	1.13
10:J:176:ARG:O	12:Z:26:ILE:HD12	1.43	1.13
5:E:224:GLN:NE2	5:E:227:HIS:ND1	1.94	1.13
14:N:26:MET:CE	14:N:186:ARG:NH1	1.81	1.13
1:O:76:ILE:HD13	1:O:114:LEU:CD1	1.78	1.13
1:A:76:ILE:HD13	1:A:114:LEU:CD1	1.78	1.12
4:D:40:ILE:HG21	4:D:211:MET:O	1.45	1.12
2:P:62:HIS:CE1	2:P:219:ARG:NH1	2.18	1.12
2:B:62:HIS:CE1	2:B:219:ARG:NH1	2.18	1.12
9:W:36:PHE:HE1	9:W:38:SER:C	1.49	1.11
13:M:17:GLY:HA3	13:M:166:LEU:HD22	1.19	1.11
5:E:42:THR:HG21	5:E:194:ALA:CB	1.81	1.11
5:E:42:THR:CG2	5:E:194:ALA:HB2	1.79	1.11
12:L:55:TRP:HZ2	12:L:95:LEU:HD13	0.98	1.10
5:S:229:PHE:HE2	5:S:233:GLU:CB	1.65	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:190:VAL:HG21	7:U:215:TRP:CZ2	1.86	1.10
2:P:73:LEU:HD22	2:P:133:LEU:HD13	1.10	1.10
12:L:55:TRP:CZ2	12:L:95:LEU:HD13	1.86	1.10
8:H:119:MET:CE	14:N:57:TYR:HD2	1.43	1.10
11:K:170:ARG:NH2	12:Z:136:TYR:CE1	2.20	1.10
7:G:190:VAL:HG21	7:G:215:TRP:CZ2	1.86	1.10
12:Z:55:TRP:CZ2	12:Z:95:LEU:HD13	1.86	1.10
7:U:190:VAL:CG1	7:U:215:TRP:CZ2	2.31	1.10
9:W:70:THR:HG23	9:W:72:ARG:H	1.16	1.10
6:F:184:LEU:HD21	6:F:214:ILE:HG21	1.34	1.09
8:H:20:THR:HG22	15:H:300:KNM:H36	1.12	1.09
7:G:75:MET:HB2	7:G:137:LEU:HD21	1.26	1.09
9:W:1:THR:HG21	15:W:300:KNM:H41	1.21	1.09
12:L:136:TYR:CE1	11:Y:170:ARG:NH2	2.20	1.09
9:I:1:THR:HG23	9:I:129:SER:H	1.05	1.09
8:H:119:MET:HE1	14:N:57:TYR:CB	1.79	1.09
3:Q:207:SER:H	3:Q:210:LYS:HD2	1.00	1.09
9:I:36:PHE:HE1	9:I:38:SER:C	1.49	1.09
14:N:6:VAL:HG22	14:N:30:TYR:HB2	1.24	1.09
2:P:41:ASN:HB2	2:P:183:LEU:HB2	1.28	1.09
5:S:42:THR:CG2	5:S:194:ALA:HB2	1.79	1.09
7:U:190:VAL:CB	7:U:215:TRP:CZ2	2.36	1.09
5:E:229:PHE:HE2	5:E:233:GLU:CB	1.65	1.09
14:N:91:TRP:CE3	14:N:94:ARG:HB2	1.88	1.09
4:D:211:MET:HB2	4:D:217:LEU:HD13	1.35	1.09
4:R:40:ILE:HG23	4:R:136:PHE:HZ	1.14	1.09
9:I:1:THR:HG21	15:I:300:KNM:H41	1.27	1.09
6:T:184:LEU:HD21	6:T:214:ILE:HG21	1.34	1.09
9:W:1:THR:HG23	9:W:129:SER:H	1.05	1.08
9:I:70:THR:HG23	9:I:72:ARG:H	1.16	1.08
13:M:99:ARG:CD	13:M:104:TYR:CZ	2.35	1.08
4:R:211:MET:HB2	4:R:217:LEU:HD13	1.35	1.08
7:U:75:MET:HB2	7:U:137:LEU:HD21	1.26	1.08
2:B:181:LEU:HD21	2:B:185:ASP:O	1.52	1.08
7:G:190:VAL:CB	7:G:215:TRP:CZ2	2.36	1.08
8:H:119:MET:HE2	14:N:57:TYR:CD2	1.84	1.08
13:M:16:ALA:HB1	13:M:119:GLY:HA3	1.22	1.08
2:P:181:LEU:HD21	2:P:185:ASP:O	1.52	1.08
9:W:1:THR:CG2	9:W:129:SER:H	1.65	1.08
13:M:100:ARG:NH1	13:M:127:VAL:HB	1.68	1.07
5:S:42:THR:HG22	5:S:194:ALA:HB2	1.36	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:THR:HG22	5:E:194:ALA:HB2	1.36	1.07
2:B:73:LEU:HD22	2:B:133:LEU:HD13	1.10	1.07
9:I:1:THR:CG2	9:I:129:SER:H	1.65	1.07
14:N:48:SER:HA	14:N:197:VAL:HG23	1.36	1.07
7:U:190:VAL:HG11	7:U:215:TRP:HZ2	0.90	1.07
14:N:91:TRP:CZ3	14:N:94:ARG:CB	2.38	1.06
12:L:50:ALA:C	13:M:97:TYR:OH	1.94	1.06
13:M:146:GLN:HB3	10:X:176:ARG:HH22	1.16	1.06
5:S:42:THR:HG21	5:S:194:ALA:CB	1.81	1.06
14:N:4:PRO:HB3	14:N:56:ASP:OD2	1.51	1.06
8:H:32:ASP:OD2	8:H:186:ARG:NH2	1.89	1.06
5:S:229:PHE:HE2	5:S:233:GLU:CG	1.61	1.06
6:F:100:ASP:OD1	14:N:90:SER:OG	1.72	1.05
5:S:42:THR:HG21	5:S:194:ALA:HB3	1.36	1.05
7:G:190:VAL:HB	7:G:215:TRP:CE2	1.91	1.05
7:U:190:VAL:HB	7:U:215:TRP:CE2	1.91	1.05
8:V:32:ASP:OD2	8:V:186:ARG:NH2	1.89	1.05
5:E:224:GLN:HE22	5:E:227:HIS:CE1	1.75	1.05
11:K:55:GLN:HG3	12:L:88:TYR:CD2	1.89	1.05
11:Y:55:GLN:HG3	12:Z:88:TYR:CD2	1.89	1.05
11:K:8:GLN:OE1	11:K:115:LEU:HD23	1.57	1.05
12:L:19:ARG:HB2	12:L:171:GLY:O	1.55	1.05
7:G:190:VAL:HB	7:G:215:TRP:HE1	1.11	1.05
13:M:15:ILE:HG22	13:M:135:PHE:HB3	1.34	1.05
5:E:229:PHE:HE2	5:E:233:GLU:CG	1.61	1.05
8:H:88:TYR:OH	14:N:62:TYR:HB2	1.51	1.04
1:A:109:ILE:CG2	1:A:114:LEU:CD2	2.14	1.04
1:A:103:TYR:C	9:I:81:ARG:NH2	2.11	1.04
10:J:157:MET:CG	10:J:161:HIS:CD2	2.23	1.04
2:P:140:GLU:HG2	2:P:141:GLY:H	1.22	1.04
7:G:72:HIS:CG	7:G:105:ASN:HD21	1.75	1.04
8:V:20:THR:HG22	15:V:300:KNM:H36	1.12	1.04
11:Y:85:ARG:NH2	11:Y:86:ARG:HH22	1.55	1.04
2:B:140:GLU:HG2	2:B:141:GLY:H	1.22	1.03
3:C:76:VAL:HG11	3:C:83:ALA:HB1	1.38	1.03
14:N:6:VAL:HG22	14:N:30:TYR:CB	1.88	1.03
5:S:224:GLN:HE22	5:S:227:HIS:CE1	1.75	1.03
8:V:7:GLN:O	8:V:8:PHE:HD1	1.40	1.03
11:K:85:ARG:NH2	11:K:86:ARG:HH22	1.55	1.03
14:N:16:PHE:CZ	14:N:166:ARG:CA	2.41	1.03
12:Z:19:ARG:HB2	12:Z:171:GLY:O	1.55	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:LYS:HB3	3:C:240:HIS:HD2	1.24	1.03
4:D:40:ILE:HG23	4:D:136:PHE:HZ	1.14	1.03
6:F:103:LEU:HD23	6:F:104:PRO:O	1.58	1.03
7:U:72:HIS:CG	7:U:105:ASN:HD21	1.75	1.03
11:Y:8:GLN:OE1	11:Y:115:LEU:HD23	1.57	1.03
3:C:24:ALA:O	3:C:28:ILE:CD1	2.07	1.03
3:Q:24:ALA:O	3:Q:28:ILE:CD1	2.07	1.03
6:T:103:LEU:HD23	6:T:104:PRO:O	1.58	1.03
8:V:1:THR:CB	15:V:300:KNM:O5	2.07	1.03
11:Y:55:GLN:HG3	12:Z:88:TYR:CE2	1.94	1.03
5:E:229:PHE:CE2	5:E:233:GLU:HB3	1.94	1.02
7:G:75:MET:HA	7:G:137:LEU:HD23	1.41	1.02
14:N:91:TRP:CZ3	14:N:94:ARG:HB2	1.93	1.02
5:E:218:ALA:HB1	5:E:226:PHE:CE1	1.95	1.02
1:O:103:TYR:C	9:W:81:ARG:NH2	2.11	1.02
3:Q:205:LYS:HB3	3:Q:240:HIS:HD2	1.24	1.02
5:S:229:PHE:HE2	5:S:233:GLU:HB3	1.22	1.02
11:K:55:GLN:HG3	12:L:88:TYR:CE2	1.94	1.02
8:V:20:THR:CG2	15:V:300:KNM:H36	1.89	1.02
8:H:119:MET:HE1	14:N:57:TYR:HB3	1.30	1.02
13:M:174:LEU:HB2	9:W:202:TYR:OH	1.57	1.02
12:Z:39:PRO:O	12:Z:184:TRP:CD1	2.13	1.02
7:G:94:GLU:OE1	7:G:115:VAL:CG2	2.08	1.02
12:L:39:PRO:O	12:L:184:TRP:CD1	2.13	1.02
8:H:20:THR:CG2	15:H:300:KNM:H36	1.89	1.01
8:H:1:THR:CB	15:H:300:KNM:O5	2.07	1.01
1:O:165:ALA:HB3	2:P:55:LEU:CD2	1.91	1.01
5:S:229:PHE:CE2	5:S:233:GLU:HB3	1.94	1.01
12:Z:45:MET:SD	15:Z:300:KNM:C20	2.49	1.01
9:I:1:THR:HG21	15:I:300:KNM:C22	1.90	1.01
7:U:75:MET:HA	7:U:137:LEU:HD23	1.41	1.01
5:E:42:THR:HG21	5:E:194:ALA:HB3	1.36	1.01
12:L:50:ALA:HB1	13:M:97:TYR:CZ	1.95	1.01
7:U:75:MET:CB	7:U:137:LEU:HD23	1.89	1.01
7:U:94:GLU:OE1	7:U:115:VAL:CG2	2.08	1.01
9:W:1:THR:HG21	15:W:300:KNM:C22	1.90	1.01
2:P:62:HIS:CE1	2:P:219:ARG:HH12	1.78	1.00
2:B:62:HIS:CE1	2:B:219:ARG:HH12	1.78	1.00
12:L:45:MET:SD	15:L:300:KNM:C20	2.49	1.00
14:N:16:PHE:CE1	14:N:165:ALA:C	2.28	1.00
3:C:205:LYS:HB3	3:C:240:HIS:CD2	1.96	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:229:PHE:CZ	5:E:233:GLU:CG	2.39	1.00
7:G:190:VAL:HG11	7:G:215:TRP:HZ2	0.90	1.00
3:Q:76:VAL:HG11	3:Q:83:ALA:HB1	1.38	1.00
13:M:18:GLU:H	13:M:166:LEU:HD13	0.89	1.00
14:N:59:ASP:C	14:N:108:ASN:HD21	1.65	1.00
5:S:218:ALA:HB1	5:S:226:PHE:CE1	1.95	1.00
7:G:190:VAL:CB	7:G:215:TRP:HZ2	1.74	1.00
14:N:46:ASN:O	14:N:48:SER:N	1.93	1.00
1:O:165:ALA:O	1:O:179:LEU:HD13	1.62	1.00
7:G:161:TRP:O	7:G:181:MET:CE	2.10	0.99
7:G:75:MET:CB	7:G:137:LEU:HD23	1.89	0.99
3:Q:205:LYS:HB3	3:Q:240:HIS:CD2	1.96	0.99
1:A:165:ALA:HB3	2:B:55:LEU:CD2	1.91	0.99
7:U:161:TRP:O	7:U:181:MET:HE1	1.62	0.99
7:U:161:TRP:O	7:U:181:MET:CE	2.10	0.99
8:V:4:MET:HB3	8:V:160:LEU:HD21	1.42	0.99
2:P:157:TRP:CE3	2:P:159:ALA:O	2.15	0.99
8:H:17:ASP:OD2	8:H:170:SER:HB2	1.63	0.99
11:K:56:PHE:HZ	11:K:84:THR:HG1	1.11	0.99
2:P:73:LEU:HD22	2:P:133:LEU:CD1	1.93	0.99
1:O:76:ILE:CD1	1:O:114:LEU:CD1	2.38	0.99
2:B:157:TRP:CE3	2:B:159:ALA:O	2.15	0.98
14:N:26:MET:SD	14:N:186:ARG:NH1	2.36	0.98
11:Y:85:ARG:NH2	11:Y:86:ARG:NH2	2.11	0.98
13:M:20:PHE:HD2	13:M:168:LEU:HD12	1.27	0.98
2:B:73:LEU:HD22	2:B:133:LEU:CD1	1.93	0.98
11:K:85:ARG:NH2	11:K:86:ARG:NH2	2.11	0.98
12:Z:55:TRP:CZ2	12:Z:95:LEU:CD1	2.43	0.98
7:G:190:VAL:CG2	7:G:215:TRP:CZ2	2.46	0.98
7:G:75:MET:CA	7:G:137:LEU:HD23	1.94	0.98
7:U:190:VAL:CG2	7:U:215:TRP:CZ2	2.46	0.98
1:A:165:ALA:O	1:A:179:LEU:HD13	1.62	0.98
2:B:68:THR:HG22	2:B:71:ILE:HB	1.46	0.98
9:I:36:PHE:CE1	9:I:39:PRO:N	2.29	0.98
7:G:72:HIS:HB2	7:G:105:ASN:HD21	1.29	0.97
7:G:94:GLU:OE1	7:G:115:VAL:HG22	1.63	0.97
8:H:4:MET:HB3	8:H:160:LEU:HD21	1.42	0.97
2:P:73:LEU:CD2	2:P:133:LEU:HD13	1.93	0.97
7:U:190:VAL:HB	7:U:215:TRP:HE1	1.11	0.97
5:E:229:PHE:HE2	5:E:233:GLU:HB3	1.22	0.97
2:P:181:LEU:HD23	2:P:186:ALA:HA	1.46	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:7:GLN:NE2	8:V:109:GLY:O	1.97	0.97
12:L:55:TRP:CZ2	12:L:95:LEU:CD1	2.43	0.97
13:M:174:LEU:HD22	9:W:202:TYR:OH	1.65	0.97
8:V:17:ASP:OD2	8:V:170:SER:HB2	1.63	0.97
9:I:47:GLY:H	15:I:300:KNM:H29	1.26	0.97
7:G:190:VAL:CG1	7:G:215:TRP:CZ2	2.31	0.97
14:N:16:PHE:HZ	14:N:166:ARG:N	1.54	0.97
7:U:94:GLU:OE1	7:U:115:VAL:HG22	1.63	0.97
7:U:72:HIS:HB2	7:U:105:ASN:HD21	1.29	0.97
2:B:181:LEU:HD23	2:B:186:ALA:HA	1.46	0.97
7:U:75:MET:CA	7:U:137:LEU:HD23	1.94	0.97
7:U:72:HIS:CB	7:U:105:ASN:HD21	1.78	0.97
12:Z:45:MET:CG	15:Z:300:KNM:H38	1.95	0.97
7:G:72:HIS:CB	7:G:105:ASN:HD21	1.78	0.96
12:L:50:ALA:CA	13:M:97:TYR:OH	2.11	0.96
10:X:157:MET:CG	10:X:161:HIS:CD2	2.24	0.96
2:B:73:LEU:CD2	2:B:133:LEU:HD13	1.93	0.96
12:L:45:MET:CG	15:L:300:KNM:H38	1.95	0.96
13:M:15:ILE:CG2	13:M:135:PHE:HB3	1.95	0.96
9:W:36:PHE:CE1	9:W:39:PRO:N	2.29	0.96
5:S:229:PHE:CZ	5:S:233:GLU:CG	2.39	0.96
14:N:16:PHE:CE1	14:N:165:ALA:HB3	2.01	0.96
9:W:47:GLY:H	15:W:300:KNM:H29	1.26	0.96
1:O:103:TYR:CA	9:W:81:ARG:HH21	1.59	0.96
2:B:38:LYS:HA	2:B:43:VAL:HG22	1.48	0.96
15:L:300:KNM:H21	15:L:300:KNM:C8	1.96	0.96
2:B:181:LEU:HD11	2:B:185:ASP:HB3	1.48	0.95
9:I:172:ASN:OD1	9:I:191:VAL:HA	1.66	0.95
2:P:38:LYS:HA	2:P:43:VAL:HG22	1.48	0.95
9:W:172:ASN:OD1	9:W:191:VAL:HA	1.66	0.95
12:L:140:ASP:OD2	11:Y:170:ARG:CD	2.15	0.95
8:V:1:THR:N	15:V:300:KNM:O5	1.99	0.95
13:M:99:ARG:CD	13:M:104:TYR:CE2	2.48	0.95
3:C:76:VAL:HG11	3:C:83:ALA:CB	1.97	0.95
2:P:181:LEU:HD11	2:P:185:ASP:HB3	1.48	0.95
2:B:51:GLN:CG	2:B:54:ILE:HA	1.97	0.95
3:Q:76:VAL:HG11	3:Q:83:ALA:CB	1.97	0.95
13:M:15:ILE:HD11	13:M:175:VAL:CG2	1.96	0.95
14:N:145:LEU:HD21	14:N:175:VAL:HG12	1.46	0.95
3:Q:198:ASN:OD1	3:Q:240:HIS:CE1	2.20	0.95
7:U:190:VAL:CB	7:U:215:TRP:HE1	1.79	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:ALA:O	3:C:28:ILE:HD12	1.64	0.95
2:P:51:GLN:CG	2:P:54:ILE:HA	1.97	0.94
11:K:170:ARG:CD	12:Z:140:ASP:OD2	2.15	0.94
8:H:1:THR:N	15:H:300:KNM:O5	1.99	0.94
1:A:76:ILE:CD1	1:A:114:LEU:CD1	2.38	0.94
2:B:137:GLY:O	2:B:144:TYR:N	2.00	0.94
11:Y:52:ASP:OD1	12:Z:88:TYR:OH	1.85	0.94
15:Z:300:KNM:C8	15:Z:300:KNM:H21	1.96	0.94
7:G:190:VAL:CB	7:G:215:TRP:HE1	1.79	0.94
8:H:88:TYR:CE2	14:N:62:TYR:HB2	2.01	0.94
7:U:190:VAL:CB	7:U:215:TRP:HZ2	1.74	0.94
2:P:157:TRP:HE3	2:P:159:ALA:O	1.49	0.94
4:R:192:ILE:CG1	4:R:228:TYR:CD1	2.50	0.94
2:P:133:LEU:CD1	2:P:135:ILE:HG12	1.98	0.94
2:P:68:THR:HG22	2:P:71:ILE:HB	1.46	0.94
3:C:198:ASN:OD1	3:C:240:HIS:CE1	2.20	0.94
14:N:59:ASP:CB	14:N:108:ASN:ND2	2.31	0.94
9:W:1:THR:N	9:W:169:SER:OG	2.01	0.94
1:A:76:ILE:HD13	1:A:114:LEU:HD12	1.50	0.94
4:D:192:ILE:CG1	4:D:228:TYR:CD1	2.50	0.94
1:A:103:TYR:C	9:I:81:ARG:HH21	1.71	0.94
13:M:152:GLN:HB3	9:W:202:TYR:CE2	2.03	0.94
1:A:161:CYS:SG	1:A:163:PHE:HE1	1.91	0.93
1:A:103:TYR:CA	9:I:81:ARG:HH21	1.59	0.93
2:B:133:LEU:CD1	2:B:135:ILE:HG12	1.98	0.93
8:V:7:GLN:O	8:V:8:PHE:CD1	2.21	0.93
10:J:16:LYS:O	10:J:18:CYS:N	2.01	0.93
11:K:52:ASP:OD1	12:L:88:TYR:OH	1.85	0.93
1:O:161:CYS:SG	1:O:163:PHE:HE1	1.91	0.93
13:M:146:GLN:HB3	10:X:176:ARG:NH2	1.83	0.93
9:I:1:THR:N	9:I:169:SER:OG	2.01	0.93
12:L:17:ASP:OD2	12:L:170:SER:HB3	1.69	0.93
10:X:16:LYS:O	10:X:18:CYS:N	2.01	0.93
12:Z:17:ASP:OD2	12:Z:170:SER:HB3	1.69	0.93
8:H:4:MET:CB	8:H:160:LEU:HD21	1.99	0.93
14:N:16:PHE:CE1	14:N:165:ALA:CA	2.52	0.93
8:H:119:MET:HE3	14:N:57:TYR:CB	1.92	0.93
1:O:109:ILE:CG2	1:O:114:LEU:CD2	2.14	0.93
3:Q:24:ALA:O	3:Q:28:ILE:HD12	1.64	0.93
2:P:137:GLY:O	2:P:144:TYR:N	2.00	0.93
13:M:152:GLN:CB	9:W:202:TYR:CE2	2.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:70:ILE:HD11	5:S:76:CYS:CB	1.99	0.92
12:L:45:MET:HG2	15:L:300:KNM:H38	1.50	0.92
2:B:157:TRP:HE3	2:B:159:ALA:O	1.48	0.92
9:I:104:ASP:O	9:I:107:GLY:N	2.03	0.92
4:D:40:ILE:HG23	4:D:136:PHE:CZ	2.04	0.92
5:E:166:ASP:HB3	5:E:185:TYR:HH	1.34	0.92
14:N:10:SER:OG	14:N:25:ASP:OD1	1.87	0.92
8:V:4:MET:CB	8:V:160:LEU:HD21	1.99	0.91
7:G:75:MET:CB	7:G:137:LEU:HD21	1.92	0.91
15:I:300:KNM:H12	10:J:124:ASP:OD1	1.71	0.91
11:K:44:LEU:HD23	11:K:102:LEU:CD1	2.01	0.91
14:N:91:TRP:CE3	14:N:94:ARG:CB	2.53	0.91
6:T:43:HIS:CG	6:T:184:LEU:HD22	2.06	0.91
4:D:36:ARG:HG3	4:D:142:PRO:HB2	1.53	0.91
5:E:70:ILE:HD11	5:E:76:CYS:CB	1.99	0.91
14:N:16:PHE:HE2	14:N:21:VAL:HB	0.76	0.91
1:A:76:ILE:HD12	1:A:114:LEU:HD11	1.52	0.91
7:G:190:VAL:CB	7:G:215:TRP:NE1	2.33	0.91
4:R:40:ILE:HG23	4:R:136:PHE:CZ	2.04	0.91
1:O:103:TYR:C	9:W:81:ARG:HH21	1.71	0.91
10:X:122:SER:HB3	10:X:136:VAL:HG11	1.52	0.91
2:B:138:TRP:NE1	2:B:143:PRO:CD	2.33	0.91
9:I:47:GLY:H	15:I:300:KNM:H28	1.35	0.91
13:M:106:VAL:HG12	13:M:108:ASN:OD1	1.70	0.91
11:Y:44:LEU:HD23	11:Y:102:LEU:CD1	2.01	0.91
11:Y:56:PHE:HZ	11:Y:84:THR:HG1	1.14	0.91
8:H:45:ARG:HE	15:H:300:KNM:C19	1.84	0.91
14:N:193:THR:O	14:N:196:GLY:N	2.04	0.91
1:O:76:ILE:HD12	1:O:114:LEU:HD11	1.52	0.90
15:W:300:KNM:H12	10:X:124:ASP:OD1	1.71	0.90
13:M:36:HIS:HB3	14:N:132:TYR:OH	1.70	0.90
14:N:48:SER:CA	14:N:197:VAL:HG23	2.01	0.90
3:C:207:SER:N	3:C:210:LYS:HD2	1.86	0.90
2:P:138:TRP:NE1	2:P:143:PRO:CD	2.33	0.90
10:J:137:VAL:CG2	10:J:146:TYR:CZ	2.54	0.90
9:W:104:ASP:O	9:W:107:GLY:N	2.03	0.90
6:F:43:HIS:CG	6:F:184:LEU:HD22	2.05	0.90
10:J:122:SER:HB3	10:J:136:VAL:HG11	1.52	0.90
14:N:21:VAL:CG2	14:N:191:THR:HG22	2.02	0.90
7:U:75:MET:CB	7:U:137:LEU:HD21	1.92	0.90
14:N:6:VAL:HG22	14:N:30:TYR:CG	2.07	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:137:VAL:CG2	10:X:146:TYR:CZ	2.54	0.90
7:G:161:TRP:O	7:G:181:MET:HE1	1.67	0.89
8:V:115:PRO:HD2	8:V:119:MET:O	1.71	0.89
1:O:76:ILE:HD13	1:O:114:LEU:HD12	1.50	0.89
5:E:229:PHE:CE2	5:E:233:GLU:CB	2.47	0.89
4:R:36:ARG:HG3	4:R:142:PRO:HB2	1.53	0.89
13:M:20:PHE:CD2	13:M:168:LEU:HD12	2.07	0.89
10:J:137:VAL:CG2	10:J:146:TYR:CE1	2.55	0.89
8:V:1:THR:OG1	15:V:300:KNM:O5	1.88	0.89
9:W:47:GLY:N	15:W:300:KNM:H28	1.88	0.89
10:X:137:VAL:CG2	10:X:146:TYR:CE1	2.55	0.89
13:M:18:GLU:N	13:M:166:LEU:CD1	2.31	0.89
8:H:115:PRO:HD2	8:H:119:MET:O	1.71	0.89
14:N:9:THR:HG22	14:N:10:SER:H	1.38	0.89
9:W:47:GLY:N	15:W:300:KNM:C16	2.35	0.89
3:C:76:VAL:HG13	3:C:134:LEU:HD21	1.55	0.89
14:N:4:PRO:HB2	14:N:56:ASP:OD2	1.71	0.89
