



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 07:19 PM UTC

PDB ID : 3OAA / pdb_00003oaa
Title : Structure of the E.coli F1-ATP synthase inhibited by subunit Epsilon
Authors : Cingolani, G.; Duncan, T.M.
Deposited on : 2010-08-05
Resolution : 3.26 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 types of validation reports are described at

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

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

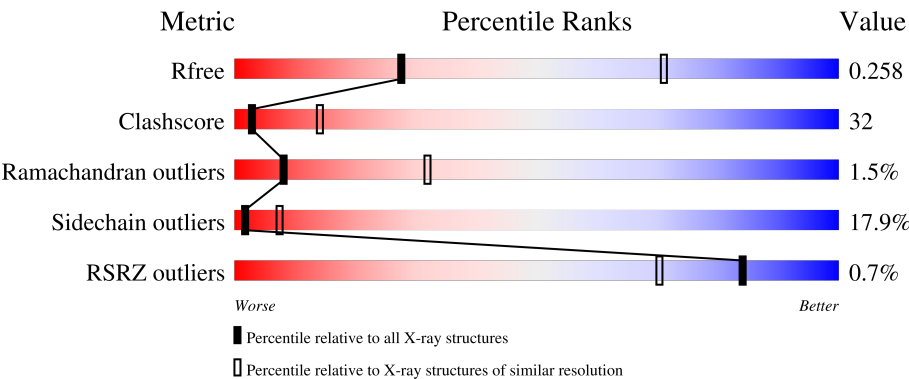
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.26 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.



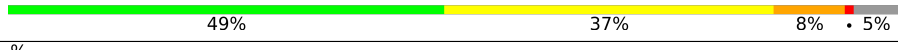
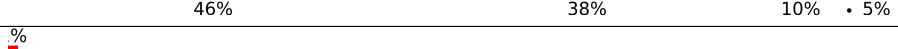
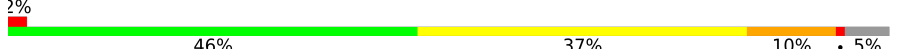
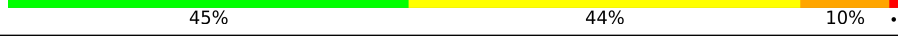
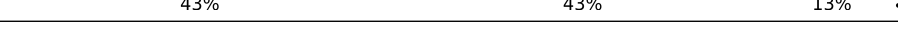
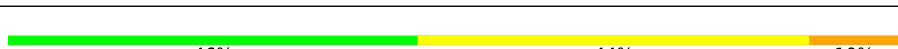
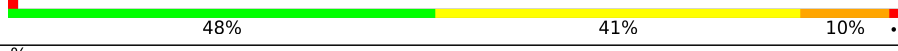
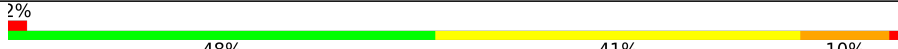
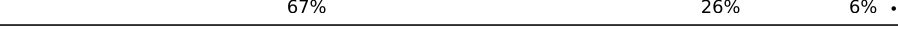
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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 of 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 $\leq 5\%$. 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	A	513	47%38%9%• 5%
1	B	513	% 46%38%10%5%
1	C	513	43%41%10%• 5%
1	I	513	% 46%39%9%• 5%
1	J	513	% 46%38%10%5%

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Mol	Chain	Length	Quality of chain
1	K	513	% 
1	Q	513	
1	R	513	% 
1	S	513	% 
1	Y	513	
1	Z	513	2% 
1	a	513	% 
2	D	459	
2	E	459	
2	F	459	
2	L	459	
2	M	459	
2	N	459	% 
2	T	459	% 
2	U	459	% 
2	V	459	2% 
2	b	459	2% 
2	c	459	
2	d	459	% 
3	G	286	
3	O	286	
3	W	286	
3	e	286	
4	H	138	
4	P	138	

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Mol	Chain	Length	Quality of chain
4	X	138	66%28%6%
4	f	138	% 64%28%7%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 99573 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 ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	B	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	C	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			
1	I	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	J	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	K	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			
1	Q	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	R	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	S	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			
1	Y	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	Z	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	a	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	E	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	L	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	M	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	N	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	T	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	U	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	V	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	b	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	c	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	d	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	81	GLU	LYS	engineered mutation	UNP C9QXA4
E	81	GLU	LYS	engineered mutation	UNP C9QXA4
F	81	GLU	LYS	engineered mutation	UNP C9QXA4
L	81	GLU	LYS	engineered mutation	UNP C9QXA4
M	81	GLU	LYS	engineered mutation	UNP C9QXA4
N	81	GLU	LYS	engineered mutation	UNP C9QXA4
T	81	GLU	LYS	engineered mutation	UNP C9QXA4
U	81	GLU	LYS	engineered mutation	UNP C9QXA4
V	81	GLU	LYS	engineered mutation	UNP C9QXA4
b	81	GLU	LYS	engineered mutation	UNP C9QXA4
c	81	GLU	LYS	engineered mutation	UNP C9QXA4
d	81	GLU	LYS	engineered mutation	UNP C9QXA4

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			

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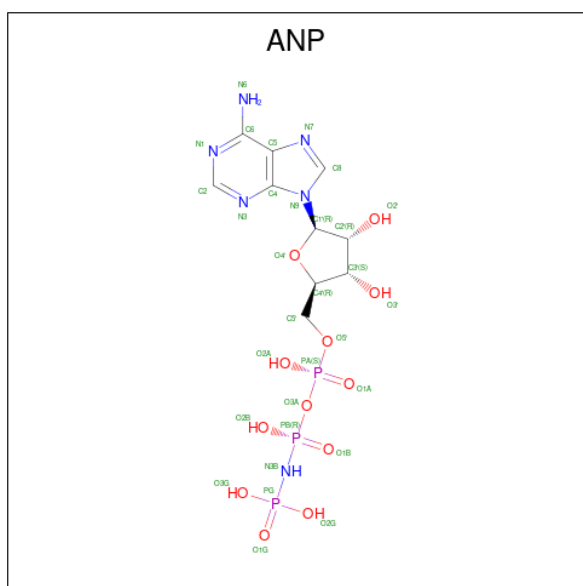
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			
3	W	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			
3	e	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	P	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	X	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	f	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	Q	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	R	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	S	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	Y	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	Z	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	a	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

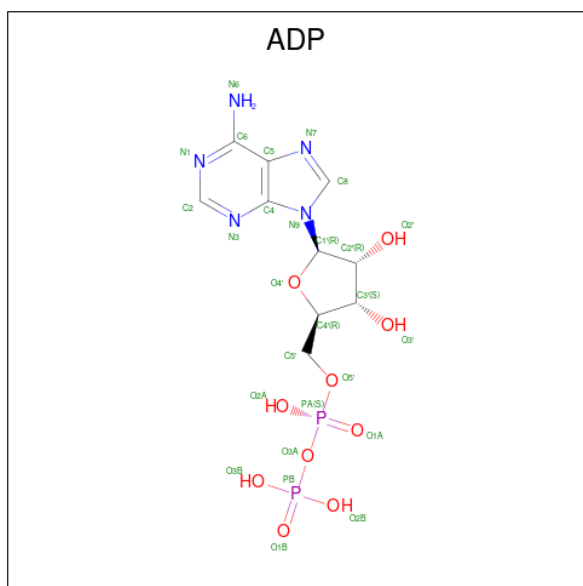
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		
6	K	1	Total	Mg	0	0
			1	1		
6	L	1	Total	Mg	0	0
			1	1		
6	Q	1	Total	Mg	0	0
			1	1		

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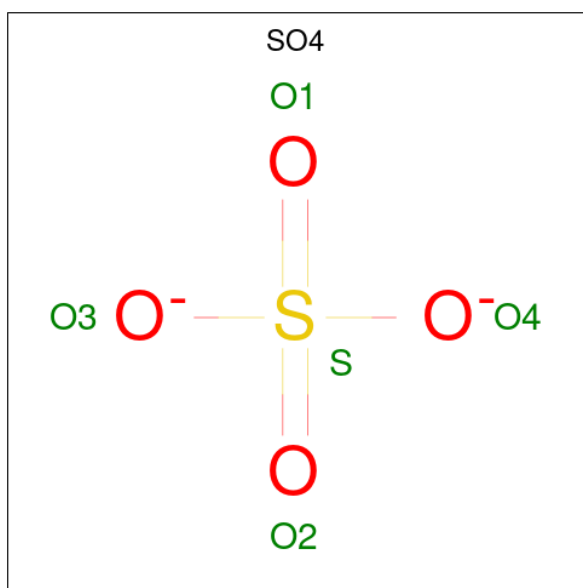
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	R	1	Total	Mg	0	0
			1	1		
6	S	1	Total	Mg	0	0
			1	1		
6	T	1	Total	Mg	0	0
			1	1		
6	Y	1	Total	Mg	0	0
			1	1		
6	Z	1	Total	Mg	0	0
			1	1		
6	a	1	Total	Mg	0	0
			1	1		
6	b	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	T	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	b	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		
8	G	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	N	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		
8	P	1	Total	O	S	0	0
			5	4	1		
8	T	1	Total	O	S	0	0
			5	4	1		
8	U	1	Total	O	S	0	0
			5	4	1		
8	V	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	W	1	Total	O	S	0	0
			5	4	1		
8	b	1	Total	O	S	0	0
			5	4	1		
8	c	1	Total	O	S	0	0
			5	4	1		
8	d	1	Total	O	S	0	0
			5	4	1		

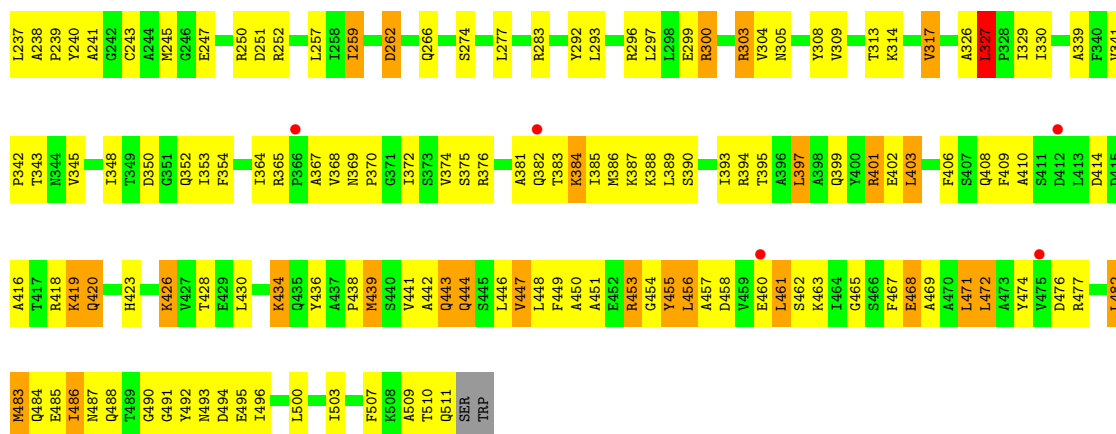
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	O	0	0
			3	3		
9	B	2	Total	O	0	0
			2	2		
9	C	2	Total	O	0	0
			2	2		
9	D	8	Total	O	0	0
			8	8		
9	E	1	Total	O	0	0
			1	1		
9	F	5	Total	O	0	0
			5	5		
9	G	10	Total	O	0	0
			10	10		
9	H	4	Total	O	0	0
			4	4		
9	J	3	Total	O	0	0
			3	3		
9	L	6	Total	O	0	0
			6	6		
9	N	3	Total	O	0	0
			3	3		
9	O	5	Total	O	0	0
			5	5		
9	P	2	Total	O	0	0
			2	2		
9	Q	1	Total	O	0	0
			1	1		
9	R	1	Total	O	0	0
			1	1		

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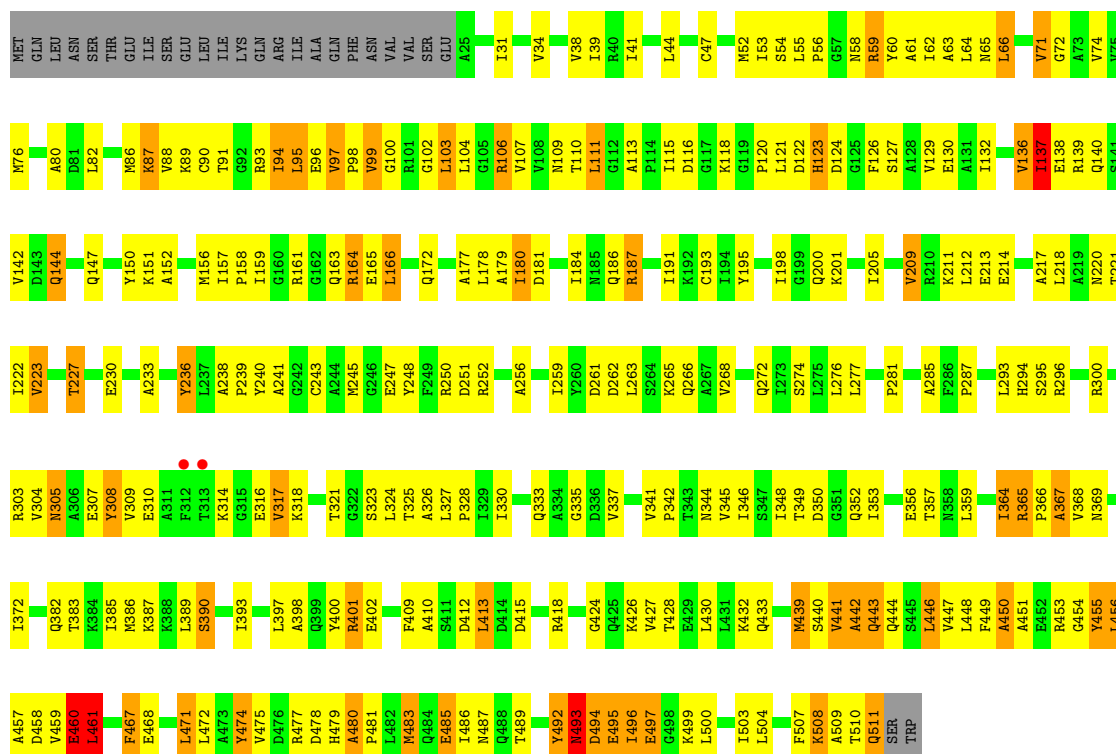
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	S	1	Total 1	O 1	0	0
9	V	2	Total 2	O 2	0	0
9	X	1	Total 1	O 1	0	0
9	a	1	Total 1	O 1	0	0
9	b	1	Total 1	O 1	0	0
9	d	2	Total 2	O 2	0	0



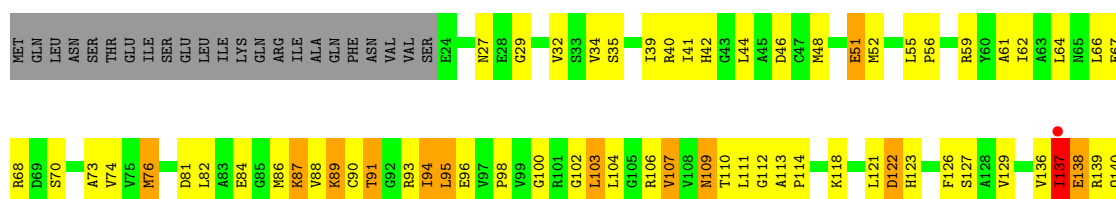
• Molecule 1: ATP synthase subunit alpha

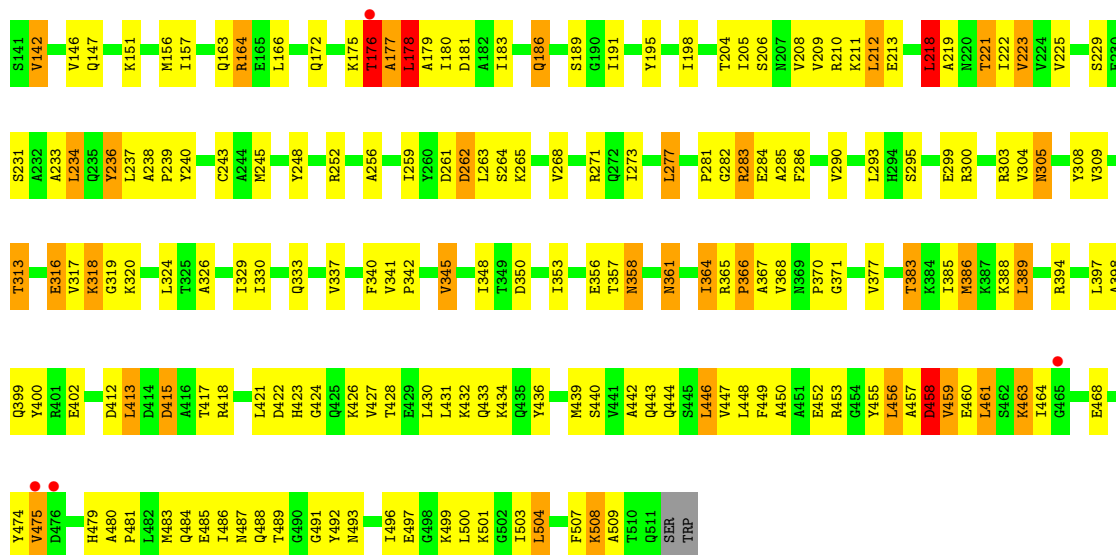
Chain C: 43% 41% 10% 5%



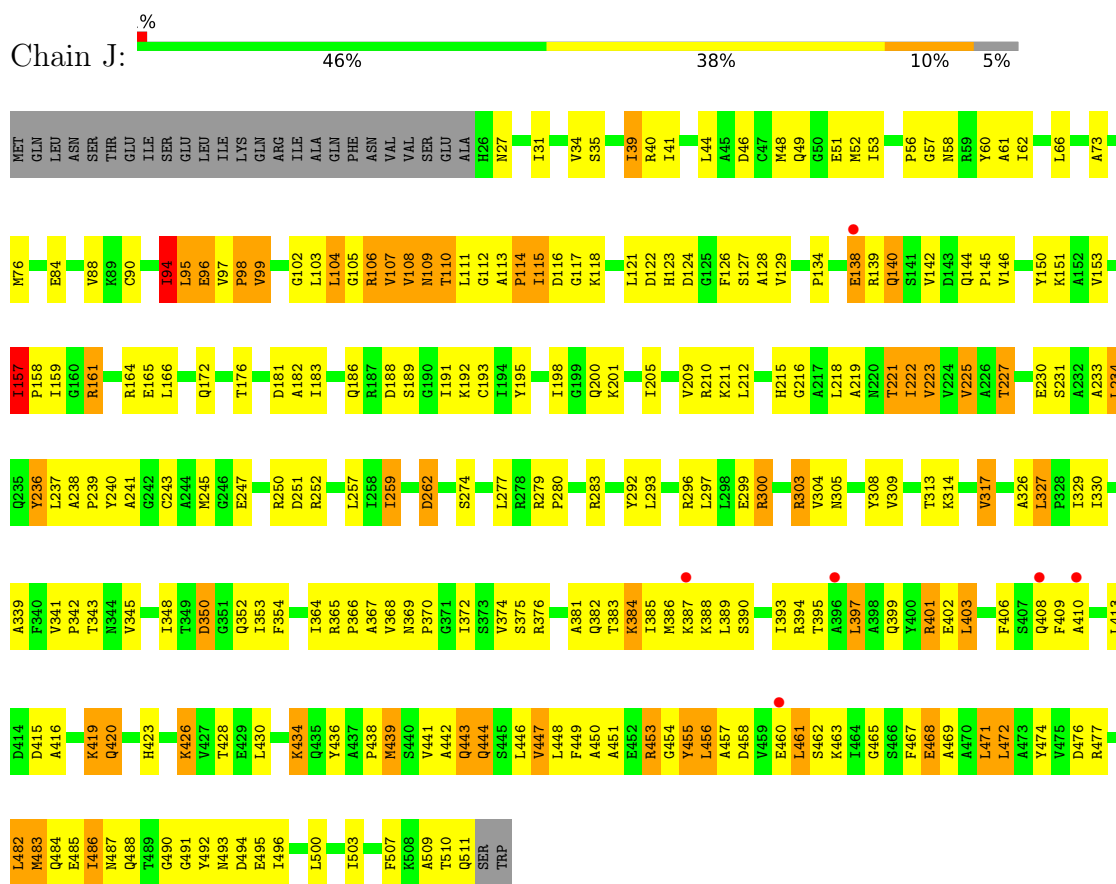
• Molecule 1: ATP synthase subunit alpha

Chain I: 46% 39% 9% 5%

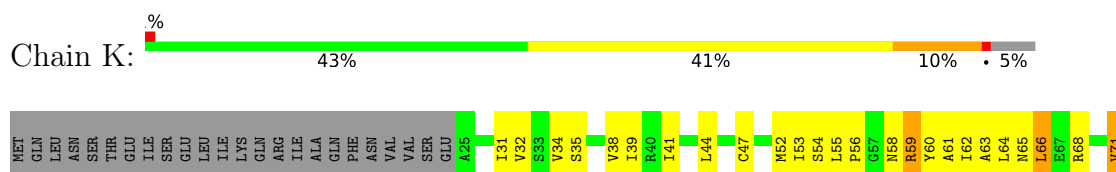


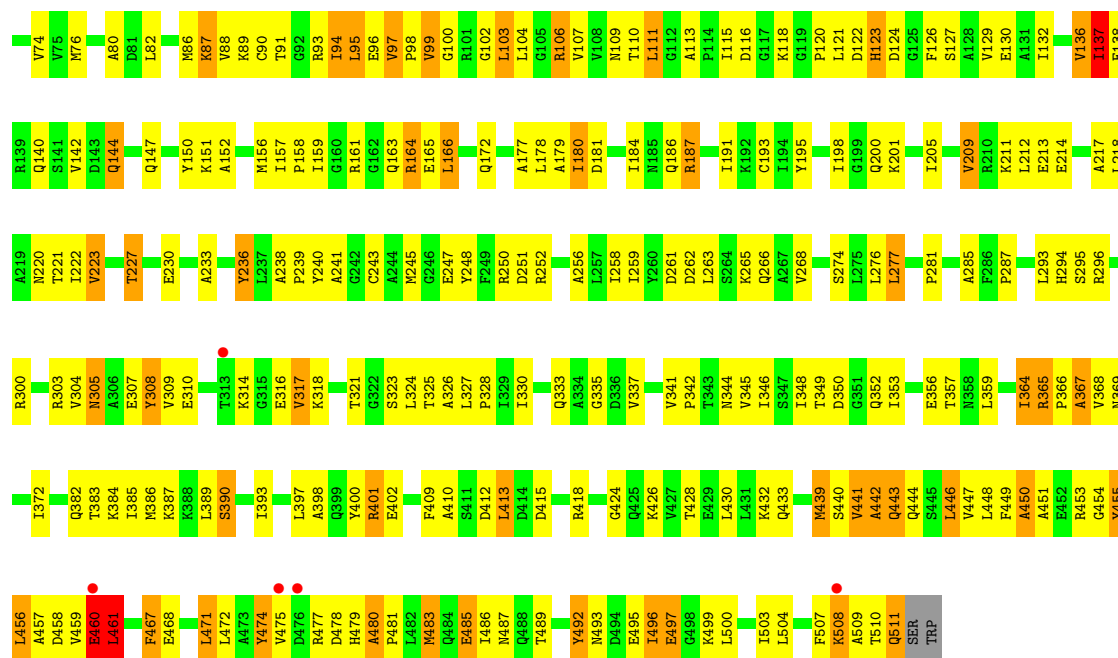


• Molecule 1: ATP synthase subunit alpha



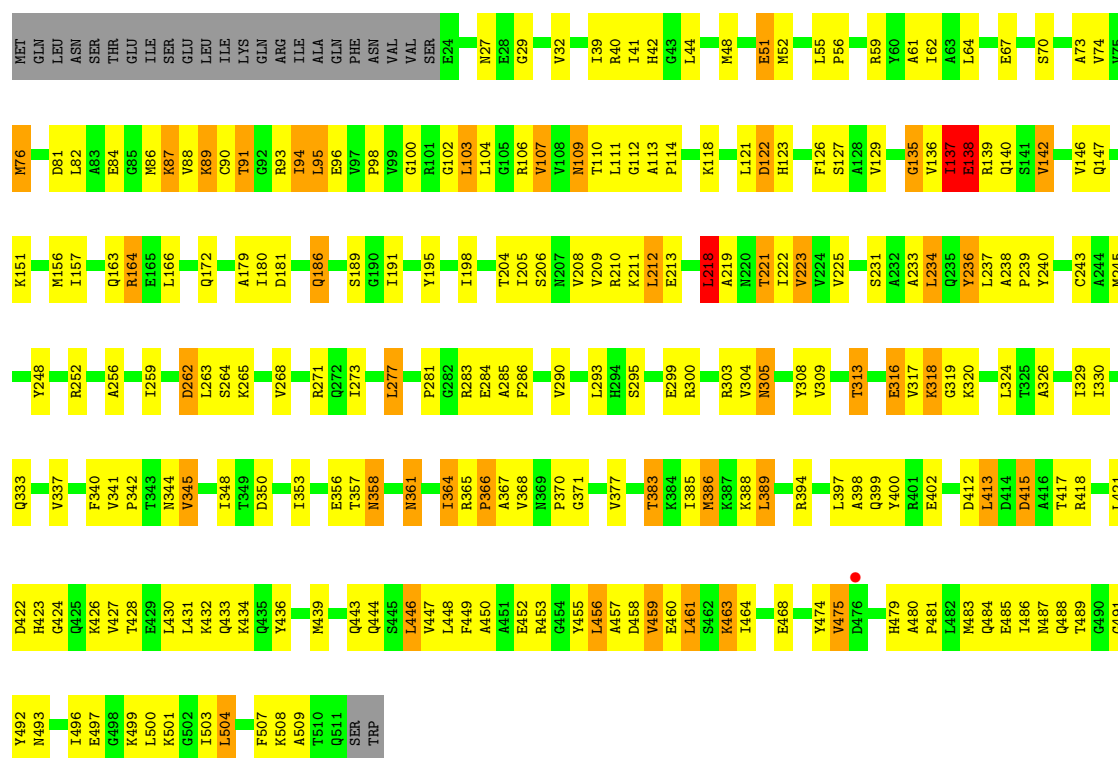
• Molecule 1: ATP synthase subunit alpha





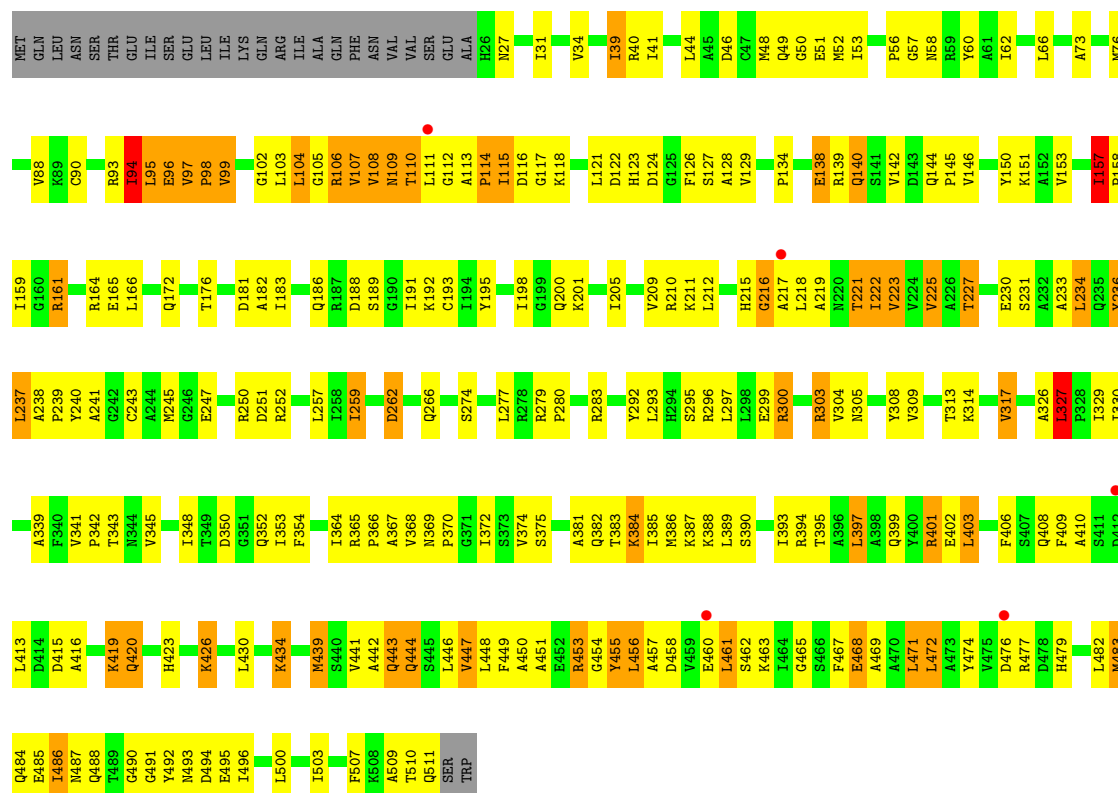
• Molecule 1: ATP synthase subunit alpha

Chain Q: 49% 37% 8% • 5%

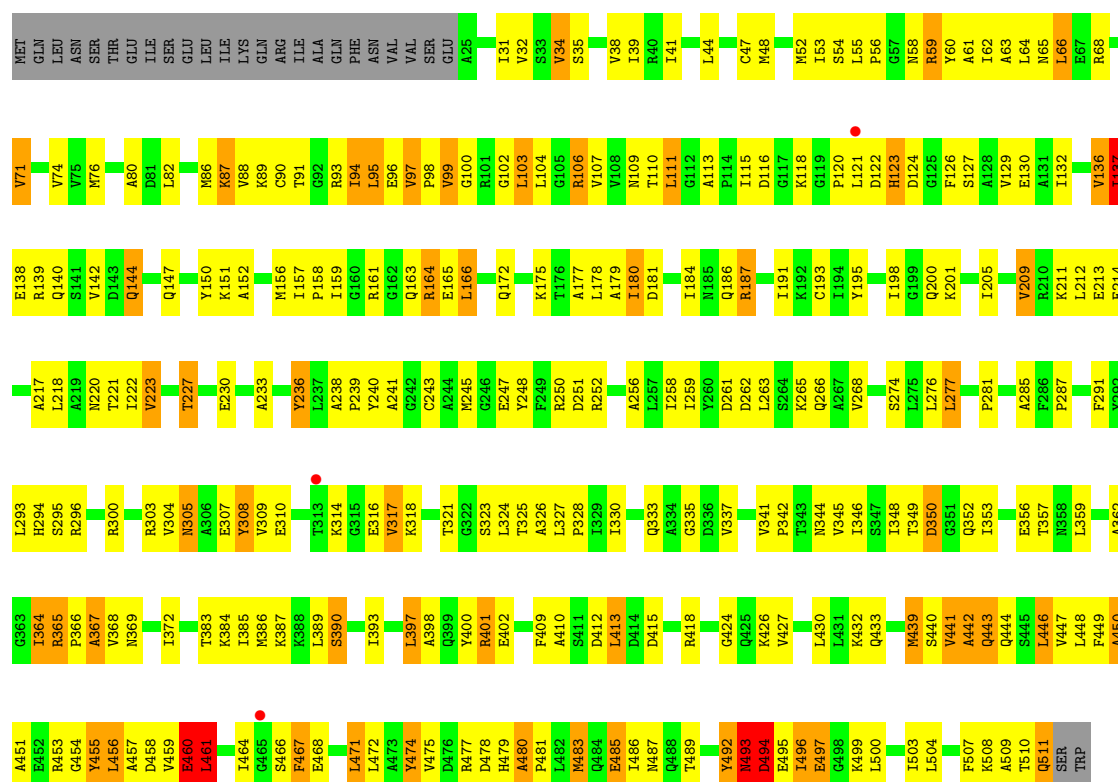
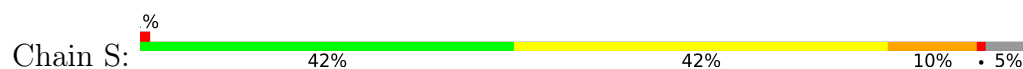


