Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:19 PM BST

PDB ID	:	2FUG
Title	:	Crystal structure of the hydrophilic domain of respiratory complex I from Thermus thermophilus
Authors	:	Sazanov, L.A.; Hinchliffe, P.
Deposited on	:	2006-01-26
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

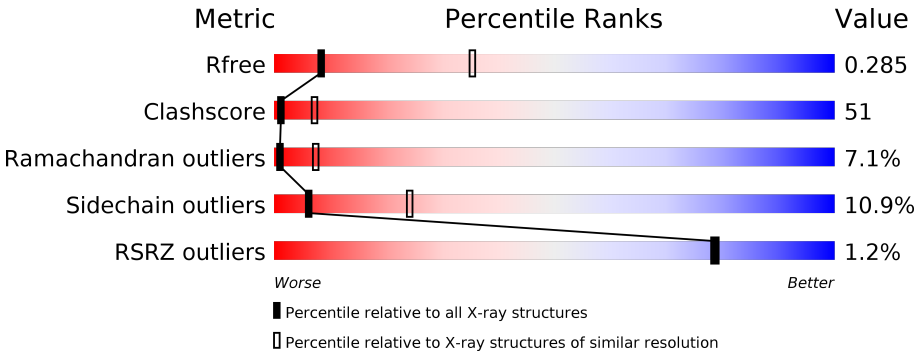
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	438	40% 49% 9%
1	A	438	40% 49% 9%
1	J	438	41% 47% 10%
1	S	438	40% 48% 10%
2	2	181	41% 48% 8%
2	B	181	45% 45% 7%

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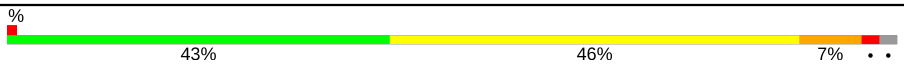
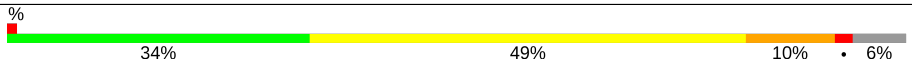
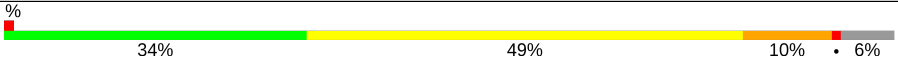
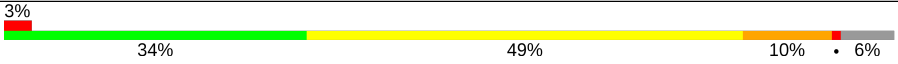
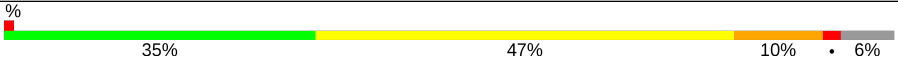
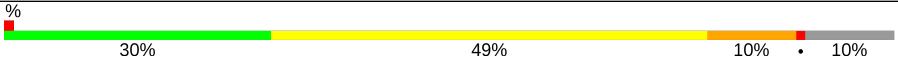
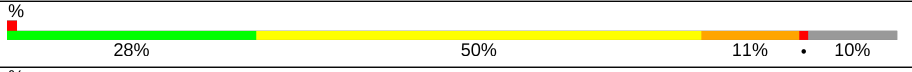
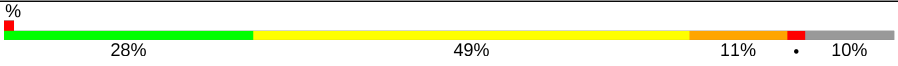
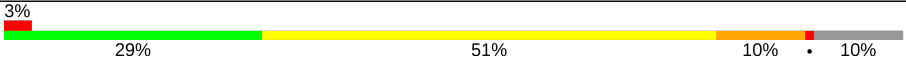
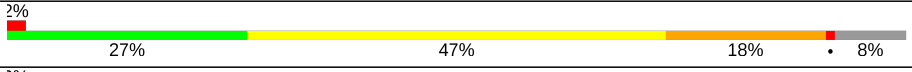
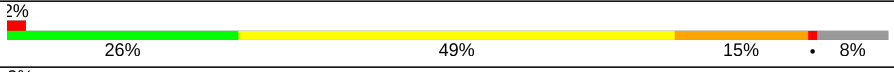
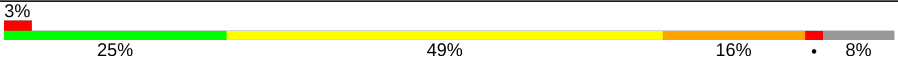
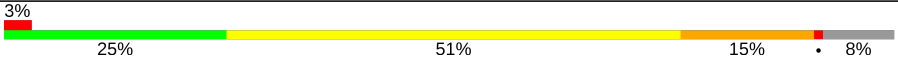
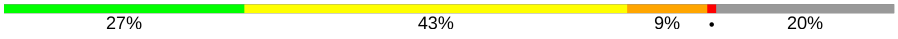
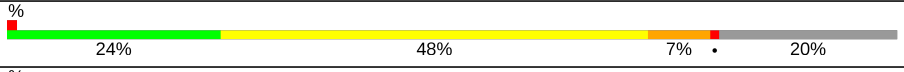
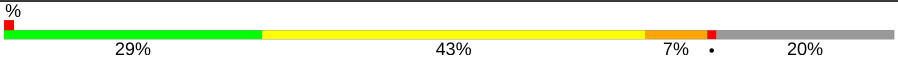
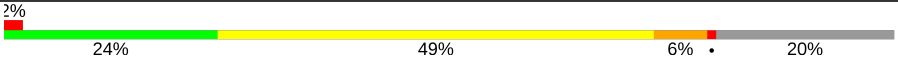
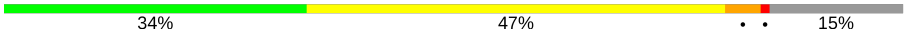
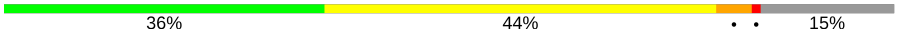
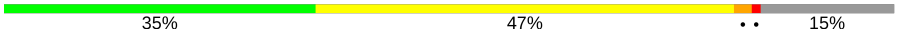
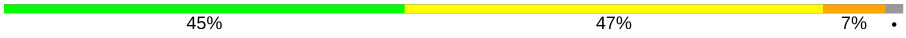
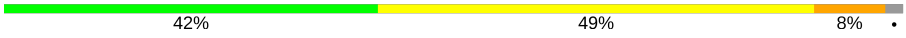
Mol	Chain	Length	Quality of chain
2	K	181	
2	T	181	
3	3	783	
3	C	783	
3	L	783	
3	U	783	
4	4	409	
4	D	409	
4	M	409	
4	V	409	
5	5	207	
5	E	207	
5	N	207	
5	W	207	
6	6	181	
6	F	181	
6	O	181	
6	X	181	
7	9	182	
7	G	182	
7	P	182	
7	Y	182	
8	7	129	
8	H	129	
8	Q	129	

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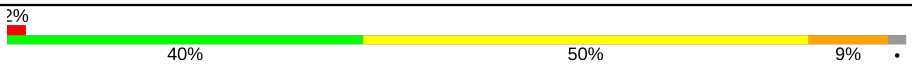
Mol	Chain	Length	Quality of chain
8	Z	129	

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
10	FES	2	182	-	-	X	-
10	FES	B	182	-	-	X	-
10	FES	K	182	-	-	X	-
9	SF4	3	786	-	-	X	-
9	SF4	C	786	-	-	X	-
9	SF4	L	786	-	-	X	-
9	SF4	U	786	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 73916 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 NADH-quinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	432	Total	C	N	O	S	0	0	0
			3383	2157	590	618	18			
1	A	432	Total	C	N	O	S	0	0	0
			3383	2157	590	618	18			
1	J	432	Total	C	N	O	S	0	0	0
			3383	2157	590	618	18			
1	S	432	Total	C	N	O	S	0	0	0
			3383	2157	590	618	18			

- Molecule 2 is a protein called NADH-quinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			
2	B	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			
2	K	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			
2	T	178	Total	C	N	O	S	0	0	0
			1406	895	238	265	8			

- Molecule 3 is a protein called NADH-quinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	737	Total	C	N	O	S	0	0	0
			5746	3657	1031	1027	31			
3	C	737	Total	C	N	O	S	0	0	0
			5746	3657	1031	1027	31			
3	L	737	Total	C	N	O	S	0	0	0
			5746	3657	1031	1027	31			
3	U	737	Total	C	N	O	S	0	0	0
			5746	3657	1031	1027	31			

- Molecule 4 is a protein called NADH-quinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	370	Total	C	N	O	S	0	0	0
			2953	1902	504	537	10			
4	D	370	Total	C	N	O	S	0	0	0
			2953	1902	504	537	10			
4	M	370	Total	C	N	O	S	0	0	0
			2953	1902	504	537	10			
4	V	370	Total	C	N	O	S	0	0	0
			2953	1902	504	537	10			

- Molecule 5 is a protein called NADH-quinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	5	191	Total	C	N	O	S	0	0	0
			1570	1018	267	282	3			
5	E	191	Total	C	N	O	S	0	0	0
			1570	1018	267	282	3			
5	N	191	Total	C	N	O	S	0	0	0
			1570	1018	267	282	3			
5	W	191	Total	C	N	O	S	0	0	0
			1570	1018	267	282	3			

- Molecule 6 is a protein called NADH-quinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	6	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			
6	F	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			
6	O	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			
6	X	144	Total	C	N	O	S	0	0	0
			1102	700	192	197	13			

- Molecule 7 is a protein called NADH-quinone oxidoreductase chain 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	9	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			
7	G	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			
7	P	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			

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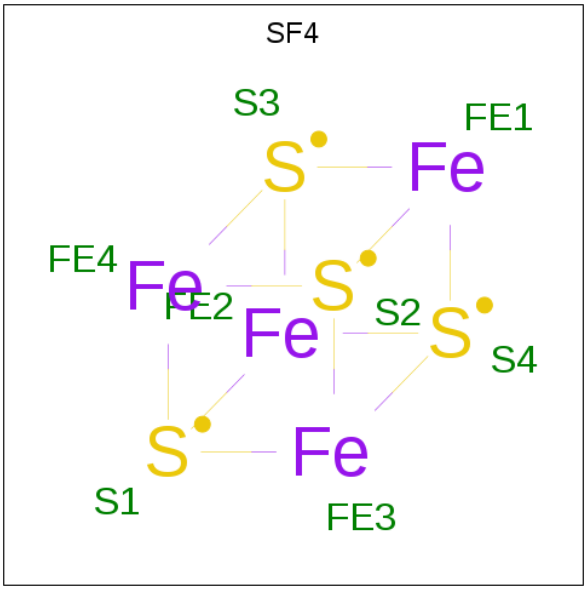
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Y	154	Total	C	N	O	S	0	0	0
			1193	759	201	222	11			

- Molecule 8 is a protein called conserved hypothetical protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	7	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	H	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	Q	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			
8	Z	127	Total	C	N	O	S	0	0	0
			1031	664	183	181	3			

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	1	1	Total	Fe	S		0	0
			8	4	4			
9	3	1	Total	Fe	S		0	0
			8	4	4			
9	3	1	Total	Fe	S		0	0
			8	4	4			
9	3	1	Total	Fe	S		0	0
			8	4	4			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	6	1	Total Fe S 8 4 4	0	0
9	9	1	Total Fe S 8 4 4	0	0
9	9	1	Total Fe S 8 4 4	0	0
9	A	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	0
9	F	1	Total Fe S 8 4 4	0	0
9	G	1	Total Fe S 8 4 4	0	0
9	G	1	Total Fe S 8 4 4	0	0
9	J	1	Total Fe S 8 4 4	0	0
9	L	1	Total Fe S 8 4 4	0	0
9	L	1	Total Fe S 8 4 4	0	0
9	L	1	Total Fe S 8 4 4	0	0
9	O	1	Total Fe S 8 4 4	0	0
9	P	1	Total Fe S 8 4 4	0	0
9	P	1	Total Fe S 8 4 4	0	0
9	S	1	Total Fe S 8 4 4	0	0
9	U	1	Total Fe S 8 4 4	0	0
9	U	1	Total Fe S 8 4 4	0	0
9	U	1	Total Fe S 8 4 4	0	0

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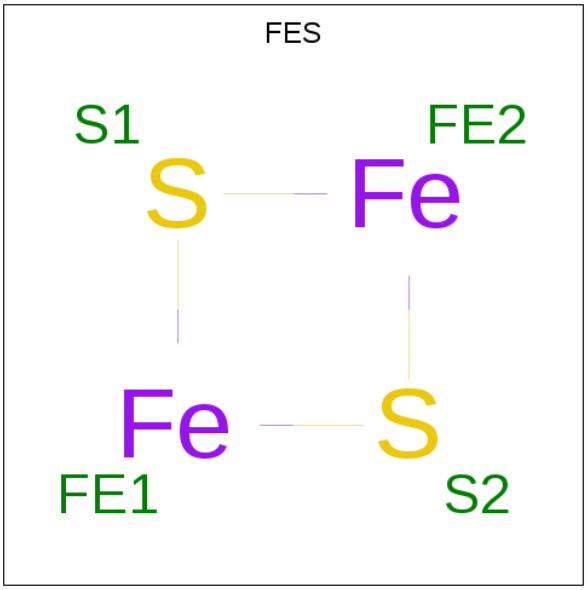
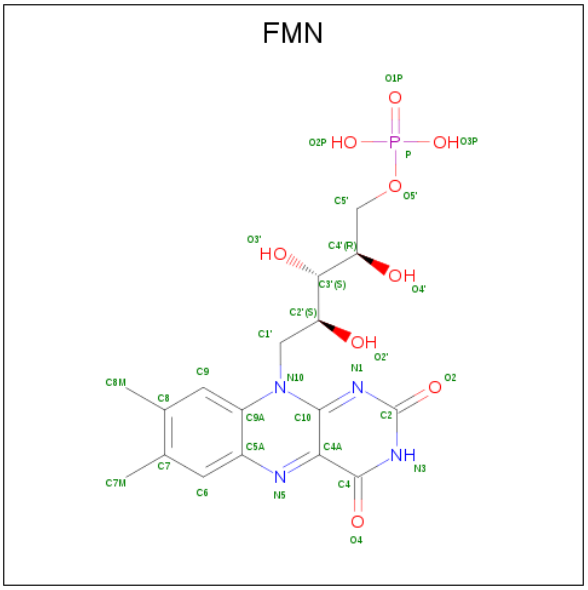
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	X	1	Total Fe S 8 4 4	0	0
9	Y	1	Total Fe S 8 4 4	0	0
9	Y	1	Total Fe S 8 4 4	0	0

- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	2	1	Total Fe S 4 2 2	0	0
10	3	1	Total Fe S 4 2 2	0	0
10	B	1	Total Fe S 4 2 2	0	0
10	C	1	Total Fe S 4 2 2	0	0
10	K	1	Total Fe S 4 2 2	0	0
10	L	1	Total Fe S 4 2 2	0	0
10	T	1	Total Fe S 4 2 2	0	0
10	U	1	Total Fe S 4 2 2	0	0

- Molecule 11 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



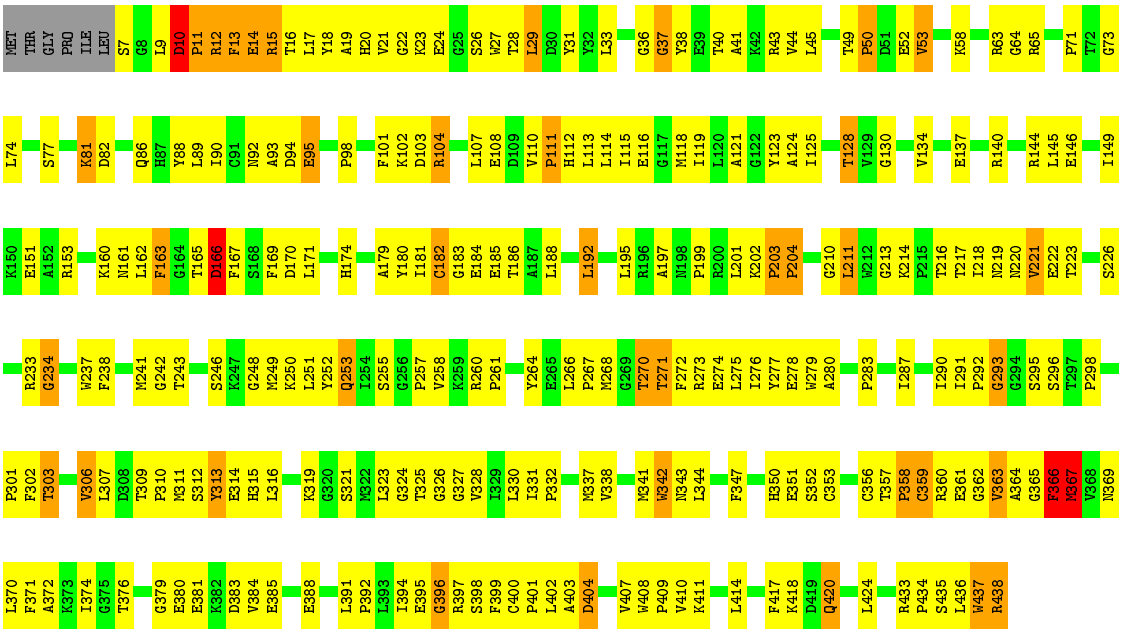
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	7	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
11	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
11	Q	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
11	Z	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

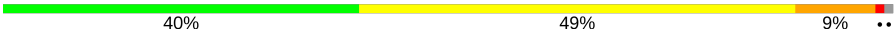
- Molecule 1: NADH-quinone oxidoreductase chain 1

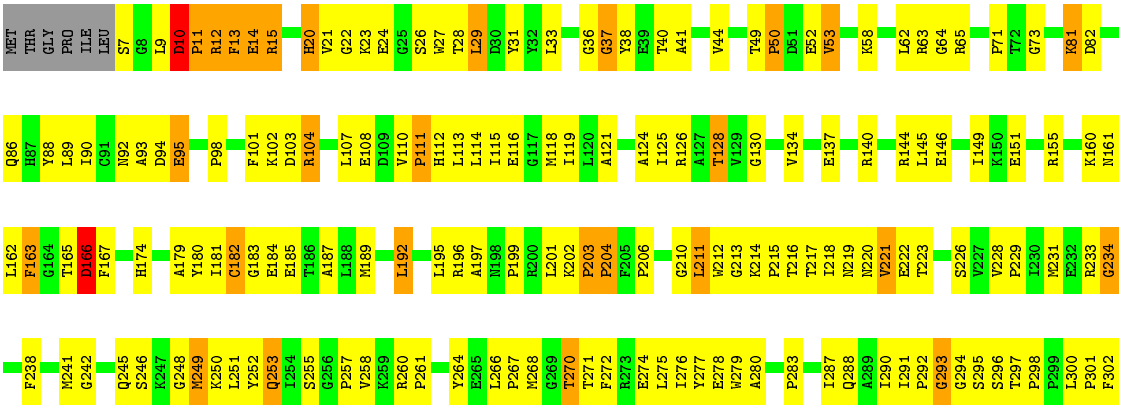
Chain 1:

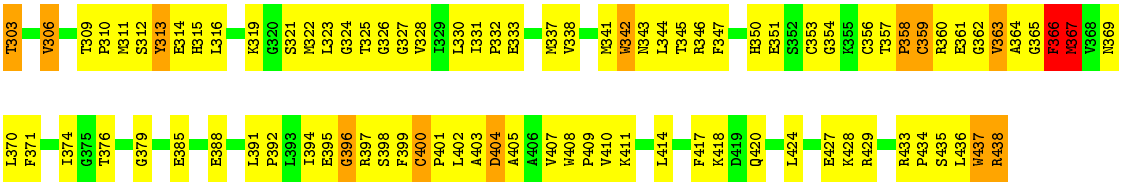


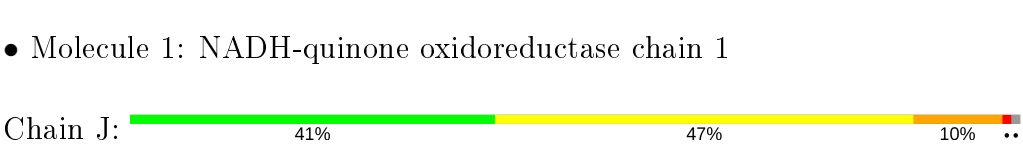
- Molecule 1: NADH-quinone oxidoreductase chain 1

Chain A:



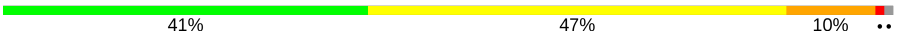


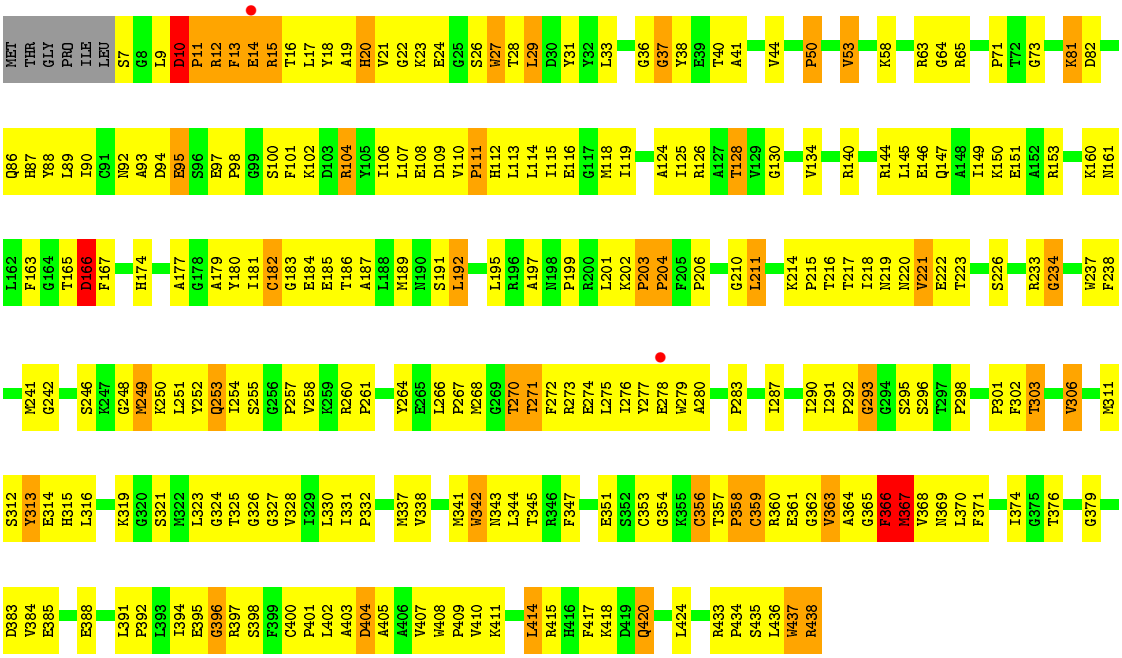




• Molecule 1: NADH-quinone oxidoreductase chain 1

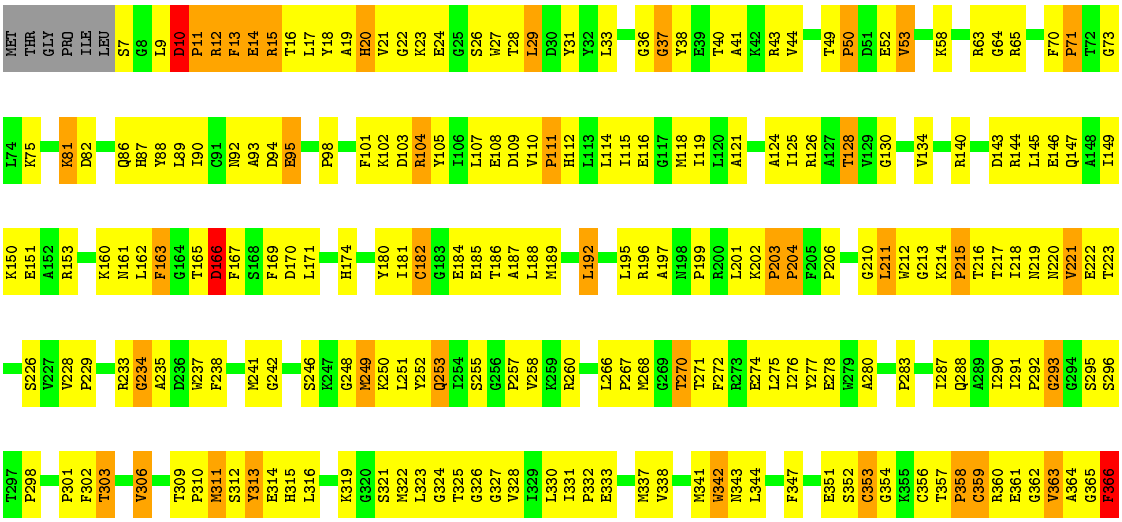
Chain J:

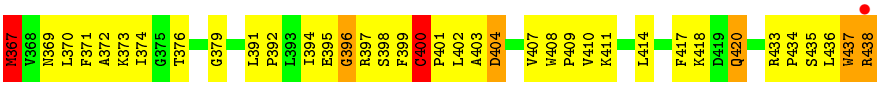




• Molecule 1: NADH-quinone oxidoreductase chain 1

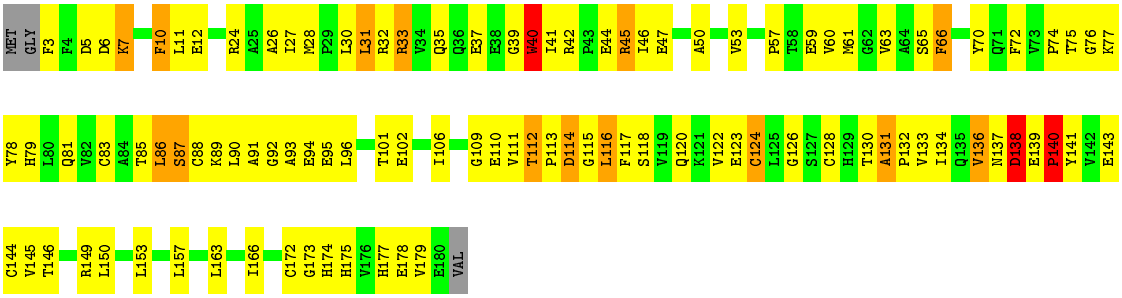
Chain S:





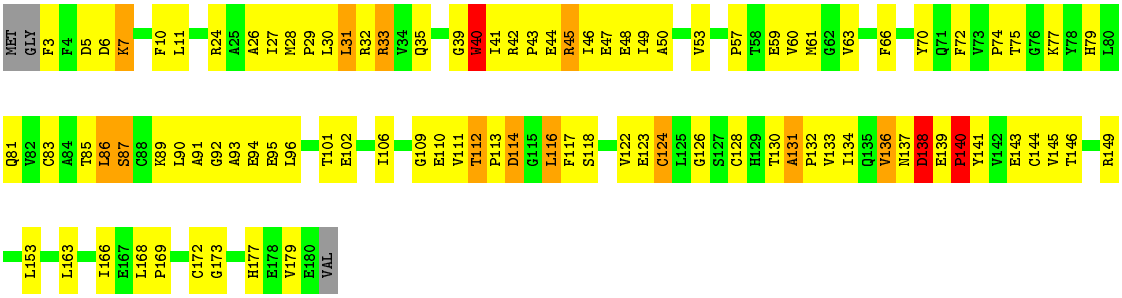
• Molecule 2: NADH-quinone oxidoreductase chain 2

Chain 2:



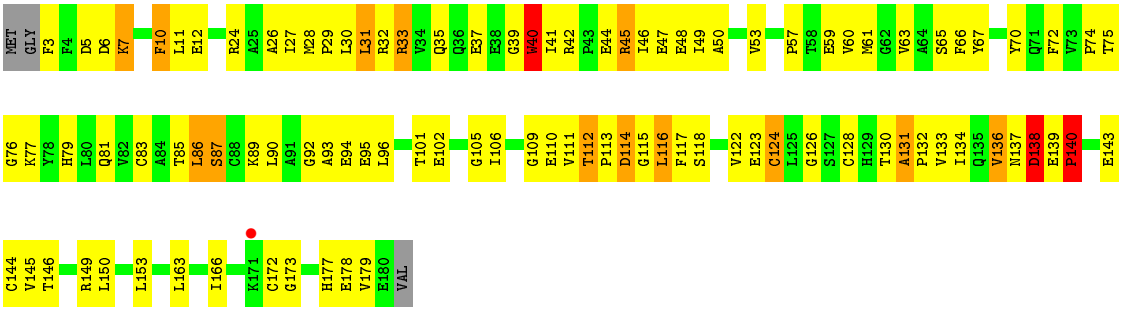
• Molecule 2: NADH-quinone oxidoreductase chain 2

Chain B:



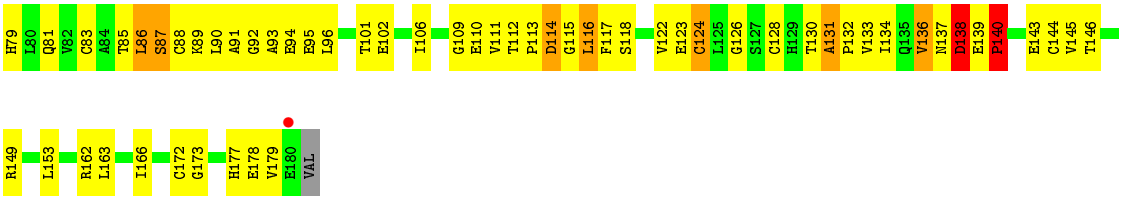
• Molecule 2: NADH-quinone oxidoreductase chain 2

Chain K:



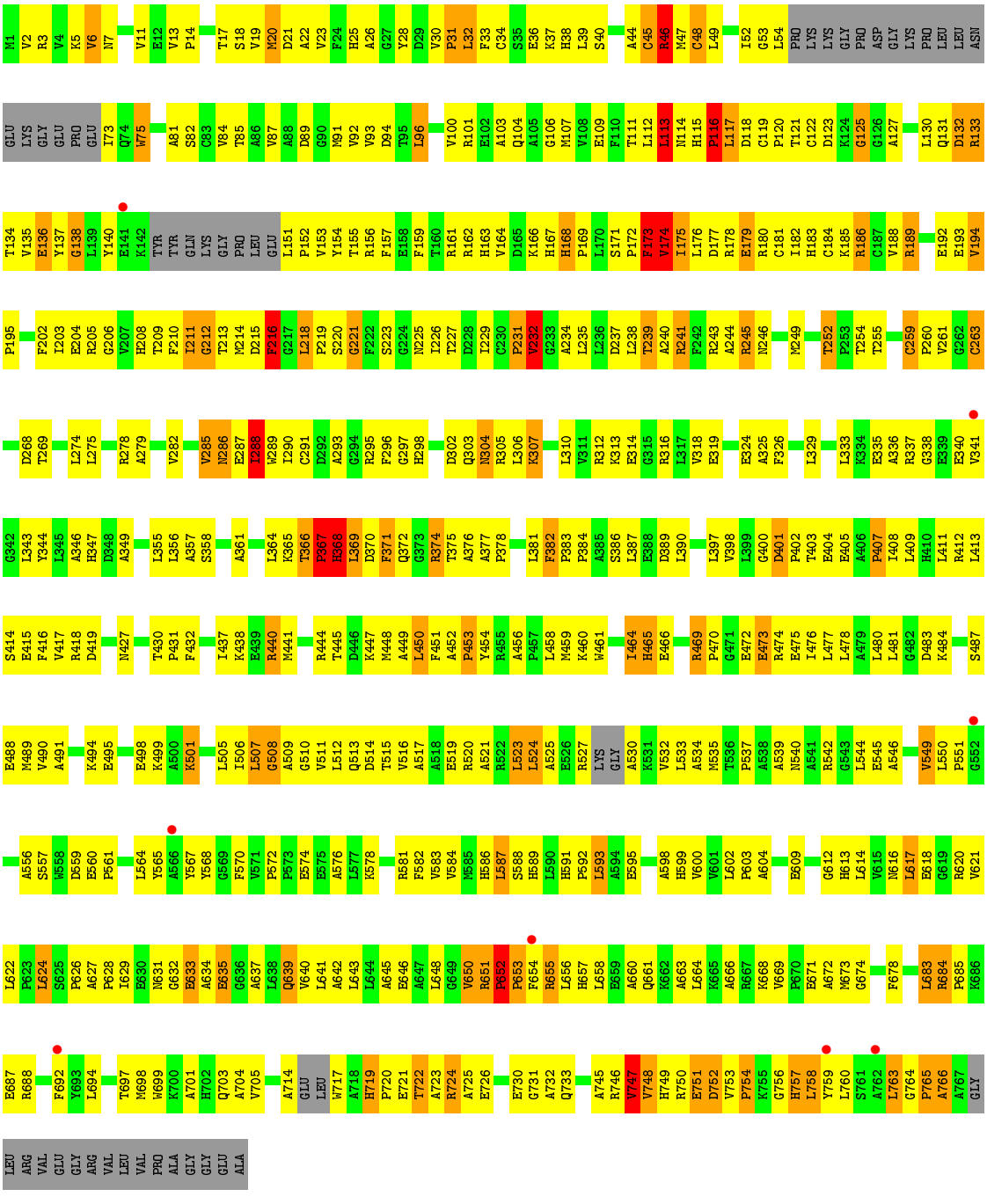
• Molecule 2: NADH-quinone oxidoreductase chain 2

Chain T:



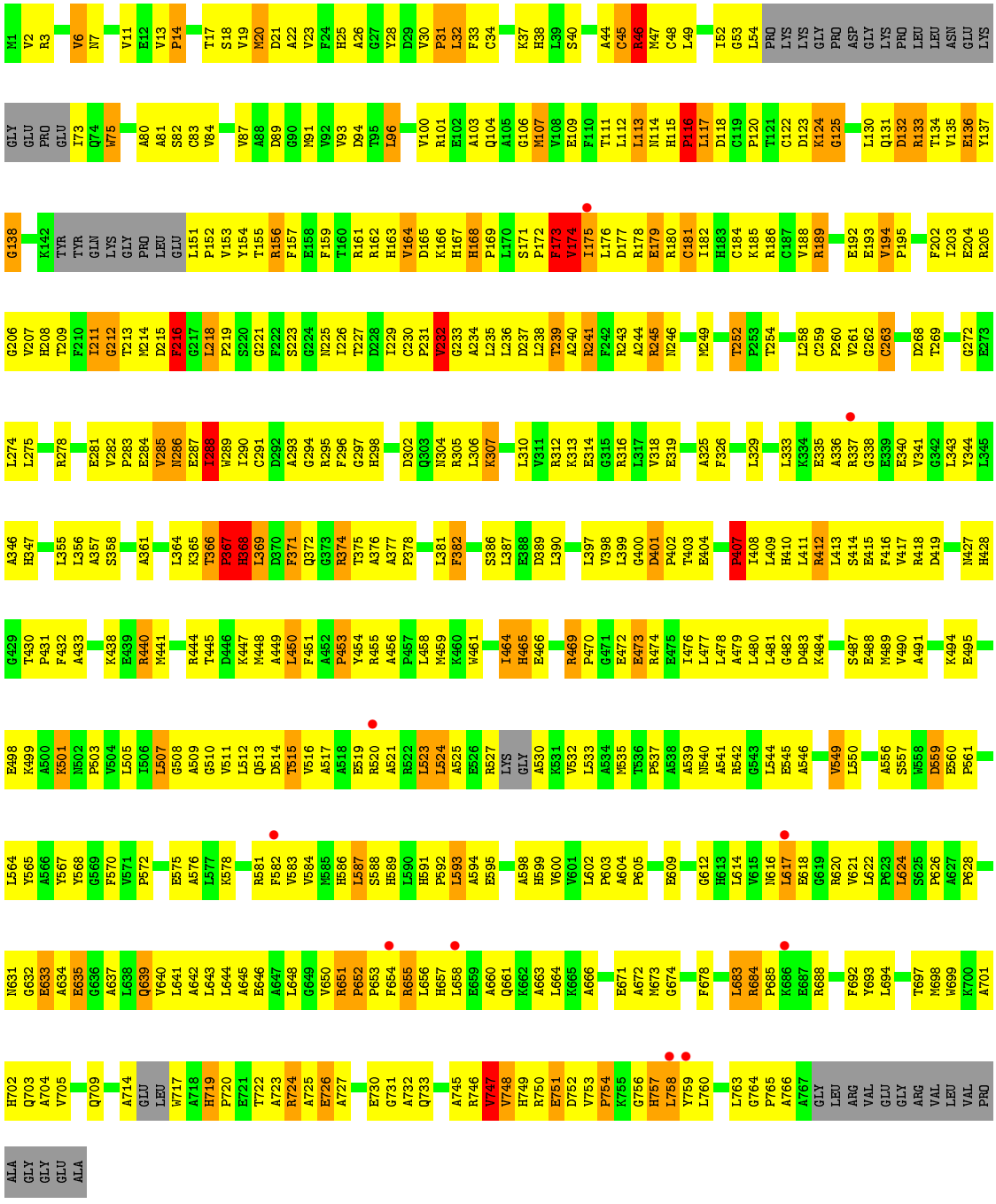
- Molecule 3: NADH-quinone oxidoreductase chain 3

Chain 3:



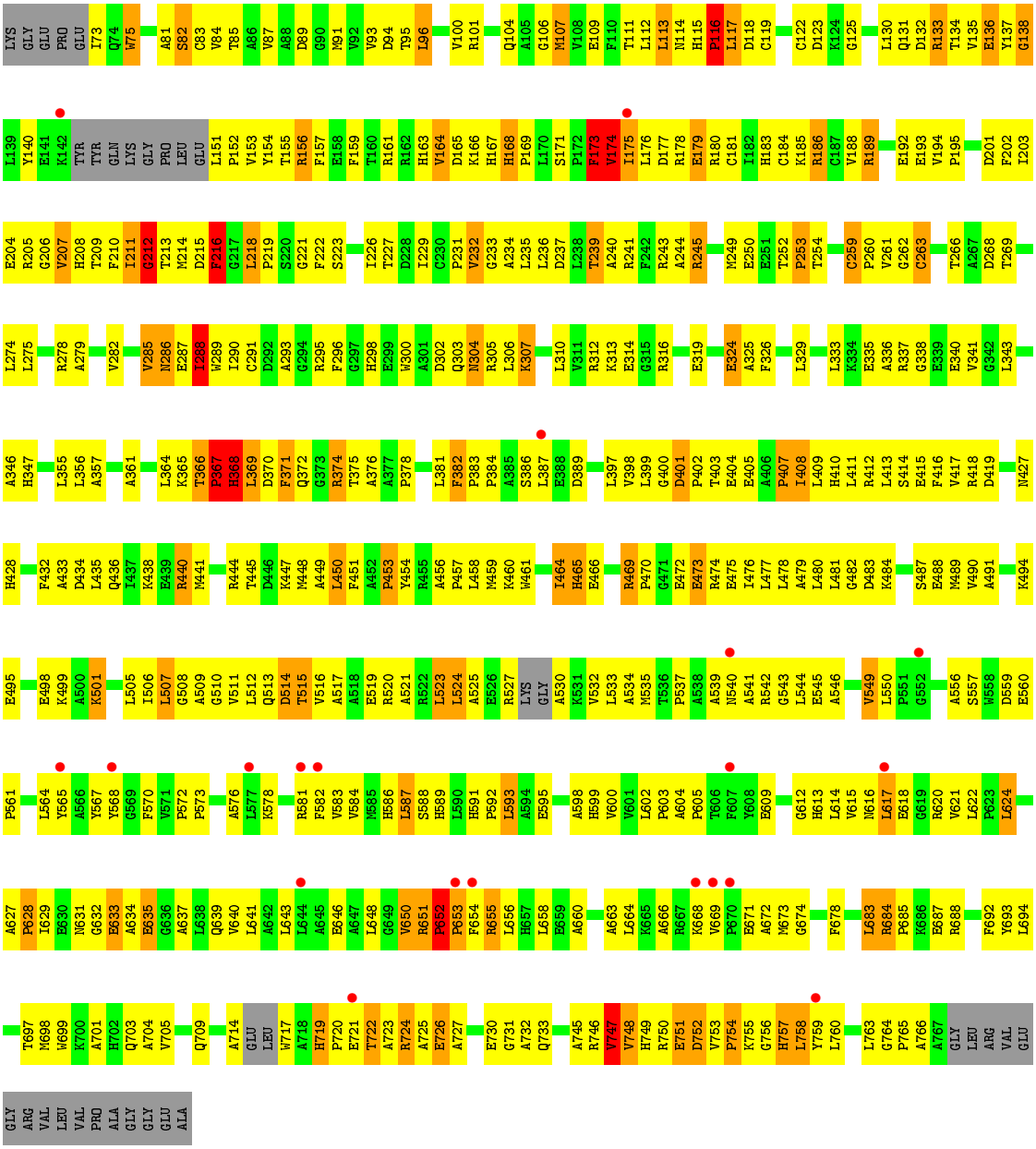
• Molecule 3: NADH-quinone oxidoreductase chain 3

Chain C:

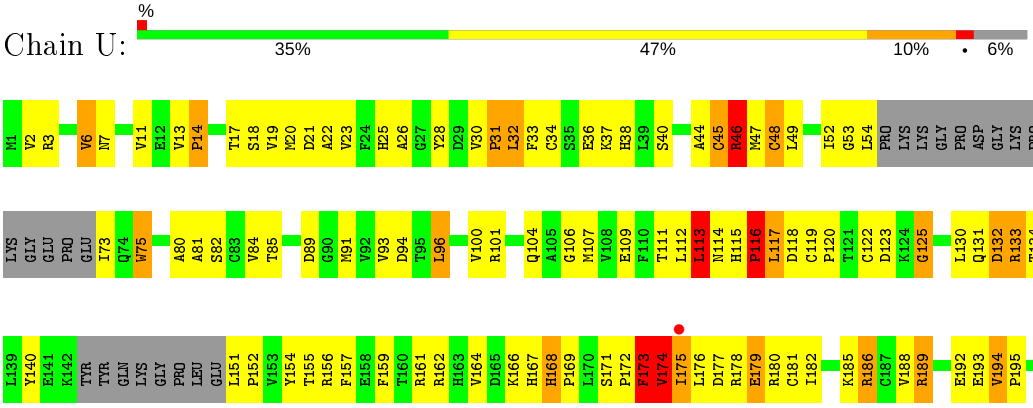


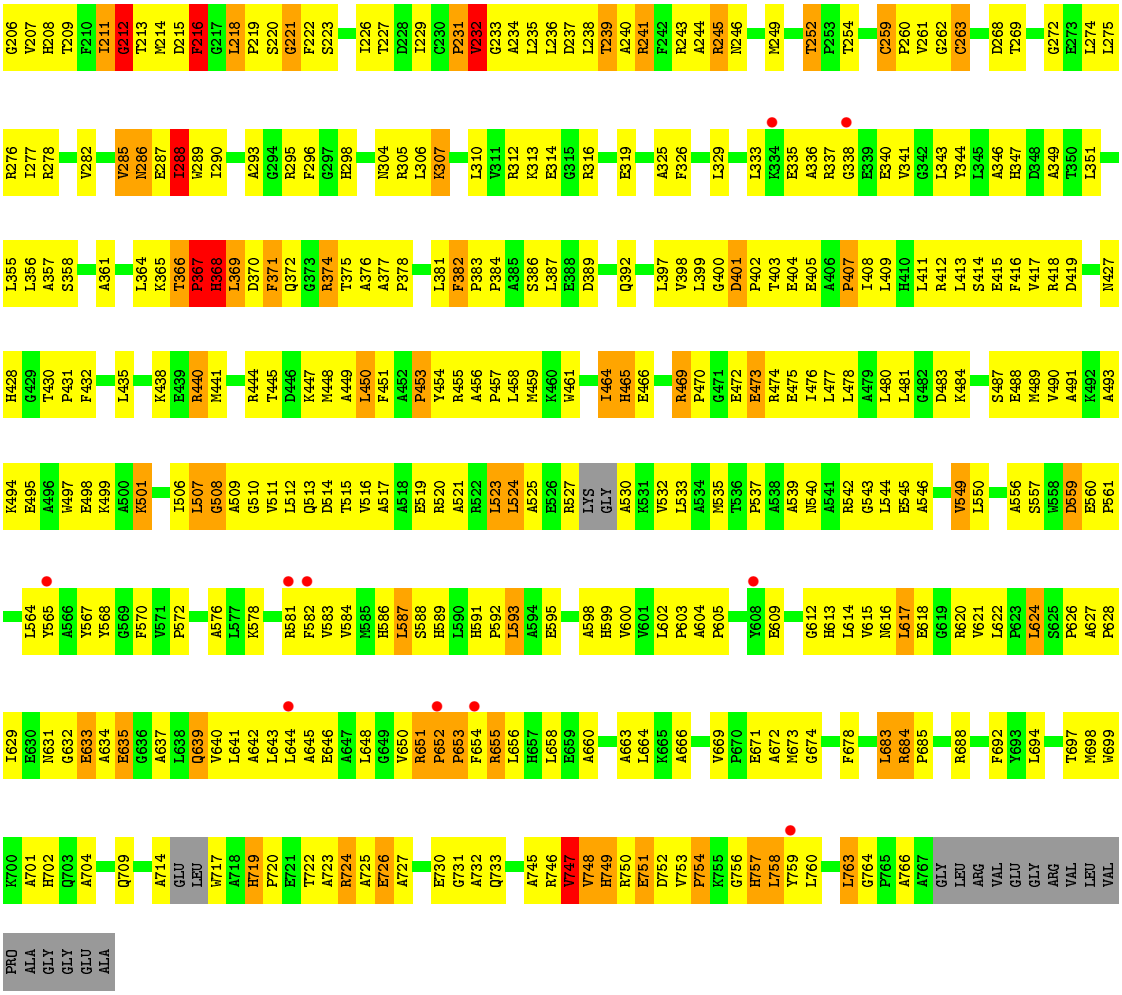
• Molecule 3: NADH-quinone oxidoreductase chain 3

Chain L:



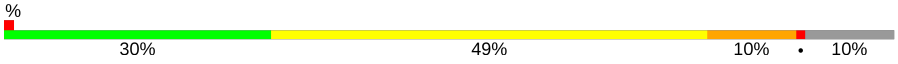
• Molecule 3: NADH-quinone oxidoreductase chain 3

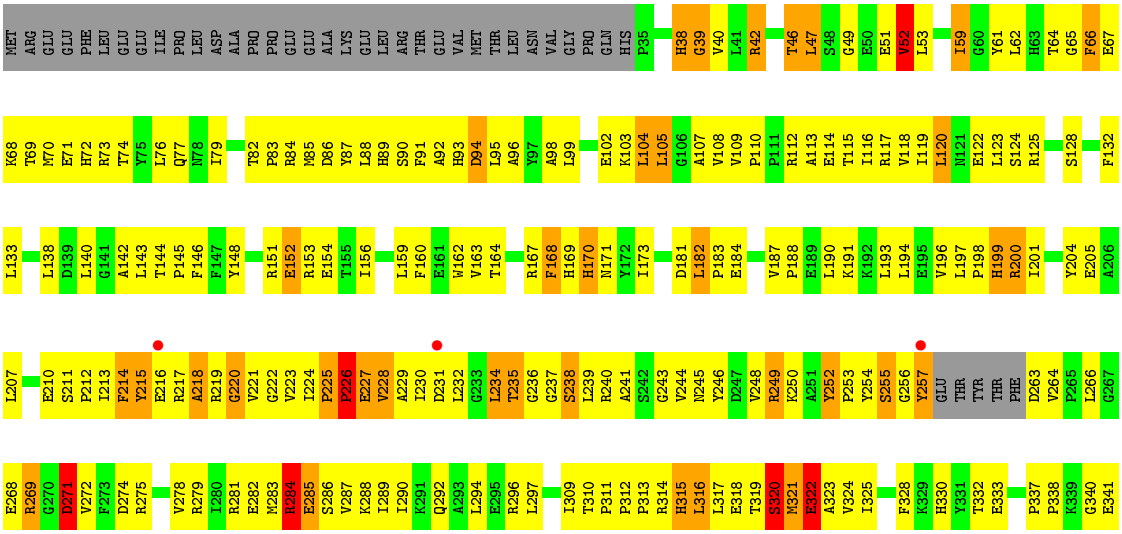


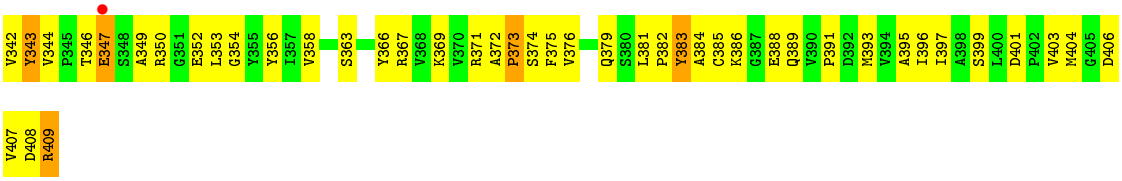


• Molecule 4: NADH-quinone oxidoreductase chain 4

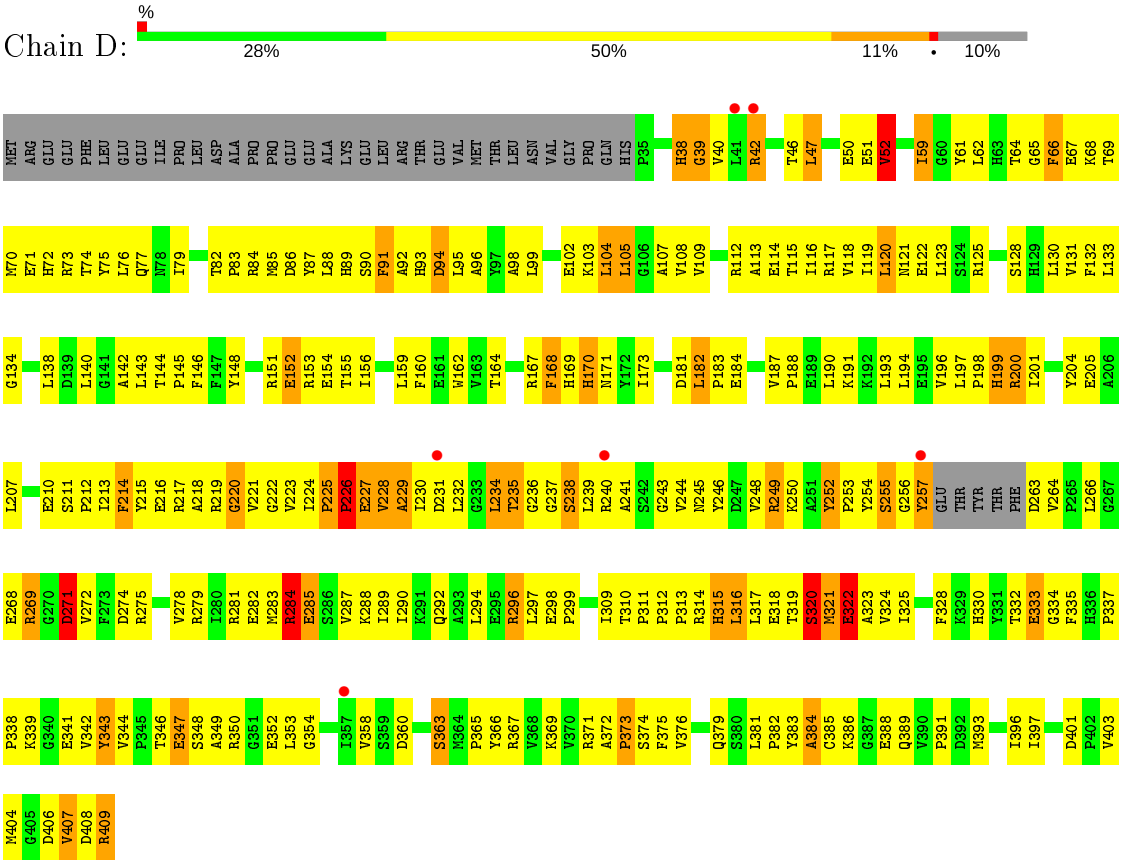
Chain 4:



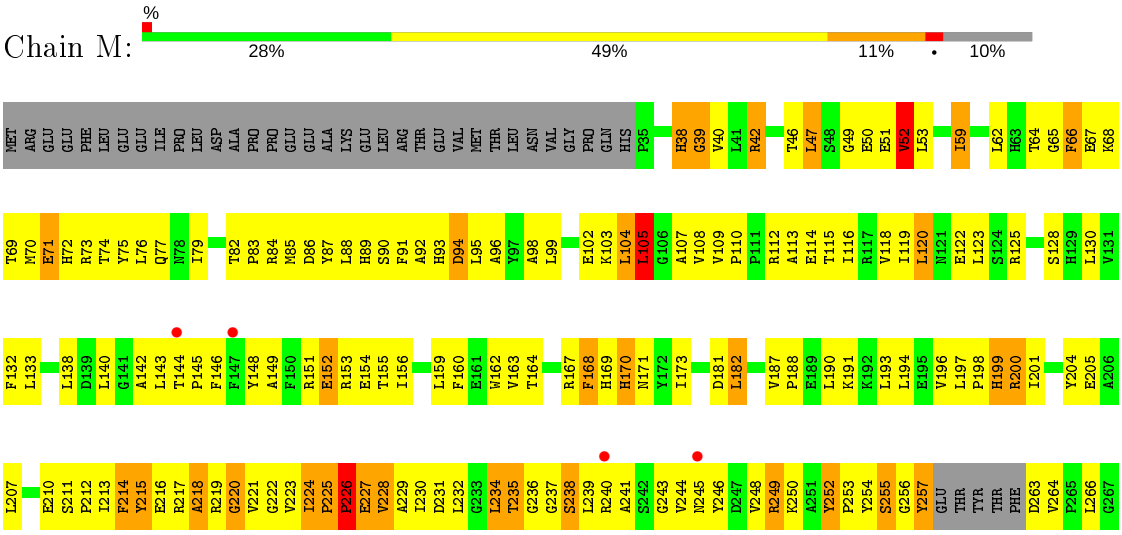


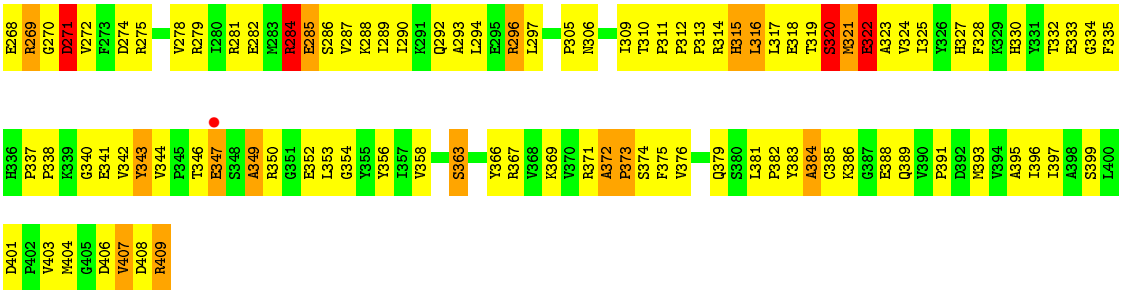


• Molecule 4: NADH-quinone oxidoreductase chain 4

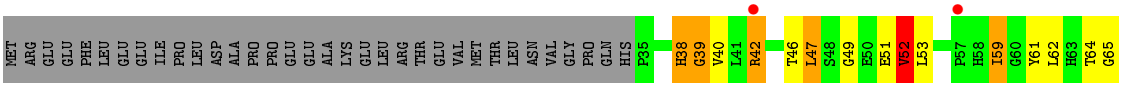


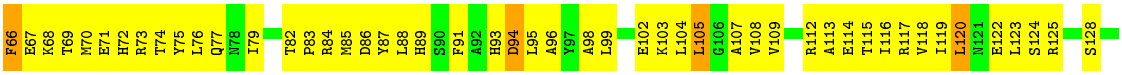
• Molecule 4: NADH-quinone oxidoreductase chain 4

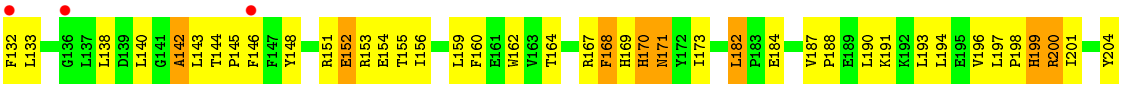


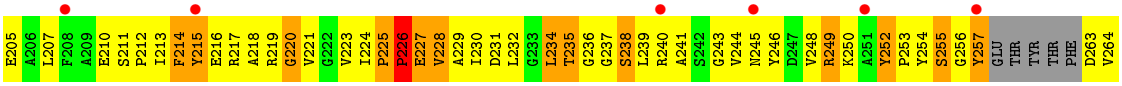


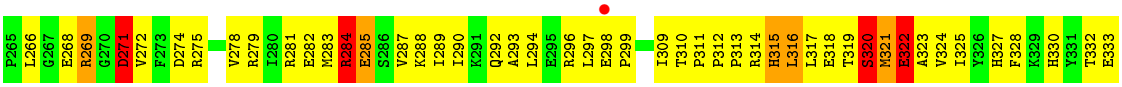
• Molecule 4: NADH-quinone oxidoreductase chain 4



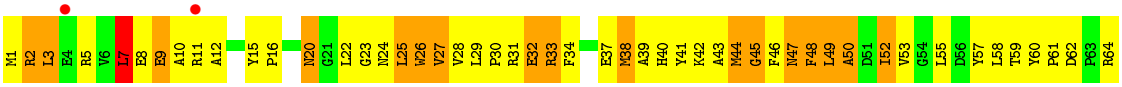


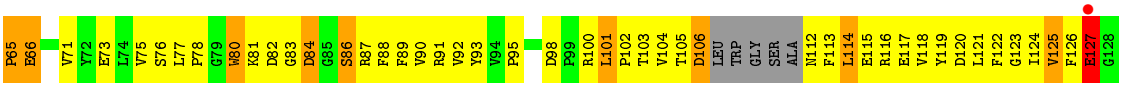


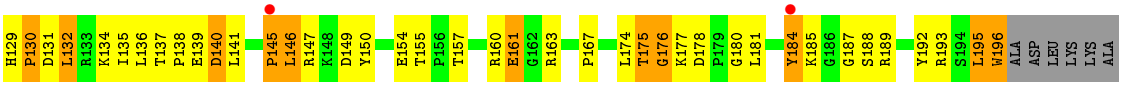




• Molecule 5: NADH-quinone oxidoreductase chain 5

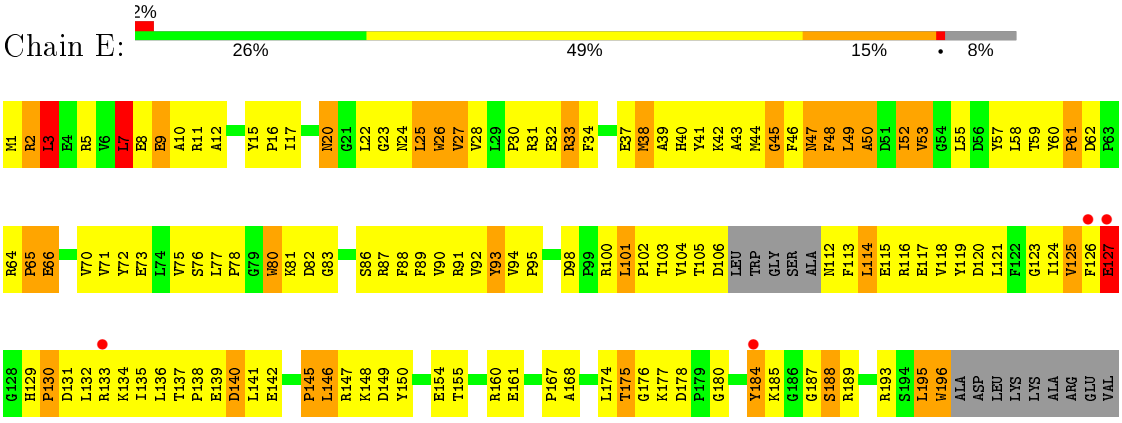






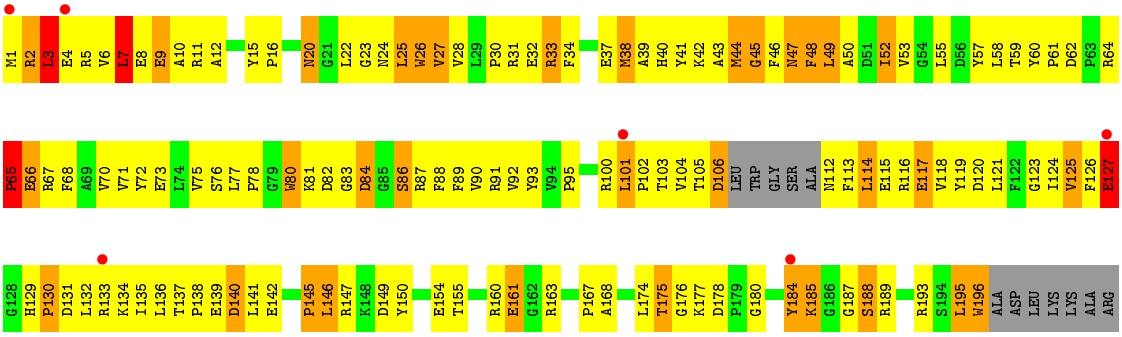
• Molecule 5: NADH-quinone oxidoreductase chain 5

Chain E:



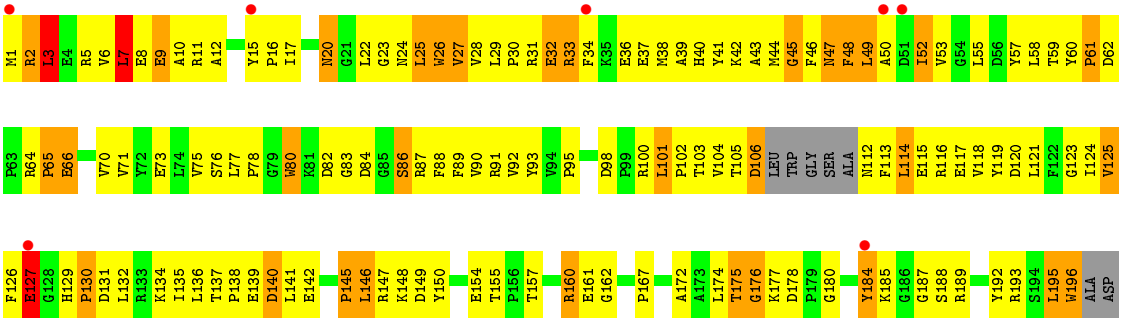
• Molecule 5: NADH-quinone oxidoreductase chain 5

Chain N:



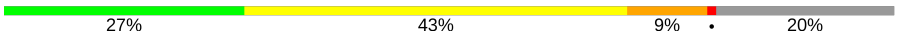
• Molecule 5: NADH-quinone oxidoreductase chain 5

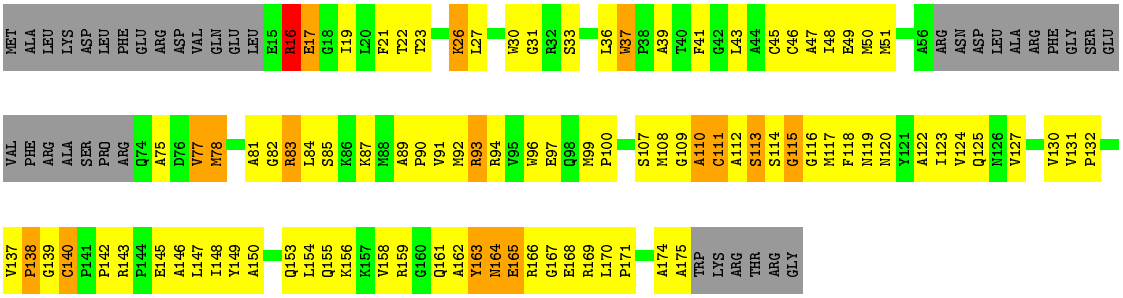
Chain W:



• Molecule 6: NADH-quinone oxidoreductase chain 6

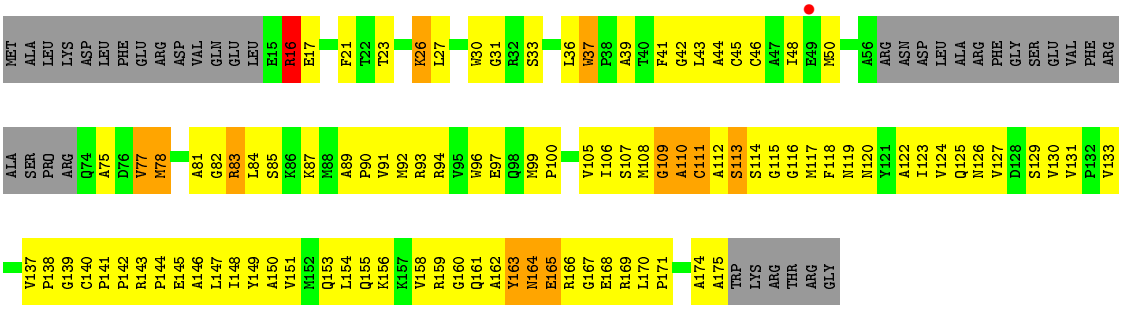
Chain 6:





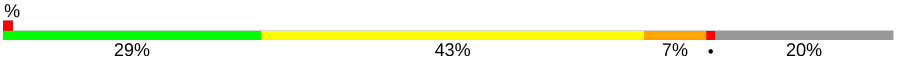
• Molecule 6: NADH-quinone oxidoreductase chain 6

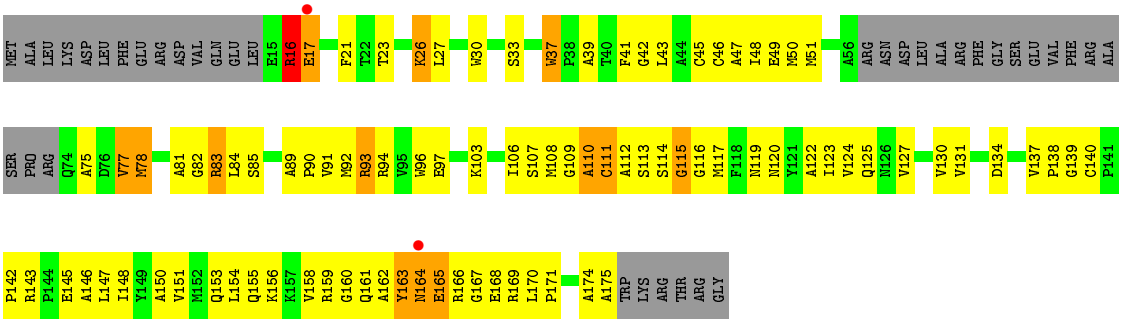
Chain F:



• Molecule 6: NADH-quinone oxidoreductase chain 6

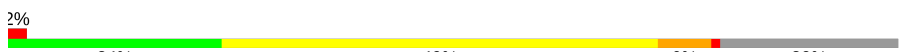
Chain O:

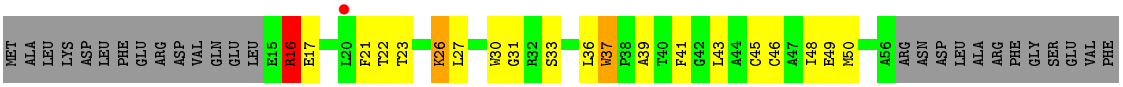


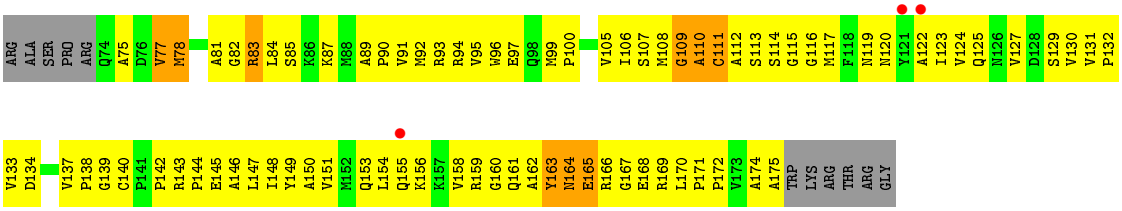


• Molecule 6: NADH-quinone oxidoreductase chain 6

Chain X:

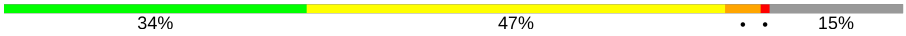


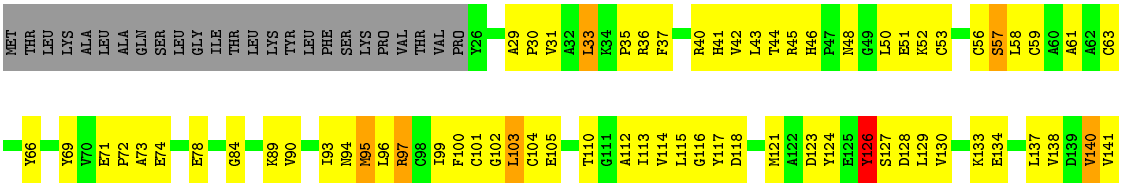


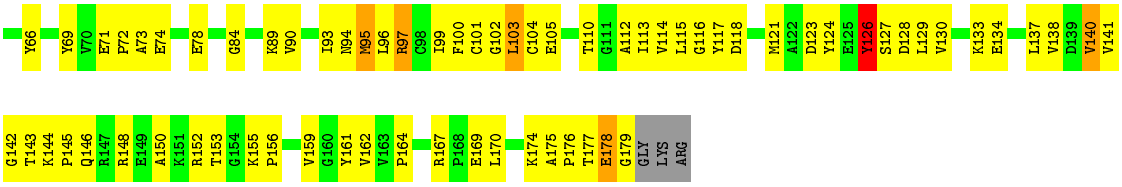


• Molecule 7: NADH-quinone oxidoreductase chain 9

Chain 9:

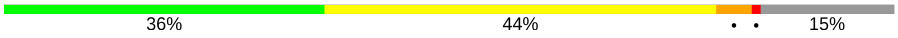


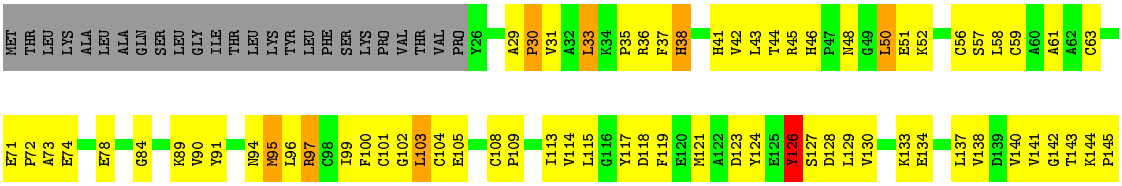


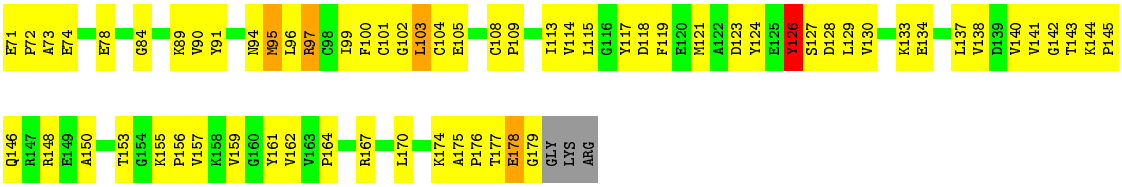


• Molecule 7: NADH-quinone oxidoreductase chain 9

Chain G:

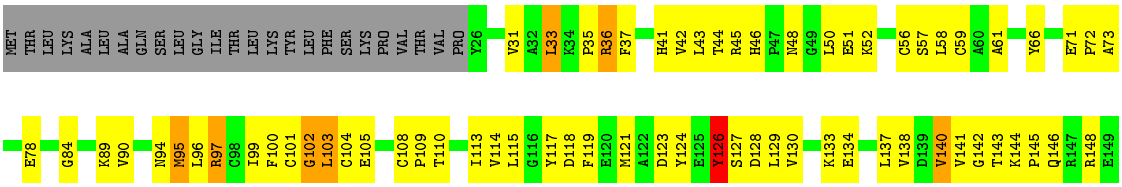


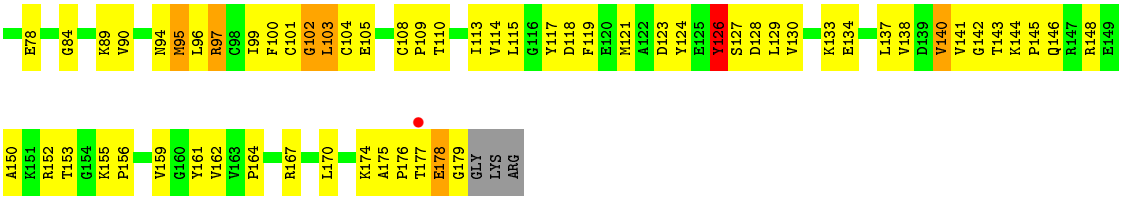




• Molecule 7: NADH-quinone oxidoreductase chain 9

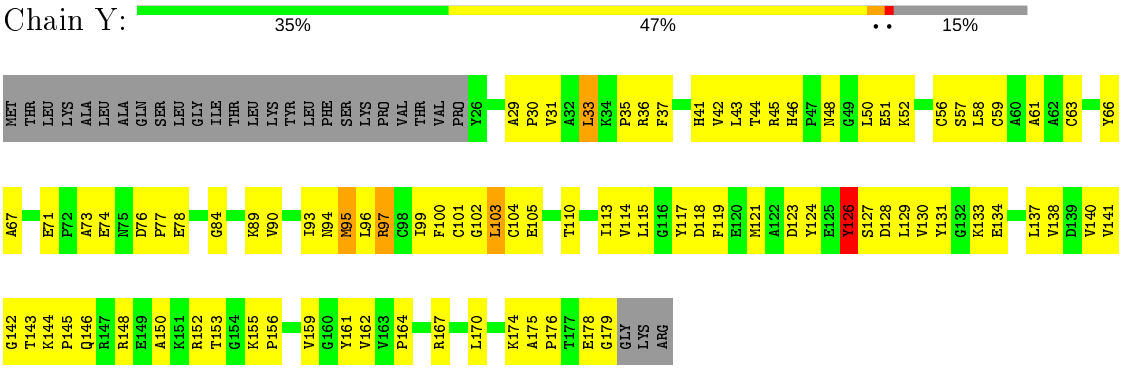
Chain P:





• Molecule 7: NADH-quinone oxidoreductase chain 9

Chain Y:



• Molecule 8: conserved hypothetical protein

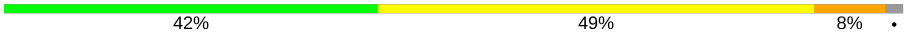
Chain 7:

• Molecule 8: conserved hypothetical protein

Chain H:

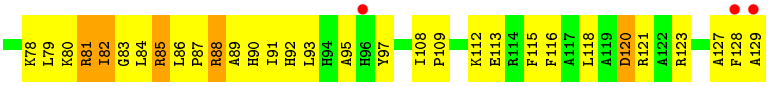
• Molecule 8: conserved hypothetical protein

Chain Q:



• Molecule 8: conserved hypothetical protein

Chain Z:


K78
L79
K80
R81
I82
G83
L84
R85
L86
P87
R88
A89
H90
I91
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L93
H94
A95
H96
Y97
I108
P109
K112
E113
R114
F115
F116
A117
L118
A119
D120
R121
A122
R123
A127
F128
A129

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.08Å 266.11Å 201.73Å 90.00° 104.71° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 29.99 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (20.00-3.30) 95.3 (29.99-3.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 3.31Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.265 , 0.298 0.251 , 0.285	Depositor DCC
R_{free} test set	3935 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	79.6	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	73916	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.47	0/3471	0.71	1/4696 (0.0%)
1	A	0.45	0/3471	0.70	1/4696 (0.0%)
1	J	0.48	1/3471 (0.0%)	0.70	1/4696 (0.0%)
1	S	0.44	1/3471 (0.0%)	0.69	1/4696 (0.0%)
2	2	0.47	0/1439	0.69	1/1953 (0.1%)
2	B	0.42	0/1439	0.68	0/1953
2	K	0.46	0/1439	0.70	1/1953 (0.1%)
2	T	0.42	0/1439	0.67	0/1953
3	3	0.46	1/5881 (0.0%)	0.73	7/7974 (0.1%)
3	C	0.45	1/5881 (0.0%)	0.72	6/7974 (0.1%)
3	L	0.44	1/5881 (0.0%)	0.73	8/7974 (0.1%)
3	U	0.44	1/5881 (0.0%)	0.72	6/7974 (0.1%)
4	4	0.46	0/3031	0.76	3/4118 (0.1%)
4	D	0.45	0/3031	0.76	3/4118 (0.1%)
4	M	0.47	0/3031	0.76	5/4118 (0.1%)
4	V	0.41	0/3031	0.73	2/4118 (0.0%)
5	5	0.43	0/1616	0.76	0/2189
5	E	0.45	0/1616	0.77	0/2189
5	N	0.46	0/1616	0.77	1/2189 (0.0%)
5	W	0.40	0/1616	0.74	0/2189
6	6	0.47	0/1126	0.77	2/1528 (0.1%)
6	F	0.49	0/1126	0.77	2/1528 (0.1%)
6	O	0.47	0/1126	0.77	2/1528 (0.1%)
6	X	0.43	0/1126	0.75	2/1528 (0.1%)
7	9	0.49	0/1224	0.72	0/1663
7	G	0.52	0/1224	0.75	1/1663 (0.1%)
7	P	0.47	0/1224	0.72	0/1663
7	Y	0.44	0/1224	0.70	0/1663
8	7	0.41	0/1059	0.70	0/1429
8	H	0.43	0/1059	0.71	0/1429
8	Q	0.44	0/1059	0.71	0/1429
8	Z	0.40	0/1059	0.69	0/1429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.45	6/75388 (0.0%)	0.73	56/102200 (0.1%)

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
7	9	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	181	CYS	CB-SG	7.59	1.95	1.82
1	J	356	CYS	CB-SG	-6.43	1.71	1.82
3	U	181	CYS	CB-SG	6.33	1.93	1.82
3	L	181	CYS	CB-SG	6.06	1.92	1.82
3	3	181	CYS	CB-SG	5.82	1.92	1.82
1	S	400	CYS	CB-SG	-5.30	1.73	1.81

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	221	GLY	N-CA-C	-7.56	94.20	113.10
3	C	221	GLY	N-CA-C	-7.31	94.82	113.10
3	L	221	GLY	N-CA-C	-7.19	95.12	113.10
3	3	221	GLY	N-CA-C	-6.92	95.80	113.10
4	D	322	GLU	N-CA-C	-6.92	92.32	111.00
4	4	322	GLU	N-CA-C	-6.88	92.44	111.00
6	F	164	ASN	N-CA-C	6.87	129.54	111.00
4	M	322	GLU	N-CA-C	-6.86	92.48	111.00
6	X	164	ASN	N-CA-C	6.85	129.49	111.00
6	O	164	ASN	N-CA-C	6.83	129.45	111.00
6	6	164	ASN	N-CA-C	6.74	129.20	111.00
4	V	322	GLU	N-CA-C	-6.70	92.92	111.00
3	3	216	PHE	N-CA-C	6.49	128.52	111.00
3	L	216	PHE	N-CA-C	6.42	128.34	111.00
3	C	211	ILE	N-CA-C	6.35	128.14	111.00
3	U	216	PHE	N-CA-C	6.29	127.99	111.00
6	O	163	TYR	N-CA-C	-6.29	94.02	111.00
4	M	238	SER	N-CA-C	-6.23	94.17	111.00
3	L	211	ILE	N-CA-C	6.16	127.63	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	U	211	ILE	N-CA-C	6.14	127.58	111.00
6	6	163	TYR	N-CA-C	-6.13	94.45	111.00
3	C	216	PHE	N-CA-C	6.12	127.52	111.00
6	X	163	TYR	N-CA-C	-6.07	94.62	111.00
3	3	211	ILE	N-CA-C	6.04	127.30	111.00
4	4	238	SER	N-CA-C	-5.93	94.98	111.00
6	F	163	TYR	N-CA-C	-5.84	95.22	111.00
3	C	181	CYS	CA-CB-SG	5.71	124.28	114.00
3	3	181	CYS	CA-CB-SG	5.65	124.16	114.00
4	D	238	SER	N-CA-C	-5.63	95.81	111.00
4	V	238	SER	N-CA-C	-5.60	95.88	111.00
3	C	116	PRO	N-CA-C	5.53	126.47	112.10
4	4	271	ASP	N-CA-C	5.40	125.58	111.00
4	M	271	ASP	N-CA-C	5.38	125.52	111.00
1	A	11	PRO	N-CA-C	5.33	125.95	112.10
3	L	212	GLY	N-CA-C	5.26	126.24	113.10
3	L	181	CYS	CA-CB-SG	5.25	123.46	114.00
3	U	212	GLY	N-CA-C	5.24	126.19	113.10
3	L	116	PRO	N-CA-C	5.19	125.60	112.10
3	3	763	LEU	CA-CB-CG	5.18	127.22	115.30
1	1	11	PRO	N-CA-C	5.17	125.56	112.10
3	3	752	ASP	N-CA-C	-5.17	97.05	111.00
3	L	184	CYS	N-CA-C	-5.16	97.07	111.00
3	L	752	ASP	N-CA-C	-5.16	97.08	111.00
2	2	40	TRP	CA-CB-CG	5.10	123.39	113.70
2	K	40	TRP	CA-CB-CG	5.08	123.36	113.70
5	N	185	LYS	N-CA-C	5.08	124.72	111.00
3	U	181	CYS	CA-CB-SG	5.07	123.12	114.00
4	M	224	ILE	N-CA-C	-5.07	97.32	111.00
1	S	11	PRO	N-CA-C	5.06	125.26	112.10
7	G	50	LEU	CA-CB-CG	5.05	126.91	115.30
4	D	333	GLU	N-CA-C	-5.04	97.38	111.00
4	M	105	LEU	CA-CB-CG	5.04	126.90	115.30
3	C	763	LEU	CA-CB-CG	5.03	126.88	115.30
3	3	116	PRO	N-CA-C	5.01	125.12	112.10
3	U	763	LEU	CA-CB-CG	5.00	126.81	115.30
1	J	11	PRO	N-CA-C	5.00	125.10	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	9	69	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	1	3383	0	3349	268	0
1	A	3383	0	3349	267	0
1	J	3383	0	3349	272	0
1	S	3383	0	3349	268	0
2	2	1406	0	1373	145	0
2	B	1406	0	1373	137	0
2	K	1406	0	1373	142	0
2	T	1406	0	1373	133	0
3	3	5746	0	5767	594	0
3	C	5746	0	5767	588	0
3	L	5746	0	5767	592	1
3	U	5746	0	5767	605	1
4	4	2953	0	2944	436	0
4	D	2953	0	2944	432	0
4	M	2953	0	2944	433	0
4	V	2953	0	2944	433	0
5	5	1570	0	1539	247	0
5	E	1570	0	1539	251	0
5	N	1570	0	1539	250	0
5	W	1570	0	1539	248	0
6	6	1102	0	1108	147	0
6	F	1102	0	1108	148	0
6	O	1102	0	1108	131	0
6	X	1102	0	1108	141	0
7	9	1193	0	1160	112	0
7	G	1193	0	1160	103	0
7	P	1193	0	1160	98	0
7	Y	1193	0	1160	109	0
8	7	1031	0	1029	73	0
8	H	1031	0	1029	85	0
8	Q	1031	0	1029	88	0
8	Z	1031	0	1029	84	0
9	1	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	3	24	0	0	3	0
9	6	8	0	0	1	0
9	9	16	0	0	2	0
9	A	8	0	0	0	0
9	C	24	0	0	3	0
9	F	8	0	0	1	0
9	G	16	0	0	2	0
9	J	8	0	0	0	0
9	L	24	0	0	3	0
9	O	8	0	0	1	0
9	P	16	0	0	1	0
9	S	8	0	0	0	0
9	U	24	0	0	3	0
9	X	8	0	0	1	0
9	Y	16	0	0	2	0
10	2	4	0	0	2	0
10	3	4	0	0	1	0
10	B	4	0	0	2	0
10	C	4	0	0	1	0
10	K	4	0	0	2	0
10	L	4	0	0	1	0
10	T	4	0	0	1	0
10	U	4	0	0	0	0
11	7	31	0	19	5	0
11	H	31	0	19	5	0
11	Q	31	0	19	7	0
11	Z	31	0	19	6	0
All	All	73916	0	73152	7497	1

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 51.