7:U:190:VAL:CB	7:U:215:TRP:NE1	2.33	0.89
8:V:45:ARG:HE	15:V:300:KNM:C19	1.84	0.89
9:W:47:GLY:H	15:W:300:KNM:H28	1.35	0.89
9:I:47:GLY:N	15:I:300:KNM:C16	2.35	0.88
9:I:1:THR:HG23	9:I:129:SER:N	1.87	0.88
14:N:6:VAL:CG2	14:N:30:TYR:HB2	2.03	0.88
5:S:35:SER:HB2	5:S:66:LYS:NZ	1.88	0.88
4:R:192:ILE:HG13	4:R:228:TYR:HD1	1.04	0.88
3:Q:207:SER:N	3:Q:210:LYS:HD2	1.86	0.88
9:W:1:THR:HG23	9:W:129:SER:N	1.87	0.88
5:E:35:SER:HB2	5:E:66:LYS:NZ	1.88	0.88
7:G:72:HIS:CG	7:G:105:ASN:ND2	2.42	0.88
14:N:25:ASP:O	14:N:41:ARG:NH1	2.07	0.88
5:S:229:PHE:CE2	5:S:233:GLU:CB	2.47	0.88
3:Q:76:VAL:HG13	3:Q:134:LEU:HD21	1.55	0.88
12:Z:45:MET:HG2	15:Z:300:KNM:H38	1.51	0.88
13:M:18:GLU:H	13:M:166:LEU:CD1	1.82	0.88
11:K:151:ILE:HG13	11:K:152:SER:H	1.40	0.87
9:I:59:ILE:HG22	9:I:63:LEU:HD13	1.57	0.87
11:K:78:THR:HG22	11:K:116:TYR:OH	1.74	0.87
13:M:49:LYS:HB3	13:M:113:LEU:H	1.40	0.87
4:D:192:ILE:HG13	4:D:228:TYR:HD1	1.04	0.87
9:I:47:GLY:N	15:I:300:KNM:H28	1.88	0.87
13:M:17:GLY:CA	13:M:166:LEU:HD22	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:GLY:O	3:C:159:TRP:HD1	1.56	0.87
14:N:26:MET:HE2	14:N:186:ARG:CZ	2.04	0.87
7:U:190:VAL:CB	7:U:215:TRP:CE2	2.56	0.87
10:J:134:ASP:OD1	10:J:135:PHE:N	2.07	0.87
14:N:9:THR:O	14:N:10:SER:OG	1.93	0.87
11:Y:46:CYS:HB2	11:Y:102:LEU:HD12	1.55	0.87
11:K:85:ARG:HH22	11:K:86:ARG:HH22	1.18	0.87
12:L:45:MET:SD	15:L:300:KNM:H36	2.14	0.87
7:U:72:HIS:CG	7:U:105:ASN:ND2	2.42	0.87
14:N:16:PHE:CD1	14:N:165:ALA:HB3	2.10	0.86
9:W:59:ILE:HG22	9:W:63:LEU:HD13	1.56	0.86
6:F:13:TRP:CD1	7:G:22:GLN:NE2	2.43	0.86
11:K:46:CYS:HB2	11:K:102:LEU:HD12	1.55	0.86
11:Y:151:ILE:HG13	11:Y:152:SER:H	1.40	0.86
1:A:103:TYR:O	9:I:81:ARG:NH2	2.08	0.86
1:O:103:TYR:O	9:W:81:ARG:NH2	2.08	0.86
9:W:1:THR:HG22	9:W:129:SER:HB2	1.57	0.86
9:I:1:THR:HG22	9:I:129:SER:CB	2.06	0.86
14:N:16:PHE:HE1	14:N:166:ARG:N	1.34	0.86
9:W:1:THR:HG22	9:W:129:SER:CB	2.06	0.86
10:J:137:VAL:HG22	10:J:146:TYR:CE1	2.11	0.86
2:B:140:GLU:CG	2:B:141:GLY:H	1.89	0.86
11:Y:78:THR:HG22	11:Y:116:TYR:OH	1.74	0.86
10:X:134:ASP:OD1	10:X:135:PHE:N	2.07	0.86
1:A:13:ILE:O	1:A:15:ILE:HG12	1.75	0.86
11:K:44:LEU:HB3	11:K:102:LEU:HD11	1.57	0.86
6:T:13:TRP:CD1	7:U:22:GLN:NE2	2.43	0.86
8:V:98:ILE:CG2	8:V:100:ILE:HG13	2.05	0.86
13:M:100:ARG:HH11	13:M:127:VAL:HB	1.40	0.86
2:P:140:GLU:OE2	2:P:144:TYR:OH	1.94	0.86
3:Q:157:GLY:O	3:Q:159:TRP:HD1	1.56	0.86
11:K:44:LEU:HG	11:K:102:LEU:HD21	1.57	0.85
8:V:20:THR:CG2	15:V:300:KNM:C20	2.49	0.85
12:Z:45:MET:SD	15:Z:300:KNM:H36	2.14	0.85
8:H:20:THR:CG2	15:H:300:KNM:C20	2.49	0.85
8:H:1:THR:OG1	15:H:300:KNM:O5	1.88	0.85
9:I:1:THR:HG22	9:I:129:SER:HB2	1.57	0.85
12:Z:45:MET:SD	15:Z:300:KNM:H38	2.15	0.85
15:L:300:KNM:H29	15:L:300:KNM:H18	1.59	0.85
7:U:181:MET:O	7:U:184:MET:N	2.09	0.85
10:X:137:VAL:HG22	10:X:146:TYR:CE1	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:44:LEU:HB3	11:Y:102:LEU:HD11	1.57	0.85
7:G:190:VAL:CB	7:G:215:TRP:CE2	2.56	0.85
1:O:13:ILE:O	1:O:15:ILE:HG12	1.76	0.85
7:G:181:MET:O	7:G:184:MET:N	2.09	0.85
2:P:216:GLY:O	2:P:218:ARG:HG3	1.77	0.85
13:M:174:LEU:CD1	9:W:202:TYR:CE2	2.59	0.85
2:P:140:GLU:CG	2:P:141:GLY:H	1.89	0.85
2:P:39:ALA:HB2	2:P:186:ALA:CB	2.07	0.85
2:P:51:GLN:HG3	2:P:54:ILE:HA	1.59	0.85
13:M:16:ALA:CB	13:M:119:GLY:HA3	2.07	0.84
9:W:1:THR:CG2	15:W:300:KNM:H41	2.06	0.84
14:N:91:TRP:CE3	14:N:94:ARG:HG3	2.11	0.84
8:H:98:ILE:CG2	8:H:100:ILE:HG13	2.05	0.84
15:I:300:KNM:H13	15:I:300:KNM:C1	2.08	0.84
8:V:45:ARG:NE	15:V:300:KNM:H33	1.92	0.84
15:Z:300:KNM:H18	15:Z:300:KNM:H29	1.59	0.84
8:H:17:ASP:OD2	8:H:170:SER:CB	2.24	0.84
2:B:181:LEU:CD2	2:B:185:ASP:O	2.25	0.84
14:N:91:TRP:CE3	14:N:94:ARG:CG	2.60	0.84
8:V:17:ASP:OD2	8:V:170:SER:CB	2.24	0.84
12:Z:149:VAL:O	12:Z:153:TYR:CD1	2.31	0.84
4:D:184:ASP:O	4:D:188:ILE:HD13	1.75	0.84
5:S:42:THR:HG23	5:S:194:ALA:CB	2.08	0.84
11:Y:85:ARG:HH22	11:Y:86:ARG:HH22	1.18	0.84
2:B:140:GLU:OE2	2:B:144:TYR:OH	1.94	0.84
8:H:22:THR:HB	15:H:300:KNM:H13	1.58	0.84
8:H:45:ARG:HE	15:H:300:KNM:H33	1.41	0.84
10:J:64:GLN:HE21	11:K:85:ARG:NH2	1.75	0.84
14:N:16:PHE:HZ	14:N:166:ARG:CA	1.87	0.84
9:I:36:PHE:CE1	9:I:38:SER:CA	2.61	0.84
8:H:47:GLY:O	15:H:300:KNM:C13	2.25	0.84
8:H:119:MET:HE3	14:N:57:TYR:HB3	1.49	0.84
8:V:9:ASP:OD2	8:V:149:LYS:HB2	1.78	0.84
9:W:36:PHE:CE1	9:W:38:SER:CA	2.61	0.84
1:A:161:CYS:SG	1:A:163:PHE:CE1	2.69	0.84
12:L:45:MET:SD	15:L:300:KNM:H38	2.15	0.84
4:R:184:ASP:O	4:R:188:ILE:HD13	1.75	0.84
11:Y:44:LEU:HG	11:Y:102:LEU:HD21	1.57	0.84
2:B:39:ALA:HB2	2:B:186:ALA:CB	2.07	0.83
2:B:216:GLY:O	2:B:218:ARG:HG3	1.77	0.83
9:I:129:SER:OG	15:I:300:KNM:C22	2.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ALA:HB3	2:B:55:LEU:HD23	1.59	0.83
12:L:149:VAL:O	12:L:153:TYR:CD1	2.31	0.83
8:V:22:THR:HB	15:V:300:KNM:H13	1.58	0.83
10:X:157:MET:HG2	10:X:161:HIS:HD2	0.67	0.83
9:W:129:SER:OG	15:W:300:KNM:C22	2.26	0.83
2:B:138:TRP:CE2	2:B:143:PRO:HD3	2.14	0.83
3:C:205:LYS:HA	3:C:240:HIS:NE2	1.94	0.83
5:E:42:THR:HG23	5:E:194:ALA:CB	2.07	0.83
6:F:13:TRP:HB2	7:G:22:GLN:NE2	1.94	0.83
8:V:45:ARG:HE	15:V:300:KNM:H33	1.41	0.83
15:W:300:KNM:H12	10:X:124:ASP:CG	1.99	0.83
15:W:300:KNM:H13	15:W:300:KNM:C1	2.08	0.83
6:T:13:TRP:HB2	7:U:22:GLN:NE2	1.94	0.83
1:A:161:CYS:HG	1:A:163:PHE:HE1	1.19	0.82
8:H:45:ARG:NE	15:H:300:KNM:H33	1.92	0.82
8:V:10:GLY:O	8:V:103:TRP:NE1	2.12	0.82
14:N:16:PHE:CE1	14:N:165:ALA:CB	2.62	0.82
14:N:26:MET:HB2	14:N:186:ARG:CZ	2.08	0.82
8:V:47:GLY:O	15:V:300:KNM:C13	2.25	0.82
2:B:51:GLN:HG3	2:B:54:ILE:HA	1.59	0.82
1:O:161:CYS:SG	1:O:163:PHE:CE1	2.69	0.82
2:P:138:TRP:CE2	2:P:143:PRO:HD3	2.14	0.82
3:Q:205:LYS:HA	3:Q:240:HIS:NE2	1.94	0.82
5:S:218:ALA:HB1	5:S:226:PHE:CZ	2.14	0.82
10:J:157:MET:HG2	10:J:161:HIS:HD2	0.67	0.82
14:N:59:ASP:CB	14:N:108:ASN:HD21	1.91	0.82
2:P:181:LEU:CD2	2:P:185:ASP:O	2.25	0.82
15:I:300:KNM:H12	10:J:124:ASP:CG	1.99	0.82
4:D:36:ARG:CG	4:D:142:PRO:HB2	2.10	0.82
6:F:49:LEU:HB2	6:F:195:LEU:HD11	1.62	0.82
11:Y:44:LEU:HD23	11:Y:102:LEU:HD13	1.61	0.82
8:H:88:TYR:OH	14:N:62:TYR:CD2	2.32	0.82
13:M:152:GLN:HG3	9:W:202:TYR:CE2	2.11	0.82
2:P:183:LEU:HD13	2:P:213:ASN:OD1	1.80	0.82
1:O:165:ALA:HB3	2:P:55:LEU:HD23	1.59	0.82
10:X:64:GLN:HE21	11:Y:85:ARG:NH2	1.75	0.82
2:B:172:PHE:CE2	2:B:196:GLU:CD	2.54	0.82
1:A:103:TYR:O	9:I:81:ARG:NE	2.13	0.81
8:H:119:MET:HE1	14:N:57:TYR:CG	2.10	0.81
4:R:36:ARG:CG	4:R:142:PRO:HB2	2.10	0.81
12:L:50:ALA:O	13:M:97:TYR:OH	1.90	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:122:LEU:HG	9:I:123:PRO:HD2	1.61	0.81
6:T:49:LEU:HB2	6:T:195:LEU:HD11	1.62	0.81
6:T:77:LEU:CD1	6:T:80:ASP:H	1.93	0.81
2:P:181:LEU:HD21	2:P:185:ASP:C	2.01	0.81
5:S:147:ASP:O	5:S:150:GLY:N	2.12	0.81
5:E:218:ALA:HB1	5:E:226:PHE:CZ	2.14	0.81
2:P:172:PHE:CE2	2:P:196:GLU:CD	2.54	0.81
4:R:192:ILE:HG13	4:R:228:TYR:CE1	2.16	0.81
2:B:183:LEU:HD13	2:B:213:ASN:OD1	1.80	0.81
8:H:10:GLY:O	8:H:103:TRP:NE1	2.14	0.81
6:F:77:LEU:CD1	6:F:80:ASP:H	1.93	0.81
2:P:39:ALA:HB1	2:P:181:LEU:O	1.81	0.81
7:G:75:MET:CG	7:G:137:LEU:HD21	2.11	0.81
1:O:103:TYR:O	9:W:81:ARG:NE	2.13	0.81
5:E:147:ASP:O	5:E:150:GLY:N	2.12	0.80
8:H:9:ASP:OD2	8:H:149:LYS:HB2	1.79	0.80
5:S:42:THR:CG2	5:S:194:ALA:HB1	2.11	0.80
9:W:129:SER:OG	15:W:300:KNM:H41	1.80	0.80
9:W:70:THR:HG23	9:W:72:ARG:N	1.96	0.80
9:I:70:THR:HG23	9:I:72:ARG:N	1.96	0.80
9:W:122:LEU:HG	9:W:123:PRO:HD2	1.61	0.80
2:B:51:GLN:O	2:B:51:GLN:NE2	2.14	0.80
4:D:192:ILE:HG13	4:D:228:TYR:CE1	2.15	0.80
14:N:59:ASP:HB3	14:N:108:ASN:ND2	1.96	0.80
2:B:181:LEU:HD21	2:B:185:ASP:C	2.01	0.80
8:H:115:PRO:HG3	14:N:36:PHE:HZ	1.44	0.80
10:J:26:ARG:HD2	10:J:33:MET:HG3	1.64	0.80
14:N:21:VAL:HG23	14:N:191:THR:HG22	1.63	0.80
14:N:91:TRP:HE3	14:N:94:ARG:CG	1.95	0.80
12:Z:42:LEU:HD11	12:Z:184:TRP:CD2	2.16	0.80
11:K:44:LEU:HD23	11:K:102:LEU:HD13	1.61	0.80
11:K:67:TYR:CE1	11:K:75:LEU:HG	2.17	0.80
12:L:42:LEU:HD11	12:L:184:TRP:CD2	2.16	0.80
13:M:27:THR:HG22	13:M:40:SER:O	1.82	0.80
13:M:46:LEU:HD23	13:M:72:LEU:HD21	1.64	0.80
2:P:51:GLN:O	2:P:51:GLN:NE2	2.14	0.80
5:S:229:PHE:HZ	5:S:233:GLU:HG2	1.39	0.80
12:Z:105:ASP:HB2	12:Z:108:GLY:O	1.82	0.80
2:B:51:GLN:HE22	2:B:56:TYR:HB2	1.47	0.79
8:H:45:ARG:NE	15:H:300:KNM:C19	2.45	0.79
8:V:45:ARG:NE	15:V:300:KNM:C19	2.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:141:ARG:HB3	11:Y:146:TYR:OH	1.82	0.79
9:I:43:CYS:SG	9:I:98:LEU:HD22	2.22	0.79
1:A:103:TYR:HA	9:I:81:ARG:HH21	1.15	0.79
5:E:229:PHE:HZ	5:E:233:GLU:HG2	1.39	0.79
7:G:190:VAL:CG2	7:G:215:TRP:CE2	2.65	0.79
9:I:1:THR:HG21	9:I:129:SER:OG	1.83	0.79
11:K:146:TYR:OH	12:Z:141:ARG:HB3	1.82	0.79
13:M:36:HIS:HB3	14:N:132:TYR:CZ	2.17	0.79
7:U:75:MET:CG	7:U:137:LEU:HD21	2.11	0.79
11:Y:67:TYR:CE1	11:Y:75:LEU:HG	2.17	0.79
9:I:1:THR:CG2	15:I:300:KNM:H41	2.10	0.79
2:P:51:GLN:HE22	2:P:56:TYR:HB2	1.47	0.79
11:Y:46:CYS:SG	11:Y:100:VAL:HB	2.23	0.79
2:B:39:ALA:HB1	2:B:181:LEU:O	1.81	0.79
10:J:154:GLU:OE2	10:J:161:HIS:NE2	2.16	0.79
7:U:94:GLU:OE1	7:U:115:VAL:HG23	1.82	0.79
10:X:55:LEU:O	10:X:59:VAL:HG23	1.83	0.79
6:F:152:ASN:HA	7:G:85:ARG:HH12	1.48	0.79
5:S:70:ILE:HD11	5:S:76:CYS:HB3	1.64	0.79
6:T:152:ASN:HA	7:U:85:ARG:HH12	1.48	0.79
9:W:1:THR:HG21	9:W:129:SER:OG	1.83	0.79
5:S:166:ASP:HB3	5:S:185:TYR:HH	1.47	0.79
13:M:174:LEU:HD13	9:W:202:TYR:HE2	1.46	0.79
2:P:42:GLY:N	2:P:183:LEU:HD12	1.98	0.79
7:U:181:MET:O	7:U:183:GLU:N	2.16	0.79
10:X:26:ARG:HD2	10:X:33:MET:HG3	1.64	0.79
10:X:154:GLU:OE2	10:X:161:HIS:NE2	2.16	0.79
2:B:181:LEU:CD2	2:B:185:ASP:C	2.52	0.78
2:B:42:GLY:N	2:B:183:LEU:HD12	1.98	0.78
12:L:105:ASP:HB2	12:L:108:GLY:O	1.82	0.78
9:I:1:THR:CG2	9:I:129:SER:OG	2.31	0.78
14:N:115:TYR:OH	14:N:118:GLY:HA2	1.83	0.78
2:P:181:LEU:CD2	2:P:185:ASP:C	2.52	0.78
7:U:190:VAL:CG2	7:U:215:TRP:CE2	2.65	0.78
9:W:43:CYS:SG	9:W:98:LEU:HD22	2.22	0.78
9:W:1:THR:CG2	9:W:129:SER:OG	2.31	0.78
11:Y:55:GLN:CG	12:Z:88:TYR:CD2	2.66	0.78
12:L:19:ARG:CB	12:L:171:GLY:O	2.31	0.78
12:Z:36:GLU:HA	12:Z:42:LEU:HD22	1.66	0.78
11:K:46:CYS:SG	11:K:100:VAL:HB	2.23	0.78
10:X:137:VAL:HG23	10:X:146:TYR:CD2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:55:TRP:HD1	12:Z:97:MET:SD	2.07	0.78
7:G:190:VAL:HB	7:G:215:TRP:CZ2	2.14	0.78
7:G:94:GLU:OE1	7:G:115:VAL:HG23	1.82	0.78
13:M:47:THR:O	13:M:203:ILE:HD11	1.84	0.78
2:P:39:ALA:HB2	2:P:186:ALA:HB3	1.66	0.78
5:S:224:GLN:NE2	5:S:227:HIS:CE1	2.46	0.78
7:G:181:MET:O	7:G:183:GLU:N	2.16	0.78
2:B:172:PHE:HE2	2:B:196:GLU:CD	1.87	0.78
10:J:137:VAL:CG2	10:J:146:TYR:CD1	2.68	0.78
14:N:26:MET:CB	14:N:186:ARG:NH2	2.46	0.78
5:S:169:ALA:O	5:S:174:SER:OG	2.02	0.78
8:V:27:ALA:O	8:V:28:ASN:HB3	1.84	0.78
12:Z:19:ARG:CB	12:Z:171:GLY:O	2.31	0.78
2:B:147:GLN:NE2	2:B:162:MET:SD	2.57	0.77
9:W:172:ASN:HD21	9:W:191:VAL:HG22	1.49	0.77
6:F:15:PRO:HD2	6:F:16:GLN:OE1	1.83	0.77
11:Y:8:GLN:OE1	11:Y:115:LEU:CD2	2.32	0.77
10:J:55:LEU:O	10:J:59:VAL:HG23	1.83	0.77
13:M:174:LEU:HD13	9:W:202:TYR:CZ	2.18	0.77
13:M:54:CYS:SG	13:M:108:ASN:ND2	2.57	0.77
3:Q:24:ALA:O	3:Q:28:ILE:HD11	1.85	0.77
8:H:27:ALA:O	8:H:28:ASN:HB3	1.84	0.77
13:M:106:VAL:CG1	13:M:108:ASN:HD21	1.97	0.77
13:M:152:GLN:CG	9:W:202:TYR:CE2	2.67	0.77
14:N:91:TRP:HE3	14:N:94:ARG:HG3	1.47	0.77
12:L:36:GLU:HA	12:L:42:LEU:HD22	1.66	0.77
13:M:152:GLN:CD	9:W:202:TYR:CD2	2.57	0.77
5:E:70:ILE:HD11	5:E:76:CYS:HB3	1.64	0.77
2:B:39:ALA:HB2	2:B:186:ALA:HB3	1.66	0.77
4:D:192:ILE:CG1	4:D:228:TYR:CE1	2.68	0.77
12:L:50:ALA:C	13:M:97:TYR:HH	1.81	0.77
5:E:169:ALA:O	5:E:174:SER:OG	2.02	0.77
8:H:98:ILE:HG21	8:H:100:ILE:HG13	1.67	0.77
10:J:137:VAL:HG23	10:J:146:TYR:CD2	2.19	0.77
14:N:16:PHE:CZ	14:N:166:ARG:HA	2.18	0.77
14:N:4:PRO:CA	14:N:56:ASP:OD2	2.32	0.77
6:T:103:LEU:CD2	6:T:104:PRO:O	2.33	0.77
2:P:133:LEU:HD12	2:P:135:ILE:HG12	1.66	0.76
5:E:42:THR:CG2	5:E:194:ALA:HB1	2.11	0.76
14:N:162:GLN:HG2	14:N:166:ARG:HH21	1.49	0.76
2:P:133:LEU:HD11	2:P:135:ILE:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:80:ASN:ND2	9:W:111:TYR:CD1	2.53	0.76
3:Q:147:LEU:HD23	3:Q:159:TRP:O	1.86	0.76
8:V:98:ILE:HG21	8:V:100:ILE:HG13	1.67	0.76
5:E:218:ALA:CB	5:E:226:PHE:CE1	2.69	0.76
12:L:42:LEU:HD11	12:L:184:TRP:CE2	2.21	0.76
12:L:55:TRP:HD1	12:L:97:MET:SD	2.07	0.76
4:R:192:ILE:CG1	4:R:228:TYR:CE1	2.68	0.76
5:S:229:PHE:CE2	5:S:233:GLU:HG3	2.20	0.76
8:H:178:ALA:O	8:H:184:VAL:HA	1.86	0.76
11:K:55:GLN:CG	12:L:88:TYR:CD2	2.66	0.76
8:H:18:SER:HB3	8:H:172:GLY:HA3	1.67	0.76
11:K:8:GLN:OE1	11:K:115:LEU:CD2	2.32	0.76
11:K:78:THR:CG2	11:K:116:TYR:OH	2.34	0.76
8:V:43:CYS:SG	8:V:98:ILE:HD12	2.26	0.76
6:F:103:LEU:CD2	6:F:104:PRO:O	2.33	0.76
2:P:172:PHE:HE2	2:P:196:GLU:CD	1.87	0.76
10:X:137:VAL:CG2	10:X:146:TYR:CD1	2.68	0.76
6:F:13:TRP:HB2	7:G:22:GLN:HE22	1.49	0.76
8:H:33:LYS:HE2	15:H:300:KNM:C20	2.16	0.76
2:P:147:GLN:NE2	2:P:162:MET:SD	2.57	0.76
10:X:137:VAL:HG23	10:X:146:TYR:CE1	2.18	0.76
1:A:120:ASP:OD2	2:B:87:HIS:HE1	1.68	0.76
7:G:75:MET:HB2	7:G:137:LEU:HD22	1.67	0.76
9:I:172:ASN:HD21	9:I:191:VAL:HG22	1.49	0.76
12:Z:42:LEU:HD11	12:Z:184:TRP:CE2	2.21	0.76
12:Z:1:THR:HG23	15:Z:300:KNM:H30	1.68	0.76
9:I:80:ASN:ND2	9:I:111:TYR:CD1	2.53	0.76
13:M:106:VAL:CG1	13:M:108:ASN:OD1	2.33	0.75
14:N:16:PHE:HB3	14:N:162:GLN:HA	1.67	0.75
2:P:51:GLN:CD	2:P:54:ILE:HA	2.07	0.75
6:T:14:SER:O	6:T:17:GLY:HA3	1.86	0.75
6:F:43:HIS:CD2	6:F:184:LEU:HD22	2.22	0.75
7:U:75:MET:CG	7:U:137:LEU:CD2	2.64	0.75
10:J:137:VAL:HG22	10:J:146:TYR:CD1	2.22	0.75
1:O:120:ASP:OD2	2:P:87:HIS:HE1	1.68	0.75
3:Q:205:LYS:CB	3:Q:240:HIS:CD2	2.69	0.75
11:Y:78:THR:CG2	11:Y:116:TYR:OH	2.34	0.75
3:C:205:LYS:CB	3:C:240:HIS:CD2	2.69	0.75
8:H:1:THR:HG22	8:H:2:THR:N	2.01	0.75
8:H:43:CYS:SG	8:H:98:ILE:HD12	2.26	0.75
1:O:109:ILE:HG23	1:O:114:LEU:CG	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:140:GLU:HG2	2:P:141:GLY:N	2.00	0.75
2:P:49:LYS:O	2:P:206:ASN:HB3	1.87	0.75
11:Y:85:ARG:HD3	11:Y:124:LEU:HB2	1.69	0.75
1:A:109:ILE:HG23	1:A:114:LEU:CG	2.17	0.75
13:M:152:GLN:CB	9:W:202:TYR:CD2	2.69	0.75
2:B:133:LEU:HD11	2:B:135:ILE:HD11	1.67	0.75
3:C:147:LEU:HD23	3:C:159:TRP:O	1.86	0.75
11:K:85:ARG:HD3	11:K:124:LEU:CB	2.17	0.75
13:M:17:GLY:C	13:M:166:LEU:HD13	2.06	0.75