• Molecule 1: ATP synthase subunit alpha

Chain R: 46% 38% 10% • 5%

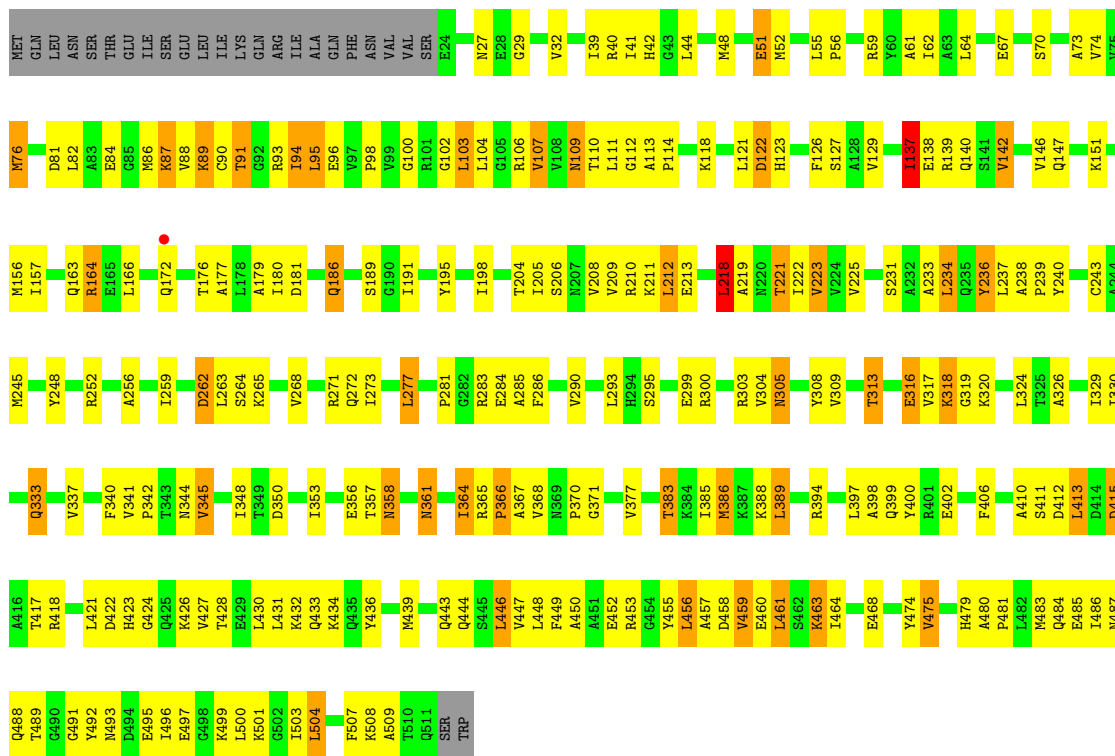


• Molecule 1: ATP synthase subunit alpha

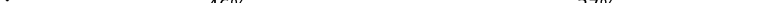


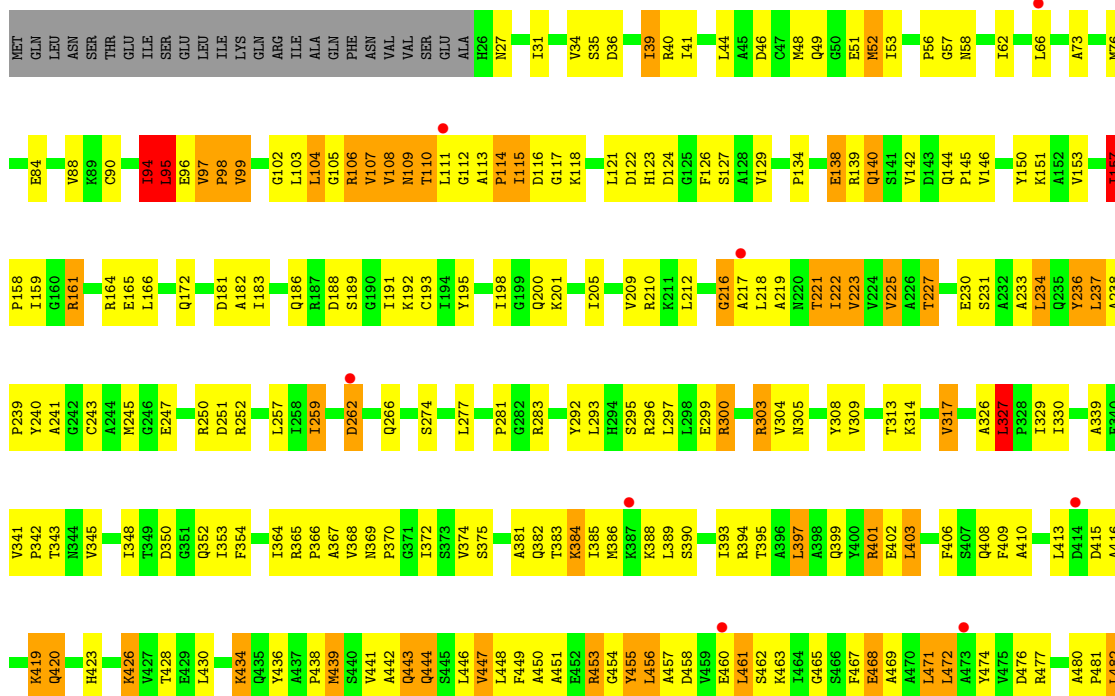
- Molecule 1: ATP synthase subunit alpha

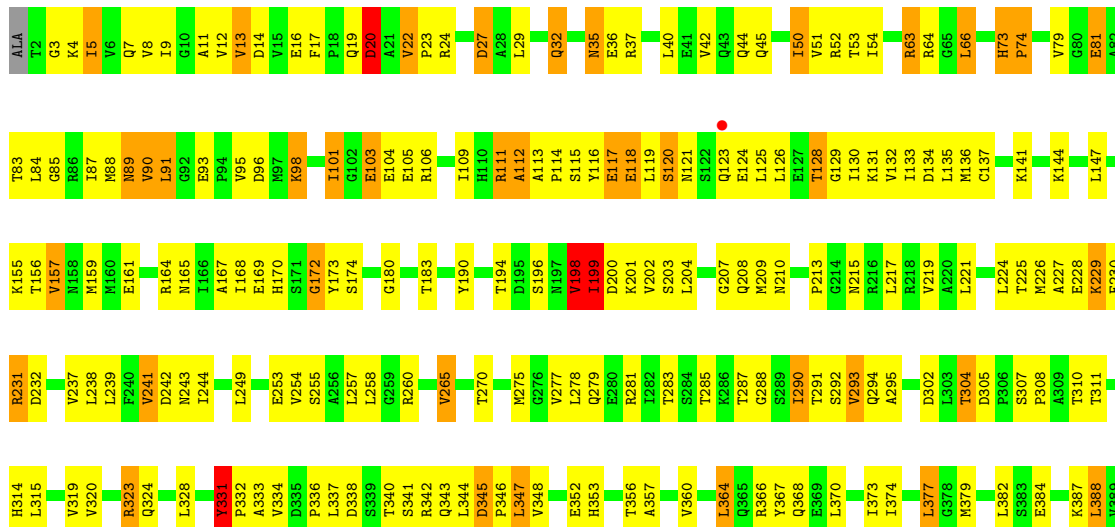
Chain Y: 48% 38% 8% 5%

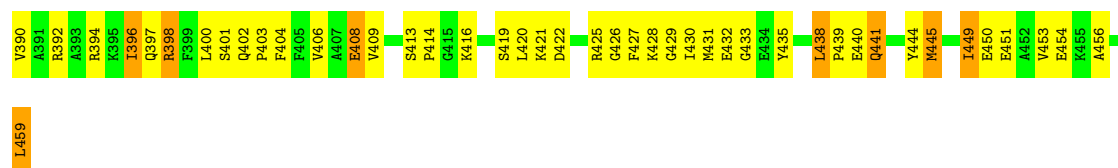


- Molecule 1: ATP synthase subunit alpha

Chain Z: 