All (7497) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:139:GLU:HB2	2:K:140:PRO:HD2	1.25	1.19
4:M:249:ARG:HB3	4:M:249:ARG:HH11	1.08	1.18
1:S:10:ASP:HB3	1:S:11:PRO:HD2	1.19	1.17
1:S:11:PRO:HB3	1:S:270:THR:HB	1.26	1.17
1:J:11:PRO:HB3	1:J:270:THR:HB	1.20	1.17
4:D:224:ILE:HB	4:D:225:PRO:HD3	1.18	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:11:PRO:HB3	1:1:270:THR:HB	1.25	1.16
3:C:205:ARG:HA	3:C:209:THR:HG22	1.24	1.15
4:V:224:ILE:HB	4:V:225:PRO:HD3	1.19	1.14
2:B:139:GLU:HB2	2:B:140:PRO:HD2	1.28	1.13
4:4:249:ARG:HB3	4:4:249:ARG:HH11	1.13	1.13
4:D:266:LEU:HD13	4:D:281:ARG:HB3	1.22	1.13
3:3:205:ARG:HA	3:3:209:THR:HG22	1.24	1.13
3:U:466:GLU:HG2	3:U:489:MET:HG3	1.30	1.13
2:2:139:GLU:HB2	2:2:140:PRO:HD2	1.26	1.12
4:D:249:ARG:HB3	4:D:249:ARG:HH11	1.11	1.12
1:A:10:ASP:HB3	1:A:11:PRO:HD2	1.14	1.12
4:4:240:ARG:HD2	4:4:243:GLY:HA3	1.27	1.11
4:M:249:ARG:HB3	4:M:249:ARG:NH1	1.64	1.11
4:V:266:LEU:HD13	4:V:281:ARG:HB3	1.26	1.11
2:T:139:GLU:HB2	2:T:140:PRO:HD2	1.28	1.11
2:2:136:VAL:HG12	2:2:137:ASN:H	1.13	1.10
4:4:266:LEU:HD13	4:4:281:ARG:HB3	1.21	1.10
1:J:10:ASP:HB3	1:J:11:PRO:HD2	1.18	1.10
4:D:249:ARG:NH1	4:D:249:ARG:HB3	1.66	1.10
3:U:205:ARG:HA	3:U:209:THR:HG22	1.23	1.10
4:M:266:LEU:HD13	4:M:281:ARG:HB3	1.21	1.09
1:A:11:PRO:HB3	1:A:270:THR:HB	1.26	1.09
4:4:224:ILE:HB	4:4:225:PRO:HD3	1.19	1.09
3:L:205:ARG:HA	3:L:209:THR:HG22	1.18	1.08
4:D:240:ARG:HD2	4:D:243:GLY:HA3	1.29	1.08
1:1:10:ASP:HB3	1:1:11:PRO:HD2	1.16	1.08
4:V:240:ARG:HD2	4:V:243:GLY:HA3	1.31	1.08
5:N:49:LEU:HB2	5:N:77:LEU:HD21	1.34	1.07
4:4:249:ARG:HB3	4:4:249:ARG:NH1	1.68	1.07
4:M:224:ILE:HB	4:M:225:PRO:HD3	1.17	1.07
4:V:249:ARG:HH11	4:V:249:ARG:HB3	1.20	1.07
5:5:119:TYR:HE1	5:5:132:LEU:HD11	1.17	1.07
4:M:240:ARG:HD2	4:M:243:GLY:HA3	1.20	1.07
2:K:136:VAL:HG12	2:K:137:ASN:H	1.17	1.06
5:5:49:LEU:HB2	5:5:77:LEU:HD21	1.37	1.06
5:W:49:LEU:HB2	5:W:77:LEU:HD21	1.34	1.06
3:U:232:VAL:HG12	9:U:784:SF4:S2	1.96	1.05
5:E:50:ALA:HB3	5:E:114:LEU:HD11	1.34	1.05
3:3:509:ALA:HA	3:3:758:LEU:HD22	1.38	1.05
4:V:249:ARG:HB3	4:V:249:ARG:NH1	1.71	1.05
3:L:466:GLU:HG2	3:L:489:MET:HG3	1.38	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:232:LEU:HD11	4:M:282:GLU:CD	1.79	1.02
3:3:232:VAL:HG12	9:3:784:SF4:S2	2.00	1.02
2:B:136:VAL:HG12	2:B:137:ASN:H	1.24	1.02
3:C:754:PRO:HD2	3:C:757:HIS:HE2	1.24	1.02
5:E:49:LEU:HB2	5:E:77:LEU:HD21	1.34	1.02
4:4:232:LEU:HD11	4:4:282:GLU:CD	1.78	1.02
1:S:201:LEU:HG	1:S:203:PRO:HD2	1.41	1.02
3:3:501:LYS:H	3:3:501:LYS:HD2	1.21	1.01
3:3:731:GLY:H	3:3:747:VAL:HG12	1.25	1.01
4:4:385:CYS:HB3	4:4:396:ILE:HG12	1.42	1.01
3:L:501:LYS:H	3:L:501:LYS:HD2	1.23	1.01
3:L:754:PRO:HD2	3:L:757:HIS:HE2	1.25	1.01
5:N:50:ALA:HB3	5:N:114:LEU:HD11	1.41	1.01
4:V:72:HIS:O	4:V:73:ARG:HD2	1.60	1.01
3:3:45:CYS:SG	3:3:45:CYS:O	2.18	1.00
3:C:285:VAL:HG13	3:C:286:ASN:H	1.26	1.00
3:L:731:GLY:H	3:L:747:VAL:HG12	1.23	1.00
3:L:285:VAL:HG13	3:L:286:ASN:H	1.26	1.00
5:N:119:TYR:HE1	5:N:132:LEU:HD11	1.24	1.00
5:N:126:PHE:HE1	5:N:147:ARG:HD2	1.24	1.00
3:C:731:GLY:H	3:C:747:VAL:HG12	1.22	1.00
3:U:501:LYS:H	3:U:501:LYS:HD2	1.22	1.00
5:E:119:TYR:HE1	5:E:132:LEU:HD11	1.23	1.00
3:C:466:GLU:HG2	3:C:489:MET:HG3	1.40	1.00
4:V:385:CYS:HB3	4:V:396:ILE:HG12	1.44	1.00
4:M:133:LEU:HD21	4:M:204:TYR:CD2	1.96	0.99
3:3:285:VAL:HG13	3:3:286:ASN:H	1.26	0.99
4:D:252:TYR:HB2	4:D:253:PRO:HD2	1.42	0.99
1:1:437:TRP:HB3	2:2:92:GLY:HA3	1.42	0.99
5:5:50:ALA:HB3	5:5:114:LEU:HD11	1.44	0.99
1:A:33:LEU:HD23	1:A:37:GLY:HA3	1.44	0.99
3:U:754:PRO:HD2	3:U:757:HIS:HE2	1.25	0.99
2:T:136:VAL:HG12	2:T:137:ASN:H	1.26	0.99
4:4:252:TYR:HB2	4:4:253:PRO:HD2	1.40	0.98
3:L:754:PRO:HD2	3:L:757:HIS:NE2	1.78	0.98
3:3:754:PRO:HD2	3:3:757:HIS:HE2	1.29	0.98
1:A:201:LEU:HG	1:A:203:PRO:HD2	1.44	0.98
3:C:232:VAL:HG12	9:C:784:SF4:S2	2.04	0.98
4:D:133:LEU:HD21	4:D:204:TYR:CD2	1.98	0.98
1:A:10:ASP:HB3	1:A:11:PRO:CD	1.93	0.98
4:D:232:LEU:HD11	4:D:282:GLU:CD	1.83	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:VAL:HG11	3:C:296:PHE:CE1	1.99	0.97
5:E:139:GLU:HG2	5:E:140:ASP:H	1.29	0.97
1:1:201:LEU:HG	1:1:203:PRO:HD2	1.43	0.97
3:3:754:PRO:HD2	3:3:757:HIS:NE2	1.79	0.97
4:D:72:HIS:O	4:D:73:ARG:HD2	1.64	0.97
3:U:754:PRO:HD2	3:U:757:HIS:NE2	1.79	0.97
1:A:10:ASP:CB	1:A:11:PRO:HD2	1.95	0.97
1:J:437:TRP:HB3	2:K:92:GLY:HA3	1.46	0.97
5:W:139:GLU:HG2	5:W:140:ASP:H	1.30	0.97
1:1:10:ASP:HB3	1:1:11:PRO:CD	1.95	0.97
1:A:316:LEU:HD12	1:A:323:LEU:HB2	1.47	0.97
4:M:72:HIS:O	4:M:73:ARG:HD2	1.63	0.97
5:W:50:ALA:HB3	5:W:114:LEU:HD11	1.45	0.97
4:V:252:TYR:HB2	4:V:253:PRO:HD2	1.46	0.97
1:S:437:TRP:HB3	2:T:92:GLY:HA3	1.43	0.96
4:4:237:GLY:CA	5:5:112:ASN:HA	1.95	0.96
4:4:72:HIS:O	4:4:73:ARG:HD2	1.64	0.96
4:M:252:TYR:HB2	4:M:253:PRO:HD2	1.44	0.96
3:U:509:ALA:HA	3:U:758:LEU:HD22	1.45	0.96
1:A:437:TRP:HB3	2:B:92:GLY:HA3	1.48	0.96
1:1:33:LEU:HD23	1:1:37:GLY:HA3	1.48	0.96
3:C:501:LYS:H	3:C:501:LYS:HD2	1.27	0.96
3:L:173:PHE:CD1	3:L:174:VAL:HG22	2.01	0.96
4:V:103:LYS:HB3	5:W:22:LEU:HD13	1.44	0.96
4:4:85:MET:HE1	4:4:409:ARG:HB2	1.48	0.96
6:F:139:GLY:HA3	6:F:142:PRO:HB3	1.45	0.96
1:J:10:ASP:HB3	1:J:11:PRO:CD	1.96	0.96
4:M:224:ILE:CB	4:M:225:PRO:HD3	1.95	0.96
7:9:141:VAL:HG13	7:9:142:GLY:H	1.30	0.95
4:M:103:LYS:HB3	5:N:22:LEU:HD13	1.46	0.95
4:V:338:PRO:HG2	5:W:193:ARG:HB2	1.48	0.95
3:L:232:VAL:HG12	9:L:784:SF4:S2	2.06	0.95
6:O:139:GLY:HA3	6:O:142:PRO:HB3	1.48	0.95
3:U:731:GLY:H	3:U:747:VAL:HG12	1.26	0.95
1:1:10:ASP:CB	1:1:11:PRO:HD2	1.97	0.95
4:V:237:GLY:CA	5:W:112:ASN:HA	1.96	0.95
5:E:125:VAL:HG12	5:E:126:PHE:H	1.29	0.95
3:3:174:VAL:HG11	3:3:296:PHE:CE1	2.02	0.95
5:5:26:TRP:HB3	5:5:89:PHE:HB2	1.49	0.95
3:C:754:PRO:HD2	3:C:757:HIS:NE2	1.80	0.95
5:W:119:TYR:HE1	5:W:132:LEU:HD11	1.30	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:33:LEU:HD23	1:J:37:GLY:HA3	1.48	0.94
3:3:466:GLU:HG2	3:3:489:MET:HG3	1.45	0.94
5:E:126:PHE:HE1	5:E:147:ARG:HD2	1.29	0.94
5:N:139:GLU:HG2	5:N:140:ASP:H	1.28	0.94
4:V:232:LEU:HD11	4:V:282:GLU:CD	1.86	0.94
5:W:126:PHE:HE1	5:W:147:ARG:HD2	1.30	0.94
1:1:266:LEU:HB3	1:1:270:THR:HG21	1.48	0.94
3:U:174:VAL:HG11	3:U:296:PHE:CE1	2.01	0.94
1:J:201:LEU:HG	1:J:203:PRO:HD2	1.47	0.94
4:4:103:LYS:HB3	5:5:22:LEU:HD13	1.49	0.94
8:7:60:SER:HB3	8:7:64:GLY:O	1.67	0.94
4:D:237:GLY:CA	5:E:112:ASN:HA	1.97	0.94
3:C:509:ALA:HA	3:C:758:LEU:HD22	1.48	0.94
5:5:126:PHE:HE1	5:5:147:ARG:HD2	1.32	0.93
2:K:137:ASN:O	2:K:138:ASP:HB3	1.66	0.93
3:L:509:ALA:HA	3:L:758:LEU:HD22	1.47	0.93
5:N:118:VAL:HG13	5:N:129:HIS:CD2	2.04	0.93
1:S:10:ASP:CB	1:S:11:PRO:HD2	1.96	0.93
4:V:133:LEU:HD21	4:V:204:TYR:CD2	2.03	0.93
3:C:173:PHE:CD1	3:C:174:VAL:HG22	2.03	0.93
5:N:125:VAL:HG12	5:N:126:PHE:H	1.32	0.93
4:V:224:ILE:CB	4:V:225:PRO:HD3	1.98	0.93
1:J:370:LEU:O	1:J:374:ILE:HG22	1.67	0.93
7:Y:141:VAL:HG13	7:Y:142:GLY:H	1.32	0.93
4:D:74:THR:HG22	4:D:76:LEU:H	1.33	0.93
4:4:224:ILE:CB	4:4:225:PRO:HD3	1.98	0.93
4:D:224:ILE:CB	4:D:225:PRO:HD3	1.97	0.93
3:C:45:CYS:O	3:C:45:CYS:SG	2.26	0.93
3:3:173:PHE:CD1	3:3:174:VAL:HG22	2.03	0.93
4:4:133:LEU:HD21	4:4:204:TYR:CD2	2.03	0.93
1:J:10:ASP:CB	1:J:11:PRO:HD2	1.99	0.93
1:S:10:ASP:HB3	1:S:11:PRO:CD	1.97	0.93
4:4:341:GLU:HG2	4:4:358:VAL:HG22	1.49	0.93
4:D:249:ARG:NH2	5:E:87:ARG:HE	1.67	0.93
2:2:136:VAL:HG12	2:2:137:ASN:N	1.82	0.92
5:5:118:VAL:HG13	5:5:129:HIS:CD2	2.05	0.92
1:J:266:LEU:HB3	1:J:270:THR:HG21	1.51	0.92
5:W:125:VAL:HG12	5:W:126:PHE:H	1.33	0.92
3:U:285:VAL:HG13	3:U:286:ASN:H	1.33	0.92
1:S:316:LEU:HD12	1:S:323:LEU:HB2	1.49	0.92
2:K:136:VAL:HG12	2:K:137:ASN:N	1.83	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:174:VAL:HG11	3:L:296:PHE:CE1	2.04	0.92
6:X:139:GLY:HA3	6:X:142:PRO:HB3	1.49	0.92
4:4:338:PRO:HG2	5:5:193:ARG:HB2	1.48	0.92
1:A:266:LEU:HB3	1:A:270:THR:HG21	1.52	0.92
3:C:288:ILE:HG12	3:C:288:ILE:O	1.70	0.92
4:4:74:THR:HB	4:4:77:GLN:HG3	1.51	0.92
5:5:139:GLU:HG2	5:5:140:ASP:H	1.31	0.92
3:U:46:ARG:O	3:U:107:MET:HG2	1.68	0.92
5:5:124:ILE:HG22	5:5:146:LEU:HB2	1.52	0.92
4:D:234:LEU:HD11	5:E:49:LEU:HD21	1.52	0.92
3:U:173:PHE:CD1	3:U:174:VAL:HG22	2.05	0.91
2:2:137:ASN:O	2:2:138:ASP:HB3	1.71	0.91
4:4:74:THR:HG22	4:4:76:LEU:H	1.36	0.91
5:5:124:ILE:HG21	5:5:146:LEU:HD23	1.52	0.91
1:J:316:LEU:HD12	1:J:323:LEU:HB2	1.51	0.91
8:H:60:SER:HB3	8:H:64:GLY:O	1.70	0.91
3:C:369:LEU:H	3:C:369:LEU:HD23	1.34	0.91
4:V:249:ARG:NH2	5:W:87:ARG:HE	1.67	0.91
4:D:385:CYS:HB3	4:D:396:ILE:HG12	1.51	0.91
1:1:185:GLU:HB2	1:1:218:ILE:HD12	1.50	0.91
4:4:234:LEU:HD11	5:5:49:LEU:HD21	1.51	0.91
5:E:26:TRP:HB3	5:E:89:PHE:HB2	1.49	0.91
5:N:26:TRP:HB3	5:N:89:PHE:HB2	1.52	0.91
7:G:141:VAL:HG13	7:G:142:GLY:H	1.35	0.91
3:C:174:VAL:HG21	3:C:296:PHE:CE2	2.05	0.90
6:F:163:TYR:HB2	6:F:168:GLU:O	1.70	0.90
3:C:194:VAL:HG12	3:C:411:LEU:HD22	1.54	0.90
3:L:748:VAL:HG22	3:L:750:ARG:O	1.72	0.90
1:S:33:LEU:HD23	1:S:37:GLY:HA3	1.50	0.90
6:F:164:ASN:HB3	7:G:148:ARG:HE	1.36	0.90
3:L:206:GLY:O	3:L:209:THR:HG23	1.71	0.90
3:C:6:VAL:HG12	3:C:7:ASN:N	1.86	0.90
5:E:52:ILE:HG23	5:E:117:GLU:HG2	1.54	0.90
3:3:288:ILE:O	3:3:288:ILE:HG12	1.69	0.90
5:W:124:ILE:HG22	5:W:146:LEU:HB2	1.54	0.90
5:5:119:TYR:CE1	5:5:132:LEU:HD11	2.06	0.90
4:V:85:MET:HE1	4:V:409:ARG:HB2	1.53	0.90
4:V:74:THR:HG22	4:V:76:LEU:H	1.36	0.90
6:6:114:SER:HB2	7:9:97:ARG:HD2	1.52	0.89
3:C:694:LEU:HB3	3:C:753:VAL:HG11	1.54	0.89
3:U:748:VAL:HG22	3:U:750:ARG:O	1.72	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:748:VAL:HG22	3:3:750:ARG:O	1.70	0.89
6:6:164:ASN:HB3	7:9:148:ARG:HE	1.38	0.89
6:X:114:SER:HB2	7:Y:97:ARG:HD2	1.53	0.89
4:M:74:THR:HG22	4:M:76:LEU:H	1.35	0.89
3:U:174:VAL:HG21	3:U:296:PHE:CE2	2.08	0.89
3:3:371:PHE:HE1	3:3:549:VAL:HB	1.38	0.89
6:O:164:ASN:HB3	7:P:148:ARG:HE	1.38	0.89
5:W:26:TRP:HB3	5:W:89:PHE:HB2	1.54	0.89
4:M:234:LEU:HD11	5:N:49:LEU:HD21	1.54	0.89
3:3:6:VAL:HG12	3:3:7:ASN:N	1.86	0.88
3:C:748:VAL:HG22	3:C:750:ARG:O	1.72	0.88
1:A:363:VAL:HG12	1:A:394:ILE:HD13	1.54	0.88
3:L:205:ARG:CA	3:L:209:THR:HG22	2.02	0.88
6:F:114:SER:HB2	7:G:97:ARG:HD2	1.53	0.88
4:M:385:CYS:HB3	4:M:396:ILE:HG12	1.55	0.88
4:V:74:THR:HB	4:V:77:GLN:HG3	1.53	0.88
2:2:131:ALA:HB1	2:2:132:PRO:CD	2.03	0.88
4:M:341:GLU:HG2	4:M:358:VAL:HG22	1.55	0.88
8:Q:60:SER:HB3	8:Q:64:GLY:O	1.73	0.88
3:3:206:GLY:O	3:3:209:THR:HG23	1.74	0.88
3:C:587:LEU:HD22	3:C:589:HIS:H	1.39	0.88
4:M:237:GLY:CA	5:N:112:ASN:HA	2.03	0.88
2:T:131:ALA:HB1	2:T:132:PRO:CD	2.04	0.88
4:D:191:LYS:NZ	3:U:730:GLU:HG3	1.86	0.88
4:V:85:MET:CE	4:V:409:ARG:HB2	2.04	0.88
4:V:234:LEU:HD11	5:W:49:LEU:HD21	1.56	0.88
3:L:587:LEU:HD22	3:L:589:HIS:H	1.39	0.88
2:T:136:VAL:HG12	2:T:137:ASN:N	1.88	0.88
2:B:136:VAL:HG12	2:B:137:ASN:N	1.89	0.88
3:U:507:LEU:HD22	3:U:520:ARG:HD3	1.56	0.88
4:D:103:LYS:HB3	5:E:22:LEU:HD13	1.54	0.87
3:L:45:CYS:O	3:L:45:CYS:SG	2.32	0.87
2:K:131:ALA:HB1	2:K:132:PRO:CD	2.04	0.87
6:F:138:PRO:HG3	7:G:121:MET:HG3	1.57	0.87
1:S:185:GLU:HB2	1:S:218:ILE:HD12	1.55	0.87
4:V:256:GLY:HA2	4:V:292:GLN:HE22	1.39	0.87
5:N:52:ILE:HG23	5:N:117:GLU:HG2	1.57	0.87
1:S:266:LEU:HB3	1:S:270:THR:HG21	1.54	0.87
3:U:45:CYS:O	3:U:45:CYS:SG	2.32	0.87
5:W:118:VAL:HG13	5:W:129:HIS:CD2	2.10	0.87
8:Z:60:SER:HB3	8:Z:64:GLY:O	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:139:GLY:HA3	6:6:142:PRO:HB3	1.57	0.87
1:A:370:LEU:O	1:A:374:ILE:HG22	1.75	0.87
1:J:11:PRO:HB3	1:J:270:THR:CB	2.03	0.87
4:D:85:MET:HE1	4:D:409:ARG:HB2	1.55	0.86
3:3:174:VAL:HG21	3:3:296:PHE:CE2	2.09	0.86
4:D:197:LEU:O	4:D:201:ILE:HD13	1.74	0.86
4:M:338:PRO:HG2	5:N:193:ARG:HB2	1.55	0.86
3:C:371:PHE:HE1	3:C:549:VAL:HB	1.39	0.86
7:P:141:VAL:HG13	7:P:142:GLY:H	1.39	0.86
6:X:164:ASN:HB3	7:Y:148:ARG:HE	1.38	0.86
5:E:124:ILE:HG22	5:E:146:LEU:HB2	1.57	0.86
3:L:6:VAL:HG12	3:L:7:ASN:N	1.89	0.86
3:U:369:LEU:H	3:U:369:LEU:HD23	1.41	0.86
6:F:84:LEU:HD11	6:F:89:ALA:HA	1.58	0.86
3:L:288:ILE:O	3:L:288:ILE:HG12	1.73	0.86
3:L:371:PHE:HE1	3:L:549:VAL:HB	1.40	0.86
6:6:163:TYR:HB2	6:6:168:GLU:O	1.75	0.85
7:9:56:CYS:SG	7:9:58:LEU:HD13	2.16	0.85
3:C:561:PRO:HB3	3:C:576:ALA:HA	1.56	0.85
3:L:243:ARG:HD3	3:L:275:LEU:HD12	1.58	0.85
4:M:249:ARG:NH2	5:N:87:ARG:HE	1.73	0.85
3:U:751:GLU:OE1	3:U:751:GLU:HA	1.76	0.85
3:3:587:LEU:HD22	3:3:589:HIS:H	1.41	0.85
4:M:74:THR:HB	4:M:77:GLN:HG3	1.58	0.85
1:S:11:PRO:HB3	1:S:270:THR:CB	2.04	0.85
7:Y:41:HIS:HB3	7:Y:113:ILE:HD11	1.57	0.85
1:1:11:PRO:HB3	1:1:270:THR:CB	2.05	0.85
1:J:108:GLU:HG2	1:J:140:ARG:HG2	1.55	0.85
2:K:114:ASP:HB2	2:K:116:LEU:CD2	2.06	0.85
3:U:371:PHE:HE1	3:U:549:VAL:HB	1.39	0.85
4:V:59:ILE:H	4:V:59:ILE:HD13	1.41	0.85
3:3:561:PRO:HB3	3:3:576:ALA:HA	1.59	0.85
2:K:139:GLU:HB2	2:K:140:PRO:CD	2.06	0.85
3:L:561:PRO:HB3	3:L:576:ALA:HA	1.59	0.85
6:O:163:TYR:HB2	6:O:168:GLU:O	1.74	0.85
6:X:138:PRO:HG3	7:Y:121:MET:HG3	1.57	0.85
1:1:108:GLU:HG2	1:1:140:ARG:HG2	1.58	0.85
7:9:56:CYS:O	7:9:56:CYS:SG	2.34	0.85
4:D:338:PRO:HG2	5:E:193:ARG:HB2	1.57	0.85
5:5:3:LEU:H	5:5:3:LEU:HD23	1.42	0.85
4:V:230:ILE:HG21	4:V:239:LEU:HB3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:85:MET:CE	4:4:409:ARG:HB2	2.06	0.84
5:W:124:ILE:HG21	5:W:146:LEU:HD23	1.57	0.84
2:B:131:ALA:HB1	2:B:132:PRO:CD	2.08	0.84
3:C:243:ARG:HD3	3:C:275:LEU:HD12	1.58	0.84
3:L:194:VAL:HG12	3:L:411:LEU:HD22	1.59	0.84
3:L:507:LEU:HD22	3:L:520:ARG:HD3	1.59	0.84
1:S:363:VAL:HG12	1:S:394:ILE:HD13	1.56	0.84
6:X:163:TYR:HB2	6:X:168:GLU:O	1.77	0.84
5:E:119:TYR:CE1	5:E:132:LEU:HD11	2.10	0.84
6:X:84:LEU:HD11	6:X:89:ALA:HA	1.59	0.84
3:3:507:LEU:HD22	3:3:520:ARG:HD3	1.59	0.84
4:D:59:ILE:HD13	4:D:59:ILE:H	1.40	0.84
4:M:249:ARG:CB	4:M:249:ARG:HH11	1.90	0.84
6:O:138:PRO:HG3	7:P:121:MET:HG3	1.58	0.84
5:W:52:ILE:HG23	5:W:117:GLU:HG2	1.59	0.84
3:C:151:LEU:HB3	3:C:152:PRO:HD3	1.59	0.84
5:N:124:ILE:HG23	5:N:145:PRO:HG2	1.57	0.84
3:U:288:ILE:HG12	3:U:288:ILE:O	1.73	0.84
3:U:205:ARG:CA	3:U:209:THR:HG22	2.07	0.84
4:4:52:VAL:HG21	4:4:388:GLU:H	1.43	0.84
3:C:206:GLY:O	3:C:209:THR:HG23	1.78	0.84
5:N:126:PHE:CE1	5:N:147:ARG:HD2	2.11	0.84
4:D:191:LYS:HZ1	3:U:730:GLU:HG3	1.41	0.84
4:D:85:MET:CE	4:D:409:ARG:HB2	2.07	0.84
5:E:118:VAL:HG13	5:E:129:HIS:CD2	2.13	0.84
1:S:88:TYR:HB2	1:S:216:THR:HG22	1.60	0.84
5:W:65:PRO:HD2	5:W:93:TYR:HE2	1.43	0.84
5:N:119:TYR:CE1	5:N:132:LEU:HD11	2.12	0.83
3:3:413:LEU:HD13	3:3:448:MET:CE	2.07	0.83
1:S:9:LEU:HB3	1:S:241:MET:HA	1.60	0.83
2:T:139:GLU:HB2	2:T:140:PRO:CD	2.09	0.83
3:3:751:GLU:OE1	3:3:751:GLU:HA	1.79	0.83
4:4:256:GLY:HA2	4:4:292:GLN:HE22	1.43	0.83
5:E:124:ILE:HG21	5:E:146:LEU:HD23	1.59	0.83
5:W:134:LYS:HE2	5:W:136:LEU:HB3	1.59	0.83
3:3:178:ARG:O	3:3:180:ARG:N	2.11	0.83
3:3:205:ARG:CA	3:3:209:THR:HG22	2.07	0.83
5:5:52:ILE:HG23	5:5:117:GLU:HG2	1.60	0.83
5:5:125:VAL:HG12	5:5:126:PHE:H	1.42	0.83
5:E:20:ASN:ND2	5:E:24:ASN:HB2	1.94	0.83
4:D:74:THR:HB	4:D:77:GLN:HG3	1.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:30:TRP:O	6:F:33:SER:HB3	1.79	0.83
5:W:3:LEU:H	5:W:3:LEU:HD23	1.42	0.83
5:5:134:LYS:HE2	5:5:136:LEU:HB3	1.61	0.83
1:A:11:PRO:HB3	1:A:270:THR:CB	2.07	0.83
2:B:139:GLU:HB2	2:B:140:PRO:CD	2.08	0.83
3:C:259:CYS:SG	3:C:261:VAL:HG22	2.18	0.83
7:P:41:HIS:HB3	7:P:113:ILE:HD11	1.60	0.83
3:3:369:LEU:H	3:3:369:LEU:HD23	1.43	0.83
2:B:137:ASN:O	2:B:138:ASP:HB3	1.77	0.83
3:C:46:ARG:O	3:C:107:MET:HG2	1.79	0.82
3:L:151:LEU:HB3	3:L:152:PRO:HD3	1.61	0.82
3:U:587:LEU:HD22	3:U:589:HIS:H	1.42	0.82
4:4:59:ILE:H	4:4:59:ILE:HD13	1.44	0.82
3:L:259:CYS:SG	3:L:261:VAL:HG22	2.18	0.82
6:6:19:ILE:HD12	1:J:274:GLU:HB2	1.60	0.82
4:4:322:GLU:O	4:4:325:ILE:HB	1.79	0.82
1:J:363:VAL:HG12	1:J:394:ILE:HD13	1.59	0.82
3:L:751:GLU:OE1	3:L:751:GLU:HA	1.79	0.82
4:M:409:ARG:HG2	4:M:409:ARG:O	1.79	0.82
1:1:88:TYR:HB2	1:1:216:THR:HG22	1.62	0.82
3:C:494:LYS:O	3:C:498:GLU:HG2	1.79	0.82
3:L:7:ASN:ND2	3:L:96:LEU:HD11	1.94	0.82
5:5:65:PRO:HD2	5:5:93:TYR:HE2	1.44	0.82
6:6:84:LEU:HD11	6:6:89:ALA:HA	1.60	0.82
4:D:64:THR:HG23	6:F:123:ILE:CD1	2.10	0.82
2:2:139:GLU:HB2	2:2:140:PRO:CD	2.08	0.82
3:C:205:ARG:CA	3:C:209:THR:HG22	2.07	0.82
1:J:11:PRO:HB2	1:J:274:GLU:OE1	1.80	0.82
4:M:52:VAL:HG21	4:M:388:GLU:H	1.45	0.82
4:V:409:ARG:O	4:V:409:ARG:HG2	1.78	0.82
5:W:25:LEU:HD23	5:W:25:LEU:H	1.45	0.82
5:E:124:ILE:HG23	5:E:145:PRO:HG2	1.62	0.82
3:U:561:PRO:HB3	3:U:576:ALA:HA	1.61	0.82
3:3:285:VAL:HG13	3:3:286:ASN:N	1.93	0.82
4:4:249:ARG:NH2	5:5:87:ARG:HE	1.77	0.82
6:O:114:SER:HB2	7:P:97:ARG:HD2	1.59	0.82
5:N:3:LEU:HD23	5:N:3:LEU:H	1.45	0.81
2:T:137:ASN:O	2:T:138:ASP:HB3	1.79	0.81
3:C:285:VAL:HG13	3:C:286:ASN:N	1.94	0.81
3:L:174:VAL:HG21	3:L:296:PHE:CE2	2.14	0.81
2:K:110:GLU:HA	8:Q:121:ARG:HH12	1.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:751:GLU:OE1	3:C:751:GLU:HA	1.80	0.81
3:L:694:LEU:HB3	3:L:753:VAL:HG11	1.62	0.81
6:6:107:SER:O	6:6:137:VAL:HG12	1.80	0.81
3:C:7:ASN:ND2	3:C:96:LEU:HD11	1.95	0.81
5:E:126:PHE:CE1	5:E:147:ARG:HD2	2.15	0.81
3:U:524:LEU:HG	3:U:525:ALA:H	1.46	0.81
3:L:157:PHE:CE1	3:L:159:PHE:HB2	2.16	0.81
3:C:178:ARG:O	3:C:180:ARG:N	2.14	0.81
4:4:225:PRO:HD2	4:4:226:PRO:HD3	1.63	0.81
2:T:114:ASP:HB2	2:T:116:LEU:CD2	2.10	0.81
6:X:81:ALA:HA	6:X:108:MET:HB3	1.62	0.81
3:3:151:LEU:HB3	3:3:152:PRO:HD3	1.63	0.81
5:E:3:LEU:H	5:E:3:LEU:HD23	1.44	0.81
3:U:202:PHE:O	3:U:203:ILE:HD13	1.81	0.81
1:1:11:PRO:HB2	1:1:274:GLU:OE1	1.81	0.81
4:M:256:GLY:HA2	4:M:292:GLN:HE22	1.46	0.81
3:U:378:PRO:O	3:U:381:LEU:HD23	1.79	0.81
1:1:363:VAL:HG12	1:1:394:ILE:HD13	1.62	0.80
2:B:114:ASP:HB2	2:B:116:LEU:CD2	2.11	0.80
1:A:95:GLU:HA	11:H:500:FMN:HN3	1.46	0.80
1:J:95:GLU:HA	11:Q:500:FMN:HN3	1.45	0.80
3:U:515:THR:HG23	3:U:516:VAL:HG23	1.62	0.80
6:6:165:GLU:HG3	7:9:128:ASP:OD1	1.82	0.80
3:C:243:ARG:HB3	3:C:275:LEU:HD12	1.61	0.80
4:M:85:MET:CE	4:M:409:ARG:HB2	2.10	0.80
5:N:124:ILE:HG21	5:N:146:LEU:HD23	1.62	0.80
3:3:46:ARG:O	3:3:107:MET:HG2	1.82	0.80
3:3:243:ARG:HD3	3:3:275:LEU:HD12	1.63	0.80
3:L:178:ARG:O	3:L:180:ARG:N	2.14	0.80
3:L:378:PRO:O	3:L:381:LEU:HD23	1.81	0.80
6:O:165:GLU:HG3	7:P:128:ASP:CG	2.02	0.80
3:U:206:GLY:O	3:U:209:THR:HG23	1.81	0.80
3:C:748:VAL:O	3:C:748:VAL:HG13	1.80	0.80
6:F:163:TYR:CB	6:F:169:ARG:HA	2.12	0.80
1:S:370:LEU:O	1:S:374:ILE:HG22	1.79	0.80
5:N:124:ILE:HG22	5:N:146:LEU:HB2	1.63	0.80
1:S:359:CYS:HA	1:S:363:VAL:HG13	1.63	0.80
5:W:119:TYR:CE1	5:W:132:LEU:HD11	2.17	0.80
1:1:316:LEU:HD12	1:1:323:LEU:HB2	1.63	0.80
5:5:65:PRO:HD2	5:5:93:TYR:CE2	2.17	0.80
7:Y:141:VAL:HG13	7:Y:142:GLY:N	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:GLU:HA	8:H:121:ARG:HH12	1.46	0.80
3:L:46:ARG:O	3:L:107:MET:HG2	1.81	0.80
4:M:59:ILE:HD13	4:M:59:ILE:H	1.47	0.80
3:3:259:CYS:SG	3:3:261:VAL:HG22	2.21	0.80
4:4:249:ARG:HH11	4:4:249:ARG:CB	1.94	0.80
5:W:124:ILE:HG23	5:W:145:PRO:HG2	1.63	0.80
1:1:253:GLN:HG2	1:1:327:GLY:HA2	1.62	0.80
5:E:134:LYS:HE2	5:E:136:LEU:HB3	1.62	0.80
6:O:84:LEU:HD11	6:O:89:ALA:HA	1.63	0.80
1:S:11:PRO:HB2	1:S:274:GLU:OE1	1.81	0.80
3:U:6:VAL:HG12	3:U:7:ASN:N	1.95	0.80
7:G:56:CYS:SG	7:G:56:CYS:O	2.39	0.79
3:L:369:LEU:HD23	3:L:369:LEU:H	1.46	0.79
4:D:256:GLY:HA2	4:D:292:GLN:HE22	1.47	0.79
1:S:253:GLN:HG2	1:S:327:GLY:HA2	1.64	0.79
5:5:25:LEU:HD23	5:5:25:LEU:H	1.47	0.79
3:L:524:LEU:HG	3:L:525:ALA:H	1.46	0.79
7:9:141:VAL:HG13	7:9:142:GLY:N	1.97	0.79
1:A:9:LEU:HB3	1:A:241:MET:HA	1.64	0.79
1:1:359:CYS:HA	1:1:363:VAL:HG13	1.62	0.79
1:A:253:GLN:HG2	1:A:327:GLY:HA2	1.63	0.79
3:L:567:TYR:HE1	3:L:586:HIS:HB2	1.47	0.79
3:U:748:VAL:O	3:U:748:VAL:HG13	1.83	0.79
4:V:341:GLU:HG2	4:V:358:VAL:HG22	1.65	0.79
4:4:409:ARG:HG2	4:4:409:ARG:O	1.80	0.79
3:L:285:VAL:HG13	3:L:286:ASN:N	1.97	0.79
3:U:376:ALA:H	3:U:512:LEU:HD12	1.47	0.79
4:V:52:VAL:HG21	4:V:388:GLU:H	1.46	0.79
3:C:567:TYR:HE1	3:C:586:HIS:HB2	1.48	0.79
3:3:186:ARG:HD3	3:3:229:ILE:HG22	1.63	0.79
4:4:59:ILE:H	4:4:59:ILE:CD1	1.96	0.79
5:E:25:LEU:H	5:E:25:LEU:HD23	1.47	0.79
6:X:145:GLU:HG2	7:Y:31:VAL:HG21	1.65	0.79
4:4:226:PRO:CD	4:4:239:LEU:HB2	2.13	0.79
4:4:52:VAL:HG21	4:4:388:GLU:N	1.98	0.79
6:6:81:ALA:HA	6:6:108:MET:HB3	1.65	0.79
7:9:41:HIS:HB3	7:9:113:ILE:HD11	1.63	0.79
1:J:88:TYR:HB2	1:J:216:THR:HG22	1.65	0.79
4:M:86:ASP:O	4:M:88:LEU:N	2.15	0.79
2:T:110:GLU:HA	8:Z:121:ARG:HH12	1.47	0.79
4:V:226:PRO:CD	4:V:239:LEU:HB2	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:515:THR:HG23	3:3:516:VAL:HG23	1.62	0.79
4:4:252:TYR:HB2	4:4:253:PRO:CD	2.13	0.79
6:6:163:TYR:CB	6:6:169:ARG:HA	2.13	0.79
4:D:249:ARG:CB	4:D:249:ARG:HH11	1.94	0.79
4:D:59:ILE:CD1	4:D:59:ILE:H	1.96	0.79
3:L:731:GLY:N	3:L:747:VAL:HG12	1.97	0.79
6:6:138:PRO:HG3	7:9:121:MET:HG3	1.63	0.78
2:B:86:LEU:O	2:B:90:LEU:HD12	1.83	0.78
3:L:374:ARG:HH21	3:L:684:ARG:HG3	1.47	0.78
5:W:80:TRP:HA	5:W:80:TRP:CE3	2.18	0.78
2:K:86:LEU:O	2:K:90:LEU:HD12	1.84	0.78
4:M:248:VAL:HG12	4:M:249:ARG:HD2	1.62	0.78
4:V:59:ILE:CD1	4:V:59:ILE:H	1.96	0.78
3:U:178:ARG:O	3:U:180:ARG:N	2.15	0.78
5:W:126:PHE:CE1	5:W:147:ARG:HD2	2.16	0.78
3:C:731:GLY:N	3:C:747:VAL:HG12	1.97	0.78
4:D:409:ARG:O	4:D:409:ARG:HG2	1.82	0.78
6:F:139:GLY:HA3	6:F:142:PRO:CB	2.14	0.78
1:1:222:GLU:CD	1:1:251:LEU:HD13	2.02	0.78
3:3:567:TYR:HE1	3:3:586:HIS:HB2	1.49	0.78
1:A:359:CYS:HA	1:A:363:VAL:HG13	1.65	0.78
1:S:222:GLU:CD	1:S:251:LEU:HD13	2.03	0.78
3:U:243:ARG:HD3	3:U:275:LEU:HD12	1.63	0.78
4:D:224:ILE:HD12	4:D:237:GLY:HA2	1.64	0.78
7:G:95:MET:HB2	7:G:129:LEU:O	1.83	0.78
2:T:40:TRP:HE3	2:T:41:ILE:N	1.82	0.78
3:U:285:VAL:HG13	3:U:286:ASN:N	1.97	0.78
3:3:537:PRO:HB3	3:3:758:LEU:HD11	1.66	0.78
2:B:136:VAL:HG21	2:B:163:LEU:HD13	1.66	0.78
7:G:117:TYR:OH	7:G:167:ARG:HG3	1.83	0.78
1:J:185:GLU:HB2	1:J:218:ILE:HD12	1.64	0.78
3:L:748:VAL:HG13	3:L:748:VAL:O	1.83	0.78
1:S:252:TYR:HB3	1:S:275:LEU:HD11	1.66	0.78
1:1:95:GLU:HA	11:7:500:FMN:HN3	1.48	0.78
4:M:226:PRO:CD	4:M:239:LEU:HB2	2.13	0.78
3:U:7:ASN:ND2	3:U:96:LEU:HD11	1.99	0.78
4:V:322:GLU:O	4:V:325:ILE:HB	1.83	0.78
1:A:11:PRO:HB2	1:A:274:GLU:OE1	1.83	0.78
1:1:9:LEU:HB3	1:1:241:MET:HA	1.65	0.77
5:5:126:PHE:CE1	5:5:147:ARG:HD2	2.18	0.77
5:W:65:PRO:HD2	5:W:93:TYR:CE2	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:398:VAL:HB	3:3:450:LEU:HD22	1.67	0.77
5:5:16:PRO:HD2	5:5:28:VAL:HG13	1.65	0.77
1:A:108:GLU:HG2	1:A:140:ARG:HG2	1.65	0.77
3:C:515:THR:HG23	3:C:516:VAL:HG23	1.66	0.77
3:C:517:ALA:HA	3:C:520:ARG:HD2	1.65	0.77
3:U:2:VAL:HG13	3:U:89:ASP:HA	1.66	0.77
7:9:96:LEU:HD21	7:9:129:LEU:HD12	1.67	0.77
3:C:586:HIS:CD2	3:C:604:ALA:HB2	2.19	0.77
6:F:81:ALA:HA	6:F:108:MET:HB3	1.66	0.77
5:W:16:PRO:HD2	5:W:28:VAL:HG13	1.65	0.77
5:5:121:LEU:N	5:5:121:LEU:HD12	2.00	0.77
1:A:185:GLU:HB2	1:A:218:ILE:HD12	1.64	0.77
3:C:378:PRO:O	3:C:381:LEU:HD23	1.83	0.77
7:G:41:HIS:HB3	7:G:113:ILE:HD11	1.67	0.77
1:J:253:GLN:HG2	1:J:327:GLY:HA2	1.65	0.77
4:M:52:VAL:HG21	4:M:388:GLU:N	1.99	0.77
3:U:567:TYR:HE1	3:U:586:HIS:HB2	1.48	0.77
1:A:88:TYR:HB2	1:A:216:THR:HG22	1.64	0.77
1:J:366:PHE:CD1	1:J:370:LEU:HD21	2.19	0.77
4:M:322:GLU:O	4:M:325:ILE:HB	1.83	0.77
3:3:194:VAL:HG12	3:3:411:LEU:HD22	1.66	0.77
4:4:237:GLY:HA2	5:5:112:ASN:HA	1.65	0.77
2:2:114:ASP:HB2	2:2:116:LEU:CD2	2.14	0.77
5:5:46:PHE:O	5:5:48:PHE:N	2.18	0.77
1:J:222:GLU:CD	1:J:251:LEU:HD13	2.04	0.77
3:L:178:ARG:HG2	3:L:178:ARG:O	1.84	0.77
2:2:110:GLU:HA	8:7:121:ARG:HH12	1.49	0.77
6:O:163:TYR:CB	6:O:169:ARG:HA	2.15	0.77
4:V:197:LEU:O	4:V:201:ILE:HD13	1.85	0.77
3:3:403:THR:OG1	3:3:458:LEU:HD11	1.85	0.77
3:3:524:LEU:HG	3:3:525:ALA:H	1.48	0.77
5:E:80:TRP:CE3	5:E:80:TRP:HA	2.20	0.77
3:L:202:PHE:O	3:L:203:ILE:HD13	1.85	0.77
1:1:252:TYR:HB3	1:1:275:LEU:HD11	1.67	0.76
4:D:322:GLU:O	4:D:325:ILE:HB	1.85	0.76
6:X:163:TYR:CB	6:X:169:ARG:HA	2.15	0.76
4:4:235:THR:HA	4:4:239:LEU:HD22	1.67	0.76
6:6:165:GLU:HG3	7:9:128:ASP:CG	2.06	0.76
3:U:524:LEU:HG	3:U:525:ALA:N	2.00	0.76
3:3:517:ALA:HA	3:3:520:ARG:HD2	1.68	0.76
3:U:243:ARG:HB3	3:U:275:LEU:HD12	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:201:LEU:O	1:1:204:PRO:HD2	1.84	0.76
3:L:356:LEU:HD13	3:L:654:PHE:HB2	1.68	0.76
3:3:731:GLY:N	3:3:747:VAL:HG12	2.00	0.76
4:4:232:LEU:HD11	4:4:282:GLU:OE2	1.85	0.76
3:C:507:LEU:HD22	3:C:520:ARG:HD3	1.65	0.76
5:E:130:PRO:HG2	5:E:131:ASP:H	1.50	0.76
5:E:65:PRO:HD2	5:E:93:TYR:HE2	1.50	0.76
2:K:86:LEU:CD1	2:K:90:LEU:HD11	2.15	0.76
6:O:107:SER:O	6:O:137:VAL:HG12	1.84	0.76
2:2:72:PHE:HB2	8:7:89:ALA:HB2	1.66	0.76
4:4:342:VAL:HG22	4:4:343:TYR:H	1.50	0.76
1:1:145:LEU:O	1:1:149:ILE:HG13	1.85	0.76
3:3:413:LEU:HD13	3:3:448:MET:HE1	1.68	0.76
3:C:202:PHE:O	3:C:203:ILE:HD13	1.85	0.76
3:C:376:ALA:H	3:C:512:LEU:HD12	1.51	0.76
5:N:48:PHE:C	5:N:50:ALA:H	1.88	0.76
3:U:403:THR:OG1	3:U:458:LEU:HD11	1.85	0.76
3:U:537:PRO:HB3	3:U:758:LEU:HD11	1.66	0.76
4:V:52:VAL:HG21	4:V:388:GLU:N	2.00	0.76
4:D:237:GLY:HA2	5:E:112:ASN:HA	1.66	0.76
5:N:46:PHE:O	5:N:48:PHE:N	2.19	0.76
4:4:168:PHE:HD1	4:4:168:PHE:N	1.84	0.76
4:4:249:ARG:NH2	5:5:87:ARG:HB2	2.01	0.76
7:G:56:CYS:SG	7:G:58:LEU:HD13	2.26	0.76
3:L:515:THR:HG23	3:L:516:VAL:HG23	1.66	0.76
4:M:59:ILE:H	4:M:59:ILE:CD1	1.99	0.76
4:V:228:VAL:HG12	4:V:271:ASP:HA	1.68	0.76
4:D:225:PRO:HD2	4:D:226:PRO:HD3	1.66	0.76
4:M:85:MET:HE1	4:M:409:ARG:HB2	1.67	0.76
6:O:81:ALA:HA	6:O:108:MET:HB3	1.66	0.76
5:W:80:TRP:HA	5:W:80:TRP:HE3	1.50	0.76
4:D:248:VAL:HG12	4:D:249:ARG:HD2	1.69	0.75
4:M:278:VAL:O	4:M:281:ARG:HB2	1.86	0.75
5:N:25:LEU:HD23	5:N:25:LEU:H	1.49	0.75
3:U:517:ALA:HA	3:U:520:ARG:HD2	1.68	0.75
4:V:237:GLY:HA2	5:W:112:ASN:HA	1.67	0.75
4:4:278:VAL:O	4:4:281:ARG:HB2	1.87	0.75
5:5:127:GLU:HA	5:5:127:GLU:OE1	1.86	0.75
3:U:151:LEU:HB3	3:U:152:PRO:HD3	1.66	0.75
1:A:366:PHE:CD1	1:A:370:LEU:HD21	2.21	0.75
4:D:226:PRO:CD	4:D:239:LEU:HB2	2.14	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:230:ILE:HG21	4:D:239:LEU:HB3	1.68	0.75
5:E:46:PHE:O	5:E:48:PHE:N	2.19	0.75
3:L:413:LEU:HD13	3:L:448:MET:CE	2.16	0.75
3:L:517:ALA:HA	3:L:520:ARG:HD2	1.67	0.75
4:M:51:GLU:O	4:M:52:VAL:HG13	1.87	0.75
1:S:90:ILE:HD11	1:S:211:LEU:HD22	1.66	0.75
1:1:438:ARG:HD2	1:1:438:ARG:H	1.52	0.75
3:L:2:VAL:HG13	3:L:89:ASP:HA	1.68	0.75
1:1:359:CYS:O	1:1:363:VAL:HG22	1.86	0.75
4:D:341:GLU:HG2	4:D:358:VAL:HG22	1.69	0.75
7:G:141:VAL:HG13	7:G:142:GLY:N	2.01	0.75
2:2:86:LEU:O	2:2:90:LEU:HD12	1.85	0.75
3:3:748:VAL:HG13	3:3:748:VAL:O	1.87	0.75
3:C:356:LEU:HD13	3:C:654:PHE:HB2	1.68	0.75
2:K:40:TRP:HE1	2:K:74:PRO:HG3	1.52	0.75
4:M:240:ARG:CD	4:M:243:GLY:HA3	2.09	0.75
7:G:35:PRO:O	7:G:36:ARG:CB	2.35	0.75
5:N:44:MET:CE	5:N:82:ASP:HB3	2.15	0.75
3:U:758:LEU:HD12	3:U:758:LEU:N	2.00	0.75
4:V:225:PRO:HD2	4:V:226:PRO:HD3	1.69	0.75
3:C:174:VAL:HG21	3:C:296:PHE:CD2	2.21	0.75
4:D:252:TYR:HB2	4:D:253:PRO:CD	2.16	0.75
4:D:52:VAL:HG21	4:D:388:GLU:H	1.51	0.75
5:E:48:PHE:C	5:E:50:ALA:H	1.88	0.75
3:L:117:LEU:HD23	4:M:322:GLU:OE2	1.86	0.75
1:S:95:GLU:HA	11:Z:500:FMN:HN3	1.51	0.75
5:5:80:TRP:HE3	5:5:80:TRP:HA	1.52	0.75
6:6:30:TRP:O	6:6:33:SER:HB3	1.85	0.75
3:C:684:ARG:HG2	3:C:684:ARG:HH11	1.52	0.75
3:L:243:ARG:HB3	3:L:275:LEU:HD12	1.68	0.75
4:V:168:PHE:HD1	4:V:168:PHE:N	1.85	0.75
2:2:39:GLY:O	2:2:75:THR:HG22	1.87	0.74
5:5:20:ASN:ND2	5:5:24:ASN:HB2	2.02	0.74
6:F:147:LEU:O	6:F:150:ALA:HB3	1.86	0.74
5:E:125:VAL:HG12	5:E:126:PHE:N	2.02	0.74
6:X:165:GLU:HG3	7:Y:128:ASP:CG	2.06	0.74
1:1:357:THR:OG1	3:3:45:CYS:HA	1.86	0.74
5:5:80:TRP:CE3	5:5:80:TRP:HA	2.20	0.74
4:D:168:PHE:HD1	4:D:168:PHE:N	1.85	0.74
4:M:235:THR:HA	4:M:239:LEU:HD22	1.70	0.74
5:N:134:LYS:HE2	5:N:136:LEU:HB3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:524:LEU:HG	3:3:525:ALA:N	2.02	0.74
5:5:139:GLU:CG	5:5:140:ASP:H	2.00	0.74
6:6:164:ASN:H	6:6:170:LEU:HD12	1.51	0.74
3:C:537:PRO:HB3	3:C:758:LEU:HD11	1.70	0.74
4:D:228:VAL:HG12	4:D:271:ASP:HA	1.69	0.74
3:L:537:PRO:HB3	3:L:758:LEU:HD11	1.70	0.74
5:N:80:TRP:HA	5:N:80:TRP:CE3	2.20	0.74
5:N:80:TRP:HA	5:N:80:TRP:HE3	1.53	0.74
3:3:174:VAL:HG21	3:3:296:PHE:CD2	2.22	0.74
3:3:307:LYS:H	3:3:307:LYS:CE	2.00	0.74
3:3:650:VAL:HG12	3:3:651:ARG:H	1.53	0.74
5:E:80:TRP:HE3	5:E:80:TRP:HA	1.53	0.74
5:N:127:GLU:HA	5:N:127:GLU:OE1	1.87	0.74
5:N:59:THR:O	5:N:59:THR:HG22	1.88	0.74
4:V:219:ARG:O	4:V:219:ARG:HD3	1.87	0.74
4:V:249:ARG:NH2	5:W:87:ARG:HB2	2.01	0.74
3:3:378:PRO:O	3:3:381:LEU:HD23	1.87	0.74
6:6:147:LEU:O	6:6:150:ALA:HB3	1.87	0.74
4:D:379:GLN:OE1	5:E:116:ARG:HG2	1.87	0.74
5:E:50:ALA:HB1	5:E:114:LEU:HD21	1.68	0.74
5:N:139:GLU:HG2	5:N:140:ASP:N	2.02	0.74
6:O:139:GLY:HA3	6:O:142:PRO:CB	2.16	0.74
1:S:219:ASN:HD22	1:S:223:THR:HG21	1.52	0.74
2:T:136:VAL:HG21	2:T:163:LEU:HD13	1.68	0.74
3:3:374:ARG:HH21	3:3:684:ARG:HG3	1.51	0.74
3:C:157:PHE:CE1	3:C:159:PHE:HB2	2.22	0.74
3:C:413:LEU:HD13	3:C:448:MET:CE	2.17	0.74
4:4:248:VAL:HG12	4:4:249:ARG:HD2	1.69	0.74
3:L:186:ARG:HD3	3:L:229:ILE:HG22	1.70	0.74
7:Y:45:ARG:HH21	7:Y:137:LEU:HD23	1.53	0.74
7:Y:56:CYS:SG	7:Y:56:CYS:O	2.45	0.74
3:3:194:VAL:HB	3:3:195:PRO:CD	2.18	0.74
1:A:252:TYR:HB3	1:A:275:LEU:HD11	1.69	0.74
6:F:120:ASN:ND2	6:F:122:ALA:HB3	2.02	0.74
1:J:357:THR:OG1	3:L:45:CYS:HA	1.87	0.74
4:M:225:PRO:HD2	4:M:226:PRO:HD3	1.69	0.74
6:O:165:GLU:HG3	7:P:128:ASP:OD1	1.88	0.74
3:U:374:ARG:HH21	3:U:684:ARG:HG3	1.52	0.74
5:W:46:PHE:O	5:W:48:PHE:N	2.21	0.74
3:3:376:ALA:H	3:3:512:LEU:HD12	1.51	0.74
1:A:214:LYS:O	1:A:216:THR:HG23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLU:CD	1:A:251:LEU:HD13	2.08	0.74
2:B:39:GLY:O	2:B:75:THR:HG22	1.88	0.74
3:C:564:LEU:HD11	3:C:581:ARG:H	1.51	0.74
1:A:201:LEU:O	1:A:204:PRO:HD2	1.88	0.73
1:J:9:LEU:HB3	1:J:241:MET:HA	1.68	0.73
3:U:174:VAL:HG21	3:U:296:PHE:CD2	2.22	0.73
3:U:413:LEU:HD13	3:U:448:MET:CE	2.18	0.73
5:W:134:LYS:CE	5:W:136:LEU:HB3	2.18	0.73
4:4:240:ARG:CD	4:4:243:GLY:HA3	2.15	0.73
3:L:524:LEU:HG	3:L:525:ALA:N	2.01	0.73
3:U:487:SER:OG	3:U:490:VAL:HG23	1.88	0.73
3:U:556:ALA:HB1	3:U:560:GLU:O	1.88	0.73
4:4:252:TYR:CB	4:4:253:PRO:HD2	2.16	0.73
3:L:403:THR:OG1	3:L:458:LEU:HD11	1.87	0.73
3:L:45:CYS:O	3:L:47:MET:N	2.22	0.73
1:S:192:LEU:HD22	1:S:211:LEU:HD11	1.69	0.73
3:3:694:LEU:HB3	3:3:753:VAL:HG11	1.68	0.73
5:5:130:PRO:HG2	5:5:131:ASP:H	1.52	0.73
2:B:106:ILE:HD11	2:B:112:THR:HB	1.71	0.73
2:B:86:LEU:CD1	2:B:90:LEU:HD11	2.17	0.73
5:E:139:GLU:HG2	5:E:140:ASP:N	2.01	0.73
5:E:175:THR:HG23	5:E:178:ASP:HB2	1.71	0.73
6:O:16:ARG:HD2	6:O:17:GLU:HG3	1.70	0.73
4:V:228:VAL:HG22	4:V:268:GLU:O	1.88	0.73
6:X:120:ASN:ND2	6:X:122:ALA:HB3	2.03	0.73
1:1:370:LEU:O	1:1:374:ILE:HG22	1.89	0.73
3:3:583:VAL:HG23	3:3:598:ALA:HA	1.70	0.73
4:4:224:ILE:HD12	4:4:237:GLY:HA2	1.70	0.73
4:4:228:VAL:HG12	4:4:271:ASP:HA	1.71	0.73
5:5:48:PHE:C	5:5:50:ALA:H	1.90	0.73
4:D:237:GLY:HA3	5:E:112:ASN:O	1.88	0.73
3:L:758:LEU:N	3:L:758:LEU:HD12	2.03	0.73
5:N:139:GLU:CG	5:N:140:ASP:H	2.01	0.73
1:S:438:ARG:HD2	1:S:438:ARG:H	1.51	0.73
3:U:398:VAL:HB	3:U:450:LEU:HD22	1.70	0.73
3:U:684:ARG:HH11	3:U:684:ARG:HG2	1.53	0.73
7:Y:95:MET:HB2	7:Y:129:LEU:O	1.89	0.73
6:6:120:ASN:ND2	6:6:122:ALA:HB3	2.04	0.73
1:A:219:ASN:HD22	1:A:223:THR:HG21	1.53	0.73
2:B:7:LYS:H	2:B:7:LYS:HD2	1.53	0.73
4:D:105:LEU:HD23	4:D:337:PRO:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:583:VAL:HG23	3:L:598:ALA:HA	1.71	0.73
4:D:116:ILE:O	4:D:120:LEU:HB2	1.89	0.73
1:J:438:ARG:HD2	1:J:438:ARG:H	1.54	0.73
3:L:398:VAL:HB	3:L:450:LEU:HD22	1.71	0.73
3:L:587:LEU:HD23	3:L:588:SER:H	1.52	0.73
4:M:320:SER:O	4:M:321:MET:C	2.25	0.73
3:3:131:GLN:HG2	4:4:325:ILE:HG12	1.71	0.73
4:4:237:GLY:HA3	5:5:112:ASN:O	1.89	0.73
5:5:124:ILE:HG23	5:5:145:PRO:HG2	1.69	0.73
3:C:171:SER:HB3	3:C:173:PHE:HB3	1.71	0.73
3:C:724:ARG:CD	3:C:724:ARG:H	2.01	0.73
3:C:2:VAL:HG13	3:C:89:ASP:HA	1.69	0.73
3:U:186:ARG:HD3	3:U:229:ILE:HG22	1.68	0.73
3:U:19:VAL:O	3:U:22:ALA:HB3	1.88	0.73
1:1:107:LEU:O	1:1:111:PRO:HG3	1.88	0.73
1:1:219:ASN:HD22	1:1:223:THR:HG21	1.54	0.73
1:A:110:VAL:N	1:A:111:PRO:HD3	2.04	0.73
4:D:320:SER:HB2	4:D:323:ALA:HB3	1.70	0.73
5:E:134:LYS:CE	5:E:136:LEU:HB3	2.18	0.73
2:K:77:LYS:H	2:K:116:LEU:HA	1.54	0.73
3:L:684:ARG:HG2	3:L:684:ARG:HH11	1.53	0.73
3:U:356:LEU:HD13	3:U:654:PHE:HB2	1.69	0.73
3:C:587:LEU:HD23	3:C:588:SER:H	1.52	0.73
1:J:252:TYR:HB3	1:J:275:LEU:HD11	1.71	0.73
1:S:201:LEU:O	1:S:204:PRO:HD2	1.89	0.73
4:V:98:ALA:O	4:V:102:GLU:HG3	1.89	0.73
2:2:40:TRP:HE3	2:2:41:ILE:N	1.87	0.72
2:B:72:PHE:HB2	8:H:89:ALA:HB2	1.71	0.72
5:E:139:GLU:CG	5:E:140:ASP:H	2.00	0.72
4:M:237:GLY:HA3	5:N:112:ASN:O	1.89	0.72
4:M:383:TYR:O	4:M:386:LYS:N	2.19	0.72
2:T:72:PHE:HB2	8:Z:89:ALA:HB2	1.71	0.72
3:U:514:ASP:OD2	3:U:685:PRO:HB3	1.89	0.72
3:3:7:ASN:ND2	3:3:96:LEU:HD11	2.04	0.72
4:D:252:TYR:CB	4:D:253:PRO:HD2	2.19	0.72
1:J:107:LEU:O	1:J:111:PRO:HG3	1.87	0.72
4:V:232:LEU:HD13	4:V:278:VAL:HG12	1.70	0.72
3:3:556:ALA:HB1	3:3:560:GLU:O	1.88	0.72
4:M:230:ILE:HG21	4:M:239:LEU:HB3	1.69	0.72
2:T:89:LYS:HA	2:T:93:ALA:HB3	1.71	0.72
3:U:194:VAL:HG12	3:U:411:LEU:HD22	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:107:SER:O	6:X:137:VAL:HG12	1.87	0.72
6:6:19:ILE:CD1	1:J:274:GLU:HB2	2.18	0.72
6:O:147:LEU:O	6:O:150:ALA:HB3	1.90	0.72
3:L:134:THR:O	3:L:138:GLY:HA3	1.89	0.72
3:U:481:LEU:HD11	3:U:519:GLU:HB2	1.70	0.72
3:U:694:LEU:HB3	3:U:753:VAL:HG11	1.71	0.72
6:X:165:GLU:HG3	7:Y:128:ASP:OD1	1.90	0.72
3:C:631:ASN:C	3:C:633:GLU:H	1.92	0.72
4:D:52:VAL:HG21	4:D:388:GLU:N	2.04	0.72
4:M:232:LEU:HD11	4:M:282:GLU:OE2	1.88	0.72
5:N:20:ASN:ND2	5:N:24:ASN:HB2	2.03	0.72
4:M:64:THR:HG23	6:O:123:ILE:CD1	2.17	0.72
2:K:72:PHE:HB2	8:Q:89:ALA:HB2	1.70	0.72
4:V:248:VAL:HG12	4:V:249:ARG:HD2	1.69	0.72
1:A:107:LEU:O	1:A:111:PRO:HG3	1.90	0.72
3:C:524:LEU:HG	3:C:525:ALA:N	2.04	0.72
3:C:374:ARG:HH21	3:C:684:ARG:HG3	1.53	0.72
3:L:115:HIS:CG	3:L:116:PRO:HD2	2.24	0.72
4:M:342:VAL:HG22	4:M:343:TYR:H	1.54	0.72
2:T:106:ILE:HD11	2:T:112:THR:HB	1.71	0.72
4:V:89:HIS:HB2	4:V:128:SER:HB2	1.70	0.72
5:5:139:GLU:HG2	5:5:140:ASP:N	2.04	0.72
2:B:39:GLY:O	2:B:40:TRP:HB2	1.88	0.72
3:C:650:VAL:HG12	3:C:651:ARG:H	1.54	0.72
4:D:393:MET:HG2	4:D:393:MET:O	1.89	0.72
4:M:266:LEU:HD13	4:M:281:ARG:CB	2.12	0.72
1:S:359:CYS:O	1:S:363:VAL:HG22	1.90	0.72
3:U:157:PHE:CE1	3:U:159:PHE:HB2	2.25	0.72
3:U:631:ASN:C	3:U:633:GLU:H	1.93	0.72
2:2:136:VAL:HG21	2:2:163:LEU:HD13	1.71	0.72
3:C:514:ASP:OD2	3:C:685:PRO:HB3	1.89	0.72
3:C:524:LEU:HG	3:C:525:ALA:H	1.55	0.72
3:L:631:ASN:C	3:L:633:GLU:H	1.93	0.72
4:M:379:GLN:OE1	5:N:116:ARG:HG2	1.90	0.72
3:3:157:PHE:CE1	3:3:159:PHE:HB2	2.25	0.72
4:4:237:GLY:HA3	5:5:112:ASN:HA	1.72	0.72
7:9:96:LEU:HD21	7:9:129:LEU:CD1	2.20	0.72
3:C:226:ILE:HD12	3:C:235:LEU:HD11	1.71	0.72
6:F:164:ASN:HB3	7:G:148:ARG:NE	2.05	0.72
3:L:376:ALA:H	3:L:512:LEU:HD12	1.54	0.72
3:L:556:ALA:HB1	3:L:560:GLU:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:121:LEU:N	5:N:121:LEU:HD12	2.03	0.72
3:3:178:ARG:HG2	3:3:178:ARG:O	1.89	0.71
3:3:2:VAL:HG13	3:3:89:ASP:HA	1.71	0.71
3:C:701:ALA:HB2	3:C:754:PRO:HG3	1.70	0.71
3:3:758:LEU:N	3:3:758:LEU:HD12	2.05	0.71
1:A:145:LEU:O	1:A:149:ILE:HG13	1.89	0.71
7:P:141:VAL:HG13	7:P:142:GLY:N	2.05	0.71
4:V:248:VAL:O	4:V:249:ARG:HG2	1.89	0.71
6:X:30:TRP:O	6:X:33:SER:HB3	1.89	0.71
3:C:186:ARG:HD3	3:C:229:ILE:HG22	1.71	0.71
3:L:584:VAL:HG12	3:L:600:VAL:HB	1.70	0.71
5:N:130:PRO:HG2	5:N:131:ASP:H	1.54	0.71
6:X:139:GLY:HA3	6:X:142:PRO:CB	2.18	0.71
3:3:587:LEU:HD23	3:3:588:SER:H	1.54	0.71
4:4:320:SER:HB2	4:4:323:ALA:HB3	1.71	0.71
4:M:116:ILE:O	4:M:120:LEU:HB2	1.90	0.71
6:X:112:ALA:O	6:X:127:VAL:HG23	1.90	0.71
3:3:567:TYR:CE1	3:3:586:HIS:HB2	2.25	0.71
4:4:266:LEU:HD13	4:4:281:ARG:CB	2.12	0.71
4:4:310:THR:HG23	4:4:311:PRO:HD2	1.72	0.71
8:7:8:GLU:HG2	8:7:97:TYR:CE2	2.26	0.71
4:D:51:GLU:O	4:D:52:VAL:HG13	1.90	0.71
1:J:342:TRP:O	1:J:342:TRP:HE3	1.73	0.71
4:M:249:ARG:NH2	5:N:87:ARG:HB2	2.05	0.71
4:V:64:THR:HG23	6:X:123:ILE:CD1	2.20	0.71
4:4:168:PHE:CD1	4:4:168:PHE:N	2.58	0.71
4:4:230:ILE:HG21	4:4:239:LEU:HB3	1.71	0.71
3:C:115:HIS:CG	3:C:116:PRO:HD2	2.26	0.71
5:E:3:LEU:HD13	5:E:44:MET:SD	2.31	0.71
5:E:47:ASN:CB	5:E:77:LEU:HG	2.21	0.71
6:F:163:TYR:HB3	6:F:169:ARG:HA	1.72	0.71
1:J:201:LEU:O	1:J:204:PRO:HD2	1.90	0.71
3:U:701:ALA:HB2	3:U:754:PRO:HG3	1.73	0.71
1:J:359:CYS:HA	1:J:363:VAL:HG13	1.70	0.71
3:L:494:LYS:O	3:L:498:GLU:HG2	1.90	0.71
3:U:263:CYS:HA	3:U:286:ASN:HB2	1.73	0.71
4:V:252:TYR:HB2	4:V:253:PRO:CD	2.21	0.71
5:W:139:GLU:CG	5:W:140:ASP:H	2.03	0.71
5:W:37:GLU:O	5:W:41:TYR:HD1	1.73	0.71
4:4:232:LEU:HD13	4:4:278:VAL:HG12	1.70	0.71
5:E:121:LEU:N	5:E:121:LEU:HD12	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:567:TYR:CE1	3:L:586:HIS:HB2	2.26	0.71
3:L:621:VAL:HG22	3:L:674:GLY:O	1.90	0.71
4:M:168:PHE:HD1	4:M:168:PHE:N	1.88	0.71
5:N:47:ASN:HD22	5:N:76:SER:HA	1.55	0.71
3:U:223:SER:O	3:U:226:ILE:HG12	1.91	0.71
3:U:494:LYS:O	3:U:498:GLU:HG2	1.91	0.71
5:W:127:GLU:OE1	5:W:127:GLU:HA	1.90	0.71
5:W:48:PHE:C	5:W:50:ALA:H	1.92	0.71
2:2:39:GLY:O	2:2:40:TRP:HB2	1.87	0.71
3:3:227:THR:HG21	3:3:237:ASP:HB2	1.73	0.71
4:4:86:ASP:O	4:4:88:LEU:N	2.23	0.71
3:C:758:LEU:N	3:C:758:LEU:HD12	2.06	0.71
4:V:224:ILE:HD12	4:V:237:GLY:HA2	1.73	0.71
4:V:342:VAL:HG22	4:V:343:TYR:H	1.56	0.71
7:Y:56:CYS:SG	7:Y:58:LEU:HD13	2.31	0.71
3:3:621:VAL:HG22	3:3:674:GLY:O	1.90	0.71
3:3:684:ARG:HG2	3:3:684:ARG:HH11	1.55	0.71
4:4:105:LEU:HD23	4:4:337:PRO:HG3	1.71	0.71
8:Q:8:GLU:HG2	8:Q:97:TYR:CE2	2.26	0.71
1:S:107:LEU:O	1:S:111:PRO:HG3	1.91	0.71
5:W:47:ASN:HB2	5:W:77:LEU:HG	1.73	0.71
3:3:243:ARG:HB3	3:3:275:LEU:HD12	1.72	0.70
5:5:134:LYS:CE	5:5:136:LEU:HB3	2.21	0.70
2:B:40:TRP:HE1	2:B:74:PRO:HG3	1.55	0.70
3:C:413:LEU:HD13	3:C:448:MET:HE1	1.73	0.70
4:M:310:THR:HG23	4:M:311:PRO:HD2	1.73	0.70
3:U:178:ARG:HG2	3:U:178:ARG:O	1.91	0.70
4:V:235:THR:HA	4:V:239:LEU:HD22	1.73	0.70
5:W:130:PRO:HG2	5:W:131:ASP:H	1.54	0.70
3:3:171:SER:HB3	3:3:173:PHE:HB3	1.73	0.70
3:3:356:LEU:HD13	3:3:654:PHE:HB2	1.73	0.70
2:B:10:PHE:CZ	2:B:33:ARG:HG3	2.26	0.70
3:C:96:LEU:N	3:C:96:LEU:HD12	2.06	0.70
1:J:192:LEU:HD22	1:J:211:LEU:HD11	1.73	0.70
4:M:367:ARG:HH11	4:M:367:ARG:HG2	1.54	0.70
2:T:114:ASP:HB2	2:T:116:LEU:HD22	1.73	0.70
3:U:259:CYS:SG	3:U:261:VAL:HG22	2.31	0.70
3:U:550:LEU:HD12	3:U:550:LEU:N	2.06	0.70
4:V:51:GLU:O	4:V:52:VAL:HG13	1.91	0.70
5:W:145:PRO:HA	5:W:150:TYR:CD2	2.25	0.70
3:3:371:PHE:CE1	3:3:549:VAL:HB	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:145:GLU:HG2	7:9:31:VAL:HG21	1.74	0.70
3:C:561:PRO:CB	3:C:576:ALA:HA	2.22	0.70
5:E:52:ILE:HG23	5:E:117:GLU:CG	2.21	0.70
5:E:47:ASN:HB2	5:E:77:LEU:HG	1.72	0.70
3:L:20:MET:HE3	3:L:32:LEU:HD21	1.72	0.70
4:M:219:ARG:O	4:M:219:ARG:HD3	1.90	0.70
1:S:214:LYS:O	1:S:216:THR:HG23	1.91	0.70
3:3:631:ASN:C	3:3:633:GLU:H	1.94	0.70
5:5:145:PRO:HA	5:5:150:TYR:CD2	2.26	0.70
3:C:166:LYS:HG3	3:C:178:ARG:HG3	1.73	0.70
4:D:219:ARG:O	4:D:219:ARG:HD3	1.91	0.70
4:D:310:THR:HG23	4:D:311:PRO:HD2	1.74	0.70
6:F:107:SER:O	6:F:137:VAL:HG12	1.92	0.70
5:N:125:VAL:HG12	5:N:126:PHE:N	2.05	0.70
3:U:583:VAL:HG23	3:U:598:ALA:HA	1.73	0.70
6:X:120:ASN:HD22	6:X:122:ALA:HB3	1.57	0.70
4:4:51:GLU:O	4:4:52:VAL:HG13	1.91	0.70
2:B:42:ARG:HB2	2:B:45:ARG:HG2	1.73	0.70
3:C:263:CYS:HA	3:C:286:ASN:HB2	1.73	0.70
1:J:145:LEU:O	1:J:149:ILE:HG13	1.91	0.70
2:K:112:THR:HG21	2:K:116:LEU:HD23	1.73	0.70
6:O:84:LEU:HD12	6:O:124:VAL:HG21	1.74	0.70
4:V:249:ARG:HH11	4:V:249:ARG:CB	2.01	0.70
4:V:320:SER:HB2	4:V:323:ALA:HB3	1.74	0.70
4:V:237:GLY:HA3	5:W:112:ASN:HA	1.74	0.70
2:2:114:ASP:HB2	2:2:116:LEU:HD22	1.74	0.70
4:4:225:PRO:HD2	4:4:226:PRO:CD	2.22	0.70
8:H:8:GLU:HG2	8:H:97:TYR:CZ	2.26	0.70
1:J:90:ILE:HD11	1:J:211:LEU:HD22	1.73	0.70
3:L:237:ASP:OD1	3:L:239:THR:HG22	1.91	0.70
1:S:108:GLU:HG2	1:S:140:ARG:HG2	1.73	0.70
3:U:178:ARG:H	3:U:234:ALA:HA	1.56	0.70
5:W:47:ASN:HD22	5:W:76:SER:HA	1.55	0.70
1:1:214:LYS:O	1:1:216:THR:HG23	1.91	0.70
4:4:379:GLN:OE1	5:5:115:GLU:HB2	1.92	0.70
6:6:19:ILE:HD11	1:J:271:THR:CG2	2.22	0.70
3:L:263:CYS:HA	3:L:286:ASN:HB2	1.74	0.70
4:M:237:GLY:HA2	5:N:112:ASN:HA	1.72	0.70
4:M:342:VAL:HG22	4:M:343:TYR:N	2.07	0.70
3:U:731:GLY:N	3:U:747:VAL:HG12	2.03	0.70
5:W:47:ASN:CB	5:W:77:LEU:HG	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:117:TYR:OH	7:Y:167:ARG:HG3	1.91	0.70
2:2:77:LYS:H	2:2:116:LEU:HA	1.56	0.70
3:3:96:LEU:N	3:3:96:LEU:HD12	2.07	0.70
7:9:35:PRO:O	7:9:36:ARG:CB	2.37	0.70
3:C:226:ILE:HD12	3:C:235:LEU:CD1	2.21	0.70
4:D:278:VAL:O	4:D:281:ARG:HB2	1.91	0.70
2:K:131:ALA:HB1	2:K:132:PRO:HD3	1.73	0.70
3:L:474:ARG:HB3	3:L:516:VAL:HG22	1.74	0.70
3:L:564:LEU:HD11	3:L:581:ARG:H	1.56	0.70
2:T:86:LEU:CD1	2:T:90:LEU:HD11	2.22	0.70
3:U:458:LEU:HD12	3:U:458:LEU:H	1.55	0.70
4:V:232:LEU:HD11	4:V:282:GLU:OE2	1.91	0.70
3:C:438:LYS:O	3:C:441:MET:HG3	1.91	0.70
4:D:168:PHE:CD1	4:D:168:PHE:N	2.59	0.70
4:D:232:LEU:HD11	4:D:282:GLU:OE2	1.90	0.70
6:F:165:GLU:HG3	7:G:128:ASP:CG	2.12	0.70
1:J:219:ASN:HD22	1:J:223:THR:HG21	1.56	0.70
3:U:171:SER:HB3	3:U:173:PHE:HB3	1.73	0.70
5:W:3:LEU:HD13	5:W:44:MET:SD	2.32	0.70
2:2:89:LYS:HA	2:2:93:ALA:HB3	1.74	0.70
3:C:134:THR:O	3:C:138:GLY:HA3	1.92	0.70
4:D:249:ARG:NH2	5:E:87:ARG:HB2	2.07	0.70
2:K:39:GLY:O	2:K:75:THR:HG22	1.92	0.70
5:W:20:ASN:ND2	5:W:24:ASN:HB2	2.06	0.70
1:1:93:ALA:HB3	1:1:134:VAL:HG12	1.73	0.69
1:1:192:LEU:HD22	1:1:211:LEU:HD11	1.73	0.69
6:6:130:VAL:HG23	6:6:131:VAL:H	1.57	0.69
3:U:612:GLY:O	3:U:624:LEU:HB2	1.91	0.69
5:5:45:GLY:O	5:5:46:PHE:C	2.28	0.69
6:6:130:VAL:HG23	6:6:131:VAL:N	2.07	0.69
7:9:123:ASP:CG	7:9:148:ARG:HH22	1.95	0.69
4:M:107:ALA:HB2	4:M:309:ILE:HD13	1.74	0.69
5:N:52:ILE:HG23	5:N:117:GLU:CG	2.21	0.69
5:N:26:TRP:CB	5:N:89:PHE:HB2	2.21	0.69
4:V:278:VAL:O	4:V:281:ARG:HB2	1.92	0.69
4:D:320:SER:O	4:D:321:MET:C	2.31	0.69
3:L:178:ARG:H	3:L:234:ALA:HA	1.57	0.69
6:O:120:ASN:ND2	6:O:122:ALA:HB3	2.07	0.69
8:Q:44:MET:O	8:Q:46:ARG:N	2.24	0.69
8:Q:8:GLU:HG2	8:Q:97:TYR:CZ	2.27	0.69
1:S:145:LEU:O	1:S:149:ILE:HG13	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:147:LEU:O	6:X:150:ALA:HB3	1.92	0.69
3:3:701:ALA:HB2	3:3:754:PRO:HG3	1.73	0.69
7:9:36:ARG:HA	7:9:167:ARG:HD3	1.75	0.69
2:B:77:LYS:H	2:B:116:LEU:HA	1.57	0.69
5:E:26:TRP:CB	5:E:89:PHE:HB2	2.21	0.69
7:G:134:GLU:CD	7:G:134:GLU:H	1.95	0.69
3:L:650:VAL:HG12	3:L:651:ARG:H	1.56	0.69
4:M:232:LEU:HD13	4:M:278:VAL:HG12	1.73	0.69
1:S:357:THR:N	1:S:358:PRO:HD2	2.07	0.69
4:V:322:GLU:C	4:V:324:VAL:N	2.44	0.69
3:3:282:VAL:O	3:3:286:ASN:O	2.11	0.69
3:3:561:PRO:CB	3:3:576:ALA:HA	2.22	0.69
2:B:40:TRP:HE3	2:B:41:ILE:N	1.90	0.69
3:C:387:LEU:HD13	3:C:618:GLU:OE1	1.92	0.69
1:S:293:GLY:O	1:S:327:GLY:N	2.25	0.69
3:U:564:LEU:HD11	3:U:581:ARG:H	1.57	0.69
1:1:90:ILE:HD11	1:1:211:LEU:HD22	1.73	0.69
3:3:347:HIS:HD2	3:3:539:ALA:H	1.40	0.69
5:5:59:THR:HG22	5:5:59:THR:O	1.93	0.69
3:C:313:LYS:O	3:C:314:GLU:HB2	1.93	0.69
1:A:357:THR:OG1	3:C:45:CYS:HA	1.91	0.69
4:D:224:ILE:CD1	4:D:237:GLY:HA2	2.23	0.69
4:D:322:GLU:C	4:D:324:VAL:H	1.94	0.69
4:D:64:THR:HG23	6:F:123:ILE:HD11	1.72	0.69
3:L:226:ILE:HD12	3:L:235:LEU:HD11	1.73	0.69
3:L:514:ASP:OD2	3:L:685:PRO:HB3	1.92	0.69
1:S:366:PHE:CD1	1:S:370:LEU:HD21	2.26	0.69
3:U:650:VAL:HG12	3:U:651:ARG:H	1.57	0.69
3:3:202:PHE:O	3:3:203:ILE:HD13	1.93	0.69
8:7:8:GLU:HG2	8:7:97:TYR:CZ	2.27	0.69
1:J:293:GLY:O	1:J:327:GLY:N	2.25	0.69
3:L:227:THR:HG21	3:L:237:ASP:HB2	1.75	0.69
3:L:751:GLU:O	3:L:753:VAL:HG13	1.92	0.69
4:M:231:ASP:HA	4:M:235:THR:HG23	1.75	0.69
5:N:50:ALA:HB1	5:N:114:LEU:HD21	1.75	0.69
7:P:56:CYS:SG	7:P:58:LEU:HD13	2.33	0.69
4:V:379:GLN:OE1	5:W:116:ARG:HG2	1.91	0.69
5:5:3:LEU:HD13	5:5:44:MET:SD	2.33	0.69
6:6:164:ASN:N	6:6:170:LEU:HD12	2.08	0.69
2:T:31:LEU:HD12	2:T:41:ILE:HD13	1.74	0.69
1:A:429:ARG:HG3	3:U:316:ARG:HH12	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:114:GLU:CG	4:V:253:PRO:HB3	2.22	0.69
4:4:320:SER:O	4:4:321:MET:C	2.29	0.69
6:6:120:ASN:HD22	6:6:122:ALA:HB3	1.57	0.69
6:6:84:LEU:HD12	6:6:124:VAL:HG21	1.75	0.69
3:U:31:PRO:HB2	3:U:47:MET:HB3	1.72	0.69
3:U:453:PRO:HB2	3:U:750:ARG:NH2	2.08	0.69
2:2:106:ILE:HD11	2:2:112:THR:HB	1.75	0.69
2:2:112:THR:HG21	2:2:116:LEU:HD23	1.75	0.69
2:2:131:ALA:HB1	2:2:132:PRO:HD3	1.75	0.69
3:3:307:LYS:HB3	3:3:632:GLY:HA3	1.73	0.69
1:A:357:THR:N	1:A:358:PRO:HD2	2.07	0.69
3:L:561:PRO:CB	3:L:576:ALA:HA	2.22	0.69
3:U:371:PHE:CE1	3:U:549:VAL:HB	2.26	0.69
1:A:115:ILE:O	1:A:119:ILE:HG13	1.92	0.69
3:C:556:ALA:HB1	3:C:560:GLU:O	1.93	0.69
3:L:171:SER:HB3	3:L:173:PHE:HB3	1.74	0.69
4:M:257:TYR:HD1	4:M:257:TYR:N	1.90	0.69
7:P:56:CYS:SG	7:P:56:CYS:O	2.50	0.69
4:V:320:SER:O	4:V:321:MET:C	2.31	0.69
3:3:550:LEU:HD12	3:3:550:LEU:N	2.08	0.68
4:4:229:ALA:HB3	4:4:241:ALA:HA	1.75	0.68
3:C:171:SER:C	3:C:173:PHE:N	2.45	0.68
8:H:8:GLU:HG2	8:H:97:TYR:CE2	2.27	0.68
1:J:110:VAL:N	1:J:111:PRO:HD3	2.07	0.68
2:K:114:ASP:HB2	2:K:116:LEU:HD22	1.74	0.68
7:P:36:ARG:HA	7:P:167:ARG:HD3	1.75	0.68
2:T:42:ARG:HB2	2:T:45:ARG:HG2	1.75	0.68
3:U:45:CYS:O	3:U:47:MET:N	2.26	0.68
3:U:477:LEU:CD2	3:U:520:ARG:HG2	2.23	0.68
4:V:225:PRO:HG2	4:V:239:LEU:H	1.58	0.68
7:9:95:MET:HB2	7:9:129:LEU:O	1.92	0.68
7:G:35:PRO:O	7:G:36:ARG:HB2	1.92	0.68
1:J:214:LYS:O	1:J:216:THR:HG23	1.93	0.68
1:J:64:GLY:HA3	11:Q:500:FMN:O1P	1.92	0.68
2:K:40:TRP:HE3	2:K:41:ILE:N	1.91	0.68
4:M:133:LEU:HD21	4:M:204:TYR:HD2	1.55	0.68
5:N:33:ARG:O	5:N:37:GLU:HB2	1.93	0.68
3:U:134:THR:O	3:U:138:GLY:HA3	1.93	0.68
3:U:724:ARG:CD	3:U:724:ARG:H	2.01	0.68
1:1:342:TRP:O	1:1:342:TRP:HE3	1.77	0.68
3:C:565:TYR:HD1	3:C:582:PHE:HB3	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:7:LYS:HD2	2:K:7:LYS:H	1.57	0.68
3:U:125:GLY:HA3	3:U:246:ASN:HD22	1.58	0.68
3:U:171:SER:C	3:U:173:PHE:N	2.43	0.68
3:U:227:THR:HG21	3:U:237:ASP:HB2	1.75	0.68
4:V:313:PRO:C	4:V:315:HIS:H	1.97	0.68
6:X:84:LEU:HD12	6:X:124:VAL:HG21	1.75	0.68
8:Z:82:ILE:HG23	8:Z:95:ALA:HB3	1.75	0.68
5:5:33:ARG:O	5:5:37:GLU:HB2	1.93	0.68
7:9:134:GLU:CD	7:9:134:GLU:H	1.97	0.68
4:D:274:ASP:O	4:D:278:VAL:HG23	1.93	0.68
4:D:322:GLU:C	4:D:324:VAL:N	2.40	0.68
7:G:101:CYS:SG	7:G:101:CYS:O	2.52	0.68
8:H:44:MET:O	8:H:46:ARG:N	2.26	0.68
3:L:387:LEU:HD13	3:L:618:GLU:OE1	1.94	0.68
4:M:252:TYR:CB	4:M:253:PRO:HD2	2.21	0.68
2:T:86:LEU:O	2:T:90:LEU:HD12	1.92	0.68
8:Z:8:GLU:HG2	8:Z:97:TYR:CZ	2.28	0.68
4:D:225:PRO:HD2	4:D:226:PRO:CD	2.24	0.68
4:D:248:VAL:O	4:D:249:ARG:HG2	1.93	0.68
4:M:228:VAL:HG12	4:M:271:ASP:HA	1.76	0.68
2:T:39:GLY:O	2:T:40:TRP:HB2	1.93	0.68
3:U:567:TYR:CE1	3:U:586:HIS:HB2	2.27	0.68
3:3:564:LEU:HD11	3:3:581:ARG:H	1.59	0.68
3:3:724:ARG:H	3:3:724:ARG:CD	2.04	0.68
3:C:282:VAL:HG22	3:C:282:VAL:O	1.92	0.68
4:D:252:TYR:OH	4:D:347:GLU:N	2.27	0.68
5:E:16:PRO:HD2	5:E:28:VAL:HG13	1.73	0.68
1:J:125:ILE:HD13	1:J:217:THR:HG21	1.75	0.68
4:M:214:PHE:C	4:M:216:GLU:H	1.96	0.68
2:T:77:LYS:H	2:T:116:LEU:HA	1.59	0.68
3:U:756:GLY:C	3:U:757:HIS:ND1	2.47	0.68
5:W:44:MET:HE2	5:W:82:ASP:HB3	1.75	0.68
3:3:514:ASP:OD2	3:3:685:PRO:HB3	1.94	0.68
1:A:20:HIS:CE1	1:A:226:SER:HA	2.29	0.68
2:K:106:ILE:HD11	2:K:112:THR:HB	1.76	0.68
4:M:353:LEU:HD12	4:M:354:GLY:H	1.57	0.68
6:O:30:TRP:O	6:O:33:SER:HB3	1.93	0.68
7:P:117:TYR:OH	7:P:167:ARG:HG3	1.94	0.68
3:3:481:LEU:HD11	3:3:519:GLU:HB2	1.74	0.68
4:4:214:PHE:C	4:4:216:GLU:H	1.97	0.68
5:E:59:THR:O	5:E:59:THR:HG22	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:436:LEU:HD23	2:T:90:LEU:HA	1.76	0.68
4:V:237:GLY:HA3	5:W:112:ASN:O	1.93	0.68
4:V:373:PRO:O	4:V:376:VAL:HG22	1.94	0.68
8:Z:8:GLU:HG2	8:Z:97:TYR:CE2	2.28	0.68
1:1:115:ILE:O	1:1:119:ILE:HG13	1.94	0.68
3:3:115:HIS:CG	3:3:116:PRO:HD2	2.28	0.68
4:4:64:THR:HG23	6:6:123:ILE:CD1	2.22	0.68
1:A:437:TRP:CH2	2:B:96:LEU:HD13	2.29	0.68
3:C:474:ARG:HB3	3:C:516:VAL:HG22	1.75	0.68
3:L:701:ALA:HB2	3:L:754:PRO:HG3	1.75	0.68
4:M:226:PRO:HD2	4:M:239:LEU:HB2	1.75	0.68
4:M:238:SER:O	4:M:239:LEU:HD23	1.94	0.68
4:M:322:GLU:C	4:M:324:VAL:N	2.45	0.68
3:U:474:ARG:HB3	3:U:516:VAL:HG22	1.75	0.68
4:V:107:ALA:HB2	4:V:309:ILE:HD13	1.75	0.68
4:V:168:PHE:CD1	4:V:168:PHE:N	2.59	0.68
3:3:545:GLU:HA	3:3:550:LEU:HD11	1.76	0.68
4:4:257:TYR:N	4:4:257:TYR:HD1	1.92	0.68
3:C:13:VAL:HG21	3:C:17:THR:HG21	1.76	0.68
3:C:751:GLU:O	3:C:753:VAL:HG13	1.93	0.68
4:D:96:ALA:HB2	4:D:346:THR:HG21	1.76	0.68
5:E:127:GLU:HA	5:E:127:GLU:OE1	1.92	0.68
3:L:282:VAL:O	3:L:286:ASN:O	2.12	0.68
4:M:168:PHE:CD1	4:M:168:PHE:N	2.61	0.68
4:M:240:ARG:HD2	4:M:243:GLY:CA	2.12	0.68
5:N:65:PRO:HD2	5:N:93:TYR:HE2	1.59	0.68
3:3:178:ARG:H	3:3:234:ALA:HA	1.58	0.67
3:3:487:SER:OG	3:3:490:VAL:HG23	1.94	0.67
3:3:509:ALA:HA	3:3:758:LEU:CD2	2.22	0.67
4:4:89:HIS:HB2	4:4:128:SER:HB2	1.76	0.67
4:4:342:VAL:HG22	4:4:343:TYR:N	2.08	0.67
3:C:20:MET:HE3	3:C:32:LEU:HD21	1.74	0.67
4:D:220:GLY:HA3	4:D:396:ILE:HD11	1.76	0.67
5:E:45:GLY:O	5:E:46:PHE:C	2.33	0.67
3:L:174:VAL:HG21	3:L:296:PHE:CD2	2.28	0.67
3:L:371:PHE:CE1	3:L:549:VAL:HB	2.28	0.67
1:1:366:PHE:CD1	1:1:370:LEU:HD21	2.29	0.67
2:B:114:ASP:HB2	2:B:116:LEU:HD22	1.74	0.67
4:D:246:TYR:CG	4:D:347:GLU:HG3	2.29	0.67
4:M:257:TYR:CD1	4:M:257:TYR:N	2.61	0.67
1:S:192:LEU:HD23	1:S:192:LEU:C	2.14	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:115:HIS:CG	3:U:116:PRO:HD2	2.28	0.67
3:U:136:GLU:O	5:W:188:SER:HB2	1.94	0.67
3:3:474:ARG:HB3	3:3:516:VAL:HG22	1.77	0.67
6:6:163:TYR:HB3	6:6:169:ARG:HA	1.76	0.67
2:K:39:GLY:O	2:K:40:TRP:HB2	1.92	0.67
4:M:252:TYR:HB2	4:M:253:PRO:CD	2.18	0.67
5:N:44:MET:HE2	5:N:82:ASP:HB3	1.75	0.67
7:P:95:MET:HB2	7:P:129:LEU:O	1.94	0.67
1:S:342:TRP:O	1:S:342:TRP:HE3	1.78	0.67
4:V:310:THR:HG23	4:V:311:PRO:HD2	1.76	0.67
7:Y:36:ARG:HA	7:Y:167:ARG:HD3	1.77	0.67
4:4:114:GLU:CG	4:4:253:PRO:HB3	2.24	0.67
4:4:197:LEU:O	4:4:201:ILE:HD13	1.94	0.67
4:4:257:TYR:N	4:4:257:TYR:CD1	2.63	0.67
8:7:44:MET:O	8:7:46:ARG:N	2.26	0.67
3:C:81:ALA:HB3	3:C:84:VAL:HG22	1.75	0.67
5:E:65:PRO:HD2	5:E:93:TYR:CE2	2.28	0.67
7:G:45:ARG:HH21	7:G:137:LEU:HD23	1.60	0.67
8:H:67:PHE:CZ	8:H:123:ARG:HG3	2.29	0.67
4:M:316:LEU:HD13	4:M:320:SER:HB2	1.76	0.67
2:2:10:PHE:CZ	2:2:33:ARG:HG3	2.30	0.67
1:A:293:GLY:O	1:A:327:GLY:N	2.28	0.67
3:C:117:LEU:HD23	4:D:322:GLU:OE2	1.94	0.67
5:E:7:LEU:HD21	5:E:41:TYR:CE2	2.29	0.67
2:T:131:ALA:HB1	2:T:132:PRO:HD3	1.74	0.67
4:V:404:MET:HA	4:V:407:VAL:CG1	2.24	0.67
5:W:121:LEU:HD12	5:W:121:LEU:N	2.10	0.67
7:Y:44:THR:OG1	7:Y:52:LYS:HD2	1.93	0.67
4:4:221:VAL:O	4:4:223:VAL:N	2.26	0.67
3:C:223:SER:O	3:C:226:ILE:HG12	1.95	0.67
3:C:31:PRO:HB2	3:C:47:MET:HB3	1.76	0.67
4:M:221:VAL:O	4:M:223:VAL:N	2.27	0.67
5:N:47:ASN:HB2	5:N:77:LEU:HG	1.75	0.67
3:U:501:LYS:H	3:U:501:LYS:CD	2.00	0.67
3:U:584:VAL:HG12	3:U:600:VAL:HB	1.76	0.67
7:Y:35:PRO:O	7:Y:36:ARG:CB	2.41	0.67
2:2:7:LYS:H	2:2:7:LYS:HD2	1.58	0.67
3:3:565:TYR:HD1	3:3:582:PHE:HB3	1.59	0.67
4:4:248:VAL:O	4:4:249:ARG:HG2	1.95	0.67
5:E:145:PRO:HA	5:E:150:TYR:CD2	2.30	0.67
5:N:116:ARG:HH11	5:N:116:ARG:HG2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:164:ASN:O	7:P:148:ARG:HD2	1.95	0.67
3:U:453:PRO:HB2	3:U:750:ARG:HH22	1.58	0.67
4:D:191:LYS:NZ	3:U:730:GLU:CG	2.58	0.67
4:V:112:ARG:O	4:V:112:ARG:HG2	1.93	0.67
5:W:45:GLY:O	5:W:46:PHE:C	2.32	0.67
1:1:293:GLY:O	1:1:327:GLY:N	2.27	0.67
4:4:219:ARG:HD3	4:4:219:ARG:O	1.95	0.67
3:C:487:SER:OG	3:C:490:VAL:HG23	1.93	0.67
3:L:307:LYS:CE	3:L:307:LYS:H	2.08	0.67
3:3:473:GLU:O	3:3:477:LEU:HD12	1.95	0.67
4:D:153:ARG:HH11	4:D:153:ARG:HG3	1.60	0.67
3:3:171:SER:C	3:3:173:PHE:N	2.46	0.67
3:3:31:PRO:HB2	3:3:47:MET:HB3	1.77	0.67
3:3:458:LEU:H	3:3:458:LEU:HD12	1.60	0.67
3:3:586:HIS:CD2	3:3:604:ALA:HB2	2.29	0.67
3:C:403:THR:OG1	3:C:458:LEU:HD11	1.94	0.67
4:M:114:GLU:CG	4:M:253:PRO:HB3	2.25	0.67
1:S:86:GLN:OE1	1:S:128:THR:HG23	1.95	0.67
3:U:751:GLU:O	3:U:753:VAL:HG13	1.95	0.67
4:V:393:MET:HG2	4:V:393:MET:O	1.93	0.67
3:3:226:ILE:HD12	3:3:235:LEU:HD11	1.75	0.66
4:4:224:ILE:CD1	4:4:237:GLY:HA2	2.25	0.66
1:A:301:PRO:O	1:A:306:VAL:HG21	1.95	0.66
3:C:719:HIS:HB2	3:C:720:PRO:HD3	1.77	0.66
7:G:123:ASP:HB2	7:G:129:LEU:HD21	1.77	0.66
5:N:45:GLY:O	5:N:46:PHE:C	2.31	0.66
4:V:322:GLU:C	4:V:324:VAL:H	1.98	0.66
8:Z:63:LEU:HD13	8:Z:129:ALA:HB2	1.77	0.66
1:1:86:GLN:OE1	1:1:128:THR:HG23	1.94	0.66
3:3:510:GLY:HA3	3:3:520:ARG:NH2	2.09	0.66
4:4:115:THR:HG21	4:4:297:LEU:HD23	1.75	0.66
3:C:584:VAL:HG12	3:C:600:VAL:HB	1.77	0.66
4:D:353:LEU:HD12	4:D:354:GLY:H	1.59	0.66
4:D:404:MET:HA	4:D:407:VAL:CG1	2.26	0.66
3:L:307:LYS:HB3	3:L:632:GLY:HA3	1.76	0.66
3:U:559:ASP:OD2	3:U:688:ARG:NH2	2.28	0.66
3:U:719:HIS:HB2	3:U:720:PRO:HD3	1.76	0.66
4:V:234:LEU:N	4:V:234:LEU:HD23	2.10	0.66
4:V:252:TYR:OH	4:V:347:GLU:N	2.28	0.66
5:W:59:THR:HG22	5:W:59:THR:O	1.94	0.66
3:3:13:VAL:HG21	3:3:17:THR:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:163:TYR:HB2	6:6:169:ARG:HA	1.78	0.66
1:A:438:ARG:H	1:A:438:ARG:HD2	1.58	0.66
3:C:178:ARG:O	3:C:178:ARG:HG2	1.94	0.66
3:C:567:TYR:CE1	3:C:586:HIS:HB2	2.29	0.66
4:D:112:ARG:HG2	4:D:112:ARG:O	1.94	0.66
3:L:13:VAL:HG21	3:L:17:THR:HG21	1.77	0.66
4:M:224:ILE:HD12	4:M:237:GLY:HA2	1.78	0.66
4:M:237:GLY:HA3	5:N:112:ASN:HA	1.78	0.66
6:O:130:VAL:HG23	6:O:131:VAL:H	1.59	0.66
7:P:134:GLU:H	7:P:134:GLU:CD	1.99	0.66
1:S:110:VAL:N	1:S:111:PRO:HD3	2.11	0.66
3:U:48:CYS:O	3:U:82:SER:HB3	1.94	0.66
2:2:42:ARG:HB2	2:2:45:ARG:HG2	1.76	0.66
2:2:59:GLU:O	2:2:63:VAL:HG23	1.95	0.66
3:3:313:LYS:O	3:3:314:GLU:HB2	1.95	0.66
6:6:16:ARG:HD2	6:6:17:GLU:HG3	1.77	0.66
1:A:342:TRP:HE3	1:A:342:TRP:O	1.78	0.66
3:C:48:CYS:O	3:C:82:SER:HB3	1.94	0.66
5:N:124:ILE:HG22	5:N:146:LEU:H	1.60	0.66
1:S:357:THR:OG1	3:U:45:CYS:HA	1.95	0.66
2:T:39:GLY:O	2:T:75:THR:HG22	1.96	0.66
3:U:100:VAL:O	3:U:104:GLN:HG3	1.96	0.66
3:U:586:HIS:HD2	3:U:602:LEU:O	1.78	0.66
1:1:110:VAL:N	1:1:111:PRO:HD3	2.10	0.66
3:3:656:LEU:H	3:3:656:LEU:HD23	1.61	0.66
4:4:320:SER:CB	4:4:323:ALA:HB3	2.25	0.66
5:5:47:ASN:HB2	5:5:77:LEU:HG	1.76	0.66
3:C:398:VAL:HB	3:C:450:LEU:HD22	1.78	0.66
3:C:45:CYS:O	3:C:47:MET:N	2.29	0.66
3:C:583:VAL:HG23	3:C:598:ALA:HA	1.76	0.66
4:D:114:GLU:CG	4:D:253:PRO:HB3	2.25	0.66
4:D:237:GLY:O	4:D:239:LEU:HG	1.95	0.66
6:F:164:ASN:O	7:G:148:ARG:HD2	1.95	0.66
6:F:164:ASN:CB	7:G:148:ARG:HE	2.08	0.66
2:K:40:TRP:HZ3	2:K:42:ARG:HA	1.59	0.66
7:P:96:LEU:HD21	7:P:129:LEU:HD12	1.77	0.66
7:P:71:GLU:HB2	7:P:90:VAL:HB	1.76	0.66
2:T:112:THR:HG21	2:T:116:LEU:HD23	1.78	0.66
3:U:365:LYS:C	3:U:367:PRO:HD3	2.15	0.66
3:U:466:GLU:CG	3:U:489:MET:HG3	2.18	0.66
4:V:214:PHE:C	4:V:216:GLU:H	1.98	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:163:TYR:HB3	6:X:169:ARG:HA	1.77	0.66
6:X:164:ASN:HB3	7:Y:148:ARG:NE	2.09	0.66
2:2:86:LEU:CD1	2:2:90:LEU:HD11	2.25	0.66
2:2:90:LEU:H	2:2:90:LEU:HD12	1.61	0.66
5:5:50:ALA:HB1	5:5:114:LEU:HD21	1.78	0.66
6:F:130:VAL:HG23	6:F:131:VAL:N	2.08	0.66
3:L:583:VAL:CG2	3:L:598:ALA:HA	2.26	0.66
4:M:404:MET:HA	4:M:407:VAL:CG1	2.25	0.66
5:W:175:THR:HG23	5:W:178:ASP:HB2	1.76	0.66
5:W:44:MET:CE	5:W:82:ASP:HB3	2.25	0.66
4:4:153:ARG:HH11	4:4:153:ARG:HG3	1.61	0.66
4:D:89:HIS:HB2	4:D:128:SER:HB2	1.77	0.66
4:D:226:PRO:HD2	4:D:239:LEU:HB2	1.76	0.66
6:O:37:TRP:HA	6:O:37:TRP:CE3	2.29	0.66
1:S:64:GLY:HA3	11:Z:500:FMN:O1P	1.96	0.66
3:U:453:PRO:HB2	3:U:750:ARG:NH1	2.10	0.66
4:V:256:GLY:CA	4:V:292:GLN:HE22	2.08	0.66
7:9:117:TYR:OH	7:9:167:ARG:HG3	1.95	0.66
3:C:307:LYS:HB3	3:C:632:GLY:HA3	1.77	0.66
4:M:226:PRO:HB3	5:N:80:TRP:CH2	2.31	0.66
5:N:124:ILE:CG2	5:N:145:PRO:HG2	2.26	0.66
7:P:35:PRO:O	7:P:36:ARG:CB	2.42	0.66
1:S:93:ALA:HB3	1:S:134:VAL:HG12	1.76	0.66
3:U:565:TYR:HD1	3:U:582:PHE:HB3	1.61	0.66
4:V:246:TYR:CG	4:V:347:GLU:HG3	2.30	0.66
7:Y:134:GLU:CD	7:Y:134:GLU:H	1.98	0.66
4:4:322:GLU:C	4:4:324:VAL:N	2.47	0.66
3:C:347:HIS:HD2	3:C:539:ALA:H	1.44	0.66
4:D:235:THR:HA	4:D:239:LEU:HD22	1.78	0.66
5:E:3:LEU:HD22	5:E:44:MET:SD	2.36	0.66
2:K:89:LYS:HA	2:K:93:ALA:HB3	1.78	0.66
3:L:477:LEU:CD2	3:L:520:ARG:HG2	2.26	0.66
3:U:131:GLN:HG2	4:V:325:ILE:HG12	1.78	0.66
5:W:7:LEU:HD21	5:W:41:TYR:CE2	2.31	0.66
6:X:16:ARG:HD2	6:X:17:GLU:HG3	1.77	0.66
2:2:130:THR:O	2:2:131:ALA:O	2.14	0.66
3:3:263:CYS:HA	3:3:286:ASN:HB2	1.78	0.66
3:3:477:LEU:CD2	3:3:520:ARG:HG2	2.26	0.66
3:3:583:VAL:CG2	3:3:598:ALA:HA	2.26	0.66
3:C:474:ARG:HA	3:C:516:VAL:HG13	1.77	0.66
4:D:346:THR:HG22	4:D:353:LEU:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:40:TRP:CZ3	2:K:42:ARG:HA	2.31	0.66
5:N:145:PRO:HA	5:N:150:TYR:CD2	2.31	0.66
3:U:347:HIS:HD2	3:U:539:ALA:H	1.44	0.66
1:1:185:GLU:HB2	1:1:218:ILE:CD1	2.25	0.65
1:1:20:HIS:CE1	1:1:226:SER:HA	2.31	0.65
4:4:249:ARG:HH22	5:5:87:ARG:CB	2.09	0.65
4:4:316:LEU:HD13	4:4:320:SER:HB2	1.78	0.65
5:5:47:ASN:HD22	5:5:76:SER:HA	1.60	0.65
6:6:155:GLN:O	6:6:158:VAL:HG22	1.96	0.65
1:A:397:ARG:HG3	3:C:46:ARG:NE	2.11	0.65
3:C:369:LEU:H	3:C:369:LEU:CD2	2.08	0.65
3:C:477:LEU:HD13	3:C:516:VAL:CG1	2.26	0.65
3:C:481:LEU:HD11	3:C:519:GLU:HB2	1.78	0.65
3:C:756:GLY:C	3:C:757:HIS:ND1	2.49	0.65
4:D:225:PRO:HG2	4:D:239:LEU:H	1.60	0.65
4:D:257:TYR:N	4:D:257:TYR:HD1	1.94	0.65
5:E:20:ASN:HD21	5:E:24:ASN:HB2	1.61	0.65
1:J:11:PRO:CB	1:J:270:THR:HB	2.12	0.65
3:L:550:LEU:N	3:L:550:LEU:HD12	2.11	0.65
4:M:252:TYR:OH	4:M:347:GLU:N	2.29	0.65
4:V:252:TYR:CB	4:V:253:PRO:HD2	2.23	0.65
3:3:584:VAL:HG12	3:3:600:VAL:HB	1.77	0.65
1:J:115:ILE:O	1:J:119:ILE:HG13	1.96	0.65
1:S:11:PRO:CB	1:S:270:THR:HB	2.15	0.65
3:U:561:PRO:CB	3:U:576:ALA:HA	2.26	0.65
4:4:228:VAL:HG22	4:4:268:GLU:O	1.95	0.65
4:4:240:ARG:NH1	5:5:78:PRO:HD2	2.12	0.65
1:A:64:GLY:HA3	11:H:500:FMN:O1P	1.97	0.65
3:C:243:ARG:HD3	3:C:275:LEU:CD1	2.25	0.65
3:C:371:PHE:CE1	3:C:549:VAL:HB	2.27	0.65
5:E:116:ARG:HG2	5:E:116:ARG:HH11	1.61	0.65
6:F:120:ASN:HD22	6:F:122:ALA:HB3	1.60	0.65
1:J:20:HIS:CE1	1:J:226:SER:HA	2.31	0.65
3:L:282:VAL:HG13	3:L:286:ASN:O	1.95	0.65
3:L:329:LEU:HD11	3:L:584:VAL:HG11	1.77	0.65
5:N:75:VAL:HG22	5:N:87:ARG:HG3	1.78	0.65
5:N:71:VAL:HG11	5:N:89:PHE:HD2	1.61	0.65
5:W:139:GLU:HG2	5:W:140:ASP:N	2.03	0.65
4:4:237:GLY:HA3	5:5:112:ASN:C	2.16	0.65
1:A:192:LEU:HD23	1:A:192:LEU:C	2.16	0.65
3:C:178:ARG:H	3:C:234:ALA:HA	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:194:VAL:HB	3:C:195:PRO:CD	2.27	0.65
5:E:47:ASN:HD22	5:E:76:SER:HA	1.61	0.65
4:V:342:VAL:HG22	4:V:343:TYR:N	2.11	0.65
5:W:7:LEU:HD13	5:W:11:ARG:HG2	1.79	0.65
4:4:226:PRO:HD2	4:4:239:LEU:HB2	1.77	0.65
4:4:266:LEU:CD1	4:4:281:ARG:HB3	2.13	0.65
4:4:96:ALA:HB2	4:4:346:THR:HG21	1.77	0.65
3:L:559:ASP:OD2	3:L:688:ARG:NH2	2.29	0.65
4:M:197:LEU:O	4:M:201:ILE:HD13	1.97	0.65
4:M:224:ILE:HB	4:M:225:PRO:CD	2.10	0.65
3:U:527:ARG:HB3	3:U:530:ALA:HB2	1.79	0.65
4:4:379:GLN:OE1	5:5:116:ARG:HG2	1.97	0.65
5:5:25:LEU:CD2	5:5:25:LEU:H	2.10	0.65
6:6:108:MET:HA	6:6:137:VAL:CG1	2.26	0.65
1:A:81:LYS:CG	1:A:82:ASP:H	2.10	0.65
4:D:342:VAL:HG22	4:D:343:TYR:N	2.10	0.65
4:D:342:VAL:HG22	4:D:343:TYR:H	1.61	0.65
5:E:55:LEU:HD12	5:E:55:LEU:N	2.12	0.65
5:E:7:LEU:HD13	5:E:11:ARG:HG2	1.79	0.65
3:L:167:HIS:C	3:L:176:LEU:HD11	2.17	0.65
3:L:414:SER:HA	3:L:461:TRP:CZ3	2.30	0.65
3:L:527:ARG:HB3	3:L:530:ALA:HB2	1.79	0.65
3:L:724:ARG:CD	3:L:724:ARG:H	2.08	0.65
4:M:320:SER:HB2	4:M:323:ALA:HB3	1.78	0.65
1:S:115:ILE:O	1:S:119:ILE:HG13	1.96	0.65
3:U:216:PHE:HZ	8:Z:128:PHE:CD2	2.15	0.65
4:V:225:PRO:HD2	4:V:226:PRO:CD	2.26	0.65
6:X:140:CYS:O	6:X:140:CYS:SG	2.54	0.65
3:3:285:VAL:HG22	3:3:286:ASN:N	2.12	0.65
3:3:329:LEU:HD11	3:3:584:VAL:HG11	1.79	0.65
3:3:559:ASP:OD2	3:3:688:ARG:NH2	2.29	0.65
4:D:223:VAL:HG13	4:D:226:PRO:O	1.97	0.65
4:D:228:VAL:HG22	4:D:268:GLU:O	1.97	0.65
4:D:350:ARG:HG2	4:D:350:ARG:O	1.97	0.65
1:J:81:LYS:CG	1:J:82:ASP:H	2.09	0.65
3:L:186:ARG:HD2	3:L:231:PRO:HD3	1.77	0.65
5:N:7:LEU:HD13	5:N:11:ARG:HG2	1.78	0.65
6:O:163:TYR:HB3	6:O:169:ARG:HA	1.78	0.65
3:U:307:LYS:H	3:U:307:LYS:CE	2.09	0.65
3:U:417:VAL:HG13	3:U:444:ARG:O	1.97	0.65
1:1:357:THR:N	1:1:358:PRO:HD2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:112:LEU:CD2	3:3:130:LEU:HD21	2.26	0.65
3:C:550:LEU:N	3:C:550:LEU:HD12	2.12	0.65
4:D:237:GLY:HA3	5:E:112:ASN:HA	1.76	0.65
3:L:313:LYS:O	3:L:314:GLU:HB2	1.96	0.65
3:L:481:LEU:HD11	3:L:519:GLU:HB2	1.77	0.65
3:L:453:PRO:HB2	3:L:750:ARG:NH1	2.11	0.65
4:M:322:GLU:O	4:M:325:ILE:N	2.29	0.65
5:N:37:GLU:O	5:N:41:TYR:HD1	1.78	0.65
6:O:145:GLU:HG2	7:P:31:VAL:HG21	1.79	0.65
7:P:73:ALA:HB2	7:P:89:LYS:HB2	1.79	0.65
3:U:313:LYS:O	3:U:314:GLU:HB2	1.95	0.65
3:U:453:PRO:HB2	3:U:750:ARG:HH12	1.61	0.65
6:X:138:PRO:CG	7:Y:121:MET:HG3	2.27	0.65
3:3:237:ASP:OD1	3:3:239:THR:HG22	1.96	0.65
3:3:45:CYS:O	3:3:47:MET:N	2.30	0.65
3:C:307:LYS:CE	3:C:307:LYS:H	2.10	0.65
3:C:701:ALA:H	3:C:754:PRO:HB3	1.62	0.65
2:T:7:LYS:HD2	2:T:7:LYS:H	1.60	0.65
4:V:240:ARG:CD	4:V:243:GLY:HA3	2.20	0.65
2:2:102:GLU:HA	8:7:108:ILE:HD11	1.79	0.65
5:5:7:LEU:HD13	5:5:11:ARG:HG2	1.79	0.65
6:6:139:GLY:HA3	6:6:142:PRO:CB	2.27	0.65
6:F:165:GLU:C	6:F:167:GLY:H	2.00	0.65
6:F:153:GLN:HG3	7:G:124:TYR:OH	1.96	0.65
3:L:565:TYR:HD1	3:L:582:PHE:HB3	1.60	0.65
3:L:453:PRO:HB2	3:L:750:ARG:HH12	1.62	0.65
4:M:59:ILE:HD11	5:N:138:PRO:HB3	1.77	0.65
5:N:134:LYS:CE	5:N:136:LEU:HB3	2.27	0.65
4:V:196:VAL:C	4:V:198:PRO:HD2	2.17	0.65
5:W:125:VAL:HG12	5:W:126:PHE:N	2.08	0.65
1:1:397:ARG:HG3	3:3:46:ARG:NE	2.12	0.64
3:3:155:THR:HB	4:4:321:MET:HB2	1.78	0.64
4:4:225:PRO:HG2	4:4:239:LEU:H	1.61	0.64
8:7:37:PHE:HD1	8:7:53:THR:O	1.80	0.64
4:M:237:GLY:O	4:M:239:LEU:HG	1.95	0.64
5:N:114:LEU:O	5:N:118:VAL:HG23	1.97	0.64
6:O:163:TYR:HB2	6:O:169:ARG:HA	1.79	0.64
1:S:20:HIS:CE1	1:S:226:SER:HA	2.32	0.64
1:S:301:PRO:O	1:S:306:VAL:HG21	1.97	0.64
3:U:237:ASP:OD1	3:U:239:THR:HG22	1.97	0.64
3:3:719:HIS:HB2	3:3:720:PRO:HD3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:124:ILE:CG2	5:5:146:LEU:HB2	2.27	0.64
2:B:89:LYS:HA	2:B:93:ALA:HB3	1.78	0.64
4:D:144:THR:HB	4:D:145:PRO:HD3	1.78	0.64
2:K:79:HIS:HD2	2:K:118:SER:HB2	1.61	0.64
3:L:229:ILE:HD11	3:L:289:TRP:CZ3	2.33	0.64
3:U:438:LYS:O	3:U:441:MET:HG3	1.97	0.64
4:V:227:GLU:HB2	4:V:269:ARG:HA	1.79	0.64
5:W:103:THR:HB	5:W:131:ASP:O	1.98	0.64
4:V:226:PRO:HB3	5:W:80:TRP:CH2	2.32	0.64
7:Y:94:ASN:HD22	7:Y:97:ARG:HB2	1.63	0.64
3:3:438:LYS:O	3:3:441:MET:HG3	1.96	0.64
4:4:112:ARG:HG2	4:4:112:ARG:O	1.97	0.64
4:4:353:LEU:HD12	4:4:354:GLY:H	1.62	0.64
5:5:121:LEU:H	5:5:121:LEU:CD1	2.10	0.64
4:4:249:ARG:HH22	5:5:87:ARG:HB2	1.62	0.64
5:5:26:TRP:CB	5:5:89:PHE:HB2	2.23	0.64
3:C:19:VAL:O	3:C:22:ALA:HB3	1.96	0.64
3:C:459:MET:HG3	3:C:465:HIS:HB2	1.79	0.64
4:D:98:ALA:O	4:D:102:GLU:HG3	1.97	0.64
4:D:227:GLU:HB2	4:D:269:ARG:HA	1.78	0.64
5:E:37:GLU:O	5:E:41:TYR:HD1	1.78	0.64
6:F:16:ARG:HD2	6:F:17:GLU:HG3	1.79	0.64
7:G:45:ARG:NH2	7:G:137:LEU:HD23	2.12	0.64
5:N:43:ALA:C	5:N:45:GLY:N	2.49	0.64
4:M:249:ARG:HH22	5:N:87:ARG:HB2	1.62	0.64
4:V:318:GLU:HB2	8:Z:39:ASP:HA	1.80	0.64
2:2:40:TRP:CZ3	2:2:42:ARG:HA	2.33	0.64
3:C:155:THR:HB	4:D:321:MET:HB2	1.77	0.64
3:C:724:ARG:HD2	3:C:724:ARG:H	1.61	0.64
6:F:165:GLU:O	6:F:167:GLY:N	2.31	0.64
3:L:205:ARG:HA	3:L:209:THR:CG2	2.11	0.64
3:L:216:PHE:HZ	8:Q:128:PHE:CD2	2.14	0.64
6:O:130:VAL:HG23	6:O:131:VAL:N	2.13	0.64
7:P:123:ASP:CG	7:P:148:ARG:HH22	2.01	0.64
8:Q:52:THR:HB	8:Q:54:ILE:HG22	1.80	0.64
4:V:193:LEU:O	4:V:193:LEU:HD23	1.97	0.64
5:W:52:ILE:HG23	5:W:117:GLU:CG	2.27	0.64
7:Y:45:ARG:NH2	7:Y:137:LEU:HD23	2.11	0.64
1:1:20:HIS:O	1:1:22:GLY:N	2.30	0.64
3:3:494:LYS:O	3:3:498:GLU:HG2	1.97	0.64
4:4:373:PRO:O	4:4:376:VAL:HG22	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:62:LEU:HD21	6:6:43:LEU:HB3	1.78	0.64
4:4:59:ILE:HD11	5:5:138:PRO:HB3	1.79	0.64
6:6:165:GLU:C	6:6:167:GLY:H	2.01	0.64
3:C:112:LEU:CD2	3:C:130:LEU:HD21	2.27	0.64
3:C:211:ILE:HG23	3:C:211:ILE:O	1.98	0.64
4:D:238:SER:O	4:D:239:LEU:HD23	1.97	0.64
4:D:313:PRO:C	4:D:315:HIS:H	2.00	0.64
6:F:165:GLU:HG3	7:G:128:ASP:OD1	1.97	0.64
7:G:36:ARG:HA	7:G:167:ARG:HD3	1.78	0.64
1:J:93:ALA:HB3	1:J:134:VAL:HG12	1.78	0.64
3:L:473:GLU:O	3:L:477:LEU:HD12	1.97	0.64
4:M:246:TYR:CG	4:M:347:GLU:HG3	2.32	0.64
4:M:64:THR:O	4:M:64:THR:HG22	1.96	0.64
8:Q:112:LYS:O	8:Q:116:PHE:HD1	1.80	0.64
5:W:124:ILE:HG22	5:W:146:LEU:H	1.63	0.64
3:3:756:GLY:C	3:3:757:HIS:ND1	2.50	0.64
4:4:322:GLU:C	4:4:324:VAL:H	2.01	0.64
3:C:177:ASP:HB3	3:C:235:LEU:HD22	1.79	0.64
4:D:317:LEU:N	4:D:317:LEU:HD12	2.11	0.64
4:D:320:SER:CB	4:D:323:ALA:HB3	2.27	0.64
3:L:38:HIS:NE2	3:L:287:GLU:HG2	2.12	0.64
4:M:322:GLU:C	4:M:324:VAL:H	2.01	0.64
4:M:62:LEU:N	4:M:408:ASP:OD2	2.28	0.64
6:X:163:TYR:HB2	6:X:169:ARG:HA	1.79	0.64
8:Z:44:MET:O	8:Z:46:ARG:N	2.31	0.64
3:3:134:THR:O	3:3:138:GLY:HA3	1.97	0.64
7:9:101:CYS:O	7:9:101:CYS:SG	2.55	0.64
3:C:33:PHE:HZ	3:C:130:LEU:HA	1.61	0.64
4:D:62:LEU:HD21	6:F:43:LEU:HB3	1.80	0.64
4:M:350:ARG:NH1	4:M:401:ASP:OD2	2.31	0.64
3:U:33:PHE:HZ	3:U:130:LEU:HA	1.61	0.64
3:U:166:LYS:HE3	3:U:180:ARG:HD2	1.80	0.64
3:U:369:LEU:CD2	3:U:369:LEU:H	2.11	0.64
3:U:307:LYS:HB3	3:U:632:GLY:HA3	1.80	0.64
3:3:307:LYS:H	3:3:307:LYS:HE3	1.63	0.64
3:3:387:LEU:HD13	3:3:618:GLU:OE1	1.98	0.64
1:A:9:LEU:HD23	1:A:10:ASP:N	2.11	0.64
1:A:434:PRO:HG2	1:A:436:LEU:CD1	2.28	0.64
2:B:40:TRP:CZ3	2:B:42:ARG:HA	2.33	0.64
5:E:53:VAL:HG22	5:E:55:LEU:HD12	1.78	0.64
6:F:108:MET:HA	6:F:137:VAL:CG1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:12:ARG:NE	1:J:12:ARG:O	2.28	0.64
4:M:227:GLU:HB2	4:M:269:ARG:HA	1.78	0.64
5:N:53:VAL:HG22	5:N:55:LEU:HD12	1.80	0.64
3:U:285:VAL:HG22	3:U:286:ASN:N	2.12	0.64
4:V:249:ARG:HH22	5:W:87:ARG:CB	2.11	0.64
4:V:313:PRO:O	4:V:315:HIS:N	2.31	0.64
3:U:155:THR:HB	4:V:321:MET:HB2	1.80	0.64
5:W:33:ARG:O	5:W:37:GLU:HB2	1.98	0.64
3:C:166:LYS:HE3	3:C:180:ARG:HD2	1.80	0.64
4:D:234:LEU:HD23	4:D:234:LEU:N	2.12	0.64
4:D:381:LEU:HA	4:D:384:ALA:HB3	1.78	0.64
6:F:115:GLY:HA3	6:F:125:GLN:OE1	1.97	0.64
6:6:19:ILE:HD11	1:J:271:THR:HG23	1.80	0.64
2:K:90:LEU:HD12	2:K:90:LEU:H	1.63	0.64
3:L:40:SER:OG	3:L:189:ARG:HD2	1.98	0.64
4:M:393:MET:HG2	4:M:393:MET:O	1.97	0.64
6:O:165:GLU:O	6:O:167:GLY:N	2.31	0.64
3:U:226:ILE:HD12	3:U:235:LEU:HD11	1.80	0.64
6:X:92:MET:HE1	6:X:127:VAL:HG13	1.79	0.64
1:1:436:LEU:HD23	2:2:90:LEU:HA	1.78	0.64
3:3:501:LYS:H	3:3:501:LYS:CD	1.98	0.64
4:4:116:ILE:O	4:4:120:LEU:HB2	1.97	0.64
4:4:240:ARG:HD3	5:5:77:LEU:HB3	1.79	0.64
6:6:164:ASN:O	7:9:148:ARG:HD2	1.98	0.64
7:9:71:GLU:HB2	7:9:90:VAL:HB	1.80	0.64
3:C:227:THR:HG21	3:C:237:ASP:HB2	1.79	0.64
3:C:621:VAL:HG22	3:C:674:GLY:O	1.98	0.64
4:D:234:LEU:CD1	5:E:49:LEU:HD21	2.28	0.64
1:J:437:TRP:CH2	2:K:96:LEU:HD13	2.32	0.64
3:L:586:HIS:CD2	3:L:604:ALA:HB2	2.32	0.64
6:O:164:ASN:HB3	7:P:148:ARG:NE	2.10	0.64
3:U:117:LEU:HD23	4:V:322:GLU:OE2	1.98	0.64
4:V:105:LEU:HD23	4:V:337:PRO:HG3	1.79	0.64
4:V:237:GLY:HA3	5:W:112:ASN:C	2.19	0.64
7:Y:56:CYS:O	9:Y:184:SF4:S3	2.56	0.64
1:1:64:GLY:HA3	11:7:500:FMN:O1P	1.97	0.63
6:6:37:TRP:CE3	6:6:37:TRP:HA	2.33	0.63
1:A:360:ARG:O	1:A:364:ALA:HB3	1.98	0.63
2:B:112:THR:HG21	2:B:116:LEU:HD23	1.79	0.63
2:B:40:TRP:HZ3	2:B:42:ARG:HA	1.63	0.63
3:C:501:LYS:H	3:C:501:LYS:CD	2.04	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:237:GLY:HA3	5:E:112:ASN:C	2.17	0.63
4:D:86:ASP:O	4:D:88:LEU:N	2.31	0.63
7:G:101:CYS:O	7:G:103:LEU:N	2.31	0.63
1:J:359:CYS:O	1:J:363:VAL:HG22	1.98	0.63
4:M:225:PRO:HD2	4:M:226:PRO:CD	2.29	0.63
5:N:25:LEU:CD2	5:N:25:LEU:H	2.11	0.63
2:T:40:TRP:HE1	2:T:74:PRO:HG3	1.62	0.63
3:U:586:HIS:CD2	3:U:604:ALA:HB2	2.33	0.63
3:U:583:VAL:CG2	3:U:598:ALA:HA	2.28	0.63
4:V:379:GLN:OE1	5:W:115:GLU:HB2	1.98	0.63
7:Y:141:VAL:CG1	7:Y:142:GLY:H	2.09	0.63
4:4:224:ILE:HB	4:4:225:PRO:CD	2.13	0.63
4:4:234:LEU:HD23	4:4:234:LEU:N	2.13	0.63
7:9:45:ARG:HH21	7:9:137:LEU:HD23	1.63	0.63
2:B:27:ILE:HG13	2:B:53:VAL:HG21	1.80	0.63
3:C:100:VAL:O	3:C:104:GLN:HG3	1.98	0.63
3:C:34:CYS:SG	3:C:44:ALA:O	2.57	0.63
3:C:402:PRO:HA	3:C:535:MET:HE1	1.81	0.63
4:D:404:MET:HA	4:D:407:VAL:HG12	1.81	0.63
5:E:103:THR:HB	5:E:131:ASP:O	1.99	0.63
4:M:266:LEU:CD1	4:M:281:ARG:HB3	2.14	0.63
3:U:341:VAL:HB	3:U:364:LEU:HD21	1.80	0.63
3:U:546:ALA:HA	3:U:678:PHE:CE2	2.34	0.63
3:U:96:LEU:N	3:U:96:LEU:HD12	2.12	0.63
3:3:32:LEU:O	3:3:33:PHE:HD1	1.80	0.63
4:4:246:TYR:CG	4:4:347:GLU:HG3	2.33	0.63
3:C:612:GLY:O	3:C:624:LEU:HB2	1.99	0.63
4:D:133:LEU:HD21	4:D:204:TYR:HD2	1.62	0.63
3:L:171:SER:C	3:L:173:PHE:N	2.50	0.63
4:M:153:ARG:HH11	4:M:153:ARG:HG3	1.64	0.63
1:S:11:PRO:HG3	1:S:270:THR:HA	1.79	0.63
4:V:68:LYS:O	4:V:71:GLU:HB2	1.98	0.63
7:Y:175:ALA:HB1	7:Y:176:PRO:HD2	1.79	0.63
4:D:221:VAL:O	4:D:223:VAL:N	2.31	0.63
1:J:434:PRO:HG2	1:J:436:LEU:CD1	2.29	0.63
3:L:155:THR:HB	4:M:321:MET:HB2	1.80	0.63
3:L:733:GLN:HA	3:L:745:ALA:O	1.98	0.63
3:L:96:LEU:HD12	3:L:96:LEU:N	2.13	0.63
1:S:125:ILE:HD13	1:S:217:THR:HG21	1.79	0.63
4:V:116:ILE:O	4:V:120:LEU:HB2	1.98	0.63
4:V:320:SER:CB	4:V:323:ALA:HB3	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:346:THR:HG22	4:4:353:LEU:O	1.97	0.63
3:C:329:LEU:HD11	3:C:584:VAL:HG11	1.80	0.63
5:E:195:LEU:H	5:E:195:LEU:HD13	1.64	0.63
2:K:79:HIS:CD2	2:K:118:SER:HB2	2.33	0.63
1:J:436:LEU:HD23	2:K:90:LEU:HA	1.79	0.63
3:L:524:LEU:CG	3:L:525:ALA:N	2.60	0.63
3:U:282:VAL:HG22	3:U:282:VAL:O	1.98	0.63
4:V:70:MET:C	4:V:72:HIS:H	2.01	0.63
4:V:74:THR:CB	4:V:77:GLN:HG3	2.27	0.63
5:W:195:LEU:H	5:W:195:LEU:HD13	1.64	0.63
5:W:25:LEU:CD2	5:W:25:LEU:H	2.12	0.63
6:X:130:VAL:HG23	6:X:131:VAL:N	2.14	0.63
1:1:13:PHE:HE1	1:1:15:ARG:HG3	1.62	0.63
4:4:159:LEU:O	4:4:162:TRP:HB2	1.98	0.63
4:4:226:PRO:HB3	5:5:80:TRP:CH2	2.34	0.63
4:4:317:LEU:N	4:4:317:LEU:HD12	2.14	0.63
4:4:404:MET:HA	4:4:407:VAL:CG1	2.28	0.63
4:M:234:LEU:N	4:M:234:LEU:HD23	2.14	0.63
4:M:375:PHE:HD1	4:M:407:VAL:HG23	1.64	0.63
6:O:138:PRO:CG	7:P:121:MET:HG3	2.28	0.63
3:U:587:LEU:HD23	3:U:588:SER:H	1.63	0.63
3:U:747:VAL:HG23	3:U:747:VAL:O	1.97	0.63
3:3:132:ASP:O	3:3:136:GLU:HG3	1.99	0.63
3:3:546:ALA:HA	3:3:678:PHE:CE2	2.33	0.63
3:3:117:LEU:HD23	4:4:322:GLU:OE2	1.99	0.63
3:C:189:ARG:HG3	3:C:193:GLU:OE2	1.98	0.63
6:X:165:GLU:O	6:X:167:GLY:N	2.32	0.63
2:2:81:GLN:HB3	2:2:122:VAL:HG21	1.81	0.63
3:3:510:GLY:CA	3:3:520:ARG:HH22	2.11	0.63
3:3:586:HIS:HD2	3:3:602:LEU:O	1.82	0.63
4:4:220:GLY:HA2	4:4:384:ALA:O	1.99	0.63
1:A:90:ILE:HD11	1:A:211:LEU:HD22	1.81	0.63
1:A:359:CYS:O	1:A:363:VAL:HG22	1.98	0.63
6:F:164:ASN:H	6:F:170:LEU:HD12	1.64	0.63
3:L:194:VAL:HB	3:L:195:PRO:CD	2.29	0.63
3:L:269:THR:HG22	3:L:274:LEU:HA	1.80	0.63
3:L:581:ARG:O	3:L:599:HIS:CE1	2.52	0.63
3:L:546:ALA:HA	3:L:678:PHE:CE2	2.34	0.63
4:M:114:GLU:HG2	4:M:253:PRO:HB3	1.79	0.63
3:U:167:HIS:C	3:U:176:LEU:HD11	2.18	0.63
1:1:13:PHE:CE1	1:1:15:ARG:HG3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:219:ARG:O	4:4:221:VAL:N	2.32	0.63
4:4:227:GLU:HB2	4:4:269:ARG:HA	1.81	0.63
5:5:7:LEU:HD21	5:5:41:TYR:CE2	2.34	0.63
5:5:44:MET:CE	5:5:82:ASP:HB3	2.29	0.63
3:C:559:ASP:OD2	3:C:688:ARG:NH2	2.32	0.63
3:C:748:VAL:O	3:C:748:VAL:CG1	2.47	0.63
4:D:114:GLU:HG2	4:D:253:PRO:HB3	1.80	0.63
4:D:214:PHE:C	4:D:216:GLU:H	2.02	0.63
6:F:163:TYR:HB2	6:F:169:ARG:HA	1.79	0.63
3:L:501:LYS:CD	3:L:501:LYS:H	2.01	0.63
4:M:98:ALA:O	4:M:102:GLU:HG3	1.98	0.63
4:M:248:VAL:O	4:M:249:ARG:HG2	1.99	0.63
4:M:373:PRO:O	4:M:376:VAL:HG22	1.98	0.63
5:N:47:ASN:CB	5:N:77:LEU:HG	2.29	0.63
5:N:65:PRO:HB2	5:N:93:TYR:HD2	1.64	0.63
6:O:120:ASN:HD22	6:O:122:ALA:HB3	1.62	0.63
3:C:186:ARG:HD2	3:C:231:PRO:HD3	1.81	0.62
4:D:257:TYR:CD1	4:D:257:TYR:N	2.66	0.62
3:L:341:VAL:HB	3:L:364:LEU:HD21	1.79	0.62
3:L:586:HIS:HD2	3:L:602:LEU:O	1.82	0.62
4:M:229:ALA:HB3	4:M:241:ALA:HA	1.80	0.62
3:U:282:VAL:O	3:U:286:ASN:O	2.16	0.62
3:U:459:MET:HG3	3:U:465:HIS:HB2	1.81	0.62
3:U:524:LEU:CG	3:U:525:ALA:N	2.62	0.62
3:U:724:ARG:HD2	3:U:724:ARG:H	1.63	0.62
3:3:413:LEU:HD13	3:3:448:MET:HE2	1.80	0.62
3:3:477:LEU:HD13	3:3:516:VAL:CG1	2.29	0.62
5:5:121:LEU:N	5:5:121:LEU:CD1	2.63	0.62
5:5:175:THR:HG23	5:5:178:ASP:HB2	1.79	0.62
6:6:164:ASN:HB3	7:9:148:ARG:NE	2.11	0.62
4:D:285:GLU:O	4:D:289:ILE:HG12	1.99	0.62
5:N:49:LEU:CB	5:N:77:LEU:HD21	2.22	0.62
5:N:65:PRO:HB2	5:N:93:TYR:CD2	2.34	0.62
4:V:226:PRO:HD2	4:V:239:LEU:HB2	1.78	0.62
1:1:360:ARG:O	1:1:364:ALA:HB3	1.99	0.62
2:2:89:LYS:HE3	2:2:94:GLU:OE1	2.00	0.62
3:C:40:SER:OG	3:C:189:ARG:HD2	1.99	0.62
5:E:116:ARG:HA	5:E:119:TYR:CD2	2.33	0.62
5:E:124:ILE:HG22	5:E:146:LEU:H	1.64	0.62
1:J:357:THR:N	1:J:358:PRO:HD2	2.14	0.62
4:M:85:MET:HE2	4:M:409:ARG:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:474:ARG:HA	3:U:516:VAL:HG13	1.81	0.62
3:U:621:VAL:HG22	3:U:674:GLY:O	1.99	0.62
5:W:187:GLY:C	5:W:189:ARG:H	2.02	0.62
5:W:53:VAL:HG22	5:W:55:LEU:HD12	1.80	0.62
6:X:114:SER:CB	7:Y:97:ARG:HD2	2.28	0.62
1:1:253:GLN:CG	1:1:327:GLY:HA2	2.30	0.62
5:5:121:LEU:H	5:5:121:LEU:HD12	1.65	0.62
2:B:116:LEU:HD23	2:B:116:LEU:H	1.64	0.62
4:D:229:ALA:HB3	4:D:241:ALA:HA	1.81	0.62
4:D:84:ARG:O	6:F:83:ARG:NH2	2.32	0.62
3:L:226:ILE:HD12	3:L:235:LEU:CD1	2.29	0.62
3:L:239:THR:HG21	3:L:298:HIS:HE1	1.65	0.62
3:L:343:LEU:O	3:L:369:LEU:HA	2.00	0.62
3:L:347:HIS:HD2	3:L:539:ALA:H	1.47	0.62
4:M:119:ILE:O	4:M:123:LEU:HB2	1.99	0.62
5:N:100:ARG:O	5:N:101:LEU:HB2	1.99	0.62
4:M:237:GLY:HA3	5:N:112:ASN:C	2.20	0.62
5:N:155:THR:O	6:O:119:ASN:ND2	2.32	0.62
3:U:387:LEU:HD13	3:U:618:GLU:OE1	1.99	0.62
3:U:409:LEU:HD12	3:U:535:MET:HE2	1.79	0.62
4:4:119:ILE:O	4:4:123:LEU:HB2	1.99	0.62
4:4:256:GLY:CA	4:4:292:GLN:HE22	2.12	0.62
3:C:305:ARG:HG2	3:C:306:LEU:N	2.15	0.62
3:L:477:LEU:HD13	3:L:516:VAL:CG1	2.29	0.62
3:L:31:PRO:HB2	3:L:47:MET:HB3	1.81	0.62
5:N:3:LEU:HD13	5:N:44:MET:SD	2.39	0.62
4:V:256:GLY:HA2	4:V:292:GLN:NE2	2.14	0.62
4:V:317:LEU:HD12	4:V:317:LEU:N	2.14	0.62
6:X:130:VAL:HG23	6:X:131:VAL:H	1.65	0.62
7:Y:123:ASP:CG	7:Y:148:ARG:HH22	2.02	0.62
3:3:166:LYS:HE3	3:3:180:ARG:HD2	1.81	0.62
3:3:501:LYS:N	3:3:501:LYS:HD2	2.05	0.62
4:4:375:PHE:HD1	4:4:407:VAL:HG23	1.64	0.62
6:6:159:ARG:HB3	6:6:161:GLN:HG3	1.81	0.62
3:C:169:PRO:HD3	3:C:176:LEU:HD13	1.82	0.62
5:E:92:VAL:O	5:E:92:VAL:HG23	2.00	0.62
3:L:223:SER:O	3:L:226:ILE:HG12	1.99	0.62
3:L:413:LEU:HD13	3:L:448:MET:HE2	1.82	0.62
4:M:120:LEU:HD13	4:M:160:PHE:HE1	1.63	0.62
4:M:317:LEU:HD12	4:M:317:LEU:N	2.14	0.62
4:V:322:GLU:O	4:V:325:ILE:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:404:MET:HA	4:V:407:VAL:HG12	1.82	0.62
6:X:153:GLN:HG3	7:Y:124:TYR:OH	2.00	0.62
7:Y:161:TYR:O	7:Y:176:PRO:HG3	2.00	0.62
4:4:237:GLY:HA3	5:5:112:ASN:CA	2.30	0.62
4:4:367:ARG:HG2	4:4:367:ARG:HH11	1.62	0.62
7:9:175:ALA:HB1	7:9:176:PRO:HD2	1.81	0.62
3:C:477:LEU:CD2	3:C:520:ARG:HG2	2.30	0.62
4:D:322:GLU:O	4:D:325:ILE:N	2.33	0.62
4:D:59:ILE:HD13	4:D:59:ILE:N	2.13	0.62
8:H:82:ILE:HG23	8:H:95:ALA:HB3	1.81	0.62
2:K:102:GLU:HA	8:Q:108:ILE:HD11	1.82	0.62
3:L:458:LEU:HD12	3:L:458:LEU:H	1.65	0.62
3:L:81:ALA:HB3	3:L:84:VAL:HG22	1.81	0.62
4:M:193:LEU:O	4:M:193:LEU:HD23	1.99	0.62
4:M:89:HIS:HB2	4:M:128:SER:HB2	1.82	0.62
5:N:116:ARG:HA	5:N:119:TYR:CD2	2.34	0.62
1:S:81:LYS:CG	1:S:82:ASP:H	2.11	0.62
4:V:224:ILE:CD1	4:V:237:GLY:HA2	2.29	0.62
4:V:367:ARG:HH11	4:V:367:ARG:HG2	1.63	0.62
6:X:163:TYR:HA	6:X:170:LEU:HB2	1.81	0.62
8:Z:52:THR:HB	8:Z:54:ILE:HG22	1.82	0.62
3:3:474:ARG:HA	3:3:516:VAL:HG13	1.82	0.62
3:3:524:LEU:CG	3:3:525:ALA:N	2.62	0.62
4:4:234:LEU:CD1	5:5:49:LEU:HD21	2.26	0.62
4:4:114:GLU:HG2	4:4:253:PRO:HB3	1.80	0.62
3:C:269:THR:HG22	3:C:274:LEU:HA	1.82	0.62
3:C:458:LEU:H	3:C:458:LEU:HD12	1.65	0.62
3:C:546:ALA:HA	3:C:678:PHE:CE2	2.35	0.62
4:D:232:LEU:HD13	4:D:278:VAL:HG12	1.81	0.62
5:E:50:ALA:CB	5:E:114:LEU:HD21	2.28	0.62
4:D:318:GLU:HB2	8:H:39:ASP:HA	1.81	0.62
1:J:301:PRO:O	1:J:306:VAL:HG21	2.00	0.62
3:L:100:VAL:O	3:L:104:GLN:HG3	2.00	0.62
3:L:32:LEU:O	3:L:33:PHE:HD1	1.82	0.62
3:L:756:GLY:C	3:L:757:HIS:ND1	2.52	0.62
5:W:124:ILE:CG2	5:W:146:LEU:HB2	2.27	0.62
2:2:40:TRP:HZ3	2:2:42:ARG:HA	1.64	0.62
3:3:369:LEU:H	3:3:369:LEU:CD2	2.13	0.62
4:4:120:LEU:HD13	4:4:160:PHE:HE1	1.63	0.62
4:4:190:LEU:O	4:4:194:LEU:HB2	1.99	0.62
4:4:107:ALA:HB2	4:4:309:ILE:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:165:GLU:O	6:6:167:GLY:N	2.33	0.62
1:A:125:ILE:HD13	1:A:217:THR:HG21	1.80	0.62
3:C:361:ALA:O	3:C:367:PRO:HG3	2.00	0.62
3:C:527:ARG:HB3	3:C:530:ALA:HB2	1.81	0.62
3:C:545:GLU:HA	3:C:550:LEU:HD11	1.81	0.62
4:D:119:ILE:O	4:D:123:LEU:HB2	1.99	0.62
2:K:59:GLU:O	2:K:63:VAL:HG23	2.00	0.62
3:L:177:ASP:HB3	3:L:235:LEU:HD22	1.80	0.62
4:M:219:ARG:O	4:M:221:VAL:N	2.33	0.62
6:O:165:GLU:C	6:O:167:GLY:H	2.01	0.62
1:S:356:CYS:HB3	1:S:358:PRO:HG2	1.80	0.62
2:T:89:LYS:HE3	2:T:94:GLU:OE1	2.00	0.62
4:V:114:GLU:HG2	4:V:253:PRO:HB3	1.82	0.62
4:4:144:THR:HB	4:4:145:PRO:HD3	1.81	0.62
1:A:93:ALA:HB3	1:A:134:VAL:HG12	1.80	0.62
6:F:130:VAL:HG23	6:F:131:VAL:H	1.65	0.62
8:H:121:ARG:HH11	8:H:121:ARG:HG3	1.63	0.62
3:L:19:VAL:O	3:L:22:ALA:HB3	2.00	0.62
3:L:413:LEU:HD13	3:L:448:MET:HE1	1.82	0.62
4:M:224:ILE:CD1	4:M:237:GLY:HA2	2.30	0.62
5:N:132:LEU:HD23	5:N:135:ILE:HG23	1.82	0.62
4:V:120:LEU:HD13	4:V:160:PHE:HE1	1.65	0.62
6:X:165:GLU:C	6:X:167:GLY:H	2.03	0.62
2:2:46:ILE:HG23	2:2:60:VAL:CG1	2.29	0.61
3:3:211:ILE:O	3:3:212:GLY:O	2.18	0.61
3:3:125:GLY:HA3	3:3:246:ASN:HD22	1.64	0.61
4:4:112:ARG:O	4:4:116:ILE:HG12	2.00	0.61
3:C:498:GLU:O	3:C:527:ARG:NH2	2.33	0.61
3:C:6:VAL:HG12	3:C:7:ASN:H	1.64	0.61
4:D:240:ARG:NH2	4:D:245:ASN:OD1	2.33	0.61
6:F:145:GLU:HG2	7:G:31:VAL:HG21	1.81	0.61
6:F:155:GLN:O	6:F:158:VAL:HG22	2.00	0.61
1:J:250:LYS:HB3	1:J:252:TYR:CE2	2.35	0.61
2:K:116:LEU:HG	2:K:117:PHE:CD2	2.35	0.61
3:L:374:ARG:NH2	3:L:684:ARG:HG3	2.14	0.61
3:L:487:SER:OG	3:L:490:VAL:HG23	2.00	0.61
3:L:7:ASN:HD21	3:L:96:LEU:HD11	1.64	0.61
4:M:321:MET:O	4:M:322:GLU:HG2	1.99	0.61
3:U:20:MET:HE3	3:U:32:LEU:HD21	1.82	0.61
5:W:26:TRP:CB	5:W:89:PHE:HB2	2.28	0.61
5:W:75:VAL:HG22	5:W:87:ARG:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:125:ILE:HD13	1:1:217:THR:HG21	1.81	0.61
3:3:307:LYS:N	3:3:307:LYS:CE	2.63	0.61
3:3:557:SER:H	3:3:560:GLU:HB3	1.64	0.61
2:B:31:LEU:HD12	2:B:41:ILE:HD13	1.81	0.61
3:C:25:HIS:ND1	3:C:427:ASN:HB2	2.15	0.61
3:C:564:LEU:CD1	3:C:581:ARG:H	2.12	0.61
4:D:226:PRO:HB3	5:E:80:TRP:CH2	2.35	0.61
4:D:227:GLU:HG3	4:D:268:GLU:O	2.00	0.61
2:K:81:GLN:HB3	2:K:122:VAL:HG21	1.82	0.61
4:M:249:ARG:HH22	5:N:87:ARG:CB	2.13	0.61
5:N:121:LEU:H	5:N:121:LEU:HD12	1.62	0.61
8:Q:27:LYS:HB3	8:Q:123:ARG:NH1	2.15	0.61
3:U:305:ARG:HG2	3:U:306:LEU:H	1.65	0.61
4:V:254:TYR:O	4:V:256:GLY:N	2.33	0.61
4:V:321:MET:O	4:V:322:GLU:HG2	2.00	0.61
1:1:81:LYS:CG	1:1:82:ASP:H	2.13	0.61
2:2:27:ILE:HG22	2:2:31:LEU:HD23	1.82	0.61
3:3:36:GLU:OE2	3:3:229:ILE:HG23	2.00	0.61
4:4:252:TYR:OH	4:4:347:GLU:N	2.33	0.61
8:7:121:ARG:HH11	8:7:121:ARG:HG3	1.66	0.61
1:A:110:VAL:N	1:A:111:PRO:CD	2.62	0.61
1:A:356:CYS:HB3	1:A:358:PRO:HG2	1.81	0.61
3:C:656:LEU:HD23	3:C:656:LEU:H	1.64	0.61
4:D:249:ARG:HH22	5:E:87:ARG:HB2	1.66	0.61
2:T:90:LEU:HD12	2:T:90:LEU:H	1.64	0.61
3:U:549:VAL:C	3:U:550:LEU:HD12	2.20	0.61
6:X:164:ASN:H	6:X:170:LEU:HD12	1.64	0.61
3:3:537:PRO:HB2	3:3:756:GLY:HA2	1.81	0.61
4:4:404:MET:HA	4:4:407:VAL:HG12	1.81	0.61
5:5:71:VAL:HG11	5:5:89:PHE:HD2	1.64	0.61
7:9:35:PRO:O	7:9:36:ARG:HB2	2.01	0.61
2:B:130:THR:HG21	2:B:143:GLU:OE1	2.00	0.61
4:D:367:ARG:HG2	4:D:367:ARG:HH11	1.65	0.61
1:J:26:SER:HB3	1:J:31:TYR:CD1	2.36	0.61
3:L:166:LYS:HG3	3:L:178:ARG:HG3	1.81	0.61
3:L:34:CYS:SG	3:L:44:ALA:O	2.59	0.61
5:N:103:THR:HB	5:N:131:ASP:O	1.99	0.61
2:T:81:GLN:HB3	2:T:122:VAL:HG21	1.82	0.61
4:V:249:ARG:HH22	5:W:87:ARG:HB2	1.62	0.61
7:Y:71:GLU:HB2	7:Y:90:VAL:HB	1.82	0.61
3:3:223:SER:O	3:3:226:ILE:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:34:CYS:SG	3:3:44:ALA:O	2.59	0.61
3:3:510:GLY:HA3	3:3:520:ARG:HH22	1.64	0.61
4:4:313:PRO:C	4:4:315:HIS:H	2.03	0.61
2:B:131:ALA:HB1	2:B:132:PRO:HD3	1.79	0.61
3:C:167:HIS:C	3:C:176:LEU:HD11	2.20	0.61
3:C:586:HIS:HD2	3:C:602:LEU:O	1.83	0.61
3:C:603:PRO:HG2	3:C:634:ALA:HB1	1.82	0.61
6:F:138:PRO:CG	7:G:121:MET:HG3	2.29	0.61
7:G:153:THR:HG22	7:G:155:LYS:HB2	1.82	0.61
7:G:33:LEU:HD22	7:G:37:PHE:CD2	2.35	0.61
3:L:112:LEU:CD2	3:L:130:LEU:HD21	2.31	0.61
3:L:656:LEU:HD23	3:L:656:LEU:H	1.65	0.61
4:M:353:LEU:HA	4:M:371:ARG:HD3	1.83	0.61
8:Q:63:LEU:HD13	8:Q:129:ALA:HB2	1.82	0.61
2:T:130:THR:O	2:T:131:ALA:O	2.17	0.61
4:V:375:PHE:HD1	4:V:407:VAL:HG23	1.65	0.61
7:Y:43:LEU:O	7:Y:138:VAL:HG13	2.00	0.61
2:T:61:MET:HE3	8:Z:88:ARG:HD3	1.83	0.61
3:3:19:VAL:O	3:3:22:ALA:HB3	2.01	0.61
3:3:371:PHE:CE1	3:3:544:LEU:HB3	2.35	0.61
5:5:52:ILE:HG23	5:5:117:GLU:CG	2.29	0.61
5:E:53:VAL:HG22	5:E:55:LEU:CD1	2.30	0.61
6:F:112:ALA:O	6:F:127:VAL:HG23	2.00	0.61
3:L:537:PRO:HB2	3:L:756:GLY:HA2	1.81	0.61
4:M:232:LEU:HD11	4:M:282:GLU:OE1	1.99	0.61
4:M:320:SER:CB	4:M:323:ALA:HB3	2.29	0.61
7:P:114:VAL:HG12	7:P:115:LEU:N	2.15	0.61
3:U:305:ARG:HG2	3:U:306:LEU:N	2.14	0.61
3:U:477:LEU:HD13	3:U:516:VAL:CG1	2.31	0.61
3:U:510:GLY:HA3	3:U:520:ARG:NH2	2.15	0.61
3:3:177:ASP:HB3	3:3:235:LEU:HD22	1.81	0.61
3:3:714:ALA:HB3	3:3:745:ALA:HB2	1.82	0.61
4:4:232:LEU:HD13	4:4:278:VAL:CG1	2.30	0.61
4:4:321:MET:O	4:4:322:GLU:HG2	2.00	0.61
5:5:116:ARG:HG2	5:5:116:ARG:HH11	1.66	0.61
6:6:115:GLY:HA3	6:6:125:GLN:OE1	2.01	0.61
8:7:52:THR:HB	8:7:54:ILE:HG22	1.83	0.61
3:C:52:ILE:HG12	3:C:93:VAL:HG22	1.83	0.61
4:D:381:LEU:HD11	4:D:397:ILE:HG12	1.82	0.61
4:M:190:LEU:O	4:M:194:LEU:HB2	1.99	0.61
4:M:59:ILE:N	4:M:59:ILE:HD13	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:58:LEU:HD12	5:N:59:THR:H	1.66	0.61
6:O:108:MET:HA	6:O:137:VAL:CG1	2.30	0.61
7:P:35:PRO:O	7:P:36:ARG:HB2	2.01	0.61
8:Q:9:LEU:HD11	8:Q:82:ILE:HG22	1.82	0.61
2:T:131:ALA:CB	2:T:132:PRO:CD	2.78	0.61
6:X:37:TRP:CE3	6:X:37:TRP:HA	2.35	0.61
2:2:87:SER:HB3	10:2:182:FES:S2	2.41	0.61
3:3:194:VAL:HB	3:3:195:PRO:HD3	1.82	0.61
3:3:453:PRO:HB2	3:3:750:ARG:NH1	2.14	0.61
4:4:225:PRO:CD	4:4:226:PRO:HD3	2.31	0.61
5:5:187:GLY:C	5:5:189:ARG:H	2.03	0.61
3:C:365:LYS:C	3:C:367:PRO:HD3	2.20	0.61
3:C:6:VAL:CG1	3:C:7:ASN:N	2.58	0.61
4:D:234:LEU:HD23	4:D:234:LEU:H	1.66	0.61
5:E:119:TYR:CD1	5:E:132:LEU:HD21	2.36	0.61
6:F:84:LEU:HD12	6:F:124:VAL:HG21	1.81	0.61
1:J:366:PHE:CE1	1:J:370:LEU:HD21	2.35	0.61
3:L:285:VAL:HG22	3:L:286:ASN:N	2.16	0.61
3:U:169:PRO:HD3	3:U:176:LEU:HD13	1.82	0.61
3:U:233:GLY:O	3:U:236:LEU:HG	2.00	0.61
3:U:413:LEU:HD13	3:U:448:MET:HE2	1.81	0.61
5:W:155:THR:H	6:X:119:ASN:HD22	1.49	0.61
5:W:49:LEU:CB	5:W:77:LEU:HD21	2.21	0.61
1:1:356:CYS:HB3	1:1:358:PRO:HG2	1.82	0.61
3:3:293:ALA:CB	3:3:698:MET:HG2	2.31	0.61
4:4:220:GLY:HA3	4:4:396:ILE:HD11	1.81	0.61
5:5:49:LEU:CB	5:5:77:LEU:HD21	2.25	0.61
8:7:112:LYS:O	8:7:116:PHE:HD1	1.84	0.61
4:4:318:GLU:HB2	8:7:39:ASP:HA	1.82	0.61
3:C:714:ALA:HB3	3:C:745:ALA:HB2	1.81	0.61
4:D:256:GLY:CA	4:D:292:GLN:HE22	2.14	0.61
5:E:75:VAL:HG22	5:E:87:ARG:HG3	1.82	0.61
2:K:136:VAL:HG21	2:K:163:LEU:HD13	1.82	0.61
5:N:50:ALA:CB	5:N:114:LEU:HD21	2.31	0.61
8:Q:82:ILE:HG23	8:Q:95:ALA:HB3	1.82	0.61
3:3:307:LYS:H	3:3:307:LYS:HE2	1.64	0.61
3:3:52:ILE:HG22	3:3:53:GLY:N	2.15	0.61
3:3:751:GLU:O	3:3:753:VAL:HG13	2.01	0.61
4:4:74:THR:CB	4:4:77:GLN:HG3	2.26	0.61
1:A:50:PRO:O	1:A:53:VAL:HG12	2.00	0.61
4:D:240:ARG:CD	4:D:243:GLY:HA3	2.19	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:2:VAL:HG12	3:U:3:ARG:N	2.16	0.61
3:U:73:ILE:HD12	3:U:73:ILE:O	2.00	0.61
4:V:232:LEU:HD13	4:V:278:VAL:CG1	2.30	0.61
4:V:381:LEU:HD11	4:V:397:ILE:HG12	1.82	0.61
4:V:86:ASP:O	4:V:88:LEU:N	2.33	0.61
6:X:108:MET:HA	6:X:137:VAL:CG1	2.30	0.61
3:3:177:ASP:HA	3:3:235:LEU:H	1.65	0.60
3:3:282:VAL:HG13	3:3:286:ASN:O	2.01	0.60
2:B:144:CYS:O	2:B:149:ARG:HD3	2.01	0.60
5:E:64:ARG:HB3	5:E:65:PRO:HD2	1.83	0.60
6:F:114:SER:CB	7:G:97:ARG:HD2	2.30	0.60
1:J:356:CYS:HB3	1:J:358:PRO:HG2	1.82	0.60
2:K:10:PHE:CZ	2:K:33:ARG:HG3	2.36	0.60
5:N:92:VAL:HG23	5:N:92:VAL:O	2.01	0.60
3:U:411:LEU:O	3:U:414:SER:HB3	2.01	0.60
4:V:159:LEU:O	4:V:162:TRP:HB2	2.00	0.60
3:3:341:VAL:HB	3:3:364:LEU:HD21	1.81	0.60
4:4:227:GLU:HG3	4:4:268:GLU:O	2.01	0.60
2:B:59:GLU:O	2:B:63:VAL:HG23	2.00	0.60
3:C:2:VAL:CG1	3:C:89:ASP:HA	2.31	0.60
5:E:195:LEU:N	5:E:195:LEU:HD13	2.15	0.60
8:H:87:PRO:O	8:H:89:ALA:N	2.32	0.60
3:L:747:VAL:HG23	3:L:747:VAL:O	2.02	0.60
6:O:163:TYR:HA	6:O:170:LEU:HB2	1.83	0.60
7:Y:96:LEU:HD21	7:Y:129:LEU:HD12	1.82	0.60
1:1:438:ARG:HD2	1:1:438:ARG:N	2.16	0.60
3:3:20:MET:HE3	3:3:32:LEU:HD21	1.82	0.60
3:3:453:PRO:HB2	3:3:750:ARG:HH12	1.66	0.60
3:3:655:ARG:HH11	3:3:655:ARG:HG3	1.65	0.60
3:C:174:VAL:HG21	3:C:296:PHE:CZ	2.37	0.60
4:D:231:ASP:HA	4:D:235:THR:HG23	1.83	0.60
4:D:240:ARG:NH1	5:E:78:PRO:HD2	2.16	0.60
4:D:218:ALA:HB3	4:D:272:VAL:HG21	1.83	0.60
6:F:37:TRP:HA	6:F:37:TRP:CE3	2.35	0.60
8:H:63:LEU:HD13	8:H:129:ALA:HB2	1.82	0.60
1:J:36:GLY:O	1:J:37:GLY:O	2.19	0.60
4:M:256:GLY:CA	4:M:292:GLN:HE22	2.13	0.60
4:M:367:ARG:HG2	4:M:367:ARG:NH1	2.16	0.60
3:U:101:ARG:HH12	3:U:140:TYR:HD1	1.48	0.60
3:U:13:VAL:HG21	3:U:17:THR:HG21	1.82	0.60
3:U:177:ASP:HB3	3:U:235:LEU:HD22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:95:LEU:HA	4:V:173:ILE:HD13	1.82	0.60
2:2:26:ALA:O	2:2:30:LEU:HG	2.01	0.60
3:3:293:ALA:HB2	3:3:698:MET:HG2	1.82	0.60
3:3:25:HIS:ND1	3:3:427:ASN:HB2	2.17	0.60
3:3:650:VAL:HG12	3:3:651:ARG:N	2.16	0.60
3:3:724:ARG:HD2	3:3:724:ARG:H	1.65	0.60
1:A:436:LEU:HD23	2:B:90:LEU:HA	1.82	0.60
4:D:375:PHE:HD1	4:D:407:VAL:HG23	1.66	0.60
5:E:121:LEU:HD12	5:E:121:LEU:H	1.65	0.60
8:H:37:PHE:HD1	8:H:53:THR:O	1.84	0.60
1:J:174:HIS:CD2	1:J:192:LEU:HG	2.36	0.60
2:K:130:THR:O	2:K:131:ALA:O	2.18	0.60
1:J:435:SER:HA	2:K:95:GLU:OE2	2.01	0.60
3:L:501:LYS:HD2	3:L:501:LYS:N	2.07	0.60
4:M:232:LEU:HD13	4:M:278:VAL:CG1	2.30	0.60
4:M:379:GLN:OE1	5:N:115:GLU:HB2	2.00	0.60
1:S:344:LEU:O	1:S:347:PHE:HB3	2.02	0.60
3:U:254:THR:HG1	3:U:624:LEU:HD23	1.67	0.60
4:V:119:ILE:O	4:V:123:LEU:HB2	2.01	0.60
2:2:144:CYS:O	2:2:149:ARG:HD3	2.02	0.60
3:3:402:PRO:HD2	3:3:458:LEU:HD13	1.82	0.60
3:3:414:SER:HA	3:3:461:TRP:CZ3	2.35	0.60
4:4:237:GLY:O	4:4:239:LEU:HG	2.01	0.60
4:4:353:LEU:HA	4:4:371:ARG:HD3	1.82	0.60
1:A:26:SER:HB3	1:A:31:TYR:CD1	2.36	0.60
5:E:33:ARG:O	5:E:37:GLU:HB2	2.01	0.60
6:F:163:TYR:HA	6:F:170:LEU:HB2	1.84	0.60
7:G:71:GLU:HB2	7:G:90:VAL:HB	1.83	0.60
2:K:116:LEU:HD23	2:K:116:LEU:H	1.65	0.60
2:K:87:SER:HB3	10:K:182:FES:S2	2.42	0.60
4:M:244:VAL:CG1	4:M:246:TYR:CD1	2.85	0.60
4:M:393:MET:O	4:M:396:ILE:HG22	2.01	0.60
6:O:114:SER:C	6:O:116:GLY:H	2.04	0.60
3:U:564:LEU:HD21	3:U:581:ARG:HD2	1.82	0.60
5:W:195:LEU:HD22	5:W:195:LEU:H	1.67	0.60
5:W:3:LEU:HD22	5:W:44:MET:SD	2.41	0.60
3:3:451:PHE:HE1	3:3:466:GLU:HB2	1.66	0.60
4:4:229:ALA:HB1	4:4:241:ALA:O	2.00	0.60
5:5:47:ASN:CB	5:5:77:LEU:HG	2.30	0.60
5:5:53:VAL:HG22	5:5:55:LEU:HD12	1.84	0.60
1:A:20:HIS:O	1:A:22:GLY:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:O	1:A:347:PHE:HB3	2.00	0.60
3:C:282:VAL:HG13	3:C:286:ASN:O	2.02	0.60
4:D:219:ARG:O	4:D:221:VAL:N	2.34	0.60
3:L:305:ARG:HG2	3:L:306:LEU:N	2.16	0.60
4:M:103:LYS:CB	5:N:22:LEU:HD13	2.28	0.60
6:O:155:GLN:O	6:O:158:VAL:HG22	2.02	0.60
6:O:117:MET:HB3	7:P:99:ILE:HD13	1.82	0.60
3:U:239:THR:HG21	3:U:298:HIS:HE1	1.65	0.60
3:U:413:LEU:HD13	3:U:448:MET:HE1	1.82	0.60
3:U:616:ASN:HD22	3:U:622:LEU:HD11	1.66	0.60
4:V:229:ALA:HB3	4:V:241:ALA:HA	1.84	0.60
5:W:60:TYR:CD1	5:W:61:PRO:HD2	2.36	0.60
2:2:116:LEU:H	2:2:116:LEU:HD23	1.66	0.60
4:4:218:ALA:HB3	4:4:272:VAL:HG21	1.84	0.60
5:5:124:ILE:HG22	5:5:146:LEU:H	1.66	0.60
5:5:37:GLU:O	5:5:41:TYR:HD1	1.84	0.60
8:7:63:LEU:HD13	8:7:129:ALA:HB2	1.84	0.60
5:E:43:ALA:C	5:E:45:GLY:N	2.52	0.60
2:K:27:ILE:HG13	2:K:53:VAL:HG21	1.84	0.60
4:M:115:THR:HG21	4:M:297:LEU:HD23	1.83	0.60
4:M:133:LEU:HD21	4:M:204:TYR:CE2	2.36	0.60
5:N:11:ARG:N	5:N:11:ARG:HD2	2.17	0.60
3:U:30:VAL:HG22	3:U:48:CYS:HA	1.84	0.60
4:V:257:TYR:HD1	4:V:257:TYR:N	2.00	0.60
5:W:116:ARG:HG2	5:W:116:ARG:HH11	1.67	0.60
5:W:43:ALA:C	5:W:45:GLY:N	2.51	0.60
4:V:62:LEU:HD21	6:X:43:LEU:HB3	1.84	0.60
2:T:102:GLU:HA	8:Z:108:ILE:HD11	1.83	0.60
4:4:232:LEU:HD11	4:4:282:GLU:OE1	2.01	0.60
5:5:44:MET:HE2	5:5:82:ASP:HB3	1.83	0.60
1:A:201:LEU:CG	1:A:203:PRO:HD2	2.27	0.60
5:E:121:LEU:HB3	5:E:127:GLU:CG	2.32	0.60
7:G:73:ALA:HB2	7:G:89:LYS:HB2	1.84	0.60
1:J:192:LEU:C	1:J:192:LEU:HD23	2.21	0.60
3:L:369:LEU:CD2	3:L:369:LEU:H	2.15	0.60
7:P:118:ASP:HA	7:P:161:TYR:CE2	2.36	0.60
1:S:323:LEU:HD23	1:S:324:GLY:N	2.17	0.60
1:S:434:PRO:HG2	1:S:436:LEU:CD1	2.32	0.60
6:X:164:ASN:N	6:X:170:LEU:HD12	2.17	0.60
3:3:527:ARG:HB3	3:3:530:ALA:HB2	1.83	0.60
3:3:307:LYS:HB3	3:3:632:GLY:CA	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:237:ASP:OD1	3:C:239:THR:HG22	2.00	0.60
4:D:266:LEU:HD13	4:D:281:ARG:CB	2.15	0.60
5:E:25:LEU:CD2	5:E:25:LEU:H	2.13	0.60
3:L:413:LEU:HA	3:L:416:PHE:HB3	1.84	0.60
3:L:474:ARG:HA	3:L:516:VAL:HG13	1.83	0.60
4:M:393:MET:C	4:M:396:ILE:HG22	2.22	0.60
5:N:187:GLY:C	5:N:189:ARG:H	2.04	0.60
6:O:83:ARG:HA	6:O:111:CYS:HB3	1.84	0.60
7:P:175:ALA:HB1	7:P:176:PRO:HD2	1.82	0.60
4:V:221:VAL:O	4:V:223:VAL:N	2.34	0.60
2:2:40:TRP:HE1	2:2:74:PRO:HG3	1.67	0.60
3:3:239:THR:HG21	3:3:298:HIS:HE1	1.67	0.60
4:4:95:LEU:HA	4:4:173:ILE:HD13	1.84	0.60
3:C:650:VAL:HG12	3:C:651:ARG:N	2.17	0.60
4:D:191:LYS:HZ2	3:U:730:GLU:CG	2.15	0.60
4:D:223:VAL:HG22	4:D:226:PRO:O	2.01	0.60
4:D:252:TYR:HE2	4:D:346:THR:HA	1.67	0.60
7:G:44:THR:OG1	7:G:52:LYS:HD2	2.02	0.60
3:L:409:LEU:HD12	3:L:535:MET:HE2	1.84	0.60
3:L:438:LYS:O	3:L:441:MET:HG3	2.01	0.60
3:U:402:PRO:HD2	3:U:458:LEU:HD13	1.83	0.60
3:U:545:GLU:HA	3:U:550:LEU:HD11	1.83	0.60
3:3:269:THR:HG22	3:3:274:LEU:HA	1.82	0.59
4:4:196:VAL:C	4:4:198:PRO:HD2	2.22	0.59
4:4:322:GLU:O	4:4:325:ILE:N	2.34	0.59
5:5:3:LEU:HD22	5:5:44:MET:SD	2.42	0.59
8:7:82:ILE:HG23	8:7:95:ALA:HB3	1.84	0.59
1:A:40:THR:O	1:A:44:VAL:HG23	2.02	0.59
1:A:86:GLN:OE1	1:A:128:THR:HG23	2.03	0.59
3:C:286:ASN:HD22	3:C:287:GLU:N	2.00	0.59
3:C:216:PHE:HZ	8:H:128:PHE:CD2	2.20	0.59
3:L:402:PRO:HA	3:L:535:MET:HE1	1.84	0.59
3:L:719:HIS:HB2	3:L:720:PRO:HD3	1.82	0.59
4:M:168:PHE:HA	4:M:170:HIS:CE1	2.36	0.59
4:M:196:VAL:C	4:M:198:PRO:HD2	2.22	0.59
4:M:228:VAL:HG11	4:M:274:ASP:HB2	1.84	0.59
6:O:37:TRP:HA	6:O:37:TRP:HE3	1.66	0.59
3:3:333:LEU:HD13	3:3:648:LEU:HD21	1.84	0.59
2:T:10:PHE:CZ	2:T:33:ARG:HG3	2.37	0.59
4:V:42:ARG:HD3	4:V:42:ARG:N	2.17	0.59
4:V:59:ILE:N	4:V:59:ILE:HD13	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:50:ALA:HB1	5:W:114:LEU:HD21	1.83	0.59
5:W:195:LEU:N	5:W:195:LEU:HD13	2.16	0.59
3:3:340:GLU:HG2	3:3:368:HIS:NE2	2.17	0.59
5:5:50:ALA:CB	5:5:114:LEU:HD21	2.32	0.59
5:5:139:GLU:CG	5:5:140:ASP:N	2.63	0.59
5:5:174:LEU:HD21	5:5:180:GLY:HA2	1.83	0.59
3:C:282:VAL:O	3:C:286:ASN:O	2.21	0.59
4:D:196:VAL:C	4:D:198:PRO:HD2	2.23	0.59
5:E:22:LEU:O	5:E:24:ASN:N	2.32	0.59
7:G:118:ASP:HA	7:G:161:TYR:CE2	2.38	0.59
4:M:228:VAL:HG22	4:M:268:GLU:O	2.01	0.59
4:V:316:LEU:HD13	4:V:320:SER:HB2	1.84	0.59
5:W:11:ARG:N	5:W:11:ARG:HD2	2.17	0.59
2:2:131:ALA:HB1	2:2:132:PRO:HD2	1.84	0.59
3:3:343:LEU:O	3:3:369:LEU:HA	2.03	0.59
3:3:459:MET:HG3	3:3:465:HIS:HB2	1.84	0.59
5:5:125:VAL:HG12	5:5:126:PHE:N	2.16	0.59
3:C:166:LYS:CG	3:C:178:ARG:HG3	2.32	0.59
3:C:340:GLU:HG2	3:C:368:HIS:NE2	2.16	0.59
3:C:748:VAL:HG23	3:C:752:ASP:OD1	2.03	0.59
4:D:225:PRO:HB2	4:D:226:PRO:HD3	1.84	0.59
8:H:112:LYS:HG2	8:H:116:PHE:CE1	2.38	0.59
2:K:40:TRP:NE1	2:K:74:PRO:HG3	2.18	0.59
4:M:225:PRO:HB2	4:M:226:PRO:HD3	1.83	0.59
4:M:99:LEU:HD13	4:M:102:GLU:OE1	2.03	0.59
6:O:174:ALA:O	6:O:175:ALA:HB2	2.03	0.59
4:M:62:LEU:HD21	6:O:43:LEU:HB3	1.83	0.59
4:V:133:LEU:HD21	4:V:204:TYR:CE2	2.36	0.59
4:4:285:GLU:O	4:4:289:ILE:HG12	2.03	0.59
4:4:369:LYS:HG2	5:5:53:VAL:HB	1.84	0.59
4:4:371:ARG:NH2	4:4:376:VAL:HG21	2.17	0.59
1:A:438:ARG:N	1:A:438:ARG:HD2	2.18	0.59
2:B:106:ILE:HD11	2:B:112:THR:CB	2.31	0.59
3:C:194:VAL:HB	3:C:195:PRO:HD3	1.84	0.59
3:C:239:THR:HG21	3:C:298:HIS:HE1	1.67	0.59
4:D:333:GLU:OE1	5:E:189:ARG:NH1	2.35	0.59
4:D:353:LEU:HA	4:D:371:ARG:HD3	1.83	0.59
4:D:408:ASP:O	4:D:409:ARG:C	2.41	0.59
6:F:48:ILE:HD12	6:F:48:ILE:N	2.16	0.59
1:J:110:VAL:N	1:J:111:PRO:CD	2.65	0.59
1:J:86:GLN:OE1	1:J:128:THR:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:169:PRO:HD3	3:L:176:LEU:HD13	1.85	0.59
3:L:545:GLU:HA	3:L:550:LEU:HD11	1.85	0.59
1:S:9:LEU:HD23	1:S:10:ASP:N	2.18	0.59
3:U:254:THR:OG1	3:U:624:LEU:HD23	2.02	0.59
1:1:36:GLY:O	1:1:37:GLY:O	2.20	0.59
3:3:81:ALA:HB3	3:3:84:VAL:HG22	1.84	0.59
4:4:193:LEU:O	4:4:193:LEU:HD23	2.03	0.59
5:5:119:TYR:CD1	5:5:132:LEU:HD21	2.38	0.59
6:6:112:ALA:O	6:6:127:VAL:HG23	2.02	0.59
3:C:285:VAL:HG22	3:C:286:ASN:N	2.16	0.59
5:E:187:GLY:C	5:E:189:ARG:H	2.06	0.59
1:J:271:THR:HG1	1:J:273:ARG:HB3	1.68	0.59
1:J:277:TYR:CE1	1:J:283:PRO:HD3	2.38	0.59
1:J:344:LEU:O	1:J:347:PHE:HB3	2.01	0.59
4:M:144:THR:HB	4:M:145:PRO:HD3	1.83	0.59
4:M:227:GLU:HG3	4:M:268:GLU:O	2.02	0.59
5:N:139:GLU:CG	5:N:140:ASP:N	2.63	0.59
6:O:174:ALA:O	6:O:175:ALA:CB	2.50	0.59
8:Q:121:ARG:HH11	8:Q:121:ARG:HG3	1.68	0.59
1:S:11:PRO:HB2	1:S:274:GLU:CD	2.22	0.59
3:U:186:ARG:HD2	3:U:231:PRO:HD3	1.83	0.59
3:U:174:VAL:HG21	3:U:296:PHE:CZ	2.36	0.59
3:U:32:LEU:O	3:U:33:PHE:HD1	1.85	0.59
3:U:748:VAL:CG1	3:U:748:VAL:O	2.49	0.59
4:V:96:ALA:HB2	4:V:346:THR:HG21	1.83	0.59
1:1:11:PRO:CB	1:1:270:THR:HB	2.16	0.59
4:4:393:MET:O	4:4:393:MET:HG2	2.03	0.59
5:5:43:ALA:C	5:5:45:GLY:N	2.55	0.59
8:7:9:LEU:HD11	8:7:82:ILE:HG22	1.84	0.59
3:C:733:GLN:HA	3:C:745:ALA:O	2.02	0.59
4:D:249:ARG:HH22	5:E:87:ARG:CB	2.15	0.59
5:E:155:THR:O	6:F:119:ASN:ND2	2.34	0.59
3:L:510:GLY:HA3	3:L:520:ARG:NH2	2.17	0.59
5:N:121:LEU:H	5:N:121:LEU:CD1	2.15	0.59
7:P:33:LEU:HD22	7:P:37:PHE:CD2	2.38	0.59
3:U:2:VAL:CG1	3:U:89:ASP:HA	2.30	0.59
5:W:71:VAL:HG11	5:W:89:PHE:HD2	1.68	0.59
3:3:186:ARG:HD2	3:3:231:PRO:HD3	1.83	0.59
3:3:365:LYS:C	3:3:367:PRO:HD3	2.23	0.59
4:4:188:PRO:O	4:4:191:LYS:HB2	2.02	0.59
1:A:323:LEU:HD23	1:A:324:GLY:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:THR:OG1	2:B:149:ARG:HB2	2.02	0.59
3:C:413:LEU:HA	3:C:416:PHE:HB3	1.85	0.59
3:C:510:GLY:HA3	3:C:520:ARG:NH2	2.17	0.59
3:C:581:ARG:O	3:C:599:HIS:CE1	2.56	0.59
4:D:200:ARG:O	4:D:200:ARG:CG	2.51	0.59
1:J:438:ARG:HD2	1:J:438:ARG:N	2.17	0.59
4:M:346:THR:HG22	4:M:353:LEU:O	2.02	0.59
3:U:194:VAL:HB	3:U:195:PRO:CD	2.32	0.59
3:U:510:GLY:CA	3:U:520:ARG:HH22	2.15	0.59
3:U:81:ALA:HB3	3:U:84:VAL:HG22	1.83	0.59
6:X:164:ASN:O	7:Y:148:ARG:HD2	2.03	0.59
8:Z:121:ARG:HH11	8:Z:121:ARG:HG3	1.67	0.59
1:1:266:LEU:HB3	1:1:267:PRO:HD2	1.84	0.59
3:3:561:PRO:HB3	3:3:576:ALA:CA	2.32	0.59
1:A:337:MET:O	1:A:341:MET:HG2	2.02	0.59
6:F:148:ILE:O	6:F:151:VAL:HG22	2.03	0.59
3:L:2:VAL:CG1	3:L:89:ASP:HA	2.33	0.59
4:M:220:GLY:HA3	4:M:396:ILE:HD11	1.83	0.59
1:S:88:TYR:HB2	1:S:216:THR:CG2	2.31	0.59
4:V:237:GLY:HA3	5:W:112:ASN:CA	2.32	0.59
4:V:115:THR:HG21	4:V:297:LEU:HD23	1.84	0.59
5:W:175:THR:O	5:W:177:LYS:N	2.35	0.59
6:X:145:GLU:HG2	7:Y:31:VAL:CG2	2.33	0.59
3:3:218:LEU:N	3:3:219:PRO:HD3	2.17	0.59
3:3:612:GLY:O	3:3:624:LEU:HB2	2.02	0.59
4:4:156:ILE:O	4:4:159:LEU:HB2	2.03	0.59
4:4:228:VAL:HG11	4:4:274:ASP:HB2	1.85	0.59
5:5:195:LEU:H	5:5:195:LEU:HD22	1.68	0.59
3:C:473:GLU:O	3:C:477:LEU:HD12	2.03	0.59
4:D:64:THR:HG23	6:F:123:ILE:HD12	1.85	0.59
7:G:150:ALA:HA	7:G:153:THR:HB	1.85	0.59
3:L:132:ASP:O	3:L:136:GLU:HG3	2.03	0.59
3:L:52:ILE:HG22	3:L:53:GLY:N	2.16	0.59
4:V:257:TYR:CD1	4:V:257:TYR:N	2.71	0.59
4:V:84:ARG:O	6:X:83:ARG:NH2	2.36	0.59
1:1:242:GLY:HA2	1:1:268:MET:O	2.03	0.58
1:1:277:TYR:CE1	1:1:283:PRO:HD3	2.38	0.58
5:5:58:LEU:HD12	5:5:59:THR:H	1.68	0.58
1:A:203:PRO:HB2	1:A:204:PRO:HD3	1.86	0.58
5:E:65:PRO:HB2	5:E:93:TYR:HD2	1.67	0.58
1:J:315:HIS:O	1:J:319:LYS:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:218:LEU:N	3:L:219:PRO:HD3	2.17	0.58
4:M:223:VAL:HG13	4:M:226:PRO:O	2.02	0.58
4:M:105:LEU:HD23	4:M:337:PRO:HG3	1.84	0.58
4:M:70:MET:C	4:M:72:HIS:H	2.06	0.58
1:S:376:THR:HG22	1:S:376:THR:O	2.02	0.58
2:T:139:GLU:CB	2:T:140:PRO:HD2	2.18	0.58
3:U:166:LYS:HG3	3:U:178:ARG:HG3	1.85	0.58
6:X:48:ILE:N	6:X:48:ILE:HD12	2.18	0.58
7:Y:35:PRO:O	7:Y:36:ARG:HB2	2.03	0.58
1:1:201:LEU:CG	1:1:203:PRO:HD2	2.25	0.58
2:2:130:THR:HG21	2:2:143:GLU:OE1	2.02	0.58
1:A:11:PRO:CB	1:A:270:THR:HB	2.17	0.58
3:C:369:LEU:HD12	3:C:549:VAL:HG13	1.84	0.58
3:C:564:LEU:HD21	3:C:581:ARG:HD2	1.84	0.58
4:D:317:LEU:N	4:D:317:LEU:CD1	2.66	0.58
2:K:27:ILE:HG22	2:K:31:LEU:HD23	1.84	0.58
4:M:125:ARG:HH11	4:M:125:ARG:HG3	1.67	0.58
3:U:216:PHE:CD2	8:Z:63:LEU:HD23	2.37	0.58
3:U:340:GLU:H	3:U:366:THR:HB	1.68	0.58
4:V:219:ARG:O	4:V:221:VAL:N	2.37	0.58
7:Y:118:ASP:HA	7:Y:161:TYR:CE2	2.38	0.58
1:1:29:LEU:O	1:1:29:LEU:HD23	2.03	0.58
1:1:434:PRO:HG2	1:1:436:LEU:CD1	2.33	0.58
3:3:52:ILE:CG2	3:3:53:GLY:N	2.66	0.58
3:3:581:ARG:O	3:3:599:HIS:CE1	2.56	0.58
4:4:125:ARG:HH11	4:4:125:ARG:HG3	1.67	0.58
5:5:116:ARG:HA	5:5:119:TYR:CD2	2.39	0.58
1:A:374:ILE:HA	1:A:379:GLY:HA3	1.85	0.58
3:C:524:LEU:CG	3:C:525:ALA:N	2.65	0.58
3:C:603:PRO:HG2	3:C:634:ALA:CB	2.32	0.58
4:D:350:ARG:NH1	4:D:401:ASP:OD2	2.36	0.58
6:F:159:ARG:HB3	6:F:161:GLN:HG3	1.85	0.58
7:G:96:LEU:HD21	7:G:129:LEU:HD12	1.84	0.58
8:H:52:THR:HB	8:H:54:ILE:HG22	1.86	0.58
1:J:376:THR:HG22	1:J:376:THR:O	2.04	0.58
3:L:564:LEU:CD1	3:L:581:ARG:H	2.15	0.58
4:M:313:PRO:C	4:M:315:HIS:H	2.06	0.58
5:N:104:VAL:C	5:N:106:ASP:H	2.06	0.58
1:S:40:THR:O	1:S:44:VAL:HG23	2.04	0.58
3:U:355:LEU:HD22	3:U:664:LEU:HD23	1.84	0.58
3:U:603:PRO:HG2	3:U:634:ALA:HB1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:537:PRO:HB2	3:U:756:GLY:HA2	1.83	0.58
4:V:190:LEU:O	4:V:194:LEU:HB2	2.04	0.58
4:V:346:THR:HG22	4:V:353:LEU:O	2.03	0.58
6:X:83:ARG:HA	6:X:111:CYS:HB3	1.85	0.58
2:2:153:LEU:C	2:2:153:LEU:HD13	2.24	0.58
3:3:386:SER:HB3	3:3:389:ASP:OD2	2.04	0.58
4:4:231:ASP:HA	4:4:235:THR:HG23	1.85	0.58
3:C:616:ASN:HD22	3:C:622:LEU:HD11	1.68	0.58
5:E:195:LEU:HD22	5:E:195:LEU:H	1.67	0.58
3:L:578:LYS:HB3	3:L:578:LYS:NZ	2.18	0.58
3:L:73:ILE:HD12	3:L:73:ILE:O	2.02	0.58
5:N:42:LYS:HA	5:N:45:GLY:HA2	1.86	0.58
8:Q:92:HIS:C	8:Q:93:LEU:HD12	2.22	0.58
1:S:242:GLY:HA2	1:S:268:MET:O	2.04	0.58
3:U:218:LEU:N	3:U:219:PRO:HD3	2.18	0.58
3:U:52:ILE:HG22	3:U:53:GLY:N	2.18	0.58
4:V:252:TYR:HE2	4:V:346:THR:HA	1.68	0.58
4:V:64:THR:HG22	4:V:64:THR:O	2.02	0.58
5:W:116:ARG:HA	5:W:119:TYR:CD2	2.39	0.58
1:1:174:HIS:CD2	1:1:192:LEU:HG	2.38	0.58
3:3:382:PHE:N	3:3:382:PHE:CD1	2.71	0.58
4:4:256:GLY:HA2	4:4:292:GLN:NE2	2.18	0.58
5:5:22:LEU:O	5:5:24:ASN:N	2.31	0.58
3:C:33:PHE:CZ	3:C:130:LEU:HA	2.37	0.58
6:F:145:GLU:N	6:F:145:GLU:OE1	2.26	0.58
4:M:200:ARG:CG	4:M:200:ARG:O	2.51	0.58
1:S:438:ARG:HD2	1:S:438:ARG:N	2.16	0.58
3:U:269:THR:HG22	3:U:274:LEU:HA	1.86	0.58
3:U:38:HIS:NE2	3:U:287:GLU:HG2	2.18	0.58
3:U:567:TYR:HA	3:U:584:VAL:HG23	1.86	0.58
3:U:746:ARG:O	3:U:748:VAL:N	2.36	0.58
6:X:26:LYS:C	6:X:26:LYS:HD2	2.24	0.58
5:5:92:VAL:O	5:5:92:VAL:HG23	2.04	0.58
1:A:291:ILE:HD11	1:A:331:ILE:HD11	1.85	0.58
3:C:652:PRO:O	3:C:654:PHE:N	2.37	0.58
4:D:237:GLY:HA3	5:E:112:ASN:CA	2.32	0.58
2:K:47:GLU:O	2:K:50:ALA:HB3	2.03	0.58
3:L:724:ARG:H	3:L:724:ARG:HD2	1.68	0.58
3:L:732:ALA:O	3:L:746:ARG:HA	2.03	0.58
4:M:52:VAL:HG11	4:M:388:GLU:O	2.03	0.58
6:O:164:ASN:H	6:O:170:LEU:HD12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:116:LEU:HD23	2:T:116:LEU:H	1.68	0.58
3:U:25:HIS:ND1	3:U:427:ASN:HB2	2.18	0.58
3:U:473:GLU:O	3:U:477:LEU:HD12	2.02	0.58
3:U:701:ALA:H	3:U:754:PRO:HB3	1.67	0.58
1:1:435:SER:HA	2:2:95:GLU:OE2	2.03	0.58
3:3:616:ASN:OD1	3:3:617:LEU:N	2.37	0.58
4:4:223:VAL:HA	4:4:226:PRO:O	2.03	0.58
2:B:102:GLU:HA	8:H:108:ILE:HD11	1.83	0.58
3:C:171:SER:C	3:C:173:PHE:H	2.07	0.58
3:C:374:ARG:NH2	3:C:684:ARG:HG3	2.19	0.58
4:D:225:PRO:CD	4:D:239:LEU:HG	2.34	0.58
4:D:379:GLN:OE1	5:E:115:GLU:HB2	2.03	0.58
4:D:47:LEU:H	4:D:47:LEU:HD12	1.68	0.58
4:M:96:ALA:HB2	4:M:346:THR:HG21	1.85	0.58
4:M:64:THR:HG23	6:O:123:ILE:HD12	1.85	0.58
3:U:477:LEU:HD21	3:U:520:ARG:HG2	1.85	0.58
3:U:714:ALA:HB3	3:U:745:ALA:HB2	1.84	0.58
6:X:114:SER:C	6:X:116:GLY:H	2.05	0.58
7:Y:101:CYS:O	7:Y:103:LEU:N	2.37	0.58
1:1:344:LEU:O	1:1:347:PHE:HB3	2.04	0.58
3:3:312:ARG:HA	3:3:316:ARG:O	2.03	0.58
4:4:350:ARG:NH1	4:4:401:ASP:OD2	2.37	0.58
8:7:67:PHE:CZ	8:7:123:ARG:HG3	2.39	0.58
7:9:33:LEU:HD22	7:9:37:PHE:CD2	2.39	0.58
2:B:40:TRP:NE1	2:B:74:PRO:HG3	2.18	0.58
2:B:90:LEU:H	2:B:90:LEU:HD12	1.69	0.58
4:D:188:PRO:O	4:D:191:LYS:HB2	2.03	0.58
4:D:220:GLY:HA2	4:D:384:ALA:O	2.03	0.58
5:E:124:ILE:CG2	5:E:146:LEU:HB2	2.30	0.58
3:L:233:GLY:O	3:L:236:LEU:HG	2.04	0.58
3:L:748:VAL:O	3:L:748:VAL:CG1	2.51	0.58
4:M:49:GLY:HA2	4:M:53:LEU:HD12	1.86	0.58
4:M:237:GLY:HA3	5:N:112:ASN:CA	2.34	0.58
7:P:101:CYS:SG	7:P:101:CYS:O	2.62	0.58
1:S:36:GLY:O	1:S:37:GLY:O	2.21	0.58
3:U:340:GLU:HG2	3:U:368:HIS:NE2	2.18	0.58
4:V:234:LEU:HD23	4:V:234:LEU:H	1.67	0.58
5:W:104:VAL:HG12	5:W:104:VAL:O	2.04	0.58
6:X:84:LEU:O	6:X:124:VAL:HG23	2.04	0.58
1:1:301:PRO:O	1:1:306:VAL:HG21	2.04	0.58
3:3:477:LEU:HD22	3:3:520:ARG:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:220:GLY:O	4:4:271:ASP:HB3	2.03	0.58
3:C:7:ASN:HD21	3:C:96:LEU:HD11	1.68	0.58
5:E:44:MET:CE	5:E:82:ASP:HB3	2.34	0.58
7:G:35:PRO:HD3	7:G:164:PRO:CG	2.34	0.58
8:H:112:LYS:O	8:H:116:PHE:HD1	1.87	0.58
3:L:340:GLU:H	3:L:366:THR:HB	1.69	0.58
3:L:731:GLY:H	3:L:747:VAL:CG1	2.08	0.58
4:M:220:GLY:HA2	4:M:384:ALA:O	2.03	0.58
4:M:234:LEU:CD1	5:N:49:LEU:HD21	2.32	0.58
5:N:60:TYR:CD1	5:N:61:PRO:HD2	2.39	0.58
1:S:10:ASP:CB	1:S:11:PRO:CD	2.71	0.58
2:T:57:PRO:HD2	3:U:215:ASP:OD1	2.02	0.58
3:U:33:PHE:CZ	3:U:130:LEU:HA	2.38	0.58
3:U:375:THR:HA	3:U:512:LEU:CD1	2.34	0.58
3:U:581:ARG:O	3:U:599:HIS:CE1	2.56	0.58
4:V:266:LEU:HD13	4:V:281:ARG:CB	2.18	0.58
1:1:12:ARG:NE	1:1:12:ARG:O	2.35	0.58
1:1:192:LEU:C	1:1:192:LEU:HD23	2.24	0.58
2:2:146:THR:OG1	2:2:149:ARG:HB2	2.04	0.58
2:2:27:ILE:HG13	2:2:53:VAL:HG21	1.86	0.58
3:3:402:PRO:HA	3:3:535:MET:HE1	1.86	0.58
5:5:175:THR:O	5:5:177:LYS:N	2.36	0.58
5:5:91:ARG:HD3	5:5:93:TYR:HE1	1.69	0.58
3:C:517:ALA:HA	3:C:520:ARG:CD	2.32	0.58
3:C:747:VAL:O	3:C:747:VAL:HG23	2.03	0.58
5:E:31:ARG:NH1	5:E:31:ARG:HG2	2.19	0.58
5:E:3:LEU:N	5:E:3:LEU:HD23	2.17	0.58
6:F:41:PHE:HE2	6:F:92:MET:HB2	1.68	0.58
7:G:141:VAL:CG1	7:G:142:GLY:H	2.14	0.58
1:J:323:LEU:HD23	1:J:324:GLY:N	2.19	0.58
2:K:114:ASP:HB2	2:K:116:LEU:HD21	1.84	0.58
2:K:89:LYS:HE3	2:K:94:GLU:OE1	2.04	0.58
3:L:514:ASP:HB2	3:L:683:LEU:HD12	1.85	0.58
5:N:65:PRO:HD2	5:N:93:TYR:CE2	2.39	0.58
5:N:91:ARG:HD3	5:N:93:TYR:HE1	1.69	0.58
1:S:201:LEU:CG	1:S:203:PRO:HD2	2.25	0.58
3:U:430:THR:HG23	3:U:431:PRO:HD2	1.86	0.58
4:V:200:ARG:O	4:V:204:TYR:CD1	2.57	0.58
8:Z:38:PRO:C	8:Z:40:PHE:H	2.06	0.58
1:1:376:THR:O	1:1:376:THR:HG22	2.04	0.57
2:2:41:ILE:HD12	2:2:70:TYR:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:64:GLY:O	8:7:65:GLU:C	2.43	0.57
6:6:153:GLN:HG3	7:9:124:TYR:OH	2.04	0.57
2:B:87:SER:HB3	10:B:182:FES:S2	2.43	0.57
3:C:173:PHE:CZ	3:C:296:PHE:HB2	2.39	0.57
4:D:220:GLY:O	4:D:271:ASP:HB3	2.04	0.57
2:K:116:LEU:HD23	2:K:116:LEU:N	2.19	0.57
3:L:340:GLU:HG2	3:L:368:HIS:NE2	2.19	0.57
3:L:453:PRO:HB2	3:L:750:ARG:NH2	2.19	0.57
5:N:75:VAL:CG2	5:N:87:ARG:HG3	2.34	0.57
1:S:13:PHE:CD1	1:S:13:PHE:C	2.78	0.57
3:U:243:ARG:HD3	3:U:275:LEU:CD1	2.34	0.57
4:V:220:GLY:HA3	4:V:396:ILE:HD11	1.84	0.57
4:V:353:LEU:HA	4:V:371:ARG:HD3	1.86	0.57
4:V:381:LEU:HA	4:V:384:ALA:HB3	1.86	0.57
5:W:55:LEU:HD12	5:W:55:LEU:N	2.18	0.57
1:1:267:PRO:HG2	1:1:270:THR:HG22	1.86	0.57
3:3:413:LEU:HA	3:3:416:PHE:HB3	1.85	0.57
4:4:225:PRO:HB2	4:4:226:PRO:HD3	1.85	0.57
4:4:381:LEU:HD11	4:4:397:ILE:HG12	1.85	0.57
5:5:104:VAL:C	5:5:106:ASP:H	2.07	0.57
6:6:114:SER:C	6:6:116:GLY:H	2.07	0.57
1:A:429:ARG:HG3	3:U:316:ARG:NH1	2.19	0.57
3:C:340:GLU:H	3:C:366:THR:HB	1.69	0.57
5:E:11:ARG:N	5:E:11:ARG:HD2	2.20	0.57
5:E:48:PHE:C	5:E:50:ALA:N	2.57	0.57
6:F:114:SER:C	6:F:116:GLY:H	2.08	0.57
7:G:123:ASP:CB	7:G:129:LEU:HD21	2.33	0.57
4:M:52:VAL:CG1	4:M:388:GLU:O	2.52	0.57
7:P:94:ASN:HD22	7:P:97:ARG:HB2	1.69	0.57
4:M:318:GLU:HB2	8:Q:39:ASP:HA	1.85	0.57
2:K:61:MET:HE3	8:Q:88:ARG:HD3	1.84	0.57
2:T:153:LEU:HD13	2:T:153:LEU:C	2.25	0.57
3:U:374:ARG:NH2	3:U:684:ARG:HG3	2.19	0.57
4:V:47:LEU:H	4:V:47:LEU:HD12	1.69	0.57
1:1:250:LYS:HB3	1:1:252:TYR:CE2	2.39	0.57
3:3:171:SER:HB2	3:3:174:VAL:O	2.04	0.57
3:3:286:ASN:ND2	3:3:287:GLU:N	2.53	0.57
3:3:6:VAL:HG12	3:3:7:ASN:H	1.69	0.57
5:5:75:VAL:HG22	5:5:87:ARG:HG3	1.86	0.57
6:6:174:ALA:O	6:6:175:ALA:CB	2.52	0.57
8:7:42:TYR:O	8:7:44:MET:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:NE	1:A:12:ARG:O	2.30	0.57
3:C:587:LEU:HD22	3:C:589:HIS:N	2.16	0.57
1:J:13:PHE:C	1:J:13:PHE:CD1	2.77	0.57
1:J:29:LEU:HB2	1:J:151:GLU:OE1	2.04	0.57
3:L:2:VAL:HG12	3:L:3:ARG:N	2.19	0.57
4:M:350:ARG:HG2	4:M:350:ARG:O	2.05	0.57
5:N:102:PRO:HA	5:N:130:PRO:CG	2.34	0.57
7:P:114:VAL:HG12	7:P:115:LEU:H	1.68	0.57
2:T:40:TRP:CZ3	2:T:42:ARG:HA	2.39	0.57
4:V:223:VAL:HG13	4:V:226:PRO:O	2.04	0.57
1:1:88:TYR:HB2	1:1:216:THR:CG2	2.34	0.57
3:3:374:ARG:NH2	3:3:684:ARG:HG3	2.18	0.57
3:3:684:ARG:NH1	3:3:684:ARG:HG2	2.19	0.57
4:4:393:MET:O	4:4:396:ILE:HG22	2.05	0.57
4:4:64:THR:HG23	6:6:123:ILE:HD11	1.84	0.57
6:6:138:PRO:CG	7:9:121:MET:HG3	2.33	0.57
7:G:94:ASN:HD22	7:G:97:ARG:HB2	1.68	0.57
3:L:561:PRO:HB3	3:L:576:ALA:CA	2.32	0.57
4:M:223:VAL:HG22	4:M:226:PRO:O	2.04	0.57
4:M:234:LEU:H	4:M:234:LEU:HD23	1.68	0.57
4:M:218:ALA:HB3	4:M:272:VAL:HG21	1.87	0.57
1:S:93:ALA:O	1:S:134:VAL:HA	2.05	0.57
3:U:684:ARG:NH1	3:U:684:ARG:HG2	2.19	0.57
4:V:381:LEU:CD1	4:V:397:ILE:HG12	2.35	0.57
5:W:31:ARG:HG2	5:W:31:ARG:NH1	2.19	0.57
7:Y:123:ASP:HB2	7:Y:129:LEU:HD21	1.87	0.57
1:1:110:VAL:N	1:1:111:PRO:CD	2.68	0.57
2:2:86:LEU:O	2:2:89:LYS:N	2.37	0.57
3:3:361:ALA:O	3:3:367:PRO:HG3	2.04	0.57
6:6:164:ASN:H	6:6:170:LEU:CD1	2.16	0.57
1:A:33:LEU:HA	1:A:37:GLY:CA	2.34	0.57
3:C:537:PRO:HB2	3:C:756:GLY:HA2	1.87	0.57
4:D:59:ILE:CD1	4:D:59:ILE:N	2.67	0.57
5:E:175:THR:O	5:E:177:LYS:N	2.38	0.57
4:M:112:ARG:O	4:M:116:ILE:HG12	2.04	0.57
4:M:225:PRO:CD	4:M:239:LEU:HG	2.34	0.57
5:N:7:LEU:HD21	5:N:41:TYR:CE2	2.39	0.57
6:O:84:LEU:O	6:O:124:VAL:HG23	2.04	0.57
7:P:45:ARG:HH21	7:P:137:LEU:HD23	1.70	0.57
3:U:414:SER:O	3:U:418:ARG:HG3	2.04	0.57
3:U:656:LEU:HD23	3:U:656:LEU:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:371:ARG:NH2	4:V:376:VAL:HG21	2.19	0.57
5:W:132:LEU:HD23	5:W:135:ILE:HG23	1.87	0.57
3:3:38:HIS:NE2	3:3:287:GLU:HG2	2.20	0.57
3:3:453:PRO:HB2	3:3:750:ARG:NH2	2.20	0.57
7:9:45:ARG:NH2	7:9:137:LEU:HD23	2.19	0.57
7:9:161:TYR:O	7:9:176:PRO:HG3	2.05	0.57
1:A:174:HIS:CD2	1:A:192:LEU:HG	2.39	0.57
6:F:92:MET:HE1	6:F:127:VAL:HG13	1.85	0.57
1:J:301:PRO:HB2	1:J:303:THR:CG2	2.35	0.57
3:L:52:ILE:CG2	3:L:53:GLY:N	2.67	0.57
3:L:603:PRO:HG2	3:L:634:ALA:HB1	1.86	0.57
4:M:379:GLN:HG2	5:N:116:ARG:NH1	2.20	0.57
1:S:266:LEU:HB3	1:S:267:PRO:HD2	1.87	0.57
3:U:171:SER:C	3:U:173:PHE:H	2.05	0.57
3:U:343:LEU:O	3:U:369:LEU:HA	2.04	0.57
4:V:231:ASP:HA	4:V:235:THR:HG23	1.85	0.57
3:3:33:PHE:HZ	3:3:130:LEU:HA	1.69	0.57
4:4:254:TYR:O	4:4:256:GLY:N	2.37	0.57
5:5:103:THR:HB	5:5:131:ASP:O	2.05	0.57
5:5:11:ARG:HD2	5:5:11:ARG:N	2.20	0.57
6:6:110:ALA:HB1	6:6:116:GLY:HA2	1.85	0.57
5:5:155:THR:O	6:6:119:ASN:ND2	2.37	0.57
1:A:13:PHE:HE1	1:A:15:ARG:HG3	1.69	0.57
1:A:13:PHE:CE1	1:A:15:ARG:HG3	2.40	0.57
2:B:41:ILE:HD12	2:B:70:TYR:HB3	1.85	0.57
3:C:414:SER:HA	3:C:461:TRP:CZ3	2.40	0.57
4:D:232:LEU:HD11	4:D:282:GLU:OE1	2.04	0.57
5:E:65:PRO:HB2	5:E:93:TYR:CD2	2.40	0.57
1:J:13:PHE:O	1:J:15:ARG:N	2.38	0.57
3:L:307:LYS:H	3:L:307:LYS:HE2	1.70	0.57
1:J:397:ARG:HG3	3:L:46:ARG:NE	2.19	0.57
3:L:717:TRP:HH2	3:L:730:GLU:OE2	1.87	0.57
4:M:224:ILE:HD12	4:M:237:GLY:O	2.03	0.57
4:M:220:GLY:O	4:M:271:ASP:HB3	2.04	0.57
5:N:3:LEU:HD12	5:N:86:SER:OG	2.05	0.57
1:S:11:PRO:CG	1:S:270:THR:HA	2.35	0.57
2:T:87:SER:HB3	10:T:182:FES:S2	2.45	0.57
4:V:223:VAL:HG22	4:V:226:PRO:O	2.04	0.57
5:W:50:ALA:CB	5:W:114:LEU:HD21	2.35	0.57
7:Y:101:CYS:SG	7:Y:101:CYS:O	2.62	0.57
7:Y:141:VAL:CG1	7:Y:142:GLY:N	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:112:LYS:O	8:Z:116:PHE:HD1	1.88	0.57
5:5:55:LEU:HD12	5:5:55:LEU:N	2.19	0.57
1:A:253:GLN:CG	1:A:327:GLY:HA2	2.34	0.57
1:A:266:LEU:HB3	1:A:267:PRO:HD2	1.87	0.57
1:A:277:TYR:CE1	1:A:283:PRO:HD3	2.40	0.57
3:L:417:VAL:HG13	3:L:444:ARG:O	2.03	0.57
3:L:477:LEU:HD22	3:L:520:ARG:HG2	1.85	0.57
4:M:404:MET:HA	4:M:407:VAL:HG12	1.86	0.57