12:Z:153:TYR:CE2	12:Z:187:VAL:CG1	2.70	0.75
12:L:1:THR:HG23	15:L:300:KNM:H30	1.68	0.75
2:B:133:LEU:HD12	2:B:135:ILE:HG12	1.67	0.75
11:Y:85:ARG:HD3	11:Y:124:LEU:CB	2.17	0.75
3:C:24:ALA:O	3:C:28:ILE:HD11	1.84	0.75
11:K:147:TYR:HD1	11:K:159:LEU:HD21	1.52	0.75
12:L:153:TYR:CE2	12:L:187:VAL:CG1	2.70	0.75
2:P:138:TRP:CD1	2:P:143:PRO:HD3	2.21	0.75
2:B:138:TRP:CD1	2:B:143:PRO:HD3	2.21	0.74
9:I:1:THR:CG2	9:I:129:SER:CB	2.66	0.74
13:M:13:LEU:HD11	13:M:149:LEU:HD11	1.69	0.74
6:T:43:HIS:CD2	6:T:184:LEU:HD22	2.22	0.74
8:V:1:THR:HG22	8:V:2:THR:N	2.01	0.74
8:V:33:LYS:HE2	15:V:300:KNM:C20	2.16	0.74
2:B:181:LEU:HD23	2:B:186:ALA:CA	2.17	0.74
11:K:44:LEU:HD23	11:K:102:LEU:HD11	1.69	0.74
8:V:178:ALA:O	8:V:184:VAL:HA	1.86	0.74
2:B:49:LYS:O	2:B:206:ASN:HB3	1.87	0.74
6:F:13:TRP:HD1	7:G:22:GLN:NE2	1.83	0.74
9:I:41:ILE:HG12	9:I:102:GLY:HA3	1.69	0.74
2:P:138:TRP:HE1	2:P:143:PRO:HD3	1.52	0.74
8:V:18:SER:HB3	8:V:172:GLY:HA3	1.67	0.74
10:X:137:VAL:HG22	10:X:146:TYR:CD1	2.22	0.74
4:D:196:LEU:HD22	4:D:232:ILE:HD13	1.69	0.74
9:I:40:ASN:HB3	9:I:73:LEU:HD21	1.69	0.74
5:S:218:ALA:CB	5:S:226:PHE:CE1	2.69	0.74
6:T:13:TRP:HD1	7:U:22:GLN:NE2	1.83	0.74
11:Y:147:TYR:HD1	11:Y:159:LEU:HD21	1.52	0.74
6:T:13:TRP:HB2	7:U:22:GLN:HE22	1.50	0.74
9:I:49:ALA:HA	9:I:52:THR:HG22	1.70	0.74
14:N:9:THR:HG22	14:N:10:SER:N	2.02	0.74
6:T:7:ASP:OD2	6:T:14:SER:HA	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ALA:O	2:B:40:ALA:CB	2.36	0.74
5:E:229:PHE:CE2	5:E:233:GLU:HG3	2.20	0.74
5:E:42:THR:HG23	5:E:194:ALA:HB1	1.70	0.74
9:I:129:SER:OG	15:I:300:KNM:H43	1.86	0.74
13:M:13:LEU:HD11	13:M:149:LEU:CD1	2.17	0.74
5:S:35:SER:HB2	5:S:66:LYS:HZ2	1.53	0.74
8:V:32:ASP:CG	8:V:186:ARG:NH2	2.41	0.74
1:A:103:TYR:O	9:I:81:ARG:CZ	2.36	0.74
9:W:41:ILE:HG12	9:W:102:GLY:HA3	1.69	0.74
11:Y:29:LYS:HD2	12:Z:122:SER:O	1.88	0.74
15:Z:300:KNM:N2	15:Z:300:KNM:H8	2.03	0.74
14:N:16:PHE:HZ	14:N:165:ALA:C	1.72	0.73
14:N:59:ASP:C	14:N:108:ASN:ND2	2.40	0.73
6:T:69:HIS:ND1	6:T:96:ARG:NH2	2.36	0.73
8:V:84:LYS:O	8:V:88:TYR:HB2	1.88	0.73
2:B:140:GLU:HG2	2:B:141:GLY:N	2.00	0.73
6:T:195:LEU:CD2	6:T:210:VAL:HG12	2.18	0.73
8:H:119:MET:HE3	14:N:57:TYR:HD2	0.94	0.73
1:A:103:TYR:CA	9:I:81:ARG:HH22	1.72	0.73
15:L:300:KNM:H8	15:L:300:KNM:N2	2.03	0.73
3:Q:76:VAL:HG13	3:Q:134:LEU:CD2	2.18	0.73
9:W:80:ASN:ND2	9:W:111:TYR:CE1	2.56	0.73
9:W:1:THR:CG2	9:W:129:SER:CB	2.66	0.73
7:G:75:MET:CG	7:G:137:LEU:CD2	2.64	0.73
8:H:84:LYS:O	8:H:88:TYR:HB2	1.88	0.73
9:I:80:ASN:ND2	9:I:111:TYR:CE1	2.56	0.73
11:K:29:LYS:HD2	12:L:122:SER:O	1.88	0.73
4:R:196:LEU:HD22	4:R:232:ILE:HD13	1.69	0.73
13:M:174:LEU:CD1	9:W:202:TYR:HE2	1.99	0.73
1:A:109:ILE:HG23	1:A:114:LEU:HD11	1.71	0.73
3:C:48:GLU:HA	3:C:210:LYS:O	1.89	0.73
8:H:32:ASP:CG	8:H:186:ARG:NH2	2.41	0.73
10:J:18:CYS:SG	10:J:162:LEU:HD22	2.28	0.73
13:M:99:ARG:HB3	13:M:104:TYR:CE2	2.23	0.73
7:U:190:VAL:HB	7:U:215:TRP:CZ2	2.14	0.73
10:X:97:LYS:HB3	10:X:100:GLY:O	1.88	0.73
2:B:138:TRP:HE1	2:B:143:PRO:HD3	1.52	0.73
8:H:88:TYR:OH	14:N:62:TYR:HB3	1.87	0.73
10:J:27:PHE:CE2	10:J:35:THR:OG1	2.42	0.73
11:K:10:PRO:HD3	11:K:151:ILE:CG2	2.18	0.73
6:F:195:LEU:CD2	6:F:210:VAL:HG12	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:97:LYS:HB3	10:J:100:GLY:O	1.88	0.73
11:K:85:ARG:HD3	11:K:124:LEU:HB2	1.68	0.73
2:P:181:LEU:HD23	2:P:186:ALA:CA	2.17	0.73
1:O:103:TYR:O	9:W:81:ARG:CZ	2.36	0.73
15:Z:300:KNM:N2	15:Z:300:KNM:H21	2.04	0.73
2:B:51:GLN:CD	2:B:54:ILE:HA	2.07	0.73
14:N:21:VAL:HG22	14:N:191:THR:CG2	2.19	0.73
3:Q:48:GLU:HA	3:Q:210:LYS:O	1.89	0.73
6:T:184:LEU:HD21	6:T:214:ILE:CG2	2.17	0.73
9:W:49:ALA:HA	9:W:52:THR:HG22	1.70	0.73
9:W:40:ASN:HB3	9:W:73:LEU:HD21	1.69	0.73
10:X:18:CYS:SG	10:X:162:LEU:HD22	2.28	0.73
12:Z:55:TRP:CD1	12:Z:97:MET:SD	2.82	0.73
6:F:69:HIS:ND1	6:F:96:ARG:NH2	2.36	0.73
9:I:39:PRO:O	9:I:183:LEU:HD21	1.88	0.73
14:N:50:MET:HE3	14:N:192:VAL:HG23	1.69	0.73
4:R:172:LEU:HD22	4:R:190:LEU:HD21	1.71	0.73
9:W:59:ILE:CG2	9:W:63:LEU:HD13	2.19	0.73
10:X:26:ARG:CD	10:X:33:MET:HG3	2.19	0.73
10:J:26:ARG:CD	10:J:33:MET:HG3	2.19	0.72
5:S:120:ALA:O	5:S:121:LEU:HD23	1.89	0.72
2:B:172:PHE:CZ	2:B:196:GLU:OE1	2.42	0.72
5:S:218:ALA:CB	5:S:226:PHE:CZ	2.72	0.72
10:X:27:PHE:CE2	10:X:35:THR:OG1	2.42	0.72
1:A:109:ILE:CG2	1:A:114:LEU:CG	2.67	0.72
2:B:133:LEU:CD1	2:B:135:ILE:CG1	2.67	0.72
3:C:76:VAL:HG13	3:C:134:LEU:CD2	2.18	0.72
8:H:51:ASP:HB3	8:H:94:LEU:HD12	1.71	0.72
14:N:21:VAL:HG22	14:N:191:THR:HG22	1.71	0.72
2:P:133:LEU:CD1	2:P:135:ILE:CG1	2.66	0.72
13:M:174:LEU:CB	9:W:202:TYR:OH	2.35	0.72
5:E:218:ALA:CB	5:E:226:PHE:CZ	2.72	0.72
9:I:21:THR:O	15:I:300:KNM:H7	1.89	0.72
14:N:91:TRP:CZ3	14:N:94:ARG:HB3	2.21	0.72
2:P:39:ALA:O	2:P:40:ALA:CB	2.36	0.72
11:Y:55:GLN:CG	12:Z:88:TYR:CE2	2.71	0.72
12:L:178:HIS:CB	12:L:187:VAL:HG21	2.20	0.72
12:L:55:TRP:CD1	12:L:97:MET:SD	2.82	0.72
13:M:17:GLY:HA3	13:M:166:LEU:HD21	1.66	0.72
8:V:51:ASP:HB3	8:V:94:LEU:HD12	1.71	0.72
9:W:39:PRO:O	9:W:183:LEU:HD21	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:44:LEU:HD23	11:Y:102:LEU:HD11	1.69	0.72
11:Y:10:PRO:HD3	11:Y:151:ILE:CG2	2.18	0.72
9:I:59:ILE:CG2	9:I:63:LEU:HD13	2.19	0.72
1:O:102:LYS:O	9:W:81:ARG:NH1	2.22	0.72
12:Z:178:HIS:CB	12:Z:187:VAL:HG21	2.20	0.72
7:G:72:HIS:HB2	7:G:105:ASN:ND2	2.05	0.72
14:N:16:PHE:HD1	14:N:161:SER:O	1.73	0.72
7:U:161:TRP:O	7:U:181:MET:SD	2.48	0.72
4:D:172:LEU:HD22	4:D:190:LEU:HD21	1.71	0.72
5:E:120:ALA:O	5:E:121:LEU:HD23	1.89	0.72
6:F:184:LEU:HD21	6:F:214:ILE:CG2	2.17	0.72
10:J:137:VAL:HG23	10:J:146:TYR:CE1	2.18	0.72
1:O:109:ILE:HG23	1:O:114:LEU:HD11	1.71	0.72
2:P:172:PHE:CZ	2:P:196:GLU:OE1	2.42	0.72
9:W:21:THR:O	15:W:300:KNM:H7	1.89	0.72
11:Y:8:GLN:O	11:Y:147:TYR:OH	2.05	0.72
5:E:70:ILE:HD11	5:E:76:CYS:HB2	1.72	0.71
8:H:115:PRO:HG3	14:N:36:PHE:CZ	2.23	0.71
15:I:300:KNM:C2	15:I:300:KNM:H6	2.20	0.71
14:N:16:PHE:CE2	14:N:21:VAL:CG2	2.73	0.71
14:N:46:ASN:O	14:N:47:ASN:C	2.27	0.71
3:C:136:TYR:O	3:C:147:LEU:HA	1.90	0.71
4:D:31:THR:HG23	4:D:165:ALA:HB2	1.71	0.71
7:U:190:VAL:HG21	7:U:215:TRP:CE2	2.25	0.71
1:A:102:LYS:O	9:I:81:ARG:NH1	2.22	0.71
2:B:132:SER:OG	2:B:149:ASP:OD1	2.08	0.71
15:L:300:KNM:H21	15:L:300:KNM:N2	2.04	0.71
9:W:63:LEU:HD11	9:W:82:MET:SD	2.31	0.71
6:F:13:TRP:CB	7:G:22:GLN:HE22	2.03	0.71
9:I:36:PHE:CD1	9:I:38:SER:C	2.64	0.71
9:W:39:PRO:O	9:W:183:LEU:CD2	2.39	0.71
13:M:174:LEU:CD2	9:W:202:TYR:OH	2.38	0.71
5:E:35:SER:HB2	5:E:66:LYS:HZ2	1.53	0.71
7:G:161:TRP:O	7:G:181:MET:SD	2.48	0.71
1:A:102:LYS:O	9:I:81:ARG:CZ	2.39	0.71
13:M:106:VAL:CG1	13:M:108:ASN:ND2	2.53	0.71
13:M:16:ALA:HB2	13:M:21:ALA:HA	1.71	0.71
3:Q:198:ASN:OD1	3:Q:240:HIS:ND1	2.22	0.71
2:P:132:SER:OG	2:P:149:ASP:OD1	2.08	0.71
4:R:31:THR:HG23	4:R:165:ALA:HB2	1.71	0.71
5:S:42:THR:HG23	5:S:194:ALA:HB1	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:70:ILE:HD11	5:S:76:CYS:HB2	1.72	0.71
15:W:300:KNM:C2	15:W:300:KNM:H6	2.20	0.71
13:M:18:GLU:O	13:M:20:PHE:N	2.24	0.71
3:Q:136:TYR:O	3:Q:147:LEU:HA	1.90	0.71
9:W:36:PHE:CD1	9:W:38:SER:C	2.64	0.71
1:A:109:ILE:CG1	1:A:114:LEU:HD23	2.21	0.71
3:C:198:ASN:OD1	3:C:240:HIS:ND1	2.22	0.71
9:I:63:LEU:HD11	9:I:82:MET:SD	2.31	0.71
12:L:178:HIS:HB2	12:L:187:VAL:HG21	1.73	0.71
1:O:109:ILE:CG2	1:O:114:LEU:CG	2.67	0.71
6:T:13:TRP:CB	7:U:22:GLN:HE22	2.03	0.71
9:W:1:THR:CG2	9:W:129:SER:N	2.49	0.71
12:Z:178:HIS:HB2	12:Z:187:VAL:HG21	1.73	0.70
3:C:183:GLU:HG2	3:C:183:GLU:O	1.91	0.70
1:O:102:LYS:O	9:W:81:ARG:CZ	2.39	0.70
9:I:1:THR:CG2	9:I:129:SER:N	2.49	0.70
11:K:55:GLN:NE2	12:L:88:TYR:HD2	1.90	0.70
1:O:103:TYR:HA	9:W:81:ARG:HH21	1.15	0.70
9:I:1:THR:HG21	15:I:300:KNM:S1	2.32	0.70
11:Y:44:LEU:HG	11:Y:102:LEU:CD2	2.22	0.70
9:I:39:PRO:O	9:I:183:LEU:CD2	2.39	0.70
4:D:8:THR:O	5:E:135:ARG:HD3	1.92	0.70
11:K:55:GLN:CG	12:L:88:TYR:CE2	2.71	0.70
4:R:196:LEU:HD13	4:R:232:ILE:HG21	1.73	0.70
9:W:1:THR:HG21	15:W:300:KNM:S1	2.32	0.70
11:Y:23:SER:O	11:Y:24:ASN:OD1	0.70	0.70
11:K:23:SER:O	11:K:24:ASN:OD1	0.70	0.70
14:N:26:MET:O	14:N:186:ARG:NH2	2.24	0.70
6:T:69:HIS:CE1	6:T:96:ARG:HH21	2.10	0.70
10:X:49:TYR:CD2	10:X:189:ILE:HD11	2.26	0.70
9:I:128:GLY:HA2	15:I:300:KNM:O4	1.92	0.70
4:R:8:THR:O	5:S:135:ARG:HD3	1.91	0.70
11:Y:55:GLN:NE2	12:Z:88:TYR:HD2	1.90	0.70
2:B:44:VAL:HG23	2:B:211:ILE:HG23	1.73	0.69
15:L:300:KNM:O2	15:L:300:KNM:H34	1.92	0.69
1:O:109:ILE:CG1	1:O:114:LEU:CD2	2.70	0.69
3:Q:183:GLU:HG2	3:Q:183:GLU:O	1.91	0.69
9:W:49:ALA:HA	15:W:300:KNM:H36	1.73	0.69
7:U:72:HIS:HB2	7:U:105:ASN:ND2	2.05	0.69
9:I:129:SER:OG	15:I:300:KNM:H41	1.90	0.69
15:Z:300:KNM:O2	15:Z:300:KNM:H34	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:59:ASP:HB2	14:N:108:ASN:ND2	2.05	0.69
6:F:69:HIS:CE1	6:F:96:ARG:HH21	2.10	0.69
13:M:19:ASP:OD1	13:M:113:LEU:HD11	1.92	0.69
9:W:1:THR:O	9:W:128:GLY:HA3	1.93	0.69
1:A:109:ILE:CG1	1:A:114:LEU:CD2	2.70	0.69
1:O:161:CYS:HG	1:O:163:PHE:HE1	1.17	0.69
2:P:133:LEU:HD12	2:P:135:ILE:CG1	2.23	0.69
5:E:43:SER:HA	5:E:151:PRO:HG3	1.75	0.69
6:F:92:CYS:HA	6:F:103:LEU:HD13	1.75	0.69
9:I:1:THR:O	9:I:128:GLY:HA3	1.93	0.69
13:M:15:ILE:HD11	13:M:175:VAL:HG22	1.74	0.69
2:P:138:TRP:CD1	2:P:143:PRO:CD	2.76	0.69
14:N:4:PRO:HB2	14:N:56:ASP:CG	2.14	0.69
8:H:117:GLY:CA	14:N:5:MET:HG3	2.23	0.69
9:W:128:GLY:HA2	15:W:300:KNM:O4	1.92	0.69
5:E:168:ARG:NH1	5:E:178:GLN:OE1	2.24	0.69
11:K:8:GLN:O	11:K:147:TYR:OH	2.05	0.69
13:M:106:VAL:HG13	13:M:108:ASN:HD21	1.57	0.69
8:H:88:TYR:OH	14:N:62:TYR:CG	2.32	0.69
9:I:47:GLY:N	15:I:300:KNM:H29	2.04	0.68
9:W:63:LEU:CD1	9:W:82:MET:SD	2.81	0.68
4:D:196:LEU:HD13	4:D:232:ILE:HG21	1.73	0.68
8:H:1:THR:HB	15:H:300:KNM:O5	1.91	0.68
9:I:63:LEU:CD1	9:I:82:MET:SD	2.81	0.68
1:O:109:ILE:CG1	1:O:114:LEU:HD23	2.21	0.68
6:T:13:TRP:H	7:U:22:GLN:HE22	1.40	0.68
11:Y:151:ILE:HG13	11:Y:152:SER:N	2.08	0.68
14:N:173:MET:HB3	14:N:187:PHE:CE2	2.28	0.68
14:N:60:PHE:N	14:N:108:ASN:HD21	1.91	0.68
5:S:147:ASP:O	5:S:149:LYS:N	2.27	0.68
6:T:92:CYS:HA	6:T:103:LEU:HD13	1.75	0.68
1:A:109:ILE:CD1	1:A:114:LEU:CD2	2.31	0.68
4:D:211:MET:CB	4:D:217:LEU:HD13	2.20	0.68
6:F:98:VAL:HG13	14:N:91:TRP:CE3	2.29	0.68
11:K:151:ILE:HG13	11:K:152:SER:N	2.08	0.68
5:E:147:ASP:O	5:E:149:LYS:N	2.27	0.68
8:H:83:PHE:CD2	8:H:100:ILE:CD1	2.77	0.68
11:K:44:LEU:HG	11:K:102:LEU:CD2	2.22	0.68
5:S:43:SER:HA	5:S:151:PRO:HG3	1.75	0.68
7:U:104:TYR:OH	8:V:70:LEU:CD2	2.41	0.68
7:G:104:TYR:OH	8:H:70:LEU:CD2	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:ALA:HA	15:I:300:KNM:H36	1.73	0.68
2:P:44:VAL:HG23	2:P:211:ILE:HG23	1.73	0.68
8:V:1:THR:HB	15:V:300:KNM:O5	1.91	0.68
7:G:190:VAL:HG21	7:G:215:TRP:CE2	2.25	0.68
2:B:133:LEU:HD12	2:B:135:ILE:CG1	2.23	0.68
11:K:85:ARG:HH22	11:K:86:ARG:NH2	1.82	0.68
13:M:19:ASP:OD2	13:M:200:LYS:HG3	1.93	0.68
9:W:47:GLY:N	15:W:300:KNM:H29	2.03	0.68
6:F:13:TRP:H	7:G:22:GLN:HE22	1.40	0.68
13:M:16:ALA:HB1	13:M:119:GLY:CA	2.15	0.68
3:Q:111:VAL:HG13	3:Q:136:TYR:CE2	2.29	0.68
8:V:83:PHE:CD2	8:V:100:ILE:CD1	2.77	0.68
13:M:106:VAL:HG13	13:M:108:ASN:ND2	2.08	0.67
11:Y:85:ARG:HH22	11:Y:86:ARG:NH2	1.82	0.67
2:B:138:TRP:CD1	2:B:143:PRO:CD	2.76	0.67
2:B:140:GLU:CG	2:B:141:GLY:N	2.55	0.67
12:Z:178:HIS:O	12:Z:184:TRP:HA	1.95	0.67
12:L:178:HIS:O	12:L:184:TRP:HA	1.95	0.67
9:I:144:PRO:O	9:I:145:ASP:HB3	1.95	0.67
14:N:16:PHE:HE2	14:N:21:VAL:CG2	2.06	0.67
3:C:111:VAL:HG13	3:C:136:TYR:CE2	2.29	0.67
2:P:140:GLU:CG	2:P:141:GLY:N	2.55	0.67
5:S:120:ALA:C	5:S:121:LEU:HD23	2.15	0.67
2:B:138:TRP:CD1	2:B:143:PRO:CG	2.78	0.67
6:F:77:LEU:HD11	6:F:80:ASP:OD2	1.95	0.67
10:J:154:GLU:CD	10:J:161:HIS:NE2	2.48	0.67
10:J:49:TYR:CD2	10:J:189:ILE:HD11	2.30	0.66
3:Q:157:GLY:O	3:Q:159:TRP:CD1	2.46	0.66
11:Y:46:CYS:CB	11:Y:102:LEU:HD12	2.26	0.66
14:N:16:PHE:HZ	14:N:166:ARG:HA	1.57	0.66
12:Z:55:TRP:CZ2	12:Z:95:LEU:HD12	2.30	0.66
2:B:181:LEU:CD1	2:B:185:ASP:HB3	2.25	0.66
1:O:109:ILE:HG23	1:O:114:LEU:CD1	2.26	0.66
6:T:77:LEU:HD11	6:T:80:ASP:OD2	1.94	0.66
8:H:115:PRO:O	8:H:118:GLY:N	2.29	0.66
13:M:47:THR:O	13:M:203:ILE:CD1	2.42	0.66
2:P:138:TRP:CD1	2:P:143:PRO:CG	2.78	0.66
8:V:115:PRO:O	8:V:118:GLY:N	2.29	0.66
9:W:49:ALA:CB	15:W:300:KNM:H36	2.26	0.66
2:B:39:ALA:O	2:B:40:ALA:HB2	1.96	0.66
8:H:47:GLY:C	15:H:300:KNM:H24	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:186:LEU:HD23	3:Q:186:LEU:O	1.95	0.66
9:W:36:PHE:HB2	9:W:42:TYR:HE1	1.60	0.66
7:U:75:MET:CE	7:U:137:LEU:HD21	2.26	0.66
6:T:13:TRP:CB	7:U:22:GLN:NE2	2.59	0.66
5:E:120:ALA:C	5:E:121:LEU:HD23	2.15	0.66
5:E:227:HIS:HE2	5:E:229:PHE:HD1	1.44	0.66
9:I:36:PHE:HB2	9:I:42:TYR:HE1	1.60	0.66
5:S:35:SER:CB	5:S:66:LYS:NZ	2.59	0.66
9:W:144:PRO:O	9:W:145:ASP:HB3	1.95	0.66
9:I:49:ALA:CB	15:I:300:KNM:H36	2.26	0.66
14:N:91:TRP:HZ3	14:N:94:ARG:CB	2.07	0.65
5:E:224:GLN:NE2	5:E:227:HIS:CE1	2.46	0.65
7:G:75:MET:CE	7:G:137:LEU:HD21	2.26	0.65
8:H:1:THR:CA	15:H:300:KNM:O5	2.44	0.65
11:K:85:ARG:CZ	11:K:86:ARG:HH22	2.09	0.65
2:P:39:ALA:O	2:P:40:ALA:HB2	1.96	0.65
1:O:109:ILE:CB	1:O:114:LEU:HD21	2.20	0.65
1:A:109:ILE:HG23	1:A:114:LEU:CD1	2.26	0.65
9:I:1:THR:N	9:I:169:SER:CB	2.59	0.65
9:I:47:GLY:O	15:I:300:KNM:N3	2.28	0.65
13:M:46:LEU:HD13	13:M:52:ILE:HG22	1.78	0.65
4:R:211:MET:CB	4:R:217:LEU:HD13	2.19	0.65
3:C:157:GLY:O	3:C:159:TRP:CD1	2.46	0.65
5:E:168:ARG:HD3	5:E:178:GLN:HE22	1.62	0.65
9:I:146:MET:HE1	9:I:154:LEU:HD23	1.77	0.65
12:L:55:TRP:CZ2	12:L:95:LEU:HD12	2.30	0.65
11:Y:147:TYR:HD1	11:Y:159:LEU:CD2	2.09	0.65
5:E:188:SER:O	5:E:189:MET:HB2	1.95	0.65
6:F:13:TRP:CB	7:G:22:GLN:NE2	2.59	0.65
1:O:109:ILE:CD1	1:O:114:LEU:CD2	2.31	0.65
8:V:47:GLY:C	15:V:300:KNM:H24	2.15	0.65
10:X:137:VAL:CG2	10:X:146:TYR:CG	2.80	0.65
10:X:154:GLU:CD	10:X:161:HIS:NE2	2.48	0.65
3:C:186:LEU:O	3:C:186:LEU:HD23	1.95	0.65
4:D:31:THR:HG23	4:D:165:ALA:CB	2.26	0.65
7:G:75:MET:HG3	7:G:137:LEU:CD2	2.27	0.65
1:A:103:TYR:HA	9:I:81:ARG:HH22	0.82	0.65
10:J:122:SER:CB	10:J:136:VAL:HG11	2.25	0.65
2:P:51:GLN:HG3	2:P:54:ILE:CA	2.27	0.65
4:R:31:THR:HG23	4:R:165:ALA:CB	2.26	0.65
6:T:14:SER:C	6:T:17:GLY:HA3	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:75:MET:HB2	7:U:137:LEU:HD22	1.67	0.65