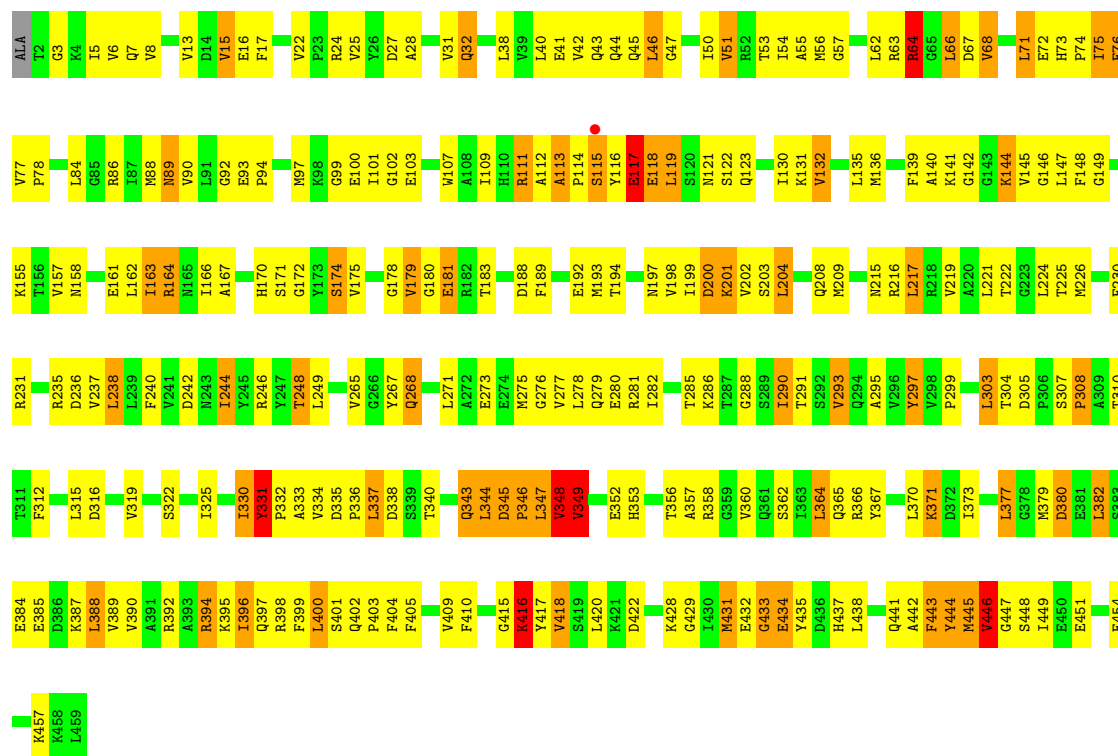






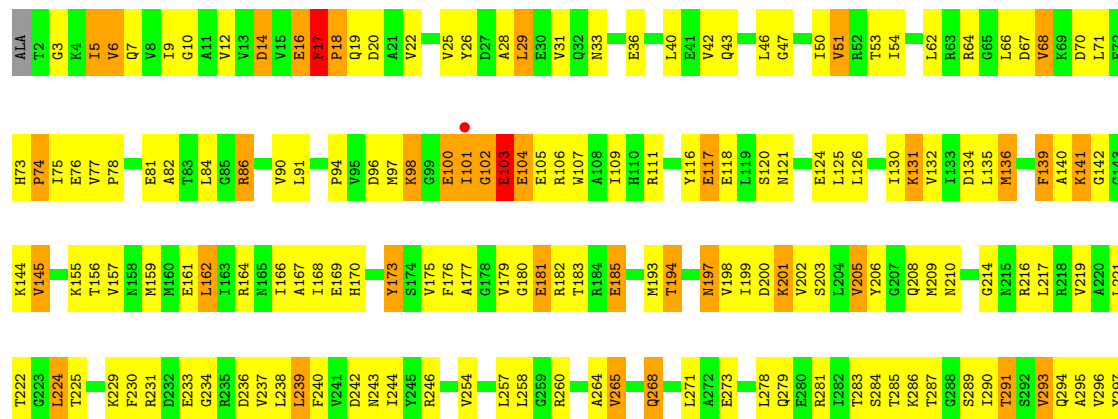
• Molecule 2: ATP synthase subunit beta

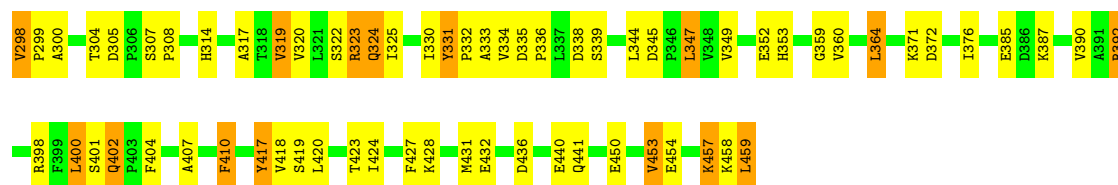
Chain E: 43% 43% 13%



• Molecule 2: ATP synthase subunit beta

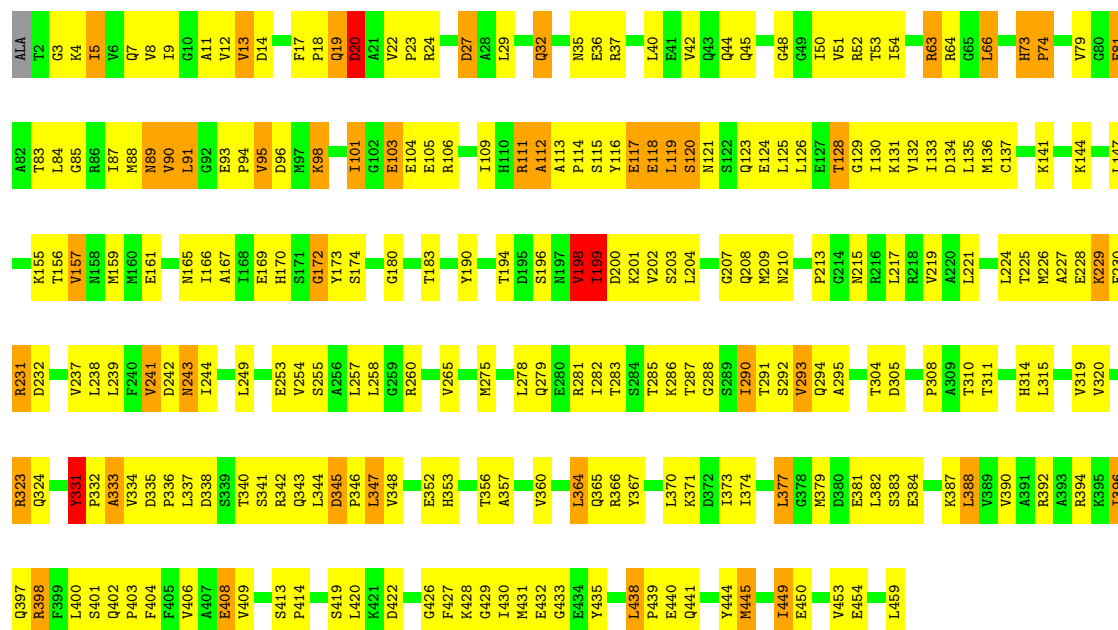
Chain F: 49% 39% 11%





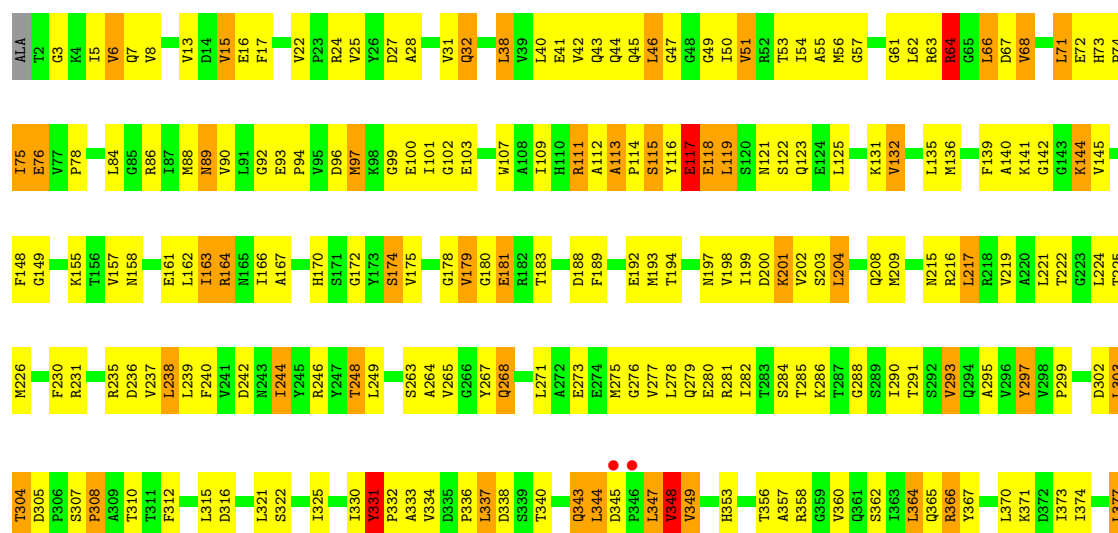
• Molecule 2: ATP synthase subunit beta

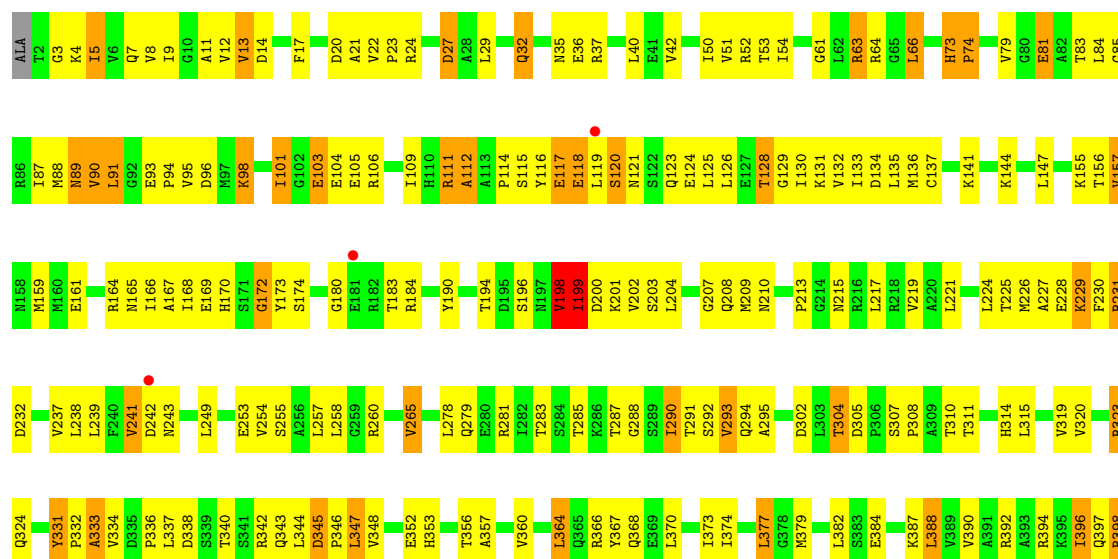
Chain L: 46% 44% 10%

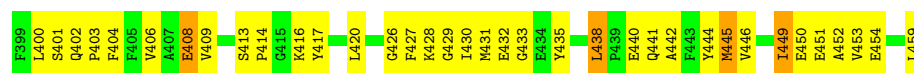


• Molecule 2: ATP synthase subunit beta

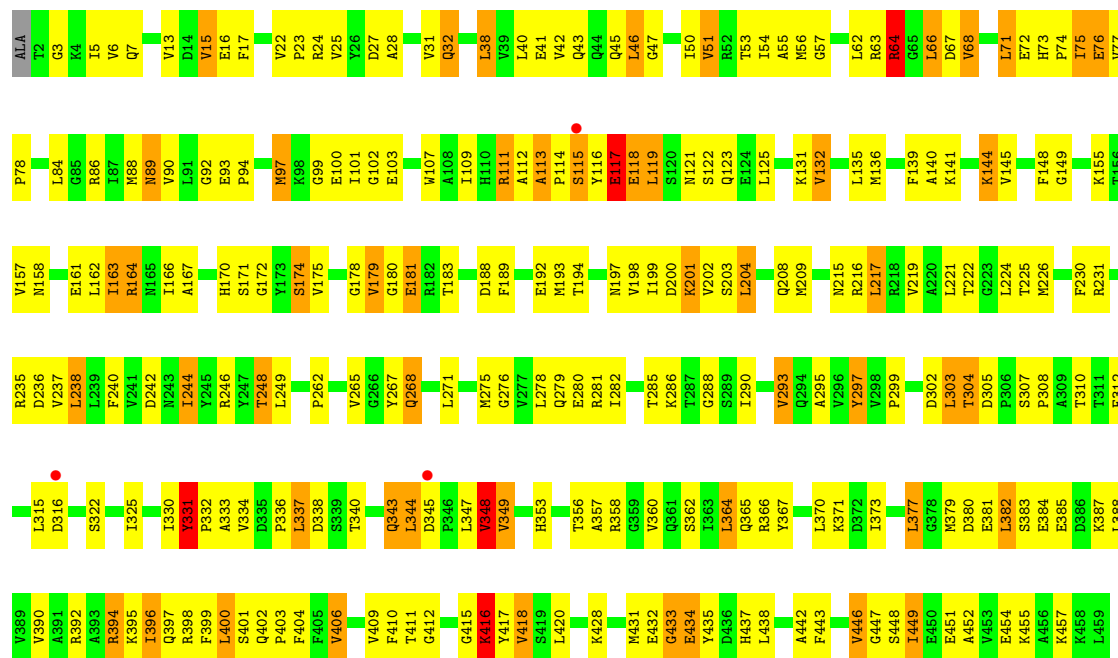
Chain M: 43% 44% 12%



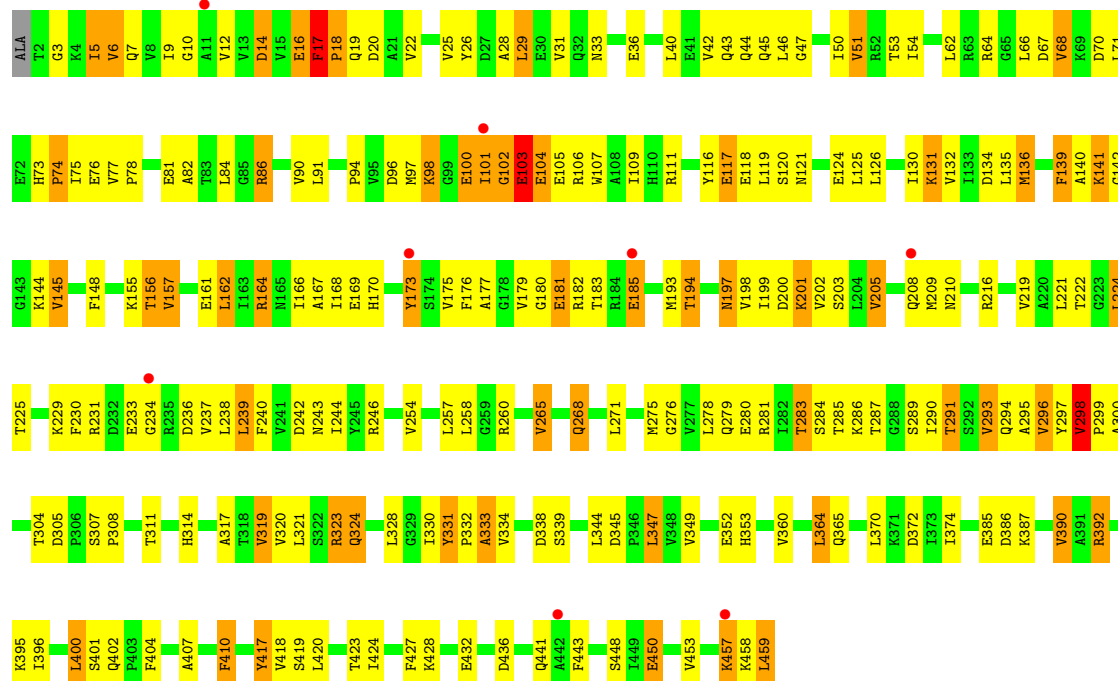




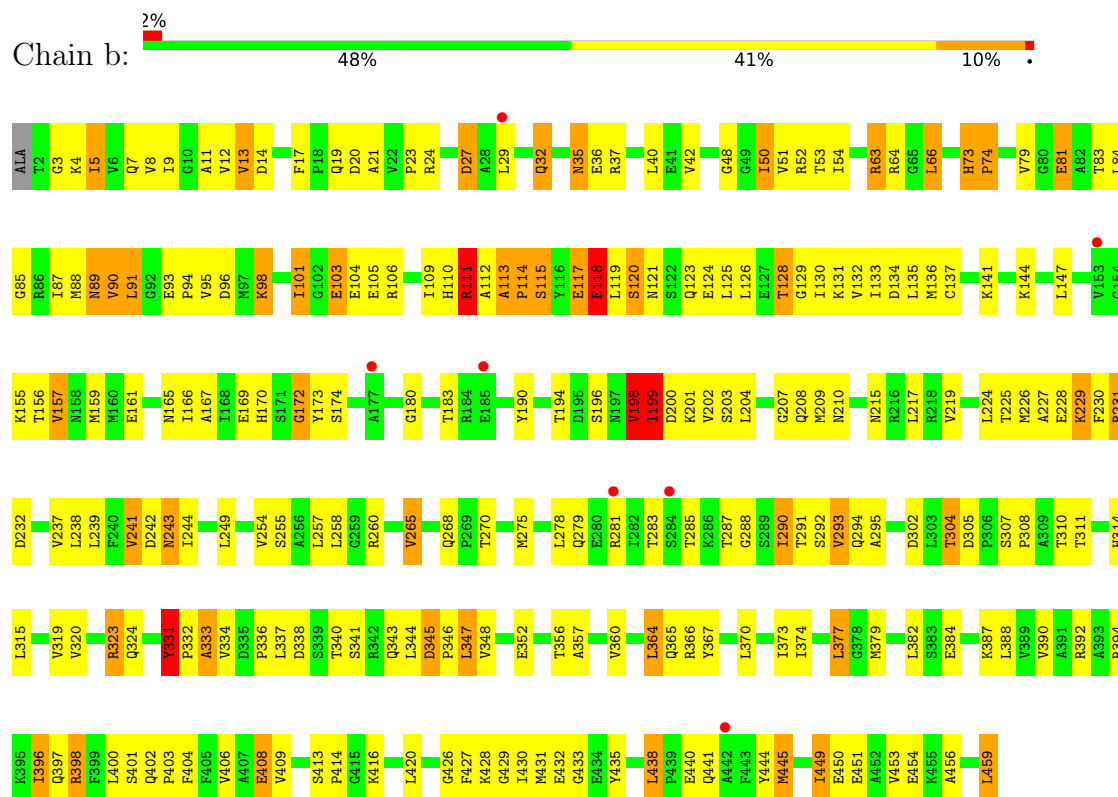
• Molecule 2: ATP synthase subunit beta



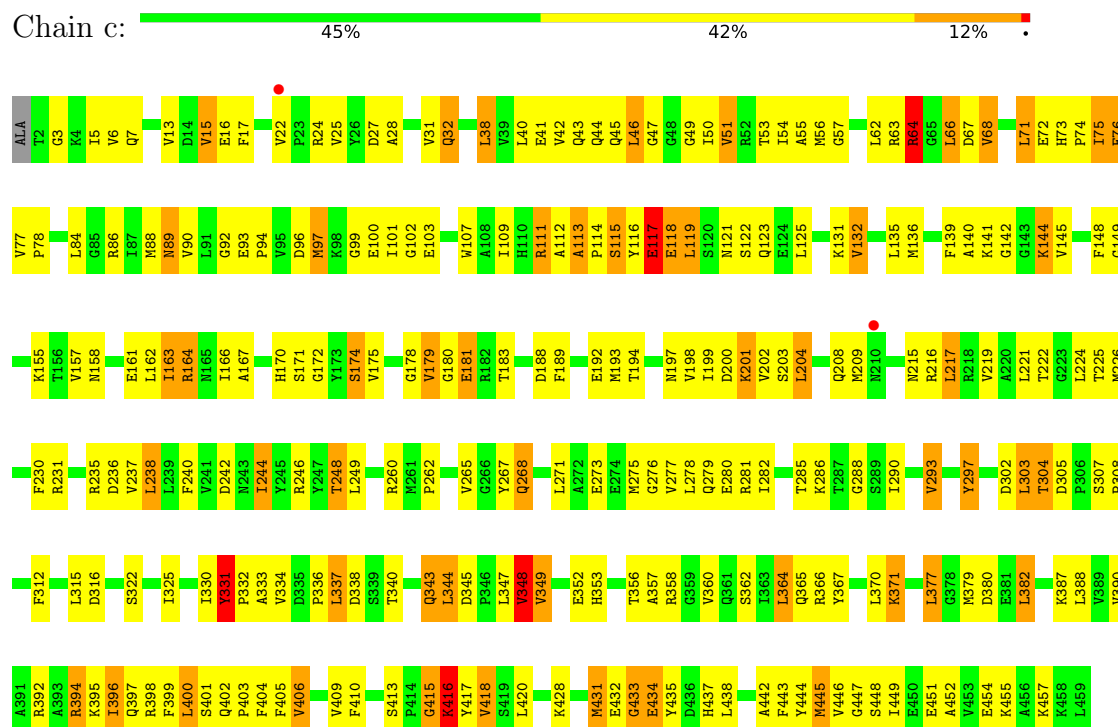
• Molecule 2: ATP synthase subunit beta



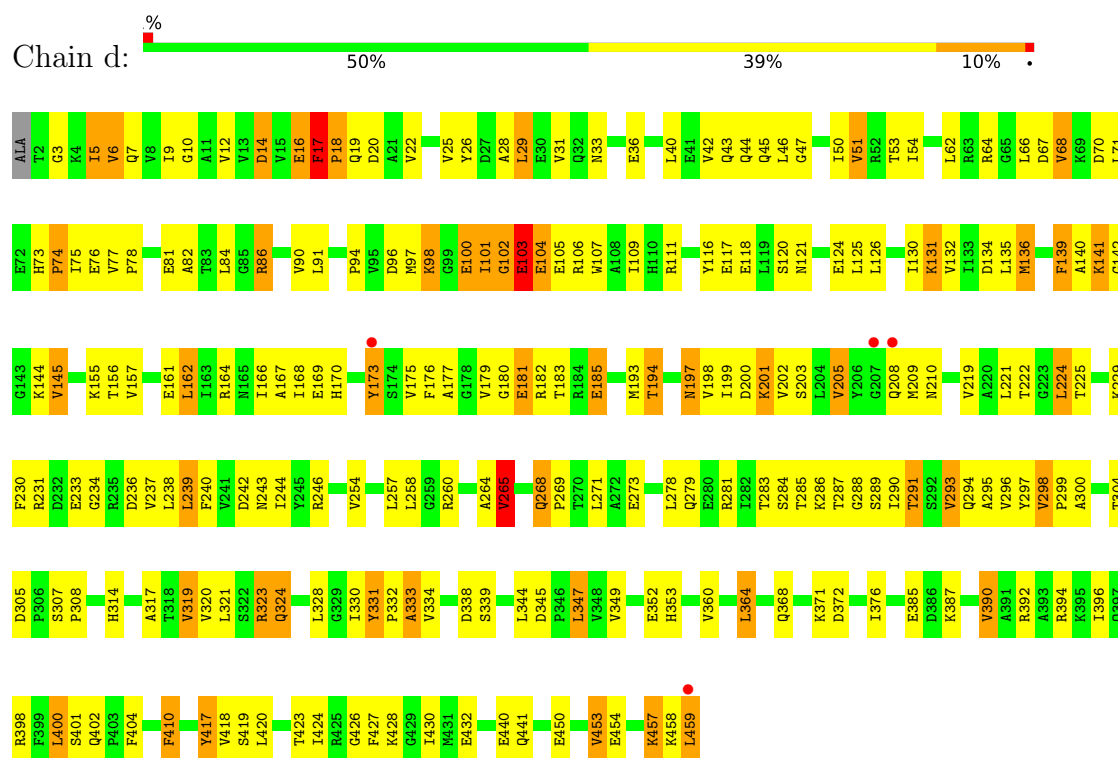
- Molecule 2: ATP synthase subunit beta



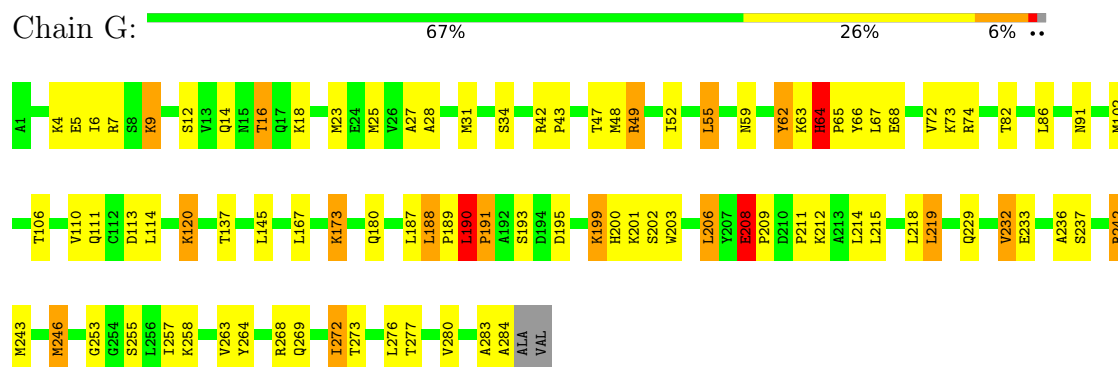
- Molecule 2: ATP synthase subunit beta



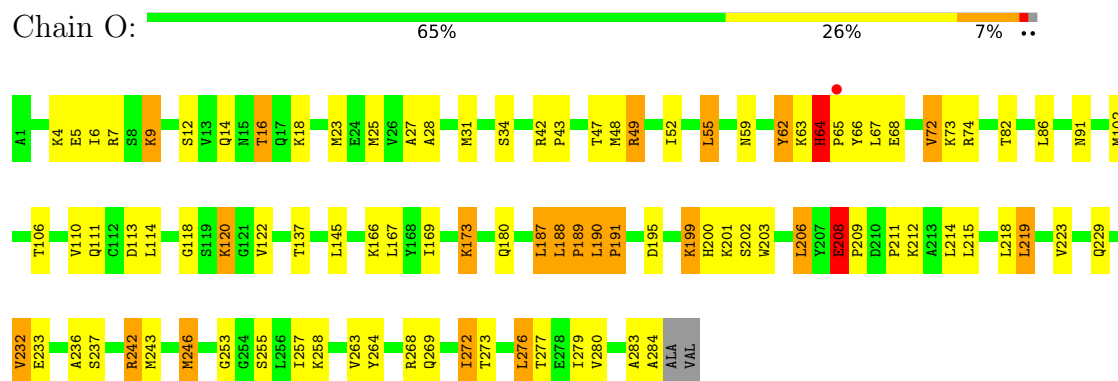
- Molecule 2: ATP synthase subunit beta



• Molecule 3: ATP synthase gamma chain

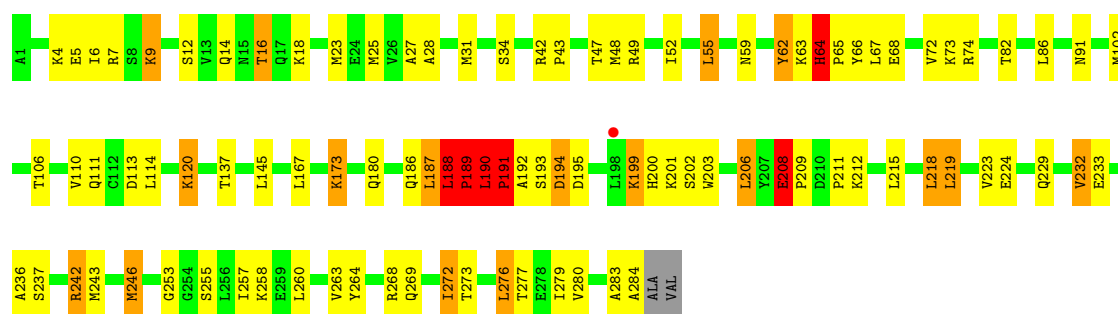


• Molecule 3: ATP synthase gamma chain



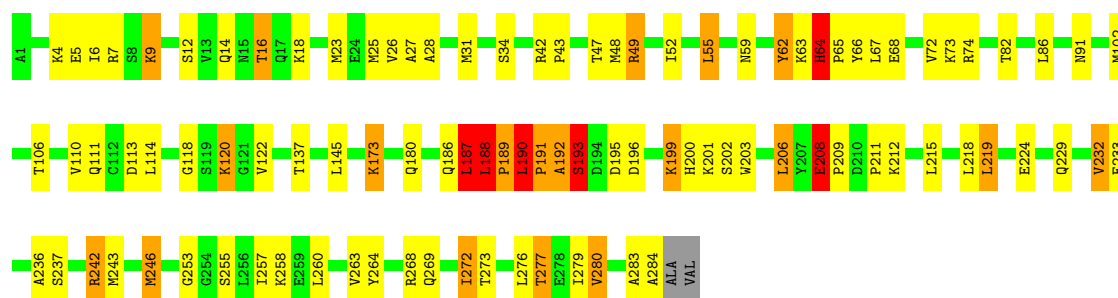
• Molecule 3: ATP synthase gamma chain

Chain W:  65% 26% 6% ..



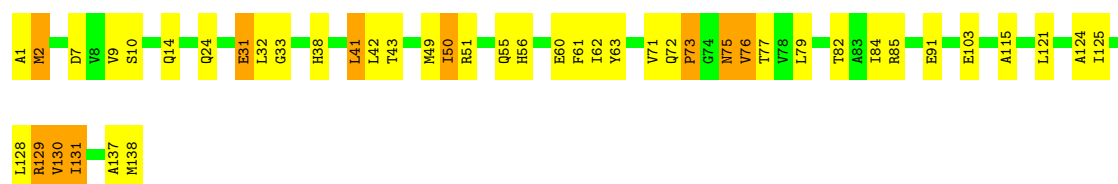
• Molecule 3: ATP synthase gamma chain

Chain e:  65% 26% 7% ..



• Molecule 4: ATP synthase epsilon chain

Chain H:  67% 25% 7%



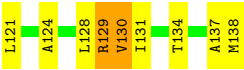
• Molecule 4: ATP synthase epsilon chain

Chain P:  67% 27% 7%

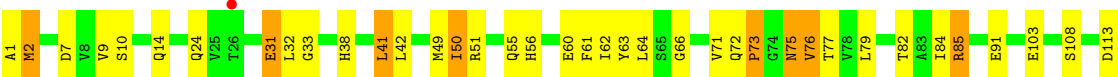


• Molecule 4: ATP synthase epsilon chain

Chain X:  66% 28% 6%



● Molecule 4: ATP synthase epsilon chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	435.97Å 183.00Å 225.39Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	15.00 – 3.26 15.00 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-3.26) 97.0 (15.00-3.26)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.6.3_473	Depositor
R, R_{free}	0.243 , 0.265 0.239 , 0.258	Depositor DCC
R_{free} test set	2000 reflections (0.79%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 82.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	99573	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ADP, MG, ANP, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	0/3720	0.80	5/5032 (0.1%)
1	B	0.33	0/3679	0.80	6/4979 (0.1%)
1	C	0.32	0/3699	0.81	6/5005 (0.1%)
1	I	0.38	0/3720	0.87	8/5032 (0.2%)
1	J	0.33	0/3679	0.79	4/4979 (0.1%)
1	K	0.33	1/3699 (0.0%)	0.81	6/5005 (0.1%)
1	Q	0.33	0/3720	0.77	3/5032 (0.1%)
1	R	0.33	0/3679	0.81	8/4979 (0.2%)
1	S	0.31	0/3699	0.81	7/5005 (0.1%)
1	Y	0.29	0/3720	0.94	5/5032 (0.1%)
1	Z	0.32	0/3679	0.80	6/4979 (0.1%)
1	a	0.30	0/3699	0.81	6/5005 (0.1%)
2	D	0.33	0/3578	0.79	7/4843 (0.1%)
2	E	0.36	1/3578 (0.0%)	0.84	8/4843 (0.2%)
2	F	0.30	0/3578	0.81	7/4843 (0.1%)
2	L	0.32	0/3578	0.81	8/4843 (0.2%)
2	M	0.33	0/3578	0.83	6/4843 (0.1%)
2	N	0.31	0/3578	0.83	9/4843 (0.2%)
2	T	0.30	0/3578	0.82	7/4843 (0.1%)
2	U	0.32	0/3578	0.83	6/4843 (0.1%)
2	V	0.29	0/3578	0.82	9/4843 (0.2%)
2	b	0.33	0/3578	0.80	7/4843 (0.1%)
2	c	0.31	0/3578	0.83	9/4843 (0.2%)
2	d	0.29	0/3578	0.81	6/4843 (0.1%)
3	G	0.44	0/2213	0.81	6/2984 (0.2%)
3	O	0.39	0/2213	0.79	5/2984 (0.2%)
3	W	0.34	0/2213	0.78	5/2984 (0.2%)
3	e	0.35	1/2213 (0.0%)	0.80	6/2984 (0.2%)
4	H	0.27	0/1062	1.00	3/1432 (0.2%)
4	P	0.28	0/1062	0.67	1/1432 (0.1%)
4	X	0.29	0/1062	0.68	1/1432 (0.1%)
4	f	0.29	0/1062	1.01	3/1432 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.33	3/100428 (0.0%)	0.82	189/135844 (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
1	A	0	1
1	C	0	2
1	I	1	1
1	J	0	1
1	K	0	1
1	Q	0	1
1	R	0	1
1	S	0	2
1	Y	1	1
1	Z	0	2
1	a	0	1
2	D	0	2
2	E	0	4
2	F	0	1
2	L	0	2
2	M	0	1
2	N	0	1
2	T	0	1
2	U	0	1
2	V	0	1
2	b	0	5
2	c	0	1
2	d	0	1
3	G	0	2
3	O	0	2
3	W	0	4
3	e	0	4
All	All	2	47

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	e	188	LEU	CA-C	-6.37	1.49	1.53
1	K	136	VAL	CA-CB	-5.72	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	446	VAL	CA-CB	-5.21	1.47	1.54

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	ALA	CB-CA-C	27.19	151.29	110.50
4	f	1	ALA	CB-CA-C	27.17	151.26	110.50
1	Y	137	ILE	CA-C-N	-24.43	80.11	121.64
1	Y	137	ILE	C-N-CA	-24.43	80.11	121.64
1	Y	137	ILE	N-CA-C	16.23	143.09	109.34
1	R	408	GLN	N-CA-C	14.06	130.80	111.39
1	A	178	LEU	N-CA-C	-13.24	96.85	111.28
1	I	138	GLU	N-CA-C	11.97	129.34	108.02
1	B	408	GLN	N-CA-C	11.81	127.54	111.24
1	Z	408	GLN	N-CA-C	11.81	127.55	111.24
1	J	408	GLN	N-CA-C	11.80	127.52	111.24
1	I	176	THR	N-CA-C	-11.51	98.76	111.07
1	I	178	LEU	N-CA-C	-11.45	98.80	111.28
1	I	458	ASP	N-CA-C	10.78	122.79	111.14
1	I	137	ILE	CA-C-N	-10.24	108.32	122.86
1	I	137	ILE	C-N-CA	-10.24	108.32	122.86
2	T	112	ALA	CB-CA-C	10.00	126.10	109.99
2	T	112	ALA	N-CA-C	-9.83	93.58	108.52
3	e	190	LEU	C-N-CD	-9.39	86.52	125.00
2	U	331	TYR	CA-C-N	-8.86	108.77	119.84
2	U	331	TYR	C-N-CA	-8.86	108.77	119.84
2	L	112	ALA	N-CA-C	-8.27	95.98	108.46
3	O	64	HIS	CA-C-N	-8.17	109.95	118.85
3	O	64	HIS	C-N-CA	-8.17	109.95	118.85
3	W	64	HIS	CA-C-N	-8.13	109.98	118.85
3	W	64	HIS	C-N-CA	-8.13	109.98	118.85
3	G	64	HIS	CA-C-N	-8.12	110.00	118.85
3	G	64	HIS	C-N-CA	-8.12	110.00	118.85
3	e	64	HIS	CA-C-N	-8.11	110.01	118.85
3	e	64	HIS	C-N-CA	-8.11	110.01	118.85
2	M	331	TYR	CA-C-N	-7.94	109.91	119.84
2	M	331	TYR	C-N-CA	-7.94	109.91	119.84
2	E	331	TYR	CA-C-N	-7.67	110.26	119.84
2	E	331	TYR	C-N-CA	-7.67	110.26	119.84
2	L	112	ALA	CB-CA-C	7.67	122.06	109.72
4	H	1	ALA	N-CA-C	-7.41	90.24	111.00
4	f	1	ALA	N-CA-C	-7.40	90.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	461	LEU	CA-C-N	7.23	130.94	120.38
1	K	461	LEU	C-N-CA	7.23	130.94	120.38
1	C	461	LEU	CA-C-N	7.23	130.93	120.38
1	C	461	LEU	C-N-CA	7.23	130.93	120.38
1	S	461	LEU	CA-C-N	7.22	130.93	120.38
1	S	461	LEU	C-N-CA	7.22	130.93	120.38
1	a	461	LEU	CA-C-N	7.22	130.92	120.38
1	a	461	LEU	C-N-CA	7.22	130.92	120.38
3	G	190	LEU	N-CA-C	-7.20	101.32	109.60
2	c	331	TYR	CA-C-N	-7.13	110.93	119.84
2	c	331	TYR	C-N-CA	-7.13	110.93	119.84
2	D	120	SER	N-CA-C	-7.07	100.02	110.48
2	b	120	SER	N-CA-C	-7.06	100.03	110.48
2	L	120	SER	N-CA-C	-7.06	100.03	110.48
2	T	120	SER	N-CA-C	-7.04	100.05	110.48
2	N	156	THR	CB-CA-C	-6.99	99.86	110.90
1	a	442	ALA	N-CA-C	-6.99	104.75	113.28
2	E	118	GLU	N-CA-C	-6.99	104.91	113.50
2	c	118	GLU	N-CA-C	-6.98	104.92	113.50
1	C	442	ALA	N-CA-C	-6.97	104.77	113.28
2	U	118	GLU	N-CA-C	-6.96	104.94	113.50
2	M	118	GLU	N-CA-C	-6.95	104.95	113.50
1	S	442	ALA	N-CA-C	-6.94	104.81	113.28
1	K	442	ALA	N-CA-C	-6.93	104.82	113.28
1	S	455	TYR	N-CA-C	-6.88	103.99	112.38
1	K	455	TYR	N-CA-C	-6.87	103.99	112.38
1	a	455	TYR	N-CA-C	-6.87	104.00	112.38
1	C	455	TYR	N-CA-C	-6.86	104.01	112.38
3	O	208	GLU	CA-C-N	-6.84	113.64	120.21
3	O	208	GLU	C-N-CA	-6.84	113.64	120.21
3	W	208	GLU	CA-C-N	-6.83	113.65	120.21
3	W	208	GLU	C-N-CA	-6.83	113.65	120.21
3	G	208	GLU	CA-C-N	-6.82	113.66	120.21
3	G	208	GLU	C-N-CA	-6.82	113.66	120.21
3	e	208	GLU	CA-C-N	-6.79	113.69	120.21
3	e	208	GLU	C-N-CA	-6.79	113.69	120.21
1	J	124	ASP	N-CA-C	-6.76	104.05	112.90
1	B	124	ASP	N-CA-C	-6.76	104.05	112.90
1	R	124	ASP	N-CA-C	-6.76	104.05	112.90
1	Z	124	ASP	N-CA-C	-6.73	104.08	112.90
2	b	21	ALA	N-CA-C	-6.59	96.75	110.80
2	T	21	ALA	N-CA-C	-6.58	96.79	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	137	ILE	CB-CA-C	-6.46	100.69	111.29
2	c	413	SER	CA-C-N	6.43	125.93	119.24
2	c	413	SER	C-N-CA	6.43	125.93	119.24
1	S	494	ASP	N-CA-C	-6.36	103.63	111.33
2	F	156	THR	CB-CA-C	-6.28	101.03	110.88
2	c	445	MET	N-CA-C	6.19	120.10	111.74
1	a	450	ALA	N-CA-C	-6.17	104.82	112.90
1	S	450	ALA	N-CA-C	-6.16	104.83	112.90
1	K	450	ALA	N-CA-C	-6.16	104.84	112.90
2	L	19	GLN	N-CA-C	-6.12	102.03	110.35
1	C	450	ALA	N-CA-C	-6.12	104.89	112.90
2	D	331	TYR	CA-C-N	-5.99	112.35	119.84
2	D	331	TYR	C-N-CA	-5.99	112.35	119.84
2	N	104	GLU	N-CA-C	-5.85	106.18	113.38
2	V	104	GLU	N-CA-C	-5.85	106.18	113.38
2	F	104	GLU	N-CA-C	-5.84	106.20	113.38
2	U	347	LEU	N-CA-C	-5.83	101.22	109.96
2	d	104	GLU	N-CA-C	-5.83	106.22	113.38
1	A	176	THR	N-CA-C	-5.82	104.94	111.28
2	T	105	GLU	N-CA-C	-5.79	105.70	112.89
2	b	105	GLU	N-CA-C	-5.77	105.74	112.89
2	D	105	GLU	N-CA-C	-5.76	105.74	112.89
2	L	105	GLU	N-CA-C	-5.76	105.74	112.89
2	b	20	ASP	N-CA-C	5.75	119.33	111.39
2	M	331	TYR	N-CA-C	5.74	122.49	109.81
2	N	103	GLU	N-CA-C	5.73	118.79	110.42
2	d	103	GLU	N-CA-C	5.73	118.79	110.42
2	T	20	ASP	N-CA-C	5.72	119.28	111.39
2	V	103	GLU	N-CA-C	5.71	118.76	110.42
2	c	347	LEU	N-CA-C	-5.70	101.41	109.96
2	F	103	GLU	N-CA-C	5.69	118.72	110.42
2	E	331	TYR	N-CA-C	5.67	122.33	109.81
2	N	298	VAL	CA-C-N	5.64	125.92	119.83
2	N	298	VAL	C-N-CA	5.64	125.92	119.83
2	D	112	ALA	N-CA-C	-5.62	98.84	110.80
1	B	157	ILE	CA-C-N	5.61	125.54	119.76
1	B	157	ILE	C-N-CA	5.61	125.54	119.76
1	R	157	ILE	CA-C-N	5.59	125.52	119.76
1	R	157	ILE	C-N-CA	5.59	125.52	119.76
2	L	331	TYR	CA-C-N	-5.58	112.87	119.84
2	L	331	TYR	C-N-CA	-5.58	112.87	119.84
2	M	416	LYS	N-CA-C	5.55	115.45	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	d	142	GLY	N-CA-C	-5.55	106.84	115.67
1	J	157	ILE	CA-C-N	5.55	125.48	119.76
1	J	157	ILE	C-N-CA	5.55	125.48	119.76
2	F	142	GLY	N-CA-C	-5.55	106.85	115.67
2	V	142	GLY	N-CA-C	-5.55	106.85	115.67
2	N	142	GLY	N-CA-C	-5.55	106.85	115.67
1	R	93	ARG	CA-C-N	-5.54	115.92	123.12
1	R	93	ARG	C-N-CA	-5.54	115.92	123.12
2	U	331	TYR	N-CA-C	5.54	122.06	109.81
2	M	347	LEU	N-CA-C	-5.54	101.65	109.96
2	V	86	ARG	N-CA-C	5.54	115.87	108.23
1	Z	157	ILE	CA-C-N	5.53	125.45	119.76
1	Z	157	ILE	C-N-CA	5.53	125.45	119.76
2	b	331	TYR	CA-C-N	-5.53	112.93	119.84
2	b	331	TYR	C-N-CA	-5.53	112.93	119.84
2	d	86	ARG	N-CA-C	5.52	115.85	108.23
2	E	416	LYS	N-CA-C	5.52	115.40	108.45
2	F	102	GLY	N-CA-C	5.52	121.11	111.78
2	V	102	GLY	N-CA-C	5.52	121.11	111.78
2	N	102	GLY	N-CA-C	5.52	121.10	111.78
2	c	331	TYR	N-CA-C	5.51	121.99	109.81
1	S	443	GLN	N-CA-C	-5.50	104.71	111.75
2	d	102	GLY	N-CA-C	5.50	121.07	111.78
1	a	443	GLN	N-CA-C	-5.49	104.72	111.75
1	A	136	VAL	CB-CA-C	-5.49	104.95	111.97
1	K	443	GLN	N-CA-C	-5.48	104.74	111.75
2	N	86	ARG	N-CA-C	5.48	115.79	108.23
2	d	156	THR	N-CA-C	5.47	117.05	111.14
2	F	86	ARG	N-CA-C	5.47	115.78	108.23
1	I	177	ALA	N-CA-C	-5.46	105.33	111.28
2	N	156	THR	N-CA-C	5.43	117.00	111.14
1	C	443	GLN	N-CA-C	-5.41	104.82	111.75
2	F	156	THR	N-CA-C	5.40	116.85	111.07
2	V	156	THR	CB-CA-C	-5.37	102.44	110.88
1	A	477	ARG	N-CA-C	-5.33	105.48	111.28
2	D	198	VAL	N-CA-C	5.24	118.41	111.17
3	G	73	LYS	N-CA-C	-5.24	108.64	114.62
2	L	198	VAL	N-CA-C	5.23	118.39	111.17
2	c	416	LYS	N-CA-C	5.23	115.04	108.45
3	O	73	LYS	N-CA-C	-5.22	108.67	114.62
3	e	73	LYS	N-CA-C	-5.22	108.67	114.62
2	V	156	THR	N-CA-C	5.22	116.65	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	198	VAL	N-CA-C	5.21	118.37	111.17
1	A	218	LEU	N-CA-C	-5.21	106.43	112.89
2	b	198	VAL	N-CA-C	5.21	118.36	111.17
3	W	73	LYS	N-CA-C	-5.20	108.69	114.62
2	D	22	VAL	N-CA-C	5.20	113.45	109.19
1	Q	218	LEU	N-CA-C	-5.19	106.45	112.89
1	Y	177	ALA	N-CA-C	-5.17	104.71	111.02
1	Y	218	LEU	N-CA-C	-5.17	106.47	112.89
1	I	218	LEU	N-CA-C	-5.17	106.48	112.89
2	E	349	VAL	N-CA-C	5.14	115.76	110.36
2	E	335	ASP	CA-C-N	5.11	125.40	119.47
2	E	335	ASP	C-N-CA	5.11	125.40	119.47
2	V	298	VAL	CA-C-N	5.06	125.22	119.90
2	V	298	VAL	C-N-CA	5.06	125.22	119.90
4	f	130	VAL	N-CA-C	5.06	115.67	110.36
4	H	130	VAL	N-CA-C	5.06	115.67	110.36
4	P	130	VAL	N-CA-C	5.06	115.67	110.36
4	X	130	VAL	N-CA-C	5.04	115.65	110.36
1	R	327	LEU	CA-C-N	5.04	125.51	120.52
1	R	327	LEU	C-N-CA	5.04	125.51	120.52
1	B	327	LEU	CA-C-N	5.04	125.50	120.52
1	B	327	LEU	C-N-CA	5.04	125.50	120.52
2	U	416	LYS	N-CA-C	5.03	114.78	108.45
1	Z	327	LEU	CA-C-N	5.02	125.49	120.52
1	Z	327	LEU	C-N-CA	5.02	125.49	120.52
1	Q	135	GLY	N-CA-C	-5.00	104.86	112.51

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	I	138	GLU	CA
1	Y	137	ILE	CA