5:N:195:LEU:N	5:N:195:LEU:HD13	2.20	0.57
7:P:101:CYS:O	7:P:103:LEU:N	2.38	0.57
6:X:159:ARG:HB3	6:X:161:GLN:HG3	1.85	0.57
3:3:193:GLU:HB3	3:3:418:ARG:HH12	1.70	0.57
3:3:336:ALA:HB3	3:3:565:TYR:CE2	2.40	0.57
3:3:746:ARG:C	3:3:748:VAL:H	2.08	0.57
2:B:131:ALA:CB	2:B:132:PRO:CD	2.82	0.57
3:C:453:PRO:HB2	3:C:750:ARG:NH2	2.20	0.57
3:C:307:LYS:HB3	3:C:632:GLY:CA	2.34	0.57
4:D:199:HIS:O	4:D:201:ILE:N	2.38	0.57
5:E:120:ASP:HB3	5:E:121:LEU:HD12	1.85	0.57
1:J:33:LEU:HA	1:J:37:GLY:CA	2.34	0.57
3:L:564:LEU:HD21	3:L:581:ARG:CD	2.35	0.57
3:U:34:CYS:SG	3:U:44:ALA:O	2.63	0.57
3:U:329:LEU:HD11	3:U:584:VAL:HG11	1.86	0.57
5:W:73:GLU:OE2	5:W:87:ARG:NH1	2.37	0.57
5:W:155:THR:O	6:X:119:ASN:ND2	2.37	0.57
6:X:155:GLN:O	6:X:158:VAL:HG22	2.04	0.57
1:1:315:HIS:O	1:1:319:LYS:HB2	2.05	0.57
4:4:274:ASP:O	4:4:278:VAL:HG23	2.04	0.57
5:5:20:ASN:OD1	5:5:22:LEU:HG	2.05	0.57
6:6:41:PHE:HE2	6:6:92:MET:HB2	1.70	0.57
3:C:305:ARG:HG2	3:C:306:LEU:H	1.70	0.57
3:C:564:LEU:HD21	3:C:581:ARG:CD	2.35	0.57
3:C:621:VAL:HG21	3:C:671:GLU:O	2.05	0.57
4:D:229:ALA:HB1	4:D:241:ALA:O	2.05	0.57
5:E:121:LEU:CD1	5:E:121:LEU:H	2.17	0.57
4:M:240:ARG:NH2	4:M:245:ASN:OD1	2.37	0.57
5:N:175:THR:HG23	5:N:178:ASP:HB2	1.86	0.57
5:N:195:LEU:HD22	5:N:195:LEU:H	1.70	0.57
5:N:55:LEU:HD12	5:N:55:LEU:N	2.19	0.57
4:M:84:ARG:O	6:O:83:ARG:NH2	2.37	0.57
4:V:188:PRO:O	4:V:191:LYS:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:224:ILE:HG21	5:W:112:ASN:HB2	1.87	0.57
6:X:174:ALA:O	6:X:175:ALA:CB	2.53	0.57
1:1:358:PRO:O	1:1:362:GLY:N	2.38	0.56
2:2:72:PHE:HB2	8:7:89:ALA:CB	2.34	0.56
3:3:567:TYR:HA	3:3:584:VAL:HG23	1.86	0.56
4:4:133:LEU:HD21	4:4:204:TYR:CE2	2.40	0.56
4:4:225:PRO:CD	4:4:239:LEU:HG	2.35	0.56
4:4:244:VAL:CG1	4:4:246:TYR:CD1	2.88	0.56
5:5:132:LEU:HD23	5:5:135:ILE:HG23	1.87	0.56
5:5:42:LYS:HA	5:5:45:GLY:HA2	1.87	0.56
4:D:120:LEU:HD13	4:D:160:PHE:HE1	1.70	0.56
4:D:74:THR:CB	4:D:77:GLN:HG3	2.31	0.56
3:L:305:ARG:HG2	3:L:306:LEU:H	1.70	0.56
3:L:54:LEU:HD13	3:L:54:LEU:C	2.24	0.56
5:N:88:PHE:CD2	5:N:89:PHE:O	2.58	0.56
6:O:114:SER:CB	7:P:97:ARG:HD2	2.34	0.56
8:Q:112:LYS:HG2	8:Q:116:PHE:CE1	2.39	0.56
8:Q:67:PHE:CZ	8:Q:123:ARG:HG3	2.40	0.56
1:S:33:LEU:HA	1:S:37:GLY:CA	2.34	0.56
3:U:340:GLU:HA	3:U:366:THR:HB	1.87	0.56
3:U:52:ILE:CG2	3:U:53:GLY:N	2.68	0.56
3:U:307:LYS:HB3	3:U:632:GLY:CA	2.36	0.56
4:V:103:LYS:CB	5:W:22:LEU:HD13	2.25	0.56
5:W:16:PRO:HB2	5:W:28:VAL:CG1	2.35	0.56
6:X:154:LEU:O	6:X:158:VAL:HG13	2.05	0.56
7:Y:130:VAL:HG13	7:Y:130:VAL:O	2.05	0.56
3:3:415:GLU:HG2	3:3:418:ARG:HH21	1.69	0.56
4:4:311:PRO:HD3	4:4:330:HIS:NE2	2.21	0.56
5:5:195:LEU:HD13	5:5:195:LEU:H	1.69	0.56
7:9:114:VAL:HG12	7:9:115:LEU:N	2.20	0.56
2:B:116:LEU:HG	2:B:117:PHE:CD2	2.40	0.56
2:B:81:GLN:HB3	2:B:122:VAL:HG21	1.87	0.56
3:C:402:PRO:HD2	3:C:458:LEU:HD13	1.85	0.56
4:D:313:PRO:O	4:D:315:HIS:N	2.38	0.56
4:D:311:PRO:HD3	4:D:330:HIS:NE2	2.20	0.56
5:E:124:ILE:CG2	5:E:145:PRO:HG2	2.34	0.56
6:F:83:ARG:HB3	6:F:123:ILE:HD13	1.87	0.56
1:J:211:LEU:HB2	1:J:216:THR:HG21	1.87	0.56
3:L:229:ILE:HD11	3:L:289:TRP:HZ3	1.69	0.56
3:L:510:GLY:CA	3:L:520:ARG:HH22	2.17	0.56
3:L:6:VAL:HG12	3:L:7:ASN:H	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:714:ALA:HB3	3:L:745:ALA:HB2	1.86	0.56
3:U:118:ASP:O	3:U:122:CYS:N	2.36	0.56
4:V:125:ARG:HH11	4:V:125:ARG:HG3	1.70	0.56
4:V:153:ARG:HH11	4:V:153:ARG:HG3	1.69	0.56
4:V:225:PRO:HB2	4:V:226:PRO:HD3	1.87	0.56
6:X:26:LYS:HD2	6:X:26:LYS:O	2.05	0.56
3:3:305:ARG:HG2	3:3:306:LEU:N	2.20	0.56
3:3:514:ASP:HB2	3:3:683:LEU:HD12	1.86	0.56
3:3:658:LEU:O	3:3:658:LEU:HD23	2.06	0.56
5:5:120:ASP:HB3	5:5:121:LEU:HD12	1.87	0.56
4:4:84:ARG:O	6:6:83:ARG:NH2	2.38	0.56
2:B:79:HIS:CD2	2:B:118:SER:HB2	2.41	0.56
3:C:286:ASN:ND2	3:C:287:GLU:N	2.54	0.56
3:C:583:VAL:CG2	3:C:598:ALA:HA	2.34	0.56
4:D:228:VAL:HG11	4:D:274:ASP:HB2	1.87	0.56
4:D:371:ARG:NH2	4:D:376:VAL:HG21	2.20	0.56
6:F:164:ASN:N	6:F:170:LEU:HD12	2.20	0.56
1:J:253:GLN:CG	1:J:327:GLY:HA2	2.36	0.56
3:L:307:LYS:HB3	3:L:632:GLY:CA	2.34	0.56
8:Q:13:TRP:CE2	8:Q:17:LEU:HD11	2.40	0.56
1:S:361:GLU:OE1	3:U:114:ASN:HB2	2.05	0.56
2:T:46:ILE:HG23	2:T:60:VAL:CG1	2.36	0.56
3:U:453:PRO:HB2	3:U:750:ARG:CZ	2.35	0.56
3:U:733:GLN:HA	3:U:745:ALA:O	2.04	0.56
3:U:746:ARG:C	3:U:748:VAL:H	2.06	0.56
4:V:220:GLY:O	4:V:271:ASP:HB3	2.05	0.56
8:Z:37:PHE:HD1	8:Z:53:THR:O	1.89	0.56
3:3:30:VAL:HG22	3:3:48:CYS:HA	1.88	0.56
3:3:355:LEU:HD22	3:3:664:LEU:HD23	1.88	0.56
5:5:114:LEU:O	5:5:118:VAL:HG23	2.05	0.56
3:3:136:GLU:O	5:5:188:SER:HB2	2.04	0.56
7:9:44:THR:OG1	7:9:52:LYS:HD2	2.04	0.56
7:G:35:PRO:HD3	7:G:164:PRO:HG3	1.86	0.56
3:L:564:LEU:HD21	3:L:581:ARG:HD2	1.87	0.56
3:L:652:PRO:O	3:L:654:PHE:N	2.38	0.56
5:N:16:PRO:HD2	5:N:28:VAL:HG13	1.86	0.56
4:M:84:ARG:HG2	9:O:182:SF4:S2	2.46	0.56
6:O:41:PHE:HE2	6:O:92:MET:HB2	1.71	0.56
1:S:290:ILE:HG22	1:S:330:LEU:HD23	1.87	0.56
3:U:501:LYS:N	3:U:501:LYS:HD2	2.05	0.56
3:U:510:GLY:HA3	3:U:520:ARG:HH22	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:2:ARG:HH21	8:Z:113:GLU:HG3	1.70	0.56
1:1:13:PHE:O	1:1:15:ARG:N	2.39	0.56
1:1:108:GLU:CG	1:1:140:ARG:HG2	2.32	0.56
3:3:136:GLU:HG2	5:5:189:ARG:HG2	1.87	0.56
3:3:409:LEU:HD12	3:3:535:MET:HE2	1.87	0.56
5:5:147:ARG:HG3	5:5:149:ASP:OD1	2.05	0.56
7:9:141:VAL:CG1	7:9:142:GLY:H	2.10	0.56
1:A:192:LEU:HD22	1:A:211:LEU:HD11	1.86	0.56
2:B:136:VAL:HG21	2:B:163:LEU:CD1	2.35	0.56
3:C:131:GLN:HG2	4:D:325:ILE:HG12	1.86	0.56
3:C:416:PHE:CE1	3:C:447:LYS:HE2	2.41	0.56
3:C:453:PRO:HB2	3:C:750:ARG:HH22	1.71	0.56
4:D:264:VAL:H	4:D:285:GLU:HG3	1.70	0.56
4:D:321:MET:O	4:D:322:GLU:HG2	2.05	0.56
5:E:104:VAL:O	5:E:104:VAL:HG12	2.05	0.56
7:G:130:VAL:O	7:G:130:VAL:HG13	2.04	0.56
2:K:153:LEU:HD13	2:K:153:LEU:C	2.26	0.56
3:L:397:LEU:HD21	3:L:480:LEU:HD13	1.87	0.56
5:N:195:LEU:H	5:N:195:LEU:HD13	1.69	0.56
5:N:44:MET:HE1	5:N:82:ASP:HB3	1.86	0.56
3:L:167:HIS:HE1	8:Q:32:GLU:OE2	1.89	0.56
3:U:229:ILE:HD11	3:U:289:TRP:CZ3	2.41	0.56
3:U:717:TRP:HH2	3:U:730:GLU:OE2	1.88	0.56
4:V:220:GLY:HA2	4:V:384:ALA:O	2.05	0.56
4:V:52:VAL:HG11	4:V:388:GLU:O	2.05	0.56
5:W:124:ILE:CG2	5:W:145:PRO:HG2	2.35	0.56
6:X:163:TYR:O	6:X:164:ASN:ND2	2.37	0.56
7:Y:113:ILE:HG23	7:Y:113:ILE:O	2.04	0.56
1:1:13:PHE:CD1	1:1:13:PHE:C	2.79	0.56
1:1:437:TRP:CH2	2:2:96:LEU:HD13	2.41	0.56
3:3:40:SER:OG	3:3:189:ARG:HD2	2.06	0.56
3:3:564:LEU:CD1	3:3:581:ARG:H	2.18	0.56
1:A:267:PRO:HG2	1:A:270:THR:HG22	1.86	0.56
2:B:24:ARG:HA	2:B:53:VAL:CG1	2.35	0.56
4:D:224:ILE:HD12	4:D:237:GLY:CA	2.33	0.56
4:D:95:LEU:HA	4:D:173:ILE:HD13	1.87	0.56
4:M:64:THR:HG23	6:O:123:ILE:HD11	1.86	0.56
4:V:224:ILE:HB	4:V:225:PRO:CD	2.13	0.56
3:3:286:ASN:HD22	3:3:287:GLU:N	2.04	0.56
4:4:207:LEU:O	4:4:211:SER:HB2	2.06	0.56
1:A:315:HIS:O	1:A:319:LYS:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:414:SER:O	3:C:418:ARG:HG3	2.04	0.56
4:D:225:PRO:CD	4:D:226:PRO:HD3	2.34	0.56
2:K:131:ALA:HB1	2:K:132:PRO:HD2	1.86	0.56
3:L:13:VAL:HG22	3:L:17:THR:OG1	2.05	0.56
6:O:140:CYS:O	6:O:140:CYS:SG	2.62	0.56
7:P:130:VAL:HG13	7:P:130:VAL:O	2.05	0.56
8:Q:89:ALA:O	8:Q:91:ILE:N	2.38	0.56
3:U:6:VAL:CG1	3:U:7:ASN:N	2.67	0.56
4:V:152:GLU:HG2	4:V:197:LEU:HD21	1.88	0.56
5:W:121:LEU:HB3	5:W:127:GLU:CG	2.35	0.56
5:5:195:LEU:HD13	5:5:195:LEU:N	2.21	0.56
1:A:427:GLU:O	3:U:316:ARG:NH1	2.39	0.56
1:A:435:SER:HA	2:B:95:GLU:OE2	2.04	0.56
4:D:125:ARG:HG3	4:D:125:ARG:HH11	1.70	0.56
1:J:9:LEU:HD23	1:J:10:ASP:N	2.19	0.56
1:J:20:HIS:O	1:J:22:GLY:N	2.37	0.56
4:M:240:ARG:NH1	5:N:78:PRO:HD2	2.21	0.56
4:M:381:LEU:HA	4:M:384:ALA:HB3	1.87	0.56
1:S:267:PRO:HG2	1:S:270:THR:HG22	1.87	0.56
1:S:397:ARG:HG3	3:U:46:ARG:NE	2.21	0.56
1:S:402:LEU:O	1:S:403:ALA:C	2.42	0.56
3:U:650:VAL:HG12	3:U:651:ARG:N	2.20	0.56
5:W:7:LEU:O	5:W:11:ARG:HG2	2.06	0.56
5:W:184:TYR:O	5:W:185:LYS:HG3	2.06	0.56
5:W:65:PRO:HB2	5:W:93:TYR:HD2	1.71	0.56
4:V:64:THR:HG23	6:X:123:ILE:HD11	1.86	0.56
1:1:11:PRO:HB2	1:1:274:GLU:CD	2.26	0.56
2:2:116:LEU:HG	2:2:117:PHE:CD2	2.40	0.56
3:3:226:ILE:HD12	3:3:235:LEU:CD1	2.34	0.56
3:3:32:LEU:O	3:3:33:PHE:CD1	2.59	0.56
3:3:36:GLU:HB3	3:3:39:LEU:HD12	1.88	0.56
3:3:701:ALA:H	3:3:754:PRO:HB3	1.70	0.56
5:5:104:VAL:HG12	5:5:104:VAL:O	2.05	0.56
7:9:118:ASP:HA	7:9:161:TYR:CE2	2.40	0.56
7:9:153:THR:HG22	7:9:155:LYS:HB2	1.87	0.56
3:C:341:VAL:HB	3:C:364:LEU:HD21	1.87	0.56
4:D:224:ILE:HB	4:D:225:PRO:CD	2.12	0.56
5:E:58:LEU:HD12	5:E:59:THR:H	1.70	0.56
1:J:11:PRO:HB2	1:J:274:GLU:CD	2.24	0.56
3:L:194:VAL:HB	3:L:195:PRO:HD3	1.86	0.56
3:L:517:ALA:HA	3:L:520:ARG:CD	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:603:PRO:HG2	3:L:634:ALA:CB	2.35	0.56
5:N:174:LEU:HD21	5:N:180:GLY:HA2	1.86	0.56
6:O:110:ALA:HB1	6:O:116:GLY:HA2	1.88	0.56
7:P:58:LEU:O	7:P:61:ALA:N	2.39	0.56
3:U:477:LEU:HD22	3:U:520:ARG:HG2	1.85	0.56
4:V:285:GLU:O	4:V:289:ILE:HG12	2.06	0.56
5:W:3:LEU:N	5:W:3:LEU:HD23	2.15	0.56
5:W:65:PRO:HB2	5:W:93:TYR:CD2	2.41	0.56
3:3:133:ARG:CZ	5:5:185:LYS:HE3	2.36	0.56
3:3:174:VAL:HG21	3:3:296:PHE:CZ	2.40	0.56
3:3:488:GLU:O	3:3:491:ALA:HB3	2.05	0.56
3:3:603:PRO:HG2	3:3:634:ALA:HB1	1.87	0.56
3:3:717:TRP:HH2	3:3:730:GLU:OE2	1.88	0.56
4:4:346:THR:N	4:4:353:LEU:O	2.25	0.56
4:4:393:MET:C	4:4:396:ILE:HG22	2.27	0.56
1:A:13:PHE:CD1	1:A:13:PHE:C	2.78	0.56
2:B:47:GLU:O	2:B:50:ALA:HB3	2.05	0.56
4:D:153:ARG:NH1	4:D:153:ARG:HG3	2.21	0.56
5:E:104:VAL:C	5:E:106:ASP:H	2.08	0.56
5:E:40:HIS:C	5:E:42:LYS:H	2.09	0.56
7:G:56:CYS:O	9:G:184:SF4:S3	2.63	0.56
2:K:133:VAL:HG12	2:K:134:ILE:N	2.21	0.56
3:L:451:PHE:HE1	3:L:466:GLU:HB2	1.71	0.56
3:L:586:HIS:HE1	3:L:637:ALA:HA	1.71	0.56
3:L:48:CYS:O	3:L:82:SER:HB3	2.06	0.56
4:M:95:LEU:HA	4:M:173:ILE:HD13	1.87	0.56
6:O:83:ARG:HB3	6:O:123:ILE:HD13	1.87	0.56
1:S:13:PHE:C	1:S:13:PHE:HD1	2.09	0.56
2:T:131:ALA:HB1	2:T:132:PRO:HD2	1.85	0.56
3:U:488:GLU:O	3:U:491:ALA:HB3	2.05	0.56
5:W:64:ARG:HB3	5:W:65:PRO:HD2	1.88	0.56
7:Y:153:THR:HG22	7:Y:155:LYS:HB2	1.86	0.56
7:Y:35:PRO:HD3	7:Y:164:PRO:CG	2.36	0.56
6:6:163:TYR:HA	6:6:170:LEU:HB2	1.87	0.56
8:7:112:LYS:HG2	8:7:116:PHE:CE1	2.41	0.56
7:9:73:ALA:HB2	7:9:89:LYS:HB2	1.88	0.56
1:A:274:GLU:HG3	1:A:278:GLU:OE1	2.06	0.56
4:D:115:THR:HG21	4:D:297:LEU:HD23	1.88	0.56
3:L:174:VAL:HG21	3:L:296:PHE:CZ	2.40	0.56
3:L:488:GLU:O	3:L:491:ALA:HB3	2.05	0.56
3:L:587:LEU:HD22	3:L:589:HIS:N	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:254:THR:HG1	3:L:624:LEU:HD23	1.71	0.56
5:N:121:LEU:CD1	5:N:121:LEU:N	2.69	0.56
1:S:94:ASP:O	1:S:95:GLU:C	2.44	0.56
4:V:369:LYS:HG2	5:W:53:VAL:HB	1.87	0.56
7:Y:58:LEU:O	7:Y:61:ALA:N	2.39	0.56
2:2:116:LEU:N	2:2:116:LEU:HD23	2.21	0.55
2:2:131:ALA:CB	2:2:132:PRO:CD	2.79	0.55
3:3:747:VAL:O	3:3:747:VAL:HG23	2.06	0.55
4:4:254:TYR:CD1	4:4:255:SER:N	2.73	0.55
1:A:29:LEU:HB2	1:A:151:GLU:OE1	2.05	0.55
2:B:79:HIS:HD2	2:B:118:SER:HB2	1.70	0.55
3:C:470:PRO:HG3	3:C:750:ARG:NH2	2.21	0.55
4:D:223:VAL:HA	4:D:226:PRO:O	2.06	0.55
7:G:58:LEU:O	7:G:61:ALA:N	2.40	0.55
3:L:134:THR:O	3:L:138:GLY:CA	2.54	0.55
3:L:549:VAL:C	3:L:550:LEU:HD12	2.26	0.55
3:L:650:VAL:HG12	3:L:651:ARG:N	2.20	0.55
4:M:224:ILE:CB	4:M:225:PRO:CD	2.77	0.55
4:M:317:LEU:CD1	4:M:317:LEU:N	2.69	0.55
4:M:333:GLU:OE1	5:N:189:ARG:NH1	2.38	0.55
5:N:3:LEU:HD22	5:N:44:MET:SD	2.46	0.55
7:P:153:THR:HG22	7:P:155:LYS:HB2	1.87	0.55
3:U:115:HIS:CD2	3:U:116:PRO:HD2	2.41	0.55
3:U:361:ALA:O	3:U:367:PRO:HG3	2.05	0.55
4:V:164:THR:CB	4:V:170:HIS:HB3	2.35	0.55
4:V:240:ARG:HD3	5:W:77:LEU:HB3	1.88	0.55
7:Y:73:ALA:HB2	7:Y:89:LYS:HB2	1.88	0.55
1:1:11:PRO:HG3	1:1:270:THR:HA	1.88	0.55
1:1:343:ASN:HD22	2:2:89:LYS:HD2	1.71	0.55
3:3:100:VAL:O	3:3:104:GLN:HG3	2.06	0.55
3:3:549:VAL:HG12	3:3:549:VAL:O	2.07	0.55
5:5:26:TRP:CD1	5:5:26:TRP:N	2.74	0.55
3:3:216:PHE:HZ	8:7:128:PHE:CD2	2.23	0.55
2:B:89:LYS:HE3	2:B:94:GLU:OE1	2.05	0.55
3:C:113:LEU:HG	3:C:157:PHE:CD2	2.41	0.55
3:C:343:LEU:O	3:C:369:LEU:HA	2.05	0.55
3:C:73:ILE:HD12	3:C:73:ILE:O	2.05	0.55
4:D:379:GLN:O	4:D:382:PRO:HD2	2.07	0.55
1:J:88:TYR:HB2	1:J:216:THR:CG2	2.36	0.55
3:L:166:LYS:HE3	3:L:180:ARG:HD2	1.87	0.55
3:L:46:ARG:NH1	3:L:46:ARG:HG2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:381:LEU:HD11	4:M:397:ILE:HG12	1.88	0.55
5:N:119:TYR:CD1	5:N:132:LEU:HD21	2.41	0.55
5:N:175:THR:O	5:N:177:LYS:N	2.39	0.55
6:O:48:ILE:N	6:O:48:ILE:HD12	2.21	0.55
7:P:123:ASP:OD2	7:P:145:PRO:HB3	2.07	0.55
4:V:218:ALA:HB3	4:V:272:VAL:HG21	1.88	0.55
4:V:317:LEU:CD1	4:V:317:LEU:N	2.68	0.55
6:X:117:MET:HB3	7:Y:99:ILE:HD13	1.86	0.55
4:4:371:ARG:HH22	4:4:376:VAL:HG21	1.71	0.55
5:5:16:PRO:HB2	5:5:28:VAL:CG1	2.35	0.55
2:B:87:SER:OG	2:B:128:CYS:HB3	2.07	0.55
1:A:357:THR:HG21	3:C:111:THR:OG1	2.07	0.55
6:F:130:VAL:HG23	6:F:131:VAL:HG13	1.87	0.55
5:N:20:ASN:OD1	5:N:22:LEU:HG	2.06	0.55
5:N:48:PHE:O	5:N:50:ALA:N	2.39	0.55
6:O:115:GLY:HA3	6:O:125:GLN:OE1	2.07	0.55
3:U:40:SER:OG	3:U:189:ARG:HD2	2.06	0.55
4:V:38:HIS:O	4:V:39:GLY:O	2.23	0.55
4:V:85:MET:HE2	4:V:409:ARG:HB2	1.84	0.55
4:V:52:VAL:CG1	4:V:388:GLU:O	2.54	0.55
6:X:41:PHE:HE2	6:X:92:MET:HB2	1.70	0.55
1:1:102:LYS:HD3	1:1:253:GLN:HE22	1.70	0.55
3:3:510:GLY:CA	3:3:520:ARG:NH2	2.69	0.55
3:3:52:ILE:HG12	3:3:93:VAL:HG22	1.88	0.55
3:3:746:ARG:O	3:3:748:VAL:N	2.40	0.55
4:4:70:MET:C	4:4:72:HIS:H	2.09	0.55
2:B:27:ILE:HG22	2:B:31:LEU:HD23	1.88	0.55
3:C:171:SER:HB2	3:C:174:VAL:O	2.05	0.55
3:C:614:LEU:HD13	3:C:624:LEU:HD12	1.87	0.55
4:D:224:ILE:HD12	4:D:237:GLY:O	2.07	0.55
4:D:373:PRO:O	4:D:376:VAL:HG22	2.07	0.55
5:E:100:ARG:O	5:E:101:LEU:HB2	2.06	0.55
1:J:195:LEU:HA	2:K:24:ARG:HH21	1.72	0.55
3:L:459:MET:HG3	3:L:465:HIS:HB2	1.88	0.55
3:L:701:ALA:H	3:L:754:PRO:HB3	1.71	0.55
1:S:301:PRO:HB2	1:S:303:THR:CG2	2.36	0.55
1:S:315:HIS:O	1:S:319:LYS:HB2	2.06	0.55
3:U:514:ASP:HB2	3:U:683:LEU:HD12	1.87	0.55
3:U:578:LYS:HB3	3:U:578:LYS:NZ	2.21	0.55
3:U:564:LEU:HD21	3:U:581:ARG:CD	2.34	0.55
3:U:2:VAL:HG13	3:U:89:ASP:CA	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:238:SER:O	4:V:239:LEU:HD23	2.07	0.55
4:V:240:ARG:NH2	4:V:245:ASN:OD1	2.40	0.55
4:V:252:TYR:CE2	4:V:346:THR:HA	2.41	0.55
4:V:125:ARG:HH21	4:V:347:GLU:HG2	1.71	0.55
5:W:139:GLU:CG	5:W:140:ASP:N	2.65	0.55
1:1:395:GLU:O	1:1:396:GLY:O	2.23	0.55
3:3:171:SER:C	3:3:173:PHE:H	2.09	0.55
3:3:293:ALA:HA	3:3:699:TRP:CZ3	2.42	0.55
5:5:103:THR:HG22	5:5:131:ASP:HB2	1.89	0.55
5:5:48:PHE:C	5:5:50:ALA:N	2.59	0.55
7:9:133:LYS:HG2	7:9:137:LEU:HD11	1.89	0.55
1:A:162:LEU:HB3	1:A:163:PHE:CE1	2.41	0.55
3:C:453:PRO:HB2	3:C:750:ARG:NH1	2.21	0.55
3:C:655:ARG:HG3	3:C:655:ARG:HH11	1.71	0.55
6:F:123:ILE:HG22	6:F:124:VAL:N	2.21	0.55
1:J:360:ARG:O	1:J:364:ALA:HB3	2.06	0.55
1:J:398:SER:C	3:L:46:ARG:HE	2.09	0.55
3:U:307:LYS:HE2	3:U:307:LYS:H	1.72	0.55
5:W:120:ASP:HB3	5:W:121:LEU:HD12	1.89	0.55
6:X:153:GLN:HG3	7:Y:124:TYR:CZ	2.41	0.55
6:X:174:ALA:O	6:X:175:ALA:HB2	2.06	0.55
5:5:124:ILE:CG2	5:5:146:LEU:HD23	2.31	0.55
6:6:78:MET:HG3	6:6:78:MET:O	2.05	0.55
7:9:35:PRO:HD3	7:9:164:PRO:CG	2.36	0.55
1:A:242:GLY:HA2	1:A:268:MET:O	2.07	0.55
3:C:2:VAL:HG12	3:C:3:ARG:N	2.22	0.55
4:D:107:ALA:HB2	4:D:309:ILE:HD13	1.87	0.55
1:J:267:PRO:HG2	1:J:270:THR:HG22	1.89	0.55
1:J:40:THR:O	1:J:44:VAL:HG23	2.07	0.55
8:Q:13:TRP:NE1	8:Q:17:LEU:HD11	2.21	0.55
2:T:106:ILE:HD11	2:T:112:THR:CB	2.35	0.55
4:V:228:VAL:HG11	4:V:274:ASP:HB2	1.88	0.55
1:1:7:SER:HB3	1:1:15:ARG:HH22	1.70	0.55
2:2:106:ILE:HD11	2:2:112:THR:CB	2.37	0.55
3:3:616:ASN:HD22	3:3:622:LEU:HD11	1.70	0.55
4:4:234:LEU:HD23	4:4:234:LEU:H	1.70	0.55
5:5:121:LEU:HB3	5:5:127:GLU:CG	2.37	0.55
8:7:9:LEU:O	8:7:12:ALA:HB3	2.07	0.55
1:A:395:GLU:O	1:A:396:GLY:O	2.25	0.55
1:A:94:ASP:O	1:A:95:GLU:C	2.45	0.55
3:C:52:ILE:CG2	3:C:53:GLY:N	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:717:TRP:HH2	3:C:730:GLU:OE2	1.89	0.55
4:D:317:LEU:CD1	4:D:317:LEU:H	2.20	0.55
5:E:134:LYS:NZ	5:E:136:LEU:HB3	2.21	0.55
3:L:365:LYS:C	3:L:367:PRO:HD3	2.27	0.55
3:L:587:LEU:CD2	3:L:589:HIS:H	2.14	0.55
4:M:38:HIS:O	4:M:39:GLY:O	2.25	0.55
3:L:216:PHE:CD2	8:Q:63:LEU:HD23	2.41	0.55
2:T:40:TRP:HZ3	2:T:42:ARG:HA	1.71	0.55
4:V:200:ARG:HG3	4:V:204:TYR:HE1	1.72	0.55
4:V:227:GLU:HG3	4:V:268:GLU:O	2.07	0.55
4:V:311:PRO:HD3	4:V:330:HIS:NE2	2.22	0.55
1:1:107:LEU:HD22	1:1:145:LEU:HD11	1.88	0.55
1:1:33:LEU:HA	1:1:37:GLY:CA	2.36	0.55
3:3:166:LYS:HG3	3:3:178:ARG:HG3	1.87	0.55
3:3:168:HIS:HE1	8:7:32:GLU:OE1	1.90	0.55
3:3:748:VAL:CG1	3:3:748:VAL:O	2.53	0.55
4:4:224:ILE:HD12	4:4:237:GLY:O	2.07	0.55
4:4:62:LEU:N	4:4:408:ASP:OD2	2.36	0.55
5:5:31:ARG:NH1	5:5:31:ARG:HG2	2.21	0.55
3:C:397:LEU:HD21	3:C:480:LEU:HD13	1.89	0.55
4:D:254:TYR:O	4:D:256:GLY:N	2.39	0.55
5:E:114:LEU:O	5:E:118:VAL:HG23	2.07	0.55
5:E:26:TRP:CD1	5:E:26:TRP:N	2.74	0.55
6:F:84:LEU:O	6:F:124:VAL:HG23	2.07	0.55
6:F:93:ARG:HD2	6:F:97:GLU:HG3	1.89	0.55
8:H:37:PHE:CD1	8:H:55:MET:HB2	2.42	0.55
3:L:481:LEU:HD23	3:L:523:LEU:HD22	1.89	0.55
7:P:161:TYR:O	7:P:176:PRO:HG3	2.07	0.55
3:U:202:PHE:C	3:U:203:ILE:HD13	2.27	0.55
3:U:430:THR:CG2	3:U:431:PRO:HD2	2.37	0.55
4:V:225:PRO:CD	4:V:239:LEU:HG	2.36	0.55
4:V:313:PRO:C	4:V:315:HIS:N	2.60	0.55
5:W:104:VAL:C	5:W:106:ASP:H	2.10	0.55
5:W:119:TYR:CD1	5:W:132:LEU:HD21	2.41	0.55
4:4:350:ARG:O	4:4:350:ARG:HG2	2.07	0.55
2:B:131:ALA:HB1	2:B:132:PRO:HD2	1.88	0.55
3:C:453:PRO:HB2	3:C:750:ARG:HH12	1.72	0.55
5:E:75:VAL:CG2	5:E:87:ARG:HG3	2.37	0.55
1:J:11:PRO:HG3	1:J:270:THR:HA	1.89	0.55
3:L:282:VAL:HG22	3:L:282:VAL:O	2.07	0.55
3:L:155:THR:HB	4:M:321:MET:CA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:47:LEU:H	4:M:47:LEU:HD12	1.72	0.55
4:M:74:THR:CB	4:M:77:GLN:HG3	2.32	0.55
4:M:79:ILE:HD13	4:M:173:ILE:O	2.06	0.55
5:N:48:PHE:C	5:N:50:ALA:N	2.59	0.55
1:S:369:ASN:O	1:S:372:ALA:HB3	2.07	0.55
3:U:33:PHE:HB2	3:U:45:CYS:SG	2.47	0.55
3:U:564:LEU:CD1	3:U:581:ARG:H	2.18	0.55
3:U:655:ARG:HG3	3:U:655:ARG:HH11	1.70	0.55
4:V:112:ARG:O	4:V:116:ILE:HG12	2.07	0.55
3:3:411:LEU:O	3:3:414:SER:HB3	2.06	0.55
3:3:254:THR:HG1	3:3:624:LEU:HD23	1.71	0.55
4:4:257:TYR:C	4:4:263:ASP:N	2.60	0.55
5:5:40:HIS:C	5:5:42:LYS:H	2.10	0.55
1:A:36:GLY:O	1:A:37:GLY:O	2.25	0.55
3:C:409:LEU:HD12	3:C:535:MET:HE2	1.89	0.55
5:E:103:THR:HG22	5:E:131:ASP:HB2	1.89	0.55
5:E:38:MET:O	5:E:41:TYR:HB2	2.07	0.55
1:J:23:LYS:O	1:J:24:GLU:CD	2.45	0.55
3:L:202:PHE:C	3:L:203:ILE:HD13	2.26	0.55
4:M:207:LEU:O	4:M:211:SER:HB2	2.07	0.55
4:M:225:PRO:CD	4:M:226:PRO:HD3	2.37	0.55
4:M:256:GLY:HA2	4:M:292:GLN:NE2	2.21	0.55
4:M:42:ARG:N	4:M:42:ARG:HD3	2.22	0.55
4:M:64:THR:HB	4:M:66:PHE:CE1	2.41	0.55
6:O:112:ALA:O	6:O:127:VAL:HG23	2.07	0.55
4:V:200:ARG:CG	4:V:200:ARG:O	2.55	0.55
5:W:92:VAL:HG23	5:W:92:VAL:O	2.07	0.55
6:X:148:ILE:O	6:X:151:VAL:HG22	2.07	0.55
7:Y:58:LEU:HD12	7:Y:58:LEU:N	2.21	0.55
7:Y:58:LEU:O	7:Y:59:CYS:C	2.45	0.55
1:1:195:LEU:HA	2:2:24:ARG:HH21	1.72	0.54
1:1:94:ASP:O	1:1:95:GLU:C	2.46	0.54
1:1:357:THR:HG21	3:3:111:THR:OG1	2.07	0.54
6:6:19:ILE:HD11	1:J:271:THR:OG1	2.06	0.54
2:B:116:LEU:HD23	2:B:116:LEU:N	2.21	0.54
3:C:132:ASP:O	3:C:135:VAL:HG12	2.06	0.54
3:C:505:LEU:O	3:C:532:VAL:HG13	2.08	0.54
3:C:564:LEU:HD11	3:C:581:ARG:N	2.20	0.54
3:C:404:GLU:HB3	3:C:697:THR:HA	1.89	0.54
3:C:757:HIS:N	3:C:757:HIS:ND1	2.55	0.54
4:D:159:LEU:O	4:D:162:TRP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:373:PRO:O	4:D:374:SER:C	2.46	0.54
6:F:117:MET:HB3	7:G:99:ILE:HD13	1.88	0.54
1:J:357:THR:HG21	3:L:111:THR:OG1	2.07	0.54
3:L:469:ARG:HD3	3:L:472:GLU:OE2	2.08	0.54
7:P:45:ARG:NH2	7:P:137:LEU:HD23	2.22	0.54
8:Q:16:LEU:HD13	8:Q:16:LEU:C	2.27	0.54
1:S:437:TRP:CH2	2:T:96:LEU:HD13	2.42	0.54
3:U:244:ALA:HB3	3:U:249:MET:CE	2.37	0.54
1:A:428:LYS:C	3:U:316:ARG:HH22	2.11	0.54
3:U:517:ALA:HA	3:U:520:ARG:CD	2.37	0.54
4:V:229:ALA:HB1	4:V:241:ALA:O	2.07	0.54
8:Z:64:GLY:O	8:Z:65:GLU:C	2.46	0.54
3:3:514:ASP:CG	3:3:685:PRO:HB3	2.27	0.54
4:4:83:PRO:HB2	4:4:169:HIS:HA	1.88	0.54
5:5:58:LEU:HD12	5:5:59:THR:N	2.22	0.54
7:9:141:VAL:CG1	7:9:142:GLY:N	2.70	0.54
7:9:43:LEU:O	7:9:138:VAL:HG13	2.08	0.54
1:A:238:PHE:HE1	1:A:249:MET:CE	2.21	0.54
3:C:549:VAL:C	3:C:550:LEU:HD12	2.27	0.54
3:C:557:SER:H	3:C:560:GLU:HB3	1.72	0.54
3:C:567:TYR:HA	3:C:584:VAL:HG23	1.89	0.54
4:D:112:ARG:O	4:D:116:ILE:HG12	2.06	0.54
4:D:381:LEU:CD1	4:D:397:ILE:HG12	2.37	0.54
5:E:42:LYS:HA	5:E:45:GLY:HA2	1.88	0.54
7:G:113:ILE:HG23	7:G:113:ILE:O	2.07	0.54
1:J:191:SER:HB2	1:J:197:ALA:HB2	1.89	0.54
3:L:293:ALA:HA	3:L:699:TRP:CZ3	2.42	0.54
3:L:567:TYR:HA	3:L:584:VAL:HG23	1.88	0.54
3:L:586:HIS:CE1	3:L:637:ALA:HA	2.42	0.54
3:L:453:PRO:HB2	3:L:750:ARG:HH22	1.72	0.54
3:L:131:GLN:HG2	4:M:325:ILE:HG12	1.89	0.54
4:M:125:ARG:HH21	4:M:347:GLU:HG2	1.73	0.54
5:N:127:GLU:HG3	5:N:129:HIS:HE1	1.72	0.54
5:N:46:PHE:C	5:N:48:PHE:N	2.59	0.54
3:U:211:ILE:O	3:U:212:GLY:O	2.23	0.54
3:U:326:PHE:O	3:U:329:LEU:HB3	2.07	0.54
3:U:603:PRO:HG2	3:U:634:ALA:CB	2.37	0.54
4:V:254:TYR:O	4:V:255:SER:C	2.46	0.54
4:V:274:ASP:O	4:V:278:VAL:HG23	2.07	0.54
5:W:147:ARG:HG2	5:W:150:TYR:HB2	1.88	0.54
1:1:291:ILE:HD11	1:1:331:ILE:HD11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:733:GLN:HA	3:3:745:ALA:O	2.07	0.54
4:4:317:LEU:N	4:4:317:LEU:CD1	2.70	0.54
4:4:42:ARG:HD3	4:4:42:ARG:N	2.23	0.54
1:A:195:LEU:HA	2:B:24:ARG:HH21	1.71	0.54
3:C:355:LEU:HD22	3:C:664:LEU:HD23	1.89	0.54
4:D:42:ARG:N	4:D:42:ARG:HD3	2.21	0.54
4:D:51:GLU:C	4:D:52:VAL:HG22	2.28	0.54
4:D:65:GLY:O	4:D:66:PHE:C	2.45	0.54
2:K:65:SER:O	3:L:204:GLU:HA	2.06	0.54
3:L:23:VAL:HG13	3:L:28:TYR:HB2	1.89	0.54
3:L:361:ALA:O	3:L:367:PRO:HG3	2.07	0.54
3:L:510:GLY:HA3	3:L:520:ARG:HH22	1.72	0.54
4:M:371:ARG:NH2	4:M:376:VAL:HG21	2.22	0.54
5:N:124:ILE:CG2	5:N:146:LEU:HB2	2.36	0.54
3:U:194:VAL:HB	3:U:195:PRO:HD3	1.89	0.54
3:U:20:MET:HE3	3:U:432:PHE:HB3	1.89	0.54
4:V:317:LEU:H	4:V:317:LEU:CD1	2.20	0.54
8:Z:87:PRO:O	8:Z:89:ALA:N	2.39	0.54
3:3:48:CYS:O	3:3:82:SER:HB3	2.08	0.54
3:3:532:VAL:HG12	3:3:533:LEU:N	2.23	0.54
3:3:634:ALA:O	3:3:635:GLU:O	2.25	0.54
4:4:89:HIS:ND1	4:4:349:ALA:HB1	2.22	0.54
3:C:285:VAL:CG1	3:C:286:ASN:N	2.65	0.54
6:F:174:ALA:O	6:F:175:ALA:HB2	2.07	0.54
1:J:433:ARG:NH1	2:K:94:GLU:OE1	2.40	0.54
3:L:132:ASP:O	3:L:135:VAL:HG12	2.07	0.54
3:L:243:ARG:HD3	3:L:275:LEU:CD1	2.31	0.54
3:L:355:LEU:HD22	3:L:664:LEU:HD23	1.90	0.54
3:L:746:ARG:C	3:L:748:VAL:H	2.10	0.54
6:O:117:MET:HG3	6:O:117:MET:O	2.08	0.54
7:P:96:LEU:HD21	7:P:129:LEU:CD1	2.38	0.54
8:Q:16:LEU:O	8:Q:16:LEU:HD13	2.07	0.54
4:V:99:LEU:HD13	4:V:102:GLU:OE1	2.07	0.54
1:1:9:LEU:HD23	1:1:10:ASP:N	2.21	0.54
3:3:113:LEU:HG	3:3:157:PHE:CD2	2.43	0.54
3:3:397:LEU:HD21	3:3:480:LEU:HD13	1.89	0.54
3:3:603:PRO:HG2	3:3:634:ALA:CB	2.37	0.54
3:3:453:PRO:HB2	3:3:750:ARG:HH22	1.73	0.54
4:4:116:ILE:HD12	4:4:182:LEU:CD2	2.38	0.54
6:6:154:LEU:O	6:6:158:VAL:HG13	2.07	0.54
6:6:114:SER:CB	7:9:97:ARG:HD2	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:430:THR:HG23	3:C:431:PRO:HD2	1.90	0.54
3:C:477:LEU:HD22	3:C:520:ARG:HG2	1.90	0.54
4:D:143:LEU:O	4:D:143:LEU:HD23	2.07	0.54
4:D:369:LYS:HG2	5:E:53:VAL:HB	1.88	0.54
4:D:85:MET:HE2	4:D:409:ARG:HB2	1.86	0.54
5:E:184:TYR:O	5:E:185:LYS:HG3	2.08	0.54
5:E:60:TYR:CD1	5:E:61:PRO:HD2	2.42	0.54
2:K:40:TRP:CD1	2:K:74:PRO:HA	2.42	0.54
3:L:2:VAL:HG13	3:L:89:ASP:CA	2.37	0.54
3:L:307:LYS:H	3:L:307:LYS:HE3	1.73	0.54
3:L:33:PHE:HZ	3:L:130:LEU:HA	1.71	0.54
3:L:514:ASP:CG	3:L:685:PRO:HB3	2.26	0.54
4:M:252:TYR:HE2	4:M:346:THR:HA	1.72	0.54
4:M:285:GLU:O	4:M:289:ILE:HG12	2.08	0.54
4:M:316:LEU:HD13	4:M:320:SER:CB	2.37	0.54
1:S:110:VAL:N	1:S:111:PRO:CD	2.70	0.54
1:S:360:ARG:O	1:S:364:ALA:HB3	2.07	0.54
3:U:166:LYS:CG	3:U:178:ARG:HG3	2.37	0.54
3:U:203:ILE:O	3:U:204:GLU:HB2	2.07	0.54
3:U:346:ALA:HA	3:U:372:GLN:HB2	1.89	0.54
3:U:550:LEU:N	3:U:550:LEU:CD1	2.70	0.54
3:U:614:LEU:HD13	3:U:624:LEU:HD12	1.89	0.54
4:V:224:ILE:CB	4:V:225:PRO:CD	2.80	0.54
6:X:37:TRP:HA	6:X:37:TRP:HE3	1.72	0.54
1:1:23:LYS:O	1:1:24:GLU:CD	2.46	0.54
2:2:31:LEU:HD12	2:2:41:ILE:HD13	1.88	0.54
3:3:269:THR:HG23	3:3:274:LEU:HD13	1.89	0.54
3:3:340:GLU:HA	3:3:366:THR:HB	1.89	0.54
3:3:19:VAL:HG23	3:3:85:THR:O	2.07	0.54
4:4:379:GLN:HG2	5:5:116:ARG:NH1	2.23	0.54
6:6:174:ALA:O	6:6:175:ALA:HB2	2.08	0.54
6:6:37:TRP:HE3	6:6:37:TRP:HA	1.70	0.54
1:A:363:VAL:HA	1:A:367:MET:HB2	1.88	0.54
3:C:631:ASN:C	3:C:633:GLU:N	2.61	0.54
3:C:746:ARG:O	3:C:748:VAL:N	2.41	0.54
5:E:102:PRO:HA	5:E:130:PRO:CG	2.37	0.54
6:F:153:GLN:HG3	7:G:124:TYR:CZ	2.42	0.54
6:F:174:ALA:O	6:F:175:ALA:CB	2.54	0.54
1:J:253:GLN:NE2	1:J:325:THR:O	2.41	0.54
1:J:371:PHE:HA	1:J:374:ILE:CG2	2.38	0.54
2:K:112:THR:CG2	2:K:116:LEU:HD23	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:73:GLU:OE2	5:N:87:ARG:HD3	2.08	0.54
6:O:164:ASN:N	6:O:170:LEU:HD12	2.23	0.54
7:P:150:ALA:HA	7:P:153:THR:HB	1.90	0.54
7:P:35:PRO:HD3	7:P:164:PRO:CG	2.38	0.54
1:S:12:ARG:O	1:S:12:ARG:NE	2.38	0.54
3:U:23:VAL:HG13	3:U:28:TYR:HB2	1.88	0.54
4:V:164:THR:OG1	4:V:170:HIS:HB3	2.07	0.54
3:U:154:TYR:O	4:V:321:MET:HB2	2.08	0.54
4:V:350:ARG:NH1	4:V:401:ASP:OD2	2.41	0.54
3:3:132:ASP:O	3:3:135:VAL:HG12	2.07	0.54
3:3:167:HIS:C	3:3:176:LEU:HD11	2.28	0.54
3:3:11:VAL:HG11	3:3:25:HIS:CD2	2.43	0.54
4:4:153:ARG:HG3	4:4:153:ARG:NH1	2.22	0.54
4:4:187:VAL:N	4:4:188:PRO:HD2	2.22	0.54
6:6:145:GLU:HG2	7:9:31:VAL:CG2	2.37	0.54
7:9:46:HIS:CD2	7:9:52:LYS:HG2	2.43	0.54
3:C:193:GLU:HB3	3:C:418:ARG:HH12	1.72	0.54
3:C:11:VAL:HG11	3:C:25:HIS:CD2	2.43	0.54
7:G:118:ASP:HA	7:G:161:TYR:HE2	1.73	0.54
1:J:10:ASP:CB	1:J:11:PRO:CD	2.72	0.54
3:L:177:ASP:HA	3:L:235:LEU:H	1.72	0.54
4:M:125:ARG:HH12	4:M:349:ALA:HA	1.72	0.54
4:M:254:TYR:CD1	4:M:255:SER:N	2.75	0.54
5:N:53:VAL:HG22	5:N:55:LEU:CD1	2.38	0.54
6:O:109:GLY:H	6:O:137:VAL:HG13	1.72	0.54
3:U:193:GLU:HB3	3:U:418:ARG:HH12	1.72	0.54
4:V:393:MET:C	4:V:396:ILE:HG22	2.28	0.54
5:W:124:ILE:CG2	5:W:146:LEU:HD23	2.35	0.54
5:W:26:TRP:N	5:W:26:TRP:CD1	2.76	0.54
1:1:272:PHE:O	1:1:276:ILE:HG13	2.08	0.54
3:3:173:PHE:CZ	3:3:296:PHE:HB2	2.42	0.54
4:4:254:TYR:O	4:4:255:SER:C	2.45	0.54
1:A:11:PRO:HB2	1:A:274:GLU:CD	2.28	0.54
3:C:293:ALA:HB2	3:C:698:MET:HG2	1.90	0.54
3:C:312:ARG:HA	3:C:316:ARG:O	2.08	0.54
3:C:469:ARG:HD3	3:C:472:GLU:OE2	2.08	0.54
4:D:211:SER:OG	4:D:212:PRO:HD2	2.08	0.54
4:D:343:TYR:CD1	4:D:344:VAL:N	2.76	0.54
6:F:106:ILE:HD11	6:F:154:LEU:HD22	1.89	0.54
8:H:108:ILE:N	8:H:108:ILE:HD12	2.23	0.54
1:J:201:LEU:CG	1:J:203:PRO:HD2	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:254:THR:OG1	3:L:624:LEU:HD23	2.08	0.54
3:L:655:ARG:HG3	3:L:655:ARG:HH11	1.71	0.54
4:M:225:PRO:HG2	4:M:239:LEU:H	1.72	0.54
4:M:320:SER:OG	4:M:323:ALA:HB3	2.07	0.54
4:M:369:LYS:HG2	5:N:53:VAL:HB	1.89	0.54
5:N:58:LEU:HD12	5:N:59:THR:N	2.22	0.54
5:N:66:GLU:HG2	5:N:95:PRO:HA	1.89	0.54
7:P:133:LYS:HG2	7:P:137:LEU:HD11	1.90	0.54
7:P:143:THR:HG23	7:P:146:GLN:OE1	2.08	0.54
1:S:13:PHE:O	1:S:15:ARG:N	2.40	0.54
2:T:27:ILE:HG13	2:T:53:VAL:HG21	1.89	0.54
3:U:307:LYS:HE3	3:U:307:LYS:H	1.72	0.54
3:U:469:ARG:HD3	3:U:472:GLU:OE2	2.07	0.54
5:W:53:VAL:HG22	5:W:55:LEU:CD1	2.38	0.54
5:W:57:TYR:OH	5:W:91:ARG:NH2	2.41	0.54
3:3:340:GLU:H	3:3:366:THR:HB	1.73	0.54
4:4:224:ILE:CB	4:4:225:PRO:CD	2.80	0.54
4:4:313:PRO:O	4:4:315:HIS:N	2.40	0.54
4:4:379:GLN:O	4:4:382:PRO:HD2	2.08	0.54
4:4:65:GLY:O	4:4:66:PHE:C	2.46	0.54
5:5:46:PHE:C	5:5:48:PHE:N	2.60	0.54
5:5:71:VAL:CG1	5:5:89:PHE:HD2	2.20	0.54
1:A:114:LEU:HD23	1:A:118:MET:HG3	1.90	0.54
1:A:376:THR:O	1:A:376:THR:HG22	2.08	0.54
3:C:23:VAL:HG13	3:C:28:TYR:HB2	1.90	0.54
3:C:570:PHE:O	3:C:572:PRO:HD3	2.08	0.54
4:D:133:LEU:HD21	4:D:204:TYR:CE2	2.40	0.54
4:D:200:ARG:O	4:D:200:ARG:HG3	2.08	0.54
5:E:121:LEU:CD1	5:E:121:LEU:N	2.70	0.54
5:E:71:VAL:HG11	5:E:89:PHE:HD2	1.72	0.54
1:J:108:GLU:HG2	1:J:140:ARG:CG	2.35	0.54
4:M:224:ILE:HD13	5:N:112:ASN:HA	1.89	0.54
1:S:195:LEU:HA	2:T:24:ARG:HH21	1.72	0.54
3:U:112:LEU:CD2	3:U:130:LEU:HD21	2.38	0.54
3:U:132:ASP:O	3:U:135:VAL:HG12	2.07	0.54
3:U:46:ARG:HG2	3:U:46:ARG:NH1	2.21	0.54
5:W:75:VAL:CG2	5:W:87:ARG:HG3	2.38	0.54
1:1:134:VAL:HG23	1:1:134:VAL:O	2.07	0.54
3:3:33:PHE:CZ	3:3:130:LEU:HA	2.43	0.54
3:3:517:ALA:HA	3:3:520:ARG:CD	2.36	0.54
3:3:586:HIS:HE1	3:3:637:ALA:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:240:ARG:NH2	4:4:245:ASN:OD1	2.40	0.54
6:6:153:GLN:HG3	7:9:124:TYR:CZ	2.42	0.54
6:6:164:ASN:CB	7:9:148:ARG:HE	2.14	0.54
3:C:459:MET:CG	3:C:465:HIS:HB2	2.37	0.54
3:C:514:ASP:CG	3:C:685:PRO:HB3	2.28	0.54
3:C:703:GLN:O	3:C:705:VAL:N	2.41	0.54
5:E:50:ALA:HB3	5:E:114:LEU:CD1	2.23	0.54
4:D:366:TYR:OH	5:E:58:LEU:O	2.26	0.54
2:K:42:ARG:HB2	2:K:45:ARG:HG2	1.89	0.54
2:K:86:LEU:O	2:K:89:LYS:N	2.41	0.54
3:L:333:LEU:HD13	3:L:648:LEU:HD21	1.90	0.54
3:L:557:SER:H	3:L:560:GLU:HB3	1.73	0.54
4:M:254:TYR:O	4:M:255:SER:C	2.45	0.54
5:N:120:ASP:HB3	5:N:121:LEU:HD12	1.89	0.54
5:N:66:GLU:CG	5:N:95:PRO:HA	2.38	0.54
7:P:56:CYS:O	9:P:184:SF4:S3	2.66	0.54
7:P:58:LEU:O	7:P:59:CYS:C	2.46	0.54
8:Q:108:ILE:N	8:Q:108:ILE:HD12	2.23	0.54
1:S:250:LYS:HB3	1:S:252:TYR:CE2	2.43	0.54
1:S:253:GLN:CG	1:S:327:GLY:HA2	2.36	0.54
3:U:454:TYR:O	3:U:456:ALA:N	2.41	0.54
4:V:144:THR:HB	4:V:145:PRO:HD3	1.90	0.54
4:V:224:ILE:HD12	4:V:237:GLY:O	2.07	0.54
4:V:240:ARG:NH1	5:W:78:PRO:HD2	2.23	0.54
4:V:274:ASP:O	4:V:275:ARG:C	2.47	0.54
5:W:31:ARG:HG2	5:W:31:ARG:HH11	1.73	0.54
7:Y:143:THR:HG23	7:Y:146:GLN:OE1	2.08	0.54
2:2:79:HIS:HD2	2:2:118:SER:HB2	1.73	0.53
3:3:346:ALA:HA	3:3:372:GLN:HB2	1.90	0.53
3:3:375:THR:HA	3:3:512:LEU:CD1	2.38	0.53
6:6:123:ILE:HG22	6:6:124:VAL:N	2.22	0.53
2:B:86:LEU:HD11	2:B:90:LEU:HD11	1.90	0.53
4:D:207:LEU:O	4:D:211:SER:HB2	2.09	0.53
4:D:132:PHE:CD2	4:D:279:ARG:HD2	2.43	0.53
1:J:102:LYS:HD3	1:J:253:GLN:HE22	1.72	0.53
3:L:268:ASP:OD2	3:L:278:ARG:NH1	2.41	0.53
3:L:338:GLY:HA2	3:L:364:LEU:HD11	1.90	0.53
2:T:116:LEU:HD23	2:T:116:LEU:N	2.22	0.53
3:U:370:ASP:OD2	3:U:557:SER:HB2	2.09	0.53
3:U:397:LEU:HD21	3:U:480:LEU:HD13	1.89	0.53
4:V:168:PHE:HA	4:V:170:HIS:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:121:LEU:HD12	5:W:121:LEU:H	1.73	0.53
5:W:42:LYS:HA	5:W:45:GLY:HA2	1.88	0.53
2:2:136:VAL:CG1	2:2:137:ASN:N	2.55	0.53
4:4:200:ARG:O	4:4:200:ARG:CG	2.55	0.53
1:A:13:PHE:HD1	1:A:13:PHE:C	2.12	0.53
1:A:272:PHE:O	1:A:276:ILE:HG13	2.07	0.53
3:C:307:LYS:HE3	3:C:307:LYS:H	1.72	0.53
3:C:319:GLU:H	3:C:319:GLU:CD	2.12	0.53
4:D:190:LEU:O	4:D:194:LEU:HB2	2.08	0.53
5:E:132:LEU:HD23	5:E:135:ILE:HG23	1.89	0.53
8:H:72:VAL:HG22	8:H:73:SER:N	2.23	0.53
2:K:106:ILE:HD11	2:K:112:THR:CB	2.38	0.53
3:L:154:TYR:CZ	4:M:312:PRO:HB3	2.43	0.53
3:L:409:LEU:HD12	3:L:535:MET:CE	2.38	0.53
3:L:414:SER:HA	3:L:461:TRP:HZ3	1.72	0.53
4:M:116:ILE:HD12	4:M:182:LEU:CD2	2.38	0.53
3:U:404:GLU:HB3	3:U:697:THR:HA	1.90	0.53
4:V:51:GLU:C	4:V:52:VAL:HG22	2.29	0.53
5:W:60:TYR:CG	5:W:61:PRO:HD2	2.43	0.53
3:3:282:VAL:O	3:3:282:VAL:HG22	2.08	0.53
3:3:307:LYS:N	3:3:307:LYS:HE2	2.22	0.53
3:3:355:LEU:O	3:3:358:SER:HB3	2.08	0.53
3:3:469:ARG:HD3	3:3:472:GLU:OE2	2.09	0.53
3:3:587:LEU:HD22	3:3:589:HIS:N	2.19	0.53
4:4:346:THR:HG22	4:4:353:LEU:C	2.29	0.53
4:4:38:HIS:O	4:4:39:GLY:O	2.27	0.53
5:5:7:LEU:O	5:5:11:ARG:HG2	2.08	0.53
6:6:92:MET:HE1	6:6:127:VAL:HG13	1.91	0.53
1:A:13:PHE:O	1:A:15:ARG:N	2.41	0.53
1:A:108:GLU:CG	1:A:140:ARG:HG2	2.38	0.53
3:C:746:ARG:C	3:C:748:VAL:H	2.10	0.53
4:D:122:GLU:HB2	4:D:290:ILE:HD11	1.90	0.53
4:D:240:ARG:HD3	5:E:77:LEU:HB3	1.89	0.53
4:D:393:MET:O	4:D:396:ILE:HG22	2.08	0.53
1:J:408:TRP:N	1:J:409:PRO:HD2	2.23	0.53
1:J:94:ASP:O	1:J:95:GLU:C	2.47	0.53
3:L:375:THR:HA	3:L:512:LEU:CD1	2.39	0.53
4:M:122:GLU:HA	4:M:122:GLU:OE1	2.09	0.53
4:M:252:TYR:O	4:M:253:PRO:C	2.43	0.53
5:N:106:ASP:O	5:N:113:PHE:CZ	2.62	0.53
5:N:57:TYR:OH	5:N:91:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:27:VAL:O	5:N:90:VAL:HA	2.09	0.53
1:S:162:LEU:HB3	1:S:163:PHE:CE1	2.42	0.53
2:T:144:CYS:O	2:T:149:ARG:HD3	2.07	0.53
1:S:435:SER:HA	2:T:95:GLU:OE2	2.08	0.53
3:U:19:VAL:HG22	3:U:91:MET:HE1	1.90	0.53
3:U:417:VAL:O	3:U:417:VAL:HG12	2.07	0.53
3:U:372:GLN:NE2	3:U:570:PHE:HB2	2.22	0.53
4:V:367:ARG:NH1	4:V:367:ARG:HG2	2.23	0.53
4:V:385:CYS:CB	4:V:396:ILE:HG12	2.28	0.53
3:U:136:GLU:HG2	5:W:189:ARG:HG2	1.91	0.53
6:X:36:LEU:HD22	6:X:77:VAL:HG21	1.90	0.53
3:3:155:THR:HB	4:4:321:MET:CA	2.38	0.53
1:A:29:LEU:O	1:A:29:LEU:HD23	2.09	0.53
3:C:218:LEU:N	3:C:219:PRO:HD3	2.23	0.53
3:C:307:LYS:CE	3:C:307:LYS:N	2.71	0.53
3:C:510:GLY:CA	3:C:520:ARG:HH22	2.21	0.53
3:C:54:LEU:C	3:C:54:LEU:HD13	2.29	0.53
3:C:684:ARG:HG2	3:C:684:ARG:NH1	2.18	0.53
4:D:313:PRO:C	4:D:315:HIS:N	2.62	0.53
5:E:15:TYR:CE1	5:E:30:PRO:HD2	2.44	0.53
6:F:165:GLU:C	6:F:167:GLY:N	2.62	0.53
6:F:42:GLY:O	6:F:43:LEU:HD23	2.09	0.53
7:G:133:LYS:HG2	7:G:137:LEU:HD11	1.90	0.53
7:G:175:ALA:HB1	7:G:176:PRO:HD2	1.88	0.53
2:K:10:PHE:C	2:K:10:PHE:CD1	2.81	0.53
3:L:275:LEU:N	3:L:275:LEU:HD22	2.24	0.53
4:M:65:GLY:O	4:M:66:PHE:C	2.47	0.53
3:U:137:TYR:CD1	3:U:137:TYR:N	2.76	0.53
3:U:244:ALA:HB3	3:U:249:MET:HE1	1.90	0.53
3:U:307:LYS:CE	3:U:307:LYS:N	2.70	0.53
3:U:621:VAL:HG21	3:U:671:GLU:O	2.09	0.53
3:U:643:LEU:O	3:U:646:GLU:HB2	2.09	0.53
4:V:51:GLU:O	4:V:52:VAL:HG22	2.08	0.53
5:W:37:GLU:O	5:W:41:TYR:CD1	2.59	0.53
7:Y:33:LEU:HD22	7:Y:37:PHE:CD2	2.44	0.53
1:1:253:GLN:NE2	1:1:325:THR:O	2.42	0.53
3:3:211:ILE:HG23	3:3:211:ILE:O	2.08	0.53
3:3:37:LYS:HE3	3:3:432:PHE:HE1	1.72	0.53
5:5:48:PHE:O	5:5:50:ALA:N	2.41	0.53
7:9:113:ILE:O	7:9:113:ILE:HG23	2.08	0.53
3:C:203:ILE:O	3:C:204:GLU:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:125:GLY:HA3	3:C:246:ASN:HD22	1.73	0.53
3:C:269:THR:CG2	3:C:274:LEU:HD13	2.38	0.53
3:C:336:ALA:HB3	3:C:565:TYR:CE2	2.43	0.53
3:C:52:ILE:HG22	3:C:53:GLY:N	2.22	0.53
4:D:367:ARG:HG2	4:D:367:ARG:NH1	2.24	0.53
6:F:83:ARG:HA	6:F:111:CYS:HB3	1.90	0.53
8:H:89:ALA:O	8:H:91:ILE:N	2.42	0.53
1:J:13:PHE:C	1:J:13:PHE:HD1	2.10	0.53
2:K:146:THR:OG1	2:K:149:ARG:HB2	2.09	0.53
4:M:112:ARG:O	4:M:112:ARG:HG2	2.08	0.53
4:M:148:TYR:O	4:M:151:ARG:N	2.42	0.53
5:N:104:VAL:O	5:N:104:VAL:HG12	2.07	0.53
5:N:7:LEU:O	5:N:11:ARG:HG2	2.09	0.53
1:S:20:HIS:HE1	1:S:226:SER:HA	1.73	0.53
2:T:112:THR:OG1	2:T:113:PRO:HD2	2.09	0.53
2:T:59:GLU:O	2:T:63:VAL:HG23	2.09	0.53
3:U:757:HIS:C	3:U:758:LEU:HD12	2.28	0.53
4:V:200:ARG:HG3	4:V:200:ARG:O	2.09	0.53
4:V:220:GLY:O	4:V:272:VAL:HG22	2.08	0.53
4:V:234:LEU:O	4:V:236:GLY:N	2.42	0.53
5:W:28:VAL:O	5:W:29:LEU:HD23	2.09	0.53
5:W:40:HIS:C	5:W:42:LYS:H	2.11	0.53
5:W:50:ALA:HA	5:W:73:GLU:O	2.09	0.53
8:Z:63:LEU:HD13	8:Z:129:ALA:CB	2.37	0.53
2:2:88:CYS:O	2:2:93:ALA:HB2	2.07	0.53
4:4:320:SER:OG	4:4:323:ALA:HB3	2.08	0.53
4:4:381:LEU:CD1	4:4:397:ILE:HG12	2.39	0.53
4:4:47:LEU:H	4:4:47:LEU:HD12	1.74	0.53
6:6:83:ARG:HA	6:6:111:CYS:HB3	1.91	0.53
4:D:393:MET:C	4:D:396:ILE:HG22	2.28	0.53
6:F:92:MET:CE	6:F:127:VAL:HG13	2.38	0.53
1:J:395:GLU:O	1:J:396:GLY:O	2.25	0.53
3:L:286:ASN:HD22	3:L:287:GLU:N	2.07	0.53
3:L:382:PHE:CD1	3:L:382:PHE:N	2.77	0.53
4:M:188:PRO:O	4:M:191:LYS:HB2	2.08	0.53
4:M:211:SER:OG	4:M:212:PRO:HD2	2.08	0.53
5:N:71:VAL:CG1	5:N:89:PHE:HD2	2.20	0.53
7:P:43:LEU:O	7:P:138:VAL:HG13	2.09	0.53
7:P:94:ASN:O	7:P:96:LEU:N	2.42	0.53
8:Q:87:PRO:O	8:Q:89:ALA:N	2.41	0.53
3:U:413:LEU:HA	3:U:416:PHE:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:561:PRO:HB3	3:U:576:ALA:CA	2.37	0.53
8:Z:67:PHE:CZ	8:Z:123:ARG:HG3	2.44	0.53
8:Z:38:PRO:C	8:Z:40:PHE:N	2.62	0.53
1:1:10:ASP:CB	1:1:11:PRO:CD	2.71	0.53
1:1:50:PRO:O	1:1:53:VAL:HG12	2.09	0.53
3:3:570:PHE:O	3:3:572:PRO:HD3	2.09	0.53
6:6:123:ILE:CG2	6:6:124:VAL:N	2.71	0.53
2:B:153:LEU:C	2:B:153:LEU:HD13	2.28	0.53
2:B:66:PHE:CE1	3:C:205:ARG:HD3	2.44	0.53
3:C:244:ALA:HB3	3:C:249:MET:CE	2.39	0.53
3:C:340:GLU:HA	3:C:366:THR:HB	1.90	0.53
4:D:109:VAL:HG12	4:D:113:ALA:HB3	1.91	0.53
4:D:232:LEU:HD13	4:D:278:VAL:CG1	2.39	0.53
4:D:371:ARG:HH22	4:D:376:VAL:HG21	1.72	0.53
8:H:116:PHE:O	8:H:120:ASP:HB2	2.09	0.53
2:K:131:ALA:CB	2:K:132:PRO:CD	2.80	0.53
3:L:25:HIS:ND1	3:L:427:ASN:HB2	2.24	0.53
3:L:495:GLU:O	3:L:499:LYS:HG3	2.08	0.53
4:M:122:GLU:HB2	4:M:290:ILE:HD11	1.91	0.53
4:M:344:VAL:HG23	4:M:344:VAL:O	2.09	0.53
5:N:26:TRP:CD1	5:N:26:TRP:N	2.77	0.53
3:U:616:ASN:OD1	3:U:617:LEU:N	2.41	0.53
5:W:58:LEU:HD12	5:W:59:THR:H	1.74	0.53
6:X:164:ASN:CB	7:Y:148:ARG:HE	2.14	0.53
4:4:290:ILE:O	4:4:294:LEU:HB2	2.08	0.53
3:C:2:VAL:HG13	3:C:89:ASP:CA	2.37	0.53
4:D:252:TYR:CE2	4:D:346:THR:HA	2.44	0.53
5:E:20:ASN:OD1	5:E:22:LEU:HG	2.07	0.53
6:F:117:MET:O	6:F:117:MET:HG3	2.08	0.53
1:J:161:ASN:OD1	1:J:166:ASP:HA	2.09	0.53
3:L:167:HIS:O	3:L:167:HIS:ND1	2.41	0.53
3:L:415:GLU:HG2	3:L:418:ARG:HH21	1.73	0.53
6:O:154:LEU:O	6:O:158:VAL:HG13	2.08	0.53
6:O:26:LYS:HD2	6:O:26:LYS:O	2.08	0.53
3:U:409:LEU:HD12	3:U:535:MET:CE	2.39	0.53
5:W:22:LEU:O	5:W:24:ASN:N	2.35	0.53
4:V:84:ARG:HG2	9:X:182:SF4:S2	2.49	0.53
7:Y:35:PRO:HD3	7:Y:164:PRO:HG3	1.91	0.53
2:2:112:THR:OG1	2:2:113:PRO:HD2	2.08	0.53
2:2:61:MET:HE3	8:7:88:ARG:HD3	1.89	0.53
4:4:138:LEU:HD11	4:4:146:PHE:CG	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:229:ALA:CB	4:4:241:ALA:O	2.57	0.53
2:B:114:ASP:HB2	2:B:116:LEU:HD21	1.90	0.53
3:C:166:LYS:HG3	3:C:178:ARG:CG	2.39	0.53
3:C:517:ALA:HA	3:C:520:ARG:CG	2.39	0.53
3:C:732:ALA:O	3:C:746:ARG:HA	2.09	0.53
6:F:164:ASN:HB3	7:G:148:ARG:HH21	1.74	0.53
2:K:134:ILE:HG13	2:K:145:VAL:HG21	1.91	0.53
3:L:477:LEU:HD21	3:L:520:ARG:HG2	1.90	0.53
4:M:274:ASP:O	4:M:278:VAL:HG23	2.08	0.53
1:S:33:LEU:HA	1:S:37:GLY:HA3	1.91	0.53
4:V:237:GLY:O	4:V:239:LEU:HG	2.09	0.53
1:1:13:PHE:HD1	1:1:13:PHE:C	2.13	0.53
1:1:184:GLU:O	1:1:185:GLU:C	2.45	0.53
4:4:367:ARG:HG2	4:4:367:ARG:NH1	2.23	0.53
4:4:52:VAL:CG1	4:4:388:GLU:O	2.57	0.53
4:4:68:LYS:O	4:4:71:GLU:HB2	2.08	0.53
6:6:91:VAL:HG22	6:6:94:ARG:HH21	1.74	0.53
3:C:293:ALA:CB	3:C:698:MET:HG2	2.38	0.53
4:D:234:LEU:O	4:D:236:GLY:N	2.41	0.53
4:D:51:GLU:O	4:D:52:VAL:HG22	2.08	0.53
5:E:49:LEU:CB	5:E:77:LEU:HD21	2.23	0.53
6:F:26:LYS:HD2	6:F:26:LYS:C	2.29	0.53
3:L:307:LYS:CE	3:L:307:LYS:N	2.72	0.53
3:L:346:ALA:HA	3:L:372:GLN:HB2	1.91	0.53
3:L:404:GLU:HB3	3:L:697:THR:HA	1.90	0.53
5:N:60:TYR:CG	5:N:61:PRO:HD2	2.44	0.53
1:S:184:GLU:O	1:S:185:GLU:C	2.48	0.53
1:S:395:GLU:O	1:S:396:GLY:O	2.25	0.53
2:T:79:HIS:CD2	2:T:118:SER:HB2	2.44	0.53
3:U:355:LEU:O	3:U:358:SER:HB3	2.08	0.53
3:U:631:ASN:C	3:U:633:GLU:N	2.61	0.53
4:V:353:LEU:HD12	4:V:354:GLY:H	1.71	0.53
5:W:71:VAL:CG1	5:W:89:PHE:HD2	2.22	0.53
3:3:167:HIS:O	3:3:167:HIS:ND1	2.42	0.52
3:3:732:ALA:O	3:3:746:ARG:HA	2.09	0.52
1:A:433:ARG:NH1	2:B:94:GLU:OE1	2.41	0.52
3:C:307:LYS:HE2	3:C:307:LYS:H	1.73	0.52
3:C:451:PHE:HE1	3:C:466:GLU:HB2	1.74	0.52
4:D:168:PHE:HA	4:D:170:HIS:CE1	2.44	0.52
8:H:16:LEU:HD21	8:H:115:PHE:CE1	2.44	0.52
1:J:337:MET:O	1:J:341:MET:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:616:ASN:OD1	3:L:618:GLU:HG2	2.09	0.52
3:L:631:ASN:OD1	3:L:633:GLU:OE2	2.27	0.52
3:L:746:ARG:O	3:L:748:VAL:N	2.42	0.52
4:M:199:HIS:O	4:M:201:ILE:N	2.42	0.52
4:M:385:CYS:CB	4:M:396:ILE:HG12	2.35	0.52
4:M:403:VAL:O	4:M:406:ASP:HB3	2.08	0.52
4:M:240:ARG:HD3	5:N:77:LEU:HB3	1.90	0.52
2:T:86:LEU:O	2:T:89:LYS:N	2.42	0.52
3:U:483:ASP:O	3:U:484:LYS:HG2	2.09	0.52
3:U:652:PRO:O	3:U:654:PHE:N	2.42	0.52
4:V:108:VAL:HG23	4:V:108:VAL:O	2.08	0.52
5:W:58:LEU:O	5:W:59:THR:HB	2.09	0.52
6:X:83:ARG:HD3	6:X:111:CYS:SG	2.49	0.52
7:Y:162:VAL:HA	7:Y:176:PRO:HG2	1.90	0.52
8:Z:38:PRO:O	8:Z:40:PHE:N	2.41	0.52
1:1:38:TYR:OH	1:1:112:HIS:CD2	2.62	0.52
1:1:323:LEU:HD23	1:1:324:GLY:N	2.23	0.52
1:1:40:THR:O	1:1:44:VAL:HG23	2.08	0.52
2:2:79:HIS:CD2	2:2:118:SER:HB2	2.44	0.52
3:3:652:PRO:O	3:3:654:PHE:N	2.42	0.52
4:4:84:ARG:HD3	6:6:117:MET:HE3	1.92	0.52
1:A:301:PRO:HB2	1:A:303:THR:CG2	2.38	0.52
1:A:391:LEU:N	1:A:392:PRO:HD2	2.24	0.52
1:A:434:PRO:HG2	1:A:436:LEU:HD11	1.91	0.52
3:C:561:PRO:HB3	3:C:576:ALA:CA	2.33	0.52
4:D:343:TYR:C	4:D:343:TYR:CD1	2.83	0.52
3:C:136:GLU:O	5:E:188:SER:HB2	2.09	0.52
5:E:39:ALA:O	5:E:42:LYS:N	2.42	0.52
7:G:31:VAL:O	7:G:161:TYR:HA	2.09	0.52
1:J:272:PHE:O	1:J:276:ILE:HG13	2.09	0.52
2:K:136:VAL:CG1	2:K:137:ASN:N	2.56	0.52
3:L:44:ALA:O	3:L:45:CYS:HB3	2.08	0.52
3:L:46:ARG:HH11	3:L:46:ARG:HG2	1.74	0.52
3:L:474:ARG:CB	3:L:516:VAL:HG22	2.38	0.52
5:N:103:THR:HG22	5:N:131:ASP:HB2	1.91	0.52
5:N:22:LEU:O	5:N:24:ASN:N	2.36	0.52
3:L:216:PHE:CZ	8:Q:128:PHE:CD2	2.95	0.52
8:Q:37:PHE:CD1	8:Q:55:MET:HB2	2.44	0.52
1:S:7:SER:HB3	1:S:15:ARG:HH22	1.73	0.52
2:T:116:LEU:HG	2:T:117:PHE:CD2	2.44	0.52
2:T:163:LEU:HA	2:T:166:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:398:VAL:C	3:U:399:LEU:HD12	2.29	0.52
4:V:350:ARG:HG2	4:V:350:ARG:O	2.08	0.52
5:W:103:THR:HG22	5:W:131:ASP:HB2	1.91	0.52
6:X:110:ALA:HB1	6:X:116:GLY:HA2	1.90	0.52
8:Z:89:ALA:O	8:Z:91:ILE:N	2.42	0.52
3:3:254:THR:OG1	3:3:624:LEU:HD23	2.09	0.52
3:3:2:VAL:HG12	3:3:3:ARG:N	2.24	0.52
4:4:224:ILE:HD13	5:5:112:ASN:HA	1.92	0.52
5:5:27:VAL:O	5:5:90:VAL:HA	2.09	0.52
2:B:136:VAL:CG1	2:B:137:ASN:N	2.62	0.52
3:C:38:HIS:NE2	3:C:287:GLU:HG2	2.24	0.52
3:C:477:LEU:HD21	3:C:520:ARG:HG2	1.92	0.52
4:D:152:GLU:HG2	4:D:197:LEU:HD21	1.91	0.52
4:D:220:GLY:HA3	4:D:396:ILE:CD1	2.40	0.52
4:D:246:TYR:CB	4:D:347:GLU:HG3	2.38	0.52
4:D:64:THR:HG22	4:D:64:THR:O	2.10	0.52
5:E:147:ARG:HG2	5:E:150:TYR:HB2	1.91	0.52
8:H:39:ASP:OD2	8:H:75:ARG:HG3	2.09	0.52
3:L:87:VAL:HA	3:L:91:MET:HE1	1.92	0.52
7:P:123:ASP:HB2	7:P:129:LEU:HD21	1.91	0.52
1:S:408:TRP:N	1:S:409:PRO:HD2	2.24	0.52
2:T:136:VAL:CG1	2:T:137:ASN:H	2.06	0.52
3:U:169:PRO:CD	3:U:176:LEU:HD13	2.39	0.52
3:U:263:CYS:CA	3:U:286:ASN:HB2	2.38	0.52
3:U:414:SER:HA	3:U:461:TRP:CZ3	2.44	0.52
4:V:338:PRO:HD3	5:W:192:TYR:O	2.10	0.52
6:X:93:ARG:HD2	6:X:97:GLU:HG3	1.91	0.52
1:1:38:TYR:OH	1:1:112:HIS:HD2	1.93	0.52
1:1:211:LEU:HB2	1:1:216:THR:HG21	1.91	0.52
1:1:408:TRP:N	1:1:409:PRO:HD2	2.24	0.52
3:3:337:ARG:HD2	3:3:338:GLY:N	2.24	0.52
3:3:46:ARG:HG2	3:3:46:ARG:NH1	2.25	0.52
4:4:109:VAL:HG12	4:4:113:ALA:HB3	1.90	0.52
4:4:85:MET:HE1	4:4:409:ARG:CB	2.31	0.52
7:9:35:PRO:HD3	7:9:164:PRO:HG3	1.91	0.52
1:A:357:THR:N	1:A:358:PRO:CD	2.72	0.52
2:B:57:PRO:HD2	3:C:215:ASP:OD1	2.10	0.52
3:C:510:GLY:HA3	3:C:520:ARG:HH22	1.75	0.52
3:C:578:LYS:HB3	3:C:578:LYS:NZ	2.24	0.52
4:D:70:MET:C	4:D:72:HIS:H	2.12	0.52
5:E:48:PHE:O	5:E:50:ALA:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:44:MET:C	8:H:46:ARG:H	2.12	0.52
8:H:6:GLU:OE1	8:H:80:LYS:HE3	2.10	0.52
3:C:208:HIS:HB3	8:H:85:ARG:NH2	2.25	0.52
1:J:9:LEU:HA	1:J:13:PHE:HZ	1.74	0.52
1:J:266:LEU:HB3	1:J:267:PRO:HD2	1.92	0.52
3:L:414:SER:O	3:L:418:ARG:HG3	2.09	0.52
3:L:643:LEU:O	3:L:646:GLU:HB2	2.08	0.52
4:M:254:TYR:O	4:M:256:GLY:N	2.42	0.52
1:S:353:CYS:SG	1:S:354:GLY:N	2.83	0.52
2:T:109:GLY:HA2	8:Z:91:ILE:HD13	1.91	0.52
3:U:19:VAL:HG23	3:U:85:THR:O	2.09	0.52
3:U:11:VAL:HG11	3:U:25:HIS:CD2	2.45	0.52
3:U:557:SER:H	3:U:560:GLU:HB3	1.74	0.52
4:V:133:LEU:HD21	4:V:204:TYR:HD2	1.69	0.52
4:V:225:PRO:CD	4:V:226:PRO:HD3	2.39	0.52
1:1:203:PRO:HB2	1:1:204:PRO:HD3	1.91	0.52
3:3:73:ILE:O	3:3:73:ILE:HD12	2.09	0.52
4:4:344:VAL:HG23	4:4:344:VAL:O	2.10	0.52
6:6:92:MET:CE	6:6:127:VAL:HG13	2.39	0.52
8:7:84:LEU:HB2	8:7:93:LEU:HB2	1.92	0.52
7:9:101:CYS:O	7:9:103:LEU:N	2.43	0.52
1:A:11:PRO:HG3	1:A:270:THR:HA	1.90	0.52
3:C:398:VAL:C	3:C:399:LEU:HD12	2.29	0.52
3:C:643:LEU:O	3:C:646:GLU:HB2	2.10	0.52
4:D:132:PHE:CE2	4:D:279:ARG:HD2	2.43	0.52
4:D:224:ILE:CB	4:D:225:PRO:CD	2.80	0.52
3:L:33:PHE:CZ	3:L:130:LEU:HA	2.44	0.52
3:L:113:LEU:O	3:L:161:ARG:NH1	2.41	0.52
4:M:244:VAL:HG13	4:M:246:TYR:CD1	2.44	0.52
1:S:357:THR:N	1:S:358:PRO:CD	2.71	0.52
1:S:337:MET:HB2	1:S:420:GLN:NE2	2.25	0.52
3:U:168:HIS:HE1	8:Z:32:GLU:OE1	1.93	0.52
3:U:173:PHE:CE1	3:U:174:VAL:HG22	2.45	0.52
3:U:226:ILE:HD12	3:U:235:LEU:CD1	2.39	0.52
3:U:340:GLU:H	3:U:366:THR:CB	2.23	0.52
1:1:374:ILE:HA	1:1:379:GLY:HA3	1.91	0.52
1:1:433:ARG:NH1	2:2:94:GLU:OE1	2.42	0.52
3:3:161:ARG:HG2	3:3:161:ARG:HH11	1.74	0.52
3:3:203:ILE:O	3:3:204:GLU:HB2	2.08	0.52
4:4:238:SER:O	4:4:239:LEU:HD23	2.09	0.52
4:4:64:THR:HG22	4:4:64:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:109:GLY:H	6:6:137:VAL:HG13	1.73	0.52
4:D:256:GLY:HA2	4:D:292:GLN:NE2	2.21	0.52
4:D:316:LEU:HD13	4:D:320:SER:HB2	1.90	0.52
4:D:347:GLU:O	4:D:349:ALA:N	2.37	0.52
4:D:52:VAL:CG1	4:D:388:GLU:O	2.58	0.52
4:D:224:ILE:HD13	5:E:112:ASN:HA	1.90	0.52
7:G:143:THR:HG23	7:G:146:GLN:OE1	2.10	0.52
1:J:291:ILE:HD11	1:J:331:ILE:HD11	1.89	0.52
2:K:57:PRO:HD2	3:L:215:ASP:OD1	2.09	0.52
3:L:466:GLU:CG	3:L:489:MET:HG3	2.27	0.52
3:L:684:ARG:HG2	3:L:684:ARG:NH1	2.18	0.52
4:M:159:LEU:O	4:M:162:TRP:HB2	2.08	0.52
4:M:234:LEU:O	4:M:236:GLY:N	2.42	0.52
4:M:343:TYR:CD1	4:M:344:VAL:N	2.78	0.52
4:M:373:PRO:O	4:M:374:SER:C	2.48	0.52
5:N:40:HIS:C	5:N:42:LYS:H	2.13	0.52
6:O:165:GLU:C	6:O:167:GLY:N	2.63	0.52
1:S:169:PHE:CE2	1:S:171:LEU:HD11	2.44	0.52
1:S:10:ASP:O	1:S:267:PRO:HG3	2.10	0.52
2:T:66:PHE:C	2:T:66:PHE:CD1	2.83	0.52
3:U:155:THR:HB	4:V:321:MET:CA	2.38	0.52
3:U:268:ASP:OD2	3:U:278:ARG:NH1	2.43	0.52
3:U:470:PRO:HG3	3:U:750:ARG:NH2	2.24	0.52
2:2:42:ARG:HB3	2:2:44:GLU:OE1	2.10	0.52
3:3:477:LEU:HD21	3:3:520:ARG:HG2	1.90	0.52
8:7:89:ALA:O	8:7:91:ILE:N	2.42	0.52
3:C:173:PHE:CZ	3:C:296:PHE:CB	2.93	0.52
3:C:587:LEU:CD2	3:C:589:HIS:H	2.16	0.52
4:D:244:VAL:CG1	4:D:246:TYR:CD1	2.93	0.52
4:D:385:CYS:CB	4:D:396:ILE:HG12	2.34	0.52
7:G:94:ASN:O	7:G:96:LEU:N	2.41	0.52
1:J:7:SER:HB3	1:J:15:ARG:HH22	1.74	0.52
4:M:153:ARG:NH1	4:M:153:ARG:HG3	2.23	0.52
4:M:200:ARG:HG3	4:M:200:ARG:O	2.10	0.52
4:M:214:PHE:C	4:M:216:GLU:N	2.63	0.52
5:N:121:LEU:HB3	5:N:127:GLU:CG	2.40	0.52
6:O:164:ASN:CB	7:P:148:ARG:HE	2.15	0.52
3:L:168:HIS:HE1	8:Q:32:GLU:OE1	1.93	0.52
8:Q:38:PRO:C	8:Q:40:PHE:H	2.13	0.52
1:S:371:PHE:HA	1:S:374:ILE:CG2	2.40	0.52
3:U:336:ALA:HB3	3:U:565:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:338:GLY:HA2	3:U:364:LEU:HD11	1.92	0.52
4:V:244:VAL:HG13	4:V:246:TYR:CD1	2.44	0.52
6:X:78:MET:HG3	6:X:78:MET:O	2.10	0.52
1:1:41:ALA:HB2	1:1:116:GLU:HG3	1.91	0.52
3:3:100:VAL:O	3:3:103:ALA:HB3	2.10	0.52
3:3:390:LEU:HD21	3:3:413:LEU:HD23	1.92	0.52
4:4:168:PHE:HA	4:4:170:HIS:CE1	2.45	0.52
4:4:225:PRO:CB	4:4:226:PRO:HD3	2.40	0.52
4:4:408:ASP:O	4:4:409:ARG:C	2.48	0.52
5:5:3:LEU:CD2	5:5:3:LEU:H	2.09	0.52
4:D:116:ILE:HD12	4:D:182:LEU:CD2	2.40	0.52
5:E:147:ARG:NH1	5:E:149:ASP:OD1	2.43	0.52
5:E:71:VAL:CG1	5:E:89:PHE:HD2	2.22	0.52
1:J:203:PRO:HB2	1:J:204:PRO:HD3	1.92	0.52
2:K:46:ILE:HG23	2:K:60:VAL:CG1	2.39	0.52
3:L:113:LEU:HG	3:L:157:PHE:CD2	2.45	0.52
3:L:211:ILE:HG23	3:L:211:ILE:O	2.08	0.52
4:M:408:ASP:O	4:M:409:ARG:C	2.47	0.52
5:N:42:LYS:HA	5:N:45:GLY:CA	2.40	0.52
7:P:126:TYR:O	7:P:128:ASP:N	2.43	0.52
8:Q:63:LEU:HD13	8:Q:129:ALA:CB	2.40	0.52
1:S:283:PRO:HB3	1:S:287:ILE:HD13	1.92	0.52
3:U:451:PHE:HE1	3:U:466:GLU:HB2	1.74	0.52
4:V:343:TYR:CD1	4:V:343:TYR:C	2.83	0.52
4:V:234:LEU:CD1	5:W:49:LEU:HD21	2.34	0.52
3:3:161:ARG:NH1	3:3:161:ARG:HG2	2.24	0.52
3:3:660:ALA:O	3:3:663:ALA:HB3	2.10	0.52
4:4:316:LEU:HD13	4:4:320:SER:CB	2.39	0.52
4:4:389:GLN:HB3	4:4:391:PRO:HD2	1.91	0.52
5:5:3:LEU:N	5:5:3:LEU:HD23	2.15	0.52
6:6:165:GLU:C	6:6:167:GLY:N	2.63	0.52
1:A:98:PRO:HA	2:B:124:CYS:SG	2.50	0.52
3:C:243:ARG:CB	3:C:275:LEU:HD12	2.37	0.52
4:D:225:PRO:CB	4:D:226:PRO:HD3	2.40	0.52
5:E:31:ARG:HH11	5:E:31:ARG:HG2	1.74	0.52
6:F:109:GLY:H	6:F:137:VAL:HG13	1.75	0.52
6:F:37:TRP:HA	6:F:37:TRP:HE3	1.72	0.52
8:H:9:LEU:HD11	8:H:82:ILE:HG22	1.92	0.52
4:M:152:GLU:HG2	4:M:197:LEU:HD21	1.92	0.52
4:M:182:LEU:HD12	4:M:182:LEU:O	2.10	0.52
4:M:231:ASP:CA	4:M:235:THR:HG23	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:132:PHE:CE2	4:M:279:ARG:HD2	2.45	0.52
4:M:343:TYR:CD1	4:M:343:TYR:C	2.83	0.52
6:O:92:MET:CE	6:O:127:VAL:HG13	2.39	0.52
3:U:333:LEU:HD13	3:U:648:LEU:HD21	1.90	0.52
3:U:514:ASP:CG	3:U:685:PRO:HB3	2.29	0.52
4:V:138:LEU:HD11	4:V:146:PHE:CG	2.44	0.52
4:V:232:LEU:HD11	4:V:282:GLU:OE1	2.10	0.52
4:V:346:THR:CG2	4:V:353:LEU:HB3	2.40	0.52
4:V:82:THR:N	4:V:83:PRO:HD2	2.25	0.52
4:V:379:GLN:HG2	5:W:116:ARG:NH1	2.24	0.52
6:X:99:MET:HB3	6:X:100:PRO:HD2	1.92	0.52
2:2:47:GLU:O	2:2:50:ALA:HB3	2.10	0.52
4:4:148:TYR:O	4:4:151:ARG:HB3	2.10	0.52
4:4:64:THR:HB	4:4:66:PHE:CE1	2.44	0.52
1:A:211:LEU:HB2	1:A:216:THR:HG21	1.91	0.52
1:A:33:LEU:HA	1:A:37:GLY:HA3	1.91	0.52
2:B:122:VAL:HG12	2:B:123:GLU:H	1.74	0.52
3:C:371:PHE:CE1	3:C:544:LEU:HB3	2.45	0.52
4:D:59:ILE:HD11	5:E:138:PRO:HB3	1.92	0.52
6:F:110:ALA:HB1	6:F:116:GLY:HA2	1.91	0.52
7:G:114:VAL:HG12	7:G:115:LEU:N	2.25	0.52
7:G:161:TYR:O	7:G:176:PRO:HG3	2.09	0.52
1:J:41:ALA:HB2	1:J:116:GLU:HG3	1.91	0.52
4:M:74:THR:HG22	4:M:75:TYR:N	2.25	0.52
4:M:89:HIS:ND1	4:M:349:ALA:HB1	2.24	0.52
5:N:77:LEU:O	5:N:83:GLY:HA3	2.10	0.52
1:S:203:PRO:HB2	1:S:204:PRO:HD3	1.91	0.52
1:S:398:SER:C	3:U:46:ARG:HE	2.12	0.52
3:U:295:ARG:HD2	3:U:296:PHE:CZ	2.45	0.52
3:U:319:GLU:CD	3:U:319:GLU:H	2.13	0.52
3:U:382:PHE:CD1	3:U:382:PHE:N	2.78	0.52
3:U:732:ALA:O	3:U:746:ARG:HA	2.09	0.52
4:V:125:ARG:HH12	4:V:349:ALA:HA	1.75	0.52
5:W:48:PHE:C	5:W:50:ALA:N	2.62	0.52
6:X:117:MET:O	6:X:117:MET:HG3	2.09	0.52
4:4:52:VAL:HG11	4:4:388:GLU:O	2.10	0.51
5:5:50:ALA:HA	5:5:73:GLU:O	2.11	0.51
1:A:63:ARG:NH1	1:A:313:TYR:HB2	2.24	0.51
2:B:130:THR:O	2:B:131:ALA:O	2.27	0.51
3:C:134:THR:O	3:C:138:GLY:CA	2.57	0.51
3:C:229:ILE:HD11	3:C:289:TRP:CZ3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:346:ALA:HA	3:C:372:GLN:HB2	1.92	0.51
1:J:108:GLU:CG	1:J:140:ARG:HG2	2.34	0.51
3:L:116:PRO:O	3:L:117:LEU:HB2	2.10	0.51
5:N:39:ALA:O	5:N:42:LYS:N	2.40	0.51
5:N:42:LYS:CA	5:N:45:GLY:HA2	2.40	0.51
6:O:26:LYS:HD2	6:O:26:LYS:C	2.31	0.51
8:Q:75:ARG:HA	8:Q:80:LYS:HZ1	1.75	0.51
2:T:146:THR:OG1	2:T:149:ARG:HB2	2.09	0.51
3:U:132:ASP:O	3:U:136:GLU:HG3	2.09	0.51
3:U:173:PHE:CZ	3:U:296:PHE:HB2	2.45	0.51
3:U:746:ARG:C	3:U:748:VAL:N	2.64	0.51
4:V:109:VAL:HG12	4:V:113:ALA:HB3	1.92	0.51
5:W:174:LEU:HD21	5:W:180:GLY:HA2	1.92	0.51
3:3:564:LEU:HD21	3:3:581:ARG:CD	2.40	0.51
4:4:152:GLU:HG2	4:4:197:LEU:HD21	1.92	0.51
6:6:48:ILE:N	6:6:48:ILE:HD12	2.25	0.51
3:3:167:HIS:HE1	8:7:32:GLU:OE2	1.93	0.51
8:7:46:ARG:HB3	8:7:47:PRO:HD2	1.91	0.51
4:4:183:PRO:HD3	7:9:36:ARG:NH2	2.25	0.51
2:B:163:LEU:HA	2:B:166:ILE:HG13	1.92	0.51
2:B:26:ALA:O	2:B:30:LEU:HG	2.11	0.51
3:C:355:LEU:O	3:C:358:SER:HB3	2.10	0.51
3:C:338:GLY:HA2	3:C:364:LEU:HD11	1.92	0.51
3:C:155:THR:HB	4:D:321:MET:CA	2.39	0.51
4:D:52:VAL:HG11	4:D:388:GLU:O	2.10	0.51
2:K:163:LEU:HA	2:K:166:ILE:HG13	1.92	0.51
3:L:137:TYR:CD1	3:L:137:TYR:N	2.78	0.51
3:L:274:LEU:O	3:L:302:ASP:OD2	2.28	0.51
6:O:159:ARG:HB3	6:O:161:GLN:HG3	1.91	0.51
7:P:35:PRO:HD3	7:P:164:PRO:HG3	1.92	0.51
1:S:114:LEU:HD23	1:S:118:MET:HG3	1.92	0.51
2:T:130:THR:HG21	2:T:143:GLU:OE1	2.09	0.51
3:U:269:THR:HG23	3:U:274:LEU:HD13	1.93	0.51
3:U:46:ARG:HH11	3:U:46:ARG:HG2	1.75	0.51
4:V:385:CYS:HB3	4:V:396:ILE:CG1	2.29	0.51
1:1:11:PRO:CG	1:1:270:THR:HA	2.40	0.51
5:5:64:ARG:HB3	5:5:65:PRO:HD2	1.92	0.51
6:6:117:MET:HB3	7:9:99:ILE:HD13	1.92	0.51
1:A:20:HIS:HE1	1:A:226:SER:HA	1.72	0.51
2:B:116:LEU:CD2	2:B:116:LEU:N	2.73	0.51
2:B:86:LEU:O	2:B:89:LYS:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:ARG:O	3:C:179:GLU:C	2.48	0.51
4:D:199:HIS:C	4:D:201:ILE:H	2.13	0.51
4:D:240:ARG:HH11	5:E:78:PRO:HD2	1.75	0.51
4:D:68:LYS:O	4:D:71:GLU:HB2	2.11	0.51
8:H:43:ARG:C	8:H:44:MET:HG3	2.31	0.51
2:B:109:GLY:HA2	8:H:91:ILE:HD13	1.92	0.51
3:L:211:ILE:O	3:L:212:GLY:O	2.29	0.51
4:M:249:ARG:CB	4:M:249:ARG:NH1	2.56	0.51
2:K:111:VAL:HG12	8:Q:121:ARG:CZ	2.40	0.51
3:U:34:CYS:HB3	3:U:45:CYS:HB3	1.91	0.51
5:W:106:ASP:O	5:W:113:PHE:CZ	2.63	0.51
5:W:121:LEU:CD1	5:W:121:LEU:H	2.22	0.51
7:Y:96:LEU:HD21	7:Y:129:LEU:CD1	2.39	0.51
1:1:424:LEU:HD12	1:1:424:LEU:N	2.25	0.51
4:4:154:GLU:CD	4:4:167:ARG:HH22	2.13	0.51
4:4:240:ARG:HH11	5:5:78:PRO:HD2	1.73	0.51
4:4:51:GLU:C	4:4:52:VAL:HG22	2.30	0.51
4:4:103:LYS:CB	5:5:22:LEU:HD13	2.32	0.51
8:7:44:MET:C	8:7:46:ARG:H	2.14	0.51
7:9:56:CYS:O	9:9:184:SF4:S3	2.68	0.51
2:B:27:ILE:CG1	2:B:53:VAL:HG21	2.40	0.51
3:C:202:PHE:C	3:C:203:ILE:HD13	2.31	0.51
3:C:263:CYS:CA	3:C:286:ASN:HB2	2.38	0.51
4:D:225:PRO:HG2	4:D:239:LEU:N	2.25	0.51
4:D:346:THR:HG22	4:D:353:LEU:C	2.31	0.51
4:D:38:HIS:O	4:D:39:GLY:O	2.27	0.51
4:D:93:HIS:O	4:D:94:ASP:C	2.49	0.51
5:E:139:GLU:CG	5:E:140:ASP:N	2.62	0.51
5:E:44:MET:HE2	5:E:82:ASP:HB3	1.91	0.51
5:E:7:LEU:O	5:E:11:ARG:HG2	2.10	0.51
6:F:145:GLU:HG2	7:G:31:VAL:CG2	2.41	0.51
2:K:31:LEU:HD12	2:K:41:ILE:HD13	1.92	0.51
3:L:312:ARG:HA	3:L:316:ARG:O	2.10	0.51
3:L:398:VAL:C	3:L:399:LEU:HD12	2.31	0.51
4:M:164:THR:CB	4:M:170:HIS:HB3	2.41	0.51
4:M:225:PRO:CB	4:M:226:PRO:HD3	2.41	0.51
4:M:389:GLN:HB3	4:M:391:PRO:HD2	1.91	0.51
4:M:395:ALA:O	4:M:399:SER:HB3	2.10	0.51
8:Q:88:ARG:NE	8:Q:128:PHE:HE1	2.08	0.51
1:S:13:PHE:CE1	1:S:15:ARG:HG3	2.46	0.51
2:T:114:ASP:HB2	2:T:116:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:20:HIS:HE1	1:1:226:SER:HA	1.75	0.51
1:1:371:PHE:HA	1:1:374:ILE:CG2	2.41	0.51
3:3:261:VAL:HG23	9:3:786:SF4:S2	2.51	0.51
4:4:211:SER:OG	4:4:212:PRO:HD2	2.10	0.51
4:4:244:VAL:HG13	4:4:246:TYR:CD1	2.46	0.51
5:5:77:LEU:O	5:5:83:GLY:HA3	2.11	0.51
8:7:63:LEU:HD13	8:7:129:ALA:CB	2.40	0.51
1:A:102:LYS:HD3	1:A:253:GLN:HE22	1.76	0.51
1:A:7:SER:HB3	1:A:15:ARG:HH22	1.75	0.51
1:A:424:LEU:HD12	1:A:424:LEU:N	2.25	0.51
3:C:488:GLU:O	3:C:491:ALA:HB3	2.10	0.51
3:C:333:LEU:HD13	3:C:648:LEU:HD21	1.92	0.51
4:D:245:ASN:ND2	4:D:352:GLU:OE1	2.43	0.51
4:D:83:PRO:HB2	4:D:169:HIS:HA	1.92	0.51
5:E:127:GLU:HG3	5:E:129:HIS:HE1	1.75	0.51
4:D:245:ASN:HD21	5:E:87:ARG:HH22	1.59	0.51
6:F:154:LEU:O	6:F:158:VAL:HG13	2.11	0.51
1:J:312:SER:C	1:J:314:GLU:H	2.13	0.51
2:K:76:GLY:N	2:K:118:SER:OG	2.21	0.51
2:K:27:ILE:CG2	2:K:31:LEU:HD23	2.41	0.51
3:L:286:ASN:ND2	3:L:287:GLU:N	2.59	0.51
3:L:378:PRO:HB2	3:L:381:LEU:CD2	2.40	0.51
3:L:614:LEU:HD13	3:L:624:LEU:HD12	1.92	0.51
3:L:293:ALA:CB	3:L:698:MET:HG2	2.40	0.51
6:O:153:GLN:HG3	7:P:124:TYR:CZ	2.45	0.51
3:U:275:LEU:HD22	3:U:275:LEU:N	2.25	0.51
3:U:459:MET:CG	3:U:465:HIS:HB2	2.40	0.51
3:U:510:GLY:CA	3:U:520:ARG:NH2	2.74	0.51
3:U:474:ARG:CB	3:U:516:VAL:HG22	2.41	0.51
7:Y:118:ASP:HA	7:Y:161:TYR:HE2	1.75	0.51
3:U:167:HIS:HE1	8:Z:32:GLU:OE2	1.93	0.51
2:2:112:THR:CG2	2:2:116:LEU:HD23	2.41	0.51
3:3:137:TYR:CD1	3:3:137:TYR:N	2.77	0.51
3:3:229:ILE:HD11	3:3:289:TRP:CZ3	2.46	0.51
3:3:550:LEU:N	3:3:550:LEU:CD1	2.74	0.51
3:3:564:LEU:HD11	3:3:581:ARG:N	2.26	0.51
4:4:133:LEU:HD21	4:4:204:TYR:HD2	1.65	0.51
4:4:320:SER:OG	4:4:323:ALA:N	2.44	0.51
5:5:155:THR:H	6:6:119:ASN:HD22	1.58	0.51
5:5:58:LEU:O	5:5:59:THR:HB	2.11	0.51
7:9:94:ASN:HD22	7:9:97:ARG:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:MET:HB2	3:C:214:MET:HG3	1.93	0.51
3:C:254:THR:HG1	3:C:624:LEU:HD23	1.75	0.51
4:D:64:THR:HB	4:D:66:PHE:CE1	2.46	0.51
5:E:106:ASP:O	5:E:113:PHE:CZ	2.63	0.51
6:F:127:VAL:C	6:F:129:SER:H	2.14	0.51
1:J:332:PRO:HD2	2:K:90:LEU:HD23	1.93	0.51
3:L:261:VAL:HG23	9:L:786:SF4:S2	2.51	0.51
4:M:109:VAL:HG12	4:M:113:ALA:HB3	1.92	0.51
4:M:229:ALA:HB1	4:M:241:ALA:O	2.09	0.51
4:M:51:GLU:O	4:M:52:VAL:HG22	2.11	0.51
1:S:277:TYR:CE1	1:S:283:PRO:HD3	2.46	0.51
1:S:101:PHE:HB2	2:T:126:GLY:O	2.10	0.51
5:W:38:MET:O	5:W:41:TYR:HB2	2.09	0.51
5:W:73:GLU:OE2	5:W:87:ARG:HD3	2.10	0.51
1:1:357:THR:N	1:1:358:PRO:CD	2.74	0.51
2:2:81:GLN:O	2:2:134:ILE:HG23	2.11	0.51
3:3:268:ASP:OD2	3:3:278:ARG:NH1	2.43	0.51
3:3:409:LEU:HD12	3:3:535:MET:CE	2.41	0.51
3:3:54:LEU:C	3:3:54:LEU:HD13	2.30	0.51
3:3:631:ASN:OD1	3:3:633:GLU:OE2	2.29	0.51
4:4:214:PHE:C	4:4:216:GLU:N	2.64	0.51
4:4:224:ILE:HD12	4:4:237:GLY:CA	2.39	0.51
4:4:381:LEU:HA	4:4:384:ALA:HB3	1.92	0.51
4:4:95:LEU:HG	4:4:99:LEU:HD23	1.93	0.51
7:9:130:VAL:HG13	7:9:130:VAL:O	2.10	0.51
6:6:140:CYS:SG	7:9:99:ILE:HG13	2.51	0.51
3:C:382:PHE:CD1	3:C:382:PHE:N	2.73	0.51
4:D:229:ALA:CB	4:D:241:ALA:O	2.59	0.51
4:D:254:TYR:O	4:D:255:SER:C	2.49	0.51
5:E:46:PHE:C	5:E:48:PHE:N	2.64	0.51
4:D:183:PRO:HD3	7:G:36:ARG:NH2	2.26	0.51
1:J:261:PRO:HD2	2:K:177:HIS:O	2.11	0.51
3:L:19:VAL:HG23	3:L:85:THR:O	2.11	0.51
3:L:336:ALA:HB3	3:L:565:TYR:CE2	2.46	0.51
4:M:116:ILE:HD12	4:M:182:LEU:HD21	1.91	0.51
5:N:73:GLU:OE2	5:N:87:ARG:NH1	2.34	0.51
3:U:189:ARG:HG3	3:U:193:GLU:OE2	2.11	0.51
4:V:70:MET:C	4:V:72:HIS:N	2.64	0.51
5:W:49:LEU:HD22	5:W:77:LEU:CD2	2.41	0.51
3:3:305:ARG:HG2	3:3:306:LEU:H	1.76	0.51
3:3:112:LEU:HD13	4:4:322:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:381:LEU:HD11	4:4:397:ILE:CD1	2.40	0.51
5:5:46:PHE:C	5:5:48:PHE:H	2.14	0.51
8:7:39:ASP:OD2	8:7:75:ARG:HG3	2.11	0.51
1:A:104:ARG:NH1	1:A:108:GLU:OE2	2.44	0.51
3:C:168:HIS:HE1	8:H:32:GLU:OE1	1.93	0.51
3:C:371:PHE:CD2	3:C:374:ARG:HB2	2.46	0.51
4:D:164:THR:CB	4:D:170:HIS:HB3	2.40	0.51
5:E:10:ALA:C	5:E:12:ALA:H	2.14	0.51
6:F:78:MET:O	6:F:78:MET:HG3	2.10	0.51
7:G:96:LEU:HD21	7:G:129:LEU:CD1	2.40	0.51
3:L:290:ILE:CG2	3:L:295:ARG:HB2	2.40	0.51
5:N:20:ASN:HD21	5:N:24:ASN:HB2	1.74	0.51
4:V:220:GLY:HA3	4:V:396:ILE:CD1	2.41	0.51
4:V:264:VAL:H	4:V:285:GLU:HG3	1.76	0.51
4:V:389:GLN:HB3	4:V:391:PRO:HD2	1.91	0.51
4:V:62:LEU:N	4:V:408:ASP:OD2	2.41	0.51
4:V:83:PRO:HB2	4:V:169:HIS:HA	1.92	0.51
5:W:46:PHE:C	5:W:48:PHE:N	2.64	0.51
7:Y:94:ASN:O	7:Y:96:LEU:N	2.44	0.51
8:Z:88:ARG:NE	8:Z:128:PHE:HE1	2.09	0.51
1:1:290:ILE:HG22	1:1:330:LEU:HD23	1.93	0.51
3:3:398:VAL:HB	3:3:450:LEU:CD2	2.37	0.51
4:4:316:LEU:O	4:4:318:GLU:N	2.44	0.51
3:3:131:GLN:HA	4:4:325:ILE:HD13	1.92	0.51
6:6:84:LEU:HD13	6:6:85:SER:O	2.10	0.51
8:7:43:ARG:C	8:7:44:MET:HG3	2.30	0.51
7:9:58:LEU:N	7:9:58:LEU:HD12	2.26	0.51
1:A:179:ALA:O	1:A:182:CYS:HB2	2.10	0.51
2:B:101:THR:HG23	2:B:106:ILE:O	2.11	0.51
3:C:211:ILE:O	3:C:212:GLY:O	2.28	0.51
3:C:507:LEU:O	3:C:507:LEU:HD12	2.10	0.51
3:C:87:VAL:HA	3:C:91:MET:CE	2.41	0.51
6:F:139:GLY:CA	6:F:142:PRO:HB3	2.31	0.51
1:J:434:PRO:HG2	1:J:436:LEU:HD11	1.93	0.51
2:K:112:THR:OG1	2:K:113:PRO:HD2	2.10	0.51
4:M:187:VAL:N	4:M:188:PRO:HD2	2.25	0.51
4:M:225:PRO:HG2	4:M:238:SER:HA	1.92	0.51
1:1:274:GLU:HG3	1:1:278:GLU:OE1	2.11	0.51
3:3:34:CYS:HB3	3:3:45:CYS:HB3	1.92	0.51
3:3:587:LEU:CD2	3:3:589:HIS:H	2.18	0.51
4:4:282:GLU:O	4:4:286:SER:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:373:PRO:O	4:4:374:SER:C	2.49	0.51
4:4:342:VAL:HG21	5:5:22:LEU:HD12	1.93	0.51
6:6:26:LYS:HD2	6:6:26:LYS:C	2.32	0.51
2:2:61:MET:CE	8:7:88:ARG:HD3	2.40	0.51
3:C:13:VAL:HG22	3:C:17:THR:OG1	2.10	0.51
3:C:169:PRO:CD	3:C:176:LEU:HD13	2.41	0.51
3:C:269:THR:HG23	3:C:274:LEU:HD13	1.92	0.51
3:C:268:ASP:OD2	3:C:278:ARG:NH1	2.44	0.51
3:C:541:ALA:O	3:C:545:GLU:HG3	2.10	0.51
4:D:266:LEU:CD1	4:D:281:ARG:HB3	2.16	0.51
5:E:60:TYR:CG	5:E:61:PRO:HD2	2.45	0.51
7:G:58:LEU:O	7:G:59:CYS:C	2.50	0.51
1:J:13:PHE:CE1	1:J:15:ARG:HG3	2.46	0.51
1:J:303:THR:OG1	1:J:306:VAL:HG23	2.10	0.51
2:K:144:CYS:O	2:K:149:ARG:HD3	2.11	0.51
2:K:87:SER:OG	2:K:128:CYS:HB3	2.11	0.51
3:L:357:ALA:HB2	3:L:641:LEU:HD11	1.91	0.51
3:L:453:PRO:HB2	3:L:750:ARG:CZ	2.40	0.51
4:M:221:VAL:HB	4:M:223:VAL:HG23	1.93	0.51
4:M:340:GLY:O	4:M:341:GLU:HG3	2.11	0.51
6:O:114:SER:O	6:O:116:GLY:N	2.44	0.51
1:S:102:LYS:HD3	1:S:253:GLN:HE22	1.76	0.51
1:S:222:GLU:OE2	1:S:251:LEU:HD13	2.10	0.51
3:U:261:VAL:HG23	9:U:786:SF4:S2	2.50	0.51
3:U:540:ASN:HB2	3:U:614:LEU:HG	1.93	0.51
4:V:59:ILE:CD1	4:V:59:ILE:N	2.67	0.51
7:Y:140:VAL:HG22	7:Y:141:VAL:H	1.76	0.51
1:1:220:ASN:O	1:1:221:VAL:C	2.50	0.50
1:1:283:PRO:HB3	1:1:287:ILE:HD13	1.92	0.50
5:5:60:TYR:CD1	5:5:61:PRO:HD2	2.46	0.50
6:6:36:LEU:HD22	6:6:77:VAL:HG21	1.93	0.50
1:A:371:PHE:HA	1:A:374:ILE:CG2	2.40	0.50
3:C:375:THR:HA	3:C:512:LEU:CD1	2.41	0.50
3:C:45:CYS:O	10:C:787:FES:S1	2.70	0.50
4:D:254:TYR:CD1	4:D:255:SER:N	2.79	0.50
6:F:160:GLY:C	6:F:162:ALA:H	2.14	0.50
7:G:58:LEU:N	7:G:58:LEU:HD12	2.25	0.50
8:H:92:HIS:C	8:H:93:LEU:HD12	2.32	0.50
1:J:33:LEU:HA	1:J:37:GLY:HA3	1.93	0.50
3:L:136:GLU:O	5:N:188:SER:HB2	2.10	0.50
4:M:200:ARG:O	4:M:204:TYR:CD1	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:257:TYR:C	4:M:263:ASP:N	2.65	0.50
4:M:383:TYR:O	4:M:384:ALA:C	2.50	0.50
5:N:104:VAL:O	5:N:106:ASP:N	2.44	0.50
6:O:108:MET:SD	6:O:147:LEU:HD23	2.51	0.50
1:S:93:ALA:CB	1:S:134:VAL:HG12	2.40	0.50
4:V:207:LEU:O	4:V:211:SER:HB2	2.10	0.50
5:W:100:ARG:O	5:W:101:LEU:HB2	2.11	0.50
5:W:155:THR:N	6:X:119:ASN:HD22	2.09	0.50
6:X:92:MET:CE	6:X:127:VAL:HG13	2.41	0.50
8:Z:108:ILE:HD12	8:Z:108:ILE:N	2.26	0.50
1:1:101:PHE:CE1	1:1:253:GLN:HB2	2.46	0.50
1:1:246:SER:HB3	1:1:268:MET:HG2	1.92	0.50
2:2:76:GLY:N	2:2:118:SER:OG	2.29	0.50
3:3:31:PRO:HG3	3:3:137:TYR:CD1	2.46	0.50
4:4:313:PRO:C	4:4:315:HIS:N	2.65	0.50
6:6:137:VAL:O	6:6:137:VAL:HG13	2.11	0.50
6:6:83:ARG:HB3	6:6:123:ILE:HD13	1.92	0.50
8:7:108:ILE:HD12	8:7:108:ILE:N	2.26	0.50
3:C:254:THR:OG1	3:C:624:LEU:HD23	2.11	0.50
4:D:82:THR:N	4:D:83:PRO:HD2	2.26	0.50
5:E:42:LYS:HA	5:E:45:GLY:CA	2.42	0.50
8:H:115:PHE:O	8:H:118:LEU:HB3	2.11	0.50
1:J:23:LYS:C	1:J:24:GLU:OE1	2.50	0.50
3:L:171:SER:C	3:L:173:PHE:H	2.12	0.50
3:L:616:ASN:HD22	3:L:622:LEU:HD11	1.75	0.50
4:M:225:PRO:HD2	4:M:239:LEU:CG	2.42	0.50
4:M:51:GLU:C	4:M:52:VAL:HG22	2.30	0.50
5:N:44:MET:O	5:N:45:GLY:C	2.49	0.50
6:O:163:TYR:CD1	6:O:163:TYR:O	2.64	0.50
1:S:38:TYR:OH	1:S:112:HIS:HD2	1.93	0.50
3:U:177:ASP:CB	3:U:235:LEU:H	2.25	0.50
4:V:223:VAL:HA	4:V:226:PRO:O	2.12	0.50
4:V:64:THR:HG23	6:X:123:ILE:HD12	1.91	0.50
6:X:123:ILE:HG22	6:X:124:VAL:N	2.26	0.50
3:3:169:PRO:HD3	3:3:176:LEU:HD13	1.93	0.50
3:3:249:MET:SD	3:3:268:ASP:HB3	2.52	0.50
3:3:290:ILE:HG22	3:3:291:CYS:O	2.11	0.50
3:3:586:HIS:CE1	3:3:637:ALA:HA	2.46	0.50
3:3:54:LEU:C	3:3:73:ILE:HG22	2.32	0.50
5:5:40:HIS:O	5:5:43:ALA:N	2.45	0.50
3:C:415:GLU:HG2	3:C:418:ARG:HH21	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:616:ASN:OD1	3:C:617:LEU:N	2.45	0.50
4:D:225:PRO:HD2	4:D:239:LEU:CG	2.42	0.50
1:J:385:GLU:O	1:J:388:GLU:HB3	2.11	0.50
3:L:44:ALA:O	3:L:45:CYS:CB	2.59	0.50
3:L:517:ALA:HA	3:L:520:ARG:CG	2.41	0.50
4:M:274:ASP:O	4:M:275:ARG:C	2.50	0.50
1:S:161:ASN:OD1	1:S:166:ASP:HA	2.11	0.50
1:S:174:HIS:CD2	1:S:192:LEU:HG	2.46	0.50
1:S:26:SER:HB3	1:S:31:TYR:CD1	2.47	0.50
4:V:79:ILE:HG22	4:V:171:ASN:ND2	2.25	0.50
4:V:228:VAL:CG2	4:V:278:VAL:HG21	2.42	0.50
4:V:244:VAL:CG1	4:V:246:TYR:CD1	2.94	0.50
5:W:147:ARG:HG3	5:W:149:ASP:OD1	2.10	0.50
5:W:91:ARG:HD3	5:W:93:TYR:HE1	1.77	0.50
3:3:269:THR:CG2	3:3:274:LEU:HD13	2.41	0.50
3:3:449:ALA:HA	3:3:464:ILE:O	2.11	0.50
4:4:200:ARG:HG3	4:4:204:TYR:HE1	1.77	0.50
5:5:31:ARG:HH11	5:5:31:ARG:HG2	1.74	0.50
6:6:140:CYS:O	6:6:140:CYS:SG	2.69	0.50
6:6:93:ARG:HD2	6:6:97:GLU:HG3	1.92	0.50
1:A:261:PRO:HD2	2:B:177:HIS:O	2.12	0.50
1:A:361:GLU:OE1	3:C:114:ASN:HB2	2.12	0.50
3:C:326:PHE:O	3:C:329:LEU:HB3	2.11	0.50
3:C:474:ARG:CB	3:C:516:VAL:HG22	2.39	0.50
3:C:605:PRO:HB2	3:C:609:GLU:HG3	1.93	0.50
4:D:220:GLY:CA	4:D:396:ILE:HD11	2.41	0.50
5:E:55:LEU:CD1	5:E:55:LEU:N	2.73	0.50
5:E:8:GLU:O	5:E:9:GLU:C	2.50	0.50
6:F:140:CYS:SG	6:F:140:CYS:O	2.69	0.50
6:F:156:LYS:O	6:F:162:ALA:HB3	2.11	0.50
7:G:100:PHE:N	7:G:100:PHE:CD1	2.79	0.50
7:G:123:ASP:CG	7:G:148:ARG:HH22	2.15	0.50
8:H:13:TRP:CE2	8:H:17:LEU:HD11	2.46	0.50
2:K:86:LEU:O	2:K:87:SER:C	2.49	0.50
5:N:31:ARG:HG2	5:N:31:ARG:NH1	2.25	0.50
6:O:145:GLU:HG2	7:P:31:VAL:CG2	2.41	0.50
4:V:257:TYR:C	4:V:263:ASP:N	2.65	0.50
4:V:343:TYR:CD1	4:V:344:VAL:N	2.79	0.50
5:W:121:LEU:CD1	5:W:121:LEU:N	2.74	0.50
6:X:23:THR:O	6:X:27:LEU:HB2	2.11	0.50
6:X:91:VAL:HG22	6:X:94:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:111:VAL:HG12	8:7:121:ARG:CZ	2.41	0.50
2:2:136:VAL:CG1	2:2:137:ASN:H	1.96	0.50
2:2:163:LEU:HA	2:2:166:ILE:HG13	1.94	0.50
3:3:757:HIS:N	3:3:757:HIS:ND1	2.60	0.50
4:4:225:PRO:HG2	4:4:239:LEU:N	2.27	0.50
4:4:281:ARG:HG3	4:4:281:ARG:HH11	1.77	0.50
5:5:42:LYS:HA	5:5:45:GLY:CA	2.42	0.50
6:6:163:TYR:O	6:6:164:ASN:ND2	2.41	0.50
8:7:37:PHE:CD1	8:7:55:MET:HB2	2.47	0.50
1:A:408:TRP:N	1:A:409:PRO:HD2	2.26	0.50
5:E:7:LEU:HD13	5:E:11:ARG:CG	2.40	0.50
3:L:402:PRO:HD2	3:L:458:LEU:HD13	1.93	0.50
3:L:6:VAL:CG1	3:L:7:ASN:N	2.61	0.50
4:M:155:THR:CG2	4:M:193:LEU:HD12	2.42	0.50
4:M:223:VAL:HA	4:M:226:PRO:O	2.11	0.50
1:S:101:PHE:CB	2:T:126:GLY:O	2.59	0.50
2:T:40:TRP:CD1	2:T:74:PRO:HA	2.46	0.50
4:V:288:LYS:O	4:V:292:GLN:HB2	2.11	0.50
6:X:165:GLU:C	6:X:167:GLY:N	2.64	0.50
6:X:84:LEU:HD13	6:X:85:SER:O	2.12	0.50
8:Z:9:LEU:HD11	8:Z:82:ILE:HG22	1.92	0.50
2:2:91:ALA:HB1	2:2:132:PRO:HD3	1.94	0.50
3:3:206:GLY:C	3:3:208:HIS:H	2.15	0.50
3:3:45:CYS:O	10:3:787:FES:S1	2.70	0.50
4:4:164:THR:CB	4:4:170:HIS:HB3	2.42	0.50
4:4:84:ARG:HG2	9:6:182:SF4:S2	2.51	0.50
5:5:53:VAL:HG22	5:5:55:LEU:CD1	2.42	0.50
1:A:410:VAL:O	1:A:411:LYS:C	2.50	0.50
3:C:233:GLY:O	3:C:236:LEU:HG	2.11	0.50
3:C:81:ALA:CB	3:C:84:VAL:HG22	2.40	0.50
4:D:200:ARG:O	4:D:204:TYR:CD1	2.64	0.50
8:H:64:GLY:O	8:H:65:GLU:C	2.50	0.50
2:K:130:THR:HG21	2:K:143:GLU:OE1	2.11	0.50
3:L:203:ILE:O	3:L:204:GLU:HB2	2.11	0.50
3:L:32:LEU:O	3:L:33:PHE:CD1	2.64	0.50
3:L:386:SER:HB3	3:L:389:ASP:OD2	2.12	0.50
4:M:328:PHE:O	4:M:332:THR:HG23	2.12	0.50
5:N:137:THR:HG23	5:N:139:GLU:CD	2.32	0.50
5:N:155:THR:H	6:O:119:ASN:HD22	1.58	0.50
5:N:195:LEU:O	5:N:196:TRP:CE3	2.65	0.50
8:Q:116:PHE:O	8:Q:120:ASP:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:44:MET:C	8:Q:46:ARG:H	2.15	0.50
1:S:410:VAL:O	1:S:411:LYS:C	2.48	0.50
2:T:40:TRP:NE1	2:T:74:PRO:HG3	2.25	0.50
3:U:14:PRO:HG2	3:U:17:THR:OG1	2.12	0.50
3:U:32:LEU:O	3:U:33:PHE:CD1	2.65	0.50
3:U:757:HIS:ND1	3:U:757:HIS:N	2.60	0.50
4:V:248:VAL:C	4:V:249:ARG:HG2	2.31	0.50
5:W:34:PHE:CE1	5:W:38:MET:HB2	2.47	0.50
7:Y:31:VAL:O	7:Y:161:TYR:HA	2.11	0.50
1:1:211:LEU:CB	1:1:216:THR:HG21	2.42	0.50
1:1:301:PRO:HB2	1:1:303:THR:CG2	2.42	0.50
2:2:24:ARG:HA	2:2:53:VAL:CG1	2.42	0.50
3:3:166:LYS:CG	3:3:178:ARG:HG3	2.41	0.50
3:3:189:ARG:HG3	3:3:193:GLU:OE2	2.12	0.50
3:3:513:GLN:O	3:3:516:VAL:N	2.35	0.50
3:3:159:PHE:HE2	8:7:79:LEU:HD22	1.76	0.50
7:9:123:ASP:OD1	7:9:148:ARG:NH2	2.44	0.50
1:A:101:PHE:CE1	1:A:253:GLN:HB2	2.46	0.50
2:B:32:ARG:O	2:B:33:ARG:C	2.49	0.50
2:B:72:PHE:HB2	8:H:89:ALA:CB	2.40	0.50
3:C:115:HIS:CD2	3:C:116:PRO:HD2	2.47	0.50
3:C:188:VAL:CG2	3:C:189:ARG:N	2.75	0.50
3:C:30:VAL:HG22	3:C:48:CYS:HA	1.94	0.50
3:C:87:VAL:HA	3:C:91:MET:HE1	1.92	0.50
4:D:229:ALA:O	4:D:232:LEU:HB3	2.12	0.50
4:D:64:THR:CG2	6:F:123:ILE:HD11	2.42	0.50
7:G:126:TYR:O	7:G:128:ASP:N	2.45	0.50
3:L:319:GLU:CD	3:L:319:GLU:H	2.15	0.50
3:L:337:ARG:HD2	3:L:338:GLY:N	2.26	0.50
3:L:456:ALA:O	3:L:459:MET:HB2	2.12	0.50
4:M:316:LEU:O	4:M:318:GLU:N	2.44	0.50
5:N:16:PRO:HB2	5:N:28:VAL:CG1	2.41	0.50
5:N:155:THR:N	6:O:119:ASN:HD22	2.10	0.50
8:Q:23:TYR:C	8:Q:23:TYR:CD1	2.85	0.50
8:Q:37:PHE:HD1	8:Q:53:THR:O	1.94	0.50
2:T:101:THR:HG23	2:T:106:ILE:O	2.12	0.50
3:U:216:PHE:CZ	8:Z:128:PHE:CD2	2.98	0.50
4:V:237:GLY:CA	5:W:112:ASN:CA	2.80	0.50
4:V:254:TYR:CD1	4:V:255:SER:N	2.80	0.50
4:V:64:THR:HB	4:V:66:PHE:CE1	2.47	0.50
4:V:79:ILE:HD13	4:V:173:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:241:ARG:HD3	7:Y:74:GLU:OE1	2.12	0.50
8:Z:72:VAL:HG22	8:Z:73:SER:N	2.27	0.50
1:1:104:ARG:NH1	1:1:108:GLU:OE2	2.44	0.50
2:2:116:LEU:CD2	2:2:116:LEU:N	2.74	0.50
3:3:746:ARG:C	3:3:748:VAL:N	2.64	0.50
4:4:246:TYR:CB	4:4:347:GLU:HG3	2.42	0.50
4:4:274:ASP:O	4:4:275:ARG:C	2.50	0.50
4:4:51:GLU:O	4:4:52:VAL:HG22	2.12	0.50
4:4:93:HIS:O	4:4:94:ASP:C	2.49	0.50
5:5:42:LYS:CA	5:5:45:GLY:HA2	2.42	0.50
5:5:60:TYR:CG	5:5:61:PRO:HD2	2.47	0.50
1:A:292:PRO:HA	1:A:328:VAL:HG22	1.94	0.50
1:A:26:SER:HB3	1:A:31:TYR:CG	2.46	0.50
3:C:34:CYS:HB3	3:C:45:CYS:HB3	1.93	0.50
4:D:62:LEU:N	4:D:408:ASP:OD2	2.39	0.50
8:H:38:PRO:C	8:H:40:PHE:H	2.15	0.50
1:J:20:HIS:HE1	1:J:226:SER:HA	1.76	0.50
4:M:199:HIS:C	4:M:201:ILE:H	2.15	0.50
4:M:381:LEU:CD1	4:M:397:ILE:HG12	2.42	0.50
5:N:37:GLU:O	5:N:41:TYR:CD1	2.63	0.50
4:M:366:TYR:OH	5:N:58:LEU:O	2.30	0.50
6:O:153:GLN:HG3	7:P:124:TYR:OH	2.12	0.50
1:J:220:ASN:N	11:Q:500:FMN:O3P	2.43	0.50
1:S:181:ILE:HG23	1:S:182:CYS:N	2.26	0.50
3:U:54:LEU:C	3:U:54:LEU:HD13	2.31	0.50
3:U:672:ALA:O	3:U:673:MET:HB2	2.12	0.50
4:V:143:LEU:O	4:V:143:LEU:HD23	2.11	0.50
5:W:27:VAL:O	5:W:90:VAL:HA	2.12	0.50
6:X:164:ASN:HB3	7:Y:148:ARG:HH21	1.77	0.50
1:1:23:LYS:C	1:1:24:GLU:OE1	2.50	0.50
3:3:202:PHE:C	3:3:203:ILE:HD13	2.31	0.50
3:3:243:ARG:HD3	3:3:275:LEU:CD1	2.37	0.50
3:3:295:ARG:HD2	3:3:296:PHE:CZ	2.46	0.50
3:3:414:SER:O	3:3:418:ARG:HG3	2.11	0.50
4:4:220:GLY:HA3	4:4:396:ILE:CD1	2.42	0.50
4:4:225:PRO:HD3	4:4:239:LEU:HG	1.94	0.50
6:6:26:LYS:HD2	6:6:26:LYS:O	2.12	0.50
8:7:16:LEU:C	8:7:16:LEU:HD13	2.32	0.50
1:A:165:THR:O	1:A:167:PHE:N	2.44	0.50
3:C:753:VAL:HB	3:C:754:PRO:CD	2.42	0.50
4:D:108:VAL:HG23	4:D:108:VAL:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:274:GLU:HG3	1:J:278:GLU:OE1	2.12	0.50
1:J:357:THR:N	1:J:358:PRO:CD	2.75	0.50
3:L:188:VAL:CG2	3:L:189:ARG:N	2.75	0.50
3:L:46:ARG:HH11	3:L:46:ARG:CG	2.25	0.50
4:M:313:PRO:O	4:M:315:HIS:N	2.45	0.50
8:Q:64:GLY:O	8:Q:65:GLU:C	2.50	0.50
1:S:357:THR:HG21	3:U:111:THR:OG1	2.12	0.50
1:S:358:PRO:O	1:S:362:GLY:N	2.45	0.50
3:U:509:ALA:HA	3:U:758:LEU:CD2	2.30	0.50
3:U:532:VAL:HG12	3:U:533:LEU:N	2.27	0.50
4:V:115:THR:O	4:V:118:VAL:HG22	2.11	0.50
4:V:116:ILE:HD12	4:V:182:LEU:CD2	2.42	0.50
4:V:250:LYS:O	4:V:250:LYS:HG3	2.11	0.50
4:V:350:ARG:HD3	4:V:401:ASP:O	2.11	0.50
4:V:49:GLY:HA2	4:V:53:LEU:HD12	1.93	0.50
6:X:46:CYS:HB3	6:X:81:ALA:HB1	1.94	0.50
2:T:109:GLY:CA	8:Z:91:ILE:HD13	2.42	0.50
1:1:108:GLU:HG2	1:1:140:ARG:CG	2.38	0.49
1:1:424:LEU:H	1:1:424:LEU:HD12	1.77	0.49
3:3:440:ARG:HH11	3:3:440:ARG:HG2	1.77	0.49
3:C:261:VAL:HG23	9:C:786:SF4:S2	2.52	0.49
4:D:252:TYR:O	4:D:253:PRO:C	2.48	0.49
5:E:174:LEU:HD21	5:E:180:GLY:HA2	1.94	0.49
8:H:88:ARG:NE	8:H:128:PHE:HE1	2.10	0.49
1:J:181:ILE:HG23	1:J:182:CYS:N	2.26	0.49
2:K:66:PHE:CD1	2:K:66:PHE:C	2.84	0.49
2:K:86:LEU:HD11	2:K:90:LEU:HD11	1.91	0.49
3:L:173:PHE:CE1	3:L:174:VAL:HG22	2.45	0.49
3:L:612:GLY:O	3:L:624:LEU:HB2	2.11	0.49
4:M:311:PRO:HD3	4:M:330:HIS:NE2	2.27	0.49
5:N:64:ARG:HB3	5:N:65:PRO:HD2	1.93	0.49
5:N:8:GLU:O	5:N:9:GLU:C	2.49	0.49
1:S:63:ARG:NH1	1:S:313:TYR:HB2	2.27	0.49
1:S:291:ILE:HD11	1:S:331:ILE:HD11	1.92	0.49
3:U:113:LEU:HG	3:U:157:PHE:CD2	2.46	0.49
3:U:564:LEU:HD11	3:U:581:ARG:N	2.26	0.49
3:U:683:LEU:N	3:U:683:LEU:HD23	2.27	0.49
4:V:224:ILE:HD13	5:W:112:ASN:HA	1.94	0.49
7:Y:133:LYS:HG2	7:Y:137:LEU:HD11	1.92	0.49
8:Z:115:PHE:O	8:Z:118:LEU:HB3	2.12	0.49
8:Z:75:ARG:HA	8:Z:80:LYS:HZ1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:92:HIS:C	8:Z:93:LEU:HD12	2.33	0.49
1:1:114:LEU:HD23	1:1:118:MET:HG3	1.93	0.49
1:1:361:GLU:OE1	3:3:114:ASN:HB2	2.12	0.49
1:1:410:VAL:O	1:1:411:LYS:C	2.50	0.49
2:2:27:ILE:CG2	2:2:31:LEU:HD23	2.42	0.49
3:3:404:GLU:HB3	3:3:697:THR:HA	1.93	0.49
3:3:578:LYS:HB3	3:3:578:LYS:NZ	2.27	0.49
4:4:200:ARG:O	4:4:204:TYR:CD1	2.64	0.49
5:5:102:PRO:HA	5:5:130:PRO:CG	2.41	0.49
1:A:10:ASP:O	1:A:267:PRO:HG3	2.13	0.49
3:C:32:LEU:O	3:C:33:PHE:HD1	1.96	0.49
4:D:379:GLN:HG2	5:E:116:ARG:NH1	2.27	0.49
6:F:77:VAL:O	6:F:77:VAL:HG12	2.12	0.49
1:J:189:MET:HE1	1:J:206:PRO:HB3	1.94	0.49
1:J:271:THR:OG1	1:J:273:ARG:HB3	2.12	0.49
1:J:9:LEU:HG	1:J:13:PHE:CZ	2.47	0.49
3:L:169:PRO:CD	3:L:176:LEU:HD13	2.42	0.49
3:L:166:LYS:CG	3:L:178:ARG:HG3	2.41	0.49
3:L:340:GLU:HA	3:L:366:THR:HB	1.93	0.49
3:L:378:PRO:HB2	3:L:381:LEU:HD23	1.94	0.49
3:L:532:VAL:HG12	3:L:533:LEU:N	2.27	0.49
3:L:550:LEU:CD1	3:L:550:LEU:N	2.76	0.49
3:L:583:VAL:HG23	3:L:583:VAL:O	2.12	0.49
4:M:74:THR:HB	4:M:77:GLN:H	1.77	0.49
5:N:38:MET:O	5:N:41:TYR:HB2	2.12	0.49
5:N:40:HIS:O	5:N:43:ALA:N	2.45	0.49
1:S:49:THR:HG23	1:S:52:GLU:OE2	2.10	0.49
3:U:658:LEU:HD23	3:U:658:LEU:O	2.12	0.49
4:V:196:VAL:HG13	4:V:197:LEU:N	2.27	0.49
4:V:65:GLY:O	4:V:66:PHE:C	2.50	0.49
8:Z:70:ALA:HA	8:Z:83:GLY:O	2.12	0.49
3:3:173:PHE:CE1	3:3:296:PHE:HB3	2.47	0.49
3:3:173:PHE:CE1	3:3:174:VAL:HG22	2.44	0.49
4:4:116:ILE:HD12	4:4:182:LEU:HD21	1.94	0.49
4:4:85:MET:HE2	4:4:409:ARG:HB2	1.93	0.49
8:7:44:MET:C	8:7:46:ARG:N	2.65	0.49
3:C:118:ASP:O	3:C:122:CYS:N	2.40	0.49
3:C:218:LEU:N	3:C:218:LEU:HD23	2.26	0.49
3:C:340:GLU:H	3:C:366:THR:CB	2.24	0.49
3:C:495:GLU:O	3:C:499:LYS:HG3	2.12	0.49
3:C:672:ALA:O	3:C:673:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:514:ASP:HB2	3:C:683:LEU:HD12	1.92	0.49
3:C:6:VAL:HG21	3:C:26:ALA:CB	2.41	0.49
4:D:79:ILE:HD13	4:D:173:ILE:O	2.12	0.49
4:D:228:VAL:O	4:D:231:ASP:N	2.46	0.49
4:D:344:VAL:HG23	4:D:344:VAL:O	2.11	0.49
8:H:46:ARG:HB3	8:H:47:PRO:HD2	1.93	0.49
1:J:291:ILE:O	1:J:328:VAL:HA	2.11	0.49
3:L:173:PHE:CE1	3:L:296:PHE:HB3	2.47	0.49
3:L:510:GLY:CA	3:L:520:ARG:NH2	2.75	0.49
3:L:616:ASN:OD1	3:L:617:LEU:N	2.45	0.49
4:M:197:LEU:O	4:M:198:PRO:C	2.50	0.49
4:M:220:GLY:HA3	4:M:396:ILE:CD1	2.41	0.49
4:M:371:ARG:HH22	4:M:376:VAL:HG21	1.78	0.49
5:N:3:LEU:N	5:N:3:LEU:HD23	2.20	0.49
3:U:285:VAL:HG22	3:U:286:ASN:H	1.77	0.49
3:U:587:LEU:HD22	3:U:589:HIS:N	2.19	0.49
4:V:153:ARG:NH1	4:V:153:ARG:HG3	2.27	0.49
4:V:317:LEU:HD21	4:V:327:HIS:CD2	2.47	0.49
1:1:436:LEU:CD2	2:2:90:LEU:HA	2.43	0.49
3:3:127:ALA:HB2	5:5:181:LEU:HD23	1.94	0.49
3:3:459:MET:CG	3:3:465:HIS:HB2	2.42	0.49
4:4:196:VAL:HG13	4:4:197:LEU:H	1.78	0.49
6:6:164:ASN:HB3	7:9:148:ARG:HH21	1.78	0.49
2:B:40:TRP:CD1	2:B:74:PRO:HA	2.46	0.49
3:C:47:MET:SD	3:C:107:MET:HB3	2.52	0.49
4:D:257:TYR:C	4:D:263:ASP:N	2.66	0.49
4:D:312:PRO:O	4:D:313:PRO:C	2.51	0.49
4:D:341:GLU:OE1	5:E:26:TRP:HH2	1.95	0.49
1:J:29:LEU:HD23	1:J:29:LEU:O	2.12	0.49
2:K:101:THR:HG23	2:K:106:ILE:O	2.13	0.49
3:L:263:CYS:CA	3:L:286:ASN:HB2	2.42	0.49
3:L:505:LEU:O	3:L:532:VAL:HG13	2.13	0.49
4:M:220:GLY:O	4:M:272:VAL:HG22	2.13	0.49
4:M:246:TYR:CB	4:M:347:GLU:HG3	2.43	0.49
8:Q:15:GLU:O	8:Q:18:SER:HB3	2.11	0.49
8:Q:44:MET:C	8:Q:46:ARG:N	2.66	0.49
8:Q:72:VAL:HG22	8:Q:73:SER:N	2.26	0.49
2:T:35:GLN:O	2:T:39:GLY:N	2.39	0.49
3:U:286:ASN:HD22	3:U:287:GLU:N	2.10	0.49
4:D:191:LYS:HZ2	3:U:730:GLU:HG3	1.71	0.49
6:X:164:ASN:H	6:X:170:LEU:CD1	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:16:LEU:HG	8:Z:82:ILE:HD11	1.95	0.49
1:1:103:ASP:OD1	1:1:221:VAL:HB	2.11	0.49
4:4:350:ARG:HD3	4:4:401:ASP:O	2.13	0.49
5:5:75:VAL:CG2	5:5:87:ARG:HG3	2.43	0.49
6:6:23:THR:O	6:6:27:LEU:HB2	2.13	0.49
7:9:94:ASN:O	7:9:96:LEU:N	2.45	0.49
1:A:11:PRO:CG	1:A:270:THR:HA	2.43	0.49
1:A:428:LYS:O	3:U:316:ARG:NH2	2.45	0.49
1:A:9:LEU:HD23	1:A:9:LEU:C	2.32	0.49
2:B:46:ILE:HG23	2:B:60:VAL:CG1	2.43	0.49
3:C:136:GLU:HG2	5:E:189:ARG:HG2	1.94	0.49
3:C:449:ALA:HA	3:C:464:ILE:O	2.12	0.49
5:E:58:LEU:HD12	5:E:59:THR:N	2.27	0.49
3:C:159:PHE:HE2	8:H:79:LEU:HD22	1.78	0.49
1:J:13:PHE:O	1:J:13:PHE:HD1	1.95	0.49
1:J:292:PRO:HA	1:J:328:VAL:HG22	1.95	0.49
2:K:61:MET:HB2	3:L:214:MET:HG3	1.95	0.49
3:L:177:ASP:CB	3:L:235:LEU:H	2.26	0.49
3:L:290:ILE:HG21	3:L:295:ARG:HB2	1.92	0.49
4:M:245:ASN:ND2	4:M:352:GLU:OE1	2.46	0.49
4:M:232:LEU:HD21	4:M:282:GLU:OE2	2.12	0.49
4:M:316:LEU:C	4:M:318:GLU:N	2.66	0.49
5:N:10:ALA:C	5:N:12:ALA:H	2.15	0.49
2:T:83:CYS:SG	2:T:124:CYS:HA	2.53	0.49
2:T:43:PRO:O	2:T:46:ILE:HB	2.12	0.49
3:U:112:LEU:HD13	4:V:322:GLU:HB2	1.94	0.49
3:U:293:ALA:HA	3:U:699:TRP:CZ3	2.48	0.49
4:V:224:ILE:HD12	4:V:237:GLY:CA	2.42	0.49
4:V:342:VAL:HG21	5:W:22:LEU:HD12	1.94	0.49
5:W:10:ALA:C	5:W:12:ALA:H	2.15	0.49
2:2:40:TRP:CD1	2:2:74:PRO:HA	2.47	0.49
3:3:14:PRO:HG2	3:3:17:THR:OG1	2.13	0.49
3:3:378:PRO:HB2	3:3:381:LEU:CD2	2.42	0.49
3:3:564:LEU:HD21	3:3:581:ARG:HD2	1.95	0.49
5:5:100:ARG:O	5:5:101:LEU:HB2	2.12	0.49
8:7:88:ARG:NE	8:7:128:PHE:HE1	2.10	0.49
3:C:173:PHE:CE1	3:C:296:PHE:HB3	2.47	0.49
4:D:274:ASP:O	4:D:275:ARG:C	2.49	0.49
5:E:137:THR:CG2	5:E:139:GLU:CD	2.81	0.49
3:C:133:ARG:CZ	5:E:185:LYS:HE3	2.43	0.49
5:E:57:TYR:OH	5:E:91:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:48:ILE:CD1	6:F:48:ILE:N	2.75	0.49
1:J:104:ARG:NH1	1:J:108:GLU:OE2	2.45	0.49
1:J:184:GLU:O	1:J:185:GLU:C	2.51	0.49
3:L:116:PRO:O	3:L:117:LEU:CB	2.60	0.49
3:L:564:LEU:HD11	3:L:581:ARG:N	2.24	0.49
4:M:383:TYR:HA	4:M:386:LYS:HB2	1.95	0.49
6:O:78:MET:O	6:O:78:MET:HG3	2.11	0.49
7:P:118:ASP:HA	7:P:161:TYR:HE2	1.76	0.49
8:Q:112:LYS:CG	8:Q:116:PHE:HE1	2.26	0.49
2:T:10:PHE:CD1	2:T:10:PHE:C	2.86	0.49
3:U:386:SER:HB3	3:U:389:ASP:OD2	2.13	0.49
3:U:583:VAL:HG23	3:U:583:VAL:O	2.13	0.49
3:U:52:ILE:HG12	3:U:93:VAL:HG22	1.95	0.49
4:V:148:TYR:O	4:V:151:ARG:HB3	2.13	0.49
5:W:8:GLU:O	5:W:9:GLU:C	2.50	0.49
1:1:89:LEU:O	1:1:130:GLY:HA2	2.13	0.49
3:3:155:THR:HB	4:4:321:MET:CB	2.42	0.49
3:3:369:LEU:HD12	3:3:549:VAL:HG13	1.94	0.49
2:B:133:VAL:HG12	2:B:134:ILE:N	2.28	0.49
3:C:216:PHE:CD1	8:H:63:LEU:HD23	2.47	0.49
3:C:290:ILE:CG2	3:C:295:ARG:HB2	2.43	0.49
6:F:26:LYS:O	6:F:26:LYS:HD2	2.12	0.49
7:G:42:VAL:HG21	7:G:170:LEU:HD22	1.95	0.49
1:J:53:VAL:HG11	1:J:124:ALA:HB2	1.94	0.49
1:J:407:VAL:HG23	1:J:408:TRP:N	2.27	0.49
3:L:269:THR:CG2	3:L:274:LEU:HD13	2.43	0.49
3:L:374:ARG:NH2	3:L:684:ARG:CG	2.75	0.49
4:M:248:VAL:C	4:M:249:ARG:HG2	2.33	0.49
4:M:256:GLY:C	4:M:257:TYR:HD1	2.16	0.49
4:M:132:PHE:CD2	4:M:279:ARG:HD2	2.48	0.49
3:L:133:ARG:CZ	5:N:185:LYS:HE3	2.43	0.49
1:S:258:VAL:HG21	1:S:280:ALA:HB1	1.94	0.49
1:S:41:ALA:HB2	1:S:116:GLU:HG3	1.93	0.49
3:U:33:PHE:CB	3:U:45:CYS:SG	3.01	0.49
3:U:449:ALA:HA	3:U:464:ILE:O	2.12	0.49
3:U:46:ARG:CG	3:U:46:ARG:HH11	2.25	0.49
8:Z:31:PHE:C	8:Z:31:PHE:CD1	2.86	0.49
8:Z:47:PRO:O	8:Z:48:TYR:HB2	2.10	0.49
1:1:266:LEU:CB	1:1:270:THR:HG21	2.34	0.49
3:3:112:LEU:HD23	3:3:130:LEU:HD21	1.93	0.49
3:3:453:PRO:HB2	3:3:750:ARG:CZ	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:549:VAL:C	3:3:550:LEU:HD12	2.32	0.49
3:3:655:ARG:HG3	3:3:656:LEU:HD23	1.95	0.49
4:4:143:LEU:O	4:4:143:LEU:HD23	2.12	0.49
4:4:197:LEU:O	4:4:198:PRO:C	2.51	0.49
4:4:225:PRO:HG2	4:4:238:SER:HA	1.94	0.49
4:4:284:ARG:HB2	4:4:284:ARG:HH11	1.77	0.49
5:5:147:ARG:HG2	5:5:150:TYR:HB2	1.94	0.49
5:5:15:TYR:CE1	5:5:30:PRO:HD2	2.48	0.49
5:5:20:ASN:HD21	5:5:24:ASN:HB2	1.77	0.49
8:7:92:HIS:C	8:7:93:LEU:HD12	2.33	0.49
1:A:38:TYR:OH	1:A:112:HIS:CD2	2.66	0.49
1:A:161:ASN:OD1	1:A:166:ASP:HA	2.13	0.49
2:B:66:PHE:CD1	3:C:205:ARG:HD3	2.48	0.49
3:C:402:PRO:HA	3:C:535:MET:CE	2.42	0.49
4:D:187:VAL:N	4:D:188:PRO:HD2	2.28	0.49
4:D:200:ARG:HG3	4:D:204:TYR:HE1	1.77	0.49
4:D:225:PRO:HD3	4:D:239:LEU:HG	1.94	0.49
4:D:284:ARG:HB2	4:D:284:ARG:HH11	1.77	0.49
1:J:38:TYR:OH	1:J:112:HIS:HD2	1.95	0.49
1:J:361:GLU:OE1	3:L:114:ASN:HB2	2.13	0.49
2:K:116:LEU:CD2	2:K:116:LEU:N	2.75	0.49
3:L:118:ASP:O	3:L:122:CYS:N	2.43	0.49
3:L:631:ASN:C	3:L:633:GLU:N	2.62	0.49
5:N:50:ALA:HA	5:N:73:GLU:O	2.13	0.49
6:O:106:ILE:HD11	6:O:154:LEU:HD22	1.94	0.49
8:Q:6:GLU:OE1	8:Q:80:LYS:HE3	2.12	0.49
1:S:303:THR:O	1:S:306:VAL:HG23	2.12	0.49
3:U:177:ASP:HA	3:U:235:LEU:H	1.78	0.49
3:U:717:TRP:NE1	3:U:747:VAL:HG23	2.28	0.49
4:V:228:VAL:CG1	4:V:271:ASP:HA	2.41	0.49
4:V:234:LEU:HD13	4:V:352:GLU:HB3	1.95	0.49
5:W:137:THR:CG2	5:W:139:GLU:CD	2.81	0.49
2:T:61:MET:CE	8:Z:88:ARG:HD3	2.41	0.49
1:1:149:ILE:O	1:1:153:ARG:HB2	2.13	0.49
1:1:9:LEU:HG	1:1:13:PHE:CZ	2.48	0.49
2:2:83:CYS:SG	2:2:124:CYS:HA	2.53	0.49
1:1:137:GLU:HB3	2:2:141:TYR:OH	2.13	0.49
4:4:122:GLU:HB2	4:4:290:ILE:HD11	1.95	0.49
4:4:230:ILE:HG12	4:4:239:LEU:HB3	1.95	0.49
5:5:88:PHE:CD2	5:5:89:PHE:O	2.66	0.49
5:E:121:LEU:HB3	5:E:127:GLU:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:103:LYS:CB	5:E:22:LEU:HD13	2.34	0.49
6:F:130:VAL:CG2	6:F:131:VAL:N	2.75	0.49
6:6:19:ILE:CD1	1:J:271:THR:HG23	2.43	0.49
2:K:24:ARG:HA	2:K:53:VAL:CG1	2.43	0.49
3:L:372:GLN:NE2	3:L:570:PHE:HB2	2.28	0.49
3:L:47:MET:SD	3:L:107:MET:HB3	2.53	0.49
4:M:252:TYR:CE2	4:M:346:THR:HA	2.48	0.49
4:M:381:LEU:HD11	4:M:397:ILE:CD1	2.42	0.49
6:O:77:VAL:O	6:O:77:VAL:HG12	2.13	0.49
1:S:260:ARG:O	1:S:260:ARG:HG3	2.13	0.49
1:S:26:SER:HB3	1:S:31:TYR:CG	2.48	0.49
2:T:24:ARG:HA	2:T:53:VAL:CG1	2.42	0.49
3:U:171:SER:O	3:U:173:PHE:N	2.46	0.49
4:V:230:ILE:HG12	4:V:239:LEU:HB3	1.95	0.49
3:U:155:THR:HB	4:V:321:MET:CB	2.42	0.49
4:V:381:LEU:HD11	4:V:397:ILE:CD1	2.42	0.49
4:V:61:TYR:CE1	6:X:87:LYS:HG2	2.48	0.49
3:3:178:ARG:O	3:3:179:GLU:C	2.51	0.49
3:3:326:PHE:O	3:3:329:LEU:HB3	2.13	0.49
3:3:451:PHE:CE1	3:3:466:GLU:HB2	2.47	0.49
3:3:514:ASP:O	3:3:515:THR:C	2.52	0.49
3:3:717:TRP:CD1	3:3:747:VAL:HG23	2.48	0.49
3:3:7:ASN:HD21	3:3:96:LEU:HD11	1.78	0.49
4:4:109:VAL:CG1	4:4:113:ALA:HB3	2.43	0.49
4:4:221:VAL:HB	4:4:223:VAL:HG23	1.95	0.49
4:4:224:ILE:HG21	5:5:112:ASN:HB2	1.94	0.49
4:4:132:PHE:CD2	4:4:279:ARG:HD2	2.48	0.49
4:4:316:LEU:C	4:4:318:GLU:N	2.67	0.49
4:4:346:THR:CG2	4:4:353:LEU:HB3	2.42	0.49
5:5:73:GLU:OE2	5:5:87:ARG:HD3	2.13	0.49
7:9:31:VAL:O	7:9:161:TYR:HA	2.12	0.49
2:B:106:ILE:CD1	2:B:112:THR:HB	2.42	0.49
3:C:132:ASP:O	3:C:136:GLU:HG3	2.13	0.49
3:C:731:GLY:H	3:C:747:VAL:CG1	2.08	0.49
1:J:165:THR:O	1:J:167:PHE:N	2.46	0.49
1:J:436:LEU:CD2	2:K:90:LEU:HA	2.43	0.49
1:J:95:GLU:HA	11:Q:500:FMN:N3	2.22	0.49
3:L:178:ARG:O	3:L:179:GLU:C	2.51	0.49
3:L:658:LEU:O	3:L:658:LEU:HD23	2.13	0.49
3:L:75:TRP:HA	3:L:75:TRP:CE3	2.47	0.49
4:M:270:GLY:O	4:M:271:ASP:OD2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:220:GLY:CA	4:M:396:ILE:HD11	2.43	0.49
6:O:123:ILE:HG22	6:O:124:VAL:N	2.27	0.49
1:S:38:TYR:OH	1:S:112:HIS:CD2	2.65	0.49
2:T:26:ALA:O	2:T:29:PRO:HG2	2.13	0.49
3:U:269:THR:CG2	3:U:274:LEU:HD13	2.43	0.49
3:U:365:LYS:O	3:U:367:PRO:HD3	2.12	0.49
3:U:753:VAL:HB	3:U:754:PRO:CD	2.42	0.49
4:V:225:PRO:HG2	4:V:239:LEU:N	2.26	0.49
4:V:93:HIS:O	4:V:94:ASP:C	2.51	0.49
4:V:68:LYS:NZ	5:W:150:TYR:O	2.40	0.49
6:X:83:ARG:HB3	6:X:123:ILE:HD13	1.95	0.49
7:Y:100:PHE:CD1	7:Y:100:PHE:N	2.80	0.49
1:1:101:PHE:CB	2:2:126:GLY:O	2.61	0.48
3:3:474:ARG:CB	3:3:516:VAL:HG22	2.42	0.48
6:6:77:VAL:O	6:6:77:VAL:HG12	2.13	0.48
1:A:41:ALA:HB2	1:A:116:GLU:HG3	1.94	0.48
3:C:137:TYR:N	3:C:137:TYR:CD1	2.80	0.48
3:C:293:ALA:HA	3:C:699:TRP:CZ3	2.48	0.48
4:D:346:THR:CG2	4:D:353:LEU:HB3	2.43	0.48
5:E:2:ARG:NH2	8:Z:113:GLU:HG3	2.28	0.48
5:E:70:VAL:HG12	5:E:71:VAL:N	2.27	0.48
5:E:88:PHE:CD2	5:E:89:PHE:O	2.65	0.48
1:J:26:SER:HB3	1:J:31:TYR:CG	2.48	0.48
2:K:26:ALA:O	2:K:29:PRO:HG2	2.13	0.48
3:L:206:GLY:C	3:L:208:HIS:H	2.16	0.48
3:L:652:PRO:C	3:L:654:PHE:H	2.17	0.48
3:L:731:GLY:HA2	3:L:747:VAL:CG1	2.43	0.48
4:M:228:VAL:CG2	4:M:278:VAL:HG21	2.43	0.48
3:L:155:THR:HB	4:M:321:MET:CB	2.43	0.48
4:M:95:LEU:HG	4:M:99:LEU:HD23	1.93	0.48
6:O:163:TYR:O	6:O:164:ASN:ND2	2.44	0.48
7:P:141:VAL:CG1	7:P:142:GLY:N	2.76	0.48
7:P:44:THR:OG1	7:P:52:LYS:HD2	2.12	0.48
8:Q:16:LEU:HD21	8:Q:115:PHE:CE1	2.47	0.48
1:J:95:GLU:CA	11:Q:500:FMN:HN3	2.22	0.48
3:U:241:ARG:HH11	7:Y:74:GLU:CD	2.17	0.48
3:U:173:PHE:CE1	3:U:296:PHE:HB3	2.48	0.48
3:U:416:PHE:CE1	3:U:447:LYS:HE2	2.48	0.48
7:Y:94:ASN:ND2	7:Y:97:ARG:HB2	2.27	0.48
8:Z:81:ARG:HD3	8:Z:81:ARG:O	2.13	0.48
1:1:10:ASP:O	1:1:267:PRO:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:177:ASP:CB	3:3:235:LEU:H	2.26	0.48
3:3:46:ARG:HH11	3:3:46:ARG:HG2	1.77	0.48
3:3:47:MET:C	3:3:49:LEU:H	2.16	0.48
3:3:751:GLU:OE1	3:3:751:GLU:CA	2.57	0.48
3:3:87:VAL:HA	3:3:91:MET:HE1	1.95	0.48
1:A:125:ILE:O	1:A:126:ARG:HB2	2.12	0.48
3:C:402:PRO:HB3	3:C:535:MET:HE3	1.95	0.48
3:C:631:ASN:OD1	3:C:633:GLU:OE2	2.32	0.48
5:E:42:LYS:CA	5:E:45:GLY:HA2	2.43	0.48
5:E:154:GLU:CB	6:F:119:ASN:HB3	2.43	0.48
1:J:11:PRO:CG	1:J:270:THR:HA	2.43	0.48
3:L:672:ALA:O	3:L:673:MET:HB2	2.13	0.48
4:M:320:SER:O	4:M:322:GLU:N	2.45	0.48
4:M:350:ARG:HD3	4:M:401:ASP:O	2.13	0.48
6:O:123:ILE:CG2	6:O:124:VAL:N	2.76	0.48
1:S:110:VAL:O	1:S:110:VAL:HG23	2.12	0.48
2:T:112:THR:HG23	2:T:115:GLY:H	1.78	0.48
2:T:66:PHE:CE1	3:U:205:ARG:HD3	2.48	0.48
3:U:206:GLY:C	3:U:208:HIS:H	2.16	0.48
4:V:225:PRO:HD2	4:V:239:LEU:CG	2.43	0.48
4:V:373:PRO:O	4:V:374:SER:C	2.52	0.48
4:V:393:MET:O	4:V:396:ILE:HG22	2.12	0.48
5:W:20:ASN:HD21	5:W:24:ASN:HB2	1.77	0.48
5:W:88:PHE:CD2	5:W:89:PHE:O	2.67	0.48
8:Z:6:GLU:OE1	8:Z:80:LYS:HE3	2.13	0.48
1:1:169:PHE:CE2	1:1:171:LEU:HD11	2.47	0.48
3:3:275:LEU:N	3:3:275:LEU:HD22	2.28	0.48
3:3:511:VAL:HG22	3:3:520:ARG:NH1	2.29	0.48
4:4:98:ALA:O	4:4:102:GLU:HG3	2.13	0.48
4:4:220:GLY:CA	4:4:396:ILE:HD11	2.43	0.48
4:4:343:TYR:CD1	4:4:343:TYR:C	2.86	0.48
8:7:72:VAL:HG22	8:7:73:SER:N	2.28	0.48
1:A:283:PRO:HB3	1:A:287:ILE:HD13	1.95	0.48
2:B:66:PHE:CD1	2:B:66:PHE:C	2.85	0.48
4:D:84:ARG:HG2	9:F:182:SF4:S2	2.54	0.48
5:E:26:TRP:CZ3	5:E:91:ARG:CZ	2.96	0.48
5:E:73:GLU:OE2	5:E:87:ARG:NH1	2.42	0.48
5:E:93:TYR:N	5:E:93:TYR:CD1	2.81	0.48
1:J:353:CYS:SG	1:J:354:GLY:N	2.86	0.48
2:K:32:ARG:O	2:K:33:ARG:C	2.50	0.48
3:L:153:VAL:HG12	3:L:153:VAL:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:33:PHE:HB2	3:L:45:CYS:SG	2.53	0.48
3:L:618:GLU:OE2	3:L:620:ARG:NE	2.46	0.48
4:M:272:VAL:HA	4:M:275:ARG:HD2	1.95	0.48
5:N:46:PHE:C	5:N:48:PHE:H	2.17	0.48
5:N:7:LEU:HD13	5:N:11:ARG:CG	2.42	0.48
6:O:163:TYR:CE1	7:P:152:ARG:CZ	2.96	0.48
8:Q:9:LEU:O	8:Q:12:ALA:HB3	2.13	0.48
1:S:370:LEU:HD22	1:S:370:LEU:N	2.29	0.48
3:U:75:TRP:CE3	3:U:75:TRP:HA	2.48	0.48
4:V:403:VAL:O	4:V:406:ASP:HB3	2.12	0.48
5:W:7:LEU:HD13	5:W:11:ARG:CG	2.43	0.48
1:1:93:ALA:CB	1:1:134:VAL:HG12	2.42	0.48
3:3:188:VAL:CG2	3:3:189:ARG:N	2.76	0.48
4:4:252:TYR:HE2	4:4:346:THR:HA	1.78	0.48
5:5:26:TRP:CZ3	5:5:91:ARG:CZ	2.97	0.48
1:1:220:ASN:N	11:7:500:FMN:O3P	2.46	0.48
1:A:424:LEU:HD12	1:A:424:LEU:H	1.79	0.48
2:B:177:HIS:NE2	2:B:179:VAL:HG22	2.29	0.48
1:A:343:ASN:HD22	2:B:89:LYS:HD2	1.78	0.48
3:C:155:THR:HB	4:D:321:MET:CB	2.42	0.48
3:C:177:ASP:HA	3:C:235:LEU:H	1.78	0.48
3:C:281:GLU:HG2	3:C:283:PRO:HD3	1.95	0.48
4:D:224:ILE:HG21	5:E:112:ASN:HB2	1.95	0.48
4:D:89:HIS:ND1	4:D:349:ALA:HB1	2.29	0.48
5:E:147:ARG:HG3	5:E:149:ASP:OD1	2.13	0.48
5:E:93:TYR:N	5:E:93:TYR:HD1	2.11	0.48
6:F:163:TYR:O	6:F:164:ASN:ND2	2.45	0.48
8:H:84:LEU:HB2	8:H:93:LEU:HB2	1.95	0.48
1:J:10:ASP:O	1:J:267:PRO:HG3	2.13	0.48
1:J:242:GLY:HA2	1:J:268:MET:O	2.13	0.48
1:J:290:ILE:O	1:J:292:PRO:HD3	2.12	0.48
2:K:10:PHE:CD1	2:K:11:LEU:N	2.82	0.48
3:L:112:LEU:HD13	4:M:322:GLU:HB2	1.95	0.48
3:L:37:LYS:HE3	3:L:432:PHE:HE1	1.76	0.48
4:M:342:VAL:CG2	4:M:343:TYR:N	2.76	0.48
7:P:141:VAL:CG1	7:P:142:GLY:H	2.17	0.48
7:P:58:LEU:N	7:P:58:LEU:HD12	2.28	0.48
1:S:104:ARG:NH2	1:S:105:TYR:OH	2.46	0.48
3:U:6:VAL:HG21	3:U:26:ALA:CB	2.43	0.48
3:U:229:ILE:HD11	3:U:289:TRP:HZ3	1.78	0.48
3:U:341:VAL:CG2	3:U:364:LEU:HD21	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:371:PHE:CE1	3:U:544:LEU:HB3	2.48	0.48
5:W:15:TYR:CE1	5:W:30:PRO:HD2	2.48	0.48
8:Z:44:MET:C	8:Z:46:ARG:N	2.67	0.48
1:1:29:LEU:HB2	1:1:151:GLU:OE1	2.13	0.48
2:2:136:VAL:HG21	2:2:163:LEU:CD1	2.43	0.48
3:3:188:VAL:HG23	3:3:189:ARG:N	2.27	0.48
3:3:319:GLU:CD	3:3:319:GLU:H	2.16	0.48
3:3:376:ALA:H	3:3:512:LEU:CD1	2.25	0.48
3:3:378:PRO:HB2	3:3:381:LEU:HD23	1.96	0.48
3:3:476:ILE:N	3:3:476:ILE:HD12	2.28	0.48
3:3:527:ARG:O	3:3:530:ALA:HB2	2.12	0.48
3:3:627:ALA:O	3:3:629:ILE:N	2.40	0.48
4:4:383:TYR:CD1	4:4:383:TYR:C	2.86	0.48
4:4:82:THR:N	4:4:83:PRO:HD2	2.27	0.48
5:5:131:ASP:O	5:5:132:LEU:HB2	2.13	0.48
6:6:84:LEU:O	6:6:124:VAL:HG23	2.13	0.48
8:7:16:LEU:HG	8:7:82:ILE:HD11	1.95	0.48
1:A:38:TYR:OH	1:A:112:HIS:HD2	1.95	0.48
1:A:260:ARG:O	1:A:260:ARG:HG3	2.14	0.48
3:C:249:MET:SD	3:C:268:ASP:HB3	2.53	0.48
3:C:263:CYS:CB	3:C:286:ASN:HB2	2.44	0.48
3:C:454:TYR:O	3:C:456:ALA:N	2.47	0.48
3:C:586:HIS:NE2	3:C:604:ALA:HB2	2.28	0.48
4:D:199:HIS:ND1	4:D:200:ARG:N	2.61	0.48
6:F:123:ILE:CG2	6:F:124:VAL:N	2.75	0.48
6:F:170:LEU:HD23	6:F:171:PRO:HD2	1.95	0.48
8:H:121:ARG:HG3	8:H:121:ARG:NH1	2.29	0.48
1:J:298:PRO:HD2	1:J:321:SER:OG	2.14	0.48
1:J:424:LEU:N	1:J:424:LEU:HD12	2.29	0.48
4:M:317:LEU:HD21	4:M:327:HIS:CD2	2.49	0.48
6:O:134:ASP:OD1	6:O:174:ALA:HB2	2.13	0.48
3:U:669:VAL:HG13	3:U:669:VAL:O	2.13	0.48
4:V:316:LEU:HD13	4:V:320:SER:CB	2.42	0.48
3:3:416:PHE:CE1	3:3:447:LYS:HE2	2.47	0.48
4:4:122:GLU:OE1	4:4:122:GLU:HA	2.12	0.48
4:4:132:PHE:CE2	4:4:279:ARG:HD2	2.48	0.48
4:4:200:ARG:O	4:4:200:ARG:HG3	2.13	0.48
3:3:241:ARG:HD3	7:9:74:GLU:OE1	2.14	0.48
1:A:401:PRO:O	1:A:404:ASP:HB2	2.13	0.48
3:C:185:LYS:HG2	3:C:188:VAL:HG22	1.96	0.48
3:C:532:VAL:HG12	3:C:533:LEU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:549:VAL:O	3:C:549:VAL:HG12	2.14	0.48
3:C:632:GLY:O	3:C:634:ALA:N	2.46	0.48
4:D:246:TYR:HB3	4:D:347:GLU:HA	1.96	0.48
4:D:288:LYS:O	4:D:292:GLN:HB2	2.13	0.48
4:D:408:ASP:O	4:D:409:ARG:OXT	2.32	0.48
4:D:99:LEU:HD13	4:D:102:GLU:OE1	2.14	0.48
5:E:155:THR:H	6:F:119:ASN:HD22	1.60	0.48
5:E:46:PHE:C	5:E:48:PHE:H	2.17	0.48
2:B:61:MET:HE3	8:H:88:ARG:HD3	1.95	0.48
1:J:184:GLU:OE1	1:J:186:THR:N	2.47	0.48
3:L:683:LEU:HD23	3:L:683:LEU:N	2.29	0.48
3:L:87:VAL:HA	3:L:91:MET:CE	2.44	0.48
4:M:112:ARG:NH1	4:M:181:ASP:OD2	2.46	0.48
4:M:217:ARG:HG3	4:M:217:ARG:HH11	1.78	0.48
5:N:60:TYR:HD2	5:N:62:ASP:O	1.94	0.48
1:S:13:PHE:HE1	1:S:15:ARG:HG3	1.77	0.48
2:T:116:LEU:N	2:T:116:LEU:CD2	2.76	0.48
2:T:72:PHE:HB2	8:Z:89:ALA:CB	2.43	0.48
3:U:591:HIS:ND1	3:U:592:PRO:HD2	2.29	0.48
4:V:221:VAL:HB	4:V:223:VAL:HG23	1.95	0.48
4:V:229:ALA:O	4:V:232:LEU:HB3	2.12	0.48
4:V:290:ILE:O	4:V:294:LEU:HB2	2.13	0.48
5:W:114:LEU:CD1	5:W:114:LEU:N	2.76	0.48
6:X:81:ALA:CA	6:X:108:MET:HB3	2.38	0.48
6:X:160:GLY:C	6:X:162:ALA:H	2.17	0.48
2:2:133:VAL:HG12	2:2:134:ILE:N	2.28	0.48
3:3:507:LEU:HD12	3:3:507:LEU:O	2.13	0.48
4:4:196:VAL:HG13	4:4:197:LEU:N	2.28	0.48
4:4:199:HIS:O	4:4:201:ILE:N	2.47	0.48
2:B:87:SER:CB	10:B:182:FES:S2	3.01	0.48
3:C:100:VAL:O	3:C:103:ALA:HB3	2.14	0.48
3:C:216:PHE:CZ	8:H:128:PHE:CD2	3.02	0.48
3:C:275:LEU:N	3:C:275:LEU:HD22	2.29	0.48
3:C:428:HIS:H	3:C:428:HIS:CD2	2.32	0.48
3:C:378:PRO:HA	3:C:545:GLU:OE2	2.13	0.48
3:C:550:LEU:CD1	3:C:550:LEU:N	2.76	0.48
3:C:693:TYR:O	3:C:750:ARG:HB3	2.14	0.48
4:D:104:LEU:O	4:D:104:LEU:HD23	2.14	0.48
1:J:114:LEU:HD23	1:J:118:MET:HG3	1.95	0.48
1:J:364:ALA:O	1:J:368:VAL:HG11	2.13	0.48
3:L:239:THR:CG2	3:L:298:HIS:HE1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:200:ARG:HG3	4:M:204:TYR:HE1	1.78	0.48
4:M:290:ILE:O	4:M:294:LEU:HB2	2.12	0.48
4:M:79:ILE:HG22	4:M:171:ASN:ND2	2.28	0.48
5:N:174:LEU:CD2	5:N:180:GLY:HA2	2.44	0.48
5:N:47:ASN:HD22	5:N:76:SER:CA	2.23	0.48
8:Q:112:LYS:HG2	8:Q:116:PHE:HE1	1.78	0.48
1:S:312:SER:C	1:S:314:GLU:H	2.17	0.48
2:T:79:HIS:HD2	2:T:118:SER:HB2	1.78	0.48
3:U:286:ASN:ND2	3:U:287:GLU:N	2.62	0.48
3:U:398:VAL:HB	3:U:450:LEU:CD2	2.42	0.48
3:U:621:VAL:O	3:U:621:VAL:HG23	2.13	0.48
4:V:82:THR:OG1	4:V:83:PRO:HD3	2.14	0.48
5:W:42:LYS:CA	5:W:45:GLY:HA2	2.43	0.48
1:1:391:LEU:N	1:1:392:PRO:HD2	2.29	0.48
3:3:173:PHE:HE2	3:3:699:TRP:CZ2	2.32	0.48
3:3:631:ASN:C	3:3:633:GLU:N	2.63	0.48
5:5:104:VAL:O	5:5:106:ASP:N	2.46	0.48
4:4:333:GLU:OE1	5:5:189:ARG:NH1	2.46	0.48
5:5:60:TYR:HD2	5:5:62:ASP:O	1.95	0.48
5:5:3:LEU:HD12	5:5:86:SER:OG	2.14	0.48
4:4:61:TYR:CE1	6:6:87:LYS:HG2	2.48	0.48
7:9:114:VAL:HG12	7:9:115:LEU:H	1.79	0.48
1:A:238:PHE:CZ	1:A:248:GLY:HA3	2.48	0.48
3:C:337:ARG:HD2	3:C:338:GLY:N	2.29	0.48
5:E:104:VAL:O	5:E:106:ASP:N	2.46	0.48
5:E:77:LEU:O	5:E:83:GLY:HA3	2.13	0.48
1:J:13:PHE:HE1	1:J:15:ARG:HG3	1.78	0.48
1:J:222:GLU:OE1	1:J:251:LEU:HB2	2.12	0.48
2:K:83:CYS:SG	2:K:124:CYS:HA	2.54	0.48
3:L:249:MET:SD	3:L:268:ASP:HB3	2.54	0.48
5:N:112:ASN:ND2	5:N:113:PHE:CD1	2.81	0.48
3:U:6:VAL:HG12	3:U:7:ASN:H	1.78	0.48
3:U:7:ASN:CG	3:U:96:LEU:HD11	2.33	0.48
4:V:199:HIS:O	4:V:201:ILE:N	2.47	0.48
4:V:249:ARG:NH2	5:W:87:ARG:NE	2.50	0.48
5:W:114:LEU:O	5:W:118:VAL:HG23	2.13	0.48
5:W:3:LEU:H	5:W:3:LEU:CD2	2.10	0.48
6:X:123:ILE:CG2	6:X:124:VAL:N	2.76	0.48
1:1:134:VAL:CG2	1:1:134:VAL:O	2.61	0.48
3:3:118:ASP:O	3:3:122:CYS:N	2.44	0.48
3:3:216:PHE:CZ	8:7:128:PHE:CD2	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:642:ALA:O	3:3:645:ALA:HB3	2.14	0.48
4:4:104:LEU:HD23	4:4:104:LEU:O	2.13	0.48
4:4:59:ILE:N	4:4:59:ILE:HD13	2.15	0.48
5:5:155:THR:N	6:6:119:ASN:HD22	2.12	0.48
1:A:398:SER:C	3:C:46:ARG:HE	2.17	0.48
4:D:115:THR:O	4:D:118:VAL:HG22	2.14	0.48
8:H:63:LEU:HD13	8:H:129:ALA:CB	2.43	0.48
1:J:238:PHE:CZ	1:J:248:GLY:HA3	2.49	0.48
2:K:153:LEU:HD21	2:K:163:LEU:CD1	2.44	0.48
3:L:173:PHE:CZ	3:L:296:PHE:HB2	2.48	0.48
3:L:586:HIS:HE1	3:L:637:ALA:CA	2.26	0.48
3:L:748:VAL:HG23	3:L:752:ASP:OD1	2.13	0.48
5:N:117:GLU:O	5:N:118:VAL:C	2.52	0.48
6:O:93:ARG:HD2	6:O:97:GLU:HG3	1.95	0.48
1:S:29:LEU:HD23	1:S:29:LEU:O	2.14	0.48
2:T:133:VAL:HG12	2:T:134:ILE:N	2.29	0.48
3:U:167:HIS:O	3:U:167:HIS:ND1	2.46	0.48
3:U:415:GLU:HG2	3:U:418:ARG:HH21	1.79	0.48
3:U:587:LEU:CD2	3:U:589:HIS:H	2.19	0.48
4:V:42:ARG:H	4:V:42:ARG:HD3	1.77	0.48
5:W:154:GLU:HB3	6:X:119:ASN:HB3	1.96	0.48
6:X:115:GLY:HA3	6:X:125:GLN:OE1	2.13	0.48
7:Y:63:CYS:HA	9:Y:183:SF4:S2	2.54	0.48
1:1:26:SER:HB3	1:1:31:TYR:CD1	2.49	0.48
1:1:293:GLY:C	1:1:324:GLY:O	2.52	0.48
1:1:342:TRP:O	1:1:342:TRP:CE3	2.64	0.48
1:1:398:SER:CA	3:3:46:ARG:HD2	2.43	0.48
2:2:46:ILE:HG23	2:2:60:VAL:HG11	1.96	0.48
3:3:177:ASP:CA	3:3:235:LEU:H	2.26	0.48
3:3:430:THR:HG23	3:3:431:PRO:HD2	1.96	0.48
1:1:398:SER:C	3:3:46:ARG:HE	2.16	0.48
4:4:125:ARG:NH1	4:4:125:ARG:HG3	2.28	0.48
4:4:343:TYR:CD1	4:4:344:VAL:N	2.82	0.48
4:4:96:ALA:HB2	4:4:346:THR:CG2	2.44	0.48
5:5:20:ASN:HD22	5:5:24:ASN:HB2	1.75	0.48
5:5:44:MET:O	5:5:45:GLY:C	2.52	0.48
4:4:84:ARG:CZ	6:6:117:MET:HE1	2.44	0.48
1:A:291:ILE:O	1:A:328:VAL:HA	2.14	0.48
3:C:33:PHE:HB2	3:C:45:CYS:SG	2.53	0.48
4:D:249:ARG:O	4:D:250:LYS:C	2.52	0.48
6:F:84:LEU:HD11	6:F:89:ALA:CA	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:72:PHE:HB2	8:Q:89:ALA:CB	2.41	0.48
3:L:293:ALA:HB2	3:L:698:MET:HG2	1.94	0.48
3:L:717:TRP:NE1	3:L:747:VAL:HG23	2.28	0.48
4:M:229:ALA:CB	4:M:241:ALA:O	2.61	0.48
4:M:70:MET:C	4:M:72:HIS:N	2.66	0.48
5:N:47:ASN:O	5:N:48:PHE:HB2	2.13	0.48
1:S:325:THR:O	1:S:327:GLY:N	2.47	0.48
2:T:27:ILE:HG22	2:T:31:LEU:HD23	1.96	0.48
3:U:185:LYS:HG2	3:U:188:VAL:HG22	1.96	0.48
3:U:312:ARG:HA	3:U:316:ARG:O	2.14	0.48
3:U:717:TRP:CD1	3:U:747:VAL:HG23	2.48	0.48
3:U:748:VAL:HG23	3:U:752:ASP:OD1	2.12	0.48
4:V:187:VAL:N	4:V:188:PRO:HD2	2.29	0.48
4:V:229:ALA:CB	4:V:241:ALA:O	2.62	0.48
4:V:246:TYR:CB	4:V:347:GLU:HG3	2.44	0.48
5:W:102:PRO:HA	5:W:130:PRO:CG	2.44	0.48
5:W:58:LEU:HD12	5:W:59:THR:N	2.28	0.48
5:W:77:LEU:O	5:W:83:GLY:HA3	2.13	0.48
7:Y:162:VAL:HG12	7:Y:176:PRO:HB2	1.94	0.48
1:1:161:ASN:OD1	1:1:166:ASP:HA	2.14	0.47
3:3:173:PHE:CZ	3:3:296:PHE:CB	2.96	0.47
4:4:403:VAL:O	4:4:406:ASP:HB3	2.14	0.47
5:5:7:LEU:HD13	5:5:11:ARG:CG	2.43	0.47
6:6:130:VAL:CG2	6:6:131:VAL:N	2.76	0.47
8:7:38:PRO:C	8:7:40:PHE:H	2.17	0.47
1:A:10:ASP:C	1:A:267:PRO:HG3	2.35	0.47
1:A:366:PHE:CE1	1:A:370:LEU:HD21	2.49	0.47
1:A:63:ARG:NH1	1:A:313:TYR:CB	2.78	0.47
2:B:10:PHE:CD1	2:B:11:LEU:N	2.82	0.47
3:C:621:VAL:CG2	3:C:671:GLU:O	2.62	0.47
4:D:228:VAL:CG1	4:D:271:ASP:HA	2.41	0.47
5:E:60:TYR:HD2	5:E:62:ASP:O	1.97	0.47
6:F:163:TYR:CD1	6:F:163:TYR:O	2.67	0.47
1:J:38:TYR:OH	1:J:112:HIS:CD2	2.66	0.47
3:L:757:HIS:ND1	3:L:757:HIS:N	2.62	0.47
4:M:104:LEU:HD23	4:M:104:LEU:O	2.14	0.47
4:M:93:HIS:O	4:M:94:ASP:C	2.52	0.47
7:P:51:GLU:OE1	7:P:133:LYS:HE3	2.14	0.47
1:S:238:PHE:HE1	1:S:249:MET:CE	2.27	0.47
1:S:374:ILE:HA	1:S:379:GLY:HA3	1.94	0.47
2:T:41:ILE:HD12	2:T:70:TYR:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:42:ARG:HB3	2:T:44:GLU:OE1	2.14	0.47
3:U:282:VAL:HG13	3:U:286:ASN:O	2.13	0.47
3:U:521:ALA:HA	3:U:524:LEU:HD23	1.95	0.47
4:V:156:ILE:O	4:V:159:LEU:HB2	2.14	0.47
4:V:214:PHE:C	4:V:216:GLU:N	2.65	0.47
5:W:42:LYS:HA	5:W:45:GLY:CA	2.44	0.47
4:V:245:ASN:HD21	5:W:87:ARG:HH22	1.60	0.47
7:Y:42:VAL:HG21	7:Y:170:LEU:CD2	2.44	0.47
8:Z:112:LYS:HG2	8:Z:116:PHE:CE1	2.49	0.47
8:Z:75:ARG:HA	8:Z:80:LYS:NZ	2.29	0.47
1:1:332:PRO:HD2	2:2:90:LEU:HD23	1.95	0.47
3:3:382:PHE:HD1	3:3:382:PHE:H	1.60	0.47
4:4:199:HIS:C	4:4:201:ILE:H	2.18	0.47
4:4:229:ALA:O	4:4:232:LEU:HB3	2.14	0.47
5:5:34:PHE:CE1	5:5:38:MET:HB2	2.49	0.47
4:4:366:TYR:OH	5:5:58:LEU:O	2.32	0.47
5:5:57:TYR:OH	5:5:91:ARG:NH2	2.46	0.47
6:6:114:SER:O	6:6:116:GLY:N	2.47	0.47
2:B:112:THR:OG1	2:B:113:PRO:HD2	2.14	0.47
3:C:285:VAL:CG1	3:C:286:ASN:H	2.02	0.47
3:C:400:GLY:O	3:C:401:ASP:C	2.52	0.47
3:C:477:LEU:HD13	3:C:516:VAL:HG12	1.96	0.47
5:E:40:HIS:O	5:E:43:ALA:N	2.44	0.47
7:G:114:VAL:HG12	7:G:115:LEU:H	1.79	0.47
3:L:188:VAL:HG11	3:L:201:ASP:HA	1.96	0.47
3:L:746:ARG:C	3:L:748:VAL:N	2.67	0.47
8:Q:68:LEU:HD13	8:Q:69:LEU:N	2.29	0.47
1:S:252:TYR:HB3	1:S:275:LEU:CD1	2.41	0.47
1:S:356:CYS:SG	1:S:399:PHE:N	2.86	0.47
3:U:632:GLY:O	3:U:634:ALA:N	2.47	0.47
3:U:635:GLU:HG2	3:U:639:GLN:HG2	1.97	0.47
4:V:252:TYR:O	4:V:253:PRO:C	2.53	0.47
4:V:346:THR:HG22	4:V:353:LEU:C	2.35	0.47
2:2:40:TRP:NE1	2:2:74:PRO:HG3	2.29	0.47
3:3:591:HIS:HE1	3:3:593:LEU:HD23	1.80	0.47
4:4:224:ILE:HB	4:4:237:GLY:O	2.13	0.47
4:4:228:VAL:CG2	4:4:278:VAL:HG21	2.44	0.47
4:4:272:VAL:HA	4:4:275:ARG:HD2	1.97	0.47
4:4:283:MET:O	4:4:287:VAL:HG23	2.13	0.47
1:A:10:ASP:CB	1:A:11:PRO:CD	2.69	0.47
1:A:250:LYS:HB3	1:A:252:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:LEU:HD23	3:C:130:LEU:HD21	1.95	0.47
3:C:417:VAL:O	3:C:417:VAL:HG12	2.14	0.47
3:C:173:PHE:HE2	3:C:699:TRP:CZ2	2.32	0.47
4:D:113:ALA:O	4:D:114:GLU:C	2.50	0.47
4:D:84:ARG:HD3	6:F:117:MET:HE3	1.95	0.47
6:F:139:GLY:C	6:F:142:PRO:HD3	2.34	0.47
7:G:42:VAL:HG21	7:G:170:LEU:CD2	2.44	0.47
1:J:211:LEU:CB	1:J:216:THR:HG21	2.44	0.47
4:M:334:GLY:N	4:M:363:SER:OG	2.48	0.47
5:N:59:THR:CG2	5:N:59:THR:O	2.59	0.47
1:S:89:LEU:O	1:S:130:GLY:HA2	2.13	0.47
1:S:391:LEU:N	1:S:392:PRO:HD2	2.29	0.47
4:V:344:VAL:O	4:V:344:VAL:HG23	2.14	0.47
4:V:379:GLN:O	4:V:382:PRO:HD2	2.15	0.47
7:Y:150:ALA:HA	7:Y:153:THR:HB	1.97	0.47
1:1:9:LEU:C	1:1:9:LEU:HD23	2.35	0.47
3:3:347:HIS:N	3:3:372:GLN:HB3	2.29	0.47
3:3:403:THR:HG22	3:3:403:THR:O	2.14	0.47
3:3:454:TYR:O	3:3:456:ALA:N	2.47	0.47
3:3:592:PRO:HA	3:3:595:GLU:HG2	1.96	0.47
4:4:288:LYS:O	4:4:292:GLN:HB2	2.14	0.47
5:5:134:LYS:NZ	5:5:136:LEU:HB3	2.29	0.47
6:6:142:PRO:HB2	6:6:146:ALA:HB3	1.97	0.47
2:B:27:ILE:CG2	2:B:31:LEU:HD23	2.44	0.47
3:C:238:LEU:C	3:C:240:ALA:N	2.68	0.47
3:C:470:PRO:HG3	3:C:750:ARG:HH21	1.79	0.47
3:C:746:ARG:C	3:C:748:VAL:N	2.67	0.47
4:D:381:LEU:C	4:D:381:LEU:HD23	2.35	0.47
4:D:383:TYR:O	4:D:386:LYS:N	2.35	0.47
6:F:99:MET:HB3	6:F:100:PRO:HD2	1.96	0.47
8:H:38:PRO:O	8:H:40:PHE:N	2.47	0.47
1:J:410:VAL:O	1:J:411:LYS:C	2.53	0.47
3:L:213:THR:OG1	3:L:214:MET:N	2.47	0.47
3:L:371:PHE:CE1	3:L:544:LEU:HB3	2.49	0.47
4:M:221:VAL:HG23	4:M:221:VAL:O	2.14	0.47
4:M:225:PRO:HD3	4:M:239:LEU:HG	1.96	0.47
1:S:165:THR:O	1:S:167:PHE:N	2.47	0.47
1:S:211:LEU:HB2	1:S:216:THR:HG21	1.96	0.47
1:S:246:SER:HB3	1:S:268:MET:HG2	1.95	0.47
1:S:238:PHE:CZ	1:S:248:GLY:HA3	2.48	0.47
2:T:86:LEU:O	2:T:87:SER:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:481:LEU:HD23	3:U:523:LEU:HD22	1.95	0.47
3:U:47:MET:C	3:U:49:LEU:H	2.18	0.47
3:U:651:ARG:O	3:U:651:ARG:HD3	2.14	0.47
4:V:199:HIS:C	4:V:201:ILE:H	2.18	0.47
4:V:320:SER:OG	4:V:323:ALA:HB3	2.14	0.47
7:Y:114:VAL:HG12	7:Y:115:LEU:N	2.30	0.47
8:Z:75:ARG:C	8:Z:80:LYS:HZ1	2.18	0.47
1:1:312:SER:C	1:1:314:GLU:H	2.18	0.47
2:2:32:ARG:O	2:2:33:ARG:C	2.51	0.47
3:3:338:GLY:HA2	3:3:364:LEU:HD11	1.96	0.47
3:3:568:TYR:CE2	3:3:572:PRO:HG2	2.50	0.47
6:6:148:ILE:HG22	6:6:149:TYR:N	2.30	0.47
7:9:123:ASP:OD2	7:9:145:PRO:HB3	2.15	0.47
7:9:42:VAL:HG21	7:9:170:LEU:CD2	2.44	0.47
2:B:86:LEU:HG	2:B:90:LEU:HD11	1.95	0.47
3:C:151:LEU:HB3	3:C:152:PRO:CD	2.39	0.47
3:C:17:THR:HG22	3:C:18:SER:N	2.29	0.47
3:C:568:TYR:CE2	3:C:572:PRO:HG2	2.50	0.47
4:D:217:ARG:HH11	4:D:217:ARG:HG3	1.79	0.47
3:L:329:LEU:CD1	3:L:584:VAL:HG11	2.45	0.47
3:L:717:TRP:CD1	3:L:747:VAL:HG23	2.49	0.47
4:M:205:GLU:C	4:M:207:LEU:H	2.17	0.47
7:P:56:CYS:O	7:P:58:LEU:N	2.43	0.47
1:S:332:PRO:HD2	2:T:90:LEU:HD23	1.97	0.47
1:S:434:PRO:HG2	1:S:436:LEU:HD11	1.94	0.47
3:U:161:ARG:HG2	3:U:161:ARG:HH11	1.78	0.47
3:U:592:PRO:HA	3:U:595:GLU:HG2	1.97	0.47
3:U:453:PRO:CB	3:U:750:ARG:HH22	2.27	0.47
4:V:250:LYS:HD2	4:V:254:TYR:CE2	2.49	0.47
4:V:228:VAL:HG21	4:V:278:VAL:HG21	1.96	0.47
5:W:2:ARG:O	5:W:5:ARG:N	2.47	0.47
5:W:39:ALA:O	5:W:42:LYS:N	2.46	0.47
7:Y:129:LEU:HA	7:Y:129:LEU:HD23	1.72	0.47
1:1:398:SER:HA	3:3:46:ARG:HD2	1.96	0.47
2:2:123:GLU:H	2:2:123:GLU:CD	2.18	0.47
3:3:174:VAL:HB	3:3:175:ILE:HG13	1.96	0.47
3:3:357:ALA:HB2	3:3:641:LEU:HD11	1.95	0.47
3:3:505:LEU:O	3:3:532:VAL:HG13	2.15	0.47
3:3:651:ARG:O	3:3:652:PRO:O	2.33	0.47
3:3:683:LEU:HD23	3:3:683:LEU:N	2.30	0.47
3:3:753:VAL:HB	3:3:754:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:114:LEU:CD1	5:5:114:LEU:N	2.78	0.47
1:A:88:TYR:HB2	1:A:216:THR:CG2	2.39	0.47
3:C:188:VAL:HG23	3:C:189:ARG:N	2.29	0.47
3:C:382:PHE:HD1	3:C:382:PHE:H	1.58	0.47
3:C:510:GLY:CA	3:C:520:ARG:NH2	2.77	0.47
3:C:592:PRO:HA	3:C:595:GLU:HG2	1.96	0.47
3:C:632:GLY:C	3:C:634:ALA:N	2.68	0.47
6:F:164:ASN:H	6:F:170:LEU:CD1	2.26	0.47
7:G:162:VAL:HA	7:G:176:PRO:HG2	1.97	0.47
1:J:50:PRO:O	1:J:53:VAL:HG12	2.14	0.47
2:K:27:ILE:CG1	2:K:53:VAL:HG21	2.44	0.47
3:L:282:VAL:HG22	3:L:285:VAL:HG12	1.95	0.47
3:L:449:ALA:HA	3:L:464:ILE:O	2.14	0.47
4:M:84:ARG:HE	4:M:169:HIS:CD2	2.33	0.47
4:M:223:VAL:HG12	4:M:223:VAL:O	2.15	0.47
4:M:220:GLY:O	4:M:272:VAL:CG2	2.63	0.47
4:M:285:GLU:O	4:M:288:LYS:N	2.47	0.47
4:M:320:SER:OG	4:M:323:ALA:N	2.48	0.47
1:S:298:PRO:HD2	1:S:321:SER:OG	2.14	0.47
2:T:123:GLU:H	2:T:123:GLU:CD	2.18	0.47
2:T:134:ILE:HG13	2:T:145:VAL:HG21	1.97	0.47
3:U:260:PRO:HB3	3:U:617:LEU:HB3	1.95	0.47
4:V:122:GLU:OE1	4:V:122:GLU:HA	2.15	0.47
4:V:408:ASP:O	4:V:409:ARG:C	2.52	0.47
5:W:20:ASN:OD1	5:W:22:LEU:HG	2.13	0.47
2:T:111:VAL:HG12	8:Z:121:ARG:CZ	2.45	0.47
1:1:287:ILE:HG22	1:1:302:PHE:CG	2.50	0.47
1:1:434:PRO:HG2	1:1:436:LEU:HD11	1.95	0.47
1:1:49:THR:HG23	1:1:52:GLU:OE2	2.14	0.47
3:3:20:MET:O	3:3:23:VAL:N	2.47	0.47
3:3:340:GLU:H	3:3:366:THR:CB	2.28	0.47
3:3:495:GLU:O	3:3:499:LYS:HG3	2.15	0.47
3:3:652:PRO:HA	3:3:653:PRO:HD3	1.76	0.47
4:4:205:GLU:C	4:4:207:LEU:H	2.17	0.47
4:4:59:ILE:N	4:4:59:ILE:CD1	2.67	0.47
5:5:10:ALA:C	5:5:12:ALA:H	2.18	0.47
5:5:174:LEU:CD2	5:5:180:GLY:HA2	2.45	0.47
2:B:85:THR:CG2	2:B:86:LEU:N	2.77	0.47
3:C:347:HIS:N	3:C:372:GLN:HB3	2.30	0.47
3:C:616:ASN:OD1	3:C:618:GLU:HG2	2.14	0.47
4:D:320:SER:OG	4:D:323:ALA:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:112:LEU:HD13	4:D:322:GLU:HB2	1.95	0.47
4:D:74:THR:HB	4:D:77:GLN:H	1.80	0.47
5:E:37:GLU:O	5:E:41:TYR:CD1	2.65	0.47
5:E:154:GLU:HB3	6:F:119:ASN:HB3	1.96	0.47
8:H:44:MET:C	8:H:46:ARG:N	2.66	0.47
6:O:92:MET:HE1	6:O:127:VAL:HG13	1.97	0.47
3:U:173:PHE:CZ	3:U:296:PHE:CB	2.97	0.47
3:U:307:LYS:HE2	3:U:307:LYS:N	2.29	0.47
3:U:655:ARG:HH11	3:U:656:LEU:CD2	2.27	0.47
4:V:85:MET:HE1	4:V:409:ARG:CB	2.36	0.47
8:Z:44:MET:C	8:Z:46:ARG:H	2.17	0.47
2:2:130:THR:O	2:2:131:ALA:C	2.51	0.47
3:3:23:VAL:HG13	3:3:28:TYR:HB2	1.97	0.47
3:3:390:LEU:HD21	3:3:413:LEU:CD2	2.45	0.47
4:4:225:PRO:HD2	4:4:239:LEU:CG	2.45	0.47
4:4:341:GLU:OE1	5:5:26:TRP:HH2	1.97	0.47
5:5:8:GLU:O	5:5:9:GLU:C	2.53	0.47
1:A:101:PHE:CB	2:B:126:GLY:O	2.63	0.47
1:A:303:THR:O	1:A:306:VAL:HG23	2.14	0.47
3:C:378:PRO:HB2	3:C:381:LEU:CD2	2.45	0.47
3:C:481:LEU:HD23	3:C:523:LEU:HD22	1.97	0.47
3:C:48:CYS:O	3:C:82:SER:CB	2.60	0.47
3:C:651:ARG:O	3:C:651:ARG:HD3	2.14	0.47
4:D:381:LEU:HA	4:D:384:ALA:CB	2.43	0.47
1:J:13:PHE:O	1:J:13:PHE:CD1	2.67	0.47
1:J:9:LEU:HA	1:J:13:PHE:CZ	2.48	0.47
1:J:260:ARG:HG3	1:J:260:ARG:O	2.15	0.47
3:L:14:PRO:HG2	3:L:17:THR:OG1	2.15	0.47
4:M:193:LEU:C	4:M:193:LEU:HD23	2.35	0.47
4:M:379:GLN:O	4:M:382:PRO:HD2	2.14	0.47
6:O:23:THR:O	6:O:27:LEU:HB2	2.14	0.47
8:Q:47:PRO:O	8:Q:48:TYR:HB2	2.14	0.47
1:S:98:PRO:HB2	1:S:295:SER:HB2	1.95	0.47
3:U:378:PRO:HB2	3:U:381:LEU:CD2	2.45	0.47
3:U:495:GLU:O	3:U:499:LYS:HG3	2.14	0.47
3:U:616:ASN:OD1	3:U:618:GLU:HG2	2.15	0.47
3:U:7:ASN:HD21	3:U:96:LEU:HD11	1.77	0.47
4:V:155:THR:CG2	4:V:193:LEU:HD12	2.45	0.47
4:V:213:ILE:CG2	4:V:215:TYR:CE2	2.98	0.47
1:1:260:ARG:HG3	1:1:260:ARG:O	2.15	0.47
1:1:385:GLU:O	1:1:388:GLU:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:27:ILE:CG1	2:2:53:VAL:HG21	2.44	0.47
3:3:106:GLY:O	3:3:109:GLU:HB3	2.14	0.47
3:3:46:ARG:HH11	3:3:46:ARG:CG	2.28	0.47
3:3:618:GLU:OE2	3:3:620:ARG:NE	2.44	0.47
4:4:385:CYS:CB	4:4:396:ILE:HG12	2.28	0.47
4:4:99:LEU:HD13	4:4:102:GLU:OE1	2.14	0.47
1:A:49:THR:HG23	1:A:52:GLU:OE2	2.13	0.47
3:C:25:HIS:CE1	3:C:427:ASN:OD1	2.68	0.47
3:C:83:CYS:O	3:C:433:ALA:HB1	2.15	0.47
4:D:316:LEU:HD13	4:D:320:SER:CB	2.45	0.47
4:D:389:GLN:HB3	4:D:391:PRO:HD2	1.97	0.47
5:E:104:VAL:C	5:E:106:ASP:N	2.69	0.47
3:L:11:VAL:HG11	3:L:25:HIS:CD2	2.49	0.47
3:L:173:PHE:CZ	3:L:296:PHE:CB	2.97	0.47
3:L:340:GLU:H	3:L:366:THR:CB	2.28	0.47
3:L:54:LEU:HD13	3:L:54:LEU:O	2.15	0.47
4:M:249:ARG:O	4:M:250:LYS:C	2.52	0.47
5:N:132:LEU:O	5:N:133:ARG:C	2.53	0.47
5:N:147:ARG:HG2	5:N:150:TYR:HB2	1.95	0.47
6:O:91:VAL:HG22	6:O:94:ARG:HH21	1.80	0.47
1:S:101:PHE:CE1	1:S:253:GLN:HB2	2.50	0.47
1:S:9:LEU:HD23	1:S:9:LEU:C	2.35	0.47
1:S:436:LEU:CD2	2:T:90:LEU:HA	2.43	0.47
3:U:185:LYS:HE3	3:U:202:PHE:HE2	1.79	0.47
4:V:196:VAL:HG13	4:V:197:LEU:H	1.79	0.47
4:V:333:GLU:OE1	5:W:189:ARG:NH1	2.48	0.47
4:V:376:VAL:O	4:V:379:GLN:HG3	2.14	0.47
3:3:239:THR:CG2	3:3:298:HIS:HE1	2.27	0.47
3:3:244:ALA:HB3	3:3:249:MET:CE	2.44	0.47
3:3:20:MET:SD	3:3:32:LEU:CD2	3.02	0.47
4:4:231:ASP:CA	4:4:235:THR:HG23	2.45	0.47
4:4:252:TYR:O	4:4:253:PRO:C	2.52	0.47
4:4:125:ARG:HH12	4:4:349:ALA:HA	1.79	0.47
5:5:106:ASP:O	5:5:113:PHE:CZ	2.68	0.47
1:A:23:LYS:O	1:A:24:GLU:CD	2.53	0.47
2:B:61:MET:CE	8:H:88:ARG:HD3	2.45	0.47
4:D:244:VAL:HG13	4:D:246:TYR:CD1	2.49	0.47
4:D:383:TYR:O	4:D:384:ALA:C	2.53	0.47
7:G:43:LEU:O	7:G:138:VAL:HG13	2.15	0.47
1:J:202:LYS:N	1:J:203:PRO:CD	2.78	0.47
1:J:283:PRO:HB3	1:J:287:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:374:ILE:HA	1:J:379:GLY:HA3	1.97	0.47
3:L:511:VAL:HG22	3:L:520:ARG:NH1	2.30	0.47
5:N:136:LEU:HD13	5:N:138:PRO:HG3	1.96	0.47
5:N:31:ARG:HH11	5:N:31:ARG:HG2	1.79	0.47
5:N:58:LEU:O	5:N:59:THR:HB	2.14	0.47
7:P:140:VAL:HG22	7:P:141:VAL:H	1.80	0.47
1:S:29:LEU:HB2	1:S:151:GLU:OE1	2.15	0.47
3:U:125:GLY:CA	3:U:246:ASN:HD22	2.26	0.47
3:U:13:VAL:CG2	3:U:14:PRO:HD2	2.45	0.47
3:U:377:ALA:HB3	3:U:511:VAL:O	2.14	0.47
4:V:223:VAL:HG12	4:V:223:VAL:O	2.15	0.47
2:2:61:MET:HB2	3:3:214:MET:HG3	1.97	0.47
3:3:717:TRP:NE1	3:3:747:VAL:HG23	2.29	0.47
4:4:115:THR:CG2	4:4:297:LEU:HD23	2.43	0.47
5:5:195:LEU:O	5:5:196:TRP:CE3	2.68	0.47
6:6:163:TYR:O	6:6:163:TYR:CD1	2.68	0.47
7:9:143:THR:HG23	7:9:146:GLN:OE1	2.15	0.47
1:A:9:LEU:HG	1:A:13:PHE:CZ	2.50	0.47
3:C:413:LEU:HD13	3:C:448:MET:HE2	1.96	0.47
3:C:513:GLN:O	3:C:516:VAL:N	2.38	0.47
3:C:260:PRO:HB3	3:C:617:LEU:HB3	1.96	0.47
3:C:692:PHE:O	3:C:760:LEU:HA	2.15	0.47
4:D:214:PHE:C	4:D:216:GLU:N	2.68	0.47
4:D:248:VAL:C	4:D:249:ARG:HG2	2.35	0.47
4:D:381:LEU:HD11	4:D:397:ILE:CD1	2.44	0.47
4:D:96:ALA:HB2	4:D:346:THR:CG2	2.44	0.47
5:E:117:GLU:O	5:E:118:VAL:C	2.54	0.47
6:F:16:ARG:HA	6:F:21:PHE:CD2	2.50	0.47
1:J:358:PRO:O	1:J:362:GLY:N	2.48	0.47
3:L:188:VAL:HG23	3:L:189:ARG:N	2.29	0.47
4:M:125:ARG:NH1	4:M:125:ARG:HG3	2.29	0.47
4:M:317:LEU:H	4:M:317:LEU:CD1	2.28	0.47
5:N:15:TYR:HA	5:N:16:PRO:HD3	1.77	0.47
6:O:114:SER:C	6:O:116:GLY:N	2.68	0.47
6:O:16:ARG:HD2	6:O:17:GLU:CG	2.41	0.47
4:V:152:GLU:OE2	4:V:200:ARG:HD3	2.15	0.47
4:V:42:ARG:N	4:V:42:ARG:CD	2.76	0.47
4:4:112:ARG:NH1	4:4:181:ASP:OD2	2.48	0.46
4:4:221:VAL:O	4:4:221:VAL:HG23	2.15	0.46
6:6:170:LEU:HD23	6:6:171:PRO:HD2	1.97	0.46
1:A:365:GLY:O	1:A:369:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:229:ILE:HD11	3:C:289:TRP:HZ3	1.79	0.46
3:C:521:ALA:HA	3:C:524:LEU:HD23	1.98	0.46
3:C:663:ALA:O	3:C:666:ALA:HB3	2.15	0.46
5:E:3:LEU:HD12	5:E:86:SER:OG	2.15	0.46
7:G:153:THR:HG22	7:G:155:LYS:CB	2.44	0.46
1:J:12:ARG:CG	1:J:12:ARG:O	2.63	0.46
3:L:173:PHE:HE2	3:L:699:TRP:CZ2	2.33	0.46
3:L:369:LEU:HD12	3:L:549:VAL:HG13	1.96	0.46
4:M:225:PRO:HD2	4:M:239:LEU:HG	1.96	0.46
4:M:371:ARG:O	4:M:372:ALA:HB3	2.15	0.46
7:P:48:ASN:HB2	7:P:50:LEU:HD23	1.97	0.46
1:S:323:LEU:HD23	1:S:323:LEU:C	2.34	0.46
1:S:365:GLY:O	1:S:369:ASN:ND2	2.46	0.46