10:X:122:SER:CB	10:X:136:VAL:HG11	2.25	0.65
2:P:172:PHE:HE2	2:P:196:GLU:CG	2.09	0.65
9:W:122:LEU:CG	9:W:123:PRO:HD2	2.26	0.65
9:W:1:THR:N	9:W:169:SER:CB	2.59	0.65
2:B:172:PHE:HE2	2:B:196:GLU:CG	2.09	0.65
2:B:51:GLN:HG3	2:B:54:ILE:CA	2.27	0.65
5:E:35:SER:CB	5:E:66:LYS:NZ	2.59	0.65
6:F:100:ASP:OD1	14:N:94:ARG:NH2	2.29	0.65
10:J:57:THR:HG22	11:K:122:ALA:O	1.97	0.65
13:M:174:LEU:HB2	9:W:202:TYR:HH	1.57	0.65
5:S:35:SER:CB	5:S:66:LYS:HZ2	2.10	0.65
11:K:46:CYS:CB	11:K:102:LEU:HD12	2.26	0.64
2:P:172:PHE:CE2	2:P:196:GLU:OE1	2.50	0.64
5:S:188:SER:O	5:S:189:MET:HB2	1.95	0.64
5:S:42:THR:OG1	5:S:45:GLY:O	2.11	0.64
1:O:103:TYR:HA	9:W:81:ARG:HH22	0.82	0.64
3:C:203:VAL:HG11	3:C:210:LYS:NZ	2.11	0.64
5:E:35:SER:CB	5:E:66:LYS:HZ2	2.09	0.64
10:J:137:VAL:CG2	10:J:146:TYR:CG	2.80	0.64
14:N:48:SER:CB	14:N:196:GLY:HA3	2.27	0.64
2:P:134:LEU:CD2	2:P:162:MET:SD	2.85	0.64
13:M:146:GLN:CB	10:X:176:ARG:HH22	2.02	0.64
11:Y:120:TYR:CE1	11:Y:121:LEU:CD2	2.80	0.64
3:C:111:VAL:HG22	3:C:136:TYR:CD2	2.32	0.64
14:N:16:PHE:HE1	14:N:166:ARG:H	0.71	0.64
3:Q:111:VAL:HG22	3:Q:136:TYR:CD2	2.32	0.64
3:Q:203:VAL:HG11	3:Q:210:LYS:NZ	2.11	0.64
5:S:168:ARG:NH1	5:S:178:GLN:OE1	2.24	0.64
6:T:195:LEU:HD23	6:T:210:VAL:HG12	1.79	0.64
8:V:45:ARG:HG3	15:V:300:KNM:H34	1.79	0.64
10:X:16:LYS:O	10:X:17:ASN:C	2.36	0.64
9:I:36:PHE:CD1	9:I:38:SER:O	2.51	0.64
5:S:50:VAL:CG2	5:S:66:LYS:HD3	2.27	0.64
2:B:134:LEU:CD2	2:B:162:MET:SD	2.85	0.64
11:K:170:ARG:NH2	12:Z:136:TYR:CG	2.66	0.64
13:M:100:ARG:NH1	13:M:127:VAL:CB	2.54	0.64
14:N:59:ASP:CA	14:N:108:ASN:HD21	2.10	0.64
8:V:1:THR:CA	15:V:300:KNM:O5	2.44	0.64
11:K:147:TYR:HD1	11:K:159:LEU:CD2	2.09	0.64
14:N:21:VAL:CG2	14:N:191:THR:CG2	2.73	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:9:THR:HG22	14:N:140:GLY:O	1.97	0.64
10:X:17:ASN:OD1	10:X:18:CYS:N	2.31	0.64
8:H:45:ARG:HG3	15:H:300:KNM:H34	1.79	0.64
1:O:13:ILE:O	1:O:13:ILE:HG13	1.97	0.64
2:P:181:LEU:CD1	2:P:185:ASP:HB3	2.25	0.64
10:X:57:THR:HG22	11:Y:122:ALA:O	1.97	0.64
11:Y:5:ILE:HD11	11:Y:143:LEU:HD22	1.80	0.64
2:B:172:PHE:CE2	2:B:196:GLU:OE1	2.50	0.64
10:J:17:ASN:OD1	10:J:18:CYS:N	2.31	0.64
14:N:16:PHE:CE1	14:N:165:ALA:N	2.66	0.64
9:W:36:PHE:CD1	9:W:38:SER:O	2.51	0.64
3:C:76:VAL:HA	3:C:134:LEU:HD23	1.79	0.64
5:E:50:VAL:CG2	5:E:66:LYS:HD3	2.27	0.64
1:O:120:ASP:OD2	2:P:87:HIS:CE1	2.51	0.64
6:T:184:LEU:CD2	6:T:214:ILE:HG21	2.22	0.64
9:W:129:SER:OG	15:W:300:KNM:H43	1.97	0.64
11:K:5:ILE:HD11	11:K:143:LEU:HD22	1.80	0.64
14:N:56:ASP:O	14:N:108:ASN:OD1	2.16	0.64
2:P:133:LEU:HD11	2:P:135:ILE:CD1	2.28	0.64
5:S:168:ARG:HD3	5:S:178:GLN:HE22	1.62	0.64
11:Y:85:ARG:CZ	11:Y:86:ARG:HH22	2.09	0.64
2:B:133:LEU:HD11	2:B:135:ILE:CD1	2.28	0.63
15:V:300:KNM:O2	15:V:300:KNM:H37	1.98	0.63
2:B:42:GLY:CA	2:B:183:LEU:HD12	2.29	0.63
15:H:300:KNM:O2	15:H:300:KNM:H37	1.98	0.63
11:K:120:TYR:CE1	11:K:121:LEU:CD2	2.80	0.63
14:N:16:PHE:CD1	14:N:162:GLN:O	2.51	0.63
2:P:42:GLY:CA	2:P:183:LEU:HD12	2.29	0.63
5:S:227:HIS:HE2	5:S:229:PHE:HD1	1.44	0.63
7:U:75:MET:HG3	7:U:137:LEU:CD2	2.27	0.63
9:W:47:GLY:O	15:W:300:KNM:N3	2.28	0.63
12:L:136:TYR:CG	11:Y:170:ARG:NH2	2.66	0.63
12:Z:153:TYR:CE2	12:Z:187:VAL:HG13	2.33	0.63
1:A:13:ILE:O	1:A:13:ILE:HG13	1.97	0.63
2:B:183:LEU:O	2:B:187:ILE:HG13	1.99	0.63
7:G:190:VAL:CG2	7:G:215:TRP:NE1	2.61	0.63
3:Q:76:VAL:HA	3:Q:134:LEU:HD23	1.79	0.63
14:N:145:LEU:HG	9:W:136:ALA:HB2	1.80	0.63
11:Y:24:ASN:HD21	11:Y:26:VAL:HG23	1.64	0.63
11:Y:24:ASN:ND2	11:Y:26:VAL:CG2	2.61	0.63
9:I:122:LEU:CG	9:I:123:PRO:HD2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:24:ASN:ND2	11:K:26:VAL:CG2	2.61	0.63
6:F:195:LEU:HD23	6:F:210:VAL:HG12	1.79	0.63
8:H:177:ALA:HA	8:H:186:ARG:HG3	1.80	0.63
10:J:16:LYS:O	10:J:17:ASN:C	2.36	0.63
11:K:67:TYR:CE2	11:K:75:LEU:HD21	2.33	0.63
13:M:104:TYR:HE1	14:N:97:TYR:OH	1.82	0.63
2:P:183:LEU:O	2:P:187:ILE:HG13	1.99	0.63
5:S:42:THR:CG2	5:S:194:ALA:HB3	2.00	0.63
1:A:120:ASP:OD2	2:B:87:HIS:CE1	2.51	0.63
15:V:300:KNM:O3	15:V:300:KNM:H18	1.98	0.63
5:E:42:THR:OG1	5:E:45:GLY:O	2.11	0.63
1:O:103:TYR:HB2	8:V:61:TYR:CD1	2.33	0.63
8:H:83:PHE:CD2	8:H:100:ILE:HD11	2.34	0.63
12:L:149:VAL:HG12	12:L:153:TYR:CZ	2.34	0.63
1:A:69:LEU:CD1	1:A:229:ILE:HG13	2.30	0.62
2:B:145:LEU:HG	9:I:136:ALA:HB2	60.82	0.62
14:N:50:MET:HE2	14:N:192:VAL:CG2	2.15	0.62
8:V:135:ILE:HG12	8:V:163:ALA:HB2	1.80	0.62
9:W:22:GLU:HA	15:W:300:KNM:H6	1.81	0.62
9:W:36:PHE:HA	9:W:42:TYR:HD1	1.64	0.62
11:Y:24:ASN:ND2	11:Y:26:VAL:HG22	2.15	0.62
8:H:135:ILE:HG12	8:H:163:ALA:HB2	1.80	0.62
11:K:56:PHE:HZ	11:K:84:THR:OG1	1.81	0.62
2:P:41:ASN:OD1	2:P:182:GLU:HA	2.00	0.62
8:V:83:PHE:CD2	8:V:100:ILE:HD11	2.34	0.62
11:Y:67:TYR:CE2	11:Y:75:LEU:HD21	2.33	0.62
4:D:6:ALA:HB2	5:E:134:SER:OG	2.00	0.62
8:H:98:ILE:HG21	8:H:100:ILE:CG1	2.29	0.62
8:V:177:ALA:HA	8:V:186:ARG:HG3	1.80	0.62
9:I:46:ALA:HA	15:I:300:KNM:H31	1.81	0.62
11:K:24:ASN:HD21	11:K:26:VAL:HG23	1.64	0.62
6:T:210:VAL:HG23	6:T:210:VAL:O	1.99	0.62
10:X:137:VAL:CG2	10:X:146:TYR:CD2	2.82	0.62
6:F:210:VAL:HG23	6:F:210:VAL:O	1.99	0.62
1:A:103:TYR:HB2	8:H:61:TYR:CD1	2.33	0.62
15:L:300:KNM:H29	15:L:300:KNM:C10	2.29	0.62
12:Z:1:THR:CG2	15:Z:300:KNM:H30	2.30	0.62
15:H:300:KNM:O3	15:H:300:KNM:H18	1.98	0.62
9:I:104:ASP:O	9:I:106:THR:N	2.32	0.62
10:J:137:VAL:CG2	10:J:146:TYR:CD2	2.82	0.62
7:U:190:VAL:CG2	7:U:215:TRP:NE1	2.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:ALA:HA	15:I:300:KNM:C20	2.30	0.62
10:X:55:LEU:HD13	10:X:103:TYR:HB2	1.82	0.62
3:C:28:ILE:HD12	3:C:28:ILE:H	1.65	0.62
9:I:36:PHE:HA	9:I:42:TYR:HD1	1.64	0.62
12:L:153:TYR:CE2	12:L:187:VAL:HG13	2.33	0.62
12:L:153:TYR:CE2	12:L:187:VAL:HG11	2.35	0.62
12:L:1:THR:CG2	15:L:300:KNM:H30	2.30	0.62
9:W:104:ASP:O	9:W:106:THR:N	2.32	0.62
9:W:46:ALA:HA	15:W:300:KNM:H31	1.81	0.62
1:A:109:ILE:CB	1:A:114:LEU:HD21	2.20	0.61
2:B:41:ASN:OD1	2:B:182:GLU:HA	2.00	0.61
8:V:28:ASN:OD1	8:V:30:VAL:N	2.21	0.61
9:W:46:ALA:HB1	15:W:300:KNM:H29	1.82	0.61
10:X:64:GLN:CD	11:Y:85:ARG:HH22	2.03	0.61
12:Z:149:VAL:HG12	12:Z:153:TYR:CZ	2.34	0.61
1:O:69:LEU:HD12	1:O:229:ILE:HG13	1.82	0.61
14:N:91:TRP:HZ3	14:N:94:ARG:HB3	1.63	0.61
2:P:138:TRP:CD1	2:P:143:PRO:HG3	2.35	0.61
3:Q:79:ILE:HG22	3:Q:80:THR:N	2.15	0.61
3:Q:12:PHE:HD2	4:R:21:TYR:CB	2.14	0.61
4:R:6:ALA:HB2	5:S:134:SER:OG	2.00	0.61
6:T:13:TRP:N	7:U:22:GLN:HE22	1.99	0.61
12:Z:153:TYR:CE2	12:Z:187:VAL:HG11	2.35	0.61
2:B:138:TRP:CD1	2:B:143:PRO:HG3	2.35	0.61
3:C:12:PHE:HD2	4:D:21:TYR:CB	2.14	0.61
5:E:191:LEU:HD13	5:E:221:GLN:HG2	1.82	0.61
6:F:13:TRP:N	7:G:22:GLN:HE22	1.99	0.61
3:C:79:ILE:HG22	3:C:80:THR:N	2.15	0.61
7:G:75:MET:CA	7:G:137:LEU:CD2	2.68	0.61
11:Y:56:PHE:HZ	11:Y:84:THR:OG1	1.81	0.61
6:F:121:GLN:HG3	7:G:122:TYR:HE2	1.66	0.61
8:H:175:ARG:HG2	8:H:188:VAL:HG22	1.81	0.61
13:M:48:ASP:O	13:M:203:ILE:CG1	2.34	0.61
13:M:49:LYS:CD	13:M:113:LEU:HB3	2.30	0.61
12:L:50:ALA:CA	13:M:97:TYR:HH	2.10	0.61
1:O:69:LEU:CD1	1:O:229:ILE:HG13	2.30	0.61
6:F:77:LEU:HD11	6:F:80:ASP:CG	2.21	0.61
14:N:16:PHE:CE2	14:N:21:VAL:CB	2.45	0.61
14:N:197:VAL:O	14:N:197:VAL:HG12	2.00	0.61
8:V:175:ARG:HG2	8:V:188:VAL:HG22	1.81	0.61
15:Z:300:KNM:H29	15:Z:300:KNM:C10	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:43:HIS:HB2	6:F:184:LEU:HD13	1.82	0.61
9:I:22:GLU:HA	15:I:300:KNM:H6	1.81	0.61
9:I:46:ALA:HB1	15:I:300:KNM:H29	1.82	0.61
5:S:166:ASP:CB	5:S:185:TYR:CZ	2.73	0.61
6:T:43:HIS:HB2	6:T:184:LEU:HD13	1.82	0.61
4:D:172:LEU:CD2	4:D:190:LEU:HD21	2.31	0.61
6:F:7:ASP:OD2	6:F:14:SER:HA	2.01	0.61
1:A:229:ILE:HD12	1:A:229:ILE:N	2.16	0.60
5:E:211:ASN:O	5:E:214:ASN:N	2.31	0.60
11:K:24:ASN:ND2	11:K:26:VAL:HG22	2.15	0.60
1:A:43:ARG:HD2	1:A:149:PRO:O	2.01	0.60
3:Q:28:ILE:HD12	3:Q:28:ILE:H	1.65	0.60
7:U:104:TYR:OH	8:V:70:LEU:HD21	2.02	0.60
8:V:98:ILE:HG21	8:V:100:ILE:CG1	2.29	0.60
1:O:103:TYR:CA	9:W:81:ARG:HH22	1.72	0.60
5:E:191:LEU:CD1	5:E:221:GLN:HG2	2.31	0.60
12:L:21:THR:O	15:L:300:KNM:H25	2.00	0.60
9:W:36:PHE:CE1	9:W:38:SER:HA	2.36	0.60
12:Z:1:THR:O	12:Z:1:THR:HG22	2.01	0.60
2:B:68:THR:CG2	2:B:71:ILE:HB	2.27	0.60
7:G:46:VAL:HG22	7:G:215:TRP:CD1	2.36	0.60
9:I:172:ASN:OD1	9:I:190:THR:O	2.18	0.60
9:I:36:PHE:CE1	9:I:38:SER:HA	2.36	0.60
12:L:1:THR:O	12:L:1:THR:HG22	2.01	0.60
11:K:55:GLN:NE2	12:L:88:TYR:CD2	2.69	0.60
14:N:38:ASN:HA	14:N:186:ARG:NH2	2.16	0.60
14:N:46:ASN:C	14:N:48:SER:N	2.51	0.60
4:R:172:LEU:CD2	4:R:190:LEU:HD21	2.31	0.60
10:J:122:SER:HB3	10:J:136:VAL:CG1	2.29	0.60
14:N:193:THR:O	14:N:194:GLU:C	2.39	0.60
11:K:48:GLY:O	11:K:53:THR:HG21	2.02	0.60
13:M:146:GLN:HB3	10:X:176:ARG:CZ	2.31	0.60
1:O:159:TYR:CD1	2:P:83:ARG:NH2	2.70	0.60
5:S:191:LEU:HD13	5:S:221:GLN:HG2	1.82	0.60
9:W:49:ALA:HA	15:W:300:KNM:C20	2.30	0.60
12:Z:21:THR:O	15:Z:300:KNM:H25	2.00	0.60
1:A:69:LEU:HD12	1:A:229:ILE:HG13	1.82	0.60
12:L:111:LEU:HD23	12:L:124:ALA:O	2.02	0.60
8:H:119:MET:SD	14:N:57:TYR:HB3	2.40	0.60
1:O:43:ARG:HD2	1:O:149:PRO:O	2.01	0.60
1:O:229:ILE:HD12	1:O:229:ILE:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:166:ASP:CB	5:E:185:TYR:CZ	2.73	0.60
7:G:104:TYR:OH	8:H:70:LEU:HD21	2.02	0.60
10:J:55:LEU:HD13	10:J:103:TYR:HB2	1.82	0.60
13:M:46:LEU:HD23	13:M:72:LEU:CD2	2.31	0.60
6:T:77:LEU:HD11	6:T:80:ASP:CG	2.21	0.60
7:U:46:VAL:HG22	7:U:215:TRP:CD1	2.36	0.60
9:W:172:ASN:OD1	9:W:190:THR:O	2.18	0.60
10:X:122:SER:HB3	10:X:136:VAL:CG1	2.29	0.60
15:I:300:KNM:H5	15:I:300:KNM:H18	1.84	0.59
5:S:191:LEU:CD1	5:S:221:GLN:HG2	2.31	0.59
2:P:38:LYS:CA	2:P:43:VAL:HG22	2.28	0.59
3:Q:139:TRP:NE1	3:Q:144:GLY:HA2	2.18	0.59
8:V:4:MET:HB2	8:V:160:LEU:HD21	1.82	0.59
8:H:47:GLY:C	15:H:300:KNM:C13	2.71	0.59
10:J:64:GLN:CD	11:K:85:ARG:HH22	2.03	0.59
13:M:152:GLN:CB	9:W:202:TYR:HE2	2.13	0.59
6:T:121:GLN:HG3	7:U:122:TYR:HE2	1.66	0.59
11:Y:147:TYR:CD1	11:Y:159:LEU:HD21	2.36	0.59
12:Z:1:THR:HG22	12:Z:46:ALA:HA	1.84	0.59
8:H:8:PHE:HE2	8:H:143:TYR:CZ	2.20	0.59
12:Z:115:ASP:HB3	12:Z:119:ASN:HB2	1.84	0.59
3:C:139:TRP:NE1	3:C:144:GLY:HA2	2.18	0.59
11:K:19:ARG:O	11:K:20:VAL:CG2	2.50	0.59
12:L:115:ASP:HB3	12:L:119:ASN:HB2	1.84	0.59
14:N:16:PHE:CZ	14:N:165:ALA:CB	2.86	0.59
8:H:117:GLY:HA3	14:N:5:MET:HG3	1.84	0.59
11:Y:19:ARG:O	11:Y:20:VAL:CG2	2.50	0.59
1:A:109:ILE:HD13	1:A:114:LEU:HD23	0.66	0.59
13:M:99:ARG:CB	13:M:104:TYR:CE2	2.86	0.59
6:T:77:LEU:HD11	6:T:80:ASP:CB	2.33	0.59
8:V:32:ASP:CG	8:V:186:ARG:HH21	2.06	0.59
11:Y:48:GLY:O	11:Y:53:THR:HG21	2.02	0.59
11:Y:67:TYR:CZ	11:Y:75:LEU:HD21	2.38	0.59
12:L:1:THR:HG22	12:L:46:ALA:HA	1.84	0.59
13:M:99:ARG:HB3	13:M:104:TYR:HE2	1.66	0.59
2:P:212:CYS:HG	2:P:217:PHE:HD2	1.46	0.59
9:W:146:MET:HE1	9:W:154:LEU:HD23	1.85	0.59
15:W:300:KNM:H5	15:W:300:KNM:H18	1.84	0.59
12:Z:111:LEU:HD23	12:Z:124:ALA:O	2.02	0.59
9:I:104:ASP:O	9:I:105:VAL:C	2.42	0.59
11:K:67:TYR:CZ	11:K:75:LEU:HD21	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:16:PHE:CZ	14:N:165:ALA:HB3	2.38	0.59
1:O:109:ILE:CG2	1:O:114:LEU:HD11	2.32	0.59
2:P:68:THR:CG2	2:P:71:ILE:HB	2.27	0.59
3:Q:76:VAL:HG12	3:Q:132:VAL:HG11	1.84	0.59
11:Y:10:PRO:HD3	11:Y:151:ILE:HG22	1.85	0.59
2:P:71:ILE:HG22	2:P:72:GLY:N	2.18	0.59
6:T:152:ASN:HD21	7:U:81:LEU:HD12	1.68	0.59
5:E:50:VAL:HG22	5:E:66:LYS:HD3	1.85	0.58
6:F:77:LEU:HD11	6:F:80:ASP:CB	2.33	0.58
7:G:120:HIS:CE1	7:G:124:LEU:HD21	2.38	0.58
11:K:147:TYR:CD1	11:K:159:LEU:HD21	2.36	0.58
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.83	0.58
1:A:159:TYR:CD1	2:B:83:ARG:NH2	2.70	0.58
13:M:19:ASP:OD1	13:M:113:LEU:CD1	2.51	0.58
7:U:181:MET:O	7:U:182:LYS:C	2.41	0.58
11:Y:55:GLN:NE2	12:Z:88:TYR:CD2	2.69	0.58
3:C:76:VAL:HG12	3:C:132:VAL:HG11	1.84	0.58
7:U:120:HIS:CE1	7:U:124:LEU:HD21	2.38	0.58
14:N:41:ARG:HG3	14:N:41:ARG:HH11	1.68	0.58
13:M:104:TYR:HE1	14:N:97:TYR:HH	1.51	0.58
7:G:181:MET:O	7:G:182:LYS:C	2.41	0.58
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.83	0.58
13:M:15:ILE:HG22	13:M:135:PHE:CB	2.22	0.58
13:M:174:LEU:HD22	9:W:202:TYR:CZ	2.38	0.58
2:P:41:ASN:CB	2:P:183:LEU:HB2	2.19	0.58
7:U:122:TYR:CD1	7:U:131:PHE:CE1	2.92	0.58
13:M:99:ARG:CD	13:M:104:TYR:OH	2.52	0.58
2:B:71:ILE:HD11	2:B:106:THR:HA	1.86	0.58
8:V:83:PHE:CE2	8:V:100:ILE:HG12	2.39	0.58
9:W:49:ALA:CA	15:W:300:KNM:H36	2.34	0.58
14:N:173:MET:CB	14:N:187:PHE:CE2	2.85	0.58
2:P:39:ALA:CB	2:P:186:ALA:CB	2.82	0.58
2:P:71:ILE:HD11	2:P:106:THR:HA	1.86	0.58
8:V:3:ILE:CG2	8:V:99:ILE:HD12	2.33	0.58
6:F:14:SER:HB2	6:F:17:GLY:H	1.69	0.58
7:G:122:TYR:CD1	7:G:131:PHE:CE1	2.92	0.58
6:F:152:ASN:HD21	7:G:81:LEU:HD12	1.68	0.58
8:H:28:ASN:OD1	8:H:30:VAL:N	2.21	0.58
8:V:175:ARG:HG2	8:V:188:VAL:HG13	1.86	0.58
3:C:237:ILE:O	3:C:240:HIS:HB3	2.04	0.58
9:I:47:GLY:CA	15:I:300:KNM:H28	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:19:ARG:O	11:K:20:VAL:HG23	2.04	0.58
14:N:145:LEU:HD21	14:N:175:VAL:CG1	2.27	0.58
5:S:221:GLN:HB3	5:S:222:PRO:HD2	1.86	0.58
11:Y:19:ARG:O	11:Y:20:VAL:HG23	2.04	0.58
5:E:221:GLN:HB3	5:E:222:PRO:HD2	1.86	0.57
9:I:49:ALA:CA	15:I:300:KNM:H36	2.34	0.57
11:K:10:PRO:HD3	11:K:151:ILE:HG22	1.85	0.57
13:M:106:VAL:CG1	13:M:108:ASN:CG	2.72	0.57
13:M:146:GLN:HB3	10:X:176:ARG:HH12	1.69	0.57
1:O:109:ILE:HD13	1:O:114:LEU:HD23	0.66	0.57
1:A:109:ILE:CG2	1:A:114:LEU:HD11	2.32	0.57
2:B:71:ILE:HG22	2:B:72:GLY:N	2.18	0.57
6:F:14:SER:HB2	6:F:17:GLY:O	2.04	0.57
11:K:44:LEU:CB	11:K:102:LEU:HD11	2.32	0.57
3:Q:237:ILE:O	3:Q:240:HIS:HB3	2.04	0.57
11:Y:45:LEU:O	11:Y:102:LEU:HG	2.05	0.57
8:H:1:THR:CG2	8:H:2:THR:N	2.67	0.57
1:A:102:LYS:O	9:I:81:ARG:NH2	2.38	0.57
8:V:38:HIS:CD2	8:V:40:ARG:H	2.22	0.57
9:W:104:ASP:O	9:W:105:VAL:C	2.42	0.57
4:D:40:ILE:HG13	4:D:212:ARG:NH1	2.20	0.57
9:I:36:PHE:HA	9:I:42:TYR:CD1	2.38	0.57
11:K:121:LEU:O	11:K:122:ALA:CB	2.52	0.57
12:L:34:VAL:HG13	12:L:43:GLY:O	2.03	0.57
5:S:229:PHE:HZ	5:S:233:GLU:CG	2.04	0.57
9:W:36:PHE:HA	9:W:42:TYR:CD1	2.38	0.57
11:Y:8:GLN:HB2	11:Y:115:LEU:CD2	2.35	0.57
11:Y:121:LEU:O	11:Y:122:ALA:CB	2.52	0.57
12:Z:34:VAL:HG13	12:Z:43:GLY:O	2.03	0.57
1:A:103:TYR:C	9:I:81:ARG:CZ	2.73	0.57
9:I:186:LEU:O	9:I:189:TYR:HB2	2.05	0.57
14:N:9:THR:CG2	14:N:10:SER:H	2.15	0.57