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	GLY	Peptide
1	C	460	GLU	Peptide
1	C	493	ASN	Peptide
2	D	119	LEU	Peptide
2	D	20	ASP	Peptide
2	E	331	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	E	346	PRO	Peptide
2	E	348	VAL	Peptide
2	E	444	TYR	Peptide
2	F	331	TYR	Peptide
3	G	188	LEU	Peptide
3	G	191	PRO	Peptide
1	I	137	ILE	Peptide
1	J	94	ILE	Mainchain
1	K	460	GLU	Peptide
2	L	119	LEU	Peptide
2	L	20	ASP	Peptide
2	M	331	TYR	Peptide
2	N	331	TYR	Peptide
3	O	188	LEU	Peptide
3	O	191	PRO	Peptide
1	Q	138	GLU	Peptide
1	R	94	ILE	Peptide
1	S	460	GLU	Peptide
1	S	493	ASN	Peptide
2	T	119	LEU	Peptide
2	U	331	TYR	Peptide
2	V	331	TYR	Peptide
3	W	188	LEU	Peptide
3	W	189	PRO	Peptide
3	W	190	LEU	Peptide
3	W	191	PRO	Peptide
1	Y	137	ILE	Peptide
1	Z	94	ILE	Peptide
1	Z	95	LEU	Peptide
1	a	460	GLU	Peptide
2	b	110	HIS	Peptide
2	b	113	ALA	Peptide
2	b	115	SER	Peptide
2	b	118	GLU	Peptide
2	b	119	LEU	Peptide
2	c	331	TYR	Peptide
2	d	331	TYR	Peptide
3	e	187	LEU	Peptide
3	e	188	LEU	Peptide
3	e	191	PRO	Peptide
3	e	193	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3667	0	3702	258	0
1	B	3627	0	3650	264	0
1	C	3646	0	3669	257	0
1	I	3667	0	3702	274	0
1	J	3627	0	3650	271	0
1	K	3646	0	3669	257	0
1	Q	3667	0	3702	234	0
1	R	3627	0	3650	277	0
1	S	3646	0	3669	262	0
1	Y	3667	0	3702	239	0
1	Z	3627	0	3650	264	0
1	a	3646	0	3669	256	0
2	D	3521	0	3523	270	0
2	E	3521	0	3524	330	0
2	F	3521	0	3524	217	0
2	L	3521	0	3523	249	0
2	M	3521	0	3524	294	0
2	N	3521	0	3524	215	0
2	T	3521	0	3523	235	0
2	U	3521	0	3524	265	0
2	V	3521	0	3524	218	0
2	b	3521	0	3523	265	0
2	c	3521	0	3524	268	0
2	d	3521	0	3524	209	0
3	G	2182	0	2227	86	0
3	O	2182	0	2227	95	0
3	W	2182	0	2227	132	0
3	e	2182	0	2227	106	0
4	H	1047	0	1058	37	0
4	P	1047	0	1058	45	0
4	X	1047	0	1058	46	0
4	f	1047	0	1058	39	0
5	A	31	0	12	2	0
5	B	31	0	12	3	0
5	C	31	0	12	3	0
5	I	31	0	12	4	0
5	J	31	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	31	0	12	2	0
5	Q	31	0	12	2	0
5	R	31	0	12	3	0
5	S	31	0	12	2	0
5	Y	31	0	12	3	0
5	Z	31	0	12	3	0
5	a	31	0	12	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0
6	T	1	0	0	0	0
6	Y	1	0	0	0	0
6	Z	1	0	0	0	0
6	a	1	0	0	0	0
6	b	1	0	0	0	0
7	D	27	0	11	5	0
7	L	27	0	11	5	0
7	T	27	0	11	4	0
7	b	27	0	11	4	0
8	D	5	0	0	1	0
8	E	5	0	0	0	0
8	F	5	0	0	1	0
8	G	5	0	0	0	0
8	H	5	0	0	0	0
8	L	5	0	0	1	0
8	M	5	0	0	0	0
8	N	5	0	0	1	0
8	O	5	0	0	0	0
8	P	5	0	0	0	0
8	T	5	0	0	0	0
8	U	5	0	0	0	0
8	V	5	0	0	0	0
8	W	5	0	0	1	0
8	b	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	c	5	0	0	1	0
8	d	5	0	0	0	0
9	A	3	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	D	8	0	0	0	0
9	E	1	0	0	0	0
9	F	5	0	0	0	0
9	G	10	0	0	0	0
9	H	4	0	0	0	0
9	J	3	0	0	0	0
9	L	6	0	0	0	0
9	N	3	0	0	0	0
9	O	5	0	0	0	0
9	P	2	0	0	0	0
9	Q	1	0	0	0	0
9	R	1	0	0	0	0
9	S	1	0	0	0	0
9	V	2	0	0	0	0
9	X	1	0	0	0	0
9	a	1	0	0	0	0
9	b	1	0	0	0	0
9	d	2	0	0	0	0
All	All	99573	0	99696	6463	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (6463) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HD13	1:A:138:GLU:CA	1.35	1.50
4:P:2:MET:HE1	2:c:197:ASN:CB	1.46	1.45
1:R:50:GLY:O	1:R:94:ILE:CG2	1.63	1.45
3:W:186:GLN:NE2	3:W:189:PRO:HG2	1.31	1.45
1:R:95:LEU:CD2	1:R:129:VAL:HG22	1.44	1.42
3:e:190:LEU:HD12	3:e:191:PRO:N	1.31	1.42
1:Y:137:ILE:CD1	1:Y:137:ILE:O	1.69	1.39
1:R:51:GLU:CA	1:R:94:ILE:HG23	1.53	1.39
1:R:50:GLY:C	1:R:94:ILE:HG21	1.46	1.37
3:W:190:LEU:HD12	3:W:191:PRO:N	1.36	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:95:LEU:HD21	1:R:129:VAL:CG2	1.58	1.34
2:E:346:PRO:HG2	2:E:348:VAL:CG1	1.59	1.32
1:I:180:ILE:HD11	1:I:211:LYS:NZ	1.45	1.31
3:W:190:LEU:HD12	3:W:190:LEU:C	1.52	1.30
4:P:2:MET:CE	2:c:197:ASN:HB3	1.60	1.30
1:Z:95:LEU:C	1:Z:95:LEU:HD12	1.53	1.28
2:E:346:PRO:CG	2:E:348:VAL:HG11	1.62	1.28
1:R:50:GLY:C	1:R:94:ILE:CG2	2.05	1.26
1:R:51:GLU:HA	1:R:94:ILE:CG2	1.63	1.26
1:Y:137:ILE:O	1:Y:137:ILE:HD13	1.08	1.26
2:b:113:ALA:CB	2:b:281:ARG:HG2	1.66	1.25
3:e:188:LEU:C	3:e:188:LEU:HD12	1.53	1.25
1:A:178:LEU:C	1:A:178:LEU:HD12	1.56	1.25
2:E:442:ALA:HB3	2:E:443:PHE:CE2	1.71	1.24
1:I:178:LEU:C	1:I:178:LEU:HD12	1.57	1.24
1:A:137:ILE:HD13	1:A:138:GLU:N	1.53	1.23
1:R:94:ILE:O	1:R:95:LEU:HD12	1.38	1.22
1:R:95:LEU:HD13	1:R:95:LEU:C	1.53	1.22
1:Z:95:LEU:HD11	1:Z:129:VAL:CG2	1.69	1.21
2:b:113:ALA:HB1	2:b:114:PRO:CD	1.68	1.21
1:R:50:GLY:O	1:R:94:ILE:HG22	1.23	1.20
1:A:137:ILE:CD1	1:A:138:GLU:HB2	1.70	1.19
2:E:347:LEU:C	2:E:347:LEU:HD12	1.65	1.18
1:K:136:VAL:C	1:K:137:ILE:HG13	1.60	1.18
3:W:187:LEU:HD12	3:W:188:LEU:N	1.60	1.16
3:G:187:LEU:HD12	3:G:187:LEU:O	1.40	1.16
1:R:95:LEU:CD2	1:R:129:VAL:CG2	2.18	1.15
2:b:111:ARG:CG	2:b:112:ALA:H	1.60	1.15
2:b:113:ALA:HB2	2:b:281:ARG:HG2	1.19	1.15
2:b:111:ARG:NH1	2:b:111:ARG:HA	1.61	1.14
1:A:137:ILE:HD11	1:A:138:GLU:HB2	1.23	1.14
2:b:113:ALA:HB2	2:b:281:ARG:CG	1.78	1.14
1:J:97:VAL:HG13	1:J:98:PRO:HD2	1.30	1.13
3:W:187:LEU:HD12	3:W:187:LEU:C	1.68	1.13
3:e:189:PRO:O	3:e:191:PRO:HD3	1.47	1.13
3:e:190:LEU:CD1	3:e:191:PRO:N	2.11	1.12
1:B:95:LEU:C	1:B:95:LEU:HD12	1.73	1.12
1:B:95:LEU:HD12	1:B:95:LEU:O	1.48	1.12
1:I:364:ILE:HD11	1:I:432:LYS:HE3	1.22	1.12
2:b:111:ARG:CD	2:b:112:ALA:H	1.61	1.11
2:U:416:LYS:HD2	2:U:417:TYR:H	1.12	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:52:MET:HE3	1:Z:95:LEU:HA	1.16	1.11
1:A:137:ILE:HD13	1:A:138:GLU:CB	1.79	1.11
2:E:347:LEU:C	2:E:348:VAL:HG12	1.66	1.11
1:Y:137:ILE:O	1:Y:138:GLU:HB2	1.46	1.11
1:S:492:TYR:C	1:S:493:ASN:HD22	1.59	1.10
2:b:117:GLU:CD	2:b:117:GLU:H	1.54	1.10
3:W:187:LEU:CD1	3:W:188:LEU:CB	2.30	1.10
2:c:416:LYS:HD2	2:c:417:TYR:H	1.14	1.10
2:b:111:ARG:HH11	2:b:111:ARG:CA	1.64	1.09
1:A:137:ILE:CD1	1:A:138:GLU:CA	2.30	1.09
1:Z:96:GLU:O	1:Z:97:VAL:HG23	1.53	1.09
3:e:187:LEU:HD23	3:e:187:LEU:H	1.07	1.09
1:Z:95:LEU:HD12	1:Z:95:LEU:O	1.53	1.09
1:A:178:LEU:HD12	1:A:178:LEU:O	1.50	1.08
1:I:136:VAL:O	1:I:137:ILE:HG22	1.53	1.08
3:W:188:LEU:C	3:W:188:LEU:HD22	1.76	1.08
1:I:364:ILE:CD1	1:I:432:LYS:HE3	1.84	1.07
1:R:95:LEU:O	1:R:95:LEU:HD22	1.54	1.07
1:A:137:ILE:CD1	1:A:138:GLU:CB	2.32	1.07
1:J:97:VAL:CG1	1:J:98:PRO:HD2	1.84	1.07
1:K:136:VAL:O	1:K:137:ILE:HG13	1.51	1.07
2:b:111:ARG:HA	2:b:111:ARG:HH11	0.90	1.07
1:R:51:GLU:CA	1:R:94:ILE:CG2	2.26	1.07
2:b:113:ALA:CA	2:b:281:ARG:HG2	1.84	1.06
3:e:191:PRO:HB3	3:e:192:ALA:HB3	1.37	1.06
3:e:188:LEU:HD12	3:e:188:LEU:O	1.55	1.06
2:E:442:ALA:HB3	2:E:443:PHE:CD2	1.90	1.05
1:S:492:TYR:O	1:S:493:ASN:ND2	1.88	1.05
1:B:95:LEU:C	1:B:95:LEU:CD1	2.30	1.05
1:Z:52:MET:O	1:Z:52:MET:HG2	1.56	1.05
1:Q:138:GLU:O	1:Q:305:ASN:HB3	1.53	1.05
1:Y:137:ILE:O	1:Y:137:ILE:CG1	2.02	1.05
1:Y:137:ILE:HD13	1:Y:137:ILE:C	1.82	1.05
3:W:187:LEU:HD12	3:W:188:LEU:CB	1.86	1.05
2:b:113:ALA:HB1	2:b:114:PRO:HD2	1.06	1.04
1:A:137:ILE:CD1	1:A:137:ILE:C	2.30	1.04
1:A:137:ILE:HD13	1:A:138:GLU:HA	1.33	1.04
2:b:113:ALA:CB	2:b:281:ARG:HA	1.87	1.04
1:B:27:ASN:HD21	1:B:46:ASP:HB2	1.22	1.03
2:M:444:TYR:O	2:M:446:VAL:HG13	1.55	1.03
3:W:187:LEU:CD1	3:W:188:LEU:HB3	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HG12	1:A:138:GLU:OE1	1.57	1.03
3:W:187:LEU:HD21	3:W:223:VAL:HG13	1.40	1.03
1:Z:95:LEU:HD11	1:Z:129:VAL:HG22	1.40	1.03
1:R:27:ASN:HD21	1:R:46:ASP:HB2	1.23	1.03
1:I:137:ILE:O	1:I:137:ILE:HD13	1.60	1.02
3:W:188:LEU:HD22	3:W:188:LEU:O	1.59	1.02
1:Z:27:ASN:HD21	1:Z:46:ASP:HB2	1.23	1.02
2:E:347:LEU:O	2:E:348:VAL:HG12	1.60	1.02
3:e:187:LEU:HD23	3:e:187:LEU:N	1.65	1.02
1:Z:52:MET:CE	1:Z:95:LEU:HA	1.88	1.01
3:e:188:LEU:C	3:e:188:LEU:CD1	2.30	1.01
3:W:188:LEU:O	3:W:188:LEU:HD13	1.59	1.01
1:J:27:ASN:HD21	1:J:46:ASP:HB2	1.23	1.01
2:E:445:MET:CE	2:E:445:MET:HA	1.89	1.01
2:T:241:VAL:HG13	2:T:294:GLN:HB3	1.42	1.01
3:W:190:LEU:CD1	3:W:191:PRO:N	2.23	1.01
1:A:178:LEU:C	1:A:178:LEU:CD1	2.33	1.00
1:I:137:ILE:HD13	1:I:137:ILE:C	1.86	1.00
1:I:178:LEU:HD12	1:I:178:LEU:O	1.61	1.00
2:U:131:LYS:H	2:U:402:GLN:HE22	1.09	1.00
2:E:443:PHE:N	2:E:443:PHE:HD2	1.54	1.00
3:W:186:GLN:NE2	3:W:189:PRO:CG	2.24	1.00
2:b:111:ARG:HD3	2:b:112:ALA:N	1.76	1.00
2:E:442:ALA:HB3	2:E:443:PHE:HE2	1.25	0.99
2:M:416:LYS:HD2	2:M:417:TYR:H	1.26	0.99
1:I:459:VAL:O	1:I:459:VAL:HG12	1.59	0.99
2:b:113:ALA:HB2	2:b:281:ARG:CB	1.92	0.99
2:F:323:ARG:HH11	2:F:323:ARG:HG3	1.24	0.98
1:I:180:ILE:CD1	1:I:211:LYS:NZ	2.27	0.98
2:U:268:GLN:HE21	2:U:268:GLN:H	0.99	0.98
1:I:178:LEU:C	1:I:178:LEU:CD1	2.30	0.98
3:G:187:LEU:HD12	3:G:187:LEU:C	1.87	0.98
1:Q:136:VAL:O	1:Q:137:ILE:HG22	1.64	0.98
3:W:186:GLN:CD	3:W:189:PRO:HG2	1.87	0.98
1:A:493:ASN:HB3	1:A:496:ILE:HD13	1.46	0.97
1:A:138:GLU:HG3	1:A:305:ASN:HB3	1.46	0.97
3:W:66:TYR:HB3	3:W:188:LEU:CD2	1.94	0.97
2:L:83:THR:HB	2:L:88:MET:HE1	1.46	0.96
2:b:83:THR:HB	2:b:88:MET:HE1	1.46	0.96
2:b:113:ALA:CB	2:b:114:PRO:HD2	1.93	0.96
1:I:493:ASN:HB3	1:I:496:ILE:HD13	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:66:TYR:HB3	3:W:188:LEU:HD23	1.47	0.96
1:R:95:LEU:C	1:R:95:LEU:CD1	2.30	0.96
2:E:349:VAL:HG21	2:E:353:HIS:CG	1.99	0.96
1:Q:493:ASN:HB3	1:Q:496:ILE:HD13	1.46	0.96
3:W:190:LEU:C	3:W:190:LEU:CD1	2.29	0.96
2:D:241:VAL:HG13	2:D:294:GLN:HB3	1.46	0.96
2:L:241:VAL:HG13	2:L:294:GLN:HB3	1.45	0.96
2:T:83:THR:HB	2:T:88:MET:HE1	1.46	0.96
1:Y:493:ASN:HB3	1:Y:496:ILE:HD13	1.47	0.95
2:U:116:TYR:HD1	2:U:117:GLU:H	1.13	0.95
2:V:323:ARG:HH11	2:V:323:ARG:HG3	1.31	0.95
2:N:323:ARG:HH11	2:N:323:ARG:HG3	1.32	0.95
2:E:416:LYS:HD2	2:E:417:TYR:H	1.30	0.94
1:J:97:VAL:HG21	1:J:111:LEU:O	1.67	0.94
3:e:187:LEU:N	3:e:187:LEU:CD2	2.30	0.94
2:b:111:ARG:HG3	2:b:112:ALA:H	1.28	0.94
2:D:22:VAL:CG2	2:D:23:PRO:HD2	1.96	0.94
1:K:137:ILE:HD11	2:L:95:VAL:O	1.67	0.94
2:c:78:PRO:HB3	2:c:103:GLU:HG2	1.50	0.94
3:e:191:PRO:CB	3:e:192:ALA:HB3	1.96	0.94
1:A:137:ILE:CD1	1:A:138:GLU:N	2.30	0.94
2:E:344:LEU:C	2:E:346:PRO:CD	2.40	0.94
2:E:116:TYR:HD1	2:E:117:GLU:H	1.13	0.94
2:E:344:LEU:C	2:E:346:PRO:HD2	1.93	0.94
2:D:83:THR:HB	2:D:88:MET:HE1	1.46	0.94
1:Z:95:LEU:HD11	1:Z:129:VAL:HG21	1.48	0.94
1:Y:179:ALA:HB1	1:Y:259:ILE:HD12	1.50	0.94
2:b:241:VAL:HG13	2:b:294:GLN:HB3	1.50	0.94
1:Z:483:MET:HG2	1:Z:483:MET:O	1.68	0.93
2:D:17:PHE:HE1	2:D:23:PRO:CG	1.80	0.93
2:b:377:LEU:HD21	4:f:115:ALA:HB2	1.49	0.93
2:M:445:MET:HE2	2:M:445:MET:HA	1.50	0.93
2:c:116:TYR:HD1	2:c:117:GLU:H	1.13	0.93
1:R:483:MET:O	1:R:483:MET:HG2	1.68	0.93
2:F:134:ASP:HB3	2:F:420:LEU:HD13	1.51	0.93
2:b:113:ALA:HB1	2:b:281:ARG:HA	1.48	0.93
2:D:17:PHE:CD1	2:D:23:PRO:HD3	2.04	0.93
2:c:265:VAL:H	3:e:273:THR:HG22	1.32	0.93
1:R:96:GLU:HB2	1:R:128:ALA:HA	1.50	0.93
1:B:195:TYR:HD1	1:B:259:ILE:HD11	1.34	0.92
1:J:140:GLN:HE21	1:J:140:GLN:HA	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:347:LEU:HD12	2:E:348:VAL:N	1.85	0.92
1:R:51:GLU:N	1:R:94:ILE:CG2	2.31	0.92
3:W:187:LEU:HD11	3:W:188:LEU:CB	1.97	0.92
1:A:137:ILE:HG23	1:A:137:ILE:O	1.70	0.92
1:B:140:GLN:HE21	1:B:140:GLN:HA	1.34	0.92
2:E:268:GLN:HE21	2:E:268:GLN:H	1.06	0.92
2:E:445:MET:HA	2:E:445:MET:HE2	1.49	0.92
1:J:483:MET:O	1:J:483:MET:HG2	1.68	0.92
3:e:186:GLN:NE2	3:e:189:PRO:HG2	1.84	0.92
1:Q:179:ALA:HB1	1:Q:259:ILE:HD12	1.50	0.91
1:R:97:VAL:HG21	1:R:111:LEU:O	1.70	0.91
3:e:191:PRO:HB3	3:e:192:ALA:CB	2.00	0.91
2:F:131:LYS:HB2	2:F:402:GLN:HE22	1.33	0.91
1:J:195:TYR:HD1	1:J:259:ILE:HD11	1.34	0.91
2:M:78:PRO:HB3	2:M:103:GLU:HG2	1.50	0.91
2:U:78:PRO:HB3	2:U:103:GLU:HG2	1.50	0.91
2:U:265:VAL:H	3:W:273:THR:HG22	1.31	0.91
1:Z:140:GLN:HE21	1:Z:140:GLN:HA	1.35	0.91
2:b:111:ARG:CD	2:b:112:ALA:N	2.30	0.91
1:B:97:VAL:HG21	1:B:111:LEU:O	1.70	0.91
1:R:195:TYR:HD1	1:R:259:ILE:HD11	1.34	0.91
1:Z:109:ASN:HB3	1:Z:114:PRO:HB2	1.52	0.91
2:E:78:PRO:HB3	2:E:103:GLU:HG2	1.49	0.91
3:G:66:TYR:HB3	3:G:188:LEU:HD12	1.53	0.91
2:M:116:TYR:HD1	2:M:117:GLU:H	1.13	0.91
2:c:268:GLN:HE21	2:c:268:GLN:H	1.16	0.91
1:B:483:MET:O	1:B:483:MET:HG2	1.68	0.91
1:S:493:ASN:O	1:S:496:ILE:HG12	1.71	0.91
3:e:190:LEU:HD12	3:e:190:LEU:C	1.93	0.91
1:J:109:ASN:HB3	1:J:114:PRO:HB2	1.52	0.90
2:E:445:MET:O	2:E:446:VAL:HG12	1.71	0.90
3:W:208:GLU:CD	3:W:209:PRO:HD2	1.97	0.90
1:Z:195:TYR:HD1	1:Z:259:ILE:HD11	1.34	0.90
1:R:430:LEU:HD22	1:R:446:LEU:HD21	1.53	0.90
1:Z:95:LEU:C	1:Z:95:LEU:CD1	2.30	0.90
3:e:208:GLU:CD	3:e:209:PRO:HD2	1.97	0.90
1:R:140:GLN:HE21	1:R:140:GLN:HA	1.35	0.90
2:L:32:GLN:HG2	2:L:37:ARG:HG2	1.54	0.90
1:R:109:ASN:HB3	1:R:114:PRO:HB2	1.52	0.90
1:Z:97:VAL:HG21	1:Z:111:LEU:O	1.70	0.90
2:b:117:GLU:CD	2:b:117:GLU:N	2.30	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:430:LEU:HD22	1:Z:446:LEU:HD21	1.53	0.90
1:a:179:ALA:HB1	1:a:259:ILE:HD12	1.54	0.90
1:C:179:ALA:HB1	1:C:259:ILE:HD12	1.54	0.90
2:E:379:MET:HB2	2:E:387:LYS:NZ	1.87	0.90
2:M:268:GLN:HE21	2:M:268:GLN:H	0.91	0.89
3:e:201:LYS:HD3	3:e:202:SER:H	1.37	0.89
3:G:208:GLU:CD	3:G:209:PRO:HD2	1.96	0.89
1:A:138:GLU:HG3	1:A:305:ASN:CB	2.01	0.89
2:D:19:GLN:HB3	2:D:20:ASP:OD2	1.73	0.89
3:O:208:GLU:CD	3:O:209:PRO:HD2	1.97	0.89
3:O:189:PRO:O	3:O:191:PRO:HD3	1.73	0.89
2:b:32:GLN:HG2	2:b:37:ARG:HG2	1.54	0.89
2:d:323:ARG:HG3	2:d:323:ARG:HH11	1.37	0.89
1:B:430:LEU:HD22	1:B:446:LEU:HD21	1.53	0.89
3:O:167:LEU:HD23	3:O:188:LEU:HD23	1.53	0.89
2:M:109:ILE:HA	2:M:225:THR:HG21	1.55	0.89
2:V:134:ASP:HB3	2:V:420:LEU:HD13	1.55	0.89
2:b:113:ALA:HB2	2:b:281:ARG:CA	2.02	0.89
2:c:379:MET:HB2	2:c:387:LYS:NZ	1.88	0.89
2:D:32:GLN:HG2	2:D:37:ARG:HG2	1.54	0.88
2:E:109:ILE:HA	2:E:225:THR:HG21	1.55	0.88
2:d:131:LYS:HD3	2:d:418:VAL:HG21	1.52	0.88
2:L:118:GLU:HB2	2:L:285:THR:HA	1.56	0.88
3:W:201:LYS:HD3	3:W:202:SER:H	1.37	0.88
2:c:109:ILE:HA	2:c:225:THR:HG21	1.55	0.88
1:I:180:ILE:CD1	1:I:211:LYS:HZ3	1.85	0.88
1:S:179:ALA:HB1	1:S:259:ILE:HD12	1.54	0.88
1:S:317:VAL:HA	1:S:318:LYS:HB2	1.54	0.88
1:J:430:LEU:HD22	1:J:446:LEU:HD21	1.53	0.88
2:c:131:LYS:H	2:c:402:GLN:HE22	1.15	0.88
1:B:94:ILE:O	1:B:94:ILE:HG12	1.68	0.88
2:U:395:LYS:HD3	2:U:443:PHE:CE2	2.08	0.88
2:F:103:GLU:HB2	2:F:105:GLU:O	1.73	0.88
1:Q:348:ILE:HG23	2:U:209:MET:HE1	1.56	0.88
2:V:103:GLU:HB2	2:V:105:GLU:O	1.73	0.88
2:d:134:ASP:HB3	2:d:420:LEU:HD13	1.56	0.88
2:U:379:MET:HB2	2:U:387:LYS:NZ	1.89	0.88
2:d:103:GLU:HB2	2:d:105:GLU:O	1.73	0.88
1:B:109:ASN:HB3	1:B:114:PRO:HB2	1.52	0.88
2:F:131:LYS:HD3	2:F:418:VAL:HG21	1.56	0.88
2:E:443:PHE:CD2	2:E:443:PHE:N	2.31	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:179:ALA:HB1	1:K:259:ILE:HD12	1.55	0.88
3:G:201:LYS:HD3	3:G:202:SER:H	1.37	0.87
2:T:32:GLN:HG2	2:T:37:ARG:HG2	1.54	0.87
2:T:118:GLU:HB2	2:T:285:THR:HA	1.54	0.87
1:Z:413:LEU:O	1:Z:415:ASP:N	2.07	0.87
2:b:42:VAL:HA	2:b:53:THR:HG22	1.56	0.87
2:D:42:VAL:HA	2:D:53:THR:HG22	1.55	0.87
2:N:103:GLU:HB2	2:N:105:GLU:O	1.73	0.87
2:d:131:LYS:HB2	2:d:402:GLN:HE22	1.39	0.87
3:O:201:LYS:HD3	3:O:202:SER:H	1.37	0.87
1:C:317:VAL:HA	1:C:318:LYS:HB2	1.54	0.87
1:a:317:VAL:HA	1:a:318:LYS:HB2	1.54	0.87
1:I:364:ILE:HD11	1:I:432:LYS:CE	2.03	0.87
1:I:180:ILE:HD11	1:I:211:LYS:HZ3	1.04	0.87
2:U:109:ILE:HA	2:U:225:THR:HG21	1.55	0.87
2:V:307:SER:HB2	2:V:308:PRO:HD3	1.56	0.87
1:R:413:LEU:O	1:R:415:ASP:N	2.07	0.87
2:E:265:VAL:H	3:G:273:THR:HG22	1.38	0.87
1:R:95:LEU:HD13	1:R:96:GLU:N	1.89	0.87
2:E:347:LEU:C	2:E:347:LEU:CD1	2.35	0.87
1:J:413:LEU:O	1:J:415:ASP:N	2.07	0.87
2:L:400:LEU:HB3	2:L:427:PHE:HZ	1.39	0.86
1:K:317:VAL:HA	1:K:318:LYS:HB2	1.54	0.86
3:W:187:LEU:CD1	3:W:188:LEU:HB2	2.04	0.86
2:F:307:SER:HB2	2:F:308:PRO:HD3	1.56	0.86
1:J:97:VAL:CG1	1:J:98:PRO:CD	2.53	0.86
1:J:193:CYS:HB2	1:J:221:THR:HB	1.58	0.86
1:K:137:ILE:CD1	2:L:95:VAL:O	2.22	0.86
2:N:307:SER:HB2	2:N:308:PRO:HD3	1.57	0.86
2:M:131:LYS:H	2:M:402:GLN:HE22	1.19	0.86
2:N:131:LYS:HB2	2:N:402:GLN:HE22	1.41	0.86
2:T:111:ARG:HD3	2:T:281:ARG:HB2	1.57	0.86
2:D:17:PHE:HE1	2:D:23:PRO:HG2	1.39	0.86
1:A:137:ILE:HD13	1:A:137:ILE:C	1.90	0.86
1:I:180:ILE:HD11	1:I:211:LYS:HZ1	1.37	0.86
2:L:42:VAL:HA	2:L:53:THR:HG22	1.56	0.86
2:d:307:SER:HB2	2:d:308:PRO:HD3	1.56	0.86
2:E:345:ASP:N	2:E:346:PRO:HD3	1.89	0.86
3:G:188:LEU:HG	3:G:188:LEU:O	1.76	0.86
2:M:268:GLN:HE21	2:M:268:GLN:N	1.74	0.86
1:R:50:GLY:O	1:R:94:ILE:HG21	1.44	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:343:GLN:HG3	2:b:348:VAL:HG11	1.58	0.86
2:M:379:MET:HB2	2:M:387:LYS:NZ	1.90	0.86
1:B:193:CYS:HB2	1:B:221:THR:HB	1.58	0.85
3:W:186:GLN:HE21	3:W:189:PRO:HG2	1.03	0.85
4:H:7:ASP:HB2	4:H:77:THR:HG22	1.58	0.85
2:M:268:GLN:H	2:M:268:GLN:NE2	1.73	0.85
2:T:377:LEU:HD21	4:X:115:ALA:HB2	1.57	0.85
1:A:138:GLU:HG2	1:A:305:ASN:CG	2.00	0.85
1:C:492:TYR:C	1:C:493:ASN:ND2	2.35	0.85
2:b:379:MET:HE1	2:b:390:VAL:HG11	1.58	0.85
2:D:17:PHE:CD1	2:D:23:PRO:CD	2.59	0.85
1:J:309:VAL:HG12	1:J:317:VAL:HG11	1.58	0.85
2:U:337:LEU:HD12	2:U:338:ASP:H	1.39	0.85
1:Z:52:MET:HE3	1:Z:95:LEU:CA	2.04	0.85
1:B:309:VAL:HG12	1:B:317:VAL:HG11	1.58	0.85
2:T:42:VAL:HA	2:T:53:THR:HG22	1.56	0.85
2:U:42:VAL:HA	2:U:53:THR:HG22	1.59	0.85
3:O:188:LEU:HG	3:O:188:LEU:O	1.76	0.85
1:R:95:LEU:HD13	1:R:95:LEU:O	1.77	0.84
2:M:265:VAL:H	3:O:273:THR:HG22	1.42	0.84
4:f:7:ASP:HB2	4:f:77:THR:HG22	1.58	0.84
3:W:187:LEU:HD11	3:W:188:LEU:HB3	1.51	0.84
1:a:461:LEU:N	1:a:461:LEU:HD23	1.93	0.84
2:E:200:ASP:OD2	4:X:2:MET:HE1	1.78	0.84
1:C:492:TYR:CD2	1:C:492:TYR:O	2.30	0.84
1:K:461:LEU:N	1:K:461:LEU:HD23	1.93	0.84
2:b:113:ALA:HA	2:b:281:ARG:HG2	1.60	0.84
2:D:118:GLU:HB2	2:D:285:THR:HA	1.60	0.84
1:R:193:CYS:HB2	1:R:221:THR:HB	1.58	0.84
3:W:187:LEU:HD12	3:W:188:LEU:CA	2.07	0.84
1:R:95:LEU:HD22	1:R:129:VAL:HG22	1.56	0.84
1:R:227:THR:HG23	1:R:230:GLU:HG3	1.60	0.84
1:R:309:VAL:HG12	1:R:317:VAL:HG11	1.58	0.84
1:Z:27:ASN:ND2	1:Z:46:ASP:HB2	1.92	0.84
1:A:138:GLU:CG	1:A:305:ASN:CG	2.51	0.84
2:E:131:LYS:H	2:E:402:GLN:HE22	1.23	0.84
2:V:161:GLU:HG3	2:V:404:PHE:HB3	1.60	0.84