2:T:136:VAL:HG21	2:T:163:LEU:CD1	2.40	0.46
3:U:13:VAL:HG22	3:U:17:THR:OG1	2.15	0.46
3:U:663:ALA:O	3:U:666:ALA:HB3	2.15	0.46
3:U:6:VAL:O	3:U:93:VAL:O	2.34	0.46
4:V:105:LEU:HD13	4:V:309:ILE:HD11	1.96	0.46
5:W:60:TYR:HD2	5:W:62:ASP:O	1.97	0.46
6:X:48:ILE:CD1	6:X:48:ILE:N	2.78	0.46
6:X:83:ARG:H	6:X:83:ARG:HG2	1.46	0.46
8:Z:16:LEU:C	8:Z:16:LEU:HD13	2.36	0.46
8:Z:86:LEU:HD12	8:Z:91:ILE:HG21	1.97	0.46
1:1:98:PRO:HA	2:2:124:CYS:SG	2.55	0.46
4:4:223:VAL:O	4:4:223:VAL:HG12	2.15	0.46
4:4:226:PRO:HD3	4:4:239:LEU:HB2	1.95	0.46
4:4:84:ARG:HD3	6:6:117:MET:CE	2.45	0.46
1:A:108:GLU:HA	1:A:144:ARG:HG3	1.97	0.46
2:B:10:PHE:C	2:B:10:PHE:CD1	2.88	0.46
3:C:382:PHE:HB3	3:C:532:VAL:HB	1.95	0.46
4:D:226:PRO:HD3	4:D:239:LEU:HB2	1.96	0.46
4:D:125:ARG:HH12	4:D:349:ALA:HA	1.79	0.46
5:E:44:MET:O	5:E:45:GLY:C	2.53	0.46
6:F:36:LEU:HD22	6:F:77:VAL:HG21	1.98	0.46
6:F:91:VAL:HG22	6:F:94:ARG:HH21	1.80	0.46
3:L:326:PHE:O	3:L:329:LEU:HB3	2.15	0.46
3:L:498:GLU:O	3:L:527:ARG:NH2	2.46	0.46
3:L:655:ARG:HG3	3:L:656:LEU:HD23	1.97	0.46
5:N:161:GLU:HB2	5:N:163:ARG:CZ	2.45	0.46
5:N:70:VAL:O	5:N:91:ARG:HA	2.15	0.46
1:S:407:VAL:HG23	1:S:408:TRP:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:120:PRO:CG	8:Z:42:TYR:OH	2.63	0.46
3:U:171:SER:O	3:U:172:PRO:C	2.54	0.46
3:U:263:CYS:CB	3:U:286:ASN:HB2	2.44	0.46
3:U:276:ARG:O	3:U:277:ILE:HD13	2.16	0.46
3:U:651:ARG:O	3:U:652:PRO:C	2.53	0.46
3:U:173:PHE:HE2	3:U:699:TRP:CZ2	2.33	0.46
4:V:225:PRO:HG2	4:V:238:SER:HA	1.98	0.46
4:V:225:PRO:HD2	4:V:239:LEU:HG	1.97	0.46
5:W:127:GLU:HG3	5:W:129:HIS:HE1	1.80	0.46
5:W:134:LYS:NZ	5:W:136:LEU:HB3	2.29	0.46
5:W:55:LEU:CD1	5:W:55:LEU:N	2.79	0.46
5:W:93:TYR:CD1	5:W:93:TYR:N	2.84	0.46
7:Y:123:ASP:CB	7:Y:129:LEU:HD21	2.45	0.46
1:1:290:ILE:HG22	1:1:330:LEU:CD2	2.45	0.46
1:1:101:PHE:HB2	2:2:126:GLY:O	2.15	0.46
3:3:166:LYS:O	3:3:167:HIS:CG	2.69	0.46
2:2:57:PRO:HD2	3:3:215:ASP:OD1	2.14	0.46
4:4:223:VAL:HG13	4:4:226:PRO:O	2.15	0.46
4:4:264:VAL:H	4:4:285:GLU:HG3	1.80	0.46
4:4:320:SER:O	4:4:322:GLU:N	2.48	0.46
7:9:162:VAL:HG12	7:9:176:PRO:HB2	1.97	0.46
1:A:195:LEU:HA	2:B:24:ARG:NH2	2.30	0.46
1:A:260:ARG:HG2	1:A:280:ALA:O	2.16	0.46
1:A:89:LEU:HB2	1:A:125:ILE:HD11	1.98	0.46
2:B:109:GLY:CA	8:H:91:ILE:HD13	2.46	0.46
2:B:112:THR:CG2	2:B:116:LEU:HD23	2.42	0.46
3:C:430:THR:CG2	3:C:431:PRO:HD2	2.44	0.46
3:C:540:ASN:HB2	3:C:614:LEU:HG	1.96	0.46
3:C:717:TRP:CD1	3:C:747:VAL:HG23	2.49	0.46
5:E:116:ARG:HG2	5:E:116:ARG:NH1	2.28	0.46
8:H:112:LYS:HG2	8:H:116:PHE:HE1	1.77	0.46
1:J:323:LEU:HD23	1:J:323:LEU:C	2.35	0.46
3:L:416:PHE:CE1	3:L:447:LYS:HE2	2.50	0.46
3:L:250:GLU:OE2	3:L:628:PRO:HG2	2.15	0.46
4:M:229:ALA:O	4:M:232:LEU:HB3	2.15	0.46
4:M:228:VAL:HG21	4:M:278:VAL:HG21	1.97	0.46
4:M:313:PRO:C	4:M:315:HIS:N	2.69	0.46
4:M:66:PHE:O	4:M:68:LYS:N	2.48	0.46
5:N:104:VAL:C	5:N:106:ASP:N	2.68	0.46
1:S:433:ARG:NH1	2:T:94:GLU:OE1	2.48	0.46
3:U:337:ARG:HD2	3:U:338:GLY:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:627:ALA:O	3:U:629:ILE:N	2.42	0.46
4:V:221:VAL:HG23	4:V:221:VAL:O	2.15	0.46
4:V:226:PRO:HD3	4:V:239:LEU:HB2	1.92	0.46
4:V:340:GLY:O	4:V:341:GLU:HG3	2.16	0.46
3:3:405:GLU:HB3	3:3:535:MET:HB3	1.98	0.46
3:3:672:ALA:O	3:3:673:MET:HB2	2.15	0.46
4:4:125:ARG:HH21	4:4:347:GLU:HG2	1.81	0.46
5:5:55:LEU:N	5:5:55:LEU:CD1	2.78	0.46
6:6:47:ALA:O	6:6:51:MET:HG3	2.15	0.46
6:6:43:LEU:HD13	6:6:83:ARG:O	2.15	0.46
7:9:56:CYS:O	7:9:58:LEU:N	2.45	0.46
1:A:246:SER:HB3	1:A:268:MET:HG2	1.97	0.46
3:C:169:PRO:HA	3:C:176:LEU:HA	1.96	0.46
3:C:181:CYS:SG	3:C:182:ILE:O	2.74	0.46
3:C:307:LYS:N	3:C:307:LYS:HE2	2.30	0.46
7:G:36:ARG:CA	7:G:167:ARG:HD3	2.45	0.46
1:J:16:THR:O	1:J:17:LEU:HB2	2.16	0.46
1:J:337:MET:HB2	1:J:420:GLN:NE2	2.30	0.46
2:K:26:ALA:O	2:K:30:LEU:HG	2.16	0.46
3:U:134:THR:O	3:U:138:GLY:CA	2.63	0.46
3:U:213:THR:OG1	3:U:214:MET:N	2.48	0.46
3:U:261:VAL:O	3:U:262:GLY:C	2.51	0.46
5:W:160:ARG:O	5:W:162:GLY:N	2.43	0.46
4:V:366:TYR:OH	5:W:58:LEU:O	2.34	0.46
6:X:77:VAL:O	6:X:77:VAL:HG12	2.15	0.46
6:X:84:LEU:HD11	6:X:89:ALA:CA	2.38	0.46
7:Y:36:ARG:CA	7:Y:167:ARG:HD3	2.44	0.46
1:1:16:THR:O	1:1:17:LEU:HB2	2.15	0.46
1:1:18:TYR:N	1:1:18:TYR:CD1	2.84	0.46
1:1:261:PRO:HD2	2:2:177:HIS:O	2.15	0.46
1:1:303:THR:OG1	1:1:306:VAL:HG23	2.15	0.46
1:1:272:PHE:CE1	1:1:311:MET:HG2	2.50	0.46
1:1:33:LEU:HA	1:1:37:GLY:HA3	1.96	0.46
2:2:177:HIS:NE2	2:2:179:VAL:HG22	2.30	0.46
2:2:81:GLN:HB3	2:2:122:VAL:CG2	2.46	0.46
3:3:113:LEU:O	3:3:161:ARG:NH1	2.47	0.46
3:3:33:PHE:CD2	3:3:182:ILE:HD12	2.50	0.46
3:3:2:VAL:HG13	3:3:89:ASP:CA	2.42	0.46
3:3:498:GLU:O	3:3:527:ARG:NH2	2.49	0.46
4:4:228:VAL:HG21	4:4:278:VAL:HG21	1.98	0.46
4:4:285:GLU:O	4:4:288:LYS:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:317:LEU:H	4:4:317:LEU:CD1	2.27	0.46
4:4:340:GLY:O	4:4:341:GLU:HG3	2.15	0.46
5:5:124:ILE:CG2	5:5:145:PRO:HG2	2.41	0.46
6:6:131:VAL:HG23	6:6:131:VAL:O	2.14	0.46
1:A:89:LEU:O	1:A:130:GLY:HA2	2.15	0.46
3:C:376:ALA:H	3:C:512:LEU:CD1	2.24	0.46
3:C:297:GLY:HA3	3:C:703:GLN:NE2	2.31	0.46
3:C:758:LEU:N	3:C:758:LEU:CD1	2.77	0.46
4:D:138:LEU:HD11	4:D:146:PHE:CG	2.50	0.46
4:D:255:SER:HG	4:D:296:ARG:HH12	1.63	0.46
5:E:40:HIS:C	5:E:42:LYS:N	2.68	0.46
6:F:84:LEU:HD13	6:F:85:SER:O	2.15	0.46
1:A:95:GLU:CA	11:H:500:FMN:HN3	2.25	0.46
1:J:417:PHE:O	1:J:418:LYS:C	2.54	0.46
3:L:527:ARG:HB3	3:L:530:ALA:CB	2.43	0.46
3:L:660:ALA:O	3:L:663:ALA:HB3	2.16	0.46
4:M:118:VAL:HG23	4:M:119:ILE:N	2.30	0.46
4:M:82:THR:OG1	4:M:83:PRO:HD3	2.16	0.46
4:M:86:ASP:C	4:M:88:LEU:H	2.18	0.46
1:S:23:LYS:O	1:S:24:GLU:CD	2.54	0.46
3:U:220:SER:C	3:U:221:GLY:O	2.54	0.46
3:U:476:ILE:HD12	3:U:476:ILE:N	2.30	0.46
3:U:252:THR:HG21	3:U:626:PRO:O	2.15	0.46
4:V:220:GLY:CA	4:V:396:ILE:HD11	2.45	0.46
2:2:109:GLY:HA2	8:7:91:ILE:HD13	1.98	0.46
2:2:10:PHE:CD1	2:2:10:PHE:C	2.88	0.46
3:3:591:HIS:CE1	3:3:593:LEU:HD23	2.51	0.46
3:3:635:GLU:HG2	3:3:639:GLN:HG2	1.97	0.46
4:4:164:THR:OG1	4:4:170:HIS:HB3	2.15	0.46
4:4:234:LEU:O	4:4:236:GLY:N	2.48	0.46
4:4:245:ASN:ND2	4:4:352:GLU:OE1	2.49	0.46
6:6:165:GLU:CG	7:9:128:ASP:CG	2.82	0.46
7:9:48:ASN:HB2	7:9:50:LEU:HD23	1.98	0.46
2:B:7:LYS:HD2	2:B:7:LYS:N	2.26	0.46
3:C:757:HIS:C	3:C:758:LEU:HD12	2.35	0.46
4:D:334:GLY:N	4:D:363:SER:OG	2.49	0.46
5:E:114:LEU:CD1	5:E:114:LEU:N	2.78	0.46
5:E:27:VAL:O	5:E:90:VAL:HA	2.15	0.46
1:J:398:SER:CA	3:L:46:ARG:HD2	2.45	0.46
2:K:139:GLU:CB	2:K:140:PRO:HD2	2.15	0.46
3:L:136:GLU:HG2	5:N:189:ARG:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:570:PHE:O	3:L:572:PRO:HD3	2.16	0.46
3:L:634:ALA:O	3:L:635:GLU:O	2.33	0.46
5:N:118:VAL:CG1	5:N:129:HIS:CD2	2.90	0.46
5:N:134:LYS:NZ	5:N:136:LEU:HB3	2.31	0.46
7:P:31:VAL:O	7:P:161:TYR:HA	2.15	0.46
8:Q:38:PRO:O	8:Q:40:PHE:N	2.49	0.46
1:S:203:PRO:N	1:S:204:PRO:HD2	2.31	0.46
1:S:272:PHE:O	1:S:276:ILE:HG13	2.15	0.46
1:S:287:ILE:HG22	1:S:302:PHE:HB2	1.97	0.46
3:U:398:VAL:HG22	3:U:506:ILE:HB	1.98	0.46
3:U:618:GLU:OE2	3:U:620:ARG:NE	2.44	0.46
4:V:371:ARG:HH22	4:V:376:VAL:HG21	1.79	0.46
5:W:40:HIS:O	5:W:43:ALA:N	2.48	0.46
5:W:47:ASN:HD22	5:W:76:SER:CA	2.24	0.46
6:X:109:GLY:H	6:X:137:VAL:HG13	1.80	0.46
6:X:170:LEU:HD23	6:X:171:PRO:HD2	1.97	0.46
6:X:22:THR:HG22	6:X:23:THR:N	2.30	0.46
6:X:49:GLU:OE1	6:X:49:GLU:HA	2.15	0.46
6:X:95:VAL:HG12	6:X:95:VAL:O	2.16	0.46
8:Z:84:LEU:HB2	8:Z:93:LEU:HB2	1.98	0.46
1:1:365:GLY:O	1:1:369:ASN:ND2	2.47	0.46
3:3:171:SER:O	3:3:172:PRO:C	2.54	0.46
4:4:228:VAL:CG1	4:4:271:ASP:HA	2.42	0.46
4:4:342:VAL:CG2	4:4:343:TYR:N	2.79	0.46
6:6:46:CYS:HB3	6:6:81:ALA:HB1	1.96	0.46
1:A:402:LEU:O	1:A:403:ALA:C	2.52	0.46
3:C:245:ARG:HA	3:C:245:ARG:HD2	1.51	0.46
3:C:683:LEU:N	3:C:683:LEU:HD23	2.31	0.46
4:D:182:LEU:HD12	4:D:182:LEU:O	2.16	0.46
4:D:316:LEU:O	4:D:318:GLU:N	2.49	0.46
5:E:124:ILE:CG2	5:E:146:LEU:HD23	2.39	0.46
5:E:2:ARG:O	5:E:5:ARG:N	2.49	0.46
6:F:137:VAL:HG13	6:F:137:VAL:O	2.15	0.46
6:F:16:ARG:O	6:F:21:PHE:HB3	2.15	0.46
7:G:178:GLU:O	7:G:179:GLY:C	2.54	0.46
1:J:89:LEU:O	1:J:130:GLY:HA2	2.16	0.46
3:L:269:THR:HG23	3:L:274:LEU:HD13	1.96	0.46
3:L:454:TYR:O	3:L:456:ALA:N	2.49	0.46
4:M:164:THR:OG1	4:M:170:HIS:HB3	2.15	0.46
4:M:213:ILE:CG2	4:M:215:TYR:CE2	2.99	0.46
4:M:381:LEU:HD23	4:M:381:LEU:C	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:2:ARG:O	5:N:5:ARG:N	2.49	0.46
6:O:164:ASN:H	6:O:170:LEU:CD1	2.29	0.46
3:U:161:ARG:NH1	3:U:161:ARG:HG2	2.30	0.46
3:U:249:MET:SD	3:U:268:ASP:HB3	2.56	0.46
3:U:652:PRO:HA	3:U:653:PRO:HD3	1.75	0.46
4:V:168:PHE:O	4:V:169:HIS:HB2	2.16	0.46
6:X:156:LYS:O	6:X:162:ALA:HB3	2.15	0.46
8:Z:29:VAL:HG21	8:Z:67:PHE:CZ	2.50	0.46
1:1:179:ALA:O	1:1:182:CYS:HB2	2.16	0.46
1:1:210:GLY:O	1:1:213:GLY:N	2.49	0.46
3:3:245:ARG:HD2	3:3:245:ARG:HA	1.53	0.46
3:3:286:ASN:ND2	3:3:286:ASN:C	2.68	0.46
3:3:414:SER:HA	3:3:461:TRP:HZ3	1.78	0.46
4:4:358:VAL:HG12	4:4:366:TYR:HB3	1.98	0.46
1:A:93:ALA:CB	1:A:134:VAL:HG12	2.46	0.46
3:C:656:LEU:N	3:C:656:LEU:HD23	2.30	0.46
3:C:717:TRP:NE1	3:C:747:VAL:HG23	2.30	0.46
4:D:197:LEU:HA	4:D:200:ARG:HB3	1.98	0.46
4:D:224:ILE:HD13	5:E:112:ASN:CA	2.45	0.46
4:D:310:THR:HG23	4:D:311:PRO:CD	2.44	0.46
4:D:403:VAL:O	4:D:406:ASP:HB3	2.15	0.46
5:E:119:TYR:HE1	5:E:132:LEU:CD1	2.12	0.46
5:E:16:PRO:HB2	5:E:28:VAL:CG1	2.46	0.46
5:E:34:PHE:CE1	5:E:38:MET:HB2	2.51	0.46
7:G:129:LEU:HD23	7:G:129:LEU:HA	1.67	0.46
8:H:112:LYS:CG	8:H:116:PHE:HE1	2.27	0.46
1:J:316:LEU:CD1	1:J:323:LEU:HB2	2.36	0.46
3:L:185:LYS:HG2	3:L:188:VAL:HG22	1.98	0.46
3:L:290:ILE:HG22	3:L:291:CYS:O	2.16	0.46
3:L:401:ASP:OD2	3:L:404:GLU:HG2	2.15	0.46
3:L:509:ALA:C	3:L:511:VAL:H	2.20	0.46
3:L:655:ARG:HH11	3:L:656:LEU:CD2	2.29	0.46
3:L:470:PRO:HG3	3:L:750:ARG:NH2	2.30	0.46
4:M:316:LEU:C	4:M:318:GLU:H	2.19	0.46
4:M:346:THR:HG22	4:M:353:LEU:C	2.36	0.46
5:N:113:PHE:HB3	5:N:114:LEU:H	1.39	0.46
6:O:84:LEU:HD13	6:O:85:SER:O	2.15	0.46
8:Q:23:TYR:O	8:Q:23:TYR:CD1	2.68	0.46
1:S:180:TYR:HB3	1:S:351:GLU:OE1	2.16	0.46
2:T:177:HIS:NE2	2:T:179:VAL:HG22	2.31	0.46
3:U:218:LEU:N	3:U:218:LEU:HD23	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:239:THR:CG2	3:U:298:HIS:HE1	2.29	0.46
3:U:428:HIS:CD2	3:U:428:HIS:H	2.33	0.46
3:U:54:LEU:O	3:U:54:LEU:HD13	2.16	0.46
3:U:631:ASN:OD1	3:U:633:GLU:OE2	2.33	0.46
3:U:651:ARG:O	3:U:652:PRO:O	2.34	0.46
3:U:550:LEU:HD23	3:U:684:ARG:NH2	2.31	0.46
4:V:125:ARG:HG3	4:V:125:ARG:NH1	2.30	0.46
4:V:225:PRO:CB	4:V:226:PRO:HD3	2.45	0.46
4:V:271:ASP:O	4:V:275:ARG:HG3	2.15	0.46
4:V:285:GLU:O	4:V:288:LYS:N	2.49	0.46
4:V:381:LEU:HD11	4:V:397:ILE:CG1	2.46	0.46
7:Y:110:THR:HG22	8:Z:41:ILE:O	2.16	0.46
8:Z:23:TYR:HD2	8:Z:116:PHE:CD2	2.34	0.46
8:Z:39:ASP:OD2	8:Z:75:ARG:HG3	2.15	0.46
3:3:112:LEU:HD22	4:4:322:GLU:HG3	1.97	0.46
3:3:285:VAL:CG1	3:3:286:ASN:N	2.64	0.46
3:3:588:SER:O	3:3:589:HIS:ND1	2.49	0.46
3:3:651:ARG:O	3:3:652:PRO:C	2.54	0.46
3:3:75:TRP:HA	3:3:75:TRP:CE3	2.51	0.46
4:4:310:THR:HG23	4:4:311:PRO:CD	2.44	0.46
6:6:16:ARG:HA	6:6:21:PHE:CD2	2.51	0.46
8:7:31:PHE:C	8:7:31:PHE:CD1	2.89	0.46
3:C:168:HIS:HA	3:C:169:PRO:HD2	1.78	0.46
3:C:173:PHE:CE1	3:C:174:VAL:HG22	2.49	0.46
3:C:237:ASP:OD1	3:C:237:ASP:C	2.55	0.46
3:C:239:THR:CG2	3:C:298:HIS:HE1	2.29	0.46
4:D:116:ILE:HD12	4:D:182:LEU:HD21	1.98	0.46
4:D:234:LEU:HD13	4:D:352:GLU:HB3	1.98	0.46
4:D:42:ARG:CD	4:D:42:ARG:N	2.79	0.46
5:E:115:GLU:HB3	5:E:119:TYR:CE2	2.51	0.46
5:E:47:ASN:HD22	5:E:76:SER:CA	2.29	0.46
5:E:26:TRP:CZ3	5:E:91:ARG:NE	2.84	0.46
7:G:143:THR:O	7:G:144:LYS:C	2.54	0.46
3:L:428:HIS:CD2	3:L:428:HIS:H	2.34	0.46
3:L:405:GLU:HB3	3:L:535:MET:HB3	1.97	0.46
3:L:549:VAL:O	3:L:549:VAL:HG12	2.15	0.46
4:M:350:ARG:HG3	4:M:350:ARG:HH11	1.81	0.46
4:M:346:THR:N	4:M:353:LEU:O	2.33	0.46
5:N:137:THR:CG2	5:N:139:GLU:CD	2.84	0.46
2:K:61:MET:CE	8:Q:88:ARG:HD3	2.45	0.46
1:S:210:GLY:O	1:S:213:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:3:PHE:HB3	2:T:48:GLU:OE1	2.15	0.46
3:U:178:ARG:O	3:U:179:GLU:C	2.53	0.46
3:U:18:SER:O	3:U:19:VAL:C	2.54	0.46
3:U:185:LYS:HG3	3:U:202:PHE:CE2	2.50	0.46
3:U:20:MET:HA	3:U:82:SER:OG	2.15	0.46
3:U:261:VAL:CG2	9:U:786:SF4:S2	3.04	0.46
3:U:605:PRO:HB2	3:U:609:GLU:HG3	1.98	0.46
4:V:217:ARG:HH11	4:V:217:ARG:HG3	1.80	0.46
5:W:44:MET:O	5:W:45:GLY:C	2.53	0.46
5:W:46:PHE:C	5:W:48:PHE:H	2.19	0.46
5:W:77:LEU:HA	5:W:78:PRO:HD3	1.72	0.46
6:X:114:SER:O	6:X:116:GLY:N	2.49	0.46
1:1:366:PHE:CE1	1:1:370:LEU:HD21	2.51	0.46
1:1:407:VAL:HG23	1:1:408:TRP:N	2.30	0.46
1:1:95:GLU:HA	11:7:500:FMN:N3	2.25	0.46
2:2:106:ILE:CD1	2:2:112:THR:HB	2.45	0.46
2:2:66:PHE:CD1	2:2:66:PHE:C	2.87	0.46
3:3:113:LEU:HG	3:3:157:PHE:CE2	2.51	0.46
3:3:616:ASN:OD1	3:3:618:GLU:HG2	2.15	0.46
3:3:586:HIS:HE1	3:3:637:ALA:CA	2.29	0.46
4:4:113:ALA:O	4:4:114:GLU:C	2.53	0.46
4:4:223:VAL:HG22	4:4:226:PRO:O	2.15	0.46
5:5:104:VAL:C	5:5:106:ASP:N	2.69	0.46
5:5:127:GLU:HG3	5:5:129:HIS:HE1	1.81	0.46
4:4:338:PRO:HD3	5:5:192:TYR:O	2.16	0.46
5:5:3:LEU:HD11	5:5:84:ASP:OD2	2.16	0.46
7:9:63:CYS:HA	9:9:183:SF4:S2	2.56	0.46
1:A:81:LYS:CG	1:A:82:ASP:N	2.79	0.46
1:A:437:TRP:CZ3	2:B:96:LEU:HD13	2.51	0.46
3:C:356:LEU:O	3:C:357:ALA:C	2.55	0.46
3:C:652:PRO:C	3:C:654:PHE:H	2.18	0.46
3:C:731:GLY:HA2	3:C:747:VAL:CG1	2.46	0.46
4:D:256:GLY:C	4:D:257:TYR:HD1	2.19	0.46
5:E:39:ALA:O	5:E:42:LYS:HG2	2.16	0.46
1:J:110:VAL:O	1:J:111:PRO:C	2.53	0.46
2:K:136:VAL:CG1	2:K:137:ASN:H	1.99	0.46
3:L:31:PRO:HG3	3:L:137:TYR:CD1	2.51	0.46
6:O:147:LEU:HD13	6:O:147:LEU:C	2.36	0.46
6:O:160:GLY:C	6:O:162:ALA:H	2.19	0.46
6:O:170:LEU:HD23	6:O:171:PRO:HD2	1.98	0.46
2:K:109:GLY:HA2	8:Q:91:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:361:GLU:OE2	3:U:162:ARG:NH2	2.49	0.46
3:U:591:HIS:CE1	3:U:593:LEU:HD23	2.51	0.46
3:U:75:TRP:HE3	3:U:75:TRP:HA	1.81	0.46
4:V:231:ASP:CA	4:V:235:THR:HG23	2.46	0.46
5:W:113:PHE:HB3	5:W:114:LEU:H	1.41	0.46
5:W:93:TYR:N	5:W:93:TYR:HD1	2.14	0.46
6:X:131:VAL:HG23	6:X:131:VAL:O	2.16	0.46
6:X:156:LYS:HA	6:X:159:ARG:HD2	1.97	0.46
3:3:13:VAL:HG22	3:3:17:THR:OG1	2.16	0.45
3:3:173:PHE:CD1	3:3:174:VAL:CG2	2.89	0.45
3:3:287:GLU:C	3:3:288:ILE:HG22	2.36	0.45
3:3:372:GLN:NE2	3:3:570:PHE:HB2	2.31	0.45
3:3:583:VAL:O	3:3:583:VAL:HG23	2.16	0.45
5:5:117:GLU:O	5:5:118:VAL:C	2.52	0.45
3:C:230:CYS:HA	3:C:231:PRO:HD2	1.86	0.45
3:C:261:VAL:CG2	9:C:786:SF4:S2	3.05	0.45
3:C:401:ASP:OD2	3:C:404:GLU:HG2	2.16	0.45
4:D:85:MET:HE1	4:D:409:ARG:CB	2.37	0.45
5:E:119:TYR:HD1	5:E:132:LEU:HD21	1.81	0.45
6:F:110:ALA:O	6:F:113:SER:N	2.49	0.45
1:J:92:ASN:HD21	1:J:94:ASP:HB3	1.81	0.45
3:L:34:CYS:HB3	3:L:45:CYS:HB3	1.98	0.45
3:L:370:ASP:OD2	3:L:557:SER:HB2	2.16	0.45
3:L:540:ASN:HB2	3:L:614:LEU:HG	1.99	0.45
4:M:113:ALA:O	4:M:114:GLU:C	2.52	0.45
4:M:138:LEU:HD11	4:M:146:PHE:CG	2.50	0.45
5:N:116:ARG:HG2	5:N:116:ARG:NH1	2.28	0.45
8:Q:31:PHE:CD1	8:Q:31:PHE:C	2.89	0.45
1:S:108:GLU:CG	1:S:140:ARG:HG2	2.43	0.45
1:S:342:TRP:O	1:S:342:TRP:CE3	2.65	0.45
1:S:65:ARG:HD3	1:S:65:ARG:HA	1.73	0.45
2:T:106:ILE:CD1	2:T:112:THR:HB	2.42	0.45
3:U:509:ALA:C	3:U:511:VAL:H	2.19	0.45
3:U:513:GLN:O	3:U:516:VAL:N	2.35	0.45
3:U:344:TYR:CD2	3:U:568:TYR:CE1	3.04	0.45
4:V:122:GLU:HB2	4:V:290:ILE:HD11	1.98	0.45
4:V:144:THR:N	4:V:145:PRO:CD	2.79	0.45
4:V:59:ILE:HD11	5:W:138:PRO:HB3	1.97	0.45
7:Y:46:HIS:CD2	7:Y:52:LYS:HG2	2.51	0.45
7:Y:48:ASN:HB2	7:Y:50:LEU:HD23	1.97	0.45
4:D:257:TYR:HE2	8:Z:127:ALA:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:350:HIS:ND1	1:1:350:HIS:C	2.69	0.45
1:1:383:ASP:O	1:1:384:VAL:C	2.53	0.45
3:3:517:ALA:HA	3:3:520:ARG:CG	2.46	0.45
3:3:643:LEU:O	3:3:646:GLU:HB2	2.15	0.45
3:3:657:HIS:CE1	3:3:661:GLN:OE1	2.69	0.45
3:3:731:GLY:HA2	3:3:747:VAL:CG1	2.46	0.45
3:3:757:HIS:C	3:3:758:LEU:HD12	2.35	0.45
4:4:244:VAL:HG12	4:4:246:TYR:H	1.81	0.45
4:4:342:VAL:CG2	4:4:343:TYR:H	2.24	0.45
5:5:119:TYR:O	5:5:120:ASP:C	2.54	0.45
6:6:89:ALA:HB3	6:6:90:PRO:CD	2.46	0.45
7:9:123:ASP:HB2	7:9:129:LEU:HD21	1.97	0.45
7:9:162:VAL:HA	7:9:176:PRO:HG2	1.98	0.45
7:9:58:LEU:O	7:9:59:CYS:C	2.53	0.45
5:5:167:PRO:HB3	7:9:66:TYR:CE2	2.51	0.45
1:A:58:LYS:HA	1:A:73:GLY:HA3	1.98	0.45
3:C:509:ALA:C	3:C:511:VAL:H	2.19	0.45
4:D:122:GLU:HA	4:D:122:GLU:OE1	2.16	0.45
6:F:41:PHE:CE2	6:F:92:MET:HB2	2.49	0.45
8:H:13:TRP:NE1	8:H:17:LEU:HD11	2.31	0.45
2:K:3:PHE:HB3	2:K:48:GLU:OE1	2.16	0.45
4:M:310:THR:CG2	4:M:311:PRO:N	2.79	0.45
7:P:100:PHE:N	7:P:100:PHE:CD1	2.84	0.45
1:S:272:PHE:CE1	1:S:311:MET:HG2	2.51	0.45
1:S:338:VAL:O	1:S:342:TRP:HB2	2.16	0.45
2:T:10:PHE:CD1	2:T:11:LEU:N	2.84	0.45
3:U:174:VAL:HB	3:U:175:ILE:HG13	1.97	0.45
3:U:340:GLU:N	3:U:366:THR:HB	2.30	0.45
3:U:44:ALA:O	3:U:45:CYS:HB3	2.16	0.45
3:U:476:ILE:O	3:U:480:LEU:HG	2.17	0.45
3:U:652:PRO:C	3:U:654:PHE:H	2.19	0.45
1:1:252:TYR:HB3	1:1:275:LEU:CD1	2.43	0.45
2:2:86:LEU:HG	2:2:90:LEU:HD11	1.98	0.45
3:3:213:THR:OG1	3:3:214:MET:N	2.49	0.45
3:3:430:THR:CG2	3:3:431:PRO:HD2	2.47	0.45
3:3:154:TYR:CZ	4:4:312:PRO:HB3	2.52	0.45
5:5:66:GLU:CG	5:5:95:PRO:HA	2.46	0.45
1:A:121:ALA:O	1:A:125:ILE:HG12	2.16	0.45
1:A:370:LEU:HD22	1:A:370:LEU:N	2.30	0.45
3:C:122:CYS:SG	3:C:124:LYS:HB2	2.56	0.45
1:A:361:GLU:OE2	3:C:162:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:225:ASN:O	3:C:229:ILE:HG13	2.16	0.45
4:D:102:GLU:CD	4:D:117:ARG:HH22	2.20	0.45
4:D:109:VAL:CG1	4:D:113:ALA:HB3	2.46	0.45
4:D:220:GLY:O	4:D:272:VAL:HG22	2.16	0.45
4:D:353:LEU:HD12	4:D:354:GLY:N	2.29	0.45
4:D:75:TYR:OH	4:D:365:PRO:HA	2.16	0.45
8:H:42:TYR:O	8:H:44:MET:HG3	2.17	0.45
1:J:222:GLU:OE2	1:J:251:LEU:HD13	2.15	0.45
1:J:58:LYS:HA	1:J:73:GLY:HA3	1.99	0.45
2:K:123:GLU:O	2:K:124:CYS:C	2.55	0.45
2:K:31:LEU:HA	2:K:31:LEU:HD13	1.85	0.45
3:L:36:GLU:O	3:L:37:LYS:C	2.54	0.45
3:L:692:PHE:CE1	3:L:763:LEU:HA	2.51	0.45
4:M:68:LYS:O	4:M:71:GLU:HB2	2.15	0.45
6:O:151:VAL:O	6:O:154:LEU:HB3	2.16	0.45
1:S:11:PRO:HB2	1:S:274:GLU:OE2	2.16	0.45
2:T:27:ILE:CG1	2:T:53:VAL:HG21	2.46	0.45
3:U:238:LEU:C	3:U:240:ALA:N	2.68	0.45
3:U:2:VAL:CG1	3:U:3:ARG:N	2.80	0.45
3:U:371:PHE:CD2	3:U:374:ARG:HB2	2.51	0.45
3:U:474:ARG:NH1	3:U:515:THR:HG21	2.31	0.45
3:U:591:HIS:HE1	3:U:593:LEU:HD23	1.80	0.45
4:V:199:HIS:ND1	4:V:200:ARG:N	2.65	0.45
6:X:90:PRO:O	6:X:93:ARG:HB3	2.16	0.45
7:Y:105:GLU:HG3	7:Y:114:VAL:HA	1.99	0.45
1:1:287:ILE:HG22	1:1:302:PHE:HB2	1.98	0.45
1:1:417:PHE:O	1:1:418:LYS:C	2.54	0.45
2:2:61:MET:HE1	8:7:128:PHE:HZ	1.81	0.45
2:2:79:HIS:HE1	2:2:120:GLN:OE1	1.99	0.45
3:3:460:LYS:HB2	3:3:460:LYS:HE2	1.80	0.45
3:3:748:VAL:HG23	3:3:752:ASP:OD1	2.16	0.45
4:4:79:ILE:HD13	4:4:173:ILE:O	2.16	0.45
4:4:182:LEU:HD12	4:4:182:LEU:O	2.16	0.45
4:4:232:LEU:HB2	4:4:278:VAL:HG11	1.97	0.45
1:A:210:GLY:O	1:A:213:GLY:N	2.47	0.45
2:B:3:PHE:CD1	2:B:3:PHE:C	2.90	0.45
2:B:81:GLN:HB3	2:B:122:VAL:CG2	2.47	0.45
3:C:167:HIS:O	3:C:167:HIS:ND1	2.49	0.45
3:C:17:THR:CG2	3:C:18:SER:N	2.79	0.45
3:C:726:GLU:O	3:C:727:ALA:HB3	2.16	0.45
4:D:125:ARG:HG3	4:D:125:ARG:NH1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:89:ALA:HB3	6:F:90:PRO:CD	2.47	0.45
1:J:149:ILE:O	1:J:153:ARG:HB2	2.16	0.45
1:J:65:ARG:HD3	1:J:65:ARG:HA	1.70	0.45
2:K:7:LYS:O	2:K:7:LYS:HG2	2.17	0.45
2:K:87:SER:CB	10:K:182:FES:S2	3.05	0.45
3:L:592:PRO:HA	3:L:595:GLU:HG2	1.99	0.45
4:M:108:VAL:O	4:M:108:VAL:HG23	2.16	0.45
4:M:115:THR:O	4:M:118:VAL:HG22	2.17	0.45
4:M:144:THR:N	4:M:145:PRO:CD	2.80	0.45
4:M:155:THR:HG22	4:M:193:LEU:HD12	1.99	0.45
4:M:285:GLU:C	4:M:287:VAL:N	2.68	0.45
5:N:34:PHE:CE1	5:N:38:MET:HB2	2.51	0.45
8:Q:43:ARG:C	8:Q:44:MET:HG3	2.37	0.45
1:S:162:LEU:HB3	1:S:163:PHE:CD1	2.51	0.45
2:T:91:ALA:HB1	2:T:132:PRO:HD3	1.97	0.45
3:U:169:PRO:HA	3:U:176:LEU:HA	1.98	0.45
3:U:188:VAL:CG2	3:U:189:ARG:N	2.79	0.45
3:U:655:ARG:HG3	3:U:656:LEU:HD23	1.99	0.45
4:V:205:GLU:C	4:V:207:LEU:H	2.19	0.45
4:V:316:LEU:O	4:V:318:GLU:N	2.50	0.45
5:W:137:THR:HG23	5:W:139:GLU:CD	2.37	0.45
7:Y:113:ILE:CG2	7:Y:113:ILE:O	2.64	0.45
7:Y:153:THR:HG22	7:Y:155:LYS:CB	2.46	0.45
1:1:98:PRO:HB2	1:1:295:SER:HB2	1.97	0.45
3:3:237:ASP:OD1	3:3:237:ASP:C	2.55	0.45
3:3:481:LEU:HD23	3:3:523:LEU:HD22	1.99	0.45
3:3:2:VAL:CG1	3:3:89:ASP:HA	2.42	0.45
4:4:227:GLU:OE2	4:4:240:ARG:O	2.33	0.45
4:4:49:GLY:HA2	4:4:53:LEU:HD12	1.98	0.45
4:4:59:ILE:HD11	5:5:138:PRO:CB	2.47	0.45
6:6:117:MET:HG3	6:6:117:MET:O	2.17	0.45
6:6:165:GLU:OE1	6:6:165:GLU:C	2.55	0.45
6:6:83:ARG:H	6:6:83:ARG:HG2	1.53	0.45
3:3:163:HIS:ND1	8:7:71:ASP:OD2	2.45	0.45
7:9:105:GLU:HG3	7:9:114:VAL:HA	1.98	0.45
1:A:385:GLU:O	1:A:388:GLU:HB3	2.16	0.45
3:C:167:HIS:HE1	8:H:32:GLU:OE2	2.00	0.45
3:C:714:ALA:O	3:C:745:ALA:HA	2.16	0.45
4:D:154:GLU:CD	4:D:167:ARG:HH22	2.19	0.45
4:D:197:LEU:N	4:D:198:PRO:CD	2.80	0.45
4:D:230:ILE:HG12	4:D:239:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:101:ARG:HH12	3:L:140:TYR:HD1	1.52	0.45
3:L:193:GLU:HB3	3:L:418:ARG:HH12	1.81	0.45
3:L:368:HIS:ND1	3:L:368:HIS:O	2.47	0.45
3:L:52:ILE:HG12	3:L:93:VAL:HG22	1.99	0.45
4:M:171:ASN:HA	4:M:171:ASN:HD22	1.63	0.45
4:M:288:LYS:O	4:M:292:GLN:HB2	2.17	0.45
4:M:371:ARG:HG3	4:M:371:ARG:HH11	1.81	0.45
6:O:30:TRP:C	6:O:30:TRP:CD1	2.89	0.45
7:P:108:CYS:HA	7:P:109:PRO:HD3	1.84	0.45
6:O:164:ASN:HB3	7:P:148:ARG:HH21	1.81	0.45
7:P:36:ARG:CA	7:P:167:ARG:HD3	2.45	0.45
7:P:51:GLU:OE2	7:P:133:LYS:NZ	2.43	0.45
7:P:94:ASN:ND2	7:P:97:ARG:HB2	2.31	0.45
8:Q:46:ARG:HB3	8:Q:47:PRO:HD2	1.96	0.45
1:S:10:ASP:C	1:S:267:PRO:HG3	2.37	0.45
1:S:337:MET:O	1:S:341:MET:HG2	2.17	0.45
1:S:50:PRO:O	1:S:53:VAL:HG12	2.16	0.45
3:U:692:PHE:O	3:U:760:LEU:HA	2.16	0.45
3:U:293:ALA:CB	3:U:698:MET:HG2	2.47	0.45
6:X:114:SER:C	6:X:116:GLY:N	2.70	0.45
7:Y:51:GLU:OE1	7:Y:133:LYS:HE3	2.16	0.45
2:2:114:ASP:HB2	2:2:116:LEU:HD21	1.96	0.45
3:3:324:GLU:O	3:3:325:ALA:C	2.54	0.45
4:4:285:GLU:C	4:4:287:VAL:N	2.69	0.45
5:5:137:THR:HG23	5:5:139:GLU:CD	2.37	0.45
5:5:65:PRO:HB2	5:5:93:TYR:CD2	2.52	0.45
7:9:33:LEU:H	7:9:33:LEU:HD12	1.80	0.45
1:A:291:ILE:HG22	1:A:294:GLY:O	2.16	0.45
1:A:303:THR:OG1	1:A:306:VAL:HG23	2.16	0.45
1:A:417:PHE:O	1:A:418:LYS:C	2.55	0.45
2:B:24:ARG:HA	2:B:53:VAL:HG13	1.99	0.45
3:C:453:PRO:HB2	3:C:750:ARG:CZ	2.47	0.45
4:D:205:GLU:C	4:D:207:LEU:H	2.19	0.45
5:E:136:LEU:HD13	5:E:138:PRO:HG3	1.98	0.45
5:E:124:ILE:O	5:E:145:PRO:HD2	2.16	0.45
6:F:164:ASN:HB3	7:G:148:ARG:NH2	2.31	0.45
7:G:51:GLU:OE1	7:G:133:LYS:HE3	2.17	0.45
1:J:108:GLU:HA	1:J:144:ARG:HG3	1.98	0.45
1:J:179:ALA:O	1:J:182:CYS:HB2	2.17	0.45
1:J:342:TRP:CE3	1:J:342:TRP:O	2.62	0.45
3:L:45:CYS:O	10:L:787:FES:S1	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:543:GLY:CA	3:L:615:VAL:HB	2.46	0.45
3:L:75:TRP:HA	3:L:75:TRP:HE3	1.80	0.45
4:M:376:VAL:O	4:M:379:GLN:HG3	2.17	0.45
4:M:40:VAL:O	4:M:40:VAL:HG12	2.17	0.45
5:N:125:VAL:CG1	5:N:126:PHE:N	2.75	0.45
4:M:68:LYS:NZ	5:N:150:TYR:O	2.42	0.45
3:U:113:LEU:O	3:U:161:ARG:NH1	2.50	0.45
4:V:184:GLU:H	4:V:184:GLU:CD	2.20	0.45
4:V:132:PHE:CD2	4:V:279:ARG:HD2	2.51	0.45
4:V:321:MET:HG3	4:V:322:GLU:N	2.31	0.45
5:W:147:ARG:NH1	5:W:149:ASP:OD1	2.50	0.45
7:Y:33:LEU:HD12	7:Y:33:LEU:H	1.82	0.45
1:1:180:TYR:HB3	1:1:351:GLU:OE1	2.16	0.45
1:1:264:TYR:CD2	1:1:279:TRP:HB3	2.51	0.45
2:2:86:LEU:O	2:2:87:SER:C	2.55	0.45
4:4:197:LEU:HA	4:4:200:ARG:HB3	1.98	0.45
4:4:312:PRO:O	4:4:313:PRO:C	2.53	0.45
4:4:245:ASN:HD21	5:5:87:ARG:HH22	1.64	0.45
6:6:142:PRO:O	6:6:143:ARG:C	2.55	0.45
1:A:323:LEU:C	1:A:323:LEU:HD23	2.37	0.45
1:A:341:MET:O	1:A:342:TRP:C	2.55	0.45
3:C:372:GLN:NE2	3:C:570:PHE:HB2	2.30	0.45
6:F:131:VAL:O	6:F:131:VAL:HG23	2.17	0.45
8:H:31:PHE:C	8:H:31:PHE:CD1	2.90	0.45
1:J:93:ALA:CB	1:J:134:VAL:HG12	2.45	0.45
1:J:398:SER:HA	3:L:46:ARG:HD2	1.98	0.45
2:K:177:HIS:NE2	2:K:179:VAL:HG22	2.31	0.45
2:K:85:THR:HG22	2:K:86:LEU:N	2.31	0.45
3:L:113:LEU:HG	3:L:157:PHE:CE2	2.52	0.45
3:L:174:VAL:HG11	3:L:296:PHE:CD1	2.51	0.45
3:L:33:PHE:CB	3:L:45:CYS:SG	3.05	0.45
3:L:154:TYR:O	4:M:321:MET:HB2	2.16	0.45
4:M:82:THR:N	4:M:83:PRO:HD2	2.31	0.45
1:S:274:GLU:HG3	1:S:278:GLU:OE1	2.16	0.45
3:U:237:ASP:OD1	3:U:237:ASP:C	2.54	0.45
3:U:400:GLY:O	3:U:401:ASP:C	2.55	0.45
3:U:514:ASP:O	3:U:515:THR:C	2.55	0.45
3:U:405:GLU:HB3	3:U:535:MET:HB3	1.99	0.45
3:U:549:VAL:HG12	3:U:549:VAL:O	2.16	0.45
3:U:632:GLY:C	3:U:634:ALA:N	2.69	0.45
4:V:182:LEU:O	4:V:182:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:193:LEU:C	4:V:193:LEU:HD23	2.37	0.45
4:V:132:PHE:CE2	4:V:279:ARG:HD2	2.52	0.45
4:V:383:TYR:O	4:V:386:LYS:N	2.37	0.45
4:V:379:GLN:CD	5:W:116:ARG:HG2	2.37	0.45
8:Z:16:LEU:HD21	8:Z:115:PHE:CE1	2.52	0.45
1:1:203:PRO:N	1:1:204:PRO:HD2	2.31	0.45
1:1:238:PHE:CZ	1:1:248:GLY:HA3	2.52	0.45
3:3:657:HIS:O	3:3:660:ALA:N	2.50	0.45
4:4:118:VAL:HG23	4:4:119:ILE:N	2.32	0.45
7:9:150:ALA:HA	7:9:153:THR:HB	1.99	0.45
7:9:42:VAL:HG21	7:9:170:LEU:HD22	1.98	0.45
1:A:110:VAL:O	1:A:113:LEU:HB3	2.17	0.45
1:A:53:VAL:HG23	1:A:231:MET:CE	2.46	0.45
1:A:101:PHE:HB2	2:B:126:GLY:O	2.16	0.45
3:C:282:VAL:HG22	3:C:285:VAL:HG12	1.99	0.45
3:C:340:GLU:N	3:C:366:THR:HB	2.31	0.45
3:C:440:ARG:HG2	3:C:440:ARG:HH11	1.81	0.45
3:C:47:MET:C	3:C:49:LEU:H	2.20	0.45
5:E:20:ASN:HD22	5:E:24:ASN:HB2	1.76	0.45
5:E:77:LEU:HA	5:E:78:PRO:HD3	1.70	0.45
7:G:108:CYS:HA	7:G:109:PRO:HD3	1.85	0.45
8:H:16:LEU:HD13	8:H:16:LEU:C	2.37	0.45
8:H:38:PRO:C	8:H:40:PHE:N	2.70	0.45
1:A:220:ASN:N	11:H:500:FMN:O3P	2.48	0.45
3:L:237:ASP:C	3:L:237:ASP:OD1	2.55	0.45
3:L:521:ALA:HA	3:L:524:LEU:HD23	1.98	0.45
3:L:568:TYR:CE2	3:L:572:PRO:HG2	2.52	0.45
3:L:635:GLU:HG2	3:L:639:GLN:HG2	1.98	0.45
4:M:154:GLU:CD	4:M:167:ARG:HH22	2.20	0.45
4:M:282:GLU:O	4:M:286:SER:HB2	2.16	0.45
5:N:22:LEU:HD23	5:N:22:LEU:N	2.32	0.45
5:N:93:TYR:N	5:N:93:TYR:HD1	2.14	0.45
6:O:148:ILE:O	6:O:151:VAL:HG22	2.16	0.45
6:O:42:GLY:O	6:O:43:LEU:HD23	2.17	0.45
7:P:110:THR:HG22	8:Q:41:ILE:O	2.16	0.45
8:Q:84:LEU:HB2	8:Q:93:LEU:HB2	1.98	0.45
1:S:195:LEU:HA	2:T:24:ARG:NH2	2.32	0.45
1:S:321:SER:OG	1:S:322:MET:N	2.47	0.45
1:S:343:ASN:HD22	2:T:89:LYS:HD2	1.82	0.45
1:S:417:PHE:O	1:S:418:LYS:C	2.55	0.45
1:S:98:PRO:HA	2:T:124:CYS:SG	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:46:ILE:HG23	2:T:60:VAL:HG11	1.99	0.45
6:X:143:ARG:O	6:X:146:ALA:HB3	2.16	0.45
1:1:199:PRO:HG3	1:1:400:CYS:HB3	1.99	0.45
1:1:276:ILE:HD12	1:1:307:LEU:CD2	2.47	0.45
1:1:402:LEU:O	1:1:403:ALA:C	2.56	0.45
2:2:112:THR:HG23	2:2:115:GLY:H	1.80	0.45
2:2:65:SER:O	3:3:204:GLU:HA	2.16	0.45
3:3:225:ASN:O	3:3:229:ILE:HG13	2.16	0.45
4:4:252:TYR:CE2	4:4:346:THR:HA	2.52	0.45
4:4:64:THR:HG23	6:6:123:ILE:HD12	1.96	0.45
5:5:28:VAL:O	5:5:29:LEU:HD23	2.17	0.45
6:6:81:ALA:CA	6:6:108:MET:HB3	2.43	0.45
1:A:228:VAL:HB	1:A:229:PRO:CD	2.47	0.45
1:A:367:MET:CE	1:A:410:VAL:HG21	2.47	0.45
2:B:86:LEU:CG	2:B:90:LEU:HD11	2.46	0.45
3:C:583:VAL:O	3:C:583:VAL:HG23	2.17	0.45
4:D:84:ARG:HE	4:D:169:HIS:CD2	2.35	0.45
5:E:15:TYR:HA	5:E:16:PRO:HD3	1.81	0.45
5:E:73:GLU:OE2	5:E:87:ARG:HD3	2.17	0.45
7:G:105:GLU:HG3	7:G:114:VAL:HA	1.98	0.45
1:J:180:TYR:HB3	1:J:351:GLU:CD	2.37	0.45
3:L:18:SER:HB3	3:L:21:ASP:OD1	2.16	0.45
3:L:613:HIS:CE1	3:L:671:GLU:OE2	2.70	0.45
4:M:143:LEU:O	4:M:143:LEU:HD23	2.17	0.45
4:M:224:ILE:HD12	4:M:237:GLY:CA	2.45	0.45
4:M:246:TYR:HB3	4:M:347:GLU:HA	1.98	0.45
5:N:41:TYR:CE2	5:N:88:PHE:HZ	2.35	0.45
5:N:93:TYR:N	5:N:93:TYR:CD1	2.84	0.45
6:O:145:GLU:N	6:O:145:GLU:OE1	2.31	0.45
6:O:142:PRO:HB2	6:O:146:ALA:HB3	1.98	0.45
8:Q:75:ARG:HA	8:Q:80:LYS:NZ	2.32	0.45
1:S:121:ALA:O	1:S:125:ILE:HG12	2.17	0.45
1:S:184:GLU:HB3	1:S:187:ALA:CB	2.47	0.45
1:S:196:ARG:NH2	3:U:204:GLU:O	2.50	0.45
3:U:614:LEU:O	3:U:621:VAL:HA	2.17	0.45
4:V:116:ILE:HD12	4:V:182:LEU:HD21	1.98	0.45
4:V:284:ARG:HB2	4:V:284:ARG:HH11	1.82	0.45
4:V:285:GLU:C	4:V:287:VAL:N	2.69	0.45
5:W:40:HIS:C	5:W:42:LYS:N	2.70	0.45
2:2:87:SER:CB	10:2:182:FES:S2	3.05	0.45
3:3:450:LEU:HB3	3:3:459:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:456:ALA:O	3:3:459:MET:HB2	2.17	0.45
3:3:521:ALA:HA	3:3:524:LEU:HD23	1.98	0.45
5:5:154:GLU:HB3	6:6:119:ASN:HB3	1.99	0.45
8:7:75:ARG:C	8:7:80:LYS:HZ1	2.21	0.45
7:9:36:ARG:CA	7:9:167:ARG:HD3	2.45	0.45
7:9:93:ILE:HB	7:9:95:MET:HE2	1.98	0.45
1:A:108:GLU:HG2	1:A:140:ARG:CG	2.44	0.45
1:A:38:TYR:HA	1:A:116:GLU:OE1	2.17	0.45
4:D:138:LEU:C	4:D:140:LEU:N	2.70	0.45
4:D:285:GLU:C	4:D:287:VAL:N	2.70	0.45
5:E:50:ALA:HA	5:E:73:GLU:O	2.17	0.45
8:H:47:PRO:O	8:H:48:TYR:HB2	2.17	0.45
8:H:75:ARG:C	8:H:80:LYS:HZ1	2.20	0.45
1:J:233:ARG:O	1:J:234:GLY:C	2.56	0.45
1:J:9:LEU:HG	1:J:13:PHE:CE1	2.52	0.45
2:K:7:LYS:HD2	2:K:7:LYS:N	2.29	0.45
3:L:38:HIS:NE2	3:L:287:GLU:CG	2.79	0.45
3:L:451:PHE:CE1	3:L:466:GLU:HB2	2.51	0.45
3:L:378:PRO:HA	3:L:545:GLU:OE2	2.16	0.45
3:L:609:GLU:OE2	3:L:631:ASN:HB3	2.15	0.45
5:N:55:LEU:CD1	5:N:55:LEU:N	2.80	0.45
5:N:80:TRP:HB3	5:N:81:LYS:H	1.55	0.45
1:S:290:ILE:O	1:S:292:PRO:HD3	2.16	0.45
3:U:159:PHE:HE2	8:Z:79:LEU:HD22	1.82	0.45
2:T:61:MET:HB2	3:U:214:MET:HG3	1.99	0.45
3:U:627:ALA:C	3:U:629:ILE:H	2.20	0.45
3:U:634:ALA:O	3:U:635:GLU:O	2.34	0.45
3:U:731:GLY:H	3:U:747:VAL:CG1	2.13	0.45
4:V:95:LEU:HA	4:V:173:ILE:CD1	2.46	0.45
4:V:173:ILE:CG2	4:V:173:ILE:O	2.65	0.45
4:V:283:MET:O	4:V:287:VAL:HG23	2.17	0.45
4:V:285:GLU:HA	4:V:288:LYS:HD3	1.99	0.45
4:V:381:LEU:C	4:V:381:LEU:HD23	2.36	0.45
5:W:114:LEU:HD12	5:W:114:LEU:N	2.32	0.45
5:W:16:PRO:O	5:W:17:ILE:HD13	2.17	0.45
6:X:137:VAL:HG13	6:X:137:VAL:O	2.16	0.45
7:Y:45:ARG:NH2	7:Y:137:LEU:CD2	2.78	0.45
1:1:110:VAL:O	1:1:111:PRO:C	2.55	0.44
1:1:65:ARG:HA	1:1:65:ARG:HD3	1.71	0.44
2:2:31:LEU:HA	2:2:31:LEU:HD13	1.88	0.44
4:4:105:LEU:HD13	4:4:309:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:246:TYR:HB3	4:4:347:GLU:HA	1.98	0.44
4:D:156:ILE:O	4:D:159:LEU:HB2	2.17	0.44
6:F:127:VAL:C	6:F:129:SER:N	2.71	0.44
1:J:267:PRO:O	1:J:268:MET:C	2.56	0.44
2:K:130:THR:O	2:K:131:ALA:C	2.55	0.44
2:K:41:ILE:HD12	2:K:70:TYR:HB3	1.98	0.44
3:L:287:GLU:C	3:L:288:ILE:HG22	2.37	0.44
3:L:651:ARG:O	3:L:652:PRO:C	2.56	0.44
3:L:757:HIS:C	3:L:758:LEU:HD12	2.36	0.44
4:M:284:ARG:HB2	4:M:284:ARG:HH11	1.81	0.44
4:M:341:GLU:OE1	5:N:26:TRP:HH2	2.00	0.44
5:N:114:LEU:N	5:N:114:LEU:CD1	2.80	0.44
5:N:115:GLU:HB3	5:N:119:TYR:CE2	2.52	0.44
5:N:124:ILE:CG2	5:N:146:LEU:HD23	2.39	0.44
5:N:3:LEU:HD11	5:N:84:ASP:OD2	2.17	0.44
2:K:109:GLY:CA	8:Q:91:ILE:HD13	2.47	0.44
1:S:210:GLY:O	1:S:211:LEU:C	2.55	0.44
3:U:347:HIS:N	3:U:372:GLN:HB3	2.31	0.44
3:U:25:HIS:CE1	3:U:427:ASN:OD1	2.70	0.44
3:U:588:SER:O	3:U:589:HIS:ND1	2.50	0.44
4:V:105:LEU:HD13	4:V:309:ILE:CD1	2.47	0.44
4:V:118:VAL:HG23	4:V:119:ILE:N	2.32	0.44
4:V:154:GLU:CD	4:V:167:ARG:HH22	2.19	0.44
4:V:197:LEU:N	4:V:198:PRO:CD	2.81	0.44
4:V:211:SER:OG	4:V:212:PRO:HD2	2.18	0.44
1:1:19:ALA:HB2	1:1:237:TRP:HH2	1.82	0.44
1:1:310:PRO:O	1:1:315:HIS:HB2	2.17	0.44
1:1:369:ASN:O	1:1:372:ALA:HB3	2.17	0.44
2:2:88:CYS:C	2:2:93:ALA:HB2	2.38	0.44
3:3:652:PRO:C	3:3:654:PHE:H	2.21	0.44
3:3:669:VAL:HG13	3:3:669:VAL:O	2.15	0.44
3:3:6:VAL:HG21	3:3:26:ALA:CB	2.47	0.44
4:4:217:ARG:HG3	4:4:217:ARG:HH11	1.82	0.44
4:4:235:THR:CA	4:4:239:LEU:HD22	2.43	0.44
1:A:95:GLU:OE1	1:A:101:PHE:HA	2.17	0.44
3:C:241:ARG:HH11	7:G:74:GLU:CD	2.21	0.44
3:C:378:PRO:HB2	3:C:381:LEU:HD23	1.99	0.44
3:C:591:HIS:HE1	3:C:593:LEU:HD23	1.81	0.44
4:D:197:LEU:O	4:D:198:PRO:C	2.55	0.44
5:E:47:ASN:ND2	5:E:77:LEU:N	2.65	0.44
6:F:81:ALA:CA	6:F:108:MET:HB3	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:101:ARG:HH11	3:L:101:ARG:HB3	1.83	0.44
3:L:286:ASN:C	3:L:286:ASN:ND2	2.70	0.44
4:M:199:HIS:ND1	4:M:200:ARG:N	2.65	0.44
4:M:226:PRO:HD3	4:M:239:LEU:HB2	1.96	0.44
5:N:52:ILE:HG13	5:N:53:VAL:N	2.32	0.44
6:O:16:ARG:HA	6:O:21:PHE:CD2	2.51	0.44
6:O:164:ASN:OD1	7:P:124:TYR:HE2	2.00	0.44
7:P:46:HIS:CD2	7:P:52:LYS:HG2	2.52	0.44
1:S:290:ILE:HG22	1:S:330:LEU:CD2	2.47	0.44
3:U:293:ALA:HB2	3:U:698:MET:HG2	1.99	0.44
4:V:113:ALA:O	4:V:114:GLU:C	2.56	0.44
6:X:163:TYR:CD1	6:X:163:TYR:O	2.70	0.44
2:2:109:GLY:CA	8:7:91:ILE:HD13	2.47	0.44
3:3:655:ARG:HH11	3:3:656:LEU:CD2	2.30	0.44
4:4:40:VAL:O	4:4:40:VAL:HG12	2.17	0.44
6:6:30:TRP:C	6:6:30:TRP:CD1	2.90	0.44
11:7:500:FMN:H9	11:7:500:FMN:O2'	2.16	0.44
7:9:100:PHE:N	7:9:100:PHE:CD1	2.85	0.44
7:9:51:GLU:OE1	7:9:133:LYS:HE3	2.16	0.44
1:A:202:LYS:N	1:A:203:PRO:CD	2.80	0.44
1:A:258:VAL:HG21	1:A:280:ALA:HB1	1.99	0.44
1:A:62:LEU:HD12	1:A:65:ARG:NH2	2.33	0.44
3:C:620:ARG:HD2	3:C:622:LEU:HD21	2.00	0.44
4:D:221:VAL:HG23	4:D:221:VAL:O	2.18	0.44
4:D:250:LYS:HG3	4:D:250:LYS:O	2.17	0.44
5:E:58:LEU:O	5:E:59:THR:HB	2.18	0.44
6:F:142:PRO:HB2	6:F:146:ALA:HB3	1.99	0.44
7:G:177:THR:O	7:G:178:GLU:C	2.55	0.44
1:J:112:HIS:O	1:J:113:LEU:C	2.54	0.44
2:K:86:LEU:HG	2:K:90:LEU:HD11	1.99	0.44
3:L:721:GLU:O	3:L:722:THR:OG1	2.32	0.44
5:N:6:VAL:O	5:N:9:GLU:HB3	2.17	0.44
1:S:370:LEU:HD22	1:S:370:LEU:H	1.83	0.44
3:U:517:ALA:HA	3:U:520:ARG:CG	2.48	0.44
3:U:261:VAL:O	3:U:616:ASN:ND2	2.51	0.44
3:U:642:ALA:O	3:U:645:ALA:HB3	2.18	0.44
4:V:140:LEU:HD23	4:V:142:ALA:H	1.83	0.44
4:V:197:LEU:O	4:V:198:PRO:C	2.56	0.44
4:V:272:VAL:HA	4:V:275:ARG:HD2	1.99	0.44
4:V:346:THR:OG1	4:V:347:GLU:N	2.51	0.44
5:W:25:LEU:CD2	5:W:25:LEU:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:30:TRP:C	6:X:30:TRP:CD1	2.90	0.44
1:1:53:VAL:HG11	1:1:124:ALA:HB2	1.98	0.44
1:1:74:LEU:HD12	1:1:77:SER:OG	2.17	0.44
3:3:171:SER:O	3:3:173:PHE:N	2.50	0.44
3:3:374:ARG:NH2	3:3:684:ARG:CG	2.80	0.44
3:3:512:LEU:HA	3:3:512:LEU:HD12	1.86	0.44
3:3:651:ARG:HD3	3:3:651:ARG:O	2.18	0.44
4:4:250:LYS:HD2	4:4:254:TYR:CE2	2.53	0.44
4:4:367:ARG:NH1	4:4:369:LYS:HB2	2.32	0.44
5:5:137:THR:CG2	5:5:139:GLU:CD	2.86	0.44
5:5:95:PRO:HB2	5:5:98:ASP:HB3	1.99	0.44
6:6:99:MET:HB3	6:6:100:PRO:HD2	1.98	0.44
8:7:121:ARG:NH1	8:7:121:ARG:HG3	2.30	0.44
7:9:53:CYS:HB2	7:9:112:ALA:HB1	1.99	0.44
1:A:184:GLU:O	1:A:185:GLU:C	2.55	0.44
1:A:312:SER:C	1:A:314:GLU:H	2.20	0.44
2:B:163:LEU:HA	2:B:166:ILE:CD1	2.47	0.44
2:B:86:LEU:O	2:B:87:SER:C	2.53	0.44
5:E:155:THR:N	6:F:119:ASN:HD22	2.15	0.44
6:F:144:PRO:O	6:F:147:LEU:N	2.50	0.44
2:B:111:VAL:HG12	8:H:121:ARG:CZ	2.48	0.44
1:J:402:LEU:O	1:J:403:ALA:C	2.55	0.44
2:K:137:ASN:O	2:K:138:ASP:CB	2.47	0.44
2:K:66:PHE:CE1	3:L:205:ARG:HD3	2.52	0.44
3:L:115:HIS:CD2	3:L:116:PRO:HD2	2.52	0.44
3:L:185:LYS:HG3	3:L:202:PHE:CE2	2.52	0.44
3:L:459:MET:CG	3:L:465:HIS:HB2	2.47	0.44
4:M:138:LEU:C	4:M:140:LEU:N	2.71	0.44
4:M:230:ILE:HG12	4:M:239:LEU:HB3	1.99	0.44
4:M:264:VAL:H	4:M:285:GLU:HG3	1.82	0.44
4:M:373:PRO:HG2	4:M:374:SER:H	1.83	0.44
7:P:119:PHE:C	7:P:119:PHE:CD1	2.90	0.44
8:Q:16:LEU:HG	8:Q:82:ILE:HD11	2.00	0.44
1:S:189:MET:HE1	1:S:206:PRO:HB3	1.99	0.44
1:S:202:LYS:N	1:S:203:PRO:CD	2.80	0.44
2:T:24:ARG:HA	2:T:53:VAL:HG13	1.99	0.44
3:U:692:PHE:CE1	3:U:763:LEU:HA	2.52	0.44
4:V:234:LEU:HD13	4:V:352:GLU:CB	2.47	0.44
4:V:358:VAL:O	4:V:366:TYR:HB3	2.17	0.44
4:V:40:VAL:HG12	4:V:40:VAL:O	2.18	0.44
5:W:47:ASN:ND2	5:W:77:LEU:N	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:123:ASP:OD1	7:Y:124:TYR:N	2.39	0.44
8:Z:42:TYR:O	8:Z:44:MET:HG3	2.18	0.44
1:1:18:TYR:HD1	1:1:18:TYR:H	1.64	0.44
1:1:26:SER:HB3	1:1:31:TYR:CG	2.53	0.44
1:1:356:CYS:SG	1:1:399:PHE:N	2.90	0.44
1:1:359:CYS:HA	1:1:363:VAL:CG1	2.40	0.44
1:1:360:ARG:CZ	3:3:183:HIS:HB2	2.48	0.44
1:1:363:VAL:HA	1:1:367:MET:HB2	1.99	0.44
2:2:163:LEU:HA	2:2:166:ILE:CD1	2.47	0.44
3:3:178:ARG:C	3:3:180:ARG:N	2.71	0.44
4:4:225:PRO:HD2	4:4:239:LEU:HG	1.98	0.44
7:9:115:LEU:HA	7:9:115:LEU:HD23	1.73	0.44
1:A:180:TYR:HB3	1:A:351:GLU:OE1	2.17	0.44
1:A:233:ARG:O	1:A:234:GLY:C	2.54	0.44
1:A:253:GLN:NE2	1:A:325:THR:O	2.51	0.44
1:A:398:SER:CA	3:C:46:ARG:HD2	2.48	0.44
3:C:31:PRO:HG3	3:C:137:TYR:CD1	2.53	0.44
3:C:46:ARG:NH1	3:C:46:ARG:HG2	2.32	0.44
3:C:377:ALA:HB3	3:C:511:VAL:O	2.17	0.44
4:D:376:VAL:O	4:D:379:GLN:HG3	2.18	0.44
5:E:167:PRO:O	5:E:168:ALA:C	2.55	0.44
6:F:46:CYS:HB3	6:F:81:ALA:HB1	1.99	0.44
7:G:46:HIS:CD2	7:G:52:LYS:HG2	2.52	0.44
1:J:184:GLU:HB3	1:J:187:ALA:CB	2.48	0.44
2:K:145:VAL:CG1	2:K:150:LEU:HB2	2.47	0.44
2:K:86:LEU:HD12	2:K:90:LEU:HD11	1.98	0.44
3:L:282:VAL:CG2	3:L:285:VAL:HG12	2.48	0.44
3:L:54:LEU:C	3:L:73:ILE:HG22	2.38	0.44
3:L:621:VAL:HG21	3:L:671:GLU:O	2.18	0.44
4:M:115:THR:CG2	4:M:297:LEU:HD23	2.47	0.44
6:O:131:VAL:O	6:O:131:VAL:HG23	2.17	0.44
1:S:149:ILE:CG2	1:S:153:ARG:HH21	2.31	0.44
1:S:401:PRO:O	1:S:404:ASP:HB2	2.18	0.44
2:T:3:PHE:CD1	2:T:3:PHE:C	2.90	0.44
2:T:86:LEU:HD11	2:T:90:LEU:HD11	1.97	0.44
3:U:527:ARG:HB3	3:U:530:ALA:CB	2.47	0.44
4:V:212:PRO:O	4:V:214:PHE:N	2.50	0.44
4:V:220:GLY:O	4:V:272:VAL:CG2	2.66	0.44
4:V:224:ILE:HB	4:V:237:GLY:O	2.17	0.44
3:U:154:TYR:CZ	4:V:312:PRO:HB3	2.52	0.44
5:W:70:VAL:O	5:W:91:ARG:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:95:PRO:HB2	5:W:98:ASP:HB3	1.99	0.44
7:Y:126:TYR:O	7:Y:128:ASP:N	2.50	0.44
1:1:112:HIS:O	1:1:113:LEU:C	2.55	0.44
3:3:202:PHE:HA	3:3:210:PHE:O	2.17	0.44
3:3:40:SER:HB3	3:3:437:ILE:HG22	2.00	0.44
3:3:640:VAL:O	3:3:641:LEU:C	2.54	0.44
3:3:719:HIS:CB	3:3:720:PRO:HD3	2.48	0.44
4:4:256:GLY:C	4:4:257:TYR:HD1	2.20	0.44
4:4:274:ASP:O	4:4:278:VAL:N	2.42	0.44
4:4:371:ARG:HH11	4:4:371:ARG:HG3	1.82	0.44
4:4:42:ARG:HD3	4:4:42:ARG:H	1.82	0.44
5:5:136:LEU:HD13	5:5:138:PRO:HG3	2.00	0.44
5:5:37:GLU:O	5:5:41:TYR:CD1	2.67	0.44
5:5:40:HIS:C	5:5:42:LYS:N	2.70	0.44
5:5:65:PRO:HB2	5:5:93:TYR:HD2	1.82	0.44
6:6:142:PRO:HB2	6:6:146:ALA:CB	2.47	0.44
8:7:116:PHE:O	8:7:120:ASP:HB2	2.16	0.44
7:9:177:THR:O	7:9:178:GLU:C	2.56	0.44
1:A:222:GLU:OE2	1:A:251:LEU:HD13	2.17	0.44
1:A:23:LYS:C	1:A:24:GLU:OE1	2.55	0.44
1:A:356:CYS:HB3	1:A:358:PRO:CG	2.47	0.44
3:C:565:TYR:CD1	3:C:582:PHE:HB3	2.46	0.44
3:C:657:HIS:O	3:C:660:ALA:N	2.50	0.44
4:D:225:PRO:HD2	4:D:239:LEU:HG	1.99	0.44
3:C:154:TYR:CZ	4:D:312:PRO:HB3	2.52	0.44
4:D:42:ARG:H	4:D:42:ARG:HD3	1.82	0.44
8:H:23:TYR:CD1	8:H:23:TYR:C	2.91	0.44
1:J:210:GLY:O	1:J:211:LEU:C	2.56	0.44
1:J:276:ILE:O	1:J:280:ALA:HB3	2.17	0.44
1:J:89:LEU:HB2	1:J:125:ILE:HD11	2.00	0.44
3:L:307:LYS:N	3:L:307:LYS:HE2	2.32	0.44
3:L:411:LEU:O	3:L:414:SER:HB3	2.18	0.44
3:L:476:ILE:N	3:L:476:ILE:HD12	2.32	0.44
4:M:240:ARG:HH11	5:N:78:PRO:HD2	1.83	0.44
4:M:393:MET:HA	4:M:396:ILE:CG2	2.48	0.44
4:M:83:PRO:HB2	4:M:169:HIS:HA	2.00	0.44
4:M:84:ARG:HD3	6:O:117:MET:HE3	2.00	0.44
6:O:83:ARG:HG2	6:O:83:ARG:H	1.53	0.44
7:P:33:LEU:H	7:P:33:LEU:HD12	1.82	0.44
1:S:366:PHE:CE1	1:S:370:LEU:HD21	2.53	0.44
1:S:370:LEU:CD2	1:S:370:LEU:H	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:243:ARG:CB	3:U:275:LEU:HD12	2.44	0.44
4:V:102:GLU:CD	4:V:117:ARG:HH22	2.20	0.44
3:3:133:ARG:NH1	5:5:185:LYS:HE3	2.33	0.44
3:3:17:THR:CG2	3:3:18:SER:N	2.80	0.44
3:3:252:THR:HG21	3:3:626:PRO:O	2.18	0.44
3:3:621:VAL:HG21	3:3:671:GLU:O	2.18	0.44
3:3:655:ARG:HG3	3:3:655:ARG:NH1	2.31	0.44
3:3:669:VAL:CG1	3:3:669:VAL:O	2.65	0.44
5:5:66:GLU:HG2	5:5:95:PRO:HA	1.99	0.44
7:9:153:THR:HG22	7:9:155:LYS:CB	2.47	0.44
7:9:178:GLU:O	7:9:179:GLY:C	2.56	0.44
7:9:40:ARG:O	7:9:116:GLY:HA3	2.18	0.44
1:A:287:ILE:HG22	1:A:302:PHE:HB2	2.00	0.44
1:A:321:SER:OG	1:A:322:MET:N	2.50	0.44
3:C:156:ARG:H	3:C:156:ARG:HG2	1.63	0.44
3:C:369:LEU:N	3:C:369:LEU:CD2	2.77	0.44
4:D:196:VAL:HG13	4:D:197:LEU:N	2.33	0.44
4:D:249:ARG:NH2	5:E:87:ARG:NE	2.50	0.44
4:D:79:ILE:HG22	4:D:171:ASN:ND2	2.33	0.44
4:D:61:TYR:CE1	6:F:87:LYS:HG2	2.52	0.44
1:J:249:MET:HE2	1:J:249:MET:H	1.81	0.44
3:L:310:LEU:HD23	3:L:319:GLU:HA	1.99	0.44
3:L:632:GLY:O	3:L:634:ALA:N	2.51	0.44
3:L:714:ALA:HA	3:L:752:ASP:CG	2.38	0.44
4:M:50:GLU:O	4:M:51:GLU:OE2	2.35	0.44
1:S:293:GLY:C	1:S:324:GLY:O	2.56	0.44
2:T:27:ILE:CG2	2:T:31:LEU:HD23	2.48	0.44
3:U:357:ALA:HB2	3:U:641:LEU:HD11	1.98	0.44
3:U:570:PHE:O	3:U:572:PRO:HD3	2.17	0.44
4:V:89:HIS:ND1	4:V:349:ALA:HB1	2.32	0.44
5:W:104:VAL:C	5:W:106:ASP:N	2.71	0.44
5:W:187:GLY:C	5:W:189:ARG:N	2.70	0.44
5:W:16:PRO:HB2	5:W:28:VAL:HG11	1.99	0.44
7:Y:137:LEU:O	7:Y:140:VAL:HG12	2.18	0.44
1:1:181:ILE:HG23	1:1:182:CYS:N	2.33	0.44
1:1:222:GLU:OE1	1:1:251:LEU:HB2	2.17	0.44
1:1:361:GLU:OE2	3:3:162:ARG:NH2	2.50	0.44
1:1:391:LEU:HB2	1:1:392:PRO:CD	2.48	0.44
3:3:177:ASP:CB	3:3:235:LEU:HD22	2.48	0.44
3:3:349:ALA:O	3:3:540:ASN:ND2	2.50	0.44
3:3:591:HIS:ND1	3:3:592:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:621:VAL:HG23	3:3:621:VAL:O	2.17	0.44
4:4:144:THR:N	4:4:145:PRO:CD	2.81	0.44
4:4:248:VAL:C	4:4:249:ARG:HG2	2.38	0.44
4:4:358:VAL:O	4:4:366:TYR:HB3	2.18	0.44
5:5:115:GLU:HB3	5:5:119:TYR:CE2	2.53	0.44
5:5:147:ARG:NH1	5:5:149:ASP:OD1	2.51	0.44
6:6:145:GLU:N	6:6:145:GLU:OE1	2.30	0.44
6:6:84:LEU:HD11	6:6:89:ALA:CA	2.39	0.44
2:B:42:ARG:HB3	2:B:44:GLU:OE1	2.18	0.44
3:C:252:THR:HG21	3:C:626:PRO:O	2.18	0.44
3:C:75:TRP:CE3	3:C:75:TRP:HA	2.52	0.44
5:E:115:GLU:HB3	5:E:119:TYR:CZ	2.53	0.44
1:J:220:ASN:O	1:J:221:VAL:C	2.57	0.44
1:J:254:ILE:HB	1:J:275:LEU:HD21	1.99	0.44
3:L:253:PRO:HA	3:L:266:THR:HA	2.00	0.44
3:L:240:ALA:HB2	3:L:275:LEU:O	2.18	0.44
3:L:402:PRO:HA	3:L:535:MET:CE	2.47	0.44
4:M:213:ILE:HG23	4:M:215:TYR:CE2	2.53	0.44
4:M:248:VAL:HG12	4:M:249:ARG:CD	2.41	0.44
4:M:310:THR:HG23	4:M:311:PRO:CD	2.46	0.44
7:P:105:GLU:HG3	7:P:114:VAL:HA	1.99	0.44
1:S:103:ASP:OD1	1:S:221:VAL:HB	2.17	0.44
1:S:110:VAL:O	1:S:111:PRO:C	2.55	0.44
1:S:352:SER:OG	1:S:353:CYS:N	2.49	0.44
2:T:112:THR:CG2	2:T:116:LEU:HD23	2.46	0.44
2:T:162:ARG:HG3	2:T:162:ARG:H	1.57	0.44
3:U:340:GLU:CA	3:U:366:THR:HB	2.47	0.44
3:U:451:PHE:CE1	3:U:466:GLU:HB2	2.51	0.44
6:X:33:SER:HA	6:X:158:VAL:HG21	2.00	0.44
2:2:10:PHE:CD1	2:2:11:LEU:N	2.86	0.44
3:3:17:THR:HG22	3:3:18:SER:N	2.32	0.44
3:3:261:VAL:CG2	9:3:786:SF4:S2	3.06	0.44
3:3:96:LEU:CD1	3:3:96:LEU:N	2.78	0.44
4:4:213:ILE:CG2	4:4:215:TYR:CE2	3.01	0.44
4:4:257:TYR:O	4:4:263:ASP:N	2.51	0.44
4:4:234:LEU:HD13	4:4:352:GLU:CB	2.48	0.44
5:5:15:TYR:HA	5:5:16:PRO:HD3	1.82	0.44
8:7:112:LYS:HG2	8:7:116:PHE:HE1	1.82	0.44
7:9:144:LYS:N	7:9:145:PRO:HD2	2.33	0.44
1:A:9:LEU:HA	1:A:13:PHE:HZ	1.83	0.44
1:A:310:PRO:O	1:A:315:HIS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:411:LEU:O	3:C:414:SER:HB3	2.18	0.44
4:D:224:ILE:HB	4:D:237:GLY:O	2.18	0.44
4:D:95:LEU:HG	4:D:99:LEU:HD23	1.99	0.44
1:J:199:PRO:HG3	1:J:400:CYS:HB3	2.00	0.44
1:J:258:VAL:HG21	1:J:280:ALA:HB1	1.98	0.44
1:J:366:PHE:CD1	1:J:370:LEU:CD2	2.97	0.44
3:L:178:ARG:CG	3:L:178:ARG:O	2.59	0.44
3:L:30:VAL:HG22	3:L:48:CYS:HA	2.00	0.44
3:L:714:ALA:HA	3:L:752:ASP:CB	2.48	0.44
3:L:692:PHE:O	3:L:760:LEU:HA	2.18	0.44
3:L:261:VAL:CG2	9:L:786:SF4:S2	3.06	0.44
4:M:212:PRO:O	4:M:214:PHE:N	2.51	0.44
5:N:147:ARG:HG3	5:N:149:ASP:OD1	2.18	0.44
1:S:134:VAL:HG23	1:S:134:VAL:O	2.17	0.44
1:S:303:THR:OG1	1:S:306:VAL:HG23	2.18	0.44
1:S:310:PRO:O	1:S:315:HIS:HB2	2.18	0.44
1:S:81:LYS:CG	1:S:82:ASP:N	2.81	0.44
2:T:72:PHE:CD1	2:T:72:PHE:N	2.86	0.44
3:U:402:PRO:HA	3:U:535:MET:HE1	1.99	0.44
3:U:568:TYR:CE2	3:U:572:PRO:HG2	2.53	0.44
4:V:246:TYR:HB3	4:V:347:GLU:HA	1.99	0.44
4:V:334:GLY:N	4:V:363:SER:OG	2.50	0.44
5:W:26:TRP:CZ3	5:W:91:ARG:CZ	3.01	0.44
1:1:291:ILE:O	1:1:328:VAL:HA	2.17	0.43
1:1:89:LEU:HB2	1:1:125:ILE:HD11	2.00	0.43
3:3:134:THR:O	3:3:138:GLY:CA	2.66	0.43
3:3:401:ASP:OD2	3:3:404:GLU:HG2	2.17	0.43
3:3:719:HIS:HB2	3:3:720:PRO:CD	2.46	0.43
4:4:171:ASN:HA	4:4:171:ASN:HD22	1.63	0.43
4:4:66:PHE:O	4:4:68:LYS:N	2.51	0.43
5:5:22:LEU:HD23	5:5:22:LEU:N	2.33	0.43
6:6:93:ARG:O	6:6:96:TRP:N	2.46	0.43
3:C:310:LEU:HD23	3:C:319:GLU:HA	2.00	0.43
4:D:148:TYR:O	4:D:151:ARG:HB3	2.18	0.43
4:D:213:ILE:CG2	4:D:215:TYR:CE2	3.01	0.43
4:D:342:VAL:HG21	5:E:22:LEU:HD12	1.99	0.43
4:D:342:VAL:CG2	4:D:343:TYR:N	2.79	0.43
6:F:130:VAL:CG2	6:F:131:VAL:H	2.30	0.43
1:J:9:LEU:HD23	1:J:9:LEU:C	2.38	0.43
2:K:10:PHE:HD1	2:K:11:LEU:N	2.16	0.43
3:L:347:HIS:N	3:L:372:GLN:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:632:GLY:C	3:L:634:ALA:N	2.72	0.43
3:L:753:VAL:HB	3:L:754:PRO:CD	2.48	0.43
4:M:103:LYS:HE3	5:N:22:LEU:HB3	2.01	0.43
4:M:281:ARG:HH11	4:M:281:ARG:HG3	1.83	0.43
3:L:131:GLN:HA	4:M:325:ILE:HD13	1.98	0.43
8:Q:40:PHE:O	8:Q:43:ARG:HB3	2.18	0.43
1:S:149:ILE:O	1:S:153:ARG:HB2	2.18	0.43
1:S:398:SER:CA	3:U:46:ARG:HD2	2.48	0.43
3:U:285:VAL:CG1	3:U:286:ASN:H	2.07	0.43
3:U:368:HIS:ND1	3:U:368:HIS:O	2.48	0.43
3:U:378:PRO:HB2	3:U:381:LEU:HD23	2.00	0.43
3:U:714:ALA:O	3:U:745:ALA:HA	2.18	0.43
4:V:138:LEU:C	4:V:140:LEU:N	2.72	0.43
4:V:316:LEU:C	4:V:318:GLU:N	2.71	0.43
4:V:320:SER:O	4:V:322:GLU:N	2.51	0.43
7:Y:42:VAL:HG21	7:Y:170:LEU:HD22	1.99	0.43
5:W:167:PRO:HB3	7:Y:66:TYR:CE2	2.53	0.43
4:4:238:SER:N	5:5:112:ASN:OD1	2.52	0.43
6:6:127:VAL:O	6:6:130:VAL:HG22	2.18	0.43
7:9:134:GLU:N	7:9:134:GLU:CD	2.70	0.43
1:A:162:LEU:C	1:A:163:PHE:CD1	2.91	0.43
1:A:20:HIS:CE1	1:A:226:SER:CA	3.01	0.43
3:C:290:ILE:HA	3:C:290:ILE:HD13	1.81	0.43
3:C:290:ILE:HG21	3:C:295:ARG:HB2	2.00	0.43
3:C:355:LEU:HG	3:C:654:PHE:CZ	2.53	0.43
3:C:417:VAL:HG13	3:C:444:ARG:O	2.18	0.43
3:C:465:HIS:O	3:C:465:HIS:CD2	2.71	0.43
4:D:184:GLU:CD	4:D:184:GLU:H	2.20	0.43
4:D:225:PRO:HG2	4:D:238:SER:HA	1.99	0.43
4:D:350:ARG:HG3	4:D:350:ARG:HH11	1.82	0.43
4:D:47:LEU:N	4:D:47:LEU:HD12	2.32	0.43
4:D:62:LEU:HD23	4:D:62:LEU:HA	1.84	0.43
5:E:139:GLU:O	5:E:140:ASP:HB2	2.17	0.43
5:E:94:VAL:HA	5:E:95:PRO:HD3	1.90	0.43
8:H:16:LEU:O	8:H:19:TRP:HB2	2.18	0.43
1:J:98:PRO:HB2	1:J:295:SER:HB2	1.99	0.43
1:J:343:ASN:HD22	2:K:89:LYS:HD2	1.83	0.43
1:J:93:ALA:O	1:J:134:VAL:HA	2.17	0.43
2:K:45:ARG:O	2:K:48:GLU:HB3	2.18	0.43
3:L:171:SER:HB2	3:L:174:VAL:O	2.18	0.43
3:L:285:VAL:CG1	3:L:286:ASN:H	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:347:HIS:CE1	3:L:755:LYS:HD2	2.53	0.43
3:L:652:PRO:HA	3:L:653:PRO:HD3	1.80	0.43
3:L:355:LEU:HG	3:L:654:PHE:CZ	2.53	0.43
3:L:731:GLY:CA	3:L:747:VAL:HG12	2.48	0.43
5:N:187:GLY:C	5:N:189:ARG:N	2.72	0.43
6:O:41:PHE:CE2	6:O:92:MET:HB2	2.52	0.43
6:O:90:PRO:O	6:O:93:ARG:HB3	2.18	0.43
8:Q:23:TYR:HD2	8:Q:116:PHE:CD2	2.36	0.43
8:Q:38:PRO:C	8:Q:40:PHE:N	2.70	0.43
8:Q:61:ASP:OD1	8:Q:63:LEU:N	2.51	0.43
1:S:170:ASP:O	1:S:171:LEU:HD12	2.17	0.43
2:T:32:ARG:O	2:T:33:ARG:C	2.57	0.43
3:U:18:SER:HB3	3:U:21:ASP:OD1	2.17	0.43
3:U:498:GLU:O	3:U:527:ARG:NH2	2.50	0.43
4:V:213:ILE:HG23	4:V:215:TYR:CE2	2.52	0.43
4:V:366:TYR:CZ	5:W:148:LYS:HE3	2.53	0.43
4:V:375:PHE:CZ	5:W:116:ARG:HB3	2.54	0.43
8:Z:13:TRP:CE2	8:Z:17:LEU:HD11	2.53	0.43
8:Z:43:ARG:C	8:Z:44:MET:HG3	2.38	0.43
1:1:203:PRO:N	1:1:204:PRO:CD	2.81	0.43
1:1:323:LEU:C	1:1:323:LEU:HD23	2.39	0.43
1:1:367:MET:CE	1:1:410:VAL:HG21	2.48	0.43
1:1:93:ALA:O	1:1:134:VAL:HA	2.17	0.43
4:4:395:ALA:O	4:4:399:SER:HB3	2.18	0.43
5:5:113:PHE:HB3	5:5:114:LEU:H	1.42	0.43
7:9:110:THR:HG22	8:7:41:ILE:O	2.17	0.43
1:A:114:LEU:CD2	1:A:118:MET:SD	3.06	0.43
3:C:13:VAL:O	3:C:13:VAL:HG13	2.17	0.43
3:C:113:LEU:HG	3:C:157:PHE:CE2	2.53	0.43
3:C:174:VAL:HG11	3:C:296:PHE:CD1	2.49	0.43
4:D:131:VAL:O	4:D:134:GLY:N	2.52	0.43
4:D:221:VAL:HB	4:D:223:VAL:HG23	2.00	0.43
4:D:40:VAL:O	4:D:40:VAL:HG12	2.18	0.43
5:E:31:ARG:HH11	5:E:31:ARG:CG	2.31	0.43
6:F:105:VAL:HB	6:F:133:VAL:HA	2.01	0.43
1:J:250:LYS:HG3	1:J:251:LEU:N	2.33	0.43
1:J:371:PHE:HA	1:J:374:ILE:HG23	2.00	0.43
2:K:86:LEU:CG	2:K:90:LEU:HD11	2.47	0.43
3:L:324:GLU:O	3:L:325:ALA:C	2.56	0.43
3:L:572:PRO:CB	3:L:573:PRO:HD2	2.49	0.43
4:M:197:LEU:N	4:M:198:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:353:LEU:HD12	4:M:354:GLY:N	2.29	0.43
5:N:132:LEU:HD23	5:N:135:ILE:CG2	2.48	0.43
5:N:46:PHE:O	5:N:47:ASN:C	2.57	0.43
1:S:53:VAL:HG11	1:S:124:ALA:HB2	1.99	0.43
1:S:87:HIS:HB2	1:S:126:ARG:O	2.18	0.43
1:S:13:PHE:HD1	1:S:13:PHE:O	2.00	0.43
1:S:162:LEU:C	1:S:163:PHE:CD1	2.92	0.43
3:U:106:GLY:O	3:U:109:GLU:HB3	2.18	0.43
3:U:310:LEU:HD23	3:U:319:GLU:HA	2.00	0.43
3:U:450:LEU:HB3	3:U:459:MET:CE	2.49	0.43
3:U:512:LEU:HA	3:U:512:LEU:HD12	1.89	0.43
3:U:527:ARG:O	3:U:530:ALA:HB2	2.17	0.43
3:U:717:TRP:CG	3:U:717:TRP:O	2.72	0.43
3:U:714:ALA:HA	3:U:752:ASP:CB	2.48	0.43
4:V:225:PRO:HD3	4:V:239:LEU:HG	2.00	0.43
4:V:383:TYR:HA	4:V:386:LYS:HB2	2.00	0.43
5:W:121:LEU:HB3	5:W:127:GLU:HG3	1.99	0.43
7:Y:76:ASP:O	7:Y:77:PRO:C	2.57	0.43
8:Z:116:PHE:O	8:Z:120:ASP:HB2	2.18	0.43
8:Z:46:ARG:HB3	8:Z:47:PRO:HD2	1.99	0.43
3:3:101:ARG:HB3	3:3:101:ARG:HH11	1.84	0.43
3:3:120:PRO:CG	8:7:42:TYR:OH	2.66	0.43
3:3:303:GLN:HB3	3:3:304:ASN:H	1.56	0.43
3:3:377:ALA:HB3	3:3:511:VAL:O	2.18	0.43
4:4:184:GLU:CD	4:4:184:GLU:H	2.20	0.43
4:4:381:LEU:HD23	4:4:381:LEU:C	2.38	0.43
4:4:79:ILE:HG22	4:4:171:ASN:ND2	2.32	0.43
5:5:34:PHE:CD1	5:5:38:MET:HB2	2.53	0.43
6:6:31:GLY:C	6:6:33:SER:N	2.71	0.43
3:3:216:PHE:CD2	8:7:63:LEU:HD23	2.53	0.43
1:A:11:PRO:HA	1:A:267:PRO:HG3	1.99	0.43
1:A:201:LEU:HG	1:A:203:PRO:CD	2.33	0.43
2:B:85:THR:HG22	2:B:86:LEU:N	2.34	0.43
3:C:112:LEU:HD22	4:D:322:GLU:HG3	2.01	0.43
3:C:120:PRO:CG	8:H:42:TYR:OH	2.66	0.43
3:C:318:VAL:HG13	3:C:319:GLU:OE2	2.18	0.43
3:C:650:VAL:CG1	3:C:651:ARG:H	2.29	0.43
4:D:330:HIS:C	4:D:330:HIS:HD1	2.22	0.43
7:G:137:LEU:HD12	7:G:137:LEU:N	2.33	0.43
7:G:48:ASN:HB2	7:G:50:LEU:HD23	2.00	0.43
1:J:272:PHE:CE1	1:J:311:MET:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:195:LEU:HA	2:K:24:ARG:NH2	2.32	0.43
3:L:507:LEU:HD12	3:L:507:LEU:O	2.18	0.43
4:M:105:LEU:HD13	4:M:309:ILE:CD1	2.49	0.43
4:M:59:ILE:N	4:M:59:ILE:CD1	2.69	0.43
5:N:167:PRO:O	5:N:168:ALA:C	2.54	0.43
6:O:130:VAL:CG2	6:O:131:VAL:N	2.81	0.43
6:O:164:ASN:O	7:P:148:ARG:CD	2.65	0.43
7:P:178:GLU:O	7:P:179:GLY:C	2.56	0.43
8:Q:39:ASP:OD2	8:Q:75:ARG:HG3	2.18	0.43
1:S:233:ARG:O	1:S:234:GLY:C	2.57	0.43
2:T:85:THR:CG2	2:T:86:LEU:N	2.82	0.43
3:U:116:PRO:O	3:U:117:LEU:CB	2.65	0.43
3:U:260:PRO:CB	3:U:617:LEU:HB3	2.48	0.43
3:U:586:HIS:HE1	3:U:637:ALA:HA	1.83	0.43
4:V:109:VAL:CG1	4:V:113:ALA:HB3	2.48	0.43
4:V:168:PHE:HZ	6:X:49:GLU:HB2	1.83	0.43
4:V:230:ILE:C	4:V:232:LEU:N	2.72	0.43
4:V:328:PHE:O	4:V:332:THR:HG23	2.18	0.43
4:V:245:ASN:ND2	4:V:352:GLU:OE1	2.51	0.43
4:V:393:MET:HA	4:V:396:ILE:CG2	2.48	0.43
6:X:93:ARG:O	6:X:96:TRP:N	2.46	0.43
8:Z:108:ILE:HA	8:Z:109:PRO:HD3	1.89	0.43
2:2:101:THR:HG23	2:2:106:ILE:O	2.18	0.43
2:2:7:LYS:HG2	2:2:7:LYS:O	2.19	0.43
3:3:115:HIS:CD2	3:3:116:PRO:HD2	2.52	0.43
3:3:260:PRO:HB3	3:3:617:LEU:HB3	2.01	0.43
3:3:692:PHE:CE1	3:3:763:LEU:HA	2.54	0.43
4:4:124:SER:O	4:4:125:ARG:C	2.56	0.43
4:4:217:ARG:HA	4:4:217:ARG:HD3	1.87	0.43
4:4:42:ARG:CD	4:4:42:ARG:N	2.80	0.43
5:5:16:PRO:HB2	5:5:28:VAL:HG11	1.99	0.43
1:A:316:LEU:HA	1:A:316:LEU:HD23	1.88	0.43
1:A:358:PRO:O	1:A:362:GLY:N	2.51	0.43
1:A:436:LEU:CD2	2:B:90:LEU:HA	2.48	0.43
3:C:386:SER:HB3	3:C:389:ASP:OD2	2.18	0.43
3:C:511:VAL:HG22	3:C:520:ARG:NH1	2.33	0.43
3:C:644:LEU:C	3:C:644:LEU:HD23	2.38	0.43
4:D:283:MET:O	4:D:287:VAL:HG23	2.18	0.43
7:G:133:LYS:O	7:G:137:LEU:CD1	2.67	0.43
1:J:287:ILE:HG22	1:J:302:PHE:CG	2.54	0.43
1:J:338:VAL:O	1:J:342:TRP:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:177:ASP:CB	3:L:235:LEU:HD22	2.48	0.43
3:L:289:TRP:O	3:L:290:ILE:HD13	2.19	0.43
3:L:303:GLN:HB3	3:L:304:ASN:H	1.56	0.43
3:L:651:ARG:O	3:L:652:PRO:O	2.37	0.43
4:M:138:LEU:O	4:M:140:LEU:N	2.52	0.43
4:M:148:TYR:O	4:M:151:ARG:HB3	2.19	0.43
4:M:342:VAL:CG2	4:M:343:TYR:H	2.25	0.43
4:M:90:SER:O	4:M:92:ALA:N	2.51	0.43
5:N:77:LEU:HA	5:N:78:PRO:HD3	1.70	0.43
6:O:48:ILE:N	6:O:48:ILE:CD1	2.81	0.43
7:P:177:THR:O	7:P:178:GLU:C	2.57	0.43
8:Q:52:THR:CB	8:Q:54:ILE:HG22	2.47	0.43
1:S:363:VAL:HA	1:S:367:MET:HB2	2.01	0.43
2:T:130:THR:HB	2:T:144:CYS:SG	2.57	0.43
2:T:81:GLN:O	2:T:134:ILE:HG23	2.17	0.43
3:U:586:HIS:CE1	3:U:637:ALA:HA	2.53	0.43
4:V:383:TYR:CD1	4:V:383:TYR:C	2.92	0.43
6:X:142:PRO:HB2	6:X:146:ALA:CB	2.48	0.43
7:Y:31:VAL:O	7:Y:162:VAL:N	2.51	0.43
1:1:121:ALA:O	1:1:124:ALA:HB3	2.19	0.43
1:1:162:LEU:HB3	1:1:163:PHE:CE1	2.53	0.43
2:2:87:SER:OG	2:2:128:CYS:HB3	2.19	0.43
3:3:263:CYS:CA	3:3:286:ASN:HB2	2.48	0.43
3:3:532:VAL:CG1	3:3:533:LEU:N	2.80	0.43
4:4:230:ILE:HD11	4:4:234:LEU:O	2.19	0.43
1:A:103:ASP:OD1	1:A:221:VAL:HB	2.19	0.43
2:B:122:VAL:HG12	2:B:123:GLU:N	2.32	0.43
3:C:116:PRO:O	3:C:117:LEU:CB	2.67	0.43
3:C:177:ASP:CB	3:C:235:LEU:HD22	2.46	0.43
3:C:414:SER:HA	3:C:461:TRP:HZ3	1.83	0.43
3:C:651:ARG:O	3:C:652:PRO:C	2.56	0.43
3:C:657:HIS:CE1	3:C:661:GLN:OE1	2.71	0.43
3:C:470:PRO:CG	3:C:750:ARG:HH21	2.32	0.43
4:D:193:LEU:HD23	4:D:193:LEU:O	2.19	0.43
4:D:152:GLU:OE2	4:D:200:ARG:HD3	2.19	0.43
6:F:118:PHE:HB3	6:F:120:ASN:OD1	2.19	0.43
6:F:165:GLU:C	6:F:165:GLU:OE1	2.57	0.43
7:G:56:CYS:O	7:G:58:LEU:N	2.49	0.43
1:J:87:HIS:HB2	1:J:126:ARG:O	2.18	0.43
1:J:238:PHE:HE1	1:J:249:MET:CE	2.32	0.43
3:L:106:GLY:O	3:L:107:MET:C	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:20:MET:HE3	3:L:432:PHE:HB3	2.00	0.43
3:L:87:VAL:HG12	3:L:91:MET:HE1	2.01	0.43
5:N:43:ALA:C	5:N:45:GLY:H	2.21	0.43
5:N:70:VAL:HG12	5:N:72:TYR:CE1	2.54	0.43
5:N:154:GLU:CB	6:O:119:ASN:HB3	2.49	0.43
1:S:16:THR:O	1:S:17:LEU:HB2	2.19	0.43
1:S:246:SER:OG	1:S:312:SER:HB2	2.18	0.43
2:T:130:THR:O	2:T:131:ALA:C	2.57	0.43
2:T:139:GLU:CB	2:T:140:PRO:CD	2.83	0.43
3:U:168:HIS:HA	3:U:169:PRO:HD2	1.75	0.43
3:U:171:SER:HB2	3:U:174:VAL:O	2.18	0.43
3:U:371:PHE:N	3:U:371:PHE:CD1	2.86	0.43
3:U:222:PHE:CD1	3:U:411:LEU:HD11	2.53	0.43
3:U:543:GLY:CA	3:U:615:VAL:HB	2.49	0.43
3:U:655:ARG:HH11	3:U:656:LEU:HD23	1.84	0.43
4:V:115:THR:CG2	4:V:297:LEU:HD23	2.47	0.43
6:X:16:ARG:O	6:X:21:PHE:HB3	2.18	0.43
3:3:310:LEU:HD23	3:3:319:GLU:HA	2.00	0.43
3:3:383:PRO:HA	3:3:384:PRO:HD3	1.87	0.43
3:3:400:GLY:O	3:3:401:ASP:C	2.57	0.43
3:3:477:LEU:HD13	3:3:516:VAL:HG12	2.01	0.43
3:3:568:TYR:CD2	3:3:572:PRO:HG2	2.54	0.43
3:3:609:GLU:OE2	3:3:631:ASN:HB3	2.18	0.43
4:4:224:ILE:HD13	5:5:112:ASN:CA	2.49	0.43
4:4:255:SER:HG	4:4:296:ARG:HH12	1.66	0.43
4:4:383:TYR:HA	4:4:386:LYS:HB2	2.01	0.43
1:A:248:GLY:O	1:A:268:MET:HB2	2.18	0.43
2:B:24:ARG:HA	2:B:53:VAL:HG11	1.99	0.43
3:C:390:LEU:HD21	3:C:413:LEU:HD23	2.00	0.43
3:C:413:LEU:HA	3:C:416:PHE:CB	2.48	0.43
3:C:586:HIS:CE1	3:C:637:ALA:HA	2.54	0.43
3:C:641:LEU:HD23	3:C:641:LEU:HA	1.81	0.43
3:C:714:ALA:HA	3:C:752:ASP:CG	2.39	0.43
3:C:7:ASN:CG	3:C:96:LEU:HD11	2.37	0.43
4:D:112:ARG:NH1	4:D:181:ASP:OD2	2.51	0.43
4:D:371:ARG:HG3	4:D:371:ARG:HH11	1.82	0.43
5:E:195:LEU:O	5:E:196:TRP:CE3	2.71	0.43
6:F:114:SER:C	6:F:116:GLY:N	2.72	0.43
6:F:139:GLY:HA3	6:F:142:PRO:CD	2.48	0.43
1:J:264:TYR:CD2	1:J:279:TRP:HB3	2.53	0.43
1:J:293:GLY:C	1:J:324:GLY:O	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:360:ARG:CZ	3:L:183:HIS:HB2	2.49	0.43
2:K:112:THR:HG23	2:K:115:GLY:H	1.82	0.43
3:L:177:ASP:CA	3:L:235:LEU:H	2.31	0.43
3:L:19:VAL:HG13	3:L:93:VAL:HG21	2.00	0.43
3:L:398:VAL:HB	3:L:450:LEU:CD2	2.44	0.43
4:M:234:LEU:HD13	4:M:352:GLU:HB3	2.00	0.43
4:M:389:GLN:NE2	4:M:389:GLN:HA	2.33	0.43
3:U:401:ASP:OD2	3:U:404:GLU:HG2	2.18	0.43
3:U:613:HIS:CE1	3:U:671:GLU:OE2	2.72	0.43
3:U:214:MET:SD	8:Z:128:PHE:HE2	2.42	0.43
1:1:180:TYR:HB3	1:1:351:GLU:CD	2.38	0.43
1:1:401:PRO:O	1:1:404:ASP:HB2	2.17	0.43
2:2:123:GLU:CD	2:2:123:GLU:N	2.71	0.43
3:3:101:ARG:HH12	3:3:140:TYR:HD1	1.53	0.43
3:3:18:SER:HB3	3:3:21:ASP:OD1	2.18	0.43
3:3:483:ASP:O	3:3:484:LYS:HG2	2.19	0.43
3:3:614:LEU:HD13	3:3:624:LEU:HD12	2.01	0.43
3:3:656:LEU:N	3:3:656:LEU:HD23	2.29	0.43
4:4:193:LEU:C	4:4:193:LEU:HD23	2.39	0.43
4:4:225:PRO:CD	4:4:226:PRO:CD	2.93	0.43
4:4:385:CYS:HB3	4:4:396:ILE:CG1	2.31	0.43
5:5:52:ILE:HG13	5:5:53:VAL:N	2.33	0.43
8:7:52:THR:CG2	8:7:54:ILE:HG22	2.49	0.43
7:9:43:LEU:HD23	7:9:113:ILE:HD12	2.01	0.43
1:A:310:PRO:HB2	1:A:315:HIS:CG	2.53	0.43
1:A:356:CYS:SG	1:A:399:PHE:N	2.88	0.43
3:C:374:ARG:NH2	3:C:684:ARG:CG	2.82	0.43
4:D:164:THR:OG1	4:D:170:HIS:HB3	2.18	0.43
4:D:234:LEU:HD13	4:D:352:GLU:CB	2.49	0.43
5:E:119:TYR:O	5:E:120:ASP:C	2.56	0.43
5:E:132:LEU:HD23	5:E:135:ILE:CG2	2.48	0.43
5:E:37:GLU:O	5:E:40:HIS:HB3	2.18	0.43
5:E:47:ASN:HD22	5:E:77:LEU:N	2.16	0.43
6:F:114:SER:HB2	7:G:97:ARG:CD	2.38	0.43
6:F:23:THR:O	6:F:27:LEU:HB2	2.18	0.43
1:J:116:GLU:O	1:J:119:ILE:HB	2.19	0.43
1:J:181:ILE:O	1:J:183:GLY:N	2.52	0.43
2:K:3:PHE:CD1	2:K:3:PHE:C	2.92	0.43
1:J:177:ALA:O	2:K:67:TYR:HB3	2.19	0.43
3:L:164:VAL:HB	3:L:165:ASP:H	1.66	0.43
3:L:290:ILE:HD13	3:L:290:ILE:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:450:LEU:HB3	3:L:459:MET:CE	2.48	0.43
3:L:483:ASP:O	3:L:484:LYS:HG2	2.19	0.43
4:M:42:ARG:N	4:M:42:ARG:CD	2.80	0.43
5:N:101:LEU:O	5:N:130:PRO:HD2	2.18	0.43
7:P:129:LEU:HD23	7:P:129:LEU:HA	1.63	0.43
1:S:104:ARG:NH1	1:S:108:GLU:OE2	2.52	0.43
1:S:58:LYS:HA	1:S:73:GLY:HA3	2.00	0.43
3:U:185:LYS:HG3	3:U:202:PHE:HE2	1.84	0.43
3:U:17:THR:CG2	3:U:18:SER:N	2.81	0.43
3:U:44:ALA:O	3:U:45:CYS:CB	2.67	0.43
3:U:465:HIS:CD2	3:U:465:HIS:O	2.72	0.43
3:U:719:HIS:HB2	3:U:720:PRO:CD	2.44	0.43
4:V:234:LEU:CD2	4:V:234:LEU:N	2.80	0.43
4:V:249:ARG:O	4:V:250:LYS:C	2.57	0.43
4:V:224:ILE:HD13	5:W:112:ASN:CA	2.48	0.43
6:X:127:VAL:C	6:X:129:SER:H	2.22	0.43
7:Y:99:ILE:O	7:Y:99:ILE:HG23	2.19	0.43
8:Z:52:THR:CB	8:Z:54:ILE:HG22	2.48	0.43
8:Z:13:TRP:CH2	8:Z:71:ASP:HA	2.53	0.43
1:1:202:LYS:N	1:1:203:PRO:CD	2.82	0.43
1:1:337:MET:HB2	1:1:420:GLN:NE2	2.34	0.43
1:1:58:LYS:HA	1:1:73:GLY:HA3	2.01	0.43
3:3:36:GLU:O	3:3:37:LYS:C	2.54	0.43
3:3:54:LEU:O	3:3:54:LEU:HD13	2.19	0.43
5:5:25:LEU:HD23	5:5:25:LEU:N	2.24	0.43
8:7:115:PHE:O	8:7:118:LEU:HB3	2.19	0.43
7:9:58:LEU:O	7:9:61:ALA:N	2.52	0.43
7:9:99:ILE:HG23	7:9:99:ILE:O	2.18	0.43
1:A:332:PRO:HD2	2:B:90:LEU:HD23	2.00	0.43
3:C:274:LEU:O	3:C:302:ASP:OD2	2.37	0.43
3:C:588:SER:O	3:C:589:HIS:ND1	2.52	0.43
3:C:591:HIS:CE1	3:C:593:LEU:HD23	2.54	0.43
4:D:123:LEU:HD12	4:D:123:LEU:HA	1.93	0.43
4:D:366:TYR:CZ	5:E:148:LYS:HE3	2.54	0.43
5:E:76:SER:OG	5:E:83:GLY:HA2	2.19	0.43
1:J:18:TYR:N	1:J:18:TYR:CD1	2.87	0.43
1:J:97:GLU:O	1:J:100:SER:HB3	2.18	0.43
2:K:101:THR:O	2:K:105:GLY:N	2.42	0.43
2:K:42:ARG:HB3	2:K:44:GLU:OE1	2.18	0.43
2:K:67:TYR:N	2:K:67:TYR:CD1	2.86	0.43
3:L:185:LYS:HG3	3:L:202:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:305:ARG:HH12	3:L:609:GLU:CD	2.22	0.43
3:L:36:GLU:HB3	3:L:39:LEU:HD12	2.01	0.43
3:L:440:ARG:HH11	3:L:440:ARG:HG2	1.84	0.43
3:L:541:ALA:O	3:L:545:GLU:HG3	2.19	0.43
3:L:621:VAL:HG23	3:L:621:VAL:O	2.17	0.43
3:L:755:LYS:O	3:L:757:HIS:CE1	2.72	0.43
3:L:19:VAL:HG22	3:L:91:MET:HE1	2.01	0.43
4:M:42:ARG:H	4:M:42:ARG:HD3	1.84	0.43
5:N:147:ARG:NH1	5:N:149:ASP:OD1	2.51	0.43
5:N:50:ALA:HB3	5:N:114:LEU:CD1	2.29	0.43
1:S:18:TYR:N	1:S:18:TYR:CD1	2.87	0.43
3:U:31:PRO:HG3	3:U:137:TYR:CD1	2.54	0.43
3:U:17:THR:HG22	3:U:18:SER:N	2.33	0.43
3:U:341:VAL:CB	3:U:364:LEU:HD21	2.47	0.43
3:U:511:VAL:HG22	3:U:520:ARG:NH1	2.34	0.43
3:U:497:TRP:CE2	3:U:523:LEU:HD11	2.54	0.43
3:U:272:GLY:HA2	3:U:628:PRO:O	2.19	0.43
3:U:54:LEU:C	3:U:73:ILE:HG22	2.38	0.43
3:U:714:ALA:HA	3:U:752:ASP:CG	2.39	0.43
4:V:103:LYS:HE3	5:W:22:LEU:HB3	2.01	0.43
5:W:157:THR:HG21	7:Y:66:TYR:HB2	2.01	0.43
4:V:84:ARG:HD3	6:X:117:MET:HE3	2.01	0.43
6:X:89:ALA:HB3	6:X:90:PRO:CD	2.49	0.43
1:1:233:ARG:O	1:1:234:GLY:C	2.57	0.43
2:2:46:ILE:HG23	2:2:60:VAL:HG12	2.00	0.43
3:3:650:VAL:CG1	3:3:651:ARG:H	2.29	0.43
4:4:350:ARG:HG3	4:4:350:ARG:HH11	1.83	0.43
5:5:132:LEU:HD23	5:5:135:ILE:CG2	2.48	0.43
1:A:110:VAL:HG23	1:A:110:VAL:O	2.17	0.43
1:A:189:MET:HE1	1:A:206:PRO:HB3	2.00	0.43
1:A:288:GLN:NE2	1:A:333:GLU:HA	2.34	0.43
1:A:338:VAL:O	1:A:342:TRP:HB2	2.19	0.43
2:B:91:ALA:HB1	2:B:132:PRO:HD3	2.01	0.43
3:C:244:ALA:HB3	3:C:249:MET:HE1	1.98	0.43
3:C:287:GLU:C	3:C:288:ILE:HG22	2.39	0.43
3:C:368:HIS:O	3:C:368:HIS:ND1	2.51	0.43
3:C:621:VAL:HG23	3:C:621:VAL:O	2.19	0.43
4:D:138:LEU:O	4:D:140:LEU:N	2.51	0.43
4:D:381:LEU:HD11	4:D:397:ILE:CG1	2.47	0.43
4:D:70:MET:C	4:D:72:HIS:N	2.73	0.43
5:E:48:PHE:CD2	5:E:113:PHE:CE2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:83:ARG:HD3	6:F:111:CYS:SG	2.59	0.43
6:F:31:GLY:C	6:F:33:SER:N	2.72	0.43
8:H:16:LEU:HG	8:H:82:ILE:HD11	2.00	0.43
1:J:303:THR:O	1:J:306:VAL:HG23	2.19	0.43
1:J:95:GLU:OE1	1:J:101:PHE:HA	2.19	0.43
3:L:402:PRO:HB3	3:L:535:MET:HE3	2.00	0.43
3:L:222:PHE:CD1	3:L:411:LEU:HD11	2.54	0.43
3:L:516:VAL:O	3:L:519:GLU:HG2	2.19	0.43
3:L:527:ARG:O	3:L:530:ALA:HB2	2.19	0.43
3:L:627:ALA:O	3:L:629:ILE:N	2.44	0.43
4:M:244:VAL:HG12	4:M:246:TYR:H	1.84	0.43
4:M:342:VAL:HG21	5:N:22:LEU:HD12	2.01	0.43
5:N:67:ARG:HD3	5:N:68:PHE:CE1	2.54	0.43
5:N:47:ASN:ND2	5:N:77:LEU:N	2.67	0.43
6:O:137:VAL:HG13	6:O:137:VAL:O	2.18	0.43
1:S:125:ILE:O	1:S:126:ARG:HB2	2.18	0.43
1:S:253:GLN:O	1:S:328:VAL:N	2.49	0.43
3:U:166:LYS:HG3	3:U:178:ARG:CG	2.47	0.43
3:U:208:HIS:HB3	8:Z:85:ARG:NH2	2.33	0.43
3:U:383:PRO:HA	3:U:384:PRO:HD3	1.93	0.43
3:U:38:HIS:NE2	3:U:287:GLU:CG	2.82	0.43
4:V:256:GLY:C	4:V:257:TYR:HD1	2.22	0.43
4:V:74:THR:HB	4:V:77:GLN:H	1.84	0.43
7:Y:67:ALA:O	7:Y:93:ILE:HA	2.19	0.43
1:1:101:PHE:CD1	1:1:101:PHE:N	2.87	0.42
1:1:248:GLY:O	1:1:268:MET:HB2	2.19	0.42
3:3:118:ASP:O	3:3:121:THR:N	2.52	0.42
3:3:220:SER:C	3:3:221:GLY:O	2.57	0.42
3:3:534:ALA:O	3:3:617:LEU:HD12	2.19	0.42
4:4:199:HIS:ND1	4:4:200:ARG:N	2.66	0.42
4:4:227:GLU:HG2	4:4:228:VAL:N	2.34	0.42
4:4:310:THR:CG2	4:4:311:PRO:N	2.81	0.42
3:3:154:TYR:O	4:4:321:MET:HB2	2.18	0.42
4:4:46:THR:O	4:4:46:THR:HG22	2.19	0.42
6:6:118:PHE:HB3	6:6:120:ASN:OD1	2.19	0.42
6:6:39:ALA:HB2	6:6:75:ALA:HB1	2.01	0.42
7:9:104:CYS:O	7:9:105:GLU:C	2.54	0.42
1:A:353:CYS:SG	1:A:354:GLY:N	2.92	0.42
3:C:243:ARG:CD	3:C:275:LEU:HD12	2.40	0.42
3:C:719:HIS:HB2	3:C:720:PRO:CD	2.46	0.42
4:D:249:ARG:NH1	4:D:249:ARG:CB	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:130:PRO:HG2	5:E:131:ASP:N	2.27	0.42
7:G:140:VAL:HG22	7:G:141:VAL:H	1.83	0.42
7:G:43:LEU:HD23	7:G:113:ILE:HD12	2.01	0.42
8:H:75:ARG:HA	8:H:80:LYS:NZ	2.34	0.42
1:J:312:SER:O	1:J:314:GLU:N	2.50	0.42
2:K:122:VAL:HG12	2:K:123:GLU:H	1.84	0.42
3:L:189:ARG:HG3	3:L:193:GLU:OE2	2.19	0.42
3:L:285:VAL:CG1	3:L:286:ASN:N	2.67	0.42
3:L:417:VAL:HG12	3:L:417:VAL:O	2.18	0.42
3:L:513:GLN:O	3:L:516:VAL:N	2.36	0.42
3:L:564:LEU:HA	3:L:564:LEU:HD12	1.87	0.42
4:M:205:GLU:C	4:M:207:LEU:N	2.72	0.42
4:M:330:HIS:C	4:M:330:HIS:HD1	2.22	0.42
5:N:116:ARG:CG	5:N:116:ARG:NH1	2.81	0.42
7:P:162:VAL:HA	7:P:176:PRO:HG2	2.01	0.42
1:S:260:ARG:HG2	1:S:280:ALA:O	2.18	0.42
1:S:29:LEU:HD22	1:S:33:LEU:CD1	2.49	0.42
3:U:188:VAL:HG23	3:U:189:ARG:N	2.34	0.42
3:U:586:HIS:HE1	3:U:637:ALA:CA	2.32	0.42
4:V:155:THR:HG22	4:V:193:LEU:HD12	1.99	0.42
5:W:36:GLU:O	5:W:39:ALA:HB3	2.18	0.42
7:Y:43:LEU:HD23	7:Y:113:ILE:HD12	2.00	0.42
7:Y:178:GLU:O	7:Y:179:GLY:C	2.57	0.42
7:Y:45:ARG:HH21	7:Y:137:LEU:CD2	2.26	0.42
1:1:162:LEU:C	1:1:163:PHE:CD1	2.92	0.42
1:1:338:VAL:O	1:1:342:TRP:HB2	2.19	0.42
2:2:134:ILE:HG13	2:2:145:VAL:HG21	2.01	0.42
3:3:263:CYS:HA	3:3:286:ASN:CB	2.48	0.42
3:3:474:ARG:NH1	3:3:515:THR:HG21	2.34	0.42
3:3:476:ILE:N	3:3:476:ILE:CD1	2.82	0.42
5:5:2:ARG:O	5:5:5:ARG:N	2.52	0.42
1:A:407:VAL:HG23	1:A:408:TRP:N	2.34	0.42
2:B:83:CYS:SG	2:B:124:CYS:HA	2.59	0.42
3:C:113:LEU:O	3:C:161:ARG:NH1	2.51	0.42
3:C:398:VAL:HB	3:C:450:LEU:CD2	2.48	0.42
3:C:19:VAL:HG22	3:C:91:MET:HE1	2.01	0.42
4:D:252:TYR:CB	4:D:253:PRO:CD	2.90	0.42
4:D:383:TYR:HA	4:D:386:LYS:HB2	2.00	0.42
5:E:59:THR:CG2	5:E:59:THR:O	2.64	0.42
7:G:38:HIS:HD2	7:G:100:PHE:O	2.02	0.42
8:H:15:GLU:O	8:H:18:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:287:ILE:HG22	1:J:302:PHE:HB2	2.00	0.42
2:K:112:THR:HG22	2:K:116:LEU:H	1.83	0.42
2:K:57:PRO:HB2	3:L:214:MET:HB3	2.00	0.42
3:L:2:VAL:CG1	3:L:3:ARG:N	2.82	0.42
3:L:754:PRO:HD2	3:L:757:HIS:CE1	2.51	0.42
4:M:152:GLU:OE2	4:M:200:ARG:HD3	2.19	0.42
4:M:225:PRO:HG2	4:M:239:LEU:N	2.34	0.42
4:M:230:ILE:C	4:M:232:LEU:N	2.72	0.42
4:M:312:PRO:O	4:M:313:PRO:C	2.57	0.42
4:M:396:ILE:CG2	4:M:397:ILE:N	2.82	0.42
4:M:408:ASP:O	4:M:409:ARG:OXT	2.37	0.42
7:P:162:VAL:HG12	7:P:176:PRO:HB2	2.01	0.42
11:Q:500:FMN:H9	11:Q:500:FMN:O2'	2.19	0.42
8:Q:69:LEU:O	8:Q:84:LEU:HA	2.20	0.42
1:S:248:GLY:O	1:S:268:MET:HB2	2.19	0.42
3:U:341:VAL:HB	3:U:364:LEU:CD2	2.47	0.42
3:U:112:LEU:HD22	4:V:322:GLU:HG3	2.02	0.42
4:V:360:ASP:HB3	4:V:366:TYR:HB2	2.00	0.42
6:X:106:ILE:HD11	6:X:154:LEU:HD22	2.01	0.42
6:X:163:TYR:CE1	7:Y:152:ARG:CZ	3.02	0.42
6:X:31:GLY:C	6:X:33:SER:N	2.73	0.42
8:Z:61:ASP:OD1	8:Z:63:LEU:N	2.52	0.42
1:1:10:ASP:C	1:1:267:PRO:HG3	2.39	0.42
1:1:11:PRO:HD3	1:1:270:THR:HA	2.01	0.42
1:1:258:VAL:HG21	1:1:280:ALA:HB1	2.00	0.42
2:2:85:THR:HG22	2:2:86:LEU:N	2.33	0.42
3:3:574:GLU:HB2	3:3:593:LEU:HD11	2.00	0.42
3:3:627:ALA:C	3:3:629:ILE:H	2.20	0.42
3:3:703:GLN:O	3:3:705:VAL:N	2.51	0.42
4:4:138:LEU:HD11	4:4:146:PHE:CD2	2.55	0.42
4:4:212:PRO:O	4:4:214:PHE:N	2.52	0.42
4:4:70:MET:C	4:4:72:HIS:N	2.72	0.42
5:5:117:GLU:O	5:5:121:LEU:HD13	2.19	0.42
7:9:169:GLU:CD	7:9:169:GLU:H	2.22	0.42
3:C:171:SER:O	3:C:172:PRO:C	2.56	0.42
3:C:18:SER:HB3	3:C:21:ASP:OD1	2.18	0.42
3:C:483:ASP:O	3:C:484:LYS:HG2	2.19	0.42
4:D:118:VAL:HG23	4:D:119:ILE:N	2.34	0.42
4:D:281:ARG:HH11	4:D:281:ARG:HG3	1.83	0.42
4:D:290:ILE:O	4:D:294:LEU:HB2	2.19	0.42
6:F:110:ALA:O	6:F:111:CYS:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:159:ARG:CB	6:F:161:GLN:HG3	2.49	0.42
4:D:61:TYR:O	6:F:85:SER:HB3	2.19	0.42
6:F:93:ARG:O	6:F:96:TRP:N	2.48	0.42
3:C:241:ARG:HD3	7:G:74:GLU:OE1	2.19	0.42
1:J:106:ILE:O	1:J:110:VAL:HG22	2.19	0.42
1:J:63:ARG:NH1	1:J:313:TYR:HB2	2.33	0.42
3:L:161:ARG:HG2	3:L:161:ARG:NH1	2.33	0.42
3:L:300:TRP:H	3:L:300:TRP:HD1	1.60	0.42
4:M:224:ILE:HB	4:M:237:GLY:O	2.18	0.42
4:M:64:THR:HB	4:M:66:PHE:CD1	2.54	0.42
4:M:70:MET:O	4:M:72:HIS:N	2.52	0.42
5:N:184:TYR:O	5:N:185:LYS:HG3	2.19	0.42
1:S:211:LEU:HG	1:S:212:TRP:CE3	2.54	0.42
3:U:263:CYS:HA	3:U:286:ASN:CB	2.46	0.42
3:U:290:ILE:CG2	3:U:295:ARG:HB2	2.49	0.42
4:V:230:ILE:C	4:V:232:LEU:H	2.20	0.42
5:W:50:ALA:HB3	5:W:114:LEU:CD1	2.32	0.42
4:V:240:ARG:HH11	5:W:78:PRO:HD2	1.84	0.42
6:X:159:ARG:CB	6:X:161:GLN:HG3	2.49	0.42
1:1:170:ASP:O	1:1:171:LEU:HD12	2.19	0.42
1:1:246:SER:OG	1:1:312:SER:HB2	2.19	0.42
1:1:271:THR:OG1	1:1:273:ARG:HB3	2.19	0.42
1:1:367:MET:HA	1:1:370:LEU:HD23	2.01	0.42
1:1:195:LEU:HA	2:2:24:ARG:NH2	2.33	0.42
1:1:343:ASN:ND2	2:2:89:LYS:HD2	2.35	0.42
3:3:169:PRO:CD	3:3:176:LEU:HD13	2.49	0.42
3:3:229:ILE:HD11	3:3:289:TRP:HZ3	1.83	0.42
3:3:241:ARG:HH11	7:9:74:GLU:CD	2.23	0.42
3:3:274:LEU:O	3:3:302:ASP:OD2	2.38	0.42
3:3:724:ARG:N	3:3:724:ARG:CD	2.78	0.42
4:4:234:LEU:HD13	4:4:352:GLU:HB3	2.00	0.42
6:6:148:ILE:C	6:6:150:ALA:N	2.72	0.42
6:6:164:ASN:O	7:9:148:ARG:CD	2.66	0.42
6:6:43:LEU:CD1	6:6:83:ARG:O	2.67	0.42
6:6:43:LEU:HB2	6:6:82:GLY:HA3	2.01	0.42
7:9:29:ALA:HA	7:9:30:PRO:HD2	1.88	0.42
1:A:181:ILE:HG23	1:A:182:CYS:N	2.35	0.42
1:A:272:PHE:CE1	1:A:311:MET:HG2	2.54	0.42
3:C:174:VAL:HG13	3:C:239:THR:HB	2.01	0.42
4:D:238:SER:N	5:E:112:ASN:OD1	2.52	0.42
4:D:310:THR:CG2	4:D:311:PRO:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:350:ARG:HD3	4:D:401:ASP:O	2.19	0.42
5:E:114:LEU:HD12	5:E:114:LEU:N	2.35	0.42
6:F:33:SER:HA	6:F:158:VAL:HG21	2.00	0.42
8:H:50:LEU:HA	8:H:51:PRO:HD3	1.94	0.42
1:J:27:TRP:C	1:J:27:TRP:CD1	2.92	0.42
1:J:363:VAL:HA	1:J:367:MET:HB2	2.00	0.42
2:K:163:LEU:HA	2:K:166:ILE:CD1	2.49	0.42
2:K:24:ARG:HH12	2:K:59:GLU:HB3	1.84	0.42
3:L:295:ARG:HD2	3:L:296:PHE:CZ	2.54	0.42
3:L:434:ASP:O	3:L:436:GLN:N	2.52	0.42
6:O:43:LEU:HB2	6:O:82:GLY:HA3	2.01	0.42
8:Q:75:ARG:C	8:Q:80:LYS:HZ1	2.22	0.42
8:Q:81:ARG:O	8:Q:81:ARG:HD3	2.20	0.42
8:Q:86:LEU:HD12	8:Q:91:ILE:HG21	2.01	0.42
2:T:123:GLU:O	2:T:124:CYS:C	2.58	0.42
3:U:376:ALA:H	3:U:512:LEU:CD1	2.24	0.42
3:U:46:ARG:CG	3:U:46:ARG:NH1	2.82	0.42
3:U:621:VAL:CG2	3:U:671:GLU:O	2.66	0.42
4:V:367:ARG:NH1	4:V:369:LYS:HB2	2.34	0.42
5:W:134:LYS:O	5:W:134:LYS:HG3	2.19	0.42
5:W:25:LEU:HD23	5:W:25:LEU:N	2.23	0.42
5:W:32:GLU:O	5:W:34:PHE:N	2.51	0.42
5:W:3:LEU:HD12	5:W:86:SER:OG	2.18	0.42
6:X:114:SER:HB2	7:Y:97:ARG:CD	2.37	0.42
7:Y:29:ALA:HA	7:Y:30:PRO:HD2	1.85	0.42
1:1:108:GLU:HA	1:1:144:ARG:HG3	2.01	0.42
4:4:120:LEU:CD1	4:4:160:PHE:HE1	2.30	0.42
4:4:90:SER:O	4:4:92:ALA:N	2.52	0.42
5:5:32:GLU:O	5:5:34:PHE:N	2.49	0.42
5:5:46:PHE:O	5:5:47:ASN:C	2.58	0.42
6:6:132:PRO:HB2	6:6:174:ALA:HB1	2.02	0.42
8:7:16:LEU:HD21	8:7:115:PHE:CE1	2.54	0.42
1:A:252:TYR:HD2	1:A:266:LEU:HB2	1.84	0.42
1:A:325:THR:O	1:A:327:GLY:N	2.52	0.42
2:B:10:PHE:O	2:B:11:LEU:C	2.56	0.42
3:C:325:ALA:O	3:C:329:LEU:HB2	2.19	0.42
4:D:316:LEU:C	4:D:318:GLU:N	2.71	0.42
4:D:82:THR:N	4:D:83:PRO:CD	2.83	0.42
5:E:137:THR:HG23	5:E:139:GLU:CD	2.40	0.42
1:J:219:ASN:HA	11:Q:500:FMN:O3P	2.20	0.42
2:K:85:THR:CG2	2:K:86:LEU:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:173:PHE:C	3:L:173:PHE:CD1	2.93	0.42
3:L:403:THR:O	3:L:403:THR:HG22	2.19	0.42
4:M:109:VAL:HA	4:M:110:PRO:HD3	1.89	0.42
4:M:148:TYR:O	4:M:149:ALA:C	2.56	0.42
5:N:42:LYS:C	5:N:45:GLY:CA	2.88	0.42
6:O:142:PRO:O	6:O:143:ARG:C	2.57	0.42
6:O:156:LYS:HA	6:O:159:ARG:HD2	2.01	0.42
1:S:63:ARG:NH1	1:S:313:TYR:CB	2.81	0.42
3:U:559:ASP:OD2	3:U:688:ARG:CZ	2.67	0.42
3:U:305:ARG:HG3	3:U:588:SER:O	2.20	0.42
4:V:217:ARG:HD3	4:V:217:ARG:HA	1.84	0.42
4:V:312:PRO:O	4:V:313:PRO:C	2.56	0.42
5:W:154:GLU:CB	6:X:119:ASN:HB3	2.49	0.42
6:X:39:ALA:HB2	6:X:75:ALA:HB1	2.00	0.42
6:X:41:PHE:CE2	6:X:92:MET:HB2	2.53	0.42
1:1:184:GLU:OE1	1:1:186:THR:N	2.53	0.42
2:2:79:HIS:H	2:2:137:ASN:HB3	1.84	0.42
3:3:290:ILE:CG2	3:3:295:ARG:HB2	2.49	0.42
3:3:651:ARG:H	3:3:651:ARG:HD2	1.83	0.42
1:A:402:LEU:O	1:A:405:ALA:HB3	2.19	0.42
3:C:177:ASP:CB	3:C:235:LEU:H	2.32	0.42
3:C:32:LEU:O	3:C:33:PHE:CD1	2.73	0.42
3:C:632:GLY:O	3:C:633:GLU:C	2.57	0.42
5:E:95:PRO:HB2	5:E:98:ASP:HB3	2.01	0.42
6:F:163:TYR:HB3	6:F:170:LEU:H	1.85	0.42
1:J:185:GLU:HB2	1:J:218:ILE:CD1	2.42	0.42
1:J:290:ILE:HG22	1:J:330:LEU:HD23	2.02	0.42
1:J:38:TYR:HA	1:J:116:GLU:OE1	2.19	0.42
3:L:405:GLU:HB2	3:L:535:MET:SD	2.60	0.42
1:S:341:MET:O	1:S:342:TRP:C	2.57	0.42
1:S:436:LEU:HD23	2:T:90:LEU:CA	2.46	0.42
3:U:245:ARG:HD2	3:U:245:ARG:HA	1.48	0.42
3:U:669:VAL:CG1	3:U:669:VAL:O	2.68	0.42
4:V:350:ARG:HG3	4:V:350:ARG:HH11	1.84	0.42
3:U:133:ARG:CZ	5:W:185:LYS:HE3	2.50	0.42
5:W:48:PHE:O	5:W:50:ALA:N	2.53	0.42
5:W:6:VAL:O	5:W:9:GLU:HB3	2.18	0.42
6:X:165:GLU:OE1	6:X:165:GLU:C	2.58	0.42
1:1:293:GLY:O	1:1:324:GLY:O	2.36	0.42
1:1:380:GLU:O	1:1:381:GLU:C	2.57	0.42
3:3:173:PHE:C	3:3:173:PHE:CD1	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:285:VAL:CG1	3:3:286:ASN:H	2.02	0.42
3:3:368:HIS:O	3:3:368:HIS:ND1	2.50	0.42
3:3:378:PRO:HA	3:3:545:GLU:OE2	2.19	0.42
3:3:75:TRP:HA	3:3:75:TRP:HE3	1.83	0.42
3:3:93:VAL:HG12	3:3:93:VAL:O	2.20	0.42
5:5:26:TRP:CZ3	5:5:91:ARG:NE	2.88	0.42
5:5:59:THR:CG2	5:5:59:THR:O	2.64	0.42
8:7:86:LEU:HD12	8:7:91:ILE:HG21	2.01	0.42
1:A:350:HIS:ND1	1:A:350:HIS:C	2.73	0.42
2:B:61:MET:HE1	8:H:128:PHE:HZ	1.84	0.42
3:C:106:GLY:O	3:C:109:GLU:HB3	2.20	0.42
3:C:20:MET:HE3	3:C:432:PHE:HB3	2.01	0.42
3:C:33:PHE:CB	3:C:45:CYS:SG	3.07	0.42
3:C:591:HIS:ND1	3:C:592:PRO:HD2	2.35	0.42
4:D:271:ASP:O	4:D:275:ARG:HG3	2.20	0.42
4:D:339:LYS:HB2	4:D:339:LYS:HE3	1.79	0.42
4:D:352:GLU:O	4:D:371:ARG:NE	2.52	0.42
5:E:16:PRO:O	5:E:17:ILE:HD13	2.20	0.42
1:J:101:PHE:CE1	1:J:253:GLN:HB2	2.55	0.42
1:J:252:TYR:HB3	1:J:275:LEU:CD1	2.46	0.42
1:J:424:LEU:HD12	1:J:424:LEU:H	1.84	0.42
3:L:161:ARG:HG2	3:L:161:ARG:HH11	1.83	0.42
3:L:534:ALA:O	3:L:617:LEU:HD12	2.19	0.42
3:L:7:ASN:ND2	3:L:96:LEU:CD1	2.76	0.42
4:M:234:LEU:N	4:M:234:LEU:CD2	2.83	0.42
5:N:15:TYR:CE1	5:N:30:PRO:HD2	2.54	0.42
5:N:40:HIS:C	5:N:42:LYS:N	2.73	0.42
6:O:33:SER:HA	6:O:158:VAL:HG21	2.01	0.42
7:P:104:CYS:O	7:P:105:GLU:C	2.58	0.42
7:P:153:THR:HG22	7:P:155:LYS:CB	2.49	0.42
1:S:11:PRO:HA	1:S:267:PRO:HG3	2.01	0.42
3:U:47:MET:SD	3:U:107:MET:HB3	2.60	0.42
2:T:66:PHE:CD1	3:U:205:ARG:HD3	2.55	0.42
3:U:660:ALA:O	3:U:663:ALA:HB3	2.20	0.42
3:U:726:GLU:O	3:U:727:ALA:HB3	2.20	0.42
4:V:230:ILE:HG21	4:V:239:LEU:CB	2.39	0.42
5:W:104:VAL:O	5:W:106:ASP:N	2.52	0.42
5:W:132:LEU:HD23	5:W:135:ILE:CG2	2.48	0.42
5:W:136:LEU:HD13	5:W:138:PRO:HG3	2.02	0.42
5:W:66:GLU:CG	5:W:95:PRO:HA	2.50	0.42
6:X:43:LEU:HB2	6:X:82:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:37:PHE:HB3	8:Z:39:ASP:HB3	2.02	0.42
1:1:181:ILE:O	1:1:183:GLY:N	2.53	0.42
2:2:153:LEU:HD21	2:2:163:LEU:CD1	2.50	0.42
3:3:116:PRO:O	3:3:117:LEU:CB	2.67	0.42
3:3:254:THR:OG1	3:3:255:THR:N	2.51	0.42
3:3:287:GLU:OE2	3:3:412:ARG:NH1	2.53	0.42
3:3:344:TYR:CD1	3:3:568:TYR:CE1	3.08	0.42
3:3:5:LYS:O	3:3:92:VAL:HA	2.19	0.42
3:3:724:ARG:HE	3:3:724:ARG:HB3	1.51	0.42
3:3:470:PRO:HG3	3:3:750:ARG:NH2	2.34	0.42
3:3:20:MET:HA	3:3:82:SER:OG	2.20	0.42
4:4:109:VAL:HA	4:4:110:PRO:HD3	1.88	0.42
4:4:249:ARG:O	4:4:250:LYS:C	2.58	0.42
4:4:310:THR:HG22	4:4:311:PRO:O	2.20	0.42
4:4:381:LEU:HD11	4:4:397:ILE:CG1	2.47	0.42
4:4:74:THR:HB	4:4:77:GLN:H	1.84	0.42
5:5:139:GLU:O	5:5:140:ASP:HB2	2.20	0.42
8:7:38:PRO:O	8:7:40:PHE:N	2.53	0.42
7:9:118:ASP:HA	7:9:161:TYR:HE2	1.83	0.42
7:9:53:CYS:HB2	7:9:112:ALA:CB	2.50	0.42
1:A:184:GLU:HB3	1:A:187:ALA:CB	2.50	0.42
1:A:92:ASN:HD21	1:A:94:ASP:HB3	1.85	0.42
3:C:290:ILE:HG22	3:C:291:CYS:O	2.19	0.42
3:C:357:ALA:HB2	3:C:641:LEU:HD11	2.01	0.42
3:C:428:HIS:CD2	3:C:428:HIS:N	2.87	0.42
3:C:474:ARG:NH1	3:C:515:THR:HG21	2.35	0.42
3:C:305:ARG:HG3	3:C:588:SER:O	2.19	0.42
3:C:634:ALA:O	3:C:635:GLU:O	2.37	0.42
3:C:753:VAL:HA	3:C:754:PRO:HD3	1.89	0.42
4:D:221:VAL:HA	4:D:271:ASP:CB	2.50	0.42
4:D:228:VAL:CG2	4:D:278:VAL:HG21	2.50	0.42
4:D:227:GLU:HG2	4:D:228:VAL:N	2.34	0.42
5:E:131:ASP:O	5:E:132:LEU:HB2	2.20	0.42
5:E:64:ARG:HB3	5:E:65:PRO:CD	2.50	0.42
7:G:63:CYS:HA	9:G:183:SF4:S2	2.60	0.42
2:K:133:VAL:CG1	2:K:134:ILE:N	2.82	0.42
2:K:40:TRP:CZ3	2:K:42:ARG:CA	3.01	0.42
3:L:13:VAL:CG2	3:L:14:PRO:HD2	2.50	0.42
3:L:169:PRO:N	3:L:176:LEU:HD13	2.35	0.42
3:L:174:VAL:HG13	3:L:239:THR:HB	2.00	0.42
4:M:84:ARG:HD3	6:O:117:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:39:ALA:HB2	6:O:75:ALA:HB1	2.01	0.42
1:S:220:ASN:O	1:S:221:VAL:C	2.58	0.42
4:V:226:PRO:HD2	4:V:239:LEU:HD12	2.02	0.42
4:V:254:TYR:C	4:V:254:TYR:CD1	2.93	0.42
5:W:39:ALA:O	5:W:42:LYS:HG2	2.19	0.42
8:Z:48:TYR:CE1	8:Z:50:LEU:HB3	2.54	0.42
8:Z:68:LEU:HD13	8:Z:69:LEU:N	2.35	0.42
1:1:298:PRO:HD2	1:1:321:SER:OG	2.20	0.42
1:1:63:ARG:NH1	1:1:313:TYR:HB2	2.35	0.42
1:1:420:GLN:O	1:1:424:LEU:HD13	2.20	0.42
1:1:92:ASN:HD21	1:1:94:ASP:HB3	1.85	0.42
3:3:279:ALA:HB2	3:3:290:ILE:HG12	2.00	0.42
4:4:148:TYR:O	4:4:151:ARG:N	2.53	0.42
4:4:197:LEU:N	4:4:198:PRO:CD	2.83	0.42
4:4:213:ILE:HG23	4:4:215:TYR:CE2	2.55	0.42
4:4:389:GLN:HA	4:4:389:GLN:NE2	2.35	0.42
5:5:184:TYR:O	5:5:185:LYS:HG3	2.20	0.42
5:5:31:ARG:CG	5:5:31:ARG:HH11	2.33	0.42
6:6:130:VAL:CG2	6:6:131:VAL:H	2.28	0.42
7:9:126:TYR:O	7:9:128:ASP:N	2.53	0.42
2:B:116:LEU:HG	2:B:117:PHE:CE2	2.55	0.42
3:C:174:VAL:HB	3:C:175:ILE:HG13	2.01	0.42
3:C:37:LYS:HE3	3:C:432:PHE:HE1	1.85	0.42
3:C:640:VAL:O	3:C:641:LEU:C	2.57	0.42
4:D:244:VAL:HG12	4:D:246:TYR:H	1.85	0.42
4:D:360:ASP:HB3	4:D:366:TYR:HB2	2.02	0.42
4:D:91:PHE:CD2	4:D:121:ASN:HA	2.55	0.42
5:E:66:GLU:CG	5:E:95:PRO:HA	2.50	0.42
1:J:290:ILE:O	1:J:290:ILE:HG13	2.18	0.42
1:J:401:PRO:O	1:J:404:ASP:HB2	2.19	0.42
1:J:81:LYS:CG	1:J:82:ASP:N	2.79	0.42
3:L:428:HIS:N	3:L:428:HIS:CD2	2.87	0.42
3:L:591:HIS:ND1	3:L:592:PRO:HD2	2.34	0.42
3:L:20:MET:HA	3:L:82:SER:OG	2.20	0.42
4:M:173:ILE:CG2	4:M:173:ILE:O	2.66	0.42
4:M:238:SER:N	5:N:112:ASN:OD1	2.53	0.42
5:N:115:GLU:HB3	5:N:119:TYR:CZ	2.54	0.42
7:P:144:LYS:N	7:P:145:PRO:HD2	2.35	0.42
1:S:293:GLY:O	1:S:324:GLY:O	2.38	0.42
1:S:199:PRO:HG3	1:S:400:CYS:HB3	2.01	0.42
2:T:131:ALA:HB3	2:T:144:CYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:218:LEU:N	3:U:219:PRO:CD	2.82	0.42
3:U:440:ARG:HG2	3:U:440:ARG:HH11	1.85	0.42
3:U:49:LEU:HA	3:U:80:ALA:O	2.19	0.42
4:V:221:VAL:HA	4:V:271:ASP:CG	2.40	0.42
4:V:358:VAL:HG12	4:V:366:TYR:HB3	2.01	0.42
4:V:47:LEU:N	4:V:47:LEU:HD12	2.33	0.42
5:W:131:ASP:O	5:W:132:LEU:HB2	2.20	0.42
5:W:174:LEU:CD2	5:W:180:GLY:HA2	2.50	0.42
6:X:148:ILE:HG22	6:X:149:TYR:N	2.35	0.42
3:3:185:LYS:HG2	3:3:188:VAL:HG22	2.02	0.42
3:3:340:GLU:CA	3:3:366:THR:HB	2.49	0.42
3:3:509:ALA:C	3:3:511:VAL:H	2.23	0.42
3:3:527:ARG:HB3	3:3:530:ALA:CB	2.47	0.42
4:4:173:ILE:CG2	4:4:173:ILE:O	2.67	0.42
4:4:316:LEU:C	4:4:318:GLU:H	2.22	0.42
4:4:82:THR:OG1	4:4:83:PRO:HD3	2.20	0.42
4:4:375:PHE:CZ	5:5:116:ARG:HB3	2.55	0.42
1:A:199:PRO:HG3	1:A:400:CYS:HB3	2.02	0.42
1:A:245:GLN:HB2	1:A:314:GLU:OE2	2.20	0.42
1:A:424:LEU:H	1:A:424:LEU:CD1	2.33	0.42
2:B:123:GLU:O	2:B:124:CYS:C	2.59	0.42
2:B:134:ILE:HG13	2:B:145:VAL:HG21	2.01	0.42
3:C:286:ASN:HD22	3:C:287:GLU:H	1.67	0.42
3:C:340:GLU:CA	3:C:366:THR:HB	2.50	0.42
5:E:3:LEU:HD22	5:E:44:MET:CE	2.50	0.42
5:E:52:ILE:HG13	5:E:53:VAL:N	2.33	0.42
6:F:114:SER:O	6:F:116:GLY:N	2.53	0.42
8:H:61:ASP:OD1	8:H:63:LEU:N	2.53	0.42
3:L:156:ARG:H	3:L:156:ARG:HG2	1.65	0.42
3:L:159:PHE:HE2	8:Q:79:LEU:HD22	1.85	0.42
3:L:36:GLU:OE2	3:L:229:ILE:HG23	2.20	0.42
3:L:408:ILE:HG23	3:L:408:ILE:O	2.19	0.42
3:L:533:LEU:HA	3:L:533:LEU:HD23	1.88	0.42
3:L:52:ILE:CG2	3:L:53:GLY:H	2.33	0.42
3:L:693:TYR:O	3:L:750:ARG:HB3	2.19	0.42
4:M:109:VAL:CG1	4:M:113:ALA:HB3	2.50	0.42
4:M:358:VAL:O	4:M:366:TYR:HB3	2.20	0.42
5:N:139:GLU:O	5:N:140:ASP:HB2	2.20	0.42
5:N:154:GLU:HB3	6:O:119:ASN:HB3	2.02	0.42
8:Q:23:TYR:HB2	8:Q:116:PHE:CE2	2.55	0.42
1:S:114:LEU:O	1:S:115:ILE:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:203:PRO:N	1:S:204:PRO:CD	2.82	0.42
2:T:31:LEU:HD22	2:T:49:ILE:HD13	2.00	0.42
3:U:389:ASP:O	3:U:392:GLN:N	2.51	0.42
3:U:632:GLY:O	3:U:633:GLU:C	2.58	0.42
3:U:374:ARG:NH2	3:U:684:ARG:CG	2.82	0.42
3:U:717:TRP:O	3:U:717:TRP:CD2	2.73	0.42
6:X:139:GLY:CA	6:X:142:PRO:HB3	2.34	0.42
6:X:144:PRO:O	6:X:147:LEU:N	2.53	0.42
1:1:110:VAL:O	1:1:110:VAL:HG23	2.20	0.41
1:1:384:VAL:O	1:1:385:GLU:C	2.58	0.41
1:1:438:ARG:CD	1:1:438:ARG:H	2.27	0.41
2:2:24:ARG:HA	2:2:53:VAL:HG13	2.01	0.41
3:3:318:VAL:HG13	3:3:319:GLU:OE2	2.20	0.41
4:4:108:VAL:O	4:4:108:VAL:HG23	2.19	0.41
4:4:343:TYR:HD2	4:4:356:TYR:HB2	1.85	0.41
5:5:49:LEU:HD22	5:5:77:LEU:CD2	2.50	0.41
6:6:110:ALA:O	6:6:113:SER:N	2.53	0.41
8:7:13:TRP:CE2	8:7:17:LEU:HD11	2.55	0.41
8:7:40:PHE:O	8:7:43:ARG:HB3	2.20	0.41
1:A:300:LEU:HA	1:A:301:PRO:HD3	1.88	0.41
2:B:24:ARG:HH12	2:B:59:GLU:HB3	1.85	0.41
3:C:586:HIS:HE1	3:C:637:ALA:HA	1.85	0.41
3:C:609:GLU:OE2	3:C:631:ASN:HB3	2.20	0.41
4:D:237:GLY:O	4:D:239:LEU:CG	2.67	0.41
6:F:160:GLY:C	6:F:162:ALA:N	2.73	0.41
7:G:119:PHE:C	7:G:119:PHE:CD1	2.93	0.41
8:H:17:LEU:O	8:H:18:SER:C	2.58	0.41
2:K:106:ILE:CD1	2:K:112:THR:HB	2.48	0.41
3:L:29:ASP:N	3:L:29:ASP:OD1	2.53	0.41
3:L:410:HIS:CG	3:L:458:LEU:HD21	2.55	0.41
4:M:396:ILE:HG23	4:M:397:ILE:N	2.35	0.41
5:N:119:TYR:O	5:N:120:ASP:C	2.58	0.41
5:N:49:LEU:HD22	5:N:77:LEU:CD2	2.50	0.41
8:Q:37:PHE:HD1	8:Q:37:PHE:H	1.68	0.41
8:Q:70:ALA:HA	8:Q:83:GLY:O	2.20	0.41
1:S:20:HIS:O	1:S:22:GLY:N	2.52	0.41
1:S:234:GLY:O	1:S:235:ALA:C	2.59	0.41
1:S:95:GLU:HA	11:Z:500:FMN:N3	2.28	0.41
2:T:7:LYS:HD2	2:T:7:LYS:N	2.32	0.41
3:U:428:HIS:CD2	3:U:428:HIS:N	2.88	0.41
4:V:339:LYS:HB2	4:V:339:LYS:HE3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:82:THR:N	4:V:83:PRO:CD	2.82	0.41
5:W:31:ARG:CG	5:W:31:ARG:HH11	2.31	0.41
1:1:114:LEU:HD23	1:1:114:LEU:C	2.41	0.41
1:1:352:SER:OG	1:1:353:CYS:N	2.53	0.41
1:1:363:VAL:CG2	1:1:364:ALA:N	2.82	0.41
2:2:66:PHE:CE1	3:3:205:ARG:HD3	2.55	0.41
3:3:119:CYS:O	3:3:120:PRO:C	2.55	0.41
2:2:66:PHE:CD1	3:3:205:ARG:HD3	2.54	0.41
3:3:25:HIS:CE1	3:3:427:ASN:OD1	2.73	0.41
3:3:341:VAL:CG2	3:3:364:LEU:HD21	2.51	0.41
3:3:516:VAL:O	3:3:519:GLU:HG2	2.21	0.41
3:3:559:ASP:OD2	3:3:688:ARG:CZ	2.68	0.41
3:3:87:VAL:HA	3:3:91:MET:CE	2.51	0.41
4:4:281:ARG:NH1	4:4:281:ARG:HG3	2.34	0.41
5:5:114:LEU:N	5:5:114:LEU:HD12	2.35	0.41
8:7:52:THR:CB	8:7:54:ILE:HG22	2.48	0.41
8:7:91:ILE:O	8:7:91:ILE:HG22	2.20	0.41
1:A:264:TYR:CD2	1:A:279:TRP:HB3	2.55	0.41
2:B:130:THR:O	2:B:131:ALA:C	2.59	0.41
3:C:164:VAL:HB	3:C:165:ASP:H	1.63	0.41
3:C:286:ASN:HD21	3:C:289:TRP:H	1.69	0.41
4:D:144:THR:N	4:D:145:PRO:CD	2.84	0.41
4:D:207:LEU:HA	4:D:207:LEU:HD23	1.90	0.41
4:D:285:GLU:HA	4:D:288:LYS:HD3	2.02	0.41
4:D:50:GLU:O	4:D:51:GLU:OE2	2.39	0.41
4:D:82:THR:OG1	4:D:83:PRO:HD3	2.20	0.41
5:E:132:LEU:O	5:E:133:ARG:C	2.58	0.41
4:D:168:PHE:CE1	6:F:141:PRO:HG3	2.56	0.41
8:H:72:VAL:CG2	8:H:73:SER:N	2.83	0.41
1:J:110:VAL:O	1:J:113:LEU:HB3	2.20	0.41
3:L:106:GLY:O	3:L:109:GLU:HB3	2.19	0.41
3:L:226:ILE:HG13	3:L:235:LEU:HD12	2.01	0.41
3:L:244:ALA:HB3	3:L:249:MET:CE	2.50	0.41
3:L:669:VAL:HG13	3:L:669:VAL:O	2.18	0.41
3:L:703:GLN:O	3:L:705:VAL:N	2.52	0.41
5:N:124:ILE:O	5:N:145:PRO:HD2	2.20	0.41
7:P:143:THR:O	7:P:144:LYS:C	2.58	0.41
7:P:46:HIS:CE1	7:P:52:LYS:HA	2.55	0.41
1:S:11:PRO:HA	1:S:267:PRO:CG	2.50	0.41
3:U:515:THR:HG23	3:U:516:VAL:N	2.35	0.41
3:U:655:ARG:HG3	3:U:655:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:753:VAL:HA	3:U:754:PRO:HD3	1.90	0.41
4:V:140:LEU:CD2	4:V:142:ALA:H	2.33	0.41
4:V:252:TYR:OH	4:V:346:THR:C	2.59	0.41
4:V:371:ARG:HG3	4:V:371:ARG:HH11	1.85	0.41
4:V:75:TYR:OH	4:V:365:PRO:HA	2.20	0.41
2:2:174:HIS:HB3	2:2:175:HIS:H	1.74	0.41
3:3:101:ARG:NH1	3:3:101:ARG:HB3	2.35	0.41
3:3:178:ARG:H	3:3:234:ALA:CA	2.28	0.41
4:4:249:ARG:HH22	5:5:87:ARG:HB3	1.81	0.41
1:A:110:VAL:O	1:A:111:PRO:C	2.57	0.41
1:A:312:SER:O	1:A:314:GLU:N	2.47	0.41
1:A:293:GLY:C	1:A:324:GLY:O	2.59	0.41
2:B:139:GLU:CB	2:B:140:PRO:CD	2.83	0.41
3:C:171:SER:O	3:C:173:PHE:N	2.51	0.41
3:C:262:GLY:O	3:C:263:CYS:O	2.38	0.41
3:C:272:GLY:HA2	3:C:628:PRO:O	2.21	0.41
3:C:527:ARG:HB3	3:C:530:ALA:CB	2.49	0.41
3:C:594:ALA:O	3:C:598:ALA:HB3	2.20	0.41
3:C:717:TRP:O	3:C:717:TRP:CD2	2.73	0.41
3:C:6:VAL:O	3:C:93:VAL:O	2.38	0.41
4:D:212:PRO:O	4:D:214:PHE:N	2.53	0.41
4:D:228:VAL:HG21	4:D:278:VAL:HG21	2.02	0.41
5:E:22:LEU:N	5:E:22:LEU:HD23	2.34	0.41
6:F:126:ASN:O	6:F:129:SER:N	2.48	0.41
6:F:164:ASN:O	7:G:148:ARG:CD	2.64	0.41
7:G:144:LYS:N	7:G:145:PRO:HD2	2.36	0.41
3:C:163:HIS:ND1	8:H:71:ASP:OD2	2.48	0.41
1:J:324:GLY:C	1:J:325:THR:HG23	2.40	0.41
1:J:383:ASP:O	1:J:384:VAL:C	2.58	0.41
1:J:417:PHE:O	1:J:420:GLN:N	2.53	0.41
1:J:101:PHE:HB2	2:K:126:GLY:O	2.20	0.41
3:L:17:THR:HG22	3:L:18:SER:N	2.35	0.41
3:L:340:GLU:N	3:L:366:THR:HB	2.33	0.41
3:L:371:PHE:CD1	3:L:371:PHE:N	2.86	0.41
3:L:460:LYS:HE2	3:L:460:LYS:HB2	1.84	0.41
4:M:397:ILE:C	4:M:399:SER:N	2.74	0.41
5:N:34:PHE:CD1	5:N:38:MET:HB2	2.56	0.41
6:O:96:TRP:CZ2	6:O:103:LYS:HE3	2.55	0.41
1:S:107:LEU:HD22	1:S:145:LEU:HD11	2.02	0.41
1:S:188:LEU:C	1:S:188:LEU:HD23	2.41	0.41
1:S:222:GLU:OE1	1:S:251:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:358:PRO:O	1:S:362:GLY:CA	2.68	0.41
3:U:351:LEU:HD13	3:U:615:VAL:HG23	2.00	0.41
3:U:355:LEU:O	3:U:356:LEU:C	2.58	0.41
3:U:564:LEU:HA	3:U:564:LEU:HD12	1.84	0.41
3:U:724:ARG:HB3	3:U:724:ARG:HE	1.46	0.41
4:V:227:GLU:HG2	4:V:228:VAL:N	2.35	0.41
4:V:376:VAL:HG23	4:V:377:ASN:N	2.34	0.41
4:V:395:ALA:O	4:V:399:SER:HB3	2.20	0.41
6:X:164:ASN:HB3	7:Y:148:ARG:NH2	2.36	0.41
7:Y:51:GLU:OE2	7:Y:133:LYS:NZ	2.50	0.41
7:Y:93:ILE:HB	7:Y:95:MET:HE2	2.01	0.41
8:Z:15:GLU:O	8:Z:18:SER:HB3	2.19	0.41
8:Z:37:PHE:CD1	8:Z:55:MET:HB2	2.54	0.41
2:2:3:PHE:CD1	2:2:3:PHE:C	2.94	0.41
3:3:260:PRO:CB	3:3:617:LEU:HB3	2.51	0.41
3:3:340:GLU:N	3:3:366:THR:HB	2.35	0.41
3:3:371:PHE:N	3:3:371:PHE:CD1	2.86	0.41
3:3:631:ASN:O	3:3:633:GLU:N	2.50	0.41
4:4:115:THR:O	4:4:118:VAL:HG22	2.21	0.41
4:4:123:LEU:HD21	4:4:159:LEU:HD12	2.02	0.41
4:4:220:GLY:O	4:4:272:VAL:CG2	2.69	0.41
4:4:220:GLY:O	4:4:272:VAL:HG22	2.21	0.41
4:4:90:SER:O	4:4:93:HIS:N	2.52	0.41
5:5:26:TRP:CH2	5:5:91:ARG:NH2	2.88	0.41
5:5:73:GLU:OE2	5:5:87:ARG:NH1	2.46	0.41
6:6:114:SER:C	6:6:116:GLY:N	2.71	0.41
7:9:140:VAL:HG22	7:9:141:VAL:H	1.85	0.41
1:A:121:ALA:O	1:A:124:ALA:HB3	2.21	0.41
2:B:48:GLU:O	2:B:49:ILE:C	2.57	0.41
3:C:313:LYS:O	3:C:314:GLU:CB	2.66	0.41
3:C:479:ALA:O	3:C:482:GLY:N	2.54	0.41
3:C:568:TYR:CD2	3:C:572:PRO:HG2	2.55	0.41
4:D:227:GLU:OE2	4:D:240:ARG:O	2.39	0.41
4:D:272:VAL:HA	4:D:275:ARG:HD2	2.01	0.41
4:D:125:ARG:HH21	4:D:347:GLU:HG2	1.85	0.41
4:D:90:SER:O	4:D:92:ALA:N	2.53	0.41
5:E:48:PHE:CE2	5:E:113:PHE:CE2	3.08	0.41
5:E:80:TRP:HB3	5:E:81:LYS:H	1.60	0.41
6:F:142:PRO:O	6:F:143:ARG:C	2.58	0.41
6:F:143:ARG:O	6:F:146:ALA:HB3	2.20	0.41
8:H:60:SER:CB	8:H:64:GLY:O	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:93:LEU:N	8:H:93:LEU:HD12	2.35	0.41
1:J:114:LEU:O	1:J:115:ILE:C	2.56	0.41
1:J:147:GLN:O	1:J:150:LYS:N	2.52	0.41
1:J:248:GLY:O	1:J:268:MET:HB2	2.21	0.41
1:J:402:LEU:O	1:J:405:ALA:HB3	2.21	0.41
1:J:433:ARG:HH12	2:K:94:GLU:CD	2.23	0.41
2:K:116:LEU:HG	2:K:117:PHE:CE2	2.55	0.41
3:L:261:VAL:O	3:L:262:GLY:C	2.59	0.41
3:L:666:ALA:C	3:L:668:LYS:H	2.24	0.41
4:M:322:GLU:C	4:M:325:ILE:H	2.20	0.41
5:N:26:TRP:CZ3	5:N:91:ARG:CZ	3.04	0.41
8:Q:115:PHE:O	8:Q:118:LEU:HB3	2.20	0.41
1:S:214:LYS:HA	1:S:215:PRO:HD3	1.95	0.41
1:S:228:VAL:HB	1:S:229:PRO:CD	2.51	0.41
1:S:287:ILE:HG22	1:S:302:PHE:CG	2.56	0.41
1:S:309:THR:HA	1:S:310:PRO:HD3	1.70	0.41
3:U:174:VAL:HG11	3:U:296:PHE:CD1	2.54	0.41
3:U:185:LYS:O	3:U:186:ARG:C	2.59	0.41
3:U:268:ASP:OD1	3:U:278:ARG:NH1	2.53	0.41
3:U:474:ARG:O	3:U:475:GLU:C	2.57	0.41
5:W:175:THR:O	5:W:176:GLY:C	2.58	0.41
5:W:52:ILE:HG13	5:W:53:VAL:N	2.35	0.41
6:X:31:GLY:C	6:X:33:SER:H	2.23	0.41
7:Y:58:LEU:CD1	7:Y:58:LEU:N	2.84	0.41
1:1:165:THR:O	1:1:167:PHE:N	2.54	0.41
1:1:246:SER:HB3	1:1:268:MET:CG	2.50	0.41
1:1:292:PRO:HA	1:1:328:VAL:HG22	2.03	0.41
3:3:641:LEU:HD23	3:3:641:LEU:HA	1.83	0.41
5:5:47:ASN:HD22	5:5:76:SER:CA	2.29	0.41
5:5:77:LEU:HA	5:5:78:PRO:HD3	1.73	0.41
6:6:156:LYS:HA	6:6:159:ARG:HD2	2.01	0.41
6:6:23:THR:HG22	6:6:23:THR:O	2.21	0.41
8:7:47:PRO:O	8:7:48:TYR:HB2	2.20	0.41
1:A:144:ARG:O	1:A:145:LEU:C	2.57	0.41
1:A:246:SER:OG	1:A:312:SER:HB2	2.20	0.41
1:A:290:ILE:O	1:A:292:PRO:HD3	2.20	0.41
2:B:123:GLU:N	2:B:123:GLU:CD	2.74	0.41
3:C:263:CYS:HA	3:C:286:ASN:CB	2.48	0.41
3:C:390:LEU:HD21	3:C:413:LEU:CD2	2.50	0.41
3:C:49:LEU:HA	3:C:80:ALA:O	2.20	0.41
3:C:618:GLU:OE2	3:C:620:ARG:NE	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:TRP:HE3	3:C:75:TRP:HA	1.85	0.41
4:D:328:PHE:O	4:D:332:THR:HG23	2.20	0.41
4:D:371:ARG:O	4:D:372:ALA:HB3	2.20	0.41
5:E:70:VAL:O	5:E:91:ARG:HA	2.20	0.41
8:H:48:TYR:OH	8:H:50:LEU:HD22	2.20	0.41
1:J:246:SER:HB3	1:J:268:MET:HG2	2.00	0.41
1:J:414:LEU:O	1:J:415:ARG:C	2.59	0.41
3:L:17:THR:CG2	3:L:18:SER:N	2.83	0.41
3:L:245:ARG:HD2	3:L:245:ARG:HA	1.55	0.41
3:L:47:MET:C	3:L:49:LEU:H	2.24	0.41
4:M:250:LYS:HD2	4:M:254:TYR:CE2	2.56	0.41
4:M:338:PRO:CG	5:N:193:ARG:HB2	2.39	0.41
5:N:20:ASN:HD22	5:N:24:ASN:HB2	1.82	0.41
6:O:84:LEU:HD11	6:O:89:ALA:CA	2.41	0.41
1:S:211:LEU:CB	1:S:216:THR:HG21	2.50	0.41
2:T:85:THR:HG22	2:T:86:LEU:N	2.35	0.41
3:U:101:ARG:HB3	3:U:101:ARG:HH11	1.85	0.41
3:U:205:ARG:HA	3:U:209:THR:CG2	2.17	0.41
3:U:286:ASN:ND2	3:U:286:ASN:C	2.73	0.41
3:U:369:LEU:CD2	3:U:369:LEU:N	2.80	0.41
3:U:456:ALA:O	3:U:459:MET:HB2	2.19	0.41
3:U:508:GLY:HA3	3:U:535:MET:HB2	2.02	0.41
1:1:201:LEU:HG	1:1:203:PRO:CD	2.32	0.41
1:1:29:LEU:O	1:1:29:LEU:CD2	2.69	0.41
1:1:341:MET:CE	1:1:409:PRO:HB2	2.50	0.41
2:2:131:ALA:HB3	2:2:144:CYS:HA	2.01	0.41
2:2:78:TYR:CZ	2:2:157:LEU:HD22	2.56	0.41
3:3:178:ARG:H	3:3:234:ALA:CB	2.34	0.41
3:3:355:LEU:O	3:3:356:LEU:C	2.59	0.41
3:3:44:ALA:O	3:3:45:CYS:CB	2.68	0.41
3:3:514:ASP:HA	3:3:517:ALA:HB3	2.02	0.41
4:4:254:TYR:C	4:4:254:TYR:CD1	2.93	0.41
4:4:328:PHE:O	4:4:332:THR:HG23	2.21	0.41
4:4:393:MET:HA	4:4:396:ILE:CG2	2.51	0.41
5:5:124:ILE:O	5:5:145:PRO:HD2	2.20	0.41
5:5:175:THR:O	5:5:176:GLY:C	2.59	0.41
7:9:46:HIS:CE1	7:9:52:LYS:HA	2.55	0.41
1:A:12:ARG:O	1:A:12:ARG:CG	2.67	0.41
1:A:211:LEU:CB	1:A:216:THR:HG21	2.49	0.41
1:A:345:THR:HG21	1:A:371:PHE:CE2	2.56	0.41
1:A:434:PRO:HG2	1:A:436:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ARG:CG	3:C:46:ARG:HH11	2.33	0.41
3:C:46:ARG:HG2	3:C:46:ARG:HH11	1.86	0.41
4:D:228:VAL:O	4:D:230:ILE:N	2.54	0.41
4:D:367:ARG:NH1	4:D:369:LYS:HB2	2.36	0.41
5:E:116:ARG:CG	5:E:116:ARG:NH1	2.83	0.41
5:E:11:ARG:HH21	5:E:15:TYR:HE2	1.68	0.41
5:E:42:LYS:C	5:E:45:GLY:CA	2.88	0.41
6:F:151:VAL:O	6:F:154:LEU:HB3	2.21	0.41
6:F:31:GLY:C	6:F:33:SER:H	2.23	0.41
8:H:75:ARG:HA	8:H:80:LYS:HZ1	1.86	0.41
1:J:11:PRO:HB2	1:J:274:GLU:OE2	2.21	0.41
1:J:370:LEU:C	1:J:374:ILE:HG22	2.37	0.41
1:J:391:LEU:N	1:J:392:PRO:HD2	2.35	0.41
2:K:31:LEU:HD22	2:K:49:ILE:HD13	2.03	0.41
3:L:587:LEU:HD23	3:L:588:SER:N	2.28	0.41
3:L:591:HIS:HE1	3:L:593:LEU:HD23	1.86	0.41
3:L:656:LEU:HD23	3:L:656:LEU:N	2.31	0.41
3:L:6:VAL:HG21	3:L:26:ALA:CB	2.51	0.41
4:M:346:THR:CG2	4:M:353:LEU:HB3	2.51	0.41
5:N:37:GLU:O	5:N:40:HIS:HB3	2.21	0.41
6:O:115:GLY:N	6:O:125:GLN:O	2.54	0.41
1:S:140:ARG:O	1:S:143:ASP:HB2	2.20	0.41
3:U:169:PRO:N	3:U:176:LEU:HD13	2.35	0.41
3:U:749:HIS:N	3:U:749:HIS:ND1	2.66	0.41
4:V:320:SER:OG	4:V:323:ALA:N	2.53	0.41
4:V:96:ALA:HB2	4:V:346:THR:CG2	2.51	0.41
5:W:115:GLU:HB3	5:W:119:TYR:CE2	2.56	0.41
5:W:3:LEU:HD11	5:W:84:ASP:OD2	2.20	0.41
6:X:132:PRO:HB2	6:X:174:ALA:HB1	2.02	0.41
8:Z:121:ARG:HG3	8:Z:121:ARG:NH1	2.33	0.41
1:1:185:GLU:O	1:1:188:LEU:HB3	2.21	0.41
3:3:584:VAL:O	3:3:584:VAL:HG23	2.21	0.41
3:3:613:HIS:CE1	3:3:671:GLU:OE2	2.73	0.41
4:4:138:LEU:C	4:4:140:LEU:N	2.73	0.41
4:4:168:PHE:HZ	6:6:49:GLU:HB2	1.85	0.41
4:4:376:VAL:O	4:4:379:GLN:HG3	2.20	0.41
5:5:157:THR:HG21	7:9:66:TYR:HB2	2.03	0.41
6:6:90:PRO:O	6:6:93:ARG:HB3	2.20	0.41
7:9:114:VAL:HB	7:9:170:LEU:HD23	2.02	0.41
7:9:42:VAL:O	7:9:42:VAL:HG23	2.19	0.41
1:A:211:LEU:HD12	1:A:211:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:SER:C	1:A:297:THR:H	2.24	0.41
1:A:309:THR:HA	1:A:310:PRO:HD3	1.66	0.41
1:A:290:ILE:HG22	1:A:330:LEU:HD23	2.03	0.41
1:A:371:PHE:HA	1:A:374:ILE:HG23	2.02	0.41
3:C:185:LYS:HE3	3:C:202:PHE:HE2	1.86	0.41
3:C:561:PRO:HG3	3:C:575:GLU:O	2.21	0.41
4:D:257:TYR:O	4:D:263:ASP:N	2.54	0.41
4:D:285:GLU:O	4:D:288:LYS:N	2.53	0.41
6:F:142:PRO:HB2	6:F:146:ALA:CB	2.50	0.41
6:F:164:ASN:HB3	7:G:148:ARG:CZ	2.50	0.41
7:G:126:TYR:C	7:G:128:ASP:H	2.24	0.41
7:G:134:GLU:CD	7:G:134:GLU:N	2.71	0.41
7:G:31:VAL:O	7:G:162:VAL:N	2.53	0.41
2:K:81:GLN:HB3	2:K:122:VAL:CG2	2.47	0.41
3:L:174:VAL:HB	3:L:175:ILE:HG13	2.01	0.41
3:L:279:ALA:HB2	3:L:290:ILE:HG12	2.02	0.41
3:L:746:ARG:O	3:L:746:ARG:HG3	2.21	0.41
4:M:235:THR:CA	4:M:239:LEU:HD22	2.46	0.41
4:M:254:TYR:C	4:M:254:TYR:CD1	2.93	0.41
4:M:358:VAL:HG12	4:M:366:TYR:HB3	2.03	0.41
5:N:47:ASN:HD22	5:N:77:LEU:N	2.19	0.41
6:O:165:GLU:OE1	6:O:165:GLU:C	2.59	0.41
6:O:16:ARG:O	6:O:21:PHE:HB3	2.20	0.41
7:P:140:VAL:HG13	7:P:141:VAL:N	2.36	0.41
8:Q:88:ARG:CZ	8:Q:128:PHE:HE1	2.34	0.41
1:S:147:GLN:O	1:S:150:LYS:N	2.54	0.41
1:S:184:GLU:OE1	1:S:186:THR:N	2.53	0.41
1:S:331:ILE:HA	1:S:332:PRO:HD2	1.91	0.41
1:S:70:PHE:HA	1:S:71:PRO:HD3	1.96	0.41
1:S:92:ASN:HD21	1:S:94:ASP:HB3	1.85	0.41
2:T:79:HIS:H	2:T:137:ASN:HB3	1.85	0.41
3:U:240:ALA:CB	3:U:276:ARG:HB3	2.51	0.41
3:U:282:VAL:HG22	3:U:285:VAL:HG12	2.02	0.41
3:U:378:PRO:HA	3:U:545:GLU:OE2	2.20	0.41
3:U:537:PRO:CB	3:U:758:LEU:HD11	2.45	0.41
4:V:95:LEU:HG	4:V:99:LEU:HD23	2.02	0.41
6:X:142:PRO:O	6:X:143:ARG:C	2.58	0.41
6:X:16:ARG:HD2	6:X:17:GLU:CG	2.50	0.41
1:1:204:PRO:HG2	1:1:204:PRO:O	2.21	0.41
1:1:316:LEU:HD23	1:1:316:LEU:HA	1.88	0.41
3:3:297:GLY:HA3	3:3:703:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:765:PRO:O	3:3:766:ALA:C	2.59	0.41
5:5:93:TYR:N	5:5:93:TYR:CD1	2.88	0.41
8:7:16:LEU:O	8:7:19:TRP:HB2	2.21	0.41
1:A:436:LEU:HD23	2:B:90:LEU:CA	2.51	0.41
2:B:131:ALA:HB3	2:B:144:CYS:HA	2.03	0.41
3:C:208:HIS:O	3:C:209:THR:C	2.59	0.41
3:C:261:VAL:O	3:C:262:GLY:C	2.58	0.41
3:C:514:ASP:O	3:C:515:THR:C	2.58	0.41
3:C:344:TYR:CD1	3:C:568:TYR:CE1	3.08	0.41
4:D:84:ARG:CZ	6:F:117:MET:HE1	2.51	0.41
6:F:39:ALA:HB2	6:F:75:ALA:HB1	2.02	0.41
1:J:19:ALA:HB2	1:J:237:TRP:HH2	1.86	0.41
3:L:20:MET:SD	3:L:32:LEU:CD2	3.09	0.41
3:L:325:ALA:O	3:L:329:LEU:HB2	2.20	0.41
3:L:83:CYS:O	3:L:433:ALA:HB1	2.21	0.41
3:L:726:GLU:O	3:L:727:ALA:HB3	2.21	0.41
4:M:130:LEU:HD23	4:M:130:LEU:HA	1.94	0.41
4:M:62:LEU:HD23	4:M:62:LEU:HA	1.84	0.41
5:N:72:TYR:N	5:N:72:TYR:CD1	2.89	0.41
6:O:47:ALA:O	6:O:51:MET:HG3	2.21	0.41
6:O:49:GLU:OE1	6:O:49:GLU:HA	2.21	0.41
7:P:42:VAL:HG21	7:P:170:LEU:CD2	2.51	0.41
1:S:13:PHE:CD1	1:S:13:PHE:O	2.73	0.41
1:S:19:ALA:HB2	1:S:237:TRP:HH2	1.86	0.41
1:S:290:ILE:O	1:S:290:ILE:HG13	2.20	0.41
1:S:288:GLN:NE2	1:S:333:GLU:HA	2.36	0.41
1:S:363:VAL:CG2	1:S:364:ALA:N	2.84	0.41
1:S:337:MET:HG3	1:S:417:PHE:CD2	2.55	0.41
3:U:33:PHE:CD2	3:U:182:ILE:HD12	2.56	0.41
3:U:549:VAL:N	3:U:550:LEU:HD12	2.35	0.41
4:V:235:THR:HA	4:V:239:LEU:CD2	2.48	0.41
4:V:266:LEU:CD1	4:V:281:ARG:HB3	2.19	0.41
2:2:145:VAL:CG1	2:2:150:LEU:HB2	2.50	0.41
3:3:238:LEU:C	3:3:240:ALA:N	2.73	0.41
3:3:307:LYS:N	3:3:307:LYS:HE3	2.29	0.41
3:3:344:TYR:HB2	3:3:568:TYR:HD1	1.86	0.41
3:3:666:ALA:C	3:3:668:LYS:H	2.24	0.41
1:A:181:ILE:O	1:A:183:GLY:N	2.53	0.41
3:C:226:ILE:CD1	3:C:235:LEU:CD1	2.97	0.41
3:C:258:LEU:HD12	3:C:294:GLY:HA2	2.02	0.41
3:C:284:GLU:H	3:C:284:GLU:CD	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:117:ARG:O	4:D:121:ASN:HB2	2.20	0.41
4:D:231:ASP:CA	4:D:235:THR:HG23	2.48	0.41
5:E:41:TYR:CE2	5:E:88:PHE:HZ	2.38	0.41
8:H:40:PHE:O	8:H:43:ARG:HB3	2.20	0.41
8:H:86:LEU:HD12	8:H:91:ILE:HG21	2.01	0.41
1:J:301:PRO:HB2	1:J:303:THR:HG23	2.02	0.41
3:L:461:TRP:CD1	3:L:461:TRP:N	2.87	0.41
3:L:260:PRO:HB3	3:L:617:LEU:HB3	2.03	0.41
3:L:640:VAL:O	3:L:641:LEU:C	2.57	0.41
3:L:719:HIS:HB2	3:L:720:PRO:CD	2.49	0.41
4:M:156:ILE:O	4:M:159:LEU:HB2	2.21	0.41
4:M:52:VAL:CG2	4:M:388:GLU:O	2.68	0.41
6:O:89:ALA:HB3	6:O:90:PRO:CD	2.51	0.41
1:S:108:GLU:C	1:S:109:ASP:OD1	2.58	0.41
1:S:291:ILE:O	1:S:328:VAL:HA	2.21	0.41
2:T:47:GLU:O	2:T:50:ALA:HB3	2.20	0.41
3:U:325:ALA:O	3:U:329:LEU:HB2	2.21	0.41
5:W:195:LEU:O	5:W:196:TRP:CE3	2.74	0.41
5:W:22:LEU:HD23	5:W:22:LEU:N	2.35	0.41
5:W:70:VAL:HG12	5:W:71:VAL:N	2.36	0.41
5:W:47:ASN:HD22	5:W:77:LEU:N	2.19	0.41
6:X:165:GLU:CG	7:Y:128:ASP:CG	2.85	0.41
2:2:139:GLU:CB	2:2:140:PRO:HD2	2.17	0.41
3:3:370:ASP:OD1	3:3:551:PRO:HD3	2.20	0.41
3:3:417:VAL:HG13	3:3:444:ARG:O	2.21	0.41
3:3:731:GLY:CA	3:3:747:VAL:HG12	2.50	0.41
4:4:105:LEU:HD13	4:4:309:ILE:CD1	2.50	0.41
4:4:152:GLU:OE2	4:4:200:ARG:HD3	2.20	0.41
4:4:235:THR:HA	4:4:239:LEU:CD2	2.45	0.41
4:4:64:THR:HB	4:4:66:PHE:CD1	2.56	0.41
4:4:68:LYS:NZ	5:5:150:TYR:O	2.47	0.41
6:6:163:TYR:HB2	6:6:169:ARG:CA	2.48	0.41
6:6:16:ARG:O	6:6:21:PHE:HB3	2.21	0.41
6:6:93:ARG:NH1	6:6:96:TRP:CZ3	2.89	0.41
8:7:112:LYS:CG	8:7:116:PHE:HE1	2.34	0.41
8:7:81:ARG:O	8:7:81:ARG:HD3	2.20	0.41
7:9:177:THR:O	7:9:179:GLY:N	2.53	0.41
2:B:43:PRO:O	2:B:46:ILE:HB	2.21	0.41
3:C:282:VAL:CG2	3:C:285:VAL:HG12	2.51	0.41
3:C:399:LEU:N	3:C:399:LEU:HD12	2.35	0.41
3:C:498:GLU:OE1	3:C:498:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:517:ALA:HA	3:C:520:ARG:HG3	2.03	0.41
3:C:516:VAL:O	3:C:519:GLU:HG2	2.21	0.41
3:C:564:LEU:HA	3:C:564:LEU:HD12	1.83	0.41
4:D:130:LEU:HA	4:D:130:LEU:HD23	1.94	0.41
4:D:316:LEU:C	4:D:318:GLU:H	2.24	0.41
4:D:342:VAL:CG2	4:D:343:TYR:H	2.29	0.41
6:F:148:ILE:C	6:F:150:ALA:N	2.73	0.41
7:G:104:CYS:O	7:G:105:GLU:C	2.56	0.41
8:H:39:ASP:OD2	8:H:75:ARG:CG	2.68	0.41
11:H:500:FMN:H9	11:H:500:FMN:O2'	2.21	0.41
1:J:125:ILE:O	1:J:126:ARG:HB2	2.21	0.41
1:J:325:THR:O	1:J:327:GLY:N	2.54	0.41
2:K:131:ALA:HB3	2:K:144:CYS:HA	2.02	0.41
3:L:173:PHE:HB3	3:L:174:VAL:H	1.62	0.41
3:L:383:PRO:HA	3:L:384:PRO:HD3	1.89	0.41
3:L:457:PRO:C	3:L:459:MET:H	2.24	0.41
3:L:479:ALA:O	3:L:482:GLY:N	2.53	0.41
4:M:224:ILE:HD13	5:N:112:ASN:CA	2.51	0.41
4:M:310:THR:HG22	4:M:311:PRO:N	2.36	0.41
4:M:385:CYS:HB3	4:M:396:ILE:CG1	2.39	0.41
1:S:250:LYS:HG3	1:S:251:LEU:N	2.36	0.41
2:T:88:CYS:C	2:T:93:ALA:HB2	2.40	0.41
3:U:116:PRO:O	3:U:117:LEU:HB2	2.21	0.41
3:U:48:CYS:O	3:U:82:SER:CB	2.66	0.41
3:U:349:ALA:O	3:U:540:ASN:ND2	2.54	0.41
3:U:627:ALA:HA	3:U:628:PRO:HD3	1.90	0.41
3:U:751:GLU:CA	3:U:751:GLU:OE1	2.53	0.41
4:V:232:LEU:HD22	4:V:266:LEU:O	2.21	0.41
4:V:298:GLU:CG	4:V:299:PRO:HD2	2.51	0.41
5:W:20:ASN:HD22	5:W:24:ASN:HB2	1.82	0.41
8:Z:16:LEU:O	8:Z:19:TRP:HB2	2.21	0.41
1:1:252:TYR:CB	1:1:275:LEU:HD11	2.45	0.41
2:2:24:ARG:HB3	2:2:24:ARG:HE	1.73	0.41
3:3:505:LEU:HB3	3:3:532:VAL:HG22	2.03	0.41
3:3:398:VAL:HG22	3:3:506:ILE:HB	2.03	0.41
4:4:115:THR:HG21	4:4:297:LEU:CD2	2.47	0.41
4:4:226:PRO:HB2	4:4:227:GLU:H	1.63	0.41
4:4:230:ILE:HB	4:4:240:ARG:H	1.86	0.41
5:5:41:TYR:CE2	5:5:88:PHE:HZ	2.39	0.41
6:6:130:VAL:HG23	6:6:131:VAL:HG13	2.03	0.41
6:6:143:ARG:O	6:6:146:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:99:ILE:CG2	7:9:101:CYS:HB3	2.51	0.41
1:A:211:LEU:HG	1:A:212:TRP:CE3	2.55	0.41
1:A:370:LEU:H	1:A:370:LEU:CD2	2.33	0.41
2:B:26:ALA:O	2:B:29:PRO:HG2	2.20	0.41
3:C:101:ARG:NH1	3:C:101:ARG:HB3	2.36	0.41
3:C:213:THR:OG1	3:C:214:MET:N	2.54	0.41
3:C:407:PRO:O	3:C:410:HIS:HB3	2.21	0.41
3:C:260:PRO:CB	3:C:617:LEU:HB3	2.51	0.41
3:C:635:GLU:HG2	3:C:639:GLN:HG2	2.03	0.41
4:D:220:GLY:O	4:D:272:VAL:CG2	2.69	0.41
7:G:29:ALA:HA	7:G:30:PRO:HD2	1.81	0.41
1:J:101:PHE:N	1:J:101:PHE:CD1	2.89	0.41
1:J:29:LEU:HD22	1:J:33:LEU:CD1	2.51	0.41
1:J:358:PRO:O	1:J:362:GLY:CA	2.69	0.41
2:K:72:PHE:N	2:K:72:PHE:CD1	2.88	0.41
3:L:205:ARG:C	3:L:209:THR:HG22	2.41	0.41
3:L:341:VAL:HB	3:L:364:LEU:CD2	2.46	0.41
3:L:371:PHE:CD2	3:L:374:ARG:HB2	2.56	0.41
3:L:495:GLU:HG2	3:L:499:LYS:HE3	2.03	0.41
4:M:168:PHE:HZ	6:O:49:GLU:HB2	1.85	0.41
4:M:271:ASP:O	4:M:275:ARG:HG3	2.21	0.41
6:O:92:MET:HE3	6:O:127:VAL:HG13	2.02	0.41
7:P:113:ILE:O	7:P:113:ILE:HG23	2.20	0.41
5:N:167:PRO:HB3	7:P:66:TYR:CE2	2.56	0.41
8:Q:121:ARG:NH1	8:Q:121:ARG:HG3	2.34	0.41
8:Q:17:LEU:O	8:Q:18:SER:C	2.59	0.41
1:S:235:ALA:O	1:S:238:PHE:N	2.54	0.41
1:S:249:MET:H	1:S:249:MET:HE2	1.87	0.41
2:T:28:MET:N	2:T:29:PRO:HD2	2.36	0.41
3:U:174:VAL:HG13	3:U:239:THR:HB	2.02	0.41
3:U:640:VAL:O	3:U:641:LEU:C	2.56	0.41
3:U:644:LEU:C	3:U:644:LEU:HD23	2.41	0.41
4:V:214:PHE:O	4:V:216:GLU:N	2.54	0.41
4:V:223:VAL:O	4:V:224:ILE:C	2.57	0.41
4:V:293:ALA:HA	4:V:296:ARG:HE	1.86	0.41
4:V:341:GLU:OE1	5:W:26:TRP:HH2	2.03	0.41
7:Y:114:VAL:HG12	7:Y:115:LEU:H	1.87	0.41
1:1:45:LEU:HD23	1:1:123:TYR:CG	2.57	0.40
1:1:369:ASN:O	1:1:370:LEU:C	2.59	0.40
1:1:436:LEU:HD23	2:2:90:LEU:CA	2.47	0.40
2:2:57:PRO:HB2	3:3:214:MET:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:402:PRO:HA	3:3:535:MET:CE	2.51	0.40
3:3:474:ARG:H	3:3:474:ARG:HG2	1.72	0.40
3:3:540:ASN:HB2	3:3:614:LEU:HG	2.03	0.40
3:3:19:VAL:HG13	3:3:93:VAL:HG21	2.02	0.40
4:4:102:GLU:CD	4:4:117:ARG:HH22	2.24	0.40
4:4:221:VAL:HB	4:4:223:VAL:CG2	2.51	0.40
5:5:154:GLU:CB	6:6:119:ASN:HB3	2.51	0.40
5:5:187:GLY:C	5:5:189:ARG:N	2.71	0.40
5:5:39:ALA:O	5:5:42:LYS:N	2.49	0.40
6:6:31:GLY:C	6:6:33:SER:H	2.23	0.40
6:6:163:TYR:CE1	7:9:152:ARG:CZ	3.04	0.40
1:A:29:LEU:HD13	1:A:155:ARG:HG3	2.04	0.40
1:A:297:THR:HA	1:A:298:PRO:HD3	1.92	0.40
2:B:45:ARG:O	2:B:48:GLU:HB3	2.21	0.40
3:C:355:LEU:O	3:C:356:LEU:C	2.59	0.40
3:C:495:GLU:HG2	3:C:499:LYS:HE3	2.02	0.40
3:C:505:LEU:HB3	3:C:532:VAL:HG22	2.03	0.40
4:D:379:GLN:CD	5:E:116:ARG:HG2	2.42	0.40
5:E:130:PRO:CG	5:E:131:ASP:H	2.24	0.40
6:F:148:ILE:HG22	6:F:149:TYR:N	2.36	0.40
6:F:43:LEU:HB2	6:F:82:GLY:HA3	2.02	0.40
7:G:94:ASN:ND2	7:G:97:ARG:HB2	2.35	0.40
6:6:19:ILE:CD1	1:J:271:THR:CG2	2.93	0.40
1:J:345:THR:HG21	1:J:371:PHE:CE2	2.56	0.40
3:L:398:VAL:HG22	3:L:506:ILE:HB	2.03	0.40
3:L:400:GLY:O	3:L:401:ASP:C	2.60	0.40
3:L:651:ARG:O	3:L:651:ARG:HD3	2.21	0.40
4:M:228:VAL:CG1	4:M:271:ASP:HA	2.48	0.40
4:M:293:ALA:HA	4:M:296:ARG:HE	1.86	0.40
4:M:321:MET:HG3	4:M:322:GLU:N	2.36	0.40
4:M:220:GLY:N	4:M:388:GLU:OE2	2.54	0.40
7:P:102:GLY:O	7:P:104:CYS:N	2.54	0.40
7:P:126:TYR:C	7:P:128:ASP:H	2.24	0.40
8:Q:72:VAL:CG2	8:Q:73:SER:N	2.84	0.40
2:T:87:SER:OG	2:T:128:CYS:HB3	2.21	0.40
2:T:7:LYS:HG2	2:T:7:LYS:O	2.21	0.40
3:U:185:LYS:HG2	3:U:188:VAL:CG2	2.52	0.40
3:U:337:ARG:NH1	3:U:648:LEU:O	2.54	0.40
4:V:230:ILE:HB	4:V:240:ARG:H	1.86	0.40
4:V:409:ARG:O	4:V:409:ARG:CG	2.58	0.40
5:W:119:TYR:O	5:W:120:ASP:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:117:GLU:O	5:W:121:LEU:HD13	2.21	0.40
6:X:171:PRO:HA	6:X:172:PRO:HD3	1.92	0.40
7:Y:104:CYS:O	7:Y:105:GLU:C	2.59	0.40
7:Y:115:LEU:HA	7:Y:115:LEU:HD23	1.72	0.40
1:1:433:ARG:HH12	2:2:94:GLU:CD	2.25	0.40
2:2:85:THR:CG2	2:2:86:LEU:N	2.83	0.40
3:3:285:VAL:HG22	3:3:286:ASN:H	1.82	0.40
3:3:290:ILE:HG21	3:3:295:ARG:HB2	2.02	0.40
3:3:20:MET:HE3	3:3:432:PHE:HB3	2.02	0.40
3:3:337:ARG:NH1	3:3:648:LEU:O	2.54	0.40
5:5:50:ALA:HB3	5:5:114:LEU:CD1	2.31	0.40
5:5:80:TRP:HB3	5:5:81:LYS:H	1.57	0.40
6:6:147:LEU:C	6:6:147:LEU:HD13	2.42	0.40
8:7:23:TYR:C	8:7:23:TYR:CD1	2.95	0.40
1:A:222:GLU:OE1	1:A:251:LEU:HB2	2.21	0.40
1:A:137:GLU:HB3	2:B:141:TYR:OH	2.20	0.40
2:B:168:LEU:HA	2:B:169:PRO:HD2	1.92	0.40
3:C:174:VAL:HG12	3:C:238:LEU:H	1.85	0.40
3:C:286:ASN:ND2	3:C:286:ASN:C	2.70	0.40
3:C:298:HIS:CD2	3:C:298:HIS:C	2.95	0.40
3:C:46:ARG:O	3:C:107:MET:HE2	2.21	0.40
4:D:223:VAL:HG12	4:D:223:VAL:O	2.21	0.40
4:D:298:GLU:CG	4:D:299:PRO:HD2	2.51	0.40
5:E:10:ALA:C	5:E:12:ALA:N	2.74	0.40
5:E:44:MET:HE1	5:E:82:ASP:HB3	2.04	0.40
6:F:156:LYS:HA	6:F:159:ARG:HD2	2.03	0.40
8:H:24:ALA:HB1	8:H:29:VAL:O	2.21	0.40
1:J:180:TYR:HB3	1:J:351:GLU:OE1	2.20	0.40
1:J:365:GLY:O	1:J:369:ASN:ND2	2.54	0.40
3:L:109:GLU:OE1	3:L:156:ARG:NH1	2.49	0.40
4:M:305:PRO:O	4:M:306:ASN:C	2.58	0.40
5:N:4:GLU:O	5:N:7:LEU:HB3	2.22	0.40
6:O:46:CYS:HB3	6:O:81:ALA:HB1	2.02	0.40
1:S:108:GLU:HA	1:S:144:ARG:HG3	2.03	0.40
4:V:138:LEU:HD11	4:V:146:PHE:CD2	2.55	0.40
4:V:257:TYR:O	4:V:263:ASP:N	2.54	0.40
4:V:99:LEU:HA	4:V:99:LEU:HD13	1.87	0.40
5:W:125:VAL:CG1	5:W:126:PHE:N	2.77	0.40
11:Z:500:FMN:O2'	11:Z:500:FMN:H9	2.20	0.40
1:1:267:PRO:O	1:1:270:THR:CG2	2.70	0.40
1:1:309:THR:HA	1:1:310:PRO:HD3	1.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:366:PHE:HB3	1:1:367:MET:H	1.65	0.40
2:2:40:TRP:CZ3	2:2:42:ARG:CA	3.02	0.40
3:3:721:GLU:O	3:3:722:THR:OG1	2.36	0.40
4:4:254:TYR:CG	4:4:255:SER:N	2.88	0.40
5:5:101:LEU:O	5:5:130:PRO:HD2	2.21	0.40
5:5:121:LEU:O	5:5:122:PHE:C	2.57	0.40
5:5:124:ILE:HG22	5:5:146:LEU:CB	2.38	0.40
5:5:119:TYR:HD1	5:5:132:LEU:HD21	1.85	0.40
6:6:156:LYS:O	6:6:162:ALA:HB3	2.20	0.40
6:6:22:THR:HG22	6:6:23:THR:N	2.36	0.40
7:9:35:PRO:O	7:9:36:ARG:HB3	2.18	0.40
1:A:221:VAL:O	1:A:222:GLU:C	2.58	0.40
2:B:139:GLU:CB	2:B:140:PRO:HD2	2.18	0.40
3:C:287:GLU:OE2	3:C:412:ARG:NH1	2.54	0.40
3:C:451:PHE:CE1	3:C:466:GLU:HB2	2.53	0.40
4:D:167:ARG:C	4:D:168:PHE:HD1	2.22	0.40
4:D:249:ARG:CZ	4:D:249:ARG:HB3	2.45	0.40
4:D:254:TYR:CG	4:D:255:SER:N	2.89	0.40
5:E:72:TYR:CD1	5:E:72:TYR:N	2.89	0.40
1:J:149:ILE:CG2	1:J:153:ARG:HH21	2.34	0.40
3:L:434:ASP:C	3:L:436:GLN:N	2.74	0.40
3:L:474:ARG:O	3:L:475:GLU:C	2.60	0.40
3:L:506:ILE:HG12	3:L:533:LEU:HB2	2.02	0.40
3:L:305:ARG:NH1	3:L:609:GLU:OE2	2.51	0.40
3:L:337:ARG:NH1	3:L:648:LEU:O	2.55	0.40
3:L:724:ARG:HB3	3:L:724:ARG:HE	1.47	0.40
4:M:228:VAL:O	4:M:231:ASP:N	2.54	0.40
4:M:59:ILE:HD11	5:N:138:PRO:CB	2.47	0.40
3:L:163:HIS:ND1	8:Q:71:ASP:OD2	2.49	0.40
1:S:147:GLN:O	1:S:150:LYS:HB2	2.21	0.40
1:S:394:ILE:O	1:S:395:GLU:C	2.59	0.40
2:T:61:MET:HE1	8:Z:128:PHE:HZ	1.87	0.40
3:U:131:GLN:O	3:U:134:THR:HB	2.22	0.40
3:U:14:PRO:HG2	3:U:17:THR:HG1	1.87	0.40
3:U:178:ARG:C	3:U:180:ARG:N	2.74	0.40
3:U:36:GLU:O	3:U:37:LYS:C	2.59	0.40
4:V:235:THR:HG22	4:V:239:LEU:HD22	2.03	0.40
4:V:294:LEU:O	4:V:294:LEU:HD23	2.21	0.40
6:X:105:VAL:HB	6:X:133:VAL:HA	2.03	0.40
6:X:160:GLY:C	6:X:162:ALA:N	2.74	0.40
8:Z:17:LEU:O	8:Z:18:SER:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:12:ARG:O	1:1:12:ARG:CG	2.68	0.40
1:1:267:PRO:HD2	1:1:270:THR:CG2	2.52	0.40
3:3:116:PRO:O	3:3:117:LEU:HB2	2.20	0.40
3:3:692:PHE:O	3:3:760:LEU:HA	2.20	0.40
3:3:714:ALA:O	3:3:745:ALA:HA	2.20	0.40
4:4:118:VAL:CG2	4:4:119:ILE:N	2.84	0.40
4:4:196:VAL:C	4:4:198:PRO:CD	2.90	0.40
5:5:116:ARG:NH1	5:5:116:ARG:HG2	2.32	0.40
8:7:38:PRO:C	8:7:40:PHE:N	2.73	0.40
8:7:61:ASP:OD1	8:7:63:LEU:N	2.54	0.40
1:A:270:THR:O	1:A:311:MET:HG3	2.22	0.40
1:A:342:TRP:O	1:A:342:TRP:CE3	2.67	0.40
1:A:9:LEU:HA	1:A:13:PHE:CZ	2.57	0.40
3:C:14:PRO:HG2	3:C:17:THR:OG1	2.21	0.40
3:C:185:LYS:HG2	3:C:188:VAL:CG2	2.52	0.40
3:C:20:MET:O	3:C:21:ASP:C	2.59	0.40
3:C:511:VAL:N	3:C:520:ARG:HH12	2.20	0.40
3:C:642:ALA:O	3:C:645:ALA:HB3	2.21	0.40
3:C:658:LEU:O	3:C:658:LEU:HD23	2.22	0.40
4:D:155:THR:CG2	4:D:193:LEU:HD12	2.51	0.40
4:D:246:TYR:HB3	4:D:347:GLU:HG3	2.03	0.40
4:D:385:CYS:HB3	4:D:396:ILE:CG1	2.36	0.40
5:E:42:LYS:C	5:E:45:GLY:H	2.24	0.40
7:G:177:THR:O	7:G:179:GLY:N	2.54	0.40
7:G:43:LEU:HD21	7:G:91:TYR:CE2	2.56	0.40
8:H:29:VAL:HG21	8:H:67:PHE:CZ	2.56	0.40
8:H:43:ARG:HG2	8:H:44:MET:N	2.36	0.40
2:K:24:ARG:HB3	2:K:24:ARG:HE	1.72	0.40
3:L:262:GLY:O	3:L:263:CYS:O	2.39	0.40
3:L:532:VAL:CG1	3:L:533:LEU:N	2.84	0.40
3:L:717:TRP:O	3:L:717:TRP:CD2	2.74	0.40
4:M:237:GLY:O	4:M:239:LEU:CG	2.67	0.40
4:M:381:LEU:HD11	4:M:397:ILE:CG1	2.50	0.40
5:N:48:PHE:HE2	5:N:104:VAL:HG12	1.87	0.40
5:N:49:LEU:O	5:N:49:LEU:HG	2.22	0.40
6:O:156:LYS:O	6:O:162:ALA:HB3	2.21	0.40
6:O:41:PHE:O	6:O:41:PHE:CG	2.72	0.40
8:Q:108:ILE:N	8:Q:108:ILE:CD1	2.84	0.40
8:Q:121:ARG:O	8:Q:124:GLU:HB2	2.22	0.40
8:Q:29:VAL:HG21	8:Q:67:PHE:CZ	2.57	0.40
1:S:111:PRO:O	1:S:112:HIS:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:18:TYR:H	1:S:18:TYR:HD1	1.70	0.40
3:U:290:ILE:HA	3:U:290:ILE:HD13	1.82	0.40
3:U:469:ARG:HG3	3:U:469:ARG:HH11	1.86	0.40
3:U:490:VAL:O	3:U:493:ALA:HB3	2.21	0.40
3:U:532:VAL:CG1	3:U:533:LEU:N	2.85	0.40
4:V:232:LEU:HB2	4:V:278:VAL:HG11	2.04	0.40
4:V:322:GLU:C	4:V:325:ILE:H	2.24	0.40
4:V:221:VAL:O	4:V:383:TYR:HE1	2.04	0.40
5:W:118:VAL:HG13	5:W:129:HIS:CG	2.55	0.40
4:V:332:THR:O	5:W:172:ALA:HB3	2.21	0.40
5:W:43:ALA:C	5:W:45:GLY:H	2.19	0.40
4:V:84:ARG:CZ	6:X:117:MET:HE1	2.52	0.40
7:Y:95:MET:HG3	7:Y:131:TYR:CD1	2.56	0.40
1:1:366:PHE:O	1:1:369:ASN:N	2.50	0.40
2:2:112:THR:HG22	2:2:116:LEU:H	1.86	0.40
2:2:123:GLU:O	2:2:124:CYS:C	2.60	0.40
2:2:86:LEU:CG	2:2:90:LEU:HD11	2.51	0.40
3:3:153:VAL:O	3:3:153:VAL:HG12	2.21	0.40
3:3:452:ALA:HB1	3:3:453:PRO:HD2	2.03	0.40
3:3:474:ARG:O	3:3:475:GLU:C	2.60	0.40
3:3:506:ILE:HG12	3:3:533:LEU:HB2	2.03	0.40
3:3:508:GLY:HA3	3:3:535:MET:HB2	2.02	0.40
3:3:578:LYS:HZ3	3:3:578:LYS:HB3	1.85	0.40
3:3:714:ALA:HA	3:3:752:ASP:CB	2.51	0.40
4:4:321:MET:HG3	4:4:322:GLU:N	2.36	0.40
4:4:61:TYR:O	6:6:85:SER:HB3	2.22	0.40
4:4:86:ASP:C	4:4:88:LEU:H	2.23	0.40
5:5:161:GLU:HB2	5:5:163:ARG:CZ	2.52	0.40
7:9:31:VAL:O	7:9:162:VAL:N	2.55	0.40
1:A:11:PRO:HA	1:A:267:PRO:CG	2.52	0.40
1:A:290:ILE:HG13	1:A:290:ILE:O	2.20	0.40
1:A:398:SER:HA	3:C:46:ARG:HD2	2.03	0.40
2:B:42:ARG:N	2:B:45:ARG:HG3	2.36	0.40
3:C:153:VAL:O	3:C:153:VAL:HG12	2.21	0.40
1:A:196:ARG:NH2	3:C:204:GLU:O	2.54	0.40
3:C:476:ILE:N	3:C:476:ILE:HD12	2.37	0.40
3:C:474:ARG:HD3	3:C:515:THR:OG1	2.21	0.40
4:D:169:HIS:O	4:D:170:HIS:C	2.60	0.40
4:D:217:ARG:HD3	4:D:217:ARG:HA	1.87	0.40
4:D:122:GLU:HB2	4:D:290:ILE:CD1	2.51	0.40
4:D:358:VAL:O	4:D:366:TYR:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:383:TYR:C	4:D:383:TYR:CD1	2.95	0.40
8:H:39:ASP:CG	8:H:75:ARG:HE	2.25	0.40
1:J:108:GLU:C	1:J:109:ASP:OD1	2.60	0.40
1:J:114:LEU:C	1:J:114:LEU:HD23	2.42	0.40
2:K:24:ARG:HA	2:K:53:VAL:HG13	2.02	0.40
3:L:101:ARG:HB3	3:L:101:ARG:NH1	2.36	0.40
3:L:118:ASP:O	3:L:119:CYS:C	2.60	0.40
3:L:185:LYS:HE3	3:L:202:PHE:HE2	1.87	0.40
3:L:202:PHE:HA	3:L:210:PHE:O	2.21	0.40
3:L:382:PHE:H	3:L:382:PHE:HD1	1.66	0.40
3:L:605:PRO:HB2	3:L:609:GLU:HG3	2.04	0.40
4:M:168:PHE:O	4:M:169:HIS:HB2	2.21	0.40
4:M:343:TYR:HD2	4:M:356:TYR:HB2	1.86	0.40
4:M:64:THR:OG1	6:O:83:ARG:NH1	2.52	0.40
4:M:82:THR:N	4:M:83:PRO:CD	2.84	0.40
5:N:11:ARG:N	5:N:11:ARG:CD	2.82	0.40
7:P:102:GLY:O	7:P:103:LEU:C	2.60	0.40
1:S:9:LEU:HA	1:S:13:PHE:HZ	1.87	0.40
2:T:112:THR:HG22	2:T:116:LEU:H	1.87	0.40
2:T:153:LEU:HD21	2:T:163:LEU:CD1	2.51	0.40
3:U:457:PRO:C	3:U:459:MET:H	2.25	0.40
4:V:124:SER:O	4:V:125:ARG:C	2.60	0.40
5:W:10:ALA:C	5:W:12:ALA:N	2.75	0.40
6:X:115:GLY:N	6:X:125:GLN:O	2.54	0.40
6:X:134:ASP:OD1	6:X:174:ALA:HB2	2.21	0.40
6:X:43:LEU:CD1	6:X:83:ARG:O	2.69	0.40
7:Y:144:LYS:N	7:Y:145:PRO:HD2	2.37	0.40
1:S:220:ASN:N	11:Z:500:FMN:O3P	2.53	0.40
1:S:75:LYS:NZ	11:Z:500:FMN:O5'	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:1:MET:N	3:U:498:GLU:OE2[2_645]	2.01	0.19