4:R:40:ILE:HG13	4:R:212:ARG:NH1	2.19	0.57
8:V:47:GLY:C	15:V:300:KNM:C13	2.71	0.57
8:H:83:PHE:CE2	8:H:100:ILE:HG12	2.39	0.57
8:H:3:ILE:CG2	8:H:99:ILE:HD12	2.33	0.57
11:K:101:ASN:ND2	11:K:132:HIS:ND1	2.53	0.57
11:K:8:GLN:HB2	11:K:115:LEU:CD2	2.35	0.57
2:P:212:CYS:SG	2:P:217:PHE:CD2	2.98	0.57
6:T:14:SER:HB2	6:T:17:GLY:CA	2.34	0.57
11:Y:55:GLN:CD	12:Z:88:TYR:HD2	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:212:CYS:SG	2:B:217:PHE:CD2	2.98	0.57
6:F:69:HIS:CE1	6:F:102:PRO:HB2	2.40	0.57
8:H:32:ASP:CG	8:H:186:ARG:HH21	2.06	0.57
15:I:300:KNM:H5	15:I:300:KNM:C10	2.34	0.57
9:I:43:CYS:SG	9:I:98:LEU:HB3	2.45	0.57
11:K:55:GLN:CD	12:L:88:TYR:HD2	2.08	0.57
6:T:19:ILE:H	6:T:19:ILE:HD12	1.69	0.57
5:E:218:ALA:HB1	5:E:226:PHE:HE1	1.66	0.57
8:H:175:ARG:HG2	8:H:188:VAL:HG13	1.86	0.57
9:I:60:SER:OG	9:I:64:GLU:OE2	2.23	0.57
8:V:7:GLN:HG2	8:V:8:PHE:N	2.19	0.57
12:Z:11:GLY:HA3	12:Z:178:HIS:NE2	2.19	0.57
15:W:300:KNM:H5	15:W:300:KNM:C10	2.34	0.57
9:W:47:GLY:CA	15:W:300:KNM:H28	2.33	0.57
15:I:300:KNM:C7	10:J:124:ASP:OD2	2.53	0.56
12:L:11:GLY:HA3	12:L:178:HIS:NE2	2.19	0.56
12:L:44:THR:HG22	12:L:45:MET:N	2.20	0.56
3:Q:198:ASN:CG	3:Q:240:HIS:CE1	2.78	0.56
5:S:50:VAL:HG22	5:S:66:LYS:HD3	1.85	0.56
8:V:33:LYS:HE2	15:V:300:KNM:H36	1.87	0.56
1:O:102:LYS:O	9:W:81:ARG:NH2	2.38	0.56
15:Z:300:KNM:H15	15:Z:300:KNM:H25	1.70	0.56
2:B:39:ALA:CB	2:B:186:ALA:CB	2.82	0.56
9:I:129:SER:N	15:I:300:KNM:O4	2.38	0.56
14:N:89:HIS:CE1	14:N:125:VAL:HG22	2.40	0.56
14:N:89:HIS:NE2	14:N:131:ALA:HB1	2.19	0.56
9:W:60:SER:OG	9:W:64:GLU:OE2	2.23	0.56
11:Y:101:ASN:ND2	11:Y:132:HIS:ND1	2.53	0.56
12:Z:42:LEU:HD11	12:Z:184:TRP:CG	2.40	0.56
6:F:184:LEU:CD2	6:F:214:ILE:HG21	2.22	0.56
8:H:38:HIS:CD2	8:H:40:ARG:H	2.22	0.56
9:I:170:GLY:O	9:I:171:SER:HB2	2.05	0.56
9:W:186:LEU:O	9:W:189:TYR:HB2	2.05	0.56
10:X:73:TYR:CZ	10:X:77:GLU:OE2	2.58	0.56
11:Y:44:LEU:CB	11:Y:102:LEU:HD11	2.32	0.56
8:H:4:MET:HB2	8:H:160:LEU:HD21	1.82	0.56
10:J:73:TYR:CZ	10:J:77:GLU:OE2	2.58	0.56
15:L:300:KNM:H15	15:L:300:KNM:H25	1.70	0.56
14:N:16:PHE:O	14:N:19:GLY:O	2.22	0.56
2:B:51:GLN:NE2	2:B:56:TYR:HB2	2.18	0.56
3:C:198:ASN:CG	3:C:240:HIS:CE1	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:66:ASP:CB	4:D:68:ASN:OD1	2.54	0.56
12:L:42:LEU:HD11	12:L:184:TRP:CG	2.40	0.56
12:L:49:ALA:HB2	15:L:300:KNM:H32	1.88	0.56
14:N:115:TYR:CZ	14:N:118:GLY:HA2	2.41	0.56
6:T:13:TRP:CG	7:U:22:GLN:NE2	2.73	0.56
6:F:13:TRP:CG	7:G:22:GLN:NE2	2.73	0.56
13:M:99:ARG:HD3	13:M:104:TYR:CE1	2.28	0.56
2:P:38:LYS:HA	2:P:43:VAL:CG2	2.31	0.56
9:W:129:SER:N	15:W:300:KNM:O4	2.38	0.56
15:W:300:KNM:C7	10:X:124:ASP:OD2	2.53	0.56
9:W:170:GLY:O	9:W:171:SER:HB2	2.05	0.56
12:Z:44:THR:HG22	12:Z:45:MET:N	2.20	0.56
2:B:118:GLN:NE2	3:C:82:ASP:OD1	2.39	0.56
12:Z:49:ALA:HB2	15:Z:300:KNM:H32	1.88	0.56
11:K:45:LEU:O	11:K:102:LEU:HG	2.05	0.56
2:P:118:GLN:NE2	3:Q:82:ASP:OD1	2.39	0.56
6:T:69:HIS:CE1	6:T:102:PRO:HB2	2.40	0.56
8:V:98:ILE:HG22	8:V:100:ILE:HG13	1.88	0.56
3:C:99:LEU:HD12	10:J:64:GLN:HB3	1.88	0.56
11:K:14:LEU:HD22	11:K:156:ALA:HB1	1.88	0.56
13:M:17:GLY:CA	13:M:166:LEU:CD2	2.61	0.56
13:M:17:GLY:HA3	13:M:166:LEU:CD1	2.36	0.56
4:R:66:ASP:CB	4:R:68:ASN:OD1	2.54	0.56
7:G:122:TYR:CE1	7:G:131:PHE:CZ	2.94	0.56
10:J:134:ASP:CG	10:J:135:PHE:H	2.07	0.56
14:N:4:PRO:HB2	14:N:56:ASP:OD1	2.06	0.56
5:S:211:ASN:O	5:S:214:ASN:N	2.31	0.56
8:V:3:ILE:O	8:V:127:ILE:HA	2.06	0.56
8:V:1:THR:CG2	8:V:2:THR:N	2.67	0.56
9:W:43:CYS:SG	9:W:98:LEU:HB3	2.45	0.56
8:H:20:THR:HG22	15:H:300:KNM:H38	1.75	0.55
9:I:49:ALA:HB2	15:I:300:KNM:H33	1.87	0.55
13:M:146:GLN:HB3	10:X:176:ARG:NH1	2.20	0.55
13:M:36:HIS:CB	14:N:132:TYR:OH	2.50	0.55
2:P:172:PHE:HE2	2:P:196:GLU:HG2	1.71	0.55
6:T:14:SER:HB2	6:T:17:GLY:HA2	1.88	0.55
11:Y:14:LEU:HD22	11:Y:156:ALA:HB1	1.88	0.55
2:B:62:HIS:ND1	2:B:219:ARG:NH1	2.53	0.55
4:D:196:LEU:O	4:D:196:LEU:HD23	2.05	0.55
12:L:178:HIS:HB3	12:L:187:VAL:HG21	1.88	0.55
13:M:13:LEU:CD1	13:M:149:LEU:HD13	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:49:ALA:HB2	15:W:300:KNM:H33	1.87	0.55
10:X:10:VAL:HG23	10:X:53:ALA:HB3	1.88	0.55
2:B:172:PHE:HE2	2:B:196:GLU:HG2	1.71	0.55
2:B:44:VAL:HG23	2:B:211:ILE:CG2	2.37	0.55
2:B:212:CYS:C	2:B:213:ASN:HD22	2.10	0.55
6:F:19:ILE:HD12	6:F:19:ILE:H	1.70	0.55
13:M:113:LEU:HD23	13:M:114:ASP:O	2.06	0.55
13:M:152:GLN:NE2	9:W:202:TYR:CD2	2.74	0.55
2:P:62:HIS:ND1	2:P:219:ARG:NH1	2.53	0.55
4:R:196:LEU:O	4:R:196:LEU:HD23	2.05	0.55
2:B:38:LYS:CA	2:B:43:VAL:HG22	2.28	0.55
3:C:41:ASP:OD1	3:C:41:ASP:N	2.40	0.55
8:H:32:ASP:OD1	8:H:186:ARG:NH2	2.40	0.55
2:P:51:GLN:NE2	2:P:56:TYR:HB2	2.18	0.55
8:H:33:LYS:HE2	15:H:300:KNM:H36	1.87	0.55
10:J:10:VAL:HG23	10:J:53:ALA:HB3	1.88	0.55
13:M:152:GLN:NE2	9:W:202:TYR:CG	2.74	0.55
13:M:19:ASP:OD2	13:M:200:LYS:N	2.40	0.55
8:V:4:MET:CB	8:V:160:LEU:CD2	2.81	0.55
11:Y:120:TYR:CE1	11:Y:121:LEU:HG	2.41	0.55
11:K:120:TYR:CE1	11:K:121:LEU:HG	2.41	0.55
13:M:97:TYR:CE2	13:M:127:VAL:O	2.59	0.55
14:N:16:PHE:HE1	14:N:165:ALA:N	2.04	0.55
9:W:59:ILE:CG2	9:W:63:LEU:CD1	2.85	0.55
12:L:21:THR:HG23	15:L:300:KNM:H24	1.89	0.55
14:N:91:TRP:CZ3	14:N:94:ARG:HG3	2.40	0.55
13:M:15:ILE:CG2	13:M:135:PHE:CB	2.78	0.55
8:H:3:ILE:O	8:H:127:ILE:HA	2.06	0.55
15:H:300:KNM:H24	15:H:300:KNM:H28	1.89	0.55
13:M:13:LEU:CD1	13:M:149:LEU:CD1	2.85	0.55
7:U:122:TYR:CE1	7:U:131:PHE:CZ	2.94	0.55
12:Z:21:THR:HG23	15:Z:300:KNM:H24	1.89	0.55
3:Q:41:ASP:N	3:Q:41:ASP:OD1	2.40	0.54
6:T:43:HIS:CB	6:T:184:LEU:HD13	2.38	0.54
9:W:144:PRO:O	9:W:145:ASP:CB	2.55	0.54
2:B:38:LYS:HA	2:B:43:VAL:CG2	2.31	0.54
13:M:15:ILE:HD11	13:M:175:VAL:HG23	1.86	0.54
8:V:7:GLN:O	8:V:8:PHE:HB2	2.06	0.54
3:C:8:ARG:C	3:C:10:THR:H	2.10	0.54
12:L:1:THR:CG2	15:L:300:KNM:C17	2.85	0.54
8:V:28:ASN:OD1	8:V:29:ARG:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:7:GLN:O	8:V:8:PHE:CB	2.55	0.54
2:B:193:THR:O	2:B:195:LYS:N	3.33	0.54
15:V:300:KNM:H24	15:V:300:KNM:H28	1.89	0.54
3:Q:99:LEU:HD12	10:X:64:GLN:HB3	1.88	0.54
11:Y:29:LYS:HD3	12:Z:121:ILE:HB	1.89	0.54
3:C:115:CYS:HB3	4:D:81:ARG:NH2	2.22	0.54
10:J:64:GLN:HE22	11:K:85:ARG:NH2	1.97	0.54
2:P:212:CYS:SG	2:P:217:PHE:HD2	2.30	0.54
2:P:44:VAL:HG23	2:P:211:ILE:CG2	2.37	0.54
2:B:212:CYS:SG	2:B:217:PHE:HD2	2.30	0.54
3:C:12:PHE:CZ	4:D:25:ALA:HB2	2.43	0.54
13:M:16:ALA:HA	13:M:20:PHE:O	2.07	0.54
14:N:91:TRP:CZ3	14:N:94:ARG:CG	2.86	0.54
2:P:212:CYS:C	2:P:213:ASN:HD22	2.10	0.54
5:S:220:VAL:HG22	5:S:226:PHE:HD1	1.73	0.54
8:V:127:ILE:HD11	8:V:136:TYR:CE1	2.43	0.54
8:V:51:ASP:HB3	8:V:94:LEU:CD1	2.38	0.54
11:Y:184:ASP:O	11:Y:185:LYS:C	2.46	0.54
7:G:190:VAL:CG2	7:G:215:TRP:HZ2	2.06	0.54
8:H:127:ILE:HD11	8:H:136:TYR:CE1	2.43	0.54
9:I:144:PRO:O	9:I:145:ASP:CB	2.55	0.54
9:I:42:TYR:CD2	9:I:178:ILE:HD11	2.43	0.54
9:I:59:ILE:CG2	9:I:63:LEU:CD1	2.85	0.54
13:M:152:GLN:HG3	9:W:202:TYR:HD2	0.51	0.54
11:Y:121:LEU:O	11:Y:122:ALA:HB3	2.08	0.54
11:K:170:ARG:CZ	12:Z:136:TYR:CD1	2.88	0.54
12:Z:178:HIS:HB3	12:Z:187:VAL:HG21	1.88	0.54
12:L:44:THR:HB	12:L:100:MET:H	1.72	0.54
9:W:42:TYR:CD2	9:W:178:ILE:HD11	2.43	0.54
15:W:300:KNM:H12	10:X:124:ASP:OD2	2.08	0.54
3:Q:115:CYS:HB3	4:R:81:ARG:NH2	2.22	0.54
11:K:102:LEU:HD23	11:K:103:LEU:N	2.23	0.54
8:V:32:ASP:OD1	8:V:186:ARG:NH2	2.40	0.54
9:W:49:ALA:CA	9:W:52:THR:HG22	2.38	0.54
2:B:172:PHE:CE2	2:B:196:GLU:CG	2.90	0.53
2:B:41:ASN:CB	2:B:183:LEU:HB2	2.20	0.53
9:I:63:LEU:HD12	9:I:82:MET:SD	2.49	0.53
2:P:133:LEU:HD13	2:P:135:ILE:HG12	1.87	0.53
3:Q:8:ARG:C	3:Q:10:THR:H	2.10	0.53
3:Q:12:PHE:CZ	4:R:25:ALA:HB2	2.43	0.53
12:Z:44:THR:CG2	12:Z:45:MET:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:44:GLY:H	7:G:146:ALA:HB2	1.73	0.53
12:L:44:THR:CG2	12:L:45:MET:N	2.71	0.53
13:M:38:ARG:HH21	14:N:151:ARG:HD3	1.74	0.53
14:N:193:THR:O	14:N:195:LYS:N	2.41	0.53
9:W:49:ALA:HA	9:W:52:THR:CG2	2.38	0.53
12:Z:44:THR:HB	12:Z:100:MET:H	1.72	0.53
5:E:220:VAL:HG22	5:E:226:PHE:HD1	1.73	0.53
6:F:43:HIS:CB	6:F:184:LEU:HD13	2.38	0.53
9:I:22:GLU:HA	15:I:300:KNM:C4	2.38	0.53
9:I:52:THR:HG21	15:I:300:KNM:H38	1.91	0.53
11:K:29:LYS:HD3	12:L:121:ILE:HB	1.89	0.53
6:T:7:ASP:OD2	6:T:14:SER:OG	2.22	0.53
9:W:22:GLU:HA	15:W:300:KNM:C4	2.38	0.53
8:H:20:THR:HG22	15:H:300:KNM:H37	1.75	0.53
13:M:20:PHE:HZ	13:M:166:LEU:O	1.91	0.53
3:Q:12:PHE:HD2	4:R:21:TYR:HB2	1.74	0.53
5:S:37:ALA:O	5:S:170:ILE:N	2.38	0.53
11:Y:102:LEU:HD23	11:Y:103:LEU:N	2.23	0.53
12:Z:36:GLU:HA	12:Z:42:LEU:CD2	2.38	0.53
2:B:70:HIS:HD2	2:B:217:PHE:N	2.07	0.53
12:L:136:TYR:CD1	11:Y:170:ARG:CZ	2.88	0.53
8:H:28:ASN:OD1	8:H:29:ARG:N	2.41	0.53
9:W:70:THR:CG2	9:W:72:ARG:H	2.04	0.53
11:K:121:LEU:O	11:K:122:ALA:HB3	2.08	0.53
14:N:16:PHE:CE1	14:N:166:ARG:CA	2.76	0.53
1:O:134:LEU:CD2	7:U:124:LEU:HD22	2.39	0.53
2:P:134:LEU:HD23	2:P:162:MET:SD	2.48	0.53
8:V:1:THR:C	8:V:2:THR:CA	2.72	0.53
12:Z:1:THR:CG2	15:Z:300:KNM:C17	2.85	0.53
3:C:111:VAL:HG22	3:C:136:TYR:CE2	2.44	0.53
3:C:31:ALA:HB1	3:C:77:ALA:O	2.09	0.53
6:F:15:PRO:O	7:G:28:LYS:HE3	2.08	0.53
9:I:70:THR:CG2	9:I:72:ARG:H	2.04	0.53
12:L:39:PRO:O	12:L:184:TRP:NE1	2.42	0.53
14:N:4:PRO:HA	14:N:56:ASP:OD2	2.09	0.53
9:W:63:LEU:HD12	9:W:82:MET:SD	2.48	0.53
12:Z:39:PRO:O	12:Z:184:TRP:NE1	2.42	0.53
8:H:103:TRP:CZ2	8:H:181:GLU:HB3	2.44	0.53
8:H:51:ASP:HB3	8:H:94:LEU:CD1	2.38	0.53
13:M:13:LEU:HD11	13:M:149:LEU:HD13	1.91	0.53
13:M:174:LEU:CG	9:W:202:TYR:OH	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:77:LEU:HD11	6:T:80:ASP:HB2	1.90	0.53
12:L:136:TYR:CZ	11:Y:170:ARG:NH2	2.76	0.53
6:F:15:PRO:HA	7:G:25:TYR:CD1	2.44	0.53
11:K:8:GLN:HB2	11:K:115:LEU:HD21	1.91	0.53
7:U:75:MET:CA	7:U:137:LEU:CD2	2.68	0.53
8:V:103:TRP:CZ2	8:V:181:GLU:HB3	2.44	0.53
2:B:134:LEU:HD23	2:B:162:MET:SD	2.48	0.52
3:C:111:VAL:CG2	3:C:136:TYR:CD2	2.92	0.52
7:G:190:VAL:HG11	7:G:215:TRP:CH2	2.37	0.52
11:Y:120:TYR:HE1	11:Y:121:LEU:CD2	2.21	0.52
5:E:37:ALA:HB3	5:E:170:ILE:CG1	2.39	0.52
15:I:300:KNM:H12	10:J:124:ASP:OD2	2.08	0.52
11:K:184:ASP:O	11:K:185:LYS:C	2.46	0.52
7:U:44:GLY:H	7:U:146:ALA:HB2	1.73	0.52
9:I:1:THR:HG22	9:I:129:SER:OG	2.04	0.52
9:I:36:PHE:HE1	9:I:39:PRO:CA	2.19	0.52
13:M:135:PHE:CZ	13:M:150:ASP:HA	2.44	0.52
1:O:103:TYR:C	9:W:81:ARG:CZ	2.73	0.52
3:Q:139:TRP:HD1	3:Q:145:PHE:N	2.08	0.52
5:S:37:ALA:HB3	5:S:170:ILE:HG13	1.92	0.52
8:V:27:ALA:O	8:V:28:ASN:CB	2.57	0.52
10:X:17:ASN:O	10:X:118:PRO:HG3	2.10	0.52
11:Y:55:GLN:CD	12:Z:88:TYR:CD2	2.83	0.52
1:A:134:LEU:CD2	7:G:124:LEU:HD22	2.39	0.52
12:L:149:VAL:CG1	12:L:153:TYR:CZ	2.93	0.52
5:E:32:LYS:O	5:E:172:SER:HB3	2.10	0.52
6:F:77:LEU:HD11	6:F:80:ASP:HB2	1.90	0.52
14:N:41:ARG:HG3	14:N:41:ARG:NH1	2.25	0.52
7:U:75:MET:CG	7:U:137:LEU:HD23	2.35	0.52
3:C:79:ILE:CG2	3:C:80:THR:N	2.73	0.52
4:D:36:ARG:HG2	4:D:142:PRO:HB2	1.89	0.52
7:G:90:ILE:O	7:G:94:GLU:HG3	2.09	0.52
10:J:17:ASN:O	10:J:118:PRO:HG3	2.10	0.52
1:O:229:ILE:CD1	1:O:229:ILE:N	2.73	0.52
5:S:37:ALA:HB3	5:S:170:ILE:CG1	2.39	0.52
9:W:45:GLY:HA3	9:W:52:THR:OG1	2.10	0.52
11:Y:8:GLN:HB2	11:Y:115:LEU:HD21	1.91	0.52
6:F:69:HIS:CE1	6:F:96:ARG:NH2	2.77	0.52
10:J:16:LYS:O	10:J:18:CYS:O	2.27	0.52
11:K:120:TYR:HE1	11:K:121:LEU:CD2	2.21	0.52
3:Q:111:VAL:HG22	3:Q:136:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:42:THR:HG22	5:S:194:ALA:CB	2.02	0.52
10:X:16:LYS:O	10:X:18:CYS:O	2.27	0.52
10:J:134:ASP:CG	10:J:135:PHE:N	2.63	0.52
3:Q:111:VAL:CG2	3:Q:136:TYR:CD2	2.92	0.52
8:V:20:THR:HG22	15:V:300:KNM:H37	1.75	0.52
9:W:52:THR:HG21	15:W:300:KNM:H38	1.91	0.52
12:Z:149:VAL:CG1	12:Z:153:TYR:CZ	2.93	0.52
3:C:139:TRP:HD1	3:C:145:PHE:N	2.08	0.51
6:F:14:SER:HB2	6:F:17:GLY:C	2.29	0.51
8:H:96:ALA:O	8:H:116:MET:HA	2.10	0.51
11:K:85:ARG:HD3	11:K:124:LEU:HB3	1.92	0.51
2:P:70:HIS:HD2	2:P:217:PHE:N	2.07	0.51
11:Y:44:LEU:CD2	11:Y:102:LEU:HD11	2.39	0.51
9:I:45:GLY:HA3	9:I:52:THR:OG1	2.10	0.51
12:L:36:GLU:HA	12:L:42:LEU:CD2	2.37	0.51
2:P:51:GLN:HE22	2:P:56:TYR:H	1.58	0.51
4:D:192:ILE:HG12	4:D:228:TYR:CE1	2.44	0.51
9:I:172:ASN:ND2	9:I:191:VAL:HG22	2.21	0.51
3:Q:31:ALA:HB1	3:Q:77:ALA:O	2.09	0.51
9:W:1:THR:HG22	9:W:129:SER:OG	2.04	0.51
9:W:172:ASN:ND2	9:W:191:VAL:HG22	2.21	0.51
4:D:36:ARG:HG2	4:D:142:PRO:CG	2.41	0.51
5:E:37:ALA:HB3	5:E:170:ILE:HG13	1.92	0.51
9:I:122:LEU:HG	9:I:123:PRO:CD	2.38	0.51
9:I:127:MET:HG2	9:I:128:GLY:H	1.75	0.51
13:M:152:GLN:CD	9:W:202:TYR:HB2	2.29	0.51
2:P:172:PHE:CE2	2:P:196:GLU:CG	2.90	0.51
4:R:36:ARG:HG2	4:R:142:PRO:CG	2.41	0.51
2:P:211:ILE:HD13	2:P:220:LEU:HG	1.92	0.51
9:W:127:MET:HG2	9:W:128:GLY:H	1.75	0.51
8:H:1:THR:C	8:H:2:THR:CA	2.72	0.51
9:I:146:MET:CE	9:I:154:LEU:HD23	2.40	0.51
9:I:49:ALA:CA	9:I:52:THR:HG22	2.38	0.51
13:M:146:GLN:CB	10:X:176:ARG:HH12	2.23	0.51
14:N:173:MET:HB3	14:N:187:PHE:CD2	2.46	0.51
1:O:165:ALA:HB3	2:P:55:LEU:HD22	1.88	0.51
3:Q:79:ILE:CG2	3:Q:80:THR:N	2.73	0.51
5:S:229:PHE:CZ	5:S:233:GLU:HG3	2.38	0.51
9:W:36:PHE:HE1	9:W:39:PRO:CA	2.19	0.51
3:C:12:PHE:HD2	4:D:21:TYR:HB2	1.74	0.51
4:R:66:ASP:HB3	4:R:68:ASN:OD1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:90:ILE:O	7:U:94:GLU:HG3	2.09	0.51
8:H:8:PHE:CE2	8:H:143:TYR:CZ	2.98	0.51
11:K:55:GLN:CD	12:L:88:TYR:CD2	2.83	0.51
3:Q:151:ASP:HB3	3:Q:155:ASN:HB3	1.93	0.51
1:A:229:ILE:CD1	1:A:229:ILE:N	2.73	0.51
13:M:99:ARG:HD2	13:M:104:TYR:OH	2.09	0.51
14:N:26:MET:HB2	14:N:186:ARG:HH22	1.70	0.51
2:P:39:ALA:CB	2:P:186:ALA:HB3	2.39	0.51
8:V:96:ALA:O	8:V:116:MET:HA	2.10	0.51
9:W:146:MET:CE	9:W:154:LEU:HD23	2.40	0.51
9:W:173:ILE:HB	9:W:190:THR:HB	1.92	0.51
5:E:218:ALA:CB	5:E:226:PHE:HE1	2.22	0.51
5:E:37:ALA:O	5:E:169:ALA:HA	2.11	0.51
11:K:189:HIS:CD2	11:K:190:ASP:O	2.64	0.51
13:M:106:VAL:HG11	13:M:108:ASN:HD21	1.73	0.51
5:S:32:LYS:O	5:S:172:SER:HB3	2.10	0.51
1:A:13:ILE:HD11	1:A:15:ILE:HD13	1.93	0.50
2:B:133:LEU:HD13	2:B:135:ILE:HG12	1.87	0.50
2:B:51:GLN:HE22	2:B:56:TYR:H	1.58	0.50
6:F:77:LEU:HD12	6:F:80:ASP:H	1.74	0.50
8:H:98:ILE:HG22	8:H:100:ILE:HG13	1.88	0.50
12:L:55:TRP:CD1	12:L:97:MET:CE	2.94	0.50
14:N:25:ASP:HA	14:N:187:PHE:HB3	1.93	0.50
5:S:37:ALA:O	5:S:169:ALA:HA	2.11	0.50
7:U:216:VAL:O	7:U:216:VAL:HG12	2.11	0.50
4:D:208:LEU:HD21	4:D:228:TYR:HE1	1.77	0.50