1:R:27:ASN:ND2	1:R:46:ASP:HB2	1.92	0.83
1:Z:309:VAL:HG12	1:Z:317:VAL:HG11	1.58	0.83
2:b:113:ALA:CB	2:b:281:ARG:CG	2.48	0.83
2:c:42:VAL:HA	2:c:53:THR:HG22	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:136:VAL:C	1:K:137:ILE:CG1	2.42	0.83
2:N:244:ILE:HD11	2:N:294:GLN:HB2	1.60	0.83
4:P:7:ASP:HB2	4:P:77:THR:HG22	1.58	0.83
1:S:107:VAL:HG11	2:V:116:TYR:HE1	1.44	0.83
1:Z:193:CYS:HB2	1:Z:221:THR:HB	1.58	0.83
2:c:337:LEU:HD12	2:c:338:ASP:H	1.43	0.83
1:J:27:ASN:ND2	1:J:46:ASP:HB2	1.92	0.83
2:M:42:VAL:HA	2:M:53:THR:HG22	1.59	0.83
1:B:27:ASN:ND2	1:B:46:ASP:HB2	1.92	0.83
2:V:131:LYS:HB2	2:V:402:GLN:HE22	1.42	0.83
2:d:161:GLU:HG3	2:d:404:PHE:HB3	1.60	0.83
2:D:22:VAL:HG23	2:D:23:PRO:HD2	1.59	0.83
4:X:7:ASP:HB2	4:X:77:THR:HG22	1.58	0.83
1:Y:348:ILE:HG23	2:c:209:MET:HE1	1.60	0.83
2:L:111:ARG:HD3	2:L:281:ARG:HB2	1.61	0.83
2:b:323:ARG:H	2:b:323:ARG:HD2	1.44	0.83
1:A:444:GLN:HA	1:A:447:VAL:HB	1.61	0.82
2:E:42:VAL:HA	2:E:53:THR:HG22	1.59	0.82
1:I:444:GLN:HA	1:I:447:VAL:HB	1.61	0.82
1:J:97:VAL:HG12	1:J:98:PRO:CD	2.08	0.82
2:M:337:LEU:HD12	2:M:338:ASP:H	1.43	0.82
1:S:461:LEU:N	1:S:461:LEU:HD23	1.93	0.82
2:D:379:MET:HE1	2:D:390:VAL:HG11	1.60	0.82
1:I:137:ILE:HG21	2:M:96:ASP:HA	1.59	0.82
3:W:187:LEU:C	3:W:187:LEU:CD1	2.44	0.82
3:O:59:ASN:HD21	3:O:211:PRO:HG2	1.45	0.82
1:Y:444:GLN:HA	1:Y:447:VAL:HB	1.60	0.82
1:Z:227:THR:HG23	1:Z:230:GLU:HG3	1.60	0.82
2:c:416:LYS:HD2	2:c:417:TYR:N	1.94	0.82
1:C:493:ASN:O	1:C:496:ILE:CD1	2.27	0.82
3:G:59:ASN:HD21	3:G:211:PRO:HG2	1.45	0.82
2:F:221:LEU:HD23	2:F:278:LEU:HD13	1.61	0.82
1:J:227:THR:HG23	1:J:230:GLU:HG3	1.60	0.82
2:L:323:ARG:H	2:L:323:ARG:HD2	1.44	0.82
2:T:400:LEU:HB3	2:T:427:PHE:HZ	1.44	0.82
2:D:111:ARG:HD3	2:D:281:ARG:HB2	1.60	0.82
1:B:227:THR:HG23	1:B:230:GLU:HG3	1.60	0.81
2:b:113:ALA:CB	2:b:281:ARG:CA	2.57	0.81
1:C:461:LEU:N	1:C:461:LEU:HD23	1.93	0.81
2:D:17:PHE:CE1	2:D:23:PRO:CG	2.62	0.81
2:F:410:PHE:H	2:F:410:PHE:HD2	1.26	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:428:THR:O	1:I:432:LYS:HG2	1.79	0.81
2:U:268:GLN:H	2:U:268:GLN:NE2	1.79	0.81
1:I:136:VAL:O	1:I:137:ILE:CG2	2.28	0.81
1:Q:444:GLN:HA	1:Q:447:VAL:HB	1.61	0.81
3:e:59:ASN:HD21	3:e:211:PRO:HG2	1.45	0.81
2:U:178:GLY:HA2	2:U:242:ASP:HB2	1.63	0.81
2:c:303:LEU:HD23	2:c:303:LEU:H	1.45	0.81
2:M:178:GLY:HA2	2:M:242:ASP:HB2	1.63	0.81
3:W:59:ASN:HD21	3:W:211:PRO:HG2	1.44	0.81
1:C:495:GLU:HG2	1:C:496:ILE:HD13	1.62	0.81
3:e:190:LEU:HD12	3:e:191:PRO:CA	2.08	0.81
3:e:191:PRO:CA	3:e:192:ALA:CB	2.58	0.81
1:C:132:ILE:H	1:C:132:ILE:HD12	1.45	0.80
1:I:383:THR:HG23	1:I:386:MET:HB2	1.63	0.80
2:M:3:GLY:HA3	2:M:17:PHE:CE2	2.17	0.80
2:T:173:TYR:HB3	2:T:237:VAL:HA	1.63	0.80
2:T:323:ARG:H	2:T:323:ARG:HD2	1.44	0.80
1:a:132:ILE:H	1:a:132:ILE:HD12	1.45	0.80
1:A:383:THR:HG23	1:A:386:MET:HB2	1.63	0.80
2:E:3:GLY:HA3	2:E:17:PHE:CE2	2.17	0.80
2:c:3:GLY:HA3	2:c:17:PHE:CE2	2.17	0.80
2:c:178:GLY:HA2	2:c:242:ASP:HB2	1.63	0.80
1:I:137:ILE:O	1:I:137:ILE:CD1	2.30	0.80
1:R:95:LEU:CD2	1:R:95:LEU:O	2.30	0.80
2:E:132:VAL:HG21	2:E:332:PRO:HB2	1.61	0.80
1:Q:135:GLY:O	1:Q:138:GLU:HG2	1.82	0.80
2:U:3:GLY:HA3	2:U:17:PHE:CE2	2.17	0.80
2:V:131:LYS:HD3	2:V:418:VAL:HG21	1.62	0.80
2:D:22:VAL:HG22	2:D:23:PRO:HD2	1.63	0.80
2:D:311:THR:HG22	2:D:315:LEU:HD21	1.63	0.80
2:E:178:GLY:HA2	2:E:242:ASP:HB2	1.63	0.80
1:a:461:LEU:HD23	1:a:461:LEU:H	1.46	0.80
2:D:19:GLN:CB	2:D:20:ASP:OD2	2.30	0.80
2:E:347:LEU:O	2:E:347:LEU:HG	1.79	0.80
2:E:445:MET:O	2:E:446:VAL:CG1	2.30	0.80
2:L:400:LEU:HB3	2:L:427:PHE:CZ	2.17	0.80
2:d:221:LEU:HD23	2:d:278:LEU:HD13	1.63	0.80
3:e:66:TYR:HB3	3:e:188:LEU:HD13	1.64	0.80
2:E:337:LEU:HD12	2:E:338:ASP:H	1.45	0.80
3:e:191:PRO:HA	3:e:192:ALA:HB2	1.62	0.80
2:E:346:PRO:HG2	2:E:348:VAL:HG11	0.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:347:LEU:O	2:E:347:LEU:CD1	2.30	0.80
1:S:76:MET:HE1	1:S:95:LEU:HD21	1.64	0.80
2:b:3:GLY:HA3	2:b:17:PHE:CE2	2.17	0.80
2:F:111:ARG:HH11	2:F:111:ARG:HG3	1.47	0.79
2:E:347:LEU:O	2:E:348:VAL:CG1	2.30	0.79
1:I:67:GLU:HA	2:M:7:GLN:HG2	1.61	0.79
2:M:402:GLN:N	2:M:445:MET:CE	2.45	0.79
1:Q:52:MET:HE3	1:Q:95:LEU:HA	1.64	0.79
2:T:3:GLY:HA3	2:T:17:PHE:CE2	2.17	0.79
2:U:268:GLN:HE21	2:U:268:GLN:N	1.79	0.79
3:W:188:LEU:O	3:W:188:LEU:CD2	2.30	0.79
1:B:138:GLU:O	1:B:139:ARG:HG2	1.82	0.79
2:D:173:TYR:HB3	2:D:237:VAL:HA	1.63	0.79
2:F:161:GLU:HG3	2:F:404:PHE:HB3	1.62	0.79
1:I:459:VAL:O	1:I:459:VAL:CG1	2.30	0.79
1:K:76:MET:HE1	1:K:95:LEU:HD21	1.64	0.79
1:Q:135:GLY:O	1:Q:138:GLU:CG	2.30	0.79
1:Y:383:THR:HG23	1:Y:386:MET:HB2	1.63	0.79
2:D:22:VAL:CG2	2:D:23:PRO:CD	2.60	0.79
2:N:410:PHE:H	2:N:410:PHE:HD2	1.27	0.79
1:Q:136:VAL:O	1:Q:137:ILE:CG2	2.30	0.79
1:S:132:ILE:H	1:S:132:ILE:HD12	1.45	0.79
1:A:179:ALA:HB1	1:A:259:ILE:HD12	1.64	0.79
2:E:161:GLU:HG3	2:E:404:PHE:HB3	1.64	0.79
1:Q:383:THR:HG23	1:Q:386:MET:HB2	1.63	0.79
3:W:188:LEU:C	3:W:188:LEU:CD2	2.52	0.79
3:e:55:LEU:HD11	3:e:215:LEU:HB2	1.64	0.79
1:A:52:MET:HE3	1:A:95:LEU:HA	1.64	0.79
2:E:347:LEU:HD12	2:E:347:LEU:O	1.81	0.79
1:J:138:GLU:O	1:J:139:ARG:HG2	1.82	0.79
3:W:188:LEU:O	3:W:188:LEU:CD1	2.30	0.79
1:B:172:GLN:HA	5:B:600:ANP:HNB1	1.48	0.79
2:D:17:PHE:HD1	2:D:23:PRO:CD	1.93	0.79
3:G:189:PRO:O	3:G:190:LEU:C	2.23	0.79
1:I:52:MET:HE3	1:I:95:LEU:HA	1.64	0.79
2:M:112:ALA:C	2:M:114:PRO:HD2	2.08	0.79
2:N:254:VAL:HG12	2:N:258:LEU:HG	1.65	0.79
1:R:467:PHE:CD1	1:R:471:LEU:HD21	2.18	0.79
2:V:111:ARG:HH11	2:V:111:ARG:HG3	1.47	0.79
2:d:111:ARG:HG3	2:d:111:ARG:HH11	1.47	0.79
3:G:55:LEU:HD11	3:G:215:LEU:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:461:LEU:HD23	1:K:461:LEU:H	1.46	0.79
2:L:3:GLY:HA3	2:L:17:PHE:CE2	2.18	0.79
1:Q:364:ILE:HG13	1:Q:432:LYS:HG2	1.65	0.79
2:d:410:PHE:H	2:d:410:PHE:HD2	1.30	0.79
2:E:112:ALA:C	2:E:114:PRO:HD2	2.08	0.79
2:F:254:VAL:HG12	2:F:258:LEU:HG	1.65	0.79
1:K:132:ILE:H	1:K:132:ILE:HD12	1.45	0.79
1:R:107:VAL:HG22	1:R:116:ASP:HB2	1.65	0.79
2:c:161:GLU:HG3	2:c:404:PHE:HB3	1.64	0.79
2:b:173:TYR:HB3	2:b:237:VAL:HA	1.63	0.78
1:J:467:PHE:CD1	1:J:471:LEU:HD21	2.18	0.78
2:V:410:PHE:H	2:V:410:PHE:HD2	1.29	0.78
3:e:191:PRO:CB	3:e:192:ALA:CB	2.61	0.78
1:C:492:TYR:O	1:C:492:TYR:HD2	1.66	0.78
2:D:374:ILE:HG12	2:D:382:LEU:HD11	1.63	0.78
2:E:347:LEU:O	2:E:347:LEU:CG	2.30	0.78
2:M:116:TYR:HD1	2:M:117:GLU:N	1.81	0.78
1:Z:138:GLU:O	1:Z:139:ARG:HG2	1.82	0.78
1:B:94:ILE:O	1:B:94:ILE:CG1	2.30	0.78
2:E:349:VAL:CG2	2:E:353:HIS:HB3	2.14	0.78
2:F:457:LYS:HA	2:F:457:LYS:HE3	1.65	0.78
2:U:112:ALA:C	2:U:114:PRO:HD2	2.08	0.78
1:B:467:PHE:CD1	1:B:471:LEU:HD21	2.18	0.78
1:C:76:MET:HE1	1:C:95:LEU:HD21	1.64	0.78
1:S:80:ALA:HA	2:V:25:VAL:HG11	1.64	0.78
2:U:131:LYS:HG3	2:U:418:VAL:HG11	1.65	0.78
2:U:416:LYS:HD2	2:U:417:TYR:N	1.94	0.78
1:Z:95:LEU:O	1:Z:95:LEU:CD1	2.30	0.78
1:Z:467:PHE:CD1	1:Z:471:LEU:HD21	2.18	0.78
2:c:112:ALA:C	2:c:114:PRO:HD2	2.08	0.78
2:N:111:ARG:HH11	2:N:111:ARG:HG3	1.47	0.78
1:Y:52:MET:HE3	1:Y:95:LEU:HA	1.64	0.78
2:d:254:VAL:HG12	2:d:258:LEU:HG	1.65	0.78
2:c:307:SER:HB3	2:c:308:PRO:HD3	1.64	0.78
1:B:107:VAL:HG22	1:B:116:ASP:HB2	1.65	0.78
2:D:323:ARG:H	2:D:323:ARG:HD2	1.47	0.78
2:E:346:PRO:CG	2:E:348:VAL:CG1	2.39	0.78
2:E:445:MET:CA	2:E:445:MET:HE3	2.14	0.78
3:G:66:TYR:CD2	3:G:188:LEU:HD11	2.18	0.78
3:O:55:LEU:HD11	3:O:215:LEU:HB2	1.64	0.78
1:Q:211:LYS:HZ2	1:Q:436:TYR:HE2	1.28	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:138:GLU:O	1:R:139:ARG:HG2	1.82	0.78
2:D:426:GLY:HA2	2:D:449:ILE:HD12	1.66	0.78
2:E:161:GLU:HG3	2:E:404:PHE:CG	2.19	0.78
1:Q:87:LYS:HE3	1:Q:89:LYS:HE3	1.66	0.78
2:c:116:TYR:HD1	2:c:117:GLU:N	1.81	0.78
2:E:416:LYS:HD2	2:E:417:TYR:N	1.98	0.78
1:I:137:ILE:O	1:I:138:GLU:HB2	1.82	0.78
1:K:136:VAL:O	1:K:137:ILE:CG1	2.30	0.78
2:M:265:VAL:HA	3:O:273:THR:HG22	1.64	0.78
2:U:116:TYR:HD1	2:U:117:GLU:N	1.81	0.78
1:C:461:LEU:HD23	1:C:461:LEU:H	1.47	0.77
2:M:161:GLU:HG3	2:M:404:PHE:HB3	1.66	0.77
2:D:400:LEU:HB3	2:D:427:PHE:HZ	1.48	0.77
2:L:173:TYR:HB3	2:L:237:VAL:HA	1.63	0.77
2:L:343:GLN:HG3	2:L:348:VAL:HG11	1.66	0.77
2:V:126:LEU:HB3	2:V:141:LYS:HD2	1.67	0.77
1:Y:87:LYS:HE3	1:Y:89:LYS:HE3	1.66	0.77
1:Q:138:GLU:O	1:Q:305:ASN:CB	2.33	0.77
1:S:459:VAL:HG12	1:S:459:VAL:O	1.84	0.77
2:E:345:ASP:N	2:E:346:PRO:CD	2.46	0.77
1:Z:96:GLU:O	1:Z:97:VAL:CG2	2.33	0.77
1:a:459:VAL:O	1:a:459:VAL:HG12	1.84	0.77
2:E:268:GLN:HE21	2:E:268:GLN:N	1.82	0.77
3:W:55:LEU:HD11	3:W:215:LEU:HB2	1.64	0.77
2:D:377:LEU:HD21	4:H:115:ALA:HB2	1.66	0.77
3:G:167:LEU:HD23	3:G:188:LEU:HD23	1.67	0.77
1:I:87:LYS:HE3	1:I:89:LYS:HE3	1.66	0.77
1:J:107:VAL:HG22	1:J:116:ASP:HB2	1.65	0.77
2:L:394:ARG:HD3	2:L:440:GLU:OE1	1.84	0.77
1:R:95:LEU:HD21	1:R:129:VAL:HG22	0.80	0.77
1:A:87:LYS:HE3	1:A:89:LYS:HE3	1.66	0.77
1:B:95:LEU:HG	1:B:129:VAL:CG2	2.15	0.77
1:C:499:LYS:O	1:C:503:ILE:HG13	1.85	0.77
2:V:233:GLU:HG3	2:V:234:GLY:H	1.50	0.77
2:E:265:VAL:HG13	2:E:267:TYR:HD2	1.49	0.77
2:M:132:VAL:HG21	2:M:332:PRO:HB2	1.67	0.77
2:M:265:VAL:CA	3:O:273:THR:HG22	2.15	0.77
1:S:461:LEU:HD23	1:S:461:LEU:H	1.47	0.77
2:T:379:MET:HE1	2:T:390:VAL:HG11	1.66	0.77
2:b:400:LEU:HB3	2:b:427:PHE:HZ	1.47	0.77
2:c:113:ALA:N	2:c:114:PRO:HD2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:233:GLU:HG3	2:d:234:GLY:H	1.49	0.77
1:A:137:ILE:CG1	1:A:138:GLU:OE1	2.32	0.77
2:E:113:ALA:N	2:E:114:PRO:HD2	2.00	0.77
2:F:7:GLN:HB2	2:F:14:ASP:OD1	1.85	0.77
1:K:499:LYS:O	1:K:503:ILE:HG13	1.85	0.77
2:M:265:VAL:N	3:O:273:THR:HG22	1.99	0.77
4:P:2:MET:HE1	2:c:197:ASN:HB3	0.78	0.77
2:E:116:TYR:HD1	2:E:117:GLU:N	1.81	0.77
2:M:113:ALA:N	2:M:114:PRO:HD2	2.00	0.77
1:Q:137:ILE:HG23	1:Q:137:ILE:O	1.81	0.77
1:R:95:LEU:HD22	1:R:129:VAL:CG2	2.14	0.77
2:T:426:GLY:HA2	2:T:449:ILE:HD12	1.67	0.77
2:U:132:VAL:HG21	2:U:332:PRO:HB2	1.67	0.77
1:a:76:MET:HE1	1:a:95:LEU:HD21	1.64	0.77
2:b:374:ILE:HG12	2:b:382:LEU:HD11	1.65	0.77
1:A:364:ILE:HG13	1:A:432:LYS:HG2	1.65	0.76
4:H:41:LEU:H	4:H:71:VAL:HG23	1.50	0.76
2:V:254:VAL:HG12	2:V:258:LEU:HG	1.65	0.76
4:X:41:LEU:H	4:X:71:VAL:HG23	1.50	0.76
1:Z:107:VAL:HG22	1:Z:116:ASP:HB2	1.65	0.76
3:G:66:TYR:HB3	3:G:188:LEU:CD1	2.15	0.76
2:M:444:TYR:O	2:M:446:VAL:CG1	2.31	0.76
1:A:138:GLU:HB3	1:A:305:ASN:ND2	2.00	0.76
2:F:233:GLU:HG3	2:F:234:GLY:H	1.50	0.76
1:Y:364:ILE:HG13	1:Y:432:LYS:HG2	1.65	0.76
2:c:132:VAL:HG21	2:c:332:PRO:HB2	1.67	0.76
2:U:113:ALA:N	2:U:114:PRO:HD2	2.00	0.76
1:Z:95:LEU:HD12	1:Z:96:GLU:N	2.00	0.76
1:Z:95:LEU:CD1	1:Z:129:VAL:HG22	2.15	0.76
1:I:138:GLU:HG3	1:I:305:ASN:HB3	1.65	0.76
2:N:233:GLU:HG3	2:N:234:GLY:H	1.50	0.76
4:X:2:MET:C	4:X:3:THR:HG23	2.11	0.76
2:d:7:GLN:HB2	2:d:14:ASP:OD1	1.85	0.76
1:a:161:ARG:HH21	1:a:191:ILE:HD11	1.50	0.76
2:b:111:ARG:HG3	2:b:112:ALA:N	1.91	0.76
3:G:66:TYR:CG	3:G:188:LEU:HD11	2.20	0.76
1:I:178:LEU:O	1:I:178:LEU:CD1	2.30	0.76
1:Q:389:LEU:HG	1:Q:448:LEU:CB	2.16	0.76
2:V:7:GLN:HB2	2:V:14:ASP:OD1	1.85	0.76
3:W:186:GLN:HE21	3:W:189:PRO:CG	1.93	0.76
2:b:113:ALA:HB2	2:b:281:ARG:HA	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:347:LEU:C	2:E:348:VAL:CG1	2.41	0.76
2:F:126:LEU:HB3	2:F:141:LYS:HD2	1.67	0.76
1:K:227:THR:HG23	1:K:230:GLU:HG3	1.68	0.76
2:N:131:LYS:HD3	2:N:418:VAL:HG21	1.67	0.76
2:N:161:GLU:HG3	2:N:404:PHE:HB3	1.67	0.76
3:O:188:LEU:O	3:O:188:LEU:CG	2.30	0.76
3:W:269:GLN:O	3:W:273:THR:HG23	1.86	0.76
4:f:41:LEU:H	4:f:71:VAL:HG23	1.51	0.76
2:E:444:TYR:O	2:E:446:VAL:HG13	1.85	0.76
1:S:499:LYS:O	1:S:503:ILE:HG13	1.85	0.76
2:T:126:LEU:HD22	2:T:126:LEU:H	1.51	0.76
2:b:19:GLN:H	2:b:19:GLN:CD	1.94	0.76
2:E:268:GLN:H	2:E:268:GLN:NE2	1.82	0.76
1:I:389:LEU:HG	1:I:448:LEU:CB	2.16	0.76
3:O:269:GLN:O	3:O:273:THR:HG23	1.86	0.76
1:Y:366:PRO:HD2	1:Y:432:LYS:HG3	1.68	0.76
1:a:499:LYS:O	1:a:503:ILE:HG13	1.85	0.76
2:b:126:LEU:H	2:b:126:LEU:HD22	1.51	0.76
2:d:428:LYS:O	2:d:432:GLU:HG2	1.86	0.76
1:A:389:LEU:HG	1:A:448:LEU:CB	2.16	0.75
1:I:136:VAL:C	1:I:137:ILE:HG22	2.11	0.75
2:V:428:LYS:O	2:V:432:GLU:HG2	1.84	0.75
2:c:265:VAL:HG23	3:e:272:ILE:HD13	1.68	0.75
3:e:269:GLN:O	3:e:273:THR:HG23	1.86	0.75
2:E:445:MET:CE	2:E:445:MET:CA	2.61	0.75
2:L:311:THR:HG22	2:L:315:LEU:HD21	1.67	0.75
2:N:109:ILE:HA	2:N:225:THR:HG21	1.69	0.75
1:S:227:THR:HG23	1:S:230:GLU:HG3	1.68	0.75
2:T:400:LEU:HB3	2:T:427:PHE:CZ	2.21	0.75
2:V:109:ILE:HA	2:V:225:THR:HG21	1.68	0.75
3:W:187:LEU:CD2	3:W:223:VAL:HG13	2.16	0.75
1:Z:112:GLY:C	1:Z:114:PRO:HD2	2.12	0.75
3:e:188:LEU:O	3:e:188:LEU:CD1	2.30	0.75
1:I:283:ARG:HG3	3:O:272:ILE:HD12	1.68	0.75
2:M:416:LYS:HD2	2:M:417:TYR:N	2.01	0.75
2:N:131:LYS:HB2	2:N:402:GLN:NE2	2.02	0.75
1:S:493:ASN:H	1:S:496:ILE:CG1	2.00	0.75
1:K:459:VAL:HG12	1:K:459:VAL:O	1.85	0.75
1:R:112:GLY:C	1:R:114:PRO:HD2	2.12	0.75
1:R:461:LEU:HD22	1:R:462:SER:H	1.52	0.75
1:B:461:LEU:HD22	1:B:462:SER:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:186:GLN:HE21	3:e:189:PRO:HG2	1.50	0.75
1:C:161:ARG:HH21	1:C:191:ILE:HD11	1.51	0.75
1:C:459:VAL:HG12	1:C:459:VAL:O	1.84	0.75
2:L:374:ILE:HG12	2:L:382:LEU:HD11	1.67	0.75
2:N:7:GLN:HB2	2:N:14:ASP:OD1	1.85	0.75
2:N:221:LEU:HD23	2:N:278:LEU:HD13	1.68	0.75
1:Q:366:PRO:HD2	1:Q:432:LYS:HG3	1.68	0.75
2:U:265:VAL:HG13	2:U:267:TYR:HD2	1.52	0.75
3:W:199:LYS:HA	3:W:199:LYS:HE3	1.69	0.75
1:a:227:THR:HG23	1:a:230:GLU:HG3	1.68	0.75
3:O:199:LYS:HA	3:O:199:LYS:HE3	1.69	0.75
2:U:161:GLU:HG3	2:U:404:PHE:HB3	1.68	0.75
2:d:126:LEU:HB3	2:d:141:LYS:HD2	1.67	0.75
3:G:269:GLN:O	3:G:273:THR:HG23	1.86	0.75
1:A:211:LYS:HZ2	1:A:436:TYR:HE2	1.35	0.74
2:D:343:GLN:HG3	2:D:348:VAL:HG11	1.68	0.74
2:L:126:LEU:HD22	2:L:126:LEU:H	1.51	0.74
2:N:126:LEU:HB3	2:N:141:LYS:HD2	1.66	0.74
2:b:113:ALA:CB	2:b:114:PRO:CD	2.38	0.74
3:G:199:LYS:HE3	3:G:199:LYS:HA	1.69	0.74
2:N:279:GLN:NE2	2:N:294:GLN:HE22	1.85	0.74
2:b:426:GLY:HA2	2:b:449:ILE:HD12	1.67	0.74
1:A:178:LEU:O	1:A:178:LEU:CD1	2.30	0.74
2:M:71:LEU:HD12	2:M:73:HIS:HD2	1.53	0.74
1:Z:461:LEU:HD22	1:Z:462:SER:H	1.52	0.74
1:K:161:ARG:HH21	1:K:191:ILE:HD11	1.51	0.74
2:N:155:LYS:HE3	2:N:297:TYR:HA	1.68	0.74
1:a:107:VAL:HG11	2:d:116:TYR:HE1	1.53	0.74
2:d:109:ILE:HA	2:d:225:THR:HG21	1.68	0.74
2:D:126:LEU:HD22	2:D:126:LEU:H	1.51	0.74
2:F:428:LYS:O	2:F:432:GLU:HG2	1.87	0.74
1:B:112:GLY:C	1:B:114:PRO:HD2	2.12	0.74
2:D:17:PHE:HD1	2:D:23:PRO:HD3	1.46	0.74
2:N:42:VAL:HA	2:N:53:THR:HG22	1.70	0.74
1:Q:456:LEU:O	1:Q:460:GLU:HA	1.88	0.74
1:Y:389:LEU:HG	1:Y:448:LEU:CB	2.16	0.74
2:E:71:LEU:HD12	2:E:73:HIS:HD2	1.53	0.74
2:F:155:LYS:HE3	2:F:297:TYR:HA	1.70	0.74
2:M:353:HIS:CE1	2:M:420:LEU:HD11	2.23	0.74
2:U:116:TYR:O	2:U:117:GLU:HG2	1.87	0.74
1:Y:76:MET:HE2	1:Y:234:LEU:HD13	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:PRO:HD2	1:A:432:LYS:HG3	1.68	0.74
2:d:131:LYS:HB2	2:d:402:GLN:NE2	2.03	0.74
1:J:195:TYR:CD1	1:J:259:ILE:HD11	2.21	0.74
2:M:307:SER:HB3	2:M:308:PRO:HD3	1.69	0.74
2:b:311:THR:HG22	2:b:315:LEU:HD21	1.68	0.74
2:c:131:LYS:HG3	2:c:418:VAL:HG11	1.69	0.74
1:C:227:THR:HG23	1:C:230:GLU:HG3	1.68	0.74
2:D:167:ALA:HA	2:D:172:GLY:HA2	1.70	0.74
2:F:285:THR:HG22	2:F:287:THR:H	1.52	0.74
1:J:461:LEU:HD22	1:J:462:SER:H	1.52	0.74
1:K:493:ASN:H	1:K:496:ILE:CG1	2.01	0.74
2:M:116:TYR:O	2:M:117:GLU:HG2	1.87	0.74
2:M:161:GLU:HG3	2:M:404:PHE:CG	2.22	0.74
2:T:167:ALA:HA	2:T:172:GLY:HA2	1.70	0.74
2:T:343:GLN:HG3	2:T:348:VAL:HG11	1.70	0.74
2:c:71:LEU:HD12	2:c:73:HIS:HD2	1.53	0.74
1:A:137:ILE:C	1:A:137:ILE:HD12	2.13	0.73
3:G:16:THR:HG22	4:H:124:ALA:HB1	1.70	0.73
1:I:456:LEU:O	1:I:460:GLU:HA	1.88	0.73
1:J:96:GLU:HB3	1:J:128:ALA:HA	1.70	0.73
1:J:112:GLY:C	1:J:114:PRO:HD2	2.12	0.73
1:Y:137:ILE:O	1:Y:137:ILE:HG12	1.87	0.73
2:c:71:LEU:HD12	2:c:73:HIS:CD2	2.23	0.73
2:c:116:TYR:O	2:c:117:GLU:HG2	1.88	0.73
1:A:76:MET:HE2	1:A:234:LEU:HD13	1.70	0.73
2:F:19:GLN:NE2	2:F:19:GLN:H	1.86	0.73
2:F:109:ILE:HA	2:F:225:THR:HG21	1.68	0.73
2:M:71:LEU:HD12	2:M:73:HIS:CD2	2.23	0.73
1:Q:76:MET:HE2	1:Q:234:LEU:HD13	1.70	0.73
1:S:161:ARG:HH21	1:S:191:ILE:HD11	1.51	0.73
2:V:19:GLN:NE2	2:V:19:GLN:H	1.86	0.73
2:E:71:LEU:HD12	2:E:73:HIS:CD2	2.23	0.73
2:F:323:ARG:HH11	2:F:323:ARG:CG	1.99	0.73
4:H:128:LEU:HB3	4:H:130:VAL:HG23	1.70	0.73
1:J:402:GLU:HG3	1:J:403:LEU:HD23	1.70	0.73
1:R:443:GLN:HE21	1:R:443:GLN:H	1.37	0.73
2:U:71:LEU:HD12	2:U:73:HIS:HD2	1.53	0.73
1:Z:453:ARG:HH11	1:Z:453:ARG:HG3	1.54	0.73
1:a:493:ASN:H	1:a:496:ILE:CG1	2.01	0.73
1:A:456:LEU:O	1:A:460:GLU:HA	1.88	0.73
2:E:116:TYR:O	2:E:117:GLU:HG2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:456:LEU:N	1:K:456:LEU:HD22	2.04	0.73
2:L:131:LYS:HG3	2:L:402:GLN:OE1	1.87	0.73
4:P:41:LEU:H	4:P:71:VAL:HG23	1.50	0.73
4:f:128:LEU:HB3	4:f:130:VAL:HG23	1.70	0.73
1:R:453:ARG:HH11	1:R:453:ARG:HG3	1.54	0.73
1:a:456:LEU:HD22	1:a:456:LEU:N	2.04	0.73
1:B:402:GLU:HG3	1:B:403:LEU:HD23	1.70	0.73
2:N:131:LYS:H	2:N:402:GLN:HE22	1.34	0.73
2:U:71:LEU:HD12	2:U:73:HIS:CD2	2.23	0.73
1:B:443:GLN:HE21	1:B:443:GLN:H	1.37	0.73
1:C:493:ASN:O	1:C:496:ILE:HD11	1.89	0.73
3:G:66:TYR:CG	3:G:188:LEU:CD1	2.72	0.73
2:M:443:PHE:CD2	2:M:443:PHE:N	2.54	0.73
1:R:195:TYR:CD1	1:R:259:ILE:HD11	2.21	0.73
2:F:131:LYS:HB2	2:F:402:GLN:NE2	2.02	0.73
1:I:76:MET:HE2	1:I:234:LEU:HD13	1.70	0.73
2:U:353:HIS:CE1	2:U:420:LEU:HD11	2.23	0.73
2:F:42:VAL:HA	2:F:53:THR:HG22	1.70	0.73
2:N:428:LYS:O	2:N:432:GLU:HG2	1.89	0.73
4:X:128:LEU:HB3	4:X:130:VAL:HG23	1.70	0.73
1:Y:456:LEU:O	1:Y:460:GLU:HA	1.88	0.73
2:D:19:GLN:C	2:D:20:ASP:OD2	2.31	0.73
2:D:394:ARG:HD3	2:D:440:GLU:OE1	1.89	0.73
2:E:445:MET:C	2:E:446:VAL:CG1	2.61	0.73
1:K:80:ALA:HA	2:N:25:VAL:HG11	1.71	0.73
4:P:128:LEU:HB3	4:P:130:VAL:HG23	1.70	0.73
2:V:42:VAL:HA	2:V:53:THR:HG22	1.70	0.73
1:Z:402:GLU:HG3	1:Z:403:LEU:HD23	1.70	0.73
2:c:161:GLU:HG3	2:c:404:PHE:CG	2.23	0.73