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	430/438 (98%)	332 (77%)	68 (16%)	30 (7%)	1	7
1	A	430/438 (98%)	330 (77%)	70 (16%)	30 (7%)	1	7
1	J	430/438 (98%)	331 (77%)	70 (16%)	29 (7%)	1	8
1	S	430/438 (98%)	332 (77%)	65 (15%)	33 (8%)	1	6
2	2	176/181 (97%)	144 (82%)	24 (14%)	8 (4%)	2	15
2	B	176/181 (97%)	142 (81%)	26 (15%)	8 (4%)	2	15
2	K	176/181 (97%)	145 (82%)	23 (13%)	8 (4%)	2	15
2	T	176/181 (97%)	144 (82%)	24 (14%)	8 (4%)	2	15
3	3	727/783 (93%)	559 (77%)	117 (16%)	51 (7%)	1	7
3	C	727/783 (93%)	564 (78%)	116 (16%)	47 (6%)	1	9
3	L	727/783 (93%)	567 (78%)	109 (15%)	51 (7%)	1	7
3	U	727/783 (93%)	565 (78%)	110 (15%)	52 (7%)	1	7
4	4	366/409 (90%)	277 (76%)	64 (18%)	25 (7%)	1	8
4	D	366/409 (90%)	283 (77%)	57 (16%)	26 (7%)	1	7
4	M	366/409 (90%)	274 (75%)	63 (17%)	29 (8%)	1	6
4	V	366/409 (90%)	280 (76%)	63 (17%)	23 (6%)	1	9
5	5	187/207 (90%)	128 (68%)	34 (18%)	25 (13%)	0	1
5	E	187/207 (90%)	126 (67%)	35 (19%)	26 (14%)	0	1
5	N	187/207 (90%)	123 (66%)	38 (20%)	26 (14%)	0	1
5	W	187/207 (90%)	123 (66%)	39 (21%)	25 (13%)	0	1
6	6	140/181 (77%)	99 (71%)	31 (22%)	10 (7%)	1	7
6	F	140/181 (77%)	99 (71%)	33 (24%)	8 (6%)	1	11
6	O	140/181 (77%)	101 (72%)	31 (22%)	8 (6%)	1	11
6	X	140/181 (77%)	100 (71%)	33 (24%)	7 (5%)	2	14
7	9	152/182 (84%)	119 (78%)	24 (16%)	9 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	G	152/182 (84%)	117 (77%)	25 (16%)	10 (7%)	1 8
7	P	152/182 (84%)	121 (80%)	22 (14%)	9 (6%)	1 10
7	Y	152/182 (84%)	116 (76%)	27 (18%)	9 (6%)	1 10
8	7	125/129 (97%)	110 (88%)	10 (8%)	5 (4%)	3 18
8	H	125/129 (97%)	110 (88%)	10 (8%)	5 (4%)	3 18
8	Q	125/129 (97%)	108 (86%)	11 (9%)	6 (5%)	2 14
8	Z	125/129 (97%)	107 (86%)	12 (10%)	6 (5%)	2 14
All	All	9212/10040 (92%)	7076 (77%)	1484 (16%)	652 (7%)	1 7