6:F:103:LEU:HD21	6:F:108:LEU:HB2	1.93	0.50
6:F:188:VAL:HG13	6:F:212:ILE:HD13	1.92	0.50
15:L:300:KNM:H25	15:L:300:KNM:N2	2.26	0.50
13:M:164:VAL:HG13	13:M:166:LEU:H	1.76	0.50
3:Q:99:LEU:CD1	10:X:64:GLN:HB3	2.41	0.50
4:R:40:ILE:HG22	4:R:41:VAL:N	2.26	0.50
6:T:16:GLN:H	6:T:16:GLN:CD	2.15	0.50
8:V:9:ASP:CB	8:V:149:LYS:HD2	2.41	0.50
4:D:40:ILE:HG22	4:D:41:VAL:N	2.26	0.50
7:G:216:VAL:O	7:G:216:VAL:HG12	2.11	0.50
9:I:49:ALA:HA	9:I:52:THR:CG2	2.38	0.50
11:K:19:ARG:C	11:K:20:VAL:HG23	2.32	0.50
8:H:117:GLY:N	14:N:5:MET:HG3	2.26	0.50
1:O:221:THR:O	1:O:224:ASN:N	2.42	0.50
3:Q:10:THR:O	4:R:125:ARG:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Z:300:KNM:N2	15:Z:300:KNM:H25	2.26	0.50
1:O:13:ILE:HD11	1:O:15:ILE:HD13	1.93	0.50
6:T:96:ARG:HA	6:T:101:ARG:O	2.11	0.50
6:T:103:LEU:HD21	6:T:108:LEU:HB2	1.93	0.50
11:Y:19:ARG:C	11:Y:20:VAL:HG23	2.32	0.50
11:Y:85:ARG:HD3	11:Y:124:LEU:HB3	1.92	0.50
2:B:43:VAL:HG11	2:B:136:CYS:HB2	1.94	0.50
3:C:139:TRP:CD1	3:C:145:PHE:N	2.79	0.50
3:C:12:PHE:HD2	4:D:21:TYR:HB3	1.75	0.50
3:Q:111:VAL:HG22	3:Q:136:TYR:CG	2.47	0.50
1:A:109:ILE:HG23	1:A:114:LEU:HG	1.94	0.50
9:I:173:ILE:HB	9:I:190:THR:HB	1.92	0.50
10:J:163:PHE:HA	10:J:188:ILE:HD11	1.94	0.50
13:M:20:PHE:HA	13:M:198:VAL:O	2.11	0.50
1:O:217:VAL:O	1:O:229:ILE:HG23	2.12	0.50
2:P:133:LEU:CD1	2:P:135:ILE:CD1	2.89	0.50
9:W:113:ILE:HA	9:W:118:SER:O	2.11	0.50
10:X:134:ASP:CG	10:X:135:PHE:H	2.07	0.50
10:X:134:ASP:CG	10:X:135:PHE:N	2.63	0.50
2:B:211:ILE:HD13	2:B:220:LEU:HG	1.92	0.50
2:B:51:GLN:HE21	2:B:51:GLN:C	2.13	0.50
8:H:4:MET:CB	8:H:160:LEU:CD2	2.81	0.50
12:L:39:PRO:O	12:L:184:TRP:HD1	1.86	0.50
1:O:175:SER:HA	1:O:205:VAL:HG21	1.94	0.50
6:T:188:VAL:HG13	6:T:212:ILE:HD13	1.92	0.50
11:Y:78:THR:HG22	11:Y:116:TYR:HH	1.76	0.50
12:Z:55:TRP:CD1	12:Z:97:MET:CE	2.94	0.50
2:B:71:ILE:CG2	2:B:72:GLY:N	2.75	0.50
4:D:36:ARG:CG	4:D:142:PRO:CB	2.88	0.50
12:L:149:VAL:HG12	12:L:153:TYR:CE1	2.47	0.50
10:X:10:VAL:HG23	10:X:53:ALA:CB	2.41	0.50
11:Y:42:ILE:HD11	11:Y:75:LEU:O	2.12	0.50
1:A:134:LEU:HD22	7:G:124:LEU:HD22	1.94	0.50
2:B:138:TRP:NE1	2:B:143:PRO:CG	2.74	0.50
2:B:51:GLN:HE21	2:B:54:ILE:H	1.59	0.50
3:C:99:LEU:CD1	10:J:64:GLN:HB3	2.41	0.50
4:D:34:GLY:O	4:D:35:VAL:HG13	2.12	0.50
9:I:113:ILE:HA	9:I:118:SER:O	2.12	0.50
11:K:67:TYR:CZ	11:K:75:LEU:CD2	2.95	0.50
3:Q:12:PHE:HD2	4:R:21:TYR:HB3	1.76	0.50
6:T:184:LEU:HA	6:T:187:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:69:HIS:CE1	6:T:96:ARG:NH2	2.77	0.50
7:U:213:LEU:O	7:U:226:ILE:HD12	2.11	0.50
12:L:26:ILE:CD1	10:X:176:ARG:O	2.38	0.50
11:Y:78:THR:HG22	11:Y:116:TYR:CZ	2.47	0.50
1:A:217:VAL:O	1:A:229:ILE:HG23	2.12	0.49
3:C:111:VAL:HG22	3:C:136:TYR:CG	2.47	0.49
3:C:205:LYS:CA	3:C:240:HIS:NE2	2.73	0.49
4:D:66:ASP:HB3	4:D:68:ASN:OD1	2.11	0.49
5:E:35:SER:HB2	5:E:66:LYS:HZ3	1.76	0.49
8:H:98:ILE:HG22	8:H:99:ILE:N	2.27	0.49
10:J:10:VAL:HG23	10:J:53:ALA:CB	2.41	0.49
2:P:51:GLN:C	2:P:51:GLN:HE21	2.13	0.49
4:R:36:ARG:CG	4:R:142:PRO:CB	2.88	0.49
7:U:190:VAL:HG11	7:U:215:TRP:CH2	2.37	0.49
6:F:43:HIS:CD2	6:F:216:GLY:HA3	2.47	0.49
11:K:44:LEU:CD2	11:K:102:LEU:HD11	2.39	0.49
14:N:26:MET:HB3	14:N:39:ILE:O	2.12	0.49
14:N:45:VAL:HG12	14:N:46:ASN:OD1	2.12	0.49
2:P:106:THR:HG21	2:P:137:GLY:HA3	1.94	0.49
2:P:138:TRP:NE1	2:P:143:PRO:CG	2.74	0.49
2:P:34:SER:N	2:P:162:MET:O	2.31	0.49
3:Q:139:TRP:CD1	3:Q:145:PHE:N	2.79	0.49
4:R:192:ILE:HG12	4:R:228:TYR:CE1	2.44	0.49
4:R:208:LEU:HD21	4:R:228:TYR:HE1	1.77	0.49
11:Y:102:LEU:HD23	11:Y:103:LEU:C	2.33	0.49
11:Y:189:HIS:CD2	11:Y:190:ASP:O	2.64	0.49
12:Z:1:THR:CG2	12:Z:46:ALA:HA	2.42	0.49
2:B:137:GLY:N	2:B:144:TYR:O	2.40	0.49
9:I:122:LEU:CD1	9:I:123:PRO:HD2	2.42	0.49
1:O:134:LEU:HD22	7:U:124:LEU:HD22	1.94	0.49
2:P:51:GLN:HE21	2:P:54:ILE:H	1.59	0.49
10:X:137:VAL:CG2	10:X:146:TYR:CE2	2.69	0.49
12:Z:149:VAL:HG12	12:Z:153:TYR:CE1	2.47	0.49
2:B:34:SER:N	2:B:162:MET:O	2.31	0.49
3:C:151:ASP:HB3	3:C:155:ASN:HB3	1.93	0.49
6:F:184:LEU:HA	6:F:187:LEU:HD12	1.94	0.49
6:F:96:ARG:HA	6:F:101:ARG:O	2.11	0.49
13:M:49:LYS:HD2	13:M:113:LEU:HB3	1.93	0.49
14:N:59:ASP:HB2	14:N:108:ASN:CG	2.31	0.49
14:N:91:TRP:HA	14:N:91:TRP:CE3	2.47	0.49
3:Q:139:TRP:CD1	3:Q:144:GLY:C	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:20:THR:HG22	15:V:300:KNM:H38	1.75	0.49
2:B:106:THR:HG21	2:B:137:GLY:HA3	1.94	0.49
3:C:139:TRP:CD1	3:C:144:GLY:C	2.86	0.49
7:G:213:LEU:O	7:G:226:ILE:HD12	2.11	0.49
8:H:33:LYS:HE2	15:H:300:KNM:H32	1.94	0.49
11:K:102:LEU:HD23	11:K:103:LEU:C	2.33	0.49
11:K:15:VAL:HB	11:K:45:LEU:HD11	1.95	0.49
11:K:42:ILE:HD11	11:K:75:LEU:O	2.12	0.49
12:L:149:VAL:CG1	12:L:153:TYR:CE1	2.96	0.49
2:P:43:VAL:HG11	2:P:136:CYS:HB2	1.94	0.49
6:T:92:CYS:HA	6:T:103:LEU:CD1	2.42	0.49
6:T:43:HIS:CD2	6:T:216:GLY:HA3	2.47	0.49
8:V:66:HIS:O	8:V:70:LEU:HD13	2.13	0.49
10:X:64:GLN:HE22	11:Y:85:ARG:NH2	1.97	0.49
12:Z:39:PRO:O	12:Z:184:TRP:HD1	1.86	0.49
2:B:133:LEU:CD1	2:B:135:ILE:CD1	2.89	0.49
3:C:10:THR:O	4:D:125:ARG:HD3	2.12	0.49
10:X:163:PHE:HA	10:X:188:ILE:HD11	1.94	0.49
10:X:10:VAL:CG2	10:X:53:ALA:CB	2.90	0.49
11:Y:15:VAL:HB	11:Y:45:LEU:HD11	1.95	0.49
8:H:66:HIS:O	8:H:70:LEU:HD13	2.13	0.49
8:H:7:GLN:O	8:H:8:PHE:HB2	2.12	0.49
13:M:93:SER:O	13:M:97:TYR:HD2	1.95	0.49
8:V:98:ILE:HG22	8:V:99:ILE:N	2.27	0.49
9:W:122:LEU:CD1	9:W:123:PRO:HD2	2.42	0.49
5:E:177:ALA:HB2	5:E:205:VAL:HG11	1.95	0.49
10:J:10:VAL:CG2	10:J:53:ALA:CB	2.90	0.49
2:P:213:ASN:ND2	2:P:213:ASN:N	2.60	0.49
9:I:104:ASP:C	9:I:106:THR:N	2.65	0.49
13:M:27:THR:CG2	13:M:40:SER:O	2.58	0.49
12:Z:149:VAL:CG1	12:Z:153:TYR:CE1	2.96	0.49
2:B:54:ILE:O	2:B:54:ILE:HG22	2.13	0.49
5:E:37:ALA:O	5:E:170:ILE:N	2.38	0.49
9:I:59:ILE:O	9:I:63:LEU:HD13	2.12	0.49
11:K:5:ILE:HD11	11:K:143:LEU:CD2	2.43	0.49
2:P:71:ILE:CG2	2:P:72:GLY:N	2.75	0.49
4:R:34:GLY:O	4:R:35:VAL:HG13	2.12	0.49
8:V:4:MET:HB2	8:V:160:LEU:CD2	2.43	0.49
11:K:170:ARG:NH2	12:Z:136:TYR:CZ	2.76	0.48
13:M:20:PHE:CZ	13:M:166:LEU:O	2.66	0.48
13:M:99:ARG:NH1	13:M:104:TYR:CD1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:147:GLN:OE1	2:P:162:MET:SD	2.71	0.48
3:Q:76:VAL:HA	3:Q:134:LEU:CD2	2.43	0.48
9:W:59:ILE:O	9:W:63:LEU:HD13	2.12	0.48
2:B:213:ASN:ND2	2:B:213:ASN:N	2.60	0.48
5:E:229:PHE:HZ	5:E:233:GLU:CG	2.04	0.48
6:F:92:CYS:HA	6:F:103:LEU:CD1	2.42	0.48
7:G:75:MET:HE2	7:G:137:LEU:HD11	1.96	0.48
1:A:165:ALA:HB3	2:B:55:LEU:HD22	1.88	0.48
2:B:106:THR:CG2	2:B:137:GLY:HA3	2.43	0.48
2:B:147:GLN:OE1	2:B:162:MET:SD	2.71	0.48
3:C:107:CYS:H	3:C:140:ASP:HB3	1.79	0.48
12:L:1:THR:CG2	12:L:46:ALA:HA	2.42	0.48
12:L:21:THR:C	15:L:300:KNM:H11	2.34	0.48
15:L:300:KNM:H17	15:L:300:KNM:O5	2.13	0.48
2:P:106:THR:CG2	2:P:137:GLY:HA3	2.43	0.48
3:Q:65:ILE:HD11	3:Q:73:ALA:HB1	1.95	0.48
9:W:104:ASP:C	9:W:106:THR:N	2.65	0.48
3:C:12:PHE:HZ	4:D:25:ALA:HB2	1.78	0.48
8:H:27:ALA:O	8:H:28:ASN:CB	2.57	0.48
14:N:47:ASN:O	14:N:197:VAL:HG23	2.13	0.48
6:T:77:LEU:HD12	6:T:80:ASP:H	1.74	0.48
1:A:175:SER:HA	1:A:205:VAL:HG21	1.94	0.48
7:G:75:MET:CG	7:G:137:LEU:HD23	2.35	0.48
9:I:52:THR:HG21	15:I:300:KNM:C20	2.43	0.48
15:Z:300:KNM:H17	15:Z:300:KNM:O5	2.14	0.48
3:C:45:LEU:CD2	3:C:65:ILE:HD13	2.44	0.48
5:E:229:PHE:CZ	5:E:233:GLU:HG3	2.38	0.48
5:E:50:VAL:HG21	5:E:66:LYS:HD3	1.93	0.48
8:H:32:ASP:OD2	8:H:35:THR:HG22	2.14	0.48
12:L:4:LEU:HA	12:L:127:SER:HA	1.95	0.48
12:L:91:LYS:HE2	12:L:117:GLU:HB3	1.95	0.48
14:N:47:ASN:O	14:N:197:VAL:CG2	2.61	0.48
2:B:70:HIS:NE2	2:B:212:CYS:O	2.46	0.48
3:C:65:ILE:HD11	3:C:73:ALA:HB1	1.95	0.48
8:H:176:LEU:HB3	8:H:187:GLN:HG2	1.95	0.48
9:I:128:GLY:CA	15:I:300:KNM:O4	2.60	0.48
1:O:109:ILE:HG23	1:O:114:LEU:HG	1.94	0.48
7:U:75:MET:HE2	7:U:137:LEU:HD11	1.95	0.48
9:W:52:THR:HG21	15:W:300:KNM:C20	2.43	0.48
11:Y:67:TYR:CZ	11:Y:75:LEU:CD2	2.95	0.48
15:Z:300:KNM:H15	15:Z:300:KNM:H8	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:THR:CG2	5:E:194:ALA:HB3	2.00	0.48
14:N:91:TRP:HE3	14:N:91:TRP:HA	1.79	0.48
6:T:7:ASP:OD2	6:T:14:SER:CA	2.58	0.48
8:V:176:LEU:HB3	8:V:187:GLN:HG2	1.95	0.48
4:D:43:LEU:HD11	4:D:217:LEU:HD21	1.96	0.48
8:H:9:ASP:CB	8:H:149:LYS:HD2	2.44	0.48
15:I:300:KNM:C7	10:J:124:ASP:CG	2.77	0.48
15:L:300:KNM:H15	15:L:300:KNM:H8	1.77	0.48
2:P:54:ILE:O	2:P:54:ILE:HG22	2.13	0.48
3:Q:107:CYS:H	3:Q:140:ASP:HB3	1.79	0.48
8:V:125:PHE:HB3	8:V:143:TYR:HE2	1.78	0.48
8:V:33:LYS:HE2	15:V:300:KNM:H32	1.94	0.48
11:Y:24:ASN:HD21	11:Y:26:VAL:CG2	2.23	0.48
3:C:197:LEU:HD13	3:C:211:VAL:HG11	1.96	0.48
8:H:4:MET:HB2	8:H:160:LEU:CD2	2.43	0.48
12:L:22:ALA:HB2	15:L:300:KNM:H11	1.96	0.48
15:L:300:KNM:C14	15:L:300:KNM:H29	2.44	0.48
13:M:34:SER:O	13:M:34:SER:OG	2.30	0.48
1:O:179:LEU:HB3	2:P:55:LEU:HD21	1.95	0.48
11:Y:5:ILE:HD11	11:Y:143:LEU:CD2	2.43	0.48
12:Z:153:TYR:CZ	12:Z:187:VAL:HG11	2.49	0.48
1:A:179:LEU:HB3	2:B:55:LEU:HD21	1.95	0.47
1:A:221:THR:O	1:A:224:ASN:N	2.42	0.47
11:K:78:THR:HG22	11:K:116:TYR:CZ	2.47	0.47
3:Q:205:LYS:CA	3:Q:240:HIS:NE2	2.73	0.47
11:Y:67:TYR:CG	11:Y:75:LEU:HD11	2.49	0.47
7:G:75:MET:HG3	7:G:137:LEU:HD23	1.96	0.47
4:R:36:ARG:HG2	4:R:142:PRO:HB2	1.89	0.47
3:Q:12:PHE:HZ	4:R:25:ALA:HB2	1.78	0.47
8:V:32:ASP:OD2	8:V:35:THR:HG22	2.14	0.47
12:Z:21:THR:C	15:Z:300:KNM:H11	2.34	0.47
12:Z:51:ASP:HB3	12:Z:97:MET:HE1	1.95	0.47
3:C:159:TRP:CD2	4:D:54:GLN:NE2	2.80	0.47
5:E:166:ASP:CG	5:E:185:TYR:OH	2.52	0.47
5:E:188:SER:OG	5:E:189:MET:N	2.46	0.47
7:G:122:TYR:CE1	7:G:131:PHE:HZ	2.31	0.47
12:L:153:TYR:CZ	12:L:187:VAL:HG11	2.49	0.47
14:N:198:GLU:HG3	14:N:199:ILE:N	2.29	0.47
4:R:66:ASP:HB2	4:R:68:ASN:OD1	2.15	0.47
5:S:218:ALA:CB	5:S:226:PHE:HE1	2.22	0.47
7:U:122:TYR:CE1	7:U:131:PHE:HZ	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:125:PHE:HB3	8:V:143:TYR:CE2	2.49	0.47
9:W:122:LEU:HG	9:W:123:PRO:CD	2.38	0.47
2:B:179:GLU:HB3	2:B:180:ASP:H	1.34	0.47
13:M:54:CYS:SG	13:M:106:VAL:HG13	2.55	0.47
13:M:20:PHE:HB2	13:M:197:ILE:HG23	1.96	0.47
5:S:177:ALA:HB2	5:S:205:VAL:HG11	1.95	0.47
12:Z:91:LYS:HE2	12:Z:117:GLU:HB3	1.95	0.47
12:Z:22:ALA:HB2	15:Z:300:KNM:H11	1.96	0.47
15:H:300:KNM:H17	15:H:300:KNM:H26	1.60	0.47
11:K:67:TYR:CG	11:K:75:LEU:HD11	2.49	0.47
2:P:211:ILE:CD1	2:P:220:LEU:HG	2.45	0.47
5:E:100:TRP:C	5:E:100:TRP:CE3	2.88	0.47
6:F:184:LEU:HD11	6:F:214:ILE:HD12	0.72	0.47
7:G:94:GLU:CD	7:G:115:VAL:HG22	2.34	0.47
12:L:50:ALA:HB3	13:M:100:ARG:HH12	1.78	0.47
14:N:16:PHE:CZ	14:N:165:ALA:CA	2.92	0.47
3:Q:45:LEU:CD2	3:Q:65:ILE:HD13	2.44	0.47
5:S:50:VAL:HG21	5:S:66:LYS:HD3	1.93	0.47
6:T:152:ASN:ND2	7:U:81:LEU:HD12	2.30	0.47
12:Z:4:LEU:HA	12:Z:127:SER:HA	1.95	0.47
6:F:195:LEU:HD23	6:F:210:VAL:CG1	2.44	0.47
5:S:218:ALA:HB1	5:S:226:PHE:HE1	1.66	0.47
11:Y:24:ASN:ND2	11:Y:26:VAL:HG23	2.26	0.47
11:K:146:TYR:HH	12:Z:141:ARG:HB3	1.79	0.47
2:B:133:LEU:O	2:B:133:LEU:HD12	2.14	0.47
3:C:76:VAL:HA	3:C:134:LEU:CD2	2.43	0.47
7:G:122:TYR:CD1	7:G:131:PHE:HE1	2.31	0.47
10:J:97:LYS:HB2	10:J:101:PRO:HA	1.97	0.47
4:R:31:THR:HG23	4:R:165:ALA:CA	2.45	0.47
4:R:43:LEU:HD11	4:R:217:LEU:HD21	1.96	0.47
5:S:188:SER:OG	5:S:189:MET:N	2.46	0.47
5:S:35:SER:HB2	5:S:66:LYS:HZ3	1.76	0.47
4:D:66:ASP:HB2	4:D:68:ASN:OD1	2.15	0.47
4:D:155:ALA:HB3	5:E:63:SER:HB3	1.97	0.47
11:K:36:PHE:CE2	11:K:46:CYS:HB3	2.50	0.47
12:L:51:ASP:HB3	12:L:97:MET:HE1	1.95	0.47
13:M:99:ARG:CG	13:M:104:TYR:CE2	2.98	0.47
1:O:76:ILE:HD12	1:O:114:LEU:CD1	2.26	0.47
3:C:159:TRP:CE2	4:D:54:GLN:NE2	2.68	0.47
14:N:26:MET:CB	14:N:186:ARG:HH22	2.26	0.47
2:P:138:TRP:NE1	2:P:143:PRO:HG3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:172:ASN:OD1	9:W:191:VAL:CA	2.52	0.47
10:X:26:ARG:CG	10:X:33:MET:HG3	2.45	0.47
15:Z:300:KNM:H29	15:Z:300:KNM:C14	2.44	0.47
9:I:1:THR:HG21	15:I:300:KNM:O4	2.15	0.46
13:M:49:LYS:HB3	13:M:113:LEU:N	2.21	0.46
2:B:211:ILE:CD1	2:B:220:LEU:HG	2.45	0.46
8:H:63:LEU:O	8:H:66:HIS:HB3	2.16	0.46
6:T:81:ALA:HB2	6:T:130:VAL:HG21	1.96	0.46
7:U:75:MET:HG3	7:U:137:LEU:HD21	1.93	0.46
15:I:300:KNM:C4	15:I:300:KNM:C2	2.86	0.46
12:L:51:ASP:O	12:L:55:TRP:CD1	2.69	0.46
4:R:155:ALA:HB3	5:S:63:SER:HB3	1.97	0.46
12:Z:51:ASP:O	12:Z:55:TRP:CD1	2.69	0.46
6:F:81:ALA:HB2	6:F:130:VAL:HG21	1.96	0.46
2:P:133:LEU:HD12	2:P:133:LEU:O	2.14	0.46
2:P:133:LEU:CD1	2:P:135:ILE:HD11	2.44	0.46
4:R:40:ILE:HG22	4:R:211:MET:O	2.03	0.46
5:S:43:SER:CA	5:S:151:PRO:HG3	2.44	0.46
15:W:300:KNM:C7	10:X:124:ASP:CG	2.77	0.46
10:J:137:VAL:CG2	10:J:146:TYR:CE2	2.69	0.46
11:K:120:TYR:HE1	11:K:121:LEU:HD21	1.80	0.46
2:P:157:TRP:NE1	3:Q:56:LEU:HD21	2.30	0.46
5:S:100:TRP:CE3	5:S:100:TRP:C	2.88	0.46
9:W:49:ALA:HB2	15:W:300:KNM:H36	1.98	0.46
2:B:6:SER:O	3:C:127:LYS:HE3	2.16	0.46
9:I:63:LEU:HD21	9:I:79:ALA:HB2	1.98	0.46
13:M:197:ILE:H	13:M:197:ILE:HD12	1.81	0.46
4:R:6:ALA:CB	5:S:134:SER:OG	2.64	0.46
6:T:14:SER:HB2	6:T:17:GLY:HA3	1.98	0.46
8:V:63:LEU:O	8:V:66:HIS:HB3	2.16	0.46
9:W:1:THR:HG21	15:W:300:KNM:O4	2.15	0.46
2:B:157:TRP:NE1	3:C:56:LEU:HD21	2.30	0.46
3:Q:197:LEU:HD13	3:Q:211:VAL:HG11	1.96	0.46
2:B:70:HIS:CD2	2:B:217:PHE:N	2.84	0.46
8:H:9:ASP:HB2	8:H:149:LYS:HD2	1.98	0.46
10:J:57:THR:HG21	11:K:121:LEU:HB3	1.98	0.46
14:N:89:HIS:HB2	14:N:112:ILE:HD13	1.98	0.46
7:U:47:PHE:HE1	7:U:216:VAL:HG21	1.80	0.46
2:B:70:HIS:HE1	2:B:213:ASN:O	1.98	0.46
4:D:31:THR:HG23	4:D:165:ALA:CA	2.45	0.46
7:G:47:PHE:HE1	7:G:216:VAL:HG21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:26:ARG:CG	10:J:33:MET:HG3	2.45	0.46
9:W:22:GLU:HG3	9:W:22:GLU:O	2.16	0.46
2:B:138:TRP:NE1	2:B:143:PRO:HG3	2.30	0.46
2:B:39:ALA:CB	2:B:186:ALA:HB3	2.39	0.46
7:G:46:VAL:HG22	7:G:215:TRP:HD1	1.79	0.46
6:F:152:ASN:ND2	7:G:81:LEU:HD12	2.30	0.46
14:N:187:PHE:HE1	14:N:189:ILE:HD11	1.80	0.46
1:O:159:TYR:HD1	2:P:83:ARG:NH2	2.14	0.46
2:P:70:HIS:HE1	2:P:213:ASN:O	1.98	0.46
9:W:128:GLY:CA	15:W:300:KNM:O4	2.60	0.46
10:X:97:LYS:HB2	10:X:101:PRO:HA	1.97	0.46
11:Y:36:PHE:CE2	11:Y:46:CYS:HB3	2.50	0.46
4:D:199:VAL:HG12	4:D:200:GLN:H	1.81	0.45
5:E:169:ALA:C	5:E:174:SER:OG	2.55	0.45
11:K:184:ASP:O	11:K:187:GLY:N	2.37	0.45
13:M:49:LYS:HD2	13:M:113:LEU:O	2.16	0.45
4:R:199:VAL:HG12	4:R:200:GLN:H	1.81	0.45
4:R:216:SER:O	4:R:217:LEU:C	2.54	0.45
6:T:14:SER:CA	6:T:17:GLY:HA3	2.47	0.45