3:e:199:LYS:HA	3:e:199:LYS:HE3	1.69	0.73
2:E:43:GLN:HG3	2:E:54:ILE:HD13	1.71	0.72
4:P:55:GLN:HG3	4:P:56:HIS:HD2	1.54	0.72
1:J:453:ARG:HH11	1:J:453:ARG:HG3	1.54	0.72
1:Q:206:SER:O	1:Q:210:ARG:HG3	1.90	0.72
1:R:94:ILE:O	1:R:95:LEU:CD1	2.30	0.72
1:R:402:GLU:HG3	1:R:403:LEU:HD23	1.70	0.72
2:T:311:THR:HG22	2:T:315:LEU:HD21	1.69	0.72
2:V:221:LEU:HD23	2:V:278:LEU:HD13	1.70	0.72
1:A:206:SER:O	1:A:210:ARG:HG3	1.90	0.72
1:B:403:LEU:HD21	1:B:420:GLN:HE22	1.55	0.72
2:T:374:ILE:HG12	2:T:382:LEU:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:187:LEU:HD11	3:W:188:LEU:HB2	1.69	0.72
4:H:55:GLN:HG3	4:H:56:HIS:HD2	1.54	0.72
1:J:158:PRO:HB3	1:J:382:GLN:HG2	1.72	0.72
2:M:303:LEU:HD23	2:M:303:LEU:H	1.54	0.72
4:P:2:MET:HE2	4:P:2:MET:HA	1.71	0.72
2:d:19:GLN:NE2	2:d:19:GLN:H	1.86	0.72
1:B:406:PHE:O	1:B:409:PHE:HD1	1.73	0.72
2:E:445:MET:HA	2:E:445:MET:HE3	1.71	0.72
1:Q:67:GLU:HA	2:U:7:GLN:HG2	1.72	0.72
1:Q:140:GLN:HG3	1:Q:305:ASN:HB2	1.72	0.72
1:Z:443:GLN:HE21	1:Z:443:GLN:H	1.37	0.72
1:a:80:ALA:HA	2:d:25:VAL:HG11	1.70	0.72
2:b:400:LEU:HB3	2:b:427:PHE:CZ	2.23	0.72
4:f:55:GLN:HG3	4:f:56:HIS:HD2	1.54	0.72
1:C:456:LEU:N	1:C:456:LEU:HD22	2.04	0.72
1:I:206:SER:O	1:I:210:ARG:HG3	1.90	0.72
2:b:111:ARG:NH1	2:b:111:ARG:CA	2.38	0.72
2:b:113:ALA:HB1	2:b:114:PRO:HD3	1.72	0.72
1:A:371:GLY:H	1:A:394:ARG:HH12	1.38	0.72
2:E:442:ALA:CB	2:E:443:PHE:CE2	2.64	0.72
3:G:187:LEU:O	3:G:187:LEU:CD1	2.30	0.72
1:I:140:GLN:HG3	1:I:305:ASN:HB2	1.72	0.72
1:S:296:ARG:HA	2:T:210:ASN:HB3	1.72	0.72
1:S:456:LEU:N	1:S:456:LEU:HD22	2.04	0.72
1:Y:206:SER:O	1:Y:210:ARG:HG3	1.90	0.72
2:c:268:GLN:H	2:c:268:GLN:NE2	1.88	0.72
2:F:244:ILE:HD11	2:F:294:GLN:HB2	1.71	0.72
1:I:211:LYS:HZ2	1:I:436:TYR:HE2	1.36	0.72
1:Y:371:GLY:H	1:Y:394:ARG:HH12	1.38	0.72
2:E:349:VAL:HG22	2:E:353:HIS:HB3	1.70	0.72
2:N:131:LYS:HG2	2:N:423:THR:HG23	1.71	0.72
1:S:492:TYR:HA	1:S:496:ILE:HG13	1.72	0.72
2:b:167:ALA:HA	2:b:172:GLY:HA2	1.70	0.72
2:c:43:GLN:HG3	2:c:54:ILE:HD13	1.71	0.72
3:e:189:PRO:O	3:e:191:PRO:CD	2.35	0.72
1:B:95:LEU:O	1:B:95:LEU:CD1	2.34	0.72
1:B:195:TYR:CD1	1:B:259:ILE:HD11	2.21	0.72
2:E:353:HIS:CE1	2:E:420:LEU:HD11	2.24	0.72
2:F:120:SER:OG	2:F:286:LYS:HE3	1.90	0.72
1:J:406:PHE:O	1:J:409:PHE:HD1	1.73	0.72
2:U:231:ARG:HD3	2:U:290:ILE:HG13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ARG:HH11	1:B:453:ARG:HG3	1.54	0.71
2:F:243:ASN:HA	2:F:295:ALA:O	1.90	0.71
2:L:167:ALA:HA	2:L:172:GLY:HA2	1.70	0.71
2:M:43:GLN:HG3	2:M:54:ILE:HD13	1.71	0.71
2:N:19:GLN:NE2	2:N:19:GLN:H	1.86	0.71
1:R:461:LEU:HD22	1:R:462:SER:N	2.05	0.71
2:D:400:LEU:HB3	2:D:427:PHE:CZ	2.24	0.71
1:J:94:ILE:O	1:J:96:GLU:HG2	1.90	0.71
2:M:224:LEU:HD12	2:M:278:LEU:HD22	1.72	0.71
2:V:323:ARG:HH11	2:V:323:ARG:CG	2.02	0.71
1:a:450:ALA:HA	1:a:456:LEU:HD21	1.72	0.71
2:d:42:VAL:HA	2:d:53:THR:HG22	1.70	0.71
2:d:244:ILE:HD11	2:d:294:GLN:HB2	1.70	0.71
1:A:140:GLN:HG3	1:A:305:ASN:HB2	1.72	0.71
2:E:442:ALA:C	2:E:443:PHE:HD2	1.99	0.71
2:M:265:VAL:HG13	2:M:267:TYR:HD2	1.55	0.71
1:Y:140:GLN:HG3	1:Y:305:ASN:HB2	1.72	0.71
1:Z:406:PHE:O	1:Z:409:PHE:HD1	1.73	0.71
1:K:426:LYS:HD3	1:K:460:GLU:HB3	1.73	0.71
1:K:492:TYR:HA	1:K:496:ILE:HG13	1.72	0.71
2:b:130:ILE:HD12	2:b:133:ILE:HD12	1.72	0.71
1:A:137:ILE:O	1:A:137:ILE:CG2	2.38	0.71
1:C:492:TYR:C	1:C:492:TYR:CD2	2.67	0.71
2:D:130:ILE:HD12	2:D:133:ILE:HD12	1.72	0.71
4:X:55:GLN:HG3	4:X:56:HIS:HD2	1.54	0.71
1:Z:195:TYR:CD1	1:Z:259:ILE:HD11	2.21	0.71
3:e:49:ARG:NH1	3:e:191:PRO:O	2.24	0.71
1:B:158:PRO:HB3	1:B:382:GLN:HG2	1.72	0.71
2:D:111:ARG:NH1	2:D:111:ARG:HB2	2.06	0.71
1:I:240:TYR:OH	1:I:293:LEU:HD12	1.90	0.71
1:J:144:GLN:HB2	1:J:161:ARG:HB2	1.73	0.71
1:J:443:GLN:HE21	1:J:443:GLN:H	1.37	0.71
1:R:406:PHE:O	1:R:409:PHE:HD1	1.73	0.71
1:S:450:ALA:HA	1:S:456:LEU:HD21	1.72	0.71
2:U:303:LEU:HD23	2:U:303:LEU:H	1.56	0.71
2:V:243:ASN:HA	2:V:295:ALA:O	1.90	0.71
1:Y:240:TYR:OH	1:Y:293:LEU:HD12	1.90	0.71
1:K:161:ARG:HA	1:K:325:THR:OG1	1.91	0.71
2:E:445:MET:C	2:E:446:VAL:HG13	2.16	0.71
2:M:113:ALA:HB3	2:M:281:ARG:HG2	1.72	0.71
2:V:244:ILE:HD11	2:V:294:GLN:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ARG:HH11	2:F:300:ALA:HB3	1.55	0.71
2:D:285:THR:HG23	2:D:288:GLY:H	1.55	0.71
2:E:360:VAL:HA	2:E:431:MET:HE1	1.73	0.71
1:J:403:LEU:HD21	1:J:420:GLN:HE22	1.55	0.71
1:K:317:VAL:CA	1:K:318:LYS:HB2	2.21	0.71
2:U:43:GLN:HG3	2:U:54:ILE:HD13	1.71	0.71
1:Z:158:PRO:HB3	1:Z:382:GLN:HG2	1.72	0.71
1:S:66:LEU:CD1	2:T:8:VAL:HB	2.21	0.71
1:J:95:LEU:HD12	1:J:96:GLU:N	2.05	0.70
1:K:107:VAL:HG11	2:N:116:TYR:HE1	1.56	0.70
2:L:130:ILE:HD12	2:L:133:ILE:HD12	1.72	0.70
2:L:323:ARG:H	2:L:323:ARG:CD	2.03	0.70
1:S:161:ARG:HA	1:S:325:THR:OG1	1.91	0.70
1:S:493:ASN:O	1:S:496:ILE:CG1	2.39	0.70
1:I:180:ILE:HD12	1:I:211:LYS:HE2	1.72	0.70
2:b:79:VAL:HB	2:b:229:LYS:HG2	1.73	0.70
1:B:144:GLN:HB2	1:B:161:ARG:HB2	1.73	0.70
1:C:161:ARG:HA	1:C:325:THR:OG1	1.91	0.70
1:C:317:VAL:CA	1:C:318:LYS:HB2	2.21	0.70
2:E:131:LYS:HG3	2:E:418:VAL:HG11	1.73	0.70
1:J:97:VAL:HG11	1:J:112:GLY:CA	2.20	0.70
1:Q:489:THR:HG23	1:Q:491:GLY:H	1.57	0.70
1:R:403:LEU:HD21	1:R:420:GLN:HE22	1.55	0.70
1:Z:403:LEU:HD21	1:Z:420:GLN:HE22	1.55	0.70
1:A:413:LEU:H	1:A:413:LEU:HD22	1.57	0.70
1:B:461:LEU:HD22	1:B:462:SER:N	2.06	0.70
1:K:449:PHE:HB3	1:K:504:LEU:HD11	1.73	0.70
2:N:134:ASP:HB3	2:N:420:LEU:HD13	1.73	0.70
3:O:167:LEU:CD2	3:O:188:LEU:HD23	2.20	0.70
2:T:130:ILE:HD12	2:T:133:ILE:HD12	1.72	0.70
1:Y:211:LYS:HZ2	1:Y:436:TYR:HE2	1.36	0.70
1:Z:144:GLN:HB2	1:Z:161:ARG:HB2	1.73	0.70
1:a:317:VAL:CA	1:a:318:LYS:HB2	2.21	0.70
1:a:492:TYR:HA	1:a:496:ILE:HG13	1.72	0.70
2:E:344:LEU:O	2:E:346:PRO:HD2	1.92	0.70
1:I:371:GLY:H	1:I:394:ARG:HH12	1.38	0.70
1:I:413:LEU:H	1:I:413:LEU:HD22	1.57	0.70
1:a:426:LYS:HD3	1:a:460:GLU:HB3	1.73	0.70
1:A:240:TYR:OH	1:A:293:LEU:HD12	1.90	0.70
1:C:450:ALA:HA	1:C:456:LEU:HD21	1.73	0.70
1:C:483:MET:O	1:C:486:ILE:HG22	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:VAL:HG22	2:D:23:PRO:CD	2.21	0.70
1:Q:240:TYR:OH	1:Q:293:LEU:HD12	1.90	0.70
1:R:158:PRO:HB3	1:R:382:GLN:HG2	1.72	0.70
1:K:317:VAL:HA	1:K:318:LYS:CB	2.20	0.70
1:K:450:ALA:HA	1:K:456:LEU:HD21	1.72	0.70
2:L:285:THR:HG23	2:L:288:GLY:H	1.57	0.70
1:Q:137:ILE:O	1:Q:137:ILE:HD13	1.92	0.70
2:T:79:VAL:HB	2:T:229:LYS:HG2	1.73	0.70
2:V:131:LYS:HB2	2:V:402:GLN:NE2	2.06	0.70
4:f:71:VAL:HG12	4:f:76:VAL:HB	1.74	0.70
1:I:489:THR:HG23	1:I:491:GLY:H	1.57	0.70
1:J:461:LEU:HD22	1:J:462:SER:N	2.06	0.70
2:L:79:VAL:HB	2:L:229:LYS:HG2	1.73	0.70
2:L:426:GLY:HA2	2:L:449:ILE:HD12	1.74	0.70
2:M:265:VAL:H	3:O:273:THR:CG2	2.03	0.70
4:P:2:MET:CE	4:P:2:MET:HA	2.21	0.70
1:R:385:ILE:HD13	1:R:444:GLN:HE22	1.56	0.70
2:b:118:GLU:HB2	2:b:285:THR:HA	1.72	0.70
1:I:208:VAL:O	1:I:212:LEU:HB2	1.91	0.70
2:U:307:SER:HB3	2:U:308:PRO:HD3	1.73	0.70
1:A:208:VAL:O	1:A:212:LEU:HB2	1.91	0.70
1:J:385:ILE:HD13	1:J:444:GLN:HE22	1.56	0.70
1:K:483:MET:O	1:K:486:ILE:HG22	1.92	0.70
2:L:199:ILE:O	2:L:202:VAL:HG22	1.92	0.70
2:L:377:LEU:HD21	4:P:115:ALA:HB2	1.74	0.70
1:Q:208:VAL:O	1:Q:212:LEU:HB2	1.91	0.70
1:S:483:MET:O	1:S:486:ILE:HG22	1.92	0.70
1:Z:461:LEU:HD22	1:Z:462:SER:N	2.06	0.70
1:a:161:ARG:HA	1:a:325:THR:OG1	1.91	0.70
3:e:191:PRO:CA	3:e:192:ALA:HB2	2.22	0.70
1:B:110:THR:HG21	1:B:234:LEU:HG	1.74	0.69
1:C:426:LYS:HD3	1:C:460:GLU:HB3	1.73	0.69
2:D:199:ILE:O	2:D:202:VAL:HG22	1.92	0.69
2:L:111:ARG:NH1	2:L:111:ARG:HB2	2.06	0.69
1:S:449:PHE:HB3	1:S:504:LEU:HD11	1.73	0.69
1:S:492:TYR:C	1:S:493:ASN:ND2	2.40	0.69
2:U:370:LEU:HD13	2:U:382:LEU:HD11	1.74	0.69
1:B:385:ILE:HD13	1:B:444:GLN:HE22	1.56	0.69
1:A:489:THR:HG23	1:A:491:GLY:H	1.57	0.69
1:J:110:THR:HG21	1:J:234:LEU:HG	1.74	0.69
1:Q:365:ARG:HG2	5:Q:600:ANP:C2	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:317:VAL:CA	1:S:318:LYS:HB2	2.21	0.69
2:T:111:ARG:NH1	2:T:111:ARG:HB2	2.06	0.69
1:Y:208:VAL:O	1:Y:212:LEU:HB2	1.91	0.69
1:Z:110:THR:HG21	1:Z:234:LEU:HG	1.74	0.69
1:C:449:PHE:HB3	1:C:504:LEU:HD11	1.73	0.69
2:D:161:GLU:HG3	2:D:404:PHE:CG	2.28	0.69
1:R:283:ARG:HH11	2:V:300:ALA:HB3	1.57	0.69
1:Q:371:GLY:H	1:Q:394:ARG:HH12	1.38	0.69
1:S:426:LYS:HD3	1:S:460:GLU:HB3	1.73	0.69
3:W:65:PRO:HB2	3:W:219:LEU:HD23	1.75	0.69
1:Z:259:ILE:O	1:Z:259:ILE:HG12	1.93	0.69
2:b:199:ILE:O	2:b:202:VAL:HG22	1.92	0.69
3:e:65:PRO:HB2	3:e:219:LEU:HD23	1.75	0.69
1:R:95:LEU:HD13	1:R:96:GLU:CA	2.22	0.69
2:T:199:ILE:O	2:T:202:VAL:HG22	1.92	0.69
2:T:403:PRO:HD3	2:T:445:MET:HG3	1.75	0.69
2:U:161:GLU:HG3	2:U:404:PHE:CG	2.28	0.69
2:V:285:THR:HG22	2:V:287:THR:H	1.56	0.69
1:a:483:MET:O	1:a:486:ILE:HG22	1.92	0.69
1:Y:489:THR:HG23	1:Y:491:GLY:H	1.57	0.69
2:b:394:ARG:HD3	2:b:440:GLU:OE1	1.93	0.69
2:D:79:VAL:HB	2:D:229:LYS:HG2	1.73	0.69
2:E:265:VAL:N	3:G:273:THR:HG22	2.08	0.69
2:E:346:PRO:CB	2:E:348:VAL:HG11	2.22	0.69
1:I:179:ALA:HB1	1:I:259:ILE:HD12	1.75	0.69
2:M:244:ILE:HD11	2:M:275:MET:HE1	1.74	0.69
2:N:243:ASN:HA	2:N:295:ALA:O	1.93	0.69
1:R:110:THR:HG21	1:R:234:LEU:HG	1.74	0.69
1:R:144:GLN:HB2	1:R:161:ARG:HB2	1.73	0.69
1:Z:385:ILE:HD13	1:Z:444:GLN:HE22	1.56	0.69
2:b:285:THR:HG23	2:b:288:GLY:H	1.55	0.69
2:d:224:LEU:HD21	2:d:278:LEU:HD12	1.74	0.69
4:H:71:VAL:HG12	4:H:76:VAL:HB	1.74	0.69
2:b:323:ARG:H	2:b:323:ARG:CD	2.05	0.69
2:D:403:PRO:HD3	2:D:445:MET:HG3	1.75	0.69
4:X:71:VAL:HG12	4:X:76:VAL:HB	1.74	0.69
1:B:259:ILE:O	1:B:259:ILE:HG12	1.93	0.68
2:E:403:PRO:HG2	2:E:415:GLY:HA2	1.75	0.68
2:F:240:PHE:HD2	2:F:293:VAL:HG22	1.58	0.68
1:Q:413:LEU:HD22	1:Q:413:LEU:H	1.57	0.68
2:c:353:HIS:CE1	2:c:420:LEU:HD11	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:PHE:CE1	2:D:23:PRO:HG2	2.26	0.68
2:D:398:ARG:HD2	2:D:440:GLU:HB3	1.75	0.68
2:E:344:LEU:C	2:E:346:PRO:HD3	2.17	0.68
1:J:259:ILE:O	1:J:259:ILE:HG12	1.93	0.68
2:M:316:ASP:HB3	2:M:343:GLN:HE22	1.56	0.68
2:b:161:GLU:HG3	2:b:404:PHE:CG	2.27	0.68
1:A:67:GLU:HA	2:E:7:GLN:HG2	1.74	0.68
1:B:384:LYS:HE2	1:B:384:LYS:H	1.59	0.68
1:C:187:ARG:O	1:C:187:ARG:HG2	1.93	0.68
2:E:316:ASP:HB3	2:E:343:GLN:HE22	1.58	0.68
1:J:384:LYS:HE2	1:J:384:LYS:H	1.58	0.68
2:M:131:LYS:HG3	2:M:418:VAL:HG11	1.74	0.68
4:P:71:VAL:HG12	4:P:76:VAL:HB	1.74	0.68
1:Q:136:VAL:O	1:Q:137:ILE:CB	2.40	0.68
1:S:47:CYS:O	2:T:63:ARG:HB2	1.93	0.68
1:S:187:ARG:O	1:S:187:ARG:HG2	1.93	0.68
3:W:59:ASN:ND2	3:W:211:PRO:HG2	2.08	0.68
1:a:187:ARG:HG2	1:a:187:ARG:O	1.93	0.68
2:D:323:ARG:H	2:D:323:ARG:CD	2.07	0.68
1:J:365:ARG:HG2	5:J:600:ANP:C2	2.24	0.68
1:Y:137:ILE:HG21	2:c:96:ASP:HA	1.76	0.68
1:a:449:PHE:HB3	1:a:504:LEU:HD11	1.73	0.68
2:d:285:THR:HG22	2:d:287:THR:H	1.57	0.68
2:N:16:GLU:HG3	2:N:18:PRO:HD3	1.76	0.68
2:U:316:ASP:HB3	2:U:343:GLN:HE22	1.59	0.68
1:Z:384:LYS:HE2	1:Z:384:LYS:H	1.59	0.68
1:R:384:LYS:HE2	1:R:384:LYS:H	1.59	0.68
2:T:207:GLY:HA3	2:T:219:VAL:HG21	1.76	0.68
1:Z:52:MET:O	1:Z:52:MET:CG	2.37	0.68
2:b:111:ARG:NH1	2:b:111:ARG:CB	2.57	0.68
1:K:480:ALA:N	1:K:481:PRO:HD2	2.09	0.68
2:U:403:PRO:HG2	2:U:415:GLY:HA2	1.76	0.68
1:Y:413:LEU:HD22	1:Y:413:LEU:H	1.57	0.68
2:E:197:ASN:HB3	4:X:2:MET:HG2	1.76	0.68
1:I:348:ILE:HG23	2:M:209:MET:HE1	1.76	0.68
1:K:177:ALA:O	1:K:181:ASP:HB2	1.94	0.68
2:L:207:GLY:HA3	2:L:219:VAL:HG21	1.76	0.68
2:M:265:VAL:HG13	2:M:267:TYR:CD2	2.28	0.68
2:M:402:GLN:H	2:M:445:MET:HE1	1.57	0.68
1:R:259:ILE:O	1:R:259:ILE:HG12	1.92	0.68
2:d:90:VAL:HG13	2:d:91:LEU:HD22	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:TYR:CD1	2:E:117:GLU:N	2.60	0.68
3:G:59:ASN:ND2	3:G:211:PRO:HG2	2.08	0.68
2:U:116:TYR:CD1	2:U:117:GLU:N	2.60	0.68
1:A:137:ILE:HD11	1:A:138:GLU:CB	2.08	0.68
1:C:440:SER:C	1:C:442:ALA:H	2.02	0.68
3:O:59:ASN:ND2	3:O:211:PRO:HG2	2.08	0.68
2:V:90:VAL:HG13	2:V:91:LEU:HD22	1.76	0.68
1:Z:34:VAL:HG12	2:c:45:GLN:HB2	1.74	0.68
1:Z:241:ALA:O	1:Z:245:MET:HG3	1.94	0.68
2:b:207:GLY:HA3	2:b:219:VAL:HG21	1.76	0.68
2:c:231:ARG:HD3	2:c:290:ILE:HG13	1.74	0.68
3:e:191:PRO:HA	3:e:192:ALA:CB	2.24	0.68
1:A:32:VAL:CG2	1:A:42:HIS:HB2	2.25	0.67
2:T:111:ARG:HH21	2:T:224:LEU:HD12	1.59	0.67
2:U:31:VAL:HG22	2:U:68:VAL:HB	1.75	0.67
1:a:480:ALA:N	1:a:481:PRO:HD2	2.09	0.67
1:B:241:ALA:O	1:B:245:MET:HG3	1.94	0.67
2:D:111:ARG:HH21	2:D:224:LEU:HD12	1.59	0.67
2:F:90:VAL:HG13	2:F:91:LEU:HD22	1.76	0.67
1:J:241:ALA:O	1:J:245:MET:HG3	1.94	0.67
1:C:480:ALA:N	1:C:481:PRO:HD2	2.09	0.67
1:I:32:VAL:CG2	1:I:42:HIS:HB2	2.25	0.67
2:N:90:VAL:HG13	2:N:91:LEU:HD22	1.76	0.67
1:S:480:ALA:N	1:S:481:PRO:HD2	2.09	0.67
3:W:66:TYR:HB3	3:W:188:LEU:HD21	1.75	0.67
1:a:177:ALA:O	1:a:181:ASP:HB2	1.94	0.67
2:c:31:VAL:HG22	2:c:68:VAL:HB	1.75	0.67
2:E:303:LEU:H	2:E:303:LEU:HD23	1.60	0.67
1:J:52:MET:CE	1:J:95:LEU:HD13	2.24	0.67
1:J:97:VAL:HG11	1:J:112:GLY:HA2	1.77	0.67
1:Z:172:GLN:HA	5:Z:600:ANP:HNB1	1.59	0.67
1:Z:402:GLU:HG3	1:Z:403:LEU:N	2.10	0.67
1:C:80:ALA:HA	2:F:25:VAL:HG11	1.76	0.67
2:E:189:PHE:O	2:E:193:MET:HG3	1.95	0.67
2:L:111:ARG:HH21	2:L:224:LEU:HD12	1.59	0.67
2:M:395:LYS:HD3	2:M:443:PHE:CZ	2.29	0.67
2:T:398:ARG:HD2	2:T:440:GLU:HB3	1.76	0.67
2:U:180:GLY:O	2:U:209:MET:HG2	1.95	0.67
2:U:189:PHE:O	2:U:193:MET:HG3	1.95	0.67
1:Y:361:ASN:H	1:Y:361:ASN:HD22	1.42	0.67
2:c:116:TYR:CD1	2:c:117:GLU:N	2.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LEU:HG	1:B:129:VAL:HG22	1.75	0.67
4:H:75:ASN:HD22	4:H:76:VAL:N	1.93	0.67
1:I:361:ASN:H	1:I:361:ASN:HD22	1.42	0.67
1:J:62:ILE:HD11	1:J:95:LEU:HD22	1.74	0.67
1:K:150:TYR:HA	1:K:433:GLN:HE22	1.60	0.67
2:M:231:ARG:HD3	2:M:290:ILE:HG13	1.77	0.67
2:M:305:ASP:O	2:M:308:PRO:HD2	1.94	0.67
2:c:189:PHE:O	2:c:193:MET:HG3	1.95	0.67
1:B:402:GLU:HG3	1:B:403:LEU:N	2.10	0.67
2:E:113:ALA:HB3	2:E:281:ARG:HG2	1.77	0.67
2:E:164:ARG:HA	2:E:201:LYS:HZ2	1.60	0.67
3:G:64:HIS:CD2	3:G:64:HIS:O	2.48	0.67
2:L:364:LEU:HD23	2:L:396:ILE:HD11	1.76	0.67
3:O:189:PRO:O	3:O:190:LEU:C	2.33	0.67
1:Y:32:VAL:CG2	1:Y:42:HIS:HB2	2.24	0.67
1:a:440:SER:C	1:a:442:ALA:H	2.02	0.67
2:c:397:GLN:HA	2:c:400:LEU:HD22	1.76	0.67
1:B:365:ARG:HG2	5:B:600:ANP:C2	2.25	0.67
2:E:265:VAL:HG13	2:E:267:TYR:CD2	2.28	0.67
2:L:398:ARG:HD2	2:L:440:GLU:HB3	1.77	0.67
3:O:188:LEU:C	3:O:188:LEU:HD12	2.18	0.67
1:R:51:GLU:HA	1:R:94:ILE:HG23	0.75	0.67
1:R:241:ALA:O	1:R:245:MET:HG3	1.94	0.67
1:S:177:ALA:O	1:S:181:ASP:HB2	1.94	0.67
2:T:279:GLN:HG2	2:T:314:HIS:CB	2.25	0.67
1:C:150:TYR:HA	1:C:433:GLN:HE22	1.60	0.67
2:E:161:GLU:HG3	2:E:404:PHE:CB	2.24	0.67
3:O:65:PRO:HB2	3:O:219:LEU:HD23	1.75	0.67
4:P:75:ASN:HD22	4:P:76:VAL:N	1.93	0.67
3:e:59:ASN:ND2	3:e:211:PRO:HG2	2.08	0.67
2:F:131:LYS:HG2	2:F:423:THR:HG23	1.76	0.67
3:G:65:PRO:HB2	3:G:219:LEU:HD23	1.75	0.67
1:K:440:SER:C	1:K:442:ALA:H	2.02	0.67
1:Q:48:MET:HB3	2:U:63:ARG:HG2	1.75	0.67
2:U:139:PHE:HE2	2:U:162:LEU:HD21	1.60	0.67
2:c:265:VAL:N	3:e:273:THR:HG22	2.09	0.67
1:A:348:ILE:HG23	2:E:209:MET:HE1	1.78	0.66
2:E:346:PRO:CB	2:E:348:VAL:CG1	2.73	0.66
2:F:305:ASP:O	2:F:308:PRO:HD2	1.94	0.66
1:I:178:LEU:HD12	1:I:179:ALA:N	2.09	0.66
2:M:139:PHE:HE2	2:M:162:LEU:HD21	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:285:THR:HG22	2:N:287:THR:H	1.60	0.66
4:P:2:MET:HE1	2:c:197:ASN:CA	2.23	0.66
2:V:131:LYS:H	2:V:402:GLN:HE22	1.41	0.66
3:e:64:HIS:CD2	3:e:64:HIS:O	2.49	0.66
1:C:493:ASN:O	1:C:496:ILE:HG12	1.95	0.66
2:E:31:VAL:HG22	2:E:68:VAL:HB	1.75	0.66
2:L:161:GLU:HG3	2:L:404:PHE:CG	2.29	0.66
2:M:349:VAL:HG21	2:M:353:HIS:ND1	2.09	0.66
1:R:402:GLU:HG3	1:R:403:LEU:N	2.10	0.66
1:R:460:GLU:CD	1:R:465:GLY:HA2	2.21	0.66
2:T:323:ARG:H	2:T:323:ARG:CD	2.07	0.66
2:V:224:LEU:HD21	2:V:278:LEU:HD12	1.76	0.66
1:Z:460:GLU:CD	1:Z:465:GLY:HA2	2.21	0.66
2:b:403:PRO:HD3	2:b:445:MET:HG3	1.75	0.66
2:c:180:GLY:O	2:c:209:MET:HG2	1.94	0.66
2:E:180:GLY:O	2:E:209:MET:HG2	1.94	0.66
2:F:132:VAL:HG11	2:F:334:VAL:HB	1.78	0.66
1:K:187:ARG:O	1:K:187:ARG:HG2	1.93	0.66
2:T:285:THR:HG23	2:T:288:GLY:H	1.60	0.66
2:U:113:ALA:HB3	2:U:281:ARG:HG2	1.76	0.66
1:a:150:TYR:HA	1:a:433:GLN:HE22	1.60	0.66
1:a:384:LYS:NZ	1:a:493:ASN:HD21	1.93	0.66
2:d:198:VAL:HA	2:d:201:LYS:HE2	1.78	0.66
1:B:460:GLU:CD	1:B:465:GLY:HA2	2.21	0.66
1:C:177:ALA:O	1:C:181:ASP:HB2	1.94	0.66
1:J:460:GLU:CD	1:J:465:GLY:HA2	2.21	0.66
1:Y:48:MET:HB3	2:c:63:ARG:HG2	1.77	0.66
2:c:163:ILE:HD13	2:c:202:VAL:HG11	1.78	0.66
2:c:403:PRO:HG2	2:c:415:GLY:HA2	1.77	0.66
2:E:307:SER:HB3	2:E:308:PRO:HD3	1.76	0.66
1:I:142:VAL:HG13	1:I:377:VAL:HG21	1.78	0.66
2:M:116:TYR:CD1	2:M:117:GLU:N	2.60	0.66
2:M:180:GLY:O	2:M:209:MET:HG2	1.95	0.66
1:Q:248:TYR:O	1:Q:252:ARG:HG2	1.96	0.66
1:R:96:GLU:HG2	1:R:97:VAL:N	2.04	0.66
3:W:64:HIS:CD2	3:W:64:HIS:O	2.49	0.66
1:Y:137:ILE:CG2	2:c:96:ASP:HA	2.26	0.66
2:M:189:PHE:O	2:M:193:MET:HG3	1.95	0.66
2:N:198:VAL:HA	2:N:201:LYS:HE2	1.78	0.66
1:S:493:ASN:O	1:S:496:ILE:CD1	2.43	0.66
1:Y:248:TYR:O	1:Y:252:ARG:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ASN:H	1:A:361:ASN:HD22	1.42	0.66
2:F:16:GLU:HG3	2:F:18:PRO:HD3	1.76	0.66
2:F:198:VAL:HA	2:F:201:LYS:HE2	1.78	0.66
1:J:402:GLU:HG3	1:J:403:LEU:N	2.10	0.66
2:M:31:VAL:HG22	2:M:68:VAL:HB	1.75	0.66
1:Q:32:VAL:CG2	1:Q:42:HIS:HB2	2.25	0.66
1:S:150:TYR:HA	1:S:433:GLN:HE22	1.60	0.66
2:b:144:LYS:HD3	2:b:279:GLN:HE21	1.61	0.66
2:c:316:ASP:HB3	2:c:343:GLN:HE22	1.61	0.66
2:d:73:HIS:HD2	2:d:74:PRO:HD2	1.61	0.66
2:d:323:ARG:HH11	2:d:323:ARG:CG	2.06	0.66
2:D:207:GLY:HA3	2:D:219:VAL:HG21	1.76	0.66
2:E:348:VAL:HG22	2:E:349:VAL:N	2.11	0.66
3:O:64:HIS:CD2	3:O:64:HIS:O	2.48	0.66
1:R:52:MET:HE2	1:R:60:TYR:CD1	2.31	0.66
2:c:164:ARG:HA	2:c:201:LYS:HZ2	1.60	0.66
2:d:16:GLU:HG3	2:d:18:PRO:HD3	1.76	0.66
1:A:248:TYR:O	1:A:252:ARG:HG2	1.96	0.66
1:A:480:ALA:N	1:A:481:PRO:HD2	2.11	0.66
2:D:22:VAL:HG23	2:D:23:PRO:CD	2.25	0.66
2:E:397:GLN:HA	2:E:400:LEU:HD22	1.78	0.66