All (652) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	14	GLU
1	1	28	THR
1	1	37	GLY
1	1	160	LYS
1	1	166	ASP
2	2	124	CYS
2	2	131	ALA
2	2	136	VAL
2	2	138	ASP
2	2	140	PRO
3	3	46	ARG
3	3	138	GLY
3	3	179	GLU
3	3	212	GLY
3	3	263	CYS
3	3	288	ILE
3	3	367	PRO
3	3	368	HIS
3	3	635	GLU
3	3	652	PRO
3	3	653	PRO
3	3	704	ALA
3	3	723	ALA
3	3	748	VAL
3	3	754	PRO
4	4	39	GLY
4	4	52	VAL
4	4	87	TYR

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Mol	Chain	Res	Type
4	4	200	ARG
4	4	225	PRO
4	4	226	PRO
4	4	284	ARG
4	4	321	MET
5	5	33	ARG
5	5	47	ASN
5	5	160	ARG
5	5	161	GLU
6	6	16	ARG
6	6	110	ALA
7	9	95	MET
7	9	102	GLY
8	7	45	GLU
8	7	90	HIS
1	A	14	GLU
1	A	37	GLY
1	A	160	LYS
1	A	166	ASP
2	B	124	CYS
2	B	131	ALA
2	B	136	VAL
2	B	138	ASP
2	B	140	PRO
3	C	46	ARG
3	C	179	GLU
3	C	212	GLY
3	C	263	CYS
3	C	288	ILE
3	C	367	PRO
3	C	368	HIS
3	C	635	GLU
3	C	653	PRO
3	C	723	ALA
3	C	748	VAL
3	C	754	PRO
4	D	52	VAL
4	D	87	TYR
4	D	200	ARG
4	D	225	PRO
4	D	226	PRO
4	D	284	ARG