6:T:195:LEU:HD23	6:T:210:VAL:CG1	2.44	0.45
7:U:122:TYR:CD1	7:U:131:PHE:HE1	2.31	0.45
8:V:33:LYS:HE2	15:V:300:KNM:C18	2.45	0.45
10:X:57:THR:HG21	11:Y:121:LEU:HB3	1.98	0.45
8:H:10:GLY:O	8:H:103:TRP:CD1	2.69	0.45
9:I:22:GLU:O	9:I:22:GLU:HG3	2.16	0.45
3:Q:76:VAL:HG11	3:Q:83:ALA:HB2	1.94	0.45
11:Y:20:VAL:HG12	11:Y:21:ALA:N	2.32	0.45
2:B:82:TYR:O	2:B:86:VAL:HG23	2.16	0.45
5:E:43:SER:CA	5:E:151:PRO:HG3	2.44	0.45
11:K:85:ARG:CZ	11:K:86:ARG:NH2	2.74	0.45
12:L:125:THR:OG1	12:L:143:TYR:CE2	2.70	0.45
2:P:181:LEU:CD1	2:P:185:ASP:CB	2.94	0.45
5:S:82:ILE:HD12	5:S:82:ILE:H	1.81	0.45
6:T:184:LEU:HD11	6:T:214:ILE:HD12	0.72	0.45
7:U:48:GLY:HA3	7:U:193:VAL:HG11	1.98	0.45
8:V:46:SER:N	8:V:97:GLY:O	2.49	0.45
9:W:36:PHE:HB2	9:W:42:TYR:CE1	2.47	0.45
8:H:33:LYS:HE2	15:H:300:KNM:C18	2.45	0.45
9:I:36:PHE:HB2	9:I:42:TYR:CE1	2.47	0.45
13:M:20:PHE:CZ	13:M:166:LEU:HB3	2.51	0.45
2:P:96:TYR:CD1	2:P:104:ILE:HB	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:70:HIS:CD2	2:P:217:PHE:N	2.84	0.45
2:P:82:TYR:O	2:P:86:VAL:HG23	2.16	0.45
15:H:300:KNM:H27	15:H:300:KNM:H38	1.77	0.45
13:M:99:ARG:CB	13:M:104:TYR:HE2	2.28	0.45
2:P:6:SER:O	3:Q:127:LYS:HE3	2.16	0.45
5:S:169:ALA:C	5:S:174:SER:OG	2.55	0.45
7:U:75:MET:HG3	7:U:137:LEU:HD23	1.96	0.45
9:W:63:LEU:HD21	9:W:79:ALA:HB2	1.98	0.45
2:B:182:GLU:O	2:B:185:ASP:N	2.50	0.45
2:B:151:SER:O	3:C:81:SER:CB	2.65	0.45
9:I:11:GLY:HA2	9:I:108:PRO:HB3	1.99	0.45
8:H:46:SER:N	8:H:97:GLY:O	2.49	0.45
10:J:26:ARG:HG3	10:J:33:MET:HG3	1.99	0.45
13:M:20:PHE:HZ	13:M:166:LEU:HB3	1.81	0.45
8:V:9:ASP:CG	8:V:149:LYS:HB2	2.37	0.45
11:Y:120:TYR:HE1	11:Y:121:LEU:HD21	1.80	0.45
12:Z:49:ALA:CB	15:Z:300:KNM:H32	2.47	0.45
3:C:41:ASP:O	3:C:145:PHE:CE2	2.70	0.45
8:H:18:SER:CB	8:H:173:VAL:H	2.30	0.45
14:N:11:VAL:HG23	14:N:54:SER:OG	2.17	0.45
7:U:75:MET:CE	7:U:137:LEU:HD11	2.47	0.45
9:W:11:GLY:HA2	9:W:108:PRO:HB3	1.99	0.45
2:B:68:THR:HG22	2:B:71:ILE:CB	2.32	0.45
11:K:44:LEU:CD2	11:K:102:LEU:CD1	2.86	0.45
11:K:120:TYR:CE1	11:K:121:LEU:HD21	2.52	0.45
12:L:19:ARG:HB3	12:L:171:GLY:H	1.82	0.45
12:L:49:ALA:CB	15:L:300:KNM:H32	2.47	0.45
14:N:190:ALA:HA	14:N:199:ILE:HA	1.98	0.45
4:R:34:GLY:O	4:R:35:VAL:CG1	2.65	0.45
10:X:116:PHE:O	10:X:116:PHE:CG	2.70	0.45
2:B:45:LEU:HD21	2:B:136:CYS:HB3	1.99	0.45
7:G:48:GLY:HA3	7:G:193:VAL:HG11	1.98	0.45
13:M:38:ARG:HH22	9:W:164:PHE:HB3	1.82	0.45
5:S:40:ILE:HG21	5:S:194:ALA:HB1	1.98	0.45
8:V:42:PHE:HB2	8:V:179:ILE:HD11	2.00	0.45
1:O:100:ASN:HA	8:V:61:TYR:HE1	1.82	0.45
9:W:36:PHE:HD1	9:W:38:SER:O	1.98	0.45
10:X:134:ASP:OD2	10:X:135:PHE:CE1	2.70	0.45
4:D:6:ALA:CB	5:E:134:SER:OG	2.64	0.44
5:E:227:HIS:O	5:E:227:HIS:CG	2.70	0.44
8:H:112:TYR:CZ	8:H:122:ARG:HD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:1:THR:H2	9:I:169:SER:CB	2.29	0.44
11:K:20:VAL:HG12	11:K:21:ALA:N	2.32	0.44
14:N:16:PHE:CD1	14:N:161:SER:O	2.61	0.44
14:N:187:PHE:CD1	14:N:187:PHE:O	2.70	0.44
1:O:109:ILE:CG2	1:O:114:LEU:CD1	2.92	0.44
2:P:85:LEU:HD22	2:P:133:LEU:CD2	2.47	0.44
2:P:151:SER:O	3:Q:81:SER:CB	2.65	0.44
8:V:135:ILE:HG22	8:V:139:VAL:HG23	2.00	0.44
12:Z:88:TYR:O	12:Z:88:TYR:CD1	2.70	0.44
2:B:172:PHE:CZ	2:B:196:GLU:CD	2.88	0.44
3:C:8:ARG:O	3:C:10:THR:N	2.50	0.44
3:C:139:TRP:O	3:C:139:TRP:CE3	2.71	0.44
7:G:75:MET:CE	7:G:137:LEU:HD11	2.47	0.44
8:H:19:ARG:HH21	8:H:21:THR:HG21	1.82	0.44
13:M:118:LYS:CG	13:M:119:GLY:N	2.80	0.44
14:N:46:ASN:O	14:N:197:VAL:HG21	2.17	0.44
6:T:77:LEU:HD13	6:T:80:ASP:H	1.80	0.44
2:B:96:TYR:CD1	2:B:104:ILE:HB	2.51	0.44
4:D:216:SER:O	4:D:217:LEU:C	2.54	0.44
4:D:34:GLY:O	4:D:35:VAL:CG1	2.65	0.44
5:E:40:ILE:HG21	5:E:194:ALA:HB1	1.98	0.44
6:F:77:LEU:O	6:F:77:LEU:HD12	2.17	0.44
14:N:26:MET:HE2	14:N:186:ARG:HH12	0.31	0.44
1:O:109:ILE:CB	1:O:114:LEU:CD2	2.89	0.44
3:Q:33:THR:HG21	3:Q:200:THR:HG21	1.99	0.44
3:Q:8:ARG:O	3:Q:10:THR:N	2.50	0.44
5:S:219:THR:O	5:S:227:HIS:ND1	2.51	0.44
6:T:15:PRO:C	6:T:17:GLY:H	2.09	0.44
2:B:214:GLU:O	2:B:214:GLU:HG3	2.18	0.44
3:C:45:LEU:HD21	3:C:75:SER:HB2	2.00	0.44
14:N:46:ASN:C	14:N:48:SER:H	2.21	0.44
3:Q:45:LEU:HD21	3:Q:75:SER:HB2	2.00	0.44
6:T:121:GLN:CG	7:U:122:TYR:HE2	2.30	0.44
8:V:125:PHE:CD1	8:V:143:TYR:CE2	3.05	0.44
10:X:116:PHE:O	10:X:116:PHE:CD2	2.70	0.44
10:X:10:VAL:CG2	10:X:53:ALA:HB3	2.47	0.44
3:C:76:VAL:HG12	3:C:132:VAL:CG1	2.48	0.44
5:E:218:ALA:CB	5:E:226:PHE:HZ	2.27	0.44
10:J:116:PHE:CD2	10:J:116:PHE:O	2.70	0.44
12:L:88:TYR:O	12:L:88:TYR:CD1	2.70	0.44
2:P:182:GLU:O	2:P:185:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:41:ASP:O	3:Q:145:PHE:CE2	2.70	0.44
6:T:77:LEU:O	6:T:77:LEU:HD12	2.18	0.44
6:T:13:TRP:HD1	7:U:22:GLN:HE21	1.45	0.44
11:Y:44:LEU:CG	11:Y:102:LEU:HD21	2.40	0.44
12:Z:125:THR:OG1	12:Z:143:TYR:CE2	2.70	0.44
12:Z:19:ARG:HB3	12:Z:171:GLY:H	1.82	0.44
5:E:219:THR:O	5:E:227:HIS:ND1	2.51	0.44
5:E:82:ILE:H	5:E:82:ILE:HD12	1.81	0.44
6:F:15:PRO:HA	7:G:25:TYR:CE1	2.52	0.44
6:F:121:GLN:NE2	7:G:122:TYR:CE2	2.75	0.44
1:A:100:ASN:HA	8:H:61:TYR:HE1	1.82	0.44
10:J:134:ASP:OD2	10:J:135:PHE:CE1	2.70	0.44
11:K:147:TYR:CD1	11:K:159:LEU:CD2	2.95	0.44
10:X:26:ARG:HG3	10:X:33:MET:HG3	1.99	0.44
12:L:140:ASP:CG	11:Y:170:ARG:HD3	2.23	0.44
2:B:51:GLN:NE2	2:B:54:ILE:H	2.15	0.44
11:K:170:ARG:HD3	12:Z:140:ASP:CG	2.23	0.44
10:J:64:GLN:HE21	11:K:85:ARG:HH22	1.38	0.44
13:M:54:CYS:CB	13:M:108:ASN:HD22	2.30	0.44
13:M:185:ARG:HH21	10:X:150:GLU:CB	2.31	0.44
2:P:61:VAL:HG21	2:P:83:ARG:HH21	1.83	0.44
5:S:100:TRP:CE3	5:S:100:TRP:O	2.71	0.44
5:S:227:HIS:CG	5:S:227:HIS:O	2.71	0.44
2:B:181:LEU:CD1	2:B:185:ASP:CB	2.94	0.44
2:B:85:LEU:HD22	2:B:133:LEU:CD2	2.47	0.44
5:E:147:ASP:C	5:E:149:LYS:N	2.70	0.44
8:H:42:PHE:CE2	8:H:186:ARG:NH1	2.86	0.44
9:I:59:ILE:HG23	9:I:63:LEU:CD1	2.47	0.44
9:I:63:LEU:HD21	9:I:79:ALA:CB	2.47	0.44
2:P:45:LEU:HD21	2:P:136:CYS:HB3	1.99	0.44
2:P:51:GLN:NE2	2:P:54:ILE:H	2.15	0.44
2:P:53:SER:O	2:P:54:ILE:HB	2.18	0.44
2:P:53:SER:OG	2:P:56:TYR:CE1	2.70	0.44
3:Q:8:ARG:C	3:Q:10:THR:N	2.71	0.44
8:V:112:TYR:CZ	8:V:122:ARG:HD2	2.52	0.44
8:V:18:SER:CB	8:V:173:VAL:H	2.30	0.44
11:Y:147:TYR:CD1	11:Y:159:LEU:CD2	2.95	0.44
11:Y:184:ASP:O	11:Y:186:ASN:N	2.51	0.44
5:E:147:ASP:O	5:E:148:GLU:C	2.56	0.44
8:H:42:PHE:HB2	8:H:179:ILE:HD11	2.00	0.44
11:K:184:ASP:O	11:K:186:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:9:THR:CG2	14:N:140:GLY:O	2.63	0.44
4:R:196:LEU:HB3	4:R:232:ILE:HD13	1.99	0.44
8:V:45:ARG:CG	15:V:300:KNM:H34	2.46	0.44
9:W:59:ILE:HG23	9:W:63:LEU:CD1	2.48	0.44
5:E:100:TRP:CE3	5:E:100:TRP:O	2.71	0.43
8:H:135:ILE:HG22	8:H:139:VAL:HG23	2.00	0.43
13:M:167:SER:O	13:M:171:ALA:HB2	2.18	0.43
13:M:17:GLY:C	13:M:166:LEU:CD1	2.79	0.43
13:M:37:THR:HG23	13:M:40:SER:OG	2.18	0.43
14:N:9:THR:CG2	14:N:10:SER:N	2.73	0.43
14:N:142:GLY:HA2	14:N:146:ALA:H	1.83	0.43
13:M:104:TYR:CE1	14:N:97:TYR:OH	2.69	0.43
3:Q:159:TRP:CD2	4:R:54:GLN:NE2	2.80	0.43
9:W:63:LEU:HD21	9:W:79:ALA:CB	2.47	0.43
4:D:40:ILE:HG22	4:D:211:MET:O	2.03	0.43
6:F:152:ASN:OD1	6:F:153:TYR:N	2.51	0.43
7:G:75:MET:HE3	7:G:137:LEU:HD21	2.00	0.43
13:M:20:PHE:O	13:M:20:PHE:HD1	2.01	0.43
14:N:48:SER:HB3	14:N:196:GLY:HA3	1.99	0.43
5:S:227:HIS:O	5:S:227:HIS:CD2	2.71	0.43
6:T:152:ASN:OD1	6:T:153:TYR:N	2.51	0.43
8:V:42:PHE:CE2	8:V:186:ARG:NH1	2.86	0.43
8:V:98:ILE:CG2	8:V:99:ILE:N	2.81	0.43
15:W:300:KNM:C7	15:W:300:KNM:C1	2.89	0.43
15:W:300:KNM:C2	15:W:300:KNM:C4	2.86	0.43
10:X:10:VAL:CG2	10:X:53:ALA:HB2	2.48	0.43
10:J:6:ASN:HB3	10:J:7:GLY:H	1.59	0.43
12:L:103:GLY:HA2	12:L:179:VAL:HG11	2.00	0.43
1:O:43:ARG:CD	1:O:149:PRO:O	2.66	0.43
2:P:214:GLU:HG3	2:P:214:GLU:O	2.18	0.43
2:P:68:THR:HG22	2:P:71:ILE:CB	2.32	0.43
3:Q:139:TRP:CE3	3:Q:139:TRP:O	2.70	0.43
12:Z:103:GLY:HA2	12:Z:179:VAL:HG11	2.00	0.43
2:B:49:LYS:HB3	2:B:206:ASN:O	2.19	0.43
5:E:227:HIS:O	5:E:227:HIS:CD2	2.70	0.43
6:F:7:ASP:OD2	6:F:14:SER:CA	2.65	0.43
8:H:98:ILE:HG21	8:H:100:ILE:CD1	2.48	0.43
2:P:53:SER:OG	2:P:56:TYR:CD1	2.71	0.43
3:Q:139:TRP:HB2	3:Q:145:PHE:CE1	2.53	0.43
5:S:211:ASN:H	5:S:214:ASN:HB3	1.83	0.43
8:V:18:SER:HB3	8:V:173:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:19:ARG:HH21	8:V:21:THR:HG21	1.82	0.43
2:B:133:LEU:CD1	2:B:135:ILE:HD11	2.44	0.43
2:B:53:SER:O	2:B:54:ILE:HB	2.18	0.43
3:C:8:ARG:C	3:C:10:THR:N	2.71	0.43
7:G:216:VAL:O	7:G:216:VAL:CG1	2.66	0.43
8:H:98:ILE:CG2	8:H:99:ILE:N	2.81	0.43
9:I:172:ASN:OD1	9:I:191:VAL:CA	2.52	0.43
10:J:10:VAL:CG2	10:J:53:ALA:HB2	2.48	0.43
1:A:109:ILE:CB	1:A:114:LEU:CD2	2.89	0.43
1:A:43:ARG:CD	1:A:149:PRO:O	2.66	0.43
3:C:76:VAL:CG1	3:C:132:VAL:HG11	2.46	0.43
5:E:42:THR:HG22	5:E:194:ALA:CB	2.02	0.43
8:H:18:SER:HB3	8:H:173:VAL:H	1.84	0.43
3:Q:76:VAL:HG12	3:Q:132:VAL:CG1	2.48	0.43
3:Q:65:ILE:HD12	3:Q:74:CYS:O	2.19	0.43
5:S:147:ASP:O	5:S:148:GLU:C	2.56	0.43
2:B:61:VAL:HG21	2:B:83:ARG:HH21	1.83	0.43
3:C:205:LYS:HA	3:C:240:HIS:CD2	2.54	0.43
6:F:14:SER:CB	6:F:17:GLY:O	2.67	0.43
6:F:210:VAL:CG2	6:F:210:VAL:O	2.66	0.43
6:F:121:GLN:CG	7:G:122:TYR:HE2	2.30	0.43
8:H:160:LEU:O	8:H:163:ALA:HB3	2.18	0.43
8:H:18:SER:HB3	8:H:173:VAL:N	2.33	0.43
10:J:10:VAL:CG2	10:J:53:ALA:HB3	2.47	0.43
13:M:63:THR:HG21	14:N:97:TYR:CE2	2.54	0.43
2:P:137:GLY:N	2:P:144:TYR:O	2.40	0.43
2:P:70:HIS:NE2	2:P:212:CYS:O	2.46	0.43
1:O:180:GLU:OE2	2:P:54:ILE:HG13	2.19	0.43
7:U:94:GLU:CD	7:U:115:VAL:HG22	2.34	0.43
8:V:98:ILE:HG21	8:V:100:ILE:CD1	2.48	0.43
3:C:139:TRP:HB2	3:C:145:PHE:CE1	2.53	0.43
3:C:33:THR:HG21	3:C:200:THR:HG21	1.99	0.43
4:D:196:LEU:HB3	4:D:232:ILE:HD13	1.99	0.43
6:F:15:PRO:HG3	7:G:25:TYR:CZ	2.53	0.43
8:H:176:LEU:O	8:H:186:ARG:HA	2.19	0.43
8:H:1:THR:HG21	15:H:300:KNM:H39	1.81	0.43
2:P:49:LYS:HB3	2:P:206:ASN:O	2.19	0.43
7:U:46:VAL:HG22	7:U:215:TRP:HD1	1.79	0.43
1:A:180:GLU:OE2	2:B:54:ILE:HG13	2.19	0.43
2:B:53:SER:OG	2:B:56:TYR:CD1	2.71	0.43
13:M:149:LEU:O	13:M:153:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:76:VAL:CG1	3:Q:132:VAL:HG11	2.46	0.43
4:R:31:THR:HG23	4:R:165:ALA:HA	2.01	0.43
7:U:216:VAL:O	7:U:216:VAL:CG1	2.66	0.43
8:V:160:LEU:O	8:V:163:ALA:HB3	2.18	0.43
8:V:7:GLN:HG2	8:V:8:PHE:H	1.81	0.43
11:Y:120:TYR:CE1	11:Y:121:LEU:HD21	2.52	0.43
5:E:211:ASN:H	5:E:214:ASN:HB3	1.83	0.43
13:M:48:ASP:C	13:M:203:ILE:HG13	2.30	0.43
14:N:60:PHE:N	14:N:108:ASN:ND2	2.61	0.43
8:V:84:LYS:O	8:V:88:TYR:CB	2.63	0.43
3:C:65:ILE:HD12	3:C:74:CYS:O	2.19	0.42
4:D:36:ARG:HG2	4:D:142:PRO:CB	2.49	0.42
6:F:32:GLY:HA3	6:F:76:GLY:H	1.84	0.42
9:I:35:HIS:HB2	9:I:56:THR:HG21	2.01	0.42
11:K:10:PRO:HD2	11:K:12:TYR:CE1	2.53	0.42
14:N:26:MET:SD	14:N:186:ARG:O	2.77	0.42
8:V:10:GLY:O	8:V:103:TRP:CD1	2.70	0.42
1:A:221:THR:HG22	1:A:222:VAL:N	2.34	0.42
8:H:18:SER:HB3	8:H:172:GLY:CA	2.44	0.42
11:K:24:ASN:HD21	11:K:26:VAL:CG2	2.22	0.42
13:M:20:PHE:O	13:M:20:PHE:CD1	2.71	0.42
14:N:50:MET:HE2	14:N:192:VAL:H	1.84	0.42
14:N:25:ASP:HA	14:N:187:PHE:CB	2.49	0.42
9:W:146:MET:CE	9:W:154:LEU:CD2	2.97	0.42
9:I:36:PHE:CZ	9:I:38:SER:HA	2.54	0.42
13:M:17:GLY:CA	13:M:166:LEU:CD1	2.97	0.42
13:M:18:GLU:O	13:M:19:ASP:C	2.57	0.42
5:S:147:ASP:C	5:S:149:LYS:N	2.70	0.42
11:Y:15:VAL:HG11	11:Y:105:ALA:HB2	2.01	0.42
2:B:181:LEU:CD2	2:B:186:ALA:N	2.82	0.42
4:D:31:THR:HG23	4:D:165:ALA:HA	2.01	0.42
3:Q:7:SER:O	3:Q:8:ARG:HB2	2.20	0.42
8:V:42:PHE:CD2	8:V:186:ARG:NH1	2.87	0.42
8:V:18:SER:HB3	8:V:173:VAL:H	1.84	0.42
12:Z:3:THR:O	12:Z:100:MET:HE1	2.18	0.42
15:I:300:KNM:H41	15:I:300:KNM:H40	1.74	0.42
11:K:166:GLU:OE1	11:K:170:ARG:HG3	2.19	0.42
13:M:153:VAL:HG22	13:M:174:LEU:CD2	2.49	0.42
13:M:36:HIS:CG	14:N:132:TYR:OH	2.73	0.42
9:W:35:HIS:HB2	9:W:56:THR:HG21	2.01	0.42
12:Z:19:ARG:CB	12:Z:171:GLY:H	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:TYR:HD1	2:B:83:ARG:NH2	2.14	0.42
8:H:42:PHE:CD2	8:H:186:ARG:NH1	2.87	0.42
10:J:97:LYS:HB3	10:J:100:GLY:C	2.40	0.42
2:P:172:PHE:CZ	2:P:196:GLU:CD	2.88	0.42
2:P:179:GLU:HB3	2:P:180:ASP:H	1.34	0.42
4:R:80:ALA:HA	4:R:129:ILE:HD13	2.01	0.42
4:R:209:ALA:O	4:R:217:LEU:HD11	2.20	0.42
6:T:121:GLN:HG3	7:U:122:TYR:CE2	2.52	0.42
8:V:176:LEU:O	8:V:186:ARG:HA	2.19	0.42
8:V:45:ARG:CD	15:V:300:KNM:H34	2.50	0.42
10:J:116:PHE:CG	10:J:116:PHE:O	2.70	0.42
11:K:120:TYR:CE1	11:K:121:LEU:HD23	2.55	0.42
1:O:159:TYR:CE1	2:P:83:ARG:NH2	2.88	0.42
11:Y:9:GLY:HA3	11:Y:12:TYR:CE1	2.55	0.42
11:Y:166:GLU:OE1	11:Y:170:ARG:HG3	2.19	0.42
11:Y:20:VAL:CG1	11:Y:21:ALA:N	2.83	0.42
7:G:69:VAL:HG21	7:G:137:LEU:CD2	2.50	0.42
13:M:113:LEU:HB2	13:M:198:VAL:CG1	2.50	0.42
13:M:148:LEU:HD22	13:M:178:VAL:HG12	2.02	0.42
1:O:13:ILE:HG22	3:Q:5:TYR:CE2	2.55	0.42
3:C:33:THR:HG22	3:C:34:CYS:N	2.35	0.42
3:C:7:SER:O	3:C:8:ARG:HB2	2.20	0.42
4:D:209:ALA:O	4:D:217:LEU:HD11	2.20	0.42
4:D:80:ALA:HA	4:D:129:ILE:HD13	2.01	0.42
6:F:40:SER:HB2	6:F:187:LEU:HD11	2.02	0.42
8:H:7:GLN:O	8:H:8:PHE:CD2	2.73	0.42
9:I:97:ALA:HB3	9:I:127:MET:SD	2.59	0.42
9:I:146:MET:CE	9:I:154:LEU:CD2	2.97	0.42
9:I:49:ALA:HB2	15:I:300:KNM:H36	1.98	0.42
13:M:17:GLY:CA	13:M:166:LEU:HD13	2.49	0.42
2:P:181:LEU:HD23	2:P:186:ALA:N	2.34	0.42
4:R:46:GLU:HG2	4:R:47:LYS:H	1.85	0.42
5:S:227:HIS:NE2	5:S:229:PHE:HD1	2.16	0.42
6:T:40:SER:HB2	6:T:187:LEU:HD11	2.02	0.42
9:W:36:PHE:CZ	9:W:38:SER:HA	2.54	0.42
9:W:97:ALA:HB3	9:W:127:MET:SD	2.59	0.42
10:X:19:VAL:HG22	10:X:118:PRO:HG3	2.02	0.42
4:D:196:LEU:HD13	4:D:232:ILE:CG2	2.44	0.42
8:H:83:PHE:CG	8:H:100:ILE:HD11	2.54	0.42
10:J:58:ASP:OD1	10:J:102:TYR:HB3	2.20	0.42
2:P:68:THR:CG2	2:P:71:ILE:HG13	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:33:THR:HG22	3:Q:34:CYS:N	2.35	0.42
7:U:119:VAL:HA	7:U:131:PHE:CE1	2.55	0.42
7:U:169:ARG:O	7:U:173:LYS:HG2	2.20	0.42
2:B:181:LEU:HD23	2:B:186:ALA:N	2.34	0.41
7:G:119:VAL:HA	7:G:131:PHE:CE1	2.55	0.41
8:H:8:PHE:HB3	8:H:9:ASP:OD1	2.20	0.41
9:I:37:ILE:HG21	9:I:63:LEU:HD22	2.02	0.41
9:I:64:GLU:O	9:I:68:LEU:HB2	2.20	0.41
11:K:15:VAL:HG11	11:K:105:ALA:HB2	2.01	0.41
11:K:56:PHE:CE2	11:K:88:LEU:HD21	2.55	0.41
12:L:19:ARG:CB	12:L:171:GLY:H	2.33	0.41
2:P:181:LEU:CD2	2:P:186:ALA:N	2.82	0.41
2:P:151:SER:O	3:Q:81:SER:HB3	2.20	0.41
6:T:32:GLY:HA3	6:T:76:GLY:H	1.84	0.41
10:X:163:PHE:CA	10:X:188:ILE:HD11	2.50	0.41
11:Y:10:PRO:HD2	11:Y:12:TYR:CE1	2.53	0.41