1:K:384:LYS:NZ	1:K:493:ASN:HD21	1.93	0.66
1:Q:142:VAL:HG13	1:Q:377:VAL:HG21	1.78	0.66
1:R:471:LEU:H	1:R:471:LEU:HD22	1.61	0.66
2:T:161:GLU:HG3	2:T:404:PHE:CG	2.31	0.66
2:U:163:ILE:HD13	2:U:202:VAL:HG11	1.78	0.66
1:Z:283:ARG:HH11	2:d:300:ALA:HB3	1.61	0.66
1:Z:446:LEU:CD1	1:Z:469:ALA:HB1	2.26	0.66
1:I:48:MET:HB3	2:M:63:ARG:HG2	1.77	0.66
1:I:364:ILE:CG1	1:I:432:LYS:HE3	2.26	0.66
1:J:52:MET:HE2	1:J:60:TYR:CD1	2.31	0.66
1:K:118:LYS:HG3	1:K:120:PRO:HD2	1.78	0.66
1:S:118:LYS:HG3	1:S:120:PRO:HD2	1.78	0.66
2:b:279:GLN:HE22	2:b:294:GLN:HE22	1.43	0.66
1:B:446:LEU:CD1	1:B:469:ALA:HB1	2.26	0.65
1:J:52:MET:HE3	1:J:95:LEU:HD13	1.78	0.65
2:M:402:GLN:N	2:M:445:MET:HE1	2.09	0.65
2:N:170:HIS:CE1	2:N:238:LEU:HD13	2.31	0.65
1:R:52:MET:HE2	1:R:60:TYR:HD1	1.61	0.65
1:Z:105:GLY:HA2	1:Z:218:LEU:HD22	1.79	0.65
2:b:157:VAL:HG11	7:b:600:ADP:C8	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ALA:O	1:A:178:LEU:C	2.34	0.65
1:B:105:GLY:HA2	1:B:218:LEU:HD22	1.79	0.65
2:E:139:PHE:HE2	2:E:162:LEU:HD21	1.60	0.65
2:F:73:HIS:HD2	2:F:74:PRO:HD2	1.61	0.65
1:J:172:GLN:HA	5:J:600:ANP:HNB1	1.62	0.65
1:K:39:ILE:HD11	1:K:82:LEU:HD13	1.78	0.65
1:R:446:LEU:CD1	1:R:469:ALA:HB1	2.26	0.65
1:S:467:PHE:HZ	1:S:511:GLN:CD	2.05	0.65
1:Z:471:LEU:H	1:Z:471:LEU:HD22	1.61	0.65
2:c:268:GLN:HE21	2:c:268:GLN:N	1.91	0.65
2:D:96:ASP:OD1	2:D:98:LYS:HB2	1.97	0.65
1:I:248:TYR:O	1:I:252:ARG:HG2	1.96	0.65
2:M:163:ILE:HD13	2:M:202:VAL:HG11	1.77	0.65
2:M:200:ASP:OD2	2:M:200:ASP:C	2.39	0.65
2:V:16:GLU:HG3	2:V:18:PRO:HD3	1.76	0.65
1:B:52:MET:HE2	1:B:60:TYR:CD1	2.31	0.65
1:B:52:MET:HE2	1:B:60:TYR:HD1	1.61	0.65
2:D:111:ARG:HB2	2:D:111:ARG:HH11	1.62	0.65
1:J:105:GLY:HA2	1:J:218:LEU:HD22	1.79	0.65
2:L:111:ARG:HB2	2:L:111:ARG:HH11	1.61	0.65
2:L:320:VAL:HG21	2:L:338:ASP:HB2	1.78	0.65
1:Q:361:ASN:H	1:Q:361:ASN:HD22	1.42	0.65
2:U:113:ALA:N	2:U:114:PRO:CD	2.60	0.65
2:V:73:HIS:HD2	2:V:74:PRO:HD2	1.61	0.65
1:Z:35:SER:HB2	2:c:44:GLN:HG2	1.77	0.65
2:d:243:ASN:HA	2:d:295:ALA:O	1.96	0.65
1:B:471:LEU:H	1:B:471:LEU:HD22	1.61	0.65
2:E:395:LYS:HD3	2:E:443:PHE:CZ	2.32	0.65
2:F:170:HIS:CE1	2:F:238:LEU:HD13	2.32	0.65
1:J:52:MET:HE2	1:J:60:TYR:HD1	1.61	0.65
1:J:471:LEU:H	1:J:471:LEU:HD22	1.61	0.65
1:S:440:SER:C	1:S:442:ALA:H	2.02	0.65
2:T:111:ARG:NH2	2:T:224:LEU:HD12	2.12	0.65
2:U:344:LEU:C	2:U:344:LEU:HD12	2.22	0.65
2:V:155:LYS:HE3	2:V:297:TYR:HA	1.79	0.65
2:L:96:ASP:OD1	2:L:98:LYS:HB2	1.97	0.65
2:N:73:HIS:HD2	2:N:74:PRO:HD2	1.61	0.65
2:U:428:LYS:O	2:U:432:GLU:HG2	1.97	0.65
2:V:31:VAL:HG22	2:V:68:VAL:HG12	1.79	0.65
1:a:118:LYS:HG3	1:a:120:PRO:HD2	1.78	0.65
2:c:161:GLU:HG3	2:c:404:PHE:CB	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ILE:HD11	1:C:82:LEU:HD13	1.78	0.65
1:C:492:TYR:O	1:C:493:ASN:ND2	2.29	0.65
2:D:20:ASP:OD2	2:D:20:ASP:N	2.30	0.65
2:D:157:VAL:HG11	7:D:600:ADP:C8	2.32	0.65
2:U:201:LYS:O	2:U:201:LYS:HG2	1.97	0.65
2:V:198:VAL:HA	2:V:201:LYS:HE2	1.78	0.65
3:W:66:TYR:CG	3:W:188:LEU:HD21	2.31	0.65
1:a:467:PHE:HZ	1:a:511:GLN:CD	2.05	0.65
2:b:96:ASP:OD1	2:b:98:LYS:HB2	1.97	0.65
2:b:157:VAL:HG11	7:b:600:ADP:H8	1.59	0.65
3:G:187:LEU:C	3:G:187:LEU:CD1	2.64	0.65
1:Q:480:ALA:N	1:Q:481:PRO:HD2	2.11	0.65
2:c:139:PHE:HE2	2:c:162:LEU:HD21	1.60	0.65
2:c:265:VAL:HG13	2:c:267:TYR:HD2	1.61	0.65
1:C:493:ASN:N	1:C:493:ASN:HD22	1.94	0.65
1:I:176:THR:O	1:I:179:ALA:N	2.30	0.65
2:L:379:MET:HE1	2:L:390:VAL:HG11	1.79	0.65
2:M:113:ALA:N	2:M:114:PRO:CD	2.60	0.65
2:M:379:MET:HB2	2:M:387:LYS:HZ3	1.62	0.65
1:S:157:ILE:HG21	1:S:353:ILE:HG12	1.79	0.65
2:b:144:LYS:HE2	2:b:279:GLN:O	1.96	0.65
2:d:170:HIS:CE1	2:d:238:LEU:HD13	2.31	0.65
1:C:467:PHE:HZ	1:C:511:GLN:CD	2.05	0.65
2:E:305:ASP:O	2:E:308:PRO:HD2	1.96	0.65
1:J:446:LEU:CD1	1:J:469:ALA:HB1	2.26	0.65
2:N:132:VAL:HG11	2:N:334:VAL:HB	1.77	0.65
1:R:105:GLY:HA2	1:R:218:LEU:HD22	1.79	0.65
2:V:131:LYS:HG2	2:V:423:THR:HG23	1.80	0.65
1:Y:485:GLU:O	1:Y:489:THR:HG22	1.97	0.65
1:a:39:ILE:HD11	1:a:82:LEU:HD13	1.78	0.65
4:f:75:ASN:HD22	4:f:76:VAL:N	1.93	0.65
1:B:493:ASN:HB2	1:B:496:ILE:HG13	1.80	0.64
2:E:163:ILE:HD13	2:E:202:VAL:HG11	1.78	0.64
1:K:157:ILE:HG21	1:K:353:ILE:HG12	1.79	0.64
2:N:31:VAL:HG22	2:N:68:VAL:HG12	1.79	0.64
1:Y:142:VAL:HG13	1:Y:377:VAL:HG21	1.78	0.64
2:c:181:GLU:O	2:c:208:GLN:HG3	1.97	0.64
1:A:142:VAL:HG13	1:A:377:VAL:HG21	1.78	0.64
2:D:111:ARG:NH2	2:D:224:LEU:HD12	2.12	0.64
2:D:387:LYS:HA	2:D:390:VAL:HG12	1.79	0.64
2:L:111:ARG:NH2	2:L:224:LEU:HD12	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:387:LYS:HA	2:L:390:VAL:HG12	1.79	0.64
2:M:161:GLU:HG3	2:M:404:PHE:CB	2.27	0.64
1:Q:485:GLU:O	1:Q:489:THR:HG22	1.97	0.64
2:V:125:LEU:H	2:V:125:LEU:HD12	1.62	0.64
1:a:104:LEU:HA	1:a:222:ILE:HG22	1.80	0.64
2:b:117:GLU:N	2:b:117:GLU:OE2	2.30	0.64
2:c:344:LEU:C	2:c:344:LEU:HD12	2.22	0.64
2:F:224:LEU:HD21	2:F:278:LEU:HD12	1.78	0.64
1:J:107:VAL:HA	1:J:223:VAL:HG13	1.79	0.64
4:P:51:ARG:HG3	4:P:61:PHE:HE2	1.62	0.64
1:R:446:LEU:HD12	1:R:469:ALA:HB1	1.79	0.64
2:V:132:VAL:HG11	2:V:334:VAL:HB	1.79	0.64
2:V:240:PHE:HD2	2:V:293:VAL:HG22	1.63	0.64
3:W:186:GLN:CG	3:W:189:PRO:HG2	2.26	0.64
4:X:51:ARG:HG3	4:X:61:PHE:HE2	1.62	0.64
1:Z:446:LEU:HD12	1:Z:469:ALA:HB1	1.79	0.64
2:c:113:ALA:N	2:c:114:PRO:CD	2.60	0.64
1:C:118:LYS:HG3	1:C:120:PRO:HD2	1.78	0.64
2:E:113:ALA:N	2:E:114:PRO:CD	2.60	0.64
2:N:125:LEU:H	2:N:125:LEU:HD12	1.63	0.64
1:S:39:ILE:HD11	1:S:82:LEU:HD13	1.78	0.64
1:Y:480:ALA:N	1:Y:481:PRO:HD2	2.11	0.64
1:A:426:LYS:HZ2	1:A:457:ALA:HB2	1.63	0.64
1:C:59:ARG:NE	1:C:59:ARG:HA	2.13	0.64
2:E:395:LYS:HD3	2:E:443:PHE:CE1	2.33	0.64
1:I:283:ARG:HG3	3:O:272:ILE:CD1	2.28	0.64
2:M:201:LYS:O	2:M:201:LYS:HG2	1.97	0.64
2:U:181:GLU:O	2:U:208:GLN:HG3	1.97	0.64
3:W:186:GLN:CD	3:W:189:PRO:CG	2.66	0.64
1:Z:41:ILE:HD13	1:Z:88:VAL:HG11	1.80	0.64
1:Z:107:VAL:HA	1:Z:223:VAL:HG13	1.79	0.64
2:c:447:GLY:H	2:c:451:GLU:HG2	1.63	0.64
4:f:51:ARG:HG3	4:f:61:PHE:HE2	1.62	0.64
1:A:357:THR:HG23	1:A:358:ASN:H	1.63	0.64
1:A:449:PHE:HB3	1:A:504:LEU:HD12	1.79	0.64
2:D:352:GLU:O	2:D:356:THR:HG23	1.98	0.64
2:E:200:ASP:OD2	4:X:2:MET:CE	2.45	0.64
2:M:181:GLU:O	2:M:208:GLN:HG3	1.97	0.64
3:O:214:LEU:HD13	4:P:42:LEU:HG	1.79	0.64
1:S:59:ARG:NE	1:S:59:ARG:HA	2.13	0.64
2:T:96:ASP:OD1	2:T:98:LYS:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:397:GLN:HA	2:U:400:LEU:HD22	1.79	0.64
2:V:90:VAL:HA	2:V:222:THR:HG21	1.79	0.64
3:W:188:LEU:O	3:W:188:LEU:CG	2.44	0.64
2:c:201:LYS:O	2:c:201:LYS:HG2	1.97	0.64
1:C:157:ILE:HG21	1:C:353:ILE:HG12	1.79	0.64
2:D:131:LYS:HG3	2:D:402:GLN:OE1	1.97	0.64
4:H:51:ARG:HG3	4:H:61:PHE:HE2	1.62	0.64
1:I:480:ALA:N	1:I:481:PRO:HD2	2.11	0.64
1:J:62:ILE:CD1	1:J:95:LEU:HD22	2.27	0.64
1:J:97:VAL:HG12	1:J:98:PRO:N	2.12	0.64
2:N:90:VAL:HA	2:N:222:THR:HG21	1.79	0.64
3:W:82:THR:HA	8:W:300:SO4:O3	1.96	0.64
1:C:104:LEU:HA	1:C:222:ILE:HG22	1.80	0.64
1:C:106:ARG:HH12	1:C:116:ASP:HB3	1.63	0.64
1:C:492:TYR:HA	1:C:496:ILE:HG13	1.79	0.64
2:E:181:GLU:O	2:E:208:GLN:HG3	1.97	0.64
2:E:442:ALA:CB	2:E:443:PHE:CD2	2.74	0.64
1:I:357:THR:HG23	1:I:358:ASN:H	1.63	0.64
1:Q:460:GLU:O	1:Q:461:LEU:C	2.41	0.64
1:R:107:VAL:HA	1:R:223:VAL:HG13	1.79	0.64
2:V:170:HIS:CE1	2:V:238:LEU:HD13	2.32	0.64
1:Z:365:ARG:HG2	5:Z:600:ANP:C2	2.27	0.64
1:Z:493:ASN:HB2	1:Z:496:ILE:HG13	1.80	0.64
2:b:118:GLU:N	2:b:118:GLU:OE1	2.30	0.64
2:D:111:ARG:CG	2:D:112:ALA:H	2.11	0.64
2:F:31:VAL:HG22	2:F:68:VAL:HG12	1.79	0.64
2:F:90:VAL:HA	2:F:222:THR:HG21	1.79	0.64
2:M:397:GLN:HA	2:M:400:LEU:HD22	1.79	0.64
1:S:494:ASP:OD2	1:S:494:ASP:N	2.31	0.64
2:T:435:TYR:HB3	2:T:438:LEU:HD21	1.80	0.64
1:Z:51:GLU:HA	1:Z:94:ILE:HG22	1.80	0.64
2:b:398:ARG:HD2	2:b:440:GLU:HB3	1.80	0.64
2:D:17:PHE:CE1	2:D:23:PRO:CD	2.81	0.64
1:J:446:LEU:HD12	1:J:469:ALA:HB1	1.79	0.64
1:J:493:ASN:HB2	1:J:496:ILE:HG13	1.80	0.64
2:M:387:LYS:HE3	2:M:390:VAL:HG11	1.80	0.64
1:R:41:ILE:HD13	1:R:88:VAL:HG11	1.80	0.64
1:S:106:ARG:HH12	1:S:116:ASP:HB3	1.62	0.64
1:Z:426:LYS:HD2	1:Z:462:SER:HA	1.80	0.64
2:c:244:ILE:HD11	2:c:275:MET:HE1	1.80	0.64
2:d:125:LEU:HD12	2:d:125:LEU:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:GLU:O	1:A:489:THR:HG22	1.97	0.63
2:D:427:PHE:HA	2:D:430:ILE:HG22	1.80	0.63
1:I:449:PHE:HB3	1:I:504:LEU:HD12	1.79	0.63
2:T:157:VAL:HG11	7:T:600:ADP:H8	1.63	0.63
2:T:157:VAL:HG11	7:T:600:ADP:C8	2.33	0.63
2:T:387:LYS:HA	2:T:390:VAL:HG12	1.80	0.63
2:V:268:GLN:NE2	2:V:268:GLN:H	1.96	0.63
3:W:187:LEU:CD1	3:W:223:VAL:HG22	2.29	0.63
1:a:317:VAL:HA	1:a:318:LYS:CB	2.20	0.63
2:d:219:VAL:HA	2:d:222:THR:HG22	1.80	0.63
2:E:201:LYS:O	2:E:201:LYS:HG2	1.96	0.63
2:E:344:LEU:C	2:E:344:LEU:HD12	2.23	0.63
2:F:126:LEU:HD12	2:F:166:ILE:HG21	1.80	0.63
1:I:177:ALA:O	1:I:178:LEU:C	2.39	0.63
1:K:59:ARG:NE	1:K:59:ARG:HA	2.13	0.63
1:K:106:ARG:HH12	1:K:116:ASP:HB3	1.63	0.63
1:K:163:GLN:HG2	1:K:164:ARG:H	1.63	0.63
2:M:5:ILE:HB	2:M:64:ARG:O	1.98	0.63
2:M:337:LEU:O	2:M:338:ASP:HB2	1.98	0.63
1:S:310:GLU:HA	1:S:314:LYS:CB	2.28	0.63
2:V:106:ARG:C	2:V:107:TRP:HD1	2.07	0.63
2:V:202:VAL:HG22	2:V:203:SER:H	1.64	0.63
1:Y:460:GLU:O	1:Y:461:LEU:C	2.41	0.63
2:d:155:LYS:HE3	2:d:297:TYR:HA	1.79	0.63
1:C:310:GLU:HA	1:C:314:LYS:CB	2.28	0.63
2:D:157:VAL:HG11	7:D:600:ADP:H8	1.63	0.63
2:E:5:ILE:HB	2:E:64:ARG:O	1.98	0.63
2:E:347:LEU:O	2:E:348:VAL:CB	2.44	0.63
2:F:125:LEU:H	2:F:125:LEU:HD12	1.63	0.63
1:K:104:LEU:HA	1:K:222:ILE:HG22	1.80	0.63
2:U:164:ARG:C	2:U:164:ARG:HD3	2.23	0.63
2:U:265:VAL:HG23	3:W:272:ILE:HD13	1.79	0.63
2:d:202:VAL:HG22	2:d:203:SER:H	1.64	0.63
1:B:426:LYS:HD2	1:B:462:SER:HA	1.81	0.63
1:C:163:GLN:HG2	1:C:164:ARG:H	1.63	0.63
2:E:265:VAL:O	2:E:265:VAL:HG22	1.99	0.63
3:G:167:LEU:CD2	3:G:188:LEU:HD23	2.27	0.63
2:M:164:ARG:C	2:M:164:ARG:HD3	2.23	0.63
2:U:131:LYS:H	2:U:402:GLN:NE2	1.90	0.63
2:U:144:LYS:HE2	2:U:282:ILE:HG13	1.80	0.63
2:U:265:VAL:HG13	2:U:267:TYR:CD2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:126:LEU:HD12	2:V:166:ILE:HG21	1.80	0.63
1:Y:426:LYS:NZ	1:Y:457:ALA:HB2	2.14	0.63
1:a:59:ARG:NE	1:a:59:ARG:HA	2.13	0.63
2:d:130:ILE:HD12	2:d:404:PHE:CE1	2.33	0.63
2:d:240:PHE:HD2	2:d:293:VAL:HG22	1.63	0.63
1:C:159:ILE:HG12	1:C:165:GLU:HG3	1.81	0.63
2:F:268:GLN:H	2:F:268:GLN:NE2	1.97	0.63
1:J:426:LYS:HD2	1:J:462:SER:HA	1.81	0.63
1:K:467:PHE:HZ	1:K:511:GLN:CD	2.05	0.63
2:M:178:GLY:HA2	2:M:242:ASP:CB	2.29	0.63
1:R:94:ILE:C	1:R:95:LEU:HD12	2.21	0.63
1:S:104:LEU:HA	1:S:222:ILE:HG22	1.80	0.63
2:T:111:ARG:HB2	2:T:111:ARG:HH11	1.62	0.63
2:T:394:ARG:HD3	2:T:440:GLU:OE1	1.98	0.63
2:b:111:ARG:HH11	2:b:111:ARG:CB	2.11	0.63
2:d:90:VAL:HA	2:d:222:THR:HG21	1.79	0.63
2:d:106:ARG:C	2:d:107:TRP:HD1	2.07	0.63
1:A:39:ILE:HD11	1:A:82:LEU:HD13	1.81	0.63
1:A:426:LYS:NZ	1:A:457:ALA:HB2	2.14	0.63
2:V:319:VAL:HA	2:V:339:SER:OG	1.99	0.63
2:c:433:GLY:O	2:c:434:GLU:HB2	1.97	0.63
2:d:31:VAL:HG22	2:d:68:VAL:HG12	1.79	0.63
1:A:106:ARG:HH12	1:A:118:LYS:HB2	1.63	0.63
1:I:106:ARG:HH12	1:I:118:LYS:HB2	1.63	0.63
1:I:443:GLN:O	1:I:446:LEU:HD13	1.99	0.63
2:L:403:PRO:HD3	2:L:445:MET:HG3	1.79	0.63
1:Q:426:LYS:NZ	1:Q:457:ALA:HB2	2.14	0.63
1:R:299:GLU:HG2	2:V:209:MET:HE3	1.81	0.63
2:U:5:ILE:HB	2:U:64:ARG:O	1.98	0.63
1:Y:357:THR:HG23	1:Y:358:ASN:H	1.63	0.63
2:d:132:VAL:HG11	2:d:334:VAL:HB	1.80	0.63
1:A:460:GLU:O	1:A:461:LEU:C	2.41	0.63
1:B:107:VAL:HA	1:B:223:VAL:HG13	1.79	0.63
1:C:317:VAL:HA	1:C:318:LYS:CB	2.20	0.63
2:E:346:PRO:HB2	2:E:348:VAL:CG1	2.29	0.63
2:E:346:PRO:HB2	2:E:348:VAL:HG12	1.81	0.63
1:I:485:GLU:O	1:I:489:THR:HG22	1.97	0.63
2:N:219:VAL:HA	2:N:222:THR:HG22	1.81	0.63
3:O:64:HIS:CG	3:O:68:GLU:HG2	2.34	0.63
1:Q:357:THR:HG23	1:Q:358:ASN:H	1.63	0.63
4:X:2:MET:O	4:X:3:THR:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:392:ARG:HD3	2:b:431:MET:HA	1.80	0.63
1:A:138:GLU:CG	1:A:305:ASN:ND2	2.62	0.63
2:F:219:VAL:HA	2:F:222:THR:HG22	1.80	0.63
2:L:111:ARG:CG	2:L:112:ALA:H	2.11	0.63
1:Q:39:ILE:HD11	1:Q:82:LEU:HD13	1.81	0.63
1:Q:449:PHE:HB3	1:Q:504:LEU:HD12	1.79	0.63
1:R:106:ARG:HH12	1:R:115:ILE:CG2	2.12	0.63
1:S:68:ARG:H	2:T:7:GLN:HG2	1.63	0.63
1:S:159:ILE:HG12	1:S:165:GLU:HG3	1.81	0.63
1:S:163:GLN:HG2	1:S:164:ARG:H	1.63	0.63
1:S:330:ILE:HD11	1:S:345:VAL:HG21	1.81	0.63
2:V:305:ASP:O	2:V:308:PRO:HD2	1.99	0.63
1:Z:403:LEU:CD2	1:Z:420:GLN:HE22	2.12	0.63
2:c:164:ARG:C	2:c:164:ARG:HD3	2.23	0.63
2:E:178:GLY:HA2	2:E:242:ASP:CB	2.29	0.62
2:F:106:ARG:C	2:F:107:TRP:HD1	2.07	0.62
2:N:126:LEU:HD12	2:N:166:ILE:HG21	1.80	0.62
1:Q:135:GLY:O	1:Q:138:GLU:HG3	1.97	0.62
1:R:31:ILE:HD13	1:R:39:ILE:HD11	1.82	0.62
1:S:460:GLU:O	1:S:461:LEU:C	2.42	0.62
2:T:111:ARG:CG	2:T:112:ALA:H	2.11	0.62
2:T:364:LEU:HD23	2:T:396:ILE:HD11	1.81	0.62
1:Y:106:ARG:HH12	1:Y:118:LYS:HB2	1.63	0.62
2:c:178:GLY:HA2	2:c:242:ASP:CB	2.29	0.62
2:E:164:ARG:C	2:E:164:ARG:HD3	2.23	0.62
2:M:403:PRO:HG2	2:M:415:GLY:HA2	1.79	0.62
1:R:157:ILE:HD11	1:R:368:VAL:HG21	1.81	0.62
1:a:157:ILE:HG21	1:a:353:ILE:HG12	1.79	0.62
1:a:310:GLU:HA	1:a:314:LYS:CB	2.29	0.62
2:b:113:ALA:CB	2:b:114:PRO:HD3	2.27	0.62
2:c:5:ILE:HB	2:c:64:ARG:O	1.98	0.62
1:A:423:HIS:O	1:A:426:LYS:HG2	2.00	0.62
2:N:202:VAL:HG22	2:N:203:SER:H	1.64	0.62
2:T:435:TYR:CZ	2:T:449:ILE:HG13	2.34	0.62
2:U:178:GLY:HA2	2:U:242:ASP:CB	2.29	0.62
1:a:106:ARG:HH12	1:a:116:ASP:HB3	1.63	0.62
1:a:330:ILE:HD11	1:a:345:VAL:HG21	1.81	0.62
1:A:443:GLN:O	1:A:446:LEU:HD13	1.99	0.62
1:B:403:LEU:CD2	1:B:420:GLN:HE22	2.12	0.62
1:B:446:LEU:HD12	1:B:469:ALA:HB1	1.79	0.62
1:C:460:GLU:O	1:C:461:LEU:C	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:237:VAL:HG23	2:E:290:ILE:HG23	1.80	0.62
1:I:426:LYS:NZ	1:I:457:ALA:HB2	2.14	0.62
1:J:106:ARG:HH12	1:J:115:ILE:CG2	2.12	0.62
2:M:148:PHE:HZ	2:M:312:PHE:HE1	1.47	0.62
1:R:493:ASN:HB2	1:R:496:ILE:HG13	1.80	0.62
2:T:320:VAL:HG21	2:T:338:ASP:HB2	1.81	0.62
2:V:130:ILE:HD12	2:V:404:PHE:CE1	2.35	0.62
1:Y:371:GLY:H	1:Y:394:ARG:NH1	1.98	0.62
1:Y:449:PHE:HB3	1:Y:504:LEU:HD12	1.79	0.62
1:a:159:ILE:HG12	1:a:165:GLU:HG3	1.81	0.62
1:A:138:GLU:CG	1:A:305:ASN:CB	2.78	0.62
1:B:41:ILE:HD13	1:B:88:VAL:HG11	1.80	0.62
1:I:460:GLU:O	1:I:461:LEU:C	2.41	0.62
1:Q:281:PRO:HG3	3:W:279:ILE:HG21	1.82	0.62
1:Q:479:HIS:C	1:Q:481:PRO:HD2	2.24	0.62
2:T:408:GLU:HG3	2:T:413:SER:O	1.99	0.62
3:W:64:HIS:CG	3:W:68:GLU:HG2	2.34	0.62
1:Y:443:GLN:O	1:Y:446:LEU:HD13	1.99	0.62
1:Z:159:ILE:HG12	1:Z:165:GLU:HG3	1.82	0.62
1:B:157:ILE:HD11	1:B:368:VAL:HG21	1.81	0.62
1:C:163:GLN:HG2	1:C:164:ARG:N	2.15	0.62
1:C:494:ASP:N	1:C:494:ASP:OD2	2.30	0.62
2:D:279:GLN:HE22	2:D:294:GLN:HE22	1.46	0.62
2:D:429:GLY:O	2:D:433:GLY:HA2	1.99	0.62
2:F:319:VAL:HA	2:F:339:SER:OG	1.99	0.62
1:K:310:GLU:HA	1:K:314:LYS:CB	2.28	0.62
2:N:106:ARG:C	2:N:107:TRP:HD1	2.07	0.62
3:O:28:ALA:HA	3:O:31:MET:HE2	1.82	0.62
1:Q:443:GLN:O	1:Q:446:LEU:HD13	1.99	0.62
2:U:367:TYR:CE2	2:U:390:VAL:HG13	2.35	0.62
1:a:163:GLN:HG2	1:a:164:ARG:H	1.63	0.62
2:d:126:LEU:HD12	2:d:166:ILE:HG21	1.80	0.62
1:I:479:HIS:C	1:I:481:PRO:HD2	2.24	0.62
1:J:159:ILE:HG12	1:J:165:GLU:HG3	1.82	0.62
1:Y:39:ILE:HD11	1:Y:82:LEU:HD13	1.81	0.62
2:F:202:VAL:HG22	2:F:203:SER:H	1.63	0.62
1:I:96:GLU:HB3	1:I:126:PHE:HD2	1.65	0.62
1:I:423:HIS:O	1:I:426:LYS:HG2	2.00	0.62
1:J:110:THR:CG2	1:J:234:LEU:HG	2.30	0.62
1:K:163:GLN:HG2	1:K:164:ARG:N	2.15	0.62
2:M:115:SER:HB2	2:M:118:GLU:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:130:ILE:HD12	2:N:404:PHE:CE1	2.34	0.62
2:N:305:ASP:O	2:N:308:PRO:HD2	2.00	0.62
1:Q:106:ARG:HH12	1:Q:118:LYS:HB2	1.64	0.62
2:U:148:PHE:HZ	2:U:312:PHE:HE1	1.48	0.62
1:Z:281:PRO:HG2	3:e:277:THR:HG23	1.82	0.62
1:Z:430:LEU:HD12	1:Z:451:ALA:HB2	1.81	0.62
1:a:163:GLN:HG2	1:a:164:ARG:N	2.15	0.62
2:c:122:SER:O	2:c:123:GLN:HB2	2.00	0.62
1:C:365:ARG:HG3	5:C:600:ANP:N1	2.15	0.62
1:R:426:LYS:HD2	1:R:462:SER:HA	1.81	0.62
3:W:28:ALA:HA	3:W:31:MET:HE2	1.82	0.62
1:Z:106:ARG:HH12	1:Z:115:ILE:CG2	2.12	0.62
2:b:111:ARG:NH1	2:b:111:ARG:HB2	2.15	0.62
2:c:113:ALA:HB3	2:c:281:ARG:HG2	1.82	0.62
2:c:115:SER:HB2	2:c:118:GLU:HB2	1.82	0.62
2:E:382:LEU:HD12	2:E:387:LYS:HD3	1.81	0.62
1:I:39:ILE:HD11	1:I:82:LEU:HD13	1.81	0.62
1:J:41:ILE:HD13	1:J:88:VAL:HG11	1.80	0.62
1:J:51:GLU:HA	1:J:94:ILE:HG22	1.80	0.62
2:L:279:GLN:HG2	2:L:314:HIS:CB	2.29	0.62
2:M:443:PHE:N	2:M:443:PHE:HD2	1.96	0.62
1:Q:423:HIS:O	1:Q:426:LYS:HG2	2.00	0.62
2:U:305:ASP:O	2:U:308:PRO:HD2	2.00	0.62
2:V:120:SER:OG	2:V:286:LYS:HE3	2.00	0.62
3:W:55:LEU:HD12	3:W:55:LEU:O	2.00	0.62
1:Y:432:LYS:HD2	1:Y:432:LYS:N	2.15	0.62
1:Y:479:HIS:C	1:Y:481:PRO:HD2	2.25	0.62
1:B:159:ILE:HG12	1:B:165:GLU:HG3	1.82	0.61
2:D:279:GLN:HG2	2:D:314:HIS:CB	2.31	0.61
1:I:103:LEU:HD12	1:I:245:MET:HE3	1.82	0.61
1:J:430:LEU:HD12	1:J:451:ALA:HB2	1.81	0.61
1:Q:96:GLU:HB3	1:Q:126:PHE:HD2	1.65	0.61
1:Q:371:GLY:H	1:Q:394:ARG:NH1	1.98	0.61
1:Y:96:GLU:HB3	1:Y:126:PHE:HD2	1.65	0.61
3:e:64:HIS:CG	3:e:68:GLU:HG2	2.34	0.61
1:B:106:ARG:HH12	1:B:115:ILE:CG2	2.12	0.61
1:C:107:VAL:HG11	2:F:116:TYR:HE1	1.64	0.61
1:J:31:ILE:HD13	1:J:39:ILE:HD11	1.82	0.61
2:M:402:GLN:C	2:M:445:MET:HE1	2.25	0.61
2:N:268:GLN:NE2	2:N:268:GLN:H	1.98	0.61
3:O:189:PRO:O	3:O:191:PRO:CD	2.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:163:GLN:HG2	1:S:164:ARG:N	2.15	0.61
2:U:115:SER:HB2	2:U:118:GLU:HB2	1.82	0.61
2:F:141:LYS:HA	2:F:291:THR:HG23	1.82	0.61
1:J:35:SER:HB2	2:M:44:GLN:HG2	1.81	0.61
1:J:283:ARG:HH11	2:N:300:ALA:HB3	1.65	0.61
1:S:493:ASN:H	1:S:496:ILE:HG13	1.64	0.61
2:U:360:VAL:HA	2:U:431:MET:HE1	1.82	0.61
2:V:219:VAL:HA	2:V:222:THR:HG22	1.80	0.61
1:Z:157:ILE:HD11	1:Z:368:VAL:HG21	1.81	0.61
2:b:279:GLN:HG2	2:b:314:HIS:CB	2.30	0.61
2:d:25:VAL:HG13	2:d:26:TYR:N	2.16	0.61
1:B:31:ILE:HD13	1:B:39:ILE:HD11	1.82	0.61