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Mol	Chain	Res	Type
4	D	321	MET
5	E	33	ARG
5	E	47	ASN
5	E	160	ARG
5	E	161	GLU
6	F	16	ARG
6	F	110	ALA
7	G	95	MET
7	G	102	GLY
8	H	45	GLU
8	H	90	HIS
1	J	14	GLU
1	J	37	GLY
1	J	160	LYS
1	J	166	ASP
2	K	124	CYS
2	K	131	ALA
2	K	136	VAL
2	K	138	ASP
2	K	140	PRO
3	L	46	ARG
3	L	138	GLY
3	L	179	GLU
3	L	212	GLY
3	L	263	CYS
3	L	288	ILE
3	L	367	PRO
3	L	368	HIS
3	L	635	GLU
3	L	652	PRO
3	L	653	PRO
3	L	704	ALA
3	L	723	ALA
3	L	748	VAL
3	L	754	PRO
4	M	39	GLY
4	M	52	VAL
4	M	87	TYR
4	M	200	ARG
4	M	225	PRO
4	M	226	PRO
4	M	284	ARG

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Mol	Chain	Res	Type
4	M	321	MET
5	N	33	ARG
5	N	47	ASN
5	N	160	ARG
5	N	161	GLU
6	O	16	ARG
6	O	110	ALA
7	P	95	MET
7	P	102	GLY
7	P	103	LEU
8	Q	45	GLU
8	Q	90	HIS
1	S	14	GLU
1	S	37	GLY
1	S	160	LYS
1	S	166	ASP
2	T	86	LEU
2	T	124	CYS
2	T	131	ALA
2	T	136	VAL
2	T	138	ASP
2	T	140	PRO
3	U	46	ARG
3	U	179	GLU
3	U	212	GLY
3	U	288	ILE
3	U	367	PRO
3	U	368	HIS
3	U	635	GLU
3	U	653	PRO
3	U	723	ALA
3	U	748	VAL
3	U	754	PRO
4	V	39	GLY
4	V	52	VAL
4	V	87	TYR
4	V	200	ARG
4	V	225	PRO
4	V	226	PRO
4	V	284	ARG
4	V	321	MET
5	W	33	ARG