5:E:43:SER:HA	5:E:151:PRO:CG	2.48	0.41
9:I:1:THR:HG23	9:I:1:THR:O	2.19	0.41
9:I:36:PHE:HD1	9:I:38:SER:O	1.98	0.41
3:Q:154:GLY:O	4:R:78:ALA:HB2	2.20	0.41
4:R:36:ARG:HG2	4:R:142:PRO:CB	2.49	0.41
8:V:38:HIS:CG	8:V:39:ASP:N	2.89	0.41
12:Z:21:THR:O	15:Z:300:KNM:H11	2.20	0.41
1:A:13:ILE:HG22	3:C:5:TYR:CE2	2.55	0.41
2:B:151:SER:O	3:C:81:SER:HB3	2.20	0.41
7:G:47:PHE:HE1	7:G:216:VAL:CG2	2.33	0.41
8:H:1:THR:HG23	8:H:33:LYS:HZ3	1.84	0.41
9:I:185:PHE:HE2	9:I:187:ARG:HD3	1.85	0.41
10:J:19:VAL:HG22	10:J:118:PRO:HG3	2.02	0.41
11:K:24:ASN:ND2	11:K:26:VAL:HG23	2.26	0.41
12:L:21:THR:O	15:L:300:KNM:H11	2.20	0.41
1:O:221:THR:HG22	1:O:222:VAL:N	2.34	0.41
2:P:147:GLN:OE1	2:P:162:MET:HG2	2.21	0.41
5:S:166:ASP:CG	5:S:185:TYR:OH	2.52	0.41
9:W:1:THR:HG23	9:W:1:THR:O	2.19	0.41
10:X:64:GLN:HE21	11:Y:85:ARG:HH22	1.38	0.41
2:B:68:THR:CG2	2:B:71:ILE:HG13	2.50	0.41
4:D:196:LEU:HD22	4:D:232:ILE:HG21	2.03	0.41
4:D:70:CYS:SG	4:D:217:LEU:HD22	2.60	0.41
7:G:169:ARG:O	7:G:173:LYS:HG2	2.20	0.41
11:K:9:GLY:HA3	11:K:12:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:210:GLY:HA2	2:P:219:ARG:HA	2.02	0.41
8:V:83:PHE:CG	8:V:100:ILE:HD11	2.54	0.41
1:A:109:ILE:CG2	1:A:114:LEU:CD1	2.92	0.41
1:A:159:TYR:CE1	2:B:83:ARG:NH2	2.88	0.41
11:K:44:LEU:CG	11:K:102:LEU:HD11	2.51	0.41
2:P:138:TRP:HE1	2:P:143:PRO:CD	2.19	0.41
10:X:27:PHE:CD2	10:X:38:PHE:CG	3.09	0.41
11:Y:85:ARG:CZ	11:Y:86:ARG:NH2	2.74	0.41
8:H:45:ARG:CD	15:H:300:KNM:H34	2.50	0.41
8:H:45:ARG:CG	15:H:300:KNM:H34	2.46	0.41
12:L:178:HIS:HB3	12:L:187:VAL:CG2	2.50	0.41
12:L:21:THR:O	15:L:300:KNM:C6	2.69	0.41
13:M:13:LEU:HD13	13:M:149:LEU:HD13	2.01	0.41
3:Q:205:LYS:HA	3:Q:240:HIS:CD2	2.54	0.41
5:S:218:ALA:CB	5:S:226:PHE:HZ	2.27	0.41
8:V:18:SER:HB3	8:V:172:GLY:CA	2.44	0.41
12:Z:21:THR:O	15:Z:300:KNM:C6	2.69	0.41
2:B:53:SER:OG	2:B:56:TYR:CE1	2.70	0.41
5:E:202:LEU:HA	5:E:205:VAL:HG22	2.03	0.41
5:E:220:VAL:HG22	5:E:226:PHE:CD1	2.55	0.41
7:G:41:CYS:SG	7:G:42:LYS:N	2.94	0.41
8:H:1:THR:CA	8:H:2:THR:N	2.77	0.41
9:I:151:ALA:HA	9:I:154:LEU:HB3	2.02	0.41
9:I:37:ILE:CG2	9:I:63:LEU:HD22	2.50	0.41
11:K:44:LEU:CG	11:K:102:LEU:HD21	2.40	0.41
12:L:3:THR:O	12:L:100:MET:HE1	2.21	0.41
3:Q:159:TRP:CE2	4:R:54:GLN:NE2	2.68	0.41
4:R:102:VAL:HG11	4:R:107:ILE:HD11	2.03	0.41
11:Y:9:GLY:HA3	11:Y:12:TYR:CZ	2.56	0.41
12:Z:49:ALA:CA	15:Z:300:KNM:H32	2.51	0.41
10:J:27:PHE:CD2	10:J:38:PHE:CG	3.09	0.41
11:K:120:TYR:CE1	11:K:121:LEU:CG	3.04	0.41
11:K:20:VAL:CG1	11:K:21:ALA:N	2.83	0.41
13:M:43:CYS:SG	13:M:43:CYS:O	2.79	0.41
4:R:70:CYS:SG	4:R:217:LEU:HD22	2.60	0.41
7:U:75:MET:HE2	7:U:137:LEU:HD21	2.03	0.41
8:V:127:ILE:HD12	8:V:132:SER:O	2.21	0.41
3:C:154:GLY:O	4:D:78:ALA:HB2	2.21	0.41
2:B:151:SER:O	3:C:81:SER:OG	2.39	0.41
4:D:46:GLU:HG2	4:D:47:LYS:H	1.85	0.41
15:I:300:KNM:C7	15:I:300:KNM:C1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:163:PHE:CA	10:J:188:ILE:HD11	2.50	0.41
13:M:100:ARG:HH12	13:M:127:VAL:HB	1.74	0.41
13:M:185:ARG:HH21	10:X:150:GLU:HB3	1.85	0.41
14:N:26:MET:SD	14:N:186:ARG:HG2	2.61	0.41
1:O:109:ILE:HG12	1:O:114:LEU:HG	2.02	0.41
2:P:151:SER:O	3:Q:81:SER:OG	2.39	0.41
4:R:144:LEU:O	4:R:144:LEU:HD23	2.21	0.41
5:S:202:LEU:HA	5:S:205:VAL:HG22	2.03	0.41
9:W:185:PHE:CE2	9:W:187:ARG:HB2	2.56	0.41
10:X:97:LYS:HB3	10:X:100:GLY:C	2.40	0.41
8:H:38:HIS:CG	8:H:39:ASP:N	2.89	0.41
9:I:129:SER:HG	15:I:300:KNM:H43	1.83	0.41
11:K:120:TYR:CD1	11:K:121:LEU:N	2.89	0.41
2:P:217:PHE:CD1	2:P:218:ARG:N	2.89	0.41
2:P:70:HIS:HA	2:P:217:PHE:HB2	2.03	0.41
9:W:185:PHE:HE2	9:W:187:ARG:HD3	1.85	0.41
9:W:37:ILE:CG2	9:W:63:LEU:HD22	2.50	0.41
10:X:58:ASP:OD1	10:X:102:TYR:HB3	2.20	0.41
11:Y:44:LEU:CG	11:Y:102:LEU:HD11	2.51	0.41
2:B:217:PHE:CD1	2:B:218:ARG:N	2.89	0.41
4:D:36:ARG:HD2	4:D:142:PRO:O	2.21	0.41
4:D:65:LEU:HD11	4:D:71:MET:HB2	2.03	0.41
9:I:185:PHE:CE2	9:I:187:ARG:HB2	2.55	0.41
11:K:184:ASP:OD2	11:K:186:ASN:OD1	2.39	0.41
4:R:196:LEU:HD22	4:R:232:ILE:HG21	2.03	0.41
8:V:178:ALA:HB3	8:V:185:GLU:H	1.86	0.41
9:W:8:TYR:CE1	9:W:13:VAL:HG23	2.56	0.41
10:X:119:PHE:CD1	10:X:119:PHE:C	2.94	0.41
10:X:154:GLU:OE2	10:X:161:HIS:CE1	2.74	0.41
1:A:77:GLY:HA3	1:A:227:PHE:CE1	2.56	0.40
2:B:133:LEU:HA	2:B:162:MET:HE1	2.03	0.40
6:F:137:TYR:CD1	6:F:216:GLY:HA2	2.56	0.40
8:H:127:ILE:HD12	8:H:132:SER:O	2.21	0.40
9:I:8:TYR:CE1	9:I:13:VAL:HG23	2.56	0.40
9:I:49:ALA:O	9:I:52:THR:HG22	2.21	0.40
12:L:20:ALA:CB	15:L:300:KNM:C19	2.99	0.40
12:L:49:ALA:CA	15:L:300:KNM:H32	2.51	0.40
14:N:48:SER:C	14:N:197:VAL:HG23	2.40	0.40
14:N:46:ASN:O	14:N:197:VAL:CG2	2.69	0.40
14:N:50:MET:HE2	14:N:192:VAL:N	2.36	0.40
14:N:7:THR:OG1	14:N:56:ASP:OD1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:43:VAL:CG1	2:P:44:VAL:N	2.84	0.40
2:P:83:ARG:O	2:P:87:HIS:CE1	2.75	0.40
7:U:41:CYS:SG	7:U:42:LYS:N	2.94	0.40
15:V:300:KNM:H17	15:V:300:KNM:H26	1.60	0.40
8:V:43:CYS:SG	8:V:98:ILE:CD1	3.06	0.40
9:W:151:ALA:HA	9:W:154:LEU:HB3	2.02	0.40
13:M:146:GLN:C	10:X:176:ARG:NH2	2.74	0.40
2:B:210:GLY:HA2	2:B:219:ARG:HA	2.02	0.40
4:D:144:LEU:O	4:D:144:LEU:HD23	2.21	0.40
5:E:227:HIS:NE2	5:E:229:PHE:HD1	2.16	0.40
7:G:87:LEU:HD13	7:G:135:PHE:CE1	2.57	0.40
8:H:84:LYS:O	8:H:88:TYR:CB	2.63	0.40
10:J:119:PHE:CD1	10:J:119:PHE:C	2.94	0.40
12:L:42:LEU:HD11	12:L:184:TRP:CD1	2.56	0.40
13:M:17:GLY:HA3	13:M:166:LEU:CG	2.41	0.40
1:O:180:GLU:OE2	2:P:54:ILE:HD12	2.22	0.40
3:Q:25:MET:HA	3:Q:28:ILE:HD13	2.02	0.40
7:U:47:PHE:HE1	7:U:216:VAL:CG2	2.33	0.40
12:Z:178:HIS:HB3	12:Z:187:VAL:CG2	2.50	0.40
2:B:147:GLN:OE1	2:B:162:MET:HG2	2.21	0.40
2:B:85:LEU:CD2	2:B:133:LEU:HD21	2.51	0.40
3:C:21:VAL:HG13	3:C:153:SER:HB3	2.04	0.40
1:A:13:ILE:CG2	3:C:5:TYR:CE2	3.05	0.40
3:C:115:CYS:CB	4:D:81:ARG:NH2	2.85	0.40
6:F:147:THR:HG22	6:F:153:TYR:HB3	2.04	0.40
9:I:8:TYR:CD1	9:I:13:VAL:HG23	2.57	0.40
11:K:9:GLY:HA3	11:K:12:TYR:CZ	2.56	0.40
12:L:149:VAL:O	12:L:153:TYR:CE1	2.74	0.40
12:L:1:THR:HG23	15:L:300:KNM:C17	2.45	0.40
14:N:147:GLN:HB3	14:N:148:PRO:HD3	2.03	0.40
3:Q:140:ASP:OD1	3:Q:143:TYR:HB2	2.21	0.40
4:R:196:LEU:HD22	4:R:232:ILE:CG2	2.51	0.40
4:R:39:ASP:O	4:R:40:ILE:HD13	2.22	0.40
5:S:187:LYS:O	5:S:188:SER:OG	2.29	0.40
5:S:70:ILE:CD1	5:S:76:CYS:HB2	2.48	0.40
7:U:69:VAL:HG21	7:U:137:LEU:CD2	2.50	0.40
10:X:17:ASN:C	10:X:17:ASN:OD1	2.60	0.40
12:Z:20:ALA:CB	15:Z:300:KNM:C19	2.99	0.40
1:A:76:ILE:HD12	1:A:114:LEU:CD1	2.26	0.40
2:B:147:GLN:CD	2:B:162:MET:SD	2.99	0.40
2:B:213:ASN:HD22	2:B:213:ASN:N	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ARG:O	2:B:87:HIS:CE1	2.75	0.40
11:K:3:TYR:CE2	11:K:167:LEU:HD11	2.57	0.40
2:P:147:GLN:CD	2:P:162:MET:SD	2.99	0.40
4:R:208:LEU:HD11	4:R:228:TYR:OH	2.22	0.40
7:U:75:MET:HE3	7:U:137:LEU:HD21	2.02	0.40
8:V:13:VAL:HG13	8:V:176:LEU:HD21	2.04	0.40
11:Y:115:LEU:HD23	11:Y:115:LEU:H	1.86	0.40
11:Y:29:LYS:HD2	12:Z:122:SER:C	2.42	0.40
2:B:134:LEU:HG	2:B:162:MET:CE	2.52	0.40
2:B:70:HIS:HA	2:B:217:PHE:HB2	2.03	0.40
6:F:103:LEU:HD23	6:F:103:LEU:C	2.42	0.40
8:H:13:VAL:HG13	8:H:176:LEU:HD21	2.04	0.40
13:M:166:LEU:O	13:M:167:SER:C	2.58	0.40
14:N:6:VAL:CG1	14:N:28:GLY:O	2.70	0.40
3:Q:12:PHE:HZ	4:R:25:ALA:CB	2.33	0.40
1:O:13:ILE:CG2	3:Q:5:TYR:CE2	3.05	0.40
5:S:220:VAL:HG22	5:S:226:PHE:CD1	2.55	0.40
9:W:37:ILE:HG21	9:W:63:LEU:HD22	2.02	0.40
11:Y:120:TYR:CD1	11:Y:121:LEU:N	2.89	0.40
11:Y:3:TYR:CE2	11:Y:167:LEU:HD11	2.57	0.40
12:Z:55:TRP:HA	12:Z:55:TRP:CE3	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	186/246 (76%)	178 (96%)	8 (4%)	0	100	100
1	O	186/246 (76%)	178 (96%)	8 (4%)	0	100	100
2	B	210/234 (90%)	198 (94%)	10 (5%)	2 (1%)	17	57
2	P	210/234 (90%)	198 (94%)	10 (5%)	2 (1%)	17	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	233/261 (89%)	225 (97%)	8 (3%)	0	100	100
3	Q	233/261 (89%)	225 (97%)	8 (3%)	0	100	100
4	D	206/248 (83%)	201 (98%)	5 (2%)	0	100	100
4	R	206/248 (83%)	201 (98%)	5 (2%)	0	100	100
5	E	211/241 (88%)	201 (95%)	9 (4%)	1 (0%)	31	71
5	S	211/241 (88%)	201 (95%)	9 (4%)	1 (0%)	31	71
6	F	187/263 (71%)	184 (98%)	3 (2%)	0	100	100
6	T	187/263 (71%)	185 (99%)	2 (1%)	0	100	100
7	G	203/255 (80%)	196 (97%)	7 (3%)	0	100	100
7	U	203/255 (80%)	196 (97%)	7 (3%)	0	100	100
8	H	179/205 (87%)	164 (92%)	13 (7%)	2 (1%)	16	56
8	V	179/205 (87%)	165 (92%)	12 (7%)	2 (1%)	16	56
9	I	194/234 (83%)	187 (96%)	6 (3%)	1 (0%)	31	71
9	W	194/234 (83%)	187 (96%)	6 (3%)	1 (0%)	31	71
10	J	168/204 (82%)	158 (94%)	10 (6%)	0	100	100
10	X	168/204 (82%)	158 (94%)	10 (6%)	0	100	100
11	K	187/201 (93%)	173 (92%)	10 (5%)	4 (2%)	8	41
11	Y	187/201 (93%)	173 (92%)	10 (5%)	4 (2%)	8	41
12	L	188/204 (92%)	182 (97%)	6 (3%)	0	100	100
12	Z	188/204 (92%)	182 (97%)	6 (3%)	0	100	100
13	M	186/213 (87%)	175 (94%)	10 (5%)	1 (0%)	31	71
13	a	186/213 (87%)	175 (94%)	10 (5%)	1 (0%)	31	71
14	N	178/219 (81%)	161 (90%)	17 (10%)	0	100	100
14	b	178/219 (81%)	161 (90%)	17 (10%)	0	100	100
All	All	5432/6456 (84%)	5168 (95%)	242 (4%)	22 (0%)	40	75

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	40	ALA
2	B	54	ILE
5	E	189	MET
8	H	8	PHE
11	K	122	ALA

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Mol	Chain	Res	Type
11	K	151	ILE
2	P	40	ALA
2	P	54	ILE
5	S	189	MET
8	V	8	PHE
11	Y	122	ALA
11	Y	151	ILE
8	H	28	ASN
11	K	176	PRO
8	V	28	ASN
11	Y	176	PRO
13	M	41	PRO
13	a	41	PRO
9	I	188	PRO
11	K	97	PRO
9	W	188	PRO
11	Y	97	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	166/210 (79%)	166 (100%)	0	100	100
1	O	166/210 (79%)	166 (100%)	0	100	100
2	B	177/191 (93%)	170 (96%)	7 (4%)	34	67
2	P	177/191 (93%)	170 (96%)	7 (4%)	34	67
3	C	199/221 (90%)	197 (99%)	2 (1%)	78	90
3	Q	199/221 (90%)	197 (99%)	2 (1%)	78	90
4	D	179/211 (85%)	177 (99%)	2 (1%)	76	89
4	R	179/211 (85%)	177 (99%)	2 (1%)	76	89
5	E	181/203 (89%)	180 (99%)	1 (1%)	87	95
5	S	181/203 (89%)	180 (99%)	1 (1%)	87	95
6	F	166/224 (74%)	166 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	T	166/224 (74%)	166 (100%)	0	100	100
7	G	170/212 (80%)	170 (100%)	0	100	100
7	U	170/212 (80%)	170 (100%)	0	100	100
8	H	142/159 (89%)	140 (99%)	2 (1%)	69	87
8	V	142/159 (89%)	140 (99%)	2 (1%)	69	87
9	I	162/195 (83%)	162 (100%)	0	100	100
9	W	162/195 (83%)	162 (100%)	0	100	100
10	J	149/173 (86%)	149 (100%)	0	100	100
10	X	149/173 (86%)	149 (100%)	0	100	100
11	K	160/171 (94%)	159 (99%)	1 (1%)	87	95
11	Y	160/171 (94%)	159 (99%)	1 (1%)	87	95
12	L	148/159 (93%)	148 (100%)	0	100	100
12	Z	148/159 (93%)	148 (100%)	0	100	100
13	M	155/178 (87%)	153 (99%)	2 (1%)	71	88
13	a	155/178 (87%)	153 (99%)	2 (1%)	71	88
14	N	152/181 (84%)	151 (99%)	1 (1%)	85	94
14	b	152/181 (84%)	151 (99%)	1 (1%)	85	94
All	All	4612/5376 (86%)	4576 (99%)	36 (1%)	84	92

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	51	GLN
2	B	70	HIS
2	B	106	THR
2	B	138	TRP
2	B	211	ILE
2	B	212	CYS
2	B	213	ASN
3	C	41	ASP
3	C	151	ASP
4	D	43	LEU
4	D	228	TYR
5	E	63	SER
8	H	9	ASP
8	H	176	LEU

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Mol	Chain	Res	Type
11	K	86	ARG
13	M	15	ILE
13	M	18	GLU
14	N	62	TYR
2	P	51	GLN
2	P	70	HIS
2	P	106	THR
2	P	138	TRP
2	P	211	ILE
2	P	212	CYS
2	P	213	ASN
3	Q	41	ASP
3	Q	151	ASP
4	R	43	LEU
4	R	228	TYR
5	S	63	SER
8	V	9	ASP
8	V	176	LEU
11	Y	86	ARG
13	a	15	ILE
13	a	18	GLU
14	b	62	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	51	GLN
2	B	62	HIS
2	B	87	HIS
2	B	206	ASN
2	B	213	ASN
3	C	84	ASN
5	E	224	GLN
7	G	22	GLN
7	G	105	ASN
8	H	38	HIS
10	J	64	GLN
10	J	161	HIS
10	J	187	HIS
11	K	101	ASN
11	K	186	ASN
11	K	189	HIS

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Mol	Chain	Res	Type
13	M	108	ASN
13	M	152	GLN
14	N	108	ASN
2	P	51	GLN
2	P	62	HIS
2	P	87	HIS
2	P	168	ASN
2	P	206	ASN
2	P	213	ASN
3	Q	84	ASN
4	R	146	GLN
4	R	154	HIS
5	S	224	GLN
7	U	22	GLN
7	U	105	ASN
8	V	38	HIS
9	W	80	ASN
10	X	64	GLN
10	X	161	HIS
10	X	187	HIS
11	Y	55	GLN
11	Y	101	ASN
11	Y	186	ASN
11	Y	189	HIS
13	a	108	ASN
13	a	152	GLN
14	b	108	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	KNM	H	300	8	30,30,68	1.73	2 (6%)	39,41,91	0.90	2 (5%)
15	KNM	I	300	9	29,29,68	1.71	2 (6%)	36,39,91	1.18	2 (5%)
15	KNM	L	300	12	30,30,68	1.72	2 (6%)	39,41,91	0.89	2 (5%)
15	KNM	V	300	8	30,30,68	1.73	2 (6%)	39,41,91	0.90	2 (5%)
15	KNM	W	300	9	29,29,68	1.70	2 (6%)	36,39,91	1.18	2 (5%)
15	KNM	Z	300	12	30,30,68	1.72	2 (6%)	39,41,91	0.88	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	KNM	H	300	8	-	0/38/38/98	0/0/0/3
15	KNM	I	300	9	-	0/37/37/98	0/0/0/3
15	KNM	L	300	12	-	0/38/38/98	0/0/0/3
15	KNM	V	300	8	-	0/38/38/98	0/0/0/3
15	KNM	W	300	9	-	0/37/37/98	0/0/0/3
15	KNM	Z	300	12	-	0/38/38/98	0/0/0/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	V	300	KNM	C16-S1	-9.06	1.66	1.78
15	H	300	KNM	C16-S1	-9.06	1.66	1.78
15	L	300	KNM	C16-S1	-8.85	1.66	1.78
15	Z	300	KNM	C16-S1	-8.83	1.66	1.78
15	I	300	KNM	C16-S1	-8.55	1.66	1.78
15	W	300	KNM	C16-S1	-8.48	1.67	1.78
15	L	300	KNM	C22-S1	-2.18	1.66	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Z	300	KNM	C22-S1	-2.18	1.66	1.75
15	V	300	KNM	C22-S1	-2.16	1.66	1.75
15	H	300	KNM	C22-S1	-2.16	1.66	1.75
15	W	300	KNM	C22-S1	-2.13	1.66	1.75
15	I	300	KNM	C22-S1	-2.11	1.66	1.75

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	300	KNM	O4-S1-O5	-3.51	108.90	116.97
15	I	300	KNM	O4-S1-O5	-3.51	108.90	116.97
15	V	300	KNM	O4-S1-O5	-3.29	109.40	116.97
15	H	300	KNM	O4-S1-O5	-3.29	109.40	116.97
15	L	300	KNM	O4-S1-O5	-3.28	109.42	116.97
15	Z	300	KNM	O4-S1-O5	-3.28	109.42	116.97
15	L	300	KNM	C15-N3-C14	-2.42	119.36	123.22
15	Z	300	KNM	C15-N3-C14	-2.38	119.42	123.22
15	V	300	KNM	O5-S1-C16	2.37	109.99	108.35
15	H	300	KNM	O5-S1-C16	2.37	109.99	108.35
15	I	300	KNM	C1-N1-C3	4.46	122.34	114.11
15	W	300	KNM	C1-N1-C3	4.48	122.36	114.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 211 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	H	300	KNM	33	0
15	I	300	KNM	45	0
15	L	300	KNM	30	0
15	V	300	KNM	31	0
15	W	300	KNM	43	0
15	Z	300	KNM	29	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
8	H	1
8	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1:THR	C	2:THR	N	1.78
1	V	1:THR	C	2:THR	N	1.78