2:D:3:GLY:HA3	2:D:17:PHE:CE2	2.34	0.61
1:J:157:ILE:HD11	1:J:368:VAL:HG21	1.81	0.61
1:J:403:LEU:CD2	1:J:420:GLN:HE22	2.12	0.61
2:M:200:ASP:OD1	4:f:2:MET:HE1	1.99	0.61
4:P:2:MET:HE1	2:c:197:ASN:HB2	1.71	0.61
1:Q:426:LYS:HZ2	1:Q:457:ALA:HB2	1.65	0.61
1:R:403:LEU:CD2	1:R:420:GLN:HE22	2.12	0.61
2:U:122:SER:O	2:U:123:GLN:HB2	1.99	0.61
1:Z:496:ILE:O	1:Z:500:LEU:HG	2.01	0.61
3:e:55:LEU:HD12	3:e:55:LEU:O	2.00	0.61
1:C:66:LEU:HB2	2:D:64:ARG:HD2	1.82	0.61
2:D:311:THR:HG22	2:D:315:LEU:CD2	2.30	0.61
3:G:64:HIS:CG	3:G:68:GLU:HG2	2.34	0.61
1:K:159:ILE:HG12	1:K:165:GLU:HG3	1.81	0.61
2:N:323:ARG:HH11	2:N:323:ARG:CG	2.09	0.61
3:O:48:MET:HE3	4:P:79:LEU:CD1	2.30	0.61
1:Q:163:GLN:HG2	1:Q:164:ARG:N	2.15	0.61
2:T:427:PHE:HA	2:T:430:ILE:HG22	1.81	0.61
1:Y:103:LEU:HD12	1:Y:245:MET:HE3	1.82	0.61
1:Z:31:ILE:HD13	1:Z:39:ILE:HD11	1.82	0.61
1:A:96:GLU:HB3	1:A:126:PHE:HD2	1.65	0.61
1:I:385:ILE:O	1:I:389:LEU:HD22	2.01	0.61
1:K:460:GLU:O	1:K:461:LEU:C	2.42	0.61
2:M:344:LEU:C	2:M:344:LEU:HD12	2.25	0.61
1:Q:156:MET:HG2	1:Q:394:ARG:HA	1.83	0.61
1:A:163:GLN:HG2	1:A:164:ARG:N	2.16	0.61
1:B:110:THR:CG2	1:B:234:LEU:HG	2.30	0.61
1:C:330:ILE:HD11	1:C:345:VAL:HG21	1.82	0.61
1:C:439:MET:HB3	1:C:443:GLN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:ASN:ND2	1:C:493:ASN:N	2.47	0.61
2:D:14:ASP:HB3	2:D:52:ARG:HD3	1.83	0.61
2:E:115:SER:HB2	2:E:118:GLU:HB2	1.81	0.61
2:E:197:ASN:HB3	4:X:2:MET:CG	2.30	0.61
3:G:201:LYS:HE2	2:U:171:SER:HA	1.82	0.61
1:I:163:GLN:HG2	1:I:164:ARG:N	2.15	0.61
1:K:195:TYR:CD1	1:K:259:ILE:HD11	2.36	0.61
3:O:6:ILE:HD13	3:O:263:VAL:HG12	1.82	0.61
1:Q:109:ASN:HD21	1:Q:113:ALA:H	1.49	0.61
2:U:164:ARG:HA	2:U:201:LYS:HZ2	1.65	0.61
2:V:25:VAL:HG13	2:V:26:TYR:N	2.16	0.61
1:Y:385:ILE:O	1:Y:389:LEU:HD22	2.01	0.61
1:Z:182:ALA:O	1:Z:186:GLN:HG2	2.01	0.61
2:d:400:LEU:HD12	2:d:427:PHE:CZ	2.35	0.61
1:A:371:GLY:H	1:A:394:ARG:NH1	1.97	0.61
1:A:479:HIS:C	1:A:481:PRO:HD2	2.25	0.61
1:C:492:TYR:C	1:C:493:ASN:HD22	2.06	0.61
1:C:493:ASN:O	1:C:496:ILE:CG1	2.49	0.61
2:M:332:PRO:HD2	2:M:401:SER:HA	1.83	0.61
2:N:25:VAL:HG13	2:N:26:TYR:N	2.16	0.61
1:R:172:GLN:HA	5:R:600:ANP:HNB1	1.65	0.61
1:S:274:SER:HB2	1:S:287:PRO:HG3	1.83	0.61
1:Y:423:HIS:O	1:Y:426:LYS:HG2	2.00	0.61
1:C:195:TYR:CD1	1:C:259:ILE:HD11	2.36	0.61
2:D:8:VAL:HG22	2:D:13:VAL:HB	1.83	0.61
2:E:231:ARG:HD3	2:E:290:ILE:HG13	1.82	0.61
1:I:371:GLY:H	1:I:394:ARG:NH1	1.97	0.61
1:R:430:LEU:HD12	1:R:451:ALA:HB2	1.81	0.61
3:W:6:ILE:HD13	3:W:263:VAL:HG12	1.82	0.61
1:Z:106:ARG:HH12	1:Z:115:ILE:HG22	1.65	0.61
1:Z:106:ARG:NH2	1:Z:118:LYS:HB2	2.16	0.61
1:Z:243:CYS:O	1:Z:247:GLU:HG3	2.01	0.61
1:B:106:ARG:HH12	1:B:115:ILE:HG22	1.65	0.61
1:B:496:ILE:O	1:B:500:LEU:HG	2.01	0.61
1:I:103:LEU:HD23	1:I:103:LEU:H	1.66	0.61
3:O:55:LEU:HD12	3:O:55:LEU:O	2.00	0.61
1:R:182:ALA:O	1:R:186:GLN:HG2	2.01	0.61
1:R:496:ILE:O	1:R:500:LEU:HG	2.01	0.61
1:S:68:ARG:N	2:T:7:GLN:HG2	2.15	0.61
1:S:186:GLN:HE21	1:S:191:ILE:HD13	1.66	0.61
1:S:195:TYR:CD1	1:S:259:ILE:HD11	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:144:LYS:HZ3	2:c:279:GLN:HB3	1.66	0.61
1:A:48:MET:HB3	2:E:63:ARG:HG2	1.83	0.60
1:A:432:LYS:HD2	1:A:432:LYS:N	2.15	0.60
2:E:447:GLY:H	2:E:451:GLU:HG2	1.66	0.60
3:G:6:ILE:HD13	3:G:263:VAL:HG12	1.82	0.60
1:I:180:ILE:CD1	1:I:211:LYS:CE	2.79	0.60
1:K:66:LEU:CD1	2:L:8:VAL:HB	2.31	0.60
1:K:136:VAL:C	1:K:138:GLU:H	2.08	0.60
1:Q:432:LYS:HD2	1:Q:432:LYS:N	2.15	0.60
1:R:110:THR:CG2	1:R:234:LEU:HG	2.30	0.60
3:W:66:TYR:CB	3:W:188:LEU:CD2	2.75	0.60
1:Z:110:THR:CG2	1:Z:234:LEU:HG	2.30	0.60
1:Z:146:VAL:HG22	1:Z:161:ARG:HD3	1.83	0.60
2:c:305:ASP:O	2:c:308:PRO:HD2	2.01	0.60
2:c:394:ARG:O	2:c:398:ARG:HG3	2.00	0.60
3:e:6:ILE:HD13	3:e:263:VAL:HG12	1.82	0.60
1:A:35:SER:HB2	2:D:44:GLN:HG2	1.82	0.60
1:A:195:TYR:HD1	1:A:259:ILE:HD11	1.66	0.60
1:A:385:ILE:O	1:A:389:LEU:HD22	2.01	0.60
1:B:182:ALA:O	1:B:186:GLN:HG2	2.01	0.60
1:B:430:LEU:HD12	1:B:451:ALA:HB2	1.81	0.60
2:E:349:VAL:CG2	2:E:353:HIS:CB	2.79	0.60
2:F:25:VAL:HG13	2:F:26:TYR:N	2.16	0.60
3:G:28:ALA:HA	3:G:31:MET:HE2	1.82	0.60
1:I:453:ARG:O	1:I:453:ARG:HD3	2.01	0.60
1:K:385:ILE:HD13	1:K:444:GLN:HG2	1.83	0.60
2:L:384:GLU:OE2	2:L:387:LYS:HD3	2.01	0.60
2:L:432:GLU:H	2:L:433:GLY:HA2	1.66	0.60
2:M:360:VAL:HA	2:M:431:MET:HE1	1.83	0.60
1:S:449:PHE:CB	1:S:504:LEU:HD11	2.31	0.60
1:Y:163:GLN:HG2	1:Y:164:ARG:N	2.15	0.60
1:a:195:TYR:CD1	1:a:259:ILE:HD11	2.36	0.60
1:a:449:PHE:CB	1:a:504:LEU:HD11	2.31	0.60
3:e:28:ALA:HA	3:e:31:MET:HE2	1.82	0.60
1:A:109:ASN:HD21	1:A:113:ALA:H	1.49	0.60
1:B:95:LEU:C	1:B:95:LEU:HD13	2.25	0.60
2:E:445:MET:HE3	2:E:445:MET:N	2.15	0.60
1:I:428:THR:O	1:I:432:LYS:CG	2.49	0.60
1:J:106:ARG:NH2	1:J:118:LYS:HB2	2.16	0.60
1:K:186:GLN:HE21	1:K:191:ILE:HD13	1.66	0.60
1:Q:103:LEU:HD12	1:Q:245:MET:HE3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:138:GLU:O	1:Q:305:ASN:ND2	2.34	0.60
1:R:106:ARG:HH12	1:R:115:ILE:HG22	1.65	0.60
1:a:460:GLU:O	1:a:461:LEU:C	2.43	0.60
2:c:265:VAL:O	2:c:265:VAL:HG22	2.00	0.60
1:A:103:LEU:HD23	1:A:103:LEU:H	1.66	0.60
1:C:385:ILE:HD13	1:C:444:GLN:HG2	1.84	0.60
2:E:387:LYS:HD2	2:E:390:VAL:HB	1.82	0.60
2:E:433:GLY:O	2:E:434:GLU:HB2	2.00	0.60
2:F:118:GLU:O	2:F:286:LYS:HG2	2.01	0.60
1:J:243:CYS:O	1:J:247:GLU:HG3	2.01	0.60
1:K:274:SER:HB2	1:K:287:PRO:HG3	1.83	0.60
1:K:485:GLU:O	1:K:489:THR:HG22	2.01	0.60
2:M:122:SER:O	2:M:123:GLN:HB2	1.99	0.60
2:M:387:LYS:HD2	2:M:390:VAL:HB	1.83	0.60
1:Q:195:TYR:HD1	1:Q:259:ILE:HD11	1.66	0.60
1:S:439:MET:HB3	1:S:443:GLN:HB3	1.83	0.60
1:Z:327:LEU:HD23	1:Z:327:LEU:H	1.67	0.60
2:b:387:LYS:HA	2:b:390:VAL:HG12	1.84	0.60
1:A:103:LEU:HD12	1:A:245:MET:HE3	1.82	0.60
1:C:186:GLN:HE21	1:C:191:ILE:HD13	1.66	0.60
1:C:485:GLU:O	1:C:489:THR:HG22	2.01	0.60
1:I:138:GLU:HG3	1:I:305:ASN:CB	2.30	0.60
1:I:449:PHE:CE2	1:I:500:LEU:HB3	2.36	0.60
2:L:427:PHE:HA	2:L:430:ILE:HG22	1.83	0.60
3:O:16:THR:HG22	4:P:124:ALA:HB1	1.83	0.60
1:Q:449:PHE:CE2	1:Q:500:LEU:HB3	2.36	0.60
1:S:471:LEU:HD13	1:S:474:TYR:CE1	2.37	0.60
2:V:229:LYS:O	2:V:233:GLU:HG2	2.02	0.60
1:Y:195:TYR:HD1	1:Y:259:ILE:HD11	1.66	0.60
2:b:8:VAL:HG22	2:b:13:VAL:HB	1.83	0.60
2:c:360:VAL:HA	2:c:431:MET:HE1	1.83	0.60
2:d:120:SER:OG	2:d:286:LYS:HE3	2.01	0.60
3:e:186:GLN:NE2	3:e:189:PRO:CG	2.60	0.60
1:B:243:CYS:O	1:B:247:GLU:HG3	2.01	0.60
2:D:174:SER:O	2:D:202:VAL:HA	2.02	0.60
2:D:432:GLU:N	2:D:433:GLY:HA2	2.16	0.60
2:E:144:LYS:HE2	2:E:282:ILE:HG13	1.84	0.60
1:R:146:VAL:HG22	1:R:161:ARG:HD3	1.84	0.60
1:S:281:PRO:HB2	1:S:285:ALA:HA	1.84	0.60
2:U:433:GLY:O	2:U:434:GLU:HB2	2.02	0.60
3:W:186:GLN:HG3	3:W:189:PRO:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:109:ASN:HD21	1:Y:113:ALA:H	1.49	0.60
1:a:471:LEU:HD13	1:a:474:TYR:CE1	2.37	0.60
1:B:106:ARG:NH2	1:B:118:LYS:HB2	2.16	0.60
1:B:327:LEU:HD23	1:B:327:LEU:H	1.67	0.60
2:F:229:LYS:O	2:F:233:GLU:HG2	2.02	0.60
1:I:365:ARG:O	1:I:367:ALA:N	2.35	0.60
2:T:84:LEU:HD22	2:T:201:LYS:HB3	1.84	0.60
1:Y:449:PHE:CE2	1:Y:500:LEU:HB3	2.36	0.60
1:a:274:SER:HB2	1:a:287:PRO:HG3	1.83	0.60
2:b:231:ARG:NH1	2:b:281:ARG:HH11	2.00	0.60
2:c:78:PRO:CB	2:c:103:GLU:HG2	2.30	0.60
2:d:131:LYS:HG2	2:d:423:THR:HG23	1.82	0.60
1:B:414:ASP:O	1:B:418:ARG:CB	2.50	0.60
1:C:236:TYR:HE1	1:C:293:LEU:HD11	1.67	0.60
2:E:276:GLY:O	2:E:280:GLU:HB2	2.02	0.60
2:E:370:LEU:HD13	2:E:382:LEU:HD11	1.84	0.60
1:J:327:LEU:HD23	1:J:327:LEU:H	1.67	0.60
1:K:471:LEU:HD13	1:K:474:TYR:CE1	2.37	0.60
2:L:8:VAL:HG22	2:L:13:VAL:HB	1.83	0.60
2:M:285:THR:HG23	2:M:288:GLY:H	1.67	0.60
1:Q:453:ARG:O	1:Q:453:ARG:HD3	2.01	0.60
1:R:51:GLU:N	1:R:94:ILE:HG23	2.02	0.60
1:S:385:ILE:HD13	1:S:444:GLN:HG2	1.84	0.60
2:U:279:GLN:O	2:U:282:ILE:HG12	2.02	0.60
2:U:337:LEU:HD12	2:U:338:ASP:N	2.15	0.60
3:W:186:GLN:CG	3:W:189:PRO:CG	2.79	0.60
1:Y:180:ILE:HD11	1:Y:211:LYS:HZ3	1.67	0.60
1:a:281:PRO:HB2	1:a:285:ALA:HA	1.84	0.60
2:b:279:GLN:HE22	2:b:294:GLN:NE2	1.99	0.60
2:b:427:PHE:HA	2:b:430:ILE:HG22	1.83	0.60
1:C:471:LEU:HD13	1:C:474:TYR:CE1	2.37	0.60
1:C:479:HIS:C	1:C:481:PRO:HD2	2.27	0.60
3:G:86:LEU:HB3	3:G:246:MET:HE2	1.84	0.60
1:J:496:ILE:O	1:J:500:LEU:HG	2.01	0.60
1:K:236:TYR:HE1	1:K:293:LEU:HD11	1.67	0.60
1:K:479:HIS:C	1:K:481:PRO:HD2	2.27	0.60
2:M:89:ASN:HD21	2:M:93:GLU:H	1.50	0.60
2:M:164:ARG:HA	2:M:201:LYS:HZ2	1.67	0.60
2:N:240:PHE:HD2	2:N:293:VAL:HG22	1.67	0.60
1:S:485:GLU:O	1:S:489:THR:HG22	2.01	0.60
2:T:157:VAL:HG12	7:T:600:ADP:O1A	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:395:LYS:CD	2:U:443:PHE:CE2	2.84	0.60
1:Y:103:LEU:HD23	1:Y:103:LEU:H	1.66	0.60
2:b:231:ARG:HD2	2:b:281:ARG:HH12	1.67	0.60
1:B:186:GLN:NE2	1:B:191:ILE:HD12	2.17	0.60
1:C:281:PRO:HB2	1:C:285:ALA:HA	1.84	0.60
2:E:297:TYR:C	2:E:297:TYR:CD2	2.80	0.60
3:G:66:TYR:CB	3:G:188:LEU:CD1	2.80	0.60
1:K:330:ILE:HD11	1:K:345:VAL:HG21	1.81	0.60
2:L:388:LEU:HD11	2:L:392:ARG:NH2	2.16	0.60
1:Q:385:ILE:O	1:Q:389:LEU:HD22	2.01	0.60
2:U:89:ASN:HD21	2:U:93:GLU:H	1.50	0.60
2:V:400:LEU:HD12	2:V:427:PHE:CZ	2.37	0.60
1:a:236:TYR:HE1	1:a:293:LEU:HD11	1.67	0.60
2:b:174:SER:O	2:b:202:VAL:HA	2.02	0.60
2:d:352:GLU:H	2:d:352:GLU:CD	2.10	0.60
2:D:320:VAL:HG21	2:D:338:ASP:HB2	1.84	0.59
1:I:137:ILE:O	1:I:138:GLU:CB	2.45	0.59
1:J:106:ARG:HH12	1:J:115:ILE:HG22	1.65	0.59
2:L:14:ASP:HB3	2:L:52:ARG:HD3	1.83	0.59
3:O:201:LYS:NZ	2:c:171:SER:HA	2.17	0.59
1:Q:103:LEU:HD23	1:Q:103:LEU:H	1.66	0.59
1:R:153:VAL:HG23	1:R:157:ILE:HG13	1.84	0.59
1:R:186:GLN:NE2	1:R:191:ILE:HD12	2.17	0.59
1:R:327:LEU:HD23	1:R:327:LEU:H	1.67	0.59
2:T:14:ASP:HB3	2:T:52:ARG:HD3	1.83	0.59
2:T:89:ASN:HD21	2:T:93:GLU:HG3	1.67	0.59
1:Y:426:LYS:HZ2	1:Y:457:ALA:HB2	1.67	0.59
1:Y:453:ARG:O	1:Y:453:ARG:HD3	2.01	0.59
2:b:14:ASP:HB3	2:b:52:ARG:HD3	1.83	0.59
2:b:84:LEU:HD22	2:b:201:LYS:HB3	1.84	0.59
1:A:106:ARG:HH21	1:A:114:PRO:HB3	1.67	0.59
1:A:137:ILE:CD1	1:A:138:GLU:OE1	2.50	0.59
1:A:453:ARG:O	1:A:453:ARG:HD3	2.01	0.59
3:G:55:LEU:HD12	3:G:55:LEU:O	2.00	0.59
1:I:156:MET:HG2	1:I:394:ARG:HA	1.83	0.59
1:J:182:ALA:O	1:J:186:GLN:HG2	2.01	0.59
1:K:449:PHE:CB	1:K:504:LEU:HD11	2.31	0.59
2:N:229:LYS:O	2:N:233:GLU:HG2	2.02	0.59
2:N:417:TYR:CD2	2:N:417:TYR:C	2.80	0.59
1:R:159:ILE:HG12	1:R:165:GLU:HG3	1.82	0.59
1:S:365:ARG:HG3	5:S:600:ANP:N1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:94:PRO:HG3	2:V:100:GLU:HB3	1.85	0.59
1:Z:84:GLU:OE1	2:c:49:GLY:HA2	2.02	0.59
1:Z:240:TYR:OH	1:Z:293:LEU:HD12	2.02	0.59
2:c:349:VAL:HG21	2:c:353:HIS:ND1	2.16	0.59
2:c:387:LYS:HD2	2:c:390:VAL:HB	1.84	0.59
1:B:111:LEU:HD12	1:B:112:GLY:N	2.17	0.59
1:B:146:VAL:HG22	1:B:161:ARG:HD3	1.83	0.59
1:C:274:SER:HB2	1:C:287:PRO:HG3	1.83	0.59
1:C:449:PHE:CB	1:C:504:LEU:HD11	2.32	0.59
2:D:435:TYR:HB3	2:D:438:LEU:HD21	1.84	0.59
2:E:122:SER:O	2:E:123:GLN:HB2	1.99	0.59
1:J:111:LEU:HD12	1:J:112:GLY:N	2.17	0.59
4:P:2:MET:HE2	4:P:2:MET:CA	2.33	0.59
4:P:9:VAL:HG12	4:P:14:GLN:HG2	1.85	0.59
1:Q:233:ALA:HA	1:Q:273:ILE:HD11	1.84	0.59
1:R:106:ARG:NH2	1:R:118:LYS:HB2	2.16	0.59
1:R:240:TYR:OH	1:R:293:LEU:HD12	2.02	0.59
1:S:136:VAL:O	1:S:137:ILE:HG12	2.02	0.59
1:S:236:TYR:HE1	1:S:293:LEU:HD11	1.67	0.59
1:Y:137:ILE:HG12	1:Y:138:GLU:OE1	2.03	0.59
1:B:262:ASP:H	1:B:329:ILE:HB	1.67	0.59
1:B:402:GLU:HG3	1:B:403:LEU:H	1.68	0.59
2:E:89:ASN:HD21	2:E:93:GLU:H	1.50	0.59
2:E:349:VAL:HG21	2:E:353:HIS:ND1	2.17	0.59
1:J:153:VAL:HG23	1:J:157:ILE:HG13	1.84	0.59
1:J:262:ASP:H	1:J:329:ILE:HB	1.68	0.59
1:Q:365:ARG:O	1:Q:367:ALA:N	2.35	0.59
1:R:51:GLU:N	1:R:94:ILE:HG21	2.03	0.59
1:S:136:VAL:C	1:S:138:GLU:H	2.11	0.59
2:U:332:PRO:HD2	2:U:401:SER:HA	1.84	0.59
1:Y:156:MET:HG2	1:Y:394:ARG:HA	1.83	0.59
1:a:479:HIS:C	1:a:481:PRO:HD2	2.27	0.59
1:a:485:GLU:O	1:a:489:THR:HG22	2.01	0.59
2:d:268:GLN:NE2	2:d:268:GLN:H	1.99	0.59
1:A:156:MET:HG2	1:A:394:ARG:HA	1.83	0.59
2:D:84:LEU:HD22	2:D:201:LYS:HB3	1.84	0.59
1:J:138:GLU:C	1:J:138:GLU:CD	2.70	0.59
1:J:186:GLN:NE2	1:J:191:ILE:HD12	2.17	0.59
1:K:281:PRO:HB2	1:K:285:ALA:HA	1.84	0.59
1:K:439:MET:HB3	1:K:443:GLN:HB3	1.83	0.59
2:N:457:LYS:HA	2:N:457:LYS:HE3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:479:HIS:C	1:S:481:PRO:HD2	2.27	0.59
1:a:453:ARG:HB3	1:a:455:TYR:CE2	2.38	0.59
2:d:229:LYS:O	2:d:233:GLU:HG2	2.02	0.59
1:B:240:TYR:OH	1:B:293:LEU:HD12	2.02	0.59
1:B:453:ARG:HH11	1:B:453:ARG:CG	2.16	0.59
2:D:196:SER:HB2	2:D:198:VAL:HG12	1.84	0.59
2:E:197:ASN:HB2	4:X:2:MET:HE3	1.84	0.59
2:F:130:ILE:HD12	2:F:404:PHE:CE1	2.37	0.59
1:I:449:PHE:HA	1:I:452:GLU:HB3	1.85	0.59
1:J:113:ALA:O	1:J:114:PRO:C	2.45	0.59
1:J:146:VAL:HG22	1:J:161:ARG:HD3	1.83	0.59
1:R:113:ALA:O	1:R:114:PRO:C	2.46	0.59
2:V:12:VAL:HG11	2:V:257:LEU:HB3	1.85	0.59
2:V:200:ASP:OD1	2:V:201:LYS:HD3	2.03	0.59
1:Y:463:LYS:HD2	1:Y:464:ILE:N	2.18	0.59
1:A:365:ARG:O	1:A:367:ALA:N	2.35	0.59
1:C:193:CYS:HB2	1:C:221:THR:HB	1.85	0.59
2:F:12:VAL:HG11	2:F:257:LEU:HB3	1.85	0.59
2:F:94:PRO:HG3	2:F:100:GLU:HB3	1.85	0.59
1:K:193:CYS:HB2	1:K:221:THR:HB	1.85	0.59
2:M:78:PRO:CB	2:M:103:GLU:HG2	2.30	0.59
1:Q:449:PHE:HA	1:Q:452:GLU:HB3	1.85	0.59
2:T:174:SER:O	2:T:202:VAL:HA	2.02	0.59
1:Y:233:ALA:HA	1:Y:273:ILE:HD11	1.84	0.59
1:Y:365:ARG:O	1:Y:367:ALA:N	2.35	0.59
1:Y:449:PHE:HA	1:Y:452:GLU:HB3	1.85	0.59
2:c:336:PRO:HG3	2:c:400:LEU:HD11	1.84	0.59
1:A:218:LEU:O	1:A:218:LEU:HD22	2.03	0.59
1:A:449:PHE:CE2	1:A:500:LEU:HB3	2.36	0.59
1:B:153:VAL:HG23	1:B:157:ILE:HG13	1.84	0.59
1:C:453:ARG:HB3	1:C:455:TYR:CE2	2.38	0.59
2:E:22:VAL:HG13	2:E:45:GLN:HE22	1.68	0.59
1:I:106:ARG:HH21	1:I:114:PRO:HB3	1.68	0.59
1:I:218:LEU:O	1:I:218:LEU:HD22	2.03	0.59
2:N:12:VAL:HG11	2:N:257:LEU:HB3	1.85	0.59
3:O:169:ILE:HB	3:O:187:LEU:HD21	1.85	0.59
1:Q:55:LEU:HB3	1:Q:56:PRO:HD2	1.85	0.59
1:R:262:ASP:H	1:R:329:ILE:HB	1.67	0.59
2:T:8:VAL:HG22	2:T:13:VAL:HB	1.83	0.59
2:T:432:GLU:N	2:T:433:GLY:HA2	2.16	0.59
2:U:337:LEU:O	2:U:338:ASP:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:67:GLU:HA	2:c:7:GLN:HG2	1.85	0.59
1:Z:111:LEU:HD12	1:Z:112:GLY:N	2.17	0.59
1:Z:113:ALA:O	1:Z:114:PRO:C	2.45	0.59
1:Z:113:ALA:O	1:Z:115:ILE:HG23	2.03	0.59
1:a:186:GLN:HE21	1:a:191:ILE:HD13	1.66	0.59
1:a:439:MET:HB3	1:a:443:GLN:HB3	1.83	0.59
2:b:157:VAL:HG12	7:b:600:ADP:O1A	2.03	0.59
2:F:240:PHE:CD2	2:F:293:VAL:HG22	2.37	0.59
2:F:279:GLN:NE2	2:F:294:GLN:HE22	2.00	0.59
1:I:55:LEU:HB3	1:I:56:PRO:HD2	1.85	0.59
1:I:195:TYR:HD1	1:I:259:ILE:HD11	1.66	0.59
1:I:463:LYS:HD2	1:I:464:ILE:N	2.18	0.59
2:L:89:ASN:HD21	2:L:93:GLU:HG3	1.67	0.59
2:L:174:SER:O	2:L:202:VAL:HA	2.02	0.59
2:L:196:SER:HB2	2:L:198:VAL:HG12	1.84	0.59
2:N:120:SER:OG	2:N:286:LYS:HE3	2.03	0.59
2:N:400:LEU:HD12	2:N:427:PHE:CZ	2.38	0.59
1:R:138:GLU:C	1:R:138:GLU:CD	2.70	0.59
1:R:453:ARG:HH11	1:R:453:ARG:CG	2.15	0.59
1:S:385:ILE:HB	1:S:492:TYR:HB3	1.85	0.59
1:S:480:ALA:N	1:S:481:PRO:CD	2.66	0.59
2:T:111:ARG:NH1	2:T:221:LEU:HD22	2.18	0.59
1:Z:186:GLN:NE2	1:Z:191:ILE:HD12	2.17	0.59
1:a:136:VAL:O	1:a:137:ILE:HG12	2.02	0.59
3:e:190:LEU:HD12	3:e:191:PRO:C	2.28	0.59
1:K:453:ARG:HB3	1:K:455:TYR:CE2	2.38	0.59
2:N:200:ASP:OD1	2:N:201:LYS:HD3	2.03	0.59
2:T:114:PRO:HD3	2:T:281:ARG:HG2	1.85	0.59
3:W:208:GLU:HB2	3:W:209:PRO:CD	2.33	0.59
1:Y:137:ILE:O	1:Y:138:GLU:CB	2.22	0.59
1:a:385:ILE:HD13	1:a:444:GLN:HG2	1.84	0.59
2:b:174:SER:HB2	2:b:202:VAL:HG12	1.85	0.59
2:b:237:VAL:HG13	2:b:290:ILE:HD13	1.85	0.59
2:b:367:TYR:CE1	2:b:390:VAL:HG23	2.38	0.59
2:d:305:ASP:O	2:d:308:PRO:HD2	2.03	0.59
1:A:180:ILE:HD11	1:A:211:LYS:HZ3	1.68	0.58
1:A:463:LYS:HD2	1:A:464:ILE:N	2.18	0.58
1:B:138:GLU:CD	1:B:138:GLU:C	2.71	0.58
2:F:200:ASP:OD1	2:F:201:LYS:HD3	2.03	0.58
1:J:48:MET:HG2	1:J:51:GLU:OE1	2.03	0.58
1:J:97:VAL:HG11	1:J:112:GLY:HA3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:262:ASP:HB3	1:K:265:LYS:HG3	1.85	0.58
2:L:84:LEU:HD22	2:L:201:LYS:HB3	1.84	0.58
1:R:243:CYS:O	1:R:247:GLU:HG3	2.01	0.58
2:T:196:SER:HB2	2:T:198:VAL:HG12	1.84	0.58
1:Z:153:VAL:HG23	1:Z:157:ILE:HG13	1.84	0.58
1:a:136:VAL:C	1:a:138:GLU:H	2.11	0.58
2:b:196:SER:HB2	2:b:198:VAL:HG12	1.84	0.58
1:A:195:TYR:CD1	1:A:259:ILE:HD11	2.38	0.58
1:B:48:MET:HG2	1:B:51:GLU:OE1	2.03	0.58
1:C:480:ALA:N	1:C:481:PRO:CD	2.66	0.58
2:F:131:LYS:H	2:F:402:GLN:HE22	1.51	0.58
3:G:208:GLU:HB2	3:G:209:PRO:CD	2.33	0.58
1:I:46:ASP:O	2:M:63:ARG:HD2	2.02	0.58
1:J:453:ARG:HH11	1:J:453:ARG:CG	2.16	0.58
1:K:106:ARG:CZ	1:K:118:LYS:HB3	2.33	0.58
2:N:94:PRO:HG3	2:N:100:GLU:HB3	1.85	0.58
1:Q:135:GLY:N	1:Q:138:GLU:OE1	2.30	0.58
1:R:48:MET:HG2	1:R:51:GLU:OE1	2.03	0.58
1:S:240:TYR:HD1	1:S:300:ARG:NH2	2.01	0.58
1:S:453:ARG:HB3	1:S:455:TYR:CE2	2.38	0.58
1:a:106:ARG:CZ	1:a:118:LYS:HB3	2.33	0.58
2:c:22:VAL:HG13	2:c:45:GLN:HE22	1.68	0.58
2:c:109:ILE:HG21	2:c:222:THR:HG22	1.85	0.58
2:d:200:ASP:OD1	2:d:201:LYS:HD3	2.03	0.58
3:e:188:LEU:O	3:e:188:LEU:CG	2.50	0.58
1:A:318:LYS:H	1:A:318:LYS:HD2	1.68	0.58
1:B:113:ALA:O	1:B:114:PRO:C	2.45	0.58
1:C:136:VAL:C	1:C:138:GLU:H	2.11	0.58
2:D:89:ASN:HD21	2:D:93:GLU:HG3	1.67	0.58
2:E:148:PHE:HZ	2:E:312:PHE:HE1	1.51	0.58
2:E:367:TYR:CE2	2:E:390:VAL:HG13	2.38	0.58
1:I:318:LYS:H	1:I:318:LYS:HD2	1.68	0.58
1:J:113:ALA:O	1:J:115:ILE:HG23	2.03	0.58
2:M:140:ALA:HB2	2:M:343:GLN:CD	2.28	0.58
3:O:86:LEU:HB3	3:O:246:MET:HE2	1.84	0.58
1:R:111:LEU:HD12	1:R:112:GLY:N	2.17	0.58
1:Z:262:ASP:H	1:Z:329:ILE:HB	1.67	0.58
1:a:240:TYR:HD1	1:a:300:ARG:NH2	2.01	0.58
1:A:449:PHE:HA	1:A:452:GLU:HB3	1.85	0.58
1:C:262:ASP:HB3	1:C:265:LYS:HG3	1.85	0.58
2:L:111:ARG:NH1	2:L:221:LEU:HD22	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:161:GLU:HG3	2:U:404:PHE:CB	2.31	0.58
2:U:244:ILE:HD11	2:U:275:MET:HE1	1.85	0.58
2:U:265:VAL:HG23	3:W:272:ILE:HG21	1.85	0.58
3:W:86:LEU:HB3	3:W:246:MET:HE2	1.84	0.58
1:Y