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Mol	Chain	Res	Type
5	W	47	ASN
5	W	160	ARG
5	W	161	GLU
6	X	16	ARG
6	X	110	ALA
7	Y	95	MET
7	Y	102	GLY
7	Y	103	LEU
8	Z	45	GLU
8	Z	90	HIS
1	1	21	VAL
1	1	27	TRP
1	1	95	GLU
1	1	204	PRO
1	1	221	VAL
1	1	234	GLY
1	1	296	SER
1	1	396	GLY
2	2	40	TRP
2	2	86	LEU
2	2	173	GLY
3	3	125	GLY
3	3	136	GLU
3	3	173	PHE
3	3	175	ILE
3	3	335	GLU
3	3	722	THR
4	4	67	GLU
4	4	91	PHE
4	4	142	ALA
4	4	220	GLY
4	4	255	SER
4	4	271	ASP
4	4	314	ARG
4	4	320	SER
4	4	322	GLU
5	5	2	ARG
5	5	23	GLY
5	5	32	GLU
5	5	45	GLY
5	5	49	LEU
5	5	105	THR

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Mol	Chain	Res	Type
5	5	125	VAL
5	5	130	PRO
5	5	176	GLY
6	6	111	CYS
6	6	113	SER
6	6	166	ARG
7	9	57	SER
7	9	84	GLY
7	9	103	LEU
7	9	127	SER
8	7	48	TYR
1	A	21	VAL
1	A	27	TRP
1	A	28	THR
1	A	95	GLU
1	A	204	PRO
1	A	221	VAL
1	A	234	GLY
1	A	296	SER
1	A	313	TYR
1	A	326	GLY
1	A	396	GLY
2	B	40	TRP
2	B	86	LEU
2	B	173	GLY
3	C	117	LEU
3	C	136	GLU
3	C	138	GLY
3	C	173	PHE
3	C	335	GLU
3	C	633	GLU
3	C	652	PRO
3	C	704	ALA
3	C	722	THR
3	C	747	VAL
3	C	766	ALA
4	D	39	GLY
4	D	91	PHE
4	D	142	ALA
4	D	220	GLY
4	D	235	THR
4	D	255	SER

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Mol	Chain	Res	Type
4	D	314	ARG
4	D	320	SER
4	D	322	GLU
5	E	2	ARG
5	E	23	GLY
5	E	45	GLY
5	E	105	THR
5	E	125	VAL
5	E	130	PRO
5	E	176	GLY
6	F	113	SER
6	F	166	ARG
7	G	57	SER
7	G	103	LEU
7	G	127	SER
8	H	39	ASP
8	H	48	TYR
8	H	88	ARG
1	J	21	VAL
1	J	27	TRP
1	J	95	GLU
1	J	204	PRO
1	J	234	GLY
1	J	313	TYR
1	J	326	GLY
1	J	396	GLY
2	K	40	TRP
2	K	86	LEU
2	K	173	GLY
3	L	117	LEU
3	L	125	GLY
3	L	136	GLU
3	L	173	PHE
3	L	175	ILE
3	L	216	PHE
3	L	335	GLU
3	L	633	GLU
3	L	722	THR
4	M	67	GLU
4	M	91	PHE
4	M	142	ALA
4	M	220	GLY

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Mol	Chain	Res	Type
4	M	255	SER
4	M	314	ARG
4	M	320	SER
4	M	322	GLU
4	M	384	ALA
5	N	2	ARG
5	N	7	LEU
5	N	23	GLY
5	N	45	GLY
5	N	49	LEU
5	N	105	THR
5	N	125	VAL
5	N	130	PRO
5	N	176	GLY
6	O	111	CYS
6	O	113	SER
6	O	166	ARG
7	P	57	SER
7	P	127	SER
8	Q	48	TYR
8	Q	88	ARG
1	S	27	TRP
1	S	28	THR
1	S	95	GLU
1	S	204	PRO
1	S	221	VAL
1	S	234	GLY
1	S	296	SER
1	S	326	GLY
1	S	396	GLY
2	T	173	GLY
3	U	125	GLY
3	U	136	GLU
3	U	138	GLY
3	U	173	PHE
3	U	175	ILE
3	U	263	CYS
3	U	335	GLU
3	U	633	GLU
3	U	652	PRO
3	U	704	ALA
3	U	722	THR

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Mol	Chain	Res	Type
3	U	725	ALA
3	U	747	VAL
4	V	142	ALA
4	V	220	GLY
4	V	235	THR
4	V	255	SER
4	V	271	ASP
4	V	314	ARG
4	V	320	SER
4	V	322	GLU
5	W	2	ARG
5	W	23	GLY
5	W	45	GLY
5	W	125	VAL
5	W	130	PRO
5	W	140	ASP
5	W	176	GLY
6	X	111	CYS
6	X	113	SER
6	X	166	ARG
7	Y	127	SER
7	Y	156	PRO
8	Z	48	TYR
8	Z	88	ARG
1	1	182	CYS
1	1	243	THR
1	1	293	GLY
1	1	313	TYR
1	1	326	GLY
1	1	358	PRO
3	3	117	LEU
3	3	304	ASN
3	3	508	GLY
3	3	633	GLU
3	3	719	HIS
3	3	725	ALA
3	3	747	VAL
3	3	766	ALA
5	5	7	LEU
5	5	9	GLU
5	5	123	GLY
5	5	127	GLU

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Mol	Chain	Res	Type
5	5	140	ASP
5	5	141	LEU
5	5	145	PRO
8	7	39	ASP
3	C	6	VAL
3	C	175	ILE
3	C	304	ASN
3	C	508	GLY
3	C	719	HIS
4	D	67	GLU
4	D	271	ASP
4	D	319	THR
5	E	7	LEU
5	E	9	GLU
5	E	32	GLU
5	E	49	LEU
5	E	65	PRO
5	E	127	GLU
5	E	140	ASP
5	E	141	LEU
5	E	145	PRO
6	F	111	CYS
7	G	84	GLY
7	G	156	PRO
1	J	182	CYS
1	J	221	VAL
1	J	296	SER
3	L	6	VAL
3	L	304	ASN
3	L	508	GLY
3	L	719	HIS
3	L	725	ALA
3	L	747	VAL
3	L	766	ALA
4	M	66	PHE
4	M	218	ALA
4	M	235	THR
4	M	271	ASP
4	M	319	THR
5	N	9	GLU
5	N	32	GLU
5	N	65	PRO

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Mol	Chain	Res	Type
5	N	127	GLU
5	N	140	ASP
5	N	141	LEU
5	N	145	PRO
7	P	126	TYR
8	Q	39	ASP
1	S	146	GLU
1	S	197	ALA
1	S	313	TYR
1	S	367	MET
1	S	373	LYS
2	T	40	TRP
3	U	113	LEU
3	U	117	LEU
3	U	304	ASN
3	U	508	GLY
3	U	719	HIS
4	V	91	PHE
5	W	7	LEU
5	W	9	GLU
5	W	32	GLU
5	W	65	PRO
5	W	105	THR
5	W	127	GLU
5	W	145	PRO
7	Y	57	SER
7	Y	126	TYR
8	Z	39	ASP
1	1	71	PRO
1	1	366	PHE
1	1	367	MET
3	3	6	VAL
3	3	453	PRO
3	3	549	VAL
3	3	687	GLU
4	4	66	PHE
4	4	215	TYR
4	4	218	ALA
4	4	235	THR
4	4	319	THR
5	5	65	PRO
5	5	86	SER

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Mol	Chain	Res	Type
7	9	156	PRO
7	9	178	GLU
1	A	20	HIS
1	A	146	GLU
1	A	182	CYS
1	A	211	LEU
1	A	367	MET
3	C	20	MET
3	C	31	PRO
3	C	216	PHE
3	C	453	PRO
3	C	725	ALA
4	D	229	ALA
5	E	123	GLY
7	G	126	TYR
7	G	178	GLU
1	J	366	PHE
3	L	31	PRO
3	L	82	SER
3	L	453	PRO
4	M	215	TYR
6	O	17	GLU
1	S	20	HIS
1	S	71	PRO
1	S	182	CYS
1	S	211	LEU
1	S	366	PHE
3	U	48	CYS
3	U	285	VAL
3	U	766	ALA
4	V	215	TYR
4	V	319	THR
5	W	49	LEU
5	W	141	LEU
1	1	10	ASP
1	1	43	ARG
1	1	146	GLU
1	1	197	ALA
1	1	211	LEU
3	3	20	MET
3	3	31	PRO
3	3	48	CYS

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Mol	Chain	Res	Type
3	3	113	LEU
3	3	194	VAL
3	3	285	VAL
3	3	401	ASP
4	4	222	GLY
5	5	50	ALA
5	5	132	LEU
6	6	17	GLU
1	A	10	ASP
1	A	71	PRO
1	A	197	ALA
1	A	293	GLY
1	A	366	PHE
3	C	549	VAL
3	C	765	PRO
4	D	66	PHE
4	D	348	SER
4	D	373	PRO
4	D	384	ALA
5	E	3	LEU
5	E	50	ALA
6	F	109	GLY
1	J	10	ASP
1	J	20	HIS
1	J	28	THR
1	J	71	PRO
1	J	146	GLU
1	J	211	LEU
1	J	367	MET
3	L	186	ARG
3	L	324	GLU
3	L	401	ASP
3	L	435	LEU
3	L	514	ASP
3	L	549	VAL
3	L	687	GLU
4	M	349	ALA
5	N	86	SER
5	N	101	LEU
5	N	188	SER
7	P	156	PRO
7	P	178	GLU

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Mol	Chain	Res	Type
1	S	10	ASP
1	S	43	ARG
1	S	358	PRO
3	U	6	VAL
3	U	186	ARG
3	U	401	ASP
3	U	435	LEU
3	U	453	PRO
3	U	455	ARG
3	U	549	VAL
3	U	702	HIS
3	U	764	GLY
4	V	66	PHE
5	W	86	SER
5	W	123	GLY
3	3	186	ARG
3	3	216	PHE
3	3	764	GLY
4	4	372	ALA
7	9	126	TYR
1	A	257	PRO
1	A	358	PRO
3	C	285	VAL
3	C	401	ASP
3	C	407	PRO
3	C	455	ARG
3	C	702	HIS
3	C	764	GLY
4	D	296	ARG
5	E	101	LEU
5	E	188	SER
6	F	44	ALA
1	J	257	PRO
3	L	285	VAL
3	L	764	GLY
4	M	71	GLU
4	M	222	GLY
4	M	296	ARG
5	N	3	LEU
5	N	117	GLU
1	S	21	VAL
1	S	311	MET

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Mol	Chain	Res	Type
3	U	14	PRO
3	U	216	PHE
3	U	231	PRO
3	U	407	PRO
4	V	67	GLU
4	V	373	PRO
5	W	3	LEU
5	W	101	LEU
7	Y	119	PHE
3	3	407	PRO
6	6	138	PRO
8	7	51	PRO
1	A	111	PRO
3	C	14	PRO
3	C	125	GLY
3	C	164	VAL
4	D	222	GLY
1	J	111	PRO
1	J	293	GLY
3	L	207	VAL
3	L	407	PRO
4	M	372	ALA
1	S	293	GLY
3	U	164	VAL
6	X	109	GLY
1	1	50	PRO
3	3	164	VAL
3	3	232	VAL
3	3	765	PRO
6	F	77	VAL
1	J	215	PRO
1	J	358	PRO
5	N	123	GLY
6	O	77	VAL
6	O	115	GLY
1	S	111	PRO
3	U	31	PRO
4	V	372	ALA
8	Z	51	PRO
1	1	111	PRO
3	3	231	PRO
4	4	373	PRO

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Mol	Chain	Res	Type
5	5	101	LEU
6	6	77	VAL
1	A	50	PRO
1	J	50	PRO
3	L	174	VAL
3	L	650	VAL
3	L	765	PRO
4	M	373	PRO
1	S	257	PRO
3	U	174	VAL
3	U	232	VAL
5	W	61	PRO
6	X	77	VAL
1	1	257	PRO
3	3	174	VAL
3	3	628	PRO
3	3	650	VAL
6	6	115	GLY
6	6	140	CYS
1	A	215	PRO
3	C	194	VAL
3	C	232	VAL
3	L	628	PRO
7	P	84	GLY
8	Q	51	PRO
1	S	50	PRO
1	S	215	PRO
3	U	119	CYS
3	U	194	VAL
7	Y	84	GLY
3	C	174	VAL
5	E	61	PRO
7	G	30	PRO
3	L	116	PRO
3	L	164	VAL
3	U	116	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	351/356 (99%)	320 (91%)	31 (9%)	10 33
1	A	351/356 (99%)	318 (91%)	33 (9%)	8 30
1	J	351/356 (99%)	320 (91%)	31 (9%)	10 33
1	S	351/356 (99%)	318 (91%)	33 (9%)	8 30
2	2	150/152 (99%)	129 (86%)	21 (14%)	3 16
2	B	150/152 (99%)	134 (89%)	16 (11%)	6 25
2	K	150/152 (99%)	130 (87%)	20 (13%)	4 17
2	T	150/152 (99%)	132 (88%)	18 (12%)	5 20
3	3	593/628 (94%)	524 (88%)	69 (12%)	5 22
3	C	593/628 (94%)	518 (87%)	75 (13%)	4 19
3	L	593/628 (94%)	520 (88%)	73 (12%)	4 20
3	U	593/628 (94%)	522 (88%)	71 (12%)	5 20
4	4	319/355 (90%)	281 (88%)	38 (12%)	5 21
4	D	319/355 (90%)	281 (88%)	38 (12%)	5 21
4	M	319/355 (90%)	280 (88%)	39 (12%)	5 20
4	V	319/355 (90%)	282 (88%)	37 (12%)	5 22
5	5	164/175 (94%)	142 (87%)	22 (13%)	4 16
5	E	164/175 (94%)	142 (87%)	22 (13%)	4 16
5	N	164/175 (94%)	140 (85%)	24 (15%)	3 14
5	W	164/175 (94%)	144 (88%)	20 (12%)	5 20
6	6	117/149 (78%)	108 (92%)	9 (8%)	13 38
6	F	117/149 (78%)	109 (93%)	8 (7%)	16 44
6	O	117/149 (78%)	108 (92%)	9 (8%)	13 38
6	X	117/149 (78%)	109 (93%)	8 (7%)	16 44
7	9	126/150 (84%)	117 (93%)	9 (7%)	14 42
7	G	126/150 (84%)	117 (93%)	9 (7%)	14 42
7	P	126/150 (84%)	117 (93%)	9 (7%)	14 42
7	Y	126/150 (84%)	120 (95%)	6 (5%)	25 56
8	7	104/106 (98%)	93 (89%)	11 (11%)	6 25
8	H	104/106 (98%)	95 (91%)	9 (9%)	10 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	Q	104/106 (98%)	94 (90%)	10 (10%)	8 29
8	Z	104/106 (98%)	94 (90%)	10 (10%)	8 29
All	All	7696/8284 (93%)	6858 (89%)	838 (11%)	6 24

All (838) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	10	ASP
1	1	12	ARG
1	1	13	PHE
1	1	14	GLU
1	1	15	ARG
1	1	29	LEU
1	1	53	VAL
1	1	81	LYS
1	1	104	ARG
1	1	128	THR
1	1	163	PHE
1	1	166	ASP
1	1	192	LEU
1	1	203	PRO
1	1	249	MET
1	1	253	GLN
1	1	255	SER
1	1	270	THR
1	1	271	THR
1	1	303	THR
1	1	306	VAL
1	1	342	TRP
1	1	359	CYS
1	1	363	VAL
1	1	366	PHE
1	1	367	MET
1	1	404	ASP
1	1	414	LEU
1	1	420	GLN
1	1	437	TRP
1	1	438	ARG
2	2	5	ASP
2	2	6	ASP
2	2	7	LYS

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Mol	Chain	Res	Type
2	2	10	PHE
2	2	12	GLU
2	2	28	MET
2	2	31	LEU
2	2	33	ARG
2	2	35	GLN
2	2	37	GLU
2	2	40	TRP
2	2	45	ARG
2	2	66	PHE
2	2	87	SER
2	2	112	THR
2	2	114	ASP
2	2	116	LEU
2	2	138	ASP
2	2	140	PRO
2	2	172	CYS
2	2	178	GLU
3	3	32	LEU
3	3	45	CYS
3	3	46	ARG
3	3	75	TRP
3	3	94	ASP
3	3	96	LEU
3	3	113	LEU
3	3	116	PRO
3	3	123	ASP
3	3	132	ASP
3	3	133	ARG
3	3	156	ARG
3	3	168	HIS
3	3	173	PHE
3	3	174	VAL
3	3	184	CYS
3	3	189	ARG
3	3	192	GLU
3	3	218	LEU
3	3	232	VAL
3	3	239	THR
3	3	241	ARG
3	3	245	ARG
3	3	252	THR

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Mol	Chain	Res	Type
3	3	259	CYS
3	3	286	ASN
3	3	288	ILE
3	3	307	LYS
3	3	366	THR
3	3	367	PRO
3	3	368	HIS
3	3	369	LEU
3	3	371	PHE
3	3	374	ARG
3	3	382	PHE
3	3	407	PRO
3	3	408	ILE
3	3	419	ASP
3	3	440	ARG
3	3	445	THR
3	3	450	LEU
3	3	464	ILE
3	3	465	HIS
3	3	469	ARG
3	3	473	GLU
3	3	478	LEU
3	3	501	LYS
3	3	507	LEU
3	3	523	LEU
3	3	524	LEU
3	3	542	ARG
3	3	587	LEU
3	3	593	LEU
3	3	617	LEU
3	3	624	LEU
3	3	639	GLN
3	3	651	ARG
3	3	652	PRO
3	3	655	ARG
3	3	683	LEU
3	3	684	ARG
3	3	724	ARG
3	3	726	GLU
3	3	747	VAL
3	3	749	HIS
3	3	751	GLU

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Mol	Chain	Res	Type
3	3	757	HIS
3	3	758	LEU
3	3	759	TYR
4	4	38	HIS
4	4	42	ARG
4	4	46	THR
4	4	47	LEU
4	4	52	VAL
4	4	59	ILE
4	4	69	THR
4	4	94	ASP
4	4	104	LEU
4	4	105	LEU
4	4	120	LEU
4	4	152	GLU
4	4	163	VAL
4	4	168	PHE
4	4	170	HIS
4	4	182	LEU
4	4	199	HIS
4	4	210	GLU
4	4	214	PHE
4	4	226	PRO
4	4	227	GLU
4	4	228	VAL
4	4	234	LEU
4	4	249	ARG
4	4	252	TYR
4	4	257	TYR
4	4	269	ARG
4	4	271	ASP
4	4	284	ARG
4	4	285	GLU
4	4	315	HIS
4	4	316	LEU
4	4	320	SER
4	4	343	TYR
4	4	347	GLU
4	4	363	SER
4	4	383	TYR
4	4	409	ARG
5	5	1	MET

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Mol	Chain	Res	Type
5	5	3	LEU
5	5	7	LEU
5	5	20	ASN
5	5	25	LEU
5	5	26	TRP
5	5	27	VAL
5	5	38	MET
5	5	44	MET
5	5	48	PHE
5	5	52	ILE
5	5	66	GLU
5	5	80	TRP
5	5	84	ASP
5	5	106	ASP
5	5	114	LEU
5	5	127	GLU
5	5	146	LEU
5	5	175	THR
5	5	184	TYR
5	5	195	LEU
5	5	196	TRP
6	6	16	ARG
6	6	26	LYS
6	6	37	TRP
6	6	45	CYS
6	6	50	MET
6	6	78	MET
6	6	83	ARG
6	6	93	ARG
6	6	165	GLU
7	9	33	LEU
7	9	57	SER
7	9	72	PRO
7	9	78	GLU
7	9	97	ARG
7	9	126	TYR
7	9	140	VAL
7	9	159	VAL
7	9	174	LYS
8	7	30	ARG
8	7	39	ASP
8	7	43	ARG

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Mol	Chain	Res	Type
8	7	44	MET
8	7	52	THR
8	7	63	LEU
8	7	78	LYS
8	7	81	ARG
8	7	82	ILE
8	7	85	ARG
8	7	120	ASP
1	A	10	ASP
1	A	12	ARG
1	A	13	PHE
1	A	14	GLU
1	A	15	ARG
1	A	29	LEU
1	A	53	VAL
1	A	81	LYS
1	A	104	ARG
1	A	128	THR
1	A	163	PHE
1	A	166	ASP
1	A	192	LEU
1	A	203	PRO
1	A	249	MET
1	A	253	GLN
1	A	255	SER
1	A	270	THR
1	A	271	THR
1	A	303	THR
1	A	306	VAL
1	A	342	TRP
1	A	346	ARG
1	A	359	CYS
1	A	363	VAL
1	A	366	PHE
1	A	367	MET
1	A	400	CYS
1	A	404	ASP
1	A	414	LEU
1	A	420	GLN
1	A	437	TRP
1	A	438	ARG
2	B	5	ASP

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Mol	Chain	Res	Type
2	B	6	ASP
2	B	7	LYS
2	B	28	MET
2	B	31	LEU
2	B	33	ARG
2	B	35	GLN
2	B	40	TRP
2	B	45	ARG
2	B	87	SER
2	B	112	THR
2	B	114	ASP
2	B	116	LEU
2	B	138	ASP
2	B	140	PRO
2	B	172	CYS
3	C	32	LEU
3	C	45	CYS
3	C	46	ARG
3	C	75	TRP
3	C	94	ASP
3	C	96	LEU
3	C	107	MET
3	C	113	LEU
3	C	116	PRO
3	C	123	ASP
3	C	124	LYS
3	C	132	ASP
3	C	133	ARG
3	C	156	ARG
3	C	168	HIS
3	C	173	PHE
3	C	174	VAL
3	C	184	CYS
3	C	189	ARG
3	C	192	GLU
3	C	207	VAL
3	C	218	LEU
3	C	232	VAL
3	C	239	THR
3	C	241	ARG
3	C	245	ARG
3	C	252	THR

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Mol	Chain	Res	Type
3	C	286	ASN
3	C	288	ILE
3	C	307	LYS
3	C	366	THR
3	C	367	PRO
3	C	368	HIS
3	C	369	LEU
3	C	371	PHE
3	C	374	ARG
3	C	382	PHE
3	C	407	PRO
3	C	408	ILE
3	C	412	ARG
3	C	419	ASP
3	C	440	ARG
3	C	445	THR
3	C	450	LEU
3	C	464	ILE
3	C	465	HIS
3	C	469	ARG
3	C	473	GLU
3	C	478	LEU
3	C	501	LYS
3	C	503	PRO
3	C	507	LEU
3	C	515	THR
3	C	523	LEU
3	C	524	LEU
3	C	542	ARG
3	C	559	ASP
3	C	587	LEU
3	C	593	LEU
3	C	617	LEU
3	C	624	LEU
3	C	639	GLN
3	C	651	ARG
3	C	655	ARG
3	C	683	LEU
3	C	684	ARG
3	C	709	GLN
3	C	724	ARG
3	C	726	GLU

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Mol	Chain	Res	Type
3	C	747	VAL
3	C	749	HIS
3	C	751	GLU
3	C	757	HIS
3	C	758	LEU
3	C	759	TYR
4	D	38	HIS
4	D	42	ARG
4	D	46	THR
4	D	47	LEU
4	D	52	VAL
4	D	59	ILE
4	D	69	THR
4	D	94	ASP
4	D	104	LEU
4	D	105	LEU
4	D	120	LEU
4	D	152	GLU
4	D	168	PHE
4	D	170	HIS
4	D	182	LEU
4	D	199	HIS
4	D	210	GLU
4	D	214	PHE
4	D	226	PRO
4	D	227	GLU
4	D	228	VAL
4	D	234	LEU
4	D	249	ARG
4	D	252	TYR
4	D	257	TYR
4	D	269	ARG
4	D	271	ASP
4	D	284	ARG
4	D	285	GLU
4	D	315	HIS
4	D	316	LEU
4	D	320	SER
4	D	335	PHE
4	D	343	TYR
4	D	347	GLU
4	D	363	SER

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Mol	Chain	Res	Type
4	D	407	VAL
4	D	409	ARG
5	E	1	MET
5	E	3	LEU
5	E	7	LEU
5	E	20	ASN
5	E	25	LEU
5	E	26	TRP
5	E	27	VAL
5	E	38	MET
5	E	48	PHE
5	E	52	ILE
5	E	53	VAL
5	E	66	GLU
5	E	80	TRP
5	E	93	TYR
5	E	114	LEU
5	E	127	GLU
5	E	142	GLU
5	E	146	LEU
5	E	175	THR
5	E	184	TYR
5	E	195	LEU
5	E	196	TRP
6	F	16	ARG
6	F	26	LYS
6	F	37	TRP
6	F	45	CYS
6	F	50	MET
6	F	78	MET
6	F	83	ARG
6	F	165	GLU
7	G	33	LEU
7	G	38	HIS
7	G	72	PRO
7	G	78	GLU
7	G	97	ARG
7	G	126	TYR
7	G	157	VAL
7	G	159	VAL
7	G	174	LYS
8	H	30	ARG

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Mol	Chain	Res	Type
8	H	43	ARG
8	H	44	MET
8	H	52	THR
8	H	78	LYS
8	H	81	ARG
8	H	82	ILE
8	H	85	ARG
8	H	120	ASP
1	J	10	ASP
1	J	12	ARG
1	J	13	PHE
1	J	14	GLU
1	J	15	ARG
1	J	29	LEU
1	J	53	VAL
1	J	81	LYS
1	J	104	ARG
1	J	128	THR
1	J	163	PHE
1	J	166	ASP
1	J	192	LEU
1	J	203	PRO
1	J	249	MET
1	J	253	GLN
1	J	255	SER
1	J	270	THR
1	J	271	THR
1	J	303	THR
1	J	306	VAL
1	J	342	TRP
1	J	359	CYS
1	J	363	VAL
1	J	366	PHE
1	J	367	MET
1	J	404	ASP
1	J	414	LEU
1	J	420	GLN
1	J	437	TRP
1	J	438	ARG
2	K	5	ASP
2	K	6	ASP
2	K	7	LYS

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Mol	Chain	Res	Type
2	K	10	PHE
2	K	12	GLU
2	K	28	MET
2	K	31	LEU
2	K	33	ARG
2	K	35	GLN
2	K	37	GLU
2	K	40	TRP
2	K	45	ARG
2	K	87	SER
2	K	112	THR
2	K	114	ASP
2	K	116	LEU
2	K	138	ASP
2	K	140	PRO
2	K	172	CYS
2	K	178	GLU
3	L	32	LEU
3	L	45	CYS
3	L	46	ARG
3	L	75	TRP
3	L	94	ASP
3	L	95	THR
3	L	96	LEU
3	L	107	MET
3	L	113	LEU
3	L	116	PRO
3	L	123	ASP
3	L	133	ARG
3	L	156	ARG
3	L	168	HIS
3	L	173	PHE
3	L	174	VAL
3	L	189	ARG
3	L	192	GLU
3	L	207	VAL
3	L	218	LEU
3	L	232	VAL
3	L	239	THR
3	L	241	ARG
3	L	245	ARG
3	L	252	THR

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Mol	Chain	Res	Type
3	L	253	PRO
3	L	259	CYS
3	L	286	ASN
3	L	288	ILE
3	L	307	LYS
3	L	366	THR
3	L	367	PRO
3	L	368	HIS
3	L	369	LEU
3	L	371	PHE
3	L	374	ARG
3	L	382	PHE
3	L	407	PRO
3	L	408	ILE
3	L	412	ARG
3	L	419	ASP
3	L	440	ARG
3	L	445	THR
3	L	450	LEU
3	L	464	ILE
3	L	465	HIS
3	L	469	ARG
3	L	473	GLU
3	L	478	LEU
3	L	501	LYS
3	L	507	LEU
3	L	515	THR
3	L	523	LEU
3	L	524	LEU
3	L	542	ARG
3	L	587	LEU
3	L	593	LEU
3	L	617	LEU
3	L	624	LEU
3	L	651	ARG
3	L	652	PRO
3	L	655	ARG
3	L	683	LEU
3	L	684	ARG
3	L	709	GLN
3	L	724	ARG
3	L	726	GLU

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Mol	Chain	Res	Type
3	L	747	VAL
3	L	749	HIS
3	L	751	GLU
3	L	757	HIS
3	L	758	LEU
3	L	759	TYR
4	M	38	HIS
4	M	42	ARG
4	M	46	THR
4	M	47	LEU
4	M	52	VAL
4	M	59	ILE
4	M	69	THR
4	M	94	ASP
4	M	104	LEU
4	M	105	LEU
4	M	120	LEU
4	M	152	GLU
4	M	163	VAL
4	M	168	PHE
4	M	170	HIS
4	M	182	LEU
4	M	199	HIS
4	M	210	GLU
4	M	214	PHE
4	M	226	PRO
4	M	227	GLU
4	M	228	VAL
4	M	234	LEU
4	M	249	ARG
4	M	252	TYR
4	M	257	TYR
4	M	269	ARG
4	M	271	ASP
4	M	284	ARG
4	M	285	GLU
4	M	315	HIS
4	M	316	LEU
4	M	320	SER
4	M	335	PHE
4	M	343	TYR
4	M	347	GLU

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Mol	Chain	Res	Type
4	M	363	SER
4	M	407	VAL
4	M	409	ARG
5	N	1	MET
5	N	3	LEU
5	N	7	LEU
5	N	20	ASN
5	N	25	LEU
5	N	26	TRP
5	N	27	VAL
5	N	38	MET
5	N	44	MET
5	N	48	PHE
5	N	52	ILE
5	N	65	PRO
5	N	66	GLU
5	N	80	TRP
5	N	84	ASP
5	N	106	ASP
5	N	114	LEU
5	N	127	GLU
5	N	142	GLU
5	N	146	LEU
5	N	175	THR
5	N	184	TYR
5	N	195	LEU
5	N	196	TRP
6	O	16	ARG
6	O	26	LYS
6	O	37	TRP
6	O	45	CYS
6	O	50	MET
6	O	78	MET
6	O	83	ARG
6	O	93	ARG
6	O	165	GLU
7	P	33	LEU
7	P	36	ARG
7	P	72	PRO
7	P	78	GLU
7	P	97	ARG
7	P	126	TYR

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Mol	Chain	Res	Type
7	P	140	VAL
7	P	159	VAL
7	P	174	LYS
8	Q	30	ARG
8	Q	43	ARG
8	Q	44	MET
8	Q	52	THR
8	Q	63	LEU
8	Q	78	LYS
8	Q	81	ARG
8	Q	82	ILE
8	Q	85	ARG
8	Q	120	ASP
1	S	10	ASP
1	S	12	ARG
1	S	13	PHE
1	S	14	GLU
1	S	15	ARG
1	S	29	LEU
1	S	53	VAL
1	S	81	LYS
1	S	104	ARG
1	S	128	THR
1	S	163	PHE
1	S	166	ASP
1	S	192	LEU
1	S	203	PRO
1	S	249	MET
1	S	253	GLN
1	S	255	SER
1	S	270	THR
1	S	271	THR
1	S	303	THR
1	S	306	VAL
1	S	342	TRP
1	S	353	CYS
1	S	359	CYS
1	S	363	VAL
1	S	366	PHE
1	S	367	MET
1	S	400	CYS
1	S	404	ASP

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Mol	Chain	Res	Type
1	S	414	LEU
1	S	420	GLN
1	S	437	TRP
1	S	438	ARG
2	T	5	ASP
2	T	6	ASP
2	T	7	LYS
2	T	28	MET
2	T	31	LEU
2	T	33	ARG
2	T	35	GLN
2	T	37	GLU
2	T	40	TRP
2	T	45	ARG
2	T	66	PHE
2	T	87	SER
2	T	114	ASP
2	T	116	LEU
2	T	138	ASP
2	T	140	PRO
2	T	172	CYS
2	T	178	GLU
3	U	32	LEU
3	U	45	CYS
3	U	46	ARG
3	U	75	TRP
3	U	94	ASP
3	U	96	LEU
3	U	113	LEU
3	U	116	PRO
3	U	123	ASP
3	U	132	ASP
3	U	133	ARG
3	U	156	ARG
3	U	168	HIS
3	U	173	PHE
3	U	174	VAL
3	U	189	ARG
3	U	192	GLU
3	U	207	VAL
3	U	218	LEU
3	U	232	VAL

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Mol	Chain	Res	Type
3	U	239	THR
3	U	241	ARG
3	U	245	ARG
3	U	252	THR
3	U	259	CYS
3	U	286	ASN
3	U	288	ILE
3	U	307	LYS
3	U	366	THR
3	U	367	PRO
3	U	368	HIS
3	U	369	LEU
3	U	371	PHE
3	U	374	ARG
3	U	382	PHE
3	U	407	PRO
3	U	408	ILE
3	U	412	ARG
3	U	419	ASP
3	U	440	ARG
3	U	445	THR
3	U	450	LEU
3	U	464	ILE
3	U	465	HIS
3	U	469	ARG
3	U	473	GLU
3	U	478	LEU
3	U	501	LYS
3	U	507	LEU
3	U	523	LEU
3	U	524	LEU
3	U	542	ARG
3	U	559	ASP
3	U	587	LEU
3	U	593	LEU
3	U	617	LEU
3	U	624	LEU
3	U	639	GLN
3	U	651	ARG
3	U	655	ARG
3	U	683	LEU
3	U	684	ARG

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Mol	Chain	Res	Type
3	U	709	GLN
3	U	724	ARG
3	U	726	GLU
3	U	747	VAL
3	U	749	HIS
3	U	751	GLU
3	U	757	HIS
3	U	758	LEU
3	U	759	TYR
4	V	38	HIS
4	V	42	ARG
4	V	46	THR
4	V	47	LEU
4	V	52	VAL
4	V	59	ILE
4	V	69	THR
4	V	94	ASP
4	V	104	LEU
4	V	105	LEU
4	V	120	LEU
4	V	152	GLU
4	V	168	PHE
4	V	170	HIS
4	V	171	ASN
4	V	182	LEU
4	V	199	HIS
4	V	210	GLU
4	V	214	PHE
4	V	226	PRO
4	V	227	GLU
4	V	228	VAL
4	V	234	LEU
4	V	249	ARG
4	V	252	TYR
4	V	257	TYR
4	V	269	ARG
4	V	271	ASP
4	V	284	ARG
4	V	285	GLU
4	V	315	HIS
4	V	316	LEU
4	V	320	SER

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Mol	Chain	Res	Type
4	V	335	PHE
4	V	343	TYR
4	V	347	GLU
4	V	409	ARG
5	W	1	MET
5	W	3	LEU
5	W	7	LEU
5	W	20	ASN
5	W	25	LEU
5	W	26	TRP
5	W	27	VAL
5	W	48	PHE
5	W	52	ILE
5	W	66	GLU
5	W	80	TRP
5	W	106	ASP
5	W	114	LEU
5	W	127	GLU
5	W	142	GLU
5	W	146	LEU
5	W	175	THR
5	W	184	TYR
5	W	195	LEU
5	W	196	TRP
6	X	16	ARG
6	X	26	LYS
6	X	37	TRP
6	X	45	CYS
6	X	50	MET
6	X	78	MET
6	X	83	ARG
6	X	165	GLU
7	Y	33	LEU
7	Y	78	GLU
7	Y	97	ARG
7	Y	126	TYR
7	Y	159	VAL
7	Y	174	LYS
8	Z	30	ARG
8	Z	43	ARG
8	Z	44	MET
8	Z	52	THR

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Mol	Chain	Res	Type
8	Z	63	LEU
8	Z	78	LYS
8	Z	81	ARG
8	Z	82	ILE
8	Z	85	ARG
8	Z	120	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	92	ASN
1	1	112	HIS
1	1	147	GLN
1	1	174	HIS
1	1	219	ASN
1	1	343	ASN
1	1	420	GLN
2	2	8	GLN
2	2	36	GLN
2	2	79	HIS
3	3	131	GLN
3	3	168	HIS
3	3	298	HIS
3	3	347	HIS
3	3	428	HIS
3	3	586	HIS
3	3	613	HIS
3	3	709	GLN
3	3	733	GLN
4	4	72	HIS
4	4	129	HIS
4	4	170	HIS
4	4	171	ASN
4	4	292	GLN
4	4	308	GLN
4	4	327	HIS
4	4	336	HIS
4	4	389	GLN
5	5	40	HIS
5	5	47	ASN
6	6	119	ASN
7	9	46	HIS

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Mol	Chain	Res	Type
7	9	94	ASN
1	A	92	ASN
1	A	112	HIS
1	A	147	GLN
1	A	174	HIS
1	A	219	ASN
1	A	288	GLN
1	A	420	GLN
2	B	8	GLN
2	B	36	GLN
2	B	79	HIS
3	C	131	GLN
3	C	168	HIS
3	C	286	ASN
3	C	298	HIS
3	C	347	HIS
3	C	428	HIS
3	C	613	HIS
3	C	661	GLN
3	C	709	GLN
3	C	733	GLN
4	D	72	HIS
4	D	169	HIS
4	D	170	HIS
4	D	171	ASN
4	D	292	GLN
4	D	308	GLN
4	D	327	HIS
4	D	336	HIS
4	D	389	GLN
5	E	24	ASN
5	E	40	HIS
5	E	47	ASN
6	F	119	ASN
7	G	38	HIS
7	G	46	HIS
7	G	94	ASN
1	J	92	ASN
1	J	112	HIS
1	J	147	GLN
1	J	174	HIS
1	J	219	ASN

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Mol	Chain	Res	Type
1	J	420	GLN
2	K	8	GLN
2	K	36	GLN
2	K	79	HIS
3	L	131	GLN
3	L	168	HIS
3	L	298	HIS
3	L	347	HIS
3	L	428	HIS
3	L	586	HIS
3	L	613	HIS
3	L	709	GLN
3	L	733	GLN
4	M	72	HIS
4	M	129	HIS
4	M	169	HIS
4	M	170	HIS
4	M	171	ASN
4	M	292	GLN
4	M	308	GLN
4	M	327	HIS
4	M	336	HIS
4	M	389	GLN
5	N	40	HIS
5	N	47	ASN
6	O	119	ASN
7	P	94	ASN
1	S	92	ASN
1	S	112	HIS
1	S	147	GLN
1	S	174	HIS
1	S	219	ASN
1	S	420	GLN
2	T	8	GLN
2	T	36	GLN
2	T	79	HIS
3	U	131	GLN
3	U	168	HIS
3	U	246	ASN
3	U	298	HIS
3	U	347	HIS
3	U	428	HIS

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Mol	Chain	Res	Type
3	U	468	HIS
3	U	613	HIS
3	U	661	GLN
3	U	709	GLN
3	U	733	GLN
4	V	72	HIS
4	V	129	HIS
4	V	169	HIS
4	V	170	HIS
4	V	171	ASN
4	V	292	GLN
4	V	308	GLN
4	V	327	HIS
4	V	336	HIS
5	W	40	HIS
5	W	47	ASN
6	X	119	ASN
7	Y	46	HIS
7	Y	94	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 monosaccharides in this entry.

5.6 Ligand geometry

40 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	$\#\|Z\| > 2$
9	SF4	G	183	7	0,12,12	0.00	-	-		
9	SF4	L	784	3	0,12,12	0.00	-	-		
9	SF4	Y	184	7	0,12,12	0.00	-	-		
9	SF4	G	184	7	0,12,12	0.00	-	-		
9	SF4	U	786	3	0,12,12	0.00	-	-		
10	FES	C	787	3	0,4,4	0.00	-	-		
9	SF4	L	786	3	0,12,12	0.00	-	-		
9	SF4	3	784	3	0,12,12	0.00	-	-		
9	SF4	U	784	3	0,12,12	0.00	-	-		
10	FES	B	182	2	0,4,4	0.00	-	-		
10	FES	3	787	3	0,4,4	0.00	-	-		
11	FMN	H	500	-	31,33,33	2.36	7 (22%)	40,50,50	4.09	13 (32%)
9	SF4	3	785	3	0,12,12	0.00	-	-		
9	SF4	C	786	3	0,12,12	0.00	-	-		
11	FMN	Z	500	-	31,33,33	2.26	6 (19%)	40,50,50	4.08	12 (30%)
9	SF4	C	785	3	0,12,12	0.00	-	-		
9	SF4	O	182	6	0,12,12	0.00	-	-		
9	SF4	J	439	1	0,12,12	0.00	-	-		
11	FMN	Q	500	-	31,33,33	2.26	6 (19%)	40,50,50	4.12	12 (30%)
10	FES	L	787	3	0,4,4	0.00	-	-		
11	FMN	7	500	-	31,33,33	2.31	7 (22%)	40,50,50	4.14	13 (32%)
9	SF4	S	439	1	0,12,12	0.00	-	-		
9	SF4	P	183	7	0,12,12	0.00	-	-		
10	FES	2	182	2	0,4,4	0.00	-	-		
10	FES	T	182	2	0,4,4	0.00	-	-		
10	FES	K	182	2	0,4,4	0.00	-	-		
9	SF4	9	183	7	0,12,12	0.00	-	-		
9	SF4	A	439	1	0,12,12	0.00	-	-		
9	SF4	9	184	7	0,12,12	0.00	-	-		
9	SF4	Y	183	7	0,12,12	0.00	-	-		
9	SF4	L	785	3	0,12,12	0.00	-	-		
9	SF4	F	182	6	0,12,12	0.00	-	-		
9	SF4	P	184	7	0,12,12	0.00	-	-		
9	SF4	1	439	1	0,12,12	0.00	-	-		
9	SF4	C	784	3	0,12,12	0.00	-	-		
9	SF4	U	785	3	0,12,12	0.00	-	-		
10	FES	U	787	3	0,4,4	0.00	-	-		
9	SF4	X	182	6	0,12,12	0.00	-	-		
9	SF4	6	182	6	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	SF4	3	786	3	0,12,12	0.00	-	-		

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
9	SF4	G	183	7	-	-	0/6/5/5
9	SF4	L	784	3	-	-	0/6/5/5
9	SF4	Y	184	7	-	-	0/6/5/5
9	SF4	G	184	7	-	-	0/6/5/5
9	SF4	U	786	3	-	-	0/6/5/5
10	FES	C	787	3	-	-	0/1/1/1
9	SF4	L	786	3	-	-	0/6/5/5
9	SF4	3	784	3	-	-	0/6/5/5
9	SF4	U	784	3	-	-	0/6/5/5
10	FES	B	182	2	-	-	0/1/1/1
10	FES	3	787	3	-	-	0/1/1/1
11	FMN	H	500	-	-	1/18/18/18	0/3/3/3
9	SF4	3	785	3	-	-	0/6/5/5
9	SF4	C	786	3	-	-	0/6/5/5
11	FMN	Z	500	-	-	1/18/18/18	0/3/3/3
9	SF4	C	785	3	-	-	0/6/5/5
9	SF4	O	182	6	-	-	0/6/5/5
9	SF4	J	439	1	-	-	0/6/5/5
11	FMN	Q	500	-	-	1/18/18/18	0/3/3/3
10	FES	L	787	3	-	-	0/1/1/1
11	FMN	7	500	-	-	1/18/18/18	0/3/3/3
9	SF4	S	439	1	-	-	0/6/5/5
9	SF4	P	183	7	-	-	0/6/5/5
10	FES	2	182	2	-	-	0/1/1/1
10	FES	T	182	2	-	-	0/1/1/1
10	FES	K	182	2	-	-	0/1/1/1
9	SF4	9	183	7	-	-	0/6/5/5
9	SF4	A	439	1	-	-	0/6/5/5
9	SF4	9	184	7	-	-	0/6/5/5
9	SF4	Y	183	7	-	-	0/6/5/5
9	SF4	L	785	3	-	-	0/6/5/5
9	SF4	F	182	6	-	-	0/6/5/5
9	SF4	P	184	7	-	-	0/6/5/5
9	SF4	1	439	1	-	-	0/6/5/5
9	SF4	C	784	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	U	785	3	-	-	0/6/5/5
10	FES	U	787	3	-	-	0/1/1/1
9	SF4	X	182	6	-	-	0/6/5/5
9	SF4	6	182	6	-	-	0/6/5/5
9	SF4	3	786	3	-	-	0/6/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	500	FMN	C4A-C10	8.99	1.47	1.38
11	Q	500	FMN	C4A-C10	8.38	1.47	1.38
11	Z	500	FMN	C4A-C10	8.22	1.47	1.38
11	7	500	FMN	C4A-C10	7.96	1.46	1.38
11	Q	500	FMN	C4-C4A	5.29	1.50	1.41
11	7	500	FMN	C4-C4A	5.15	1.50	1.41
11	7	500	FMN	C1'-N10	-4.87	1.43	1.48
11	Z	500	FMN	C4-C4A	4.67	1.49	1.41
11	H	500	FMN	C4-C4A	4.66	1.49	1.41
11	Z	500	FMN	C1'-N10	-3.95	1.44	1.48
11	H	500	FMN	C1'-N10	-3.74	1.44	1.48
11	Z	500	FMN	C4-N3	3.61	1.39	1.33
11	Q	500	FMN	C1'-N10	-3.59	1.44	1.48
11	H	500	FMN	C4-N3	3.44	1.39	1.33
11	Q	500	FMN	C4-N3	3.29	1.38	1.33
11	7	500	FMN	C2-N1	-2.95	1.32	1.38
11	7	500	FMN	C4-N3	2.94	1.38	1.33
11	H	500	FMN	C9A-N10	2.87	1.42	1.38
11	Z	500	FMN	C9A-N10	2.84	1.42	1.38
11	H	500	FMN	C2-N1	-2.74	1.32	1.38
11	7	500	FMN	C9A-N10	2.68	1.42	1.38
11	Z	500	FMN	C2-N1	-2.60	1.33	1.38
11	Q	500	FMN	C2-N1	-2.58	1.33	1.38
11	7	500	FMN	C2'-C3'	-2.39	1.49	1.53
11	H	500	FMN	C2'-C3'	-2.30	1.49	1.53
11	Q	500	FMN	C9A-N10	2.26	1.41	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	7	500	FMN	C1'-N10-C9A	16.46	131.25	118.29
11	Z	500	FMN	C1'-N10-C9A	16.36	131.17	118.29
11	H	500	FMN	C1'-N10-C9A	16.34	131.15	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Q	500	FMN	C1'-N10-C9A	16.32	131.14	118.29
11	7	500	FMN	C1'-N10-C10	-10.90	108.65	118.41
11	Z	500	FMN	C1'-N10-C10	-10.46	109.04	118.41
11	Q	500	FMN	C1'-N10-C10	-10.36	109.13	118.41
11	H	500	FMN	C1'-N10-C10	-10.08	109.38	118.41
11	Q	500	FMN	C4-N3-C2	8.17	122.04	115.14
11	H	500	FMN	C4-N3-C2	7.80	121.73	115.14
11	Z	500	FMN	C4-N3-C2	7.74	121.67	115.14
11	7	500	FMN	C4-N3-C2	7.31	121.31	115.14
11	Z	500	FMN	P-O5'-C5'	-7.09	98.77	118.30
11	H	500	FMN	P-O5'-C5'	-6.95	99.15	118.30
11	7	500	FMN	P-O5'-C5'	-6.94	99.17	118.30
11	Q	500	FMN	P-O5'-C5'	-6.94	99.18	118.30
11	Q	500	FMN	C5'-C4'-C3'	-6.00	100.61	112.20
11	H	500	FMN	C5'-C4'-C3'	-5.86	100.89	112.20
11	7	500	FMN	C5'-C4'-C3'	-5.74	101.11	112.20
11	Z	500	FMN	C5'-C4'-C3'	-5.57	101.45	112.20
11	Q	500	FMN	C4-C4A-C10	-5.54	116.28	119.95
11	7	500	FMN	C4-C4A-C10	-5.48	116.32	119.95
11	H	500	FMN	C4-C4A-C10	-5.27	116.46	119.95
11	Z	500	FMN	C4-C4A-C10	-5.17	116.53	119.95
11	7	500	FMN	C4A-N5-C5A	5.10	121.87	116.77
11	Q	500	FMN	C4A-N5-C5A	4.87	121.64	116.77
11	H	500	FMN	C4A-N5-C5A	4.78	121.55	116.77
11	7	500	FMN	C4-C4A-N5	4.71	123.98	118.60
11	Z	500	FMN	C4A-N5-C5A	4.66	121.43	116.77
11	Z	500	FMN	C4A-C4-N3	-4.62	117.11	123.43
11	Q	500	FMN	C4A-C4-N3	-4.60	117.14	123.43
11	H	500	FMN	C4-C4A-N5	4.50	123.74	118.60
11	H	500	FMN	C4A-C4-N3	-4.50	117.28	123.43
11	7	500	FMN	C4A-C4-N3	-4.45	117.34	123.43
11	Q	500	FMN	C4-C4A-N5	4.38	123.61	118.60
11	Z	500	FMN	C4-C4A-N5	4.20	123.40	118.60
11	7	500	FMN	C1'-C2'-C3'	-4.17	98.13	109.79
11	H	500	FMN	C1'-C2'-C3'	-4.09	98.36	109.79
11	Q	500	FMN	C1'-C2'-C3'	-4.03	98.53	109.79
11	Z	500	FMN	C1'-C2'-C3'	-3.92	98.83	109.79
11	7	500	FMN	O5'-C5'-C4'	3.70	119.23	109.36
11	H	500	FMN	O5'-C5'-C4'	3.69	119.21	109.36
11	Q	500	FMN	O5'-C5'-C4'	3.68	119.19	109.36
11	Z	500	FMN	O5'-C5'-C4'	3.52	118.74	109.36
11	Z	500	FMN	C4'-C3'-C2'	2.49	118.55	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	500	FMN	C4'-C3'-C2'	2.42	118.40	113.36
11	7	500	FMN	C4'-C3'-C2'	2.32	118.19	113.36
11	7	500	FMN	C10-C4A-N5	-2.27	119.69	121.26
11	Q	500	FMN	C4'-C3'-C2'	2.12	117.77	113.36
11	H	500	FMN	C10-C4A-N5	-2.12	119.79	121.26

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	H	500	FMN	C2'-C1'-N10-C10
11	Q	500	FMN	C2'-C1'-N10-C10
11	Z	500	FMN	C2'-C1'-N10-C10
11	7	500	FMN	C2'-C1'-N10-C10

There are no ring outliers.

30 monomers are involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	G	183	SF4	1	0
9	L	784	SF4	1	0
9	Y	184	SF4	1	0
9	G	184	SF4	1	0
9	U	786	SF4	2	0
10	C	787	FES	1	0
9	L	786	SF4	2	0
9	3	784	SF4	1	0
9	U	784	SF4	1	0
10	B	182	FES	2	0
10	3	787	FES	1	0
11	H	500	FMN	5	0
9	C	786	SF4	2	0
11	Z	500	FMN	6	0
9	O	182	SF4	1	0
11	Q	500	FMN	7	0
10	L	787	FES	1	0
11	7	500	FMN	5	0
10	2	182	FES	2	0
10	T	182	FES	1	0
10	K	182	FES	2	0
9	9	183	SF4	1	0

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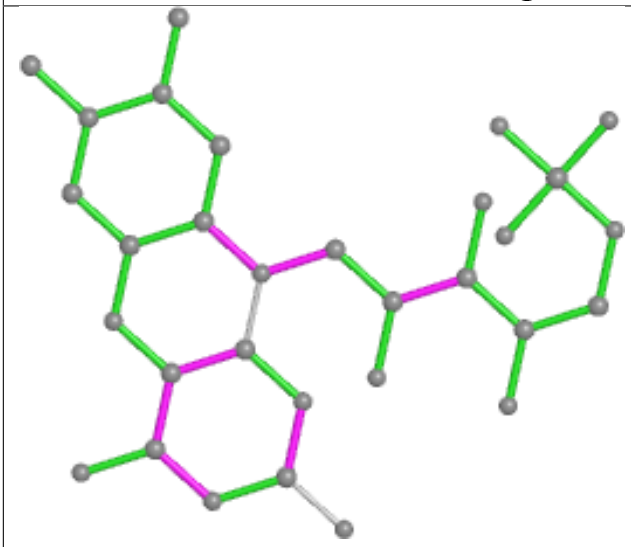
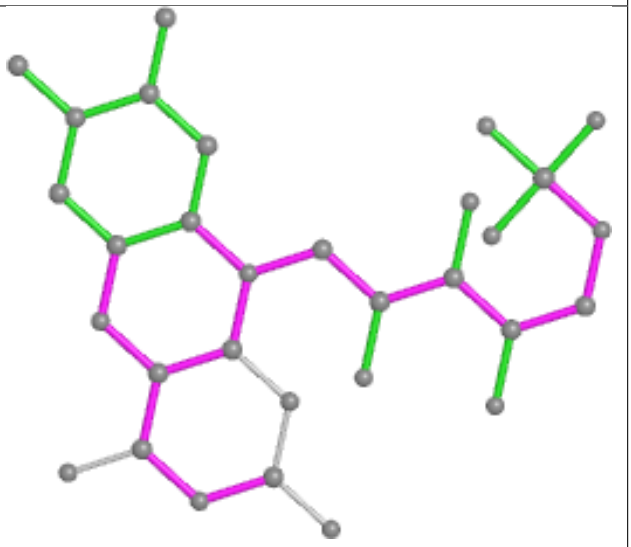
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	9	184	SF4	1	0
9	Y	183	SF4	1	0
9	F	182	SF4	1	0
9	P	184	SF4	1	0
9	C	784	SF4	1	0
9	X	182	SF4	1	0
9	6	182	SF4	1	0
9	3	786	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

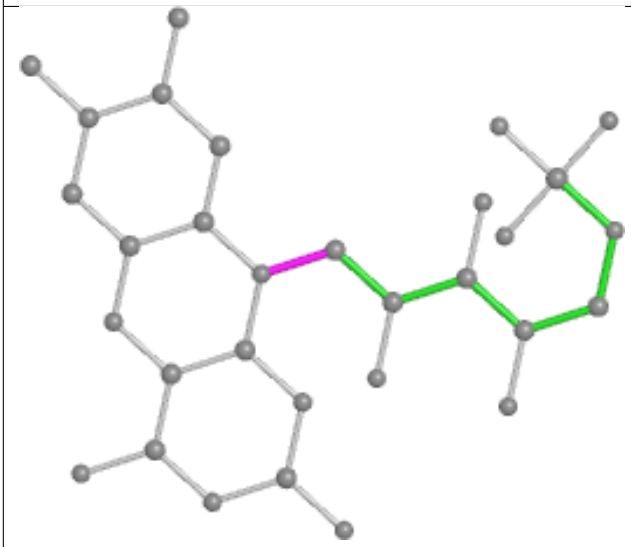
Ligand FMN H 500



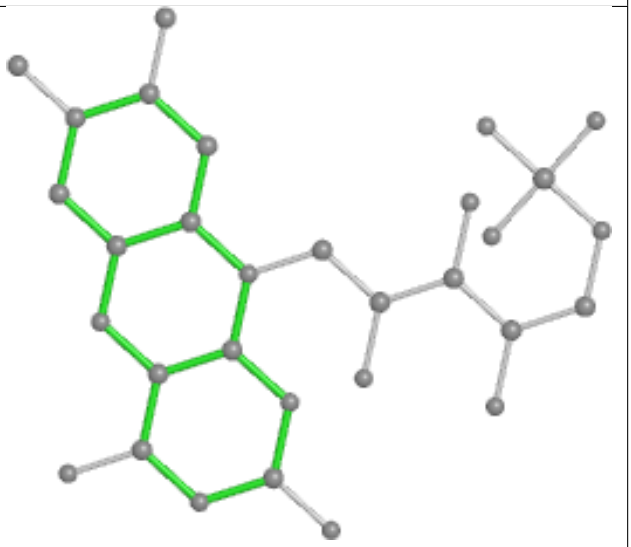
Bond lengths



Bond angles

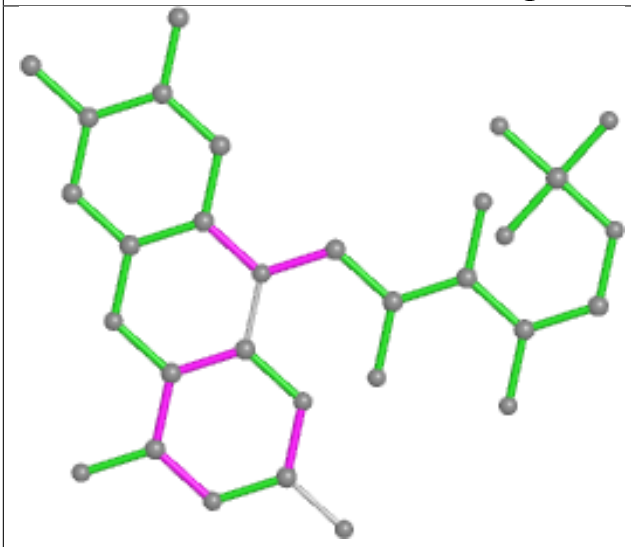


Torsions

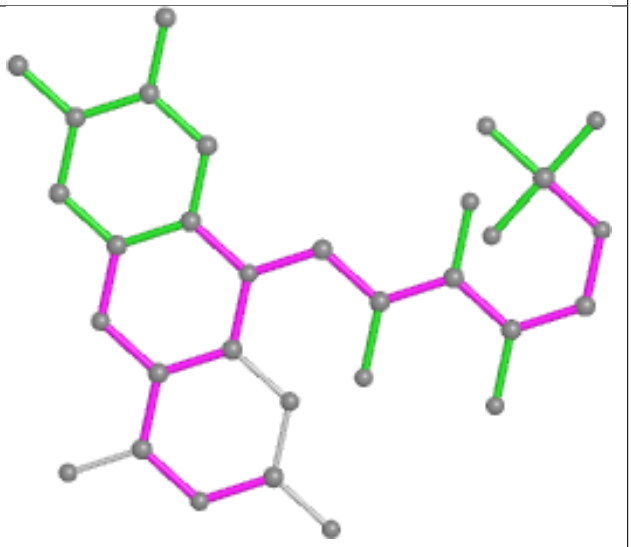


Rings

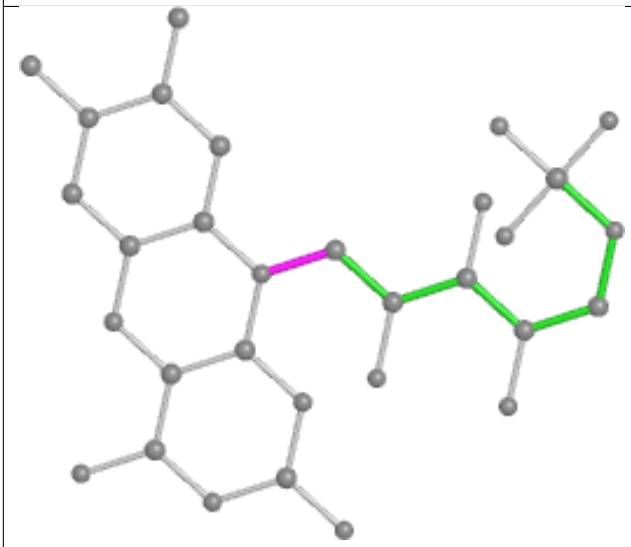
Ligand FMN Z 500



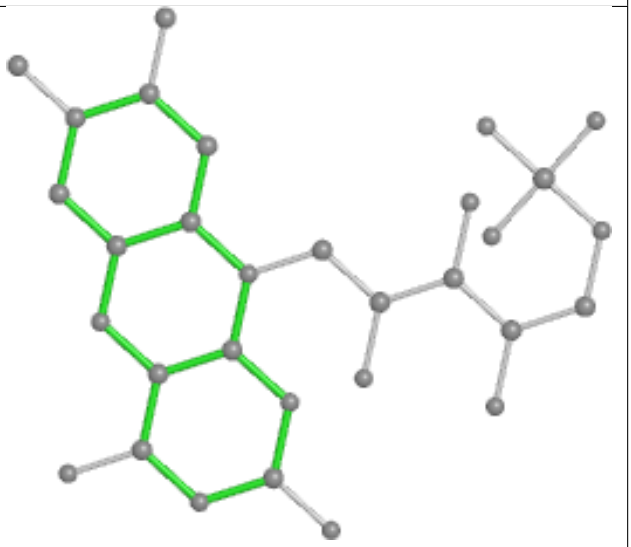
Bond lengths



Bond angles

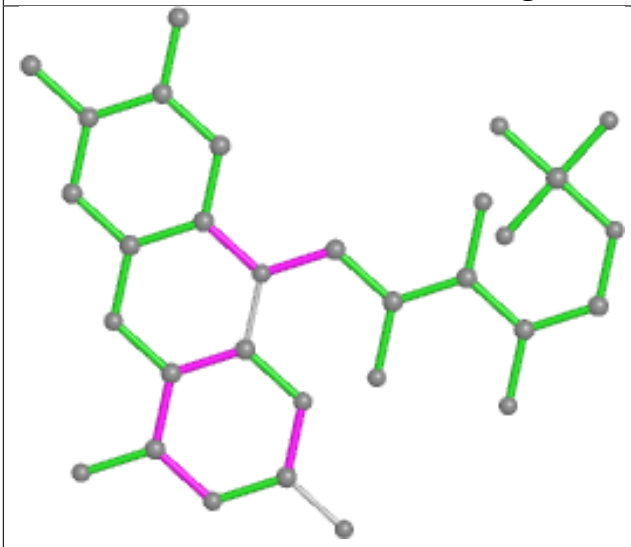


Torsions

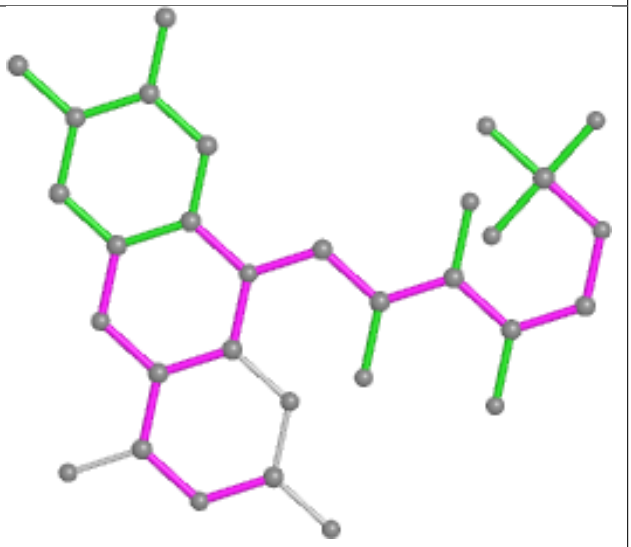


Rings

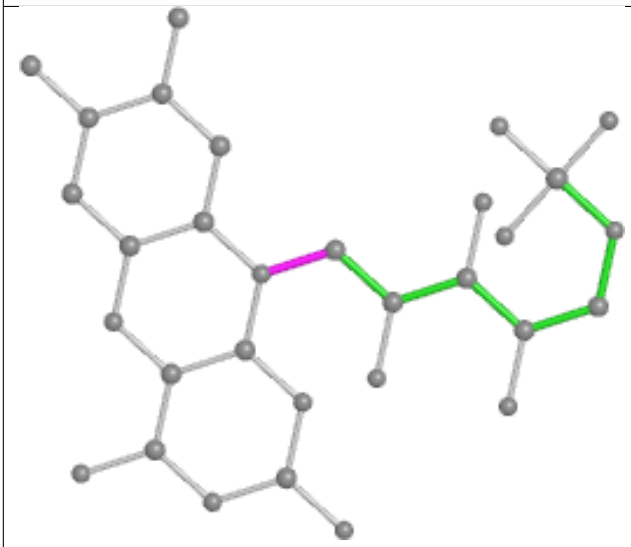
Ligand FMN Q 500



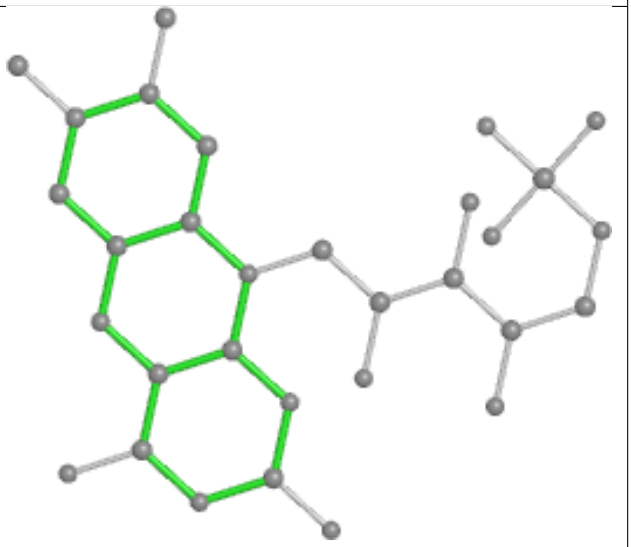
Bond lengths



Bond angles

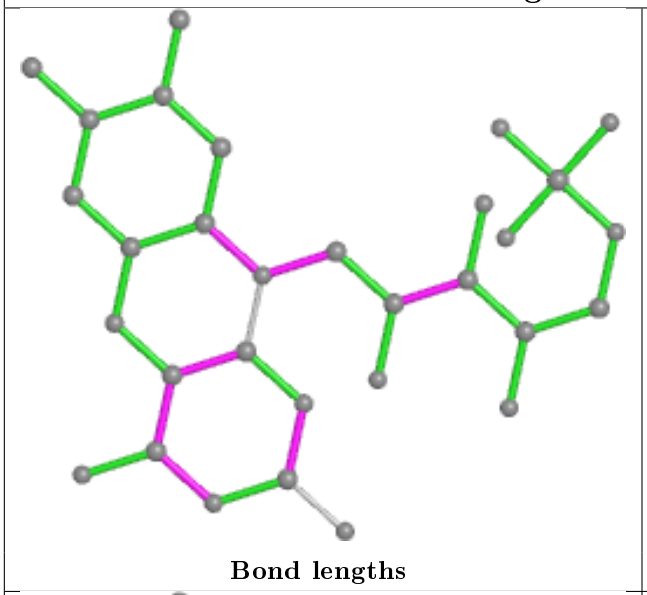


Torsions

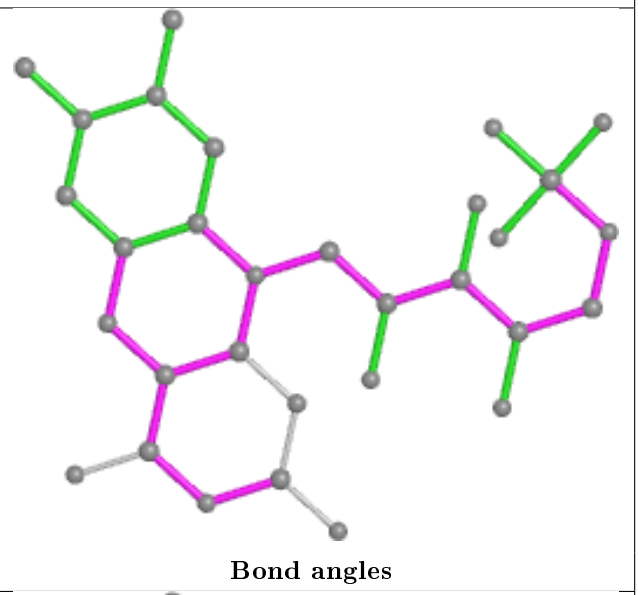


Rings

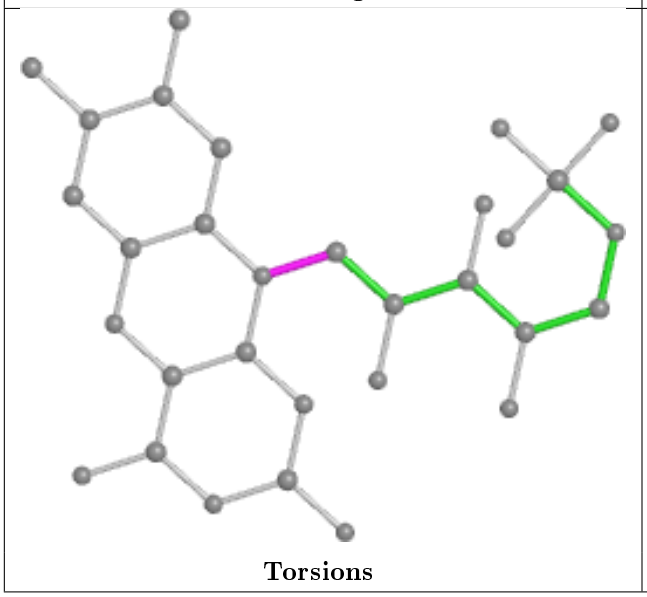
Ligand FMN 7 500



Bond lengths



Bond angles



Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	1	432/438 (98%)	-0.14	0 100 100	14, 52, 90, 114	0
1	A	432/438 (98%)	-0.11	0 100 100	25, 57, 91, 115	0
1	J	432/438 (98%)	-0.13	2 (0%) 91 91	17, 52, 91, 113	0
1	S	432/438 (98%)	-0.16	1 (0%) 95 96	23, 58, 93, 115	0
2	2	178/181 (98%)	-0.15	0 100 100	26, 59, 98, 140	0
2	B	178/181 (98%)	-0.11	0 100 100	29, 64, 100, 141	0
2	K	178/181 (98%)	-0.08	1 (0%) 89 90	29, 60, 97, 143	0
2	T	178/181 (98%)	-0.20	1 (0%) 89 90	32, 66, 100, 146	0
3	3	737/783 (94%)	-0.02	8 (1%) 80 81	20, 65, 110, 130	0
3	C	737/783 (94%)	0.02	10 (1%) 75 75	23, 67, 111, 137	0
3	L	737/783 (94%)	0.10	20 (2%) 54 52	22, 69, 114, 137	0
3	U	737/783 (94%)	-0.00	11 (1%) 73 72	23, 68, 113, 135	0
4	4	370/409 (90%)	-0.00	4 (1%) 80 81	26, 67, 109, 167	0
4	D	370/409 (90%)	0.01	6 (1%) 72 70	26, 65, 109, 165	0
4	M	370/409 (90%)	0.02	5 (1%) 75 75	24, 65, 109, 158	0
4	V	370/409 (90%)	0.16	14 (3%) 40 37	32, 75, 113, 169	0
5	5	191/207 (92%)	-0.03	5 (2%) 56 53	35, 76, 112, 144	0
5	E	191/207 (92%)	0.02	4 (2%) 63 62	36, 76, 117, 138	0
5	N	191/207 (92%)	0.11	6 (3%) 49 48	36, 75, 114, 141	0
5	W	191/207 (92%)	0.15	7 (3%) 41 38	43, 83, 119, 143	0
6	6	144/181 (79%)	-0.05	0 100 100	34, 64, 110, 118	0
6	F	144/181 (79%)	0.01	1 (0%) 87 88	31, 62, 110, 119	0
6	O	144/181 (79%)	-0.01	2 (1%) 75 75	31, 62, 111, 116	0
6	X	144/181 (79%)	0.15	4 (2%) 53 51	45, 71, 113, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
7	9	154/182 (84%)	-0.11	0 100 100	20, 56, 98, 118	0
7	G	154/182 (84%)	-0.11	0 100 100	26, 53, 95, 115	0
7	P	154/182 (84%)	-0.05	1 (0%) 89 90	26, 56, 96, 117	0
7	Y	154/182 (84%)	-0.05	0 100 100	31, 63, 100, 122	0
8	7	127/129 (98%)	-0.13	0 100 100	33, 62, 101, 116	0
8	H	127/129 (98%)	-0.12	0 100 100	35, 62, 102, 119	0
8	Q	127/129 (98%)	-0.01	0 100 100	32, 63, 104, 116	0
8	Z	127/129 (98%)	0.00	3 (2%) 59 56	34, 68, 105, 119	0
All	All	9332/10040 (92%)	-0.02	116 (1%) 79 78	14, 64, 109, 169	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	759	TYR	5.5
5	N	184	TYR	4.6
3	L	653	PRO	4.4
3	L	654	PHE	4.3
5	N	1	MET	4.3
3	C	654	PHE	4.2
3	L	582	PHE	4.2
4	V	245	ASN	4.2
4	V	385	CYS	4.1
5	E	127	GLU	4.0
5	W	127	GLU	3.9
4	V	240	ARG	3.7
3	3	759	TYR	3.6
4	V	208	PHE	3.4
5	E	184	TYR	3.4
3	3	566	ALA	3.4
4	4	257	TYR	3.3
3	C	759	TYR	3.3
3	U	581	ARG	3.2
6	X	122	ALA	3.2
5	W	50	ALA	3.2
3	U	654	PHE	3.1
3	3	552	GLY	3.1
5	W	184	TYR	3.0
5	N	4	GLU	3.0
6	X	121	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	240	ARG	2.9
3	U	759	TYR	2.9
3	L	670	PRO	2.9
4	V	392	ASP	2.8
3	L	142	LYS	2.8
4	M	147	PHE	2.8
4	4	231	ASP	2.8
4	D	41	LEU	2.8
3	U	582	PHE	2.8
3	L	669	VAL	2.8
4	V	251	ALA	2.8
5	W	51	ASP	2.7
5	5	11	ARG	2.7
3	U	338	GLY	2.7
4	V	57	PRO	2.7
3	L	552	GLY	2.7
4	V	136	GLY	2.7
3	L	565	TYR	2.6
6	X	20	LEU	2.6
4	M	245	ASN	2.6
6	O	164	ASN	2.6
3	C	658	LEU	2.6
3	3	341	VAL	2.6
3	3	654	PHE	2.6
7	P	177	THR	2.6
4	D	231	ASP	2.6
3	U	652	PRO	2.6
1	J	14	GLU	2.6
3	L	577	LEU	2.6
5	N	133	ARG	2.5
4	D	257	TYR	2.5
3	C	617	LEU	2.5
4	M	240	ARG	2.5
4	V	215	TYR	2.5
3	C	582	PHE	2.5
3	U	334	LYS	2.5
3	3	762	ALA	2.5
4	M	347	GLU	2.4
2	T	180	GLU	2.4
3	L	540	ASN	2.4
3	L	607	PHE	2.4
6	O	17	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
6	X	155	GLN	2.3
4	V	132	PHE	2.3
3	U	608	TYR	2.3
3	L	175	ILE	2.3
4	4	216	GLU	2.3
8	Z	96	HIS	2.3
4	D	42	ARG	2.3
5	5	145	PRO	2.3
5	W	34	PHE	2.2
3	U	565	TYR	2.2
3	C	686	LYS	2.2
8	Z	128	PHE	2.2
4	D	357	ILE	2.2
8	Z	129	ALA	2.2
4	V	146	PHE	2.2
3	C	758	LEU	2.2
3	U	644	LEU	2.2
1	J	278	GLU	2.2
3	C	520	ARG	2.2
5	E	133	ARG	2.2
3	3	141	GLU	2.2
1	S	438	ARG	2.2
3	L	721	GLU	2.1
3	L	581	ARG	2.1
6	F	49	GLU	2.1
5	5	184	TYR	2.1
5	N	127	GLU	2.1
5	W	1	MET	2.1
5	5	4	GLU	2.1
3	L	617	LEU	2.1
3	3	692	PHE	2.1
5	E	126	PHE	2.1
3	L	568	TYR	2.1
4	4	347	GLU	2.1
5	N	101	LEU	2.1
3	L	668	LYS	2.1
4	V	257	TYR	2.1
2	K	171	LYS	2.0
5	W	15	TYR	2.0
4	V	42	ARG	2.0
3	L	387	LEU	2.0
4	M	144	THR	2.0

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Mol	Chain	Res	Type	RSRZ
3	U	175	ILE	2.0
4	V	298	GLU	2.0
3	C	175	ILE	2.0
5	5	127	GLU	2.0
3	C	337	ARG	2.0
3	L	644	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	FMN	H	500	31/31	0.88	0.29	80,87,88,90	0
11	FMN	Q	500	31/31	0.90	0.29	79,86,88,91	0
11	FMN	Z	500	31/31	0.91	0.32	99,103,105,106	0
11	FMN	7	500	31/31	0.92	0.28	75,80,83,87	0
9	SF4	Y	183	8/8	0.98	0.19	20,27,29,44	0
9	SF4	X	182	8/8	0.98	0.17	21,42,47,61	0
9	SF4	3	784	8/8	0.99	0.18	1,12,15,16	0
9	SF4	U	784	8/8	0.99	0.17	1,17,19,19	0
10	FES	3	787	4/4	0.99	0.14	1,1,12,15	0
9	SF4	G	183	8/8	0.99	0.18	1,23,24,25	0
9	SF4	3	785	8/8	0.99	0.20	1,17,21,21	0
9	SF4	Y	184	8/8	0.99	0.17	7,20,22,22	0
9	SF4	G	184	8/8	0.99	0.17	1,16,19,21	0
9	SF4	U	786	8/8	0.99	0.19	19,40,45,45	0
9	SF4	C	785	8/8	0.99	0.19	1,16,17,18	0
9	SF4	O	182	8/8	0.99	0.17	4,14,18,18	0
9	SF4	J	439	8/8	0.99	0.19	1,8,14,18	0

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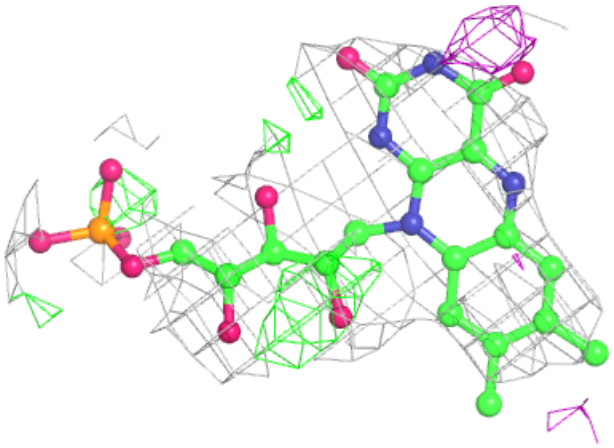
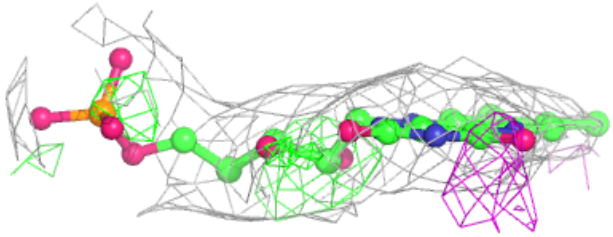
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SF4	C	786	8/8	0.99	0.19	12,31,36,38	0
10	FES	L	787	4/4	0.99	0.14	1,1,9,14	0
10	FES	C	787	4/4	0.99	0.12	1,4,16,18	0
9	SF4	S	439	8/8	0.99	0.19	14,30,33,34	0
9	SF4	P	183	8/8	0.99	0.19	1,25,26,32	0
10	FES	2	182	4/4	0.99	0.13	1,4,19,19	0
10	FES	T	182	4/4	0.99	0.11	2,9,29,30	0
9	SF4	9	183	8/8	0.99	0.18	1,17,18,29	0
9	SF4	A	439	8/8	0.99	0.17	1,17,22,24	0
9	SF4	9	184	8/8	0.99	0.18	1,15,24,25	0
9	SF4	L	785	8/8	0.99	0.20	1,13,15,16	0
9	SF4	F	182	8/8	0.99	0.17	1,16,16,17	0
9	SF4	P	184	8/8	0.99	0.20	3,18,20,20	0
9	SF4	1	439	8/8	0.99	0.18	1,9,17,17	0
9	SF4	C	784	8/8	0.99	0.18	1,10,19,20	0
9	SF4	U	785	8/8	0.99	0.19	9,18,20,21	0
10	FES	U	787	4/4	0.99	0.12	4,5,15,17	0
9	SF4	L	786	8/8	0.99	0.15	17,28,31,35	0
9	SF4	6	182	8/8	0.99	0.18	12,32,33,34	0
9	SF4	3	786	8/8	0.99	0.18	5,31,32,34	0
10	FES	B	182	4/4	1.00	0.13	2,13,32,33	0
10	FES	K	182	4/4	1.00	0.12	2,5,21,23	0
9	SF4	L	784	8/8	1.00	0.18	1,8,15,17	0

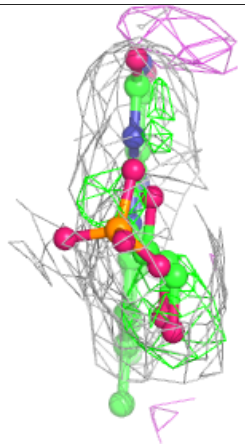
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FMN H 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

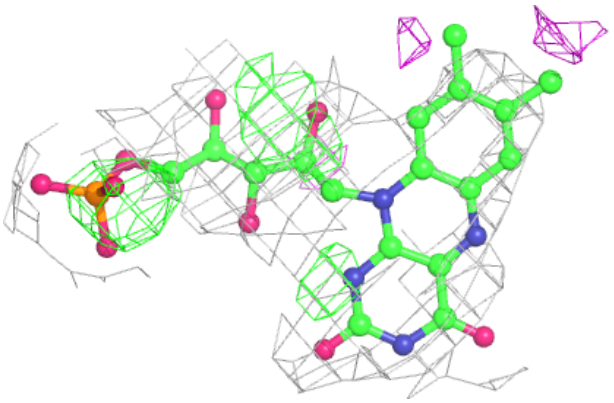


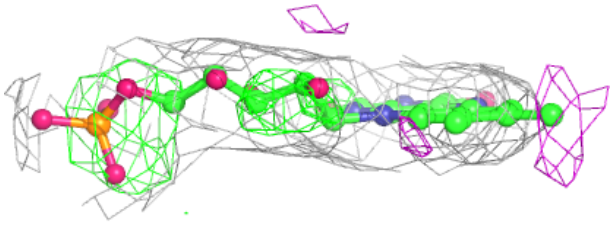


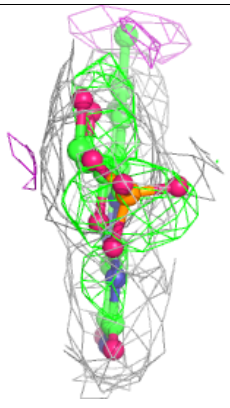


Electron density around FMN Q 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

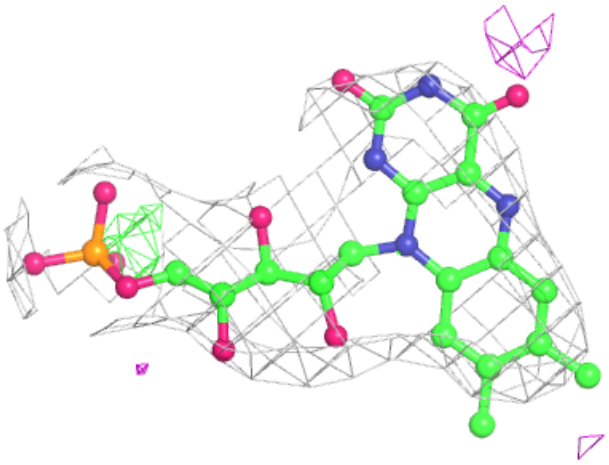


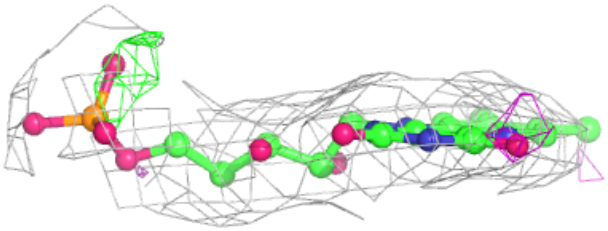


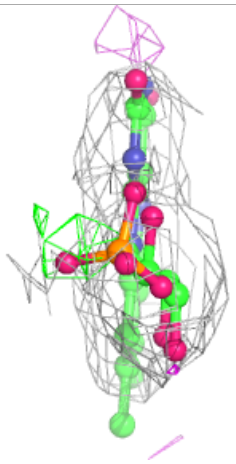


Electron density around FMN Z 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

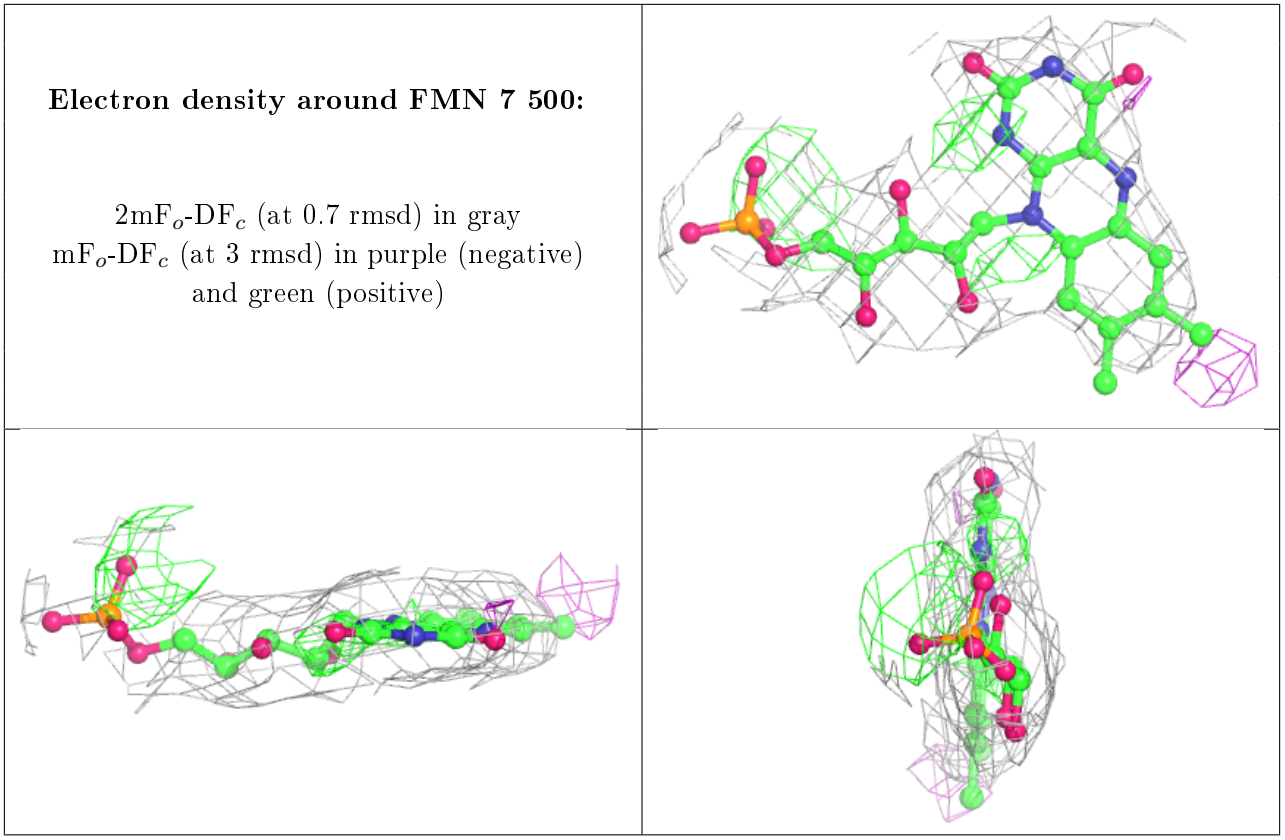






Electron density around FMN 7 500:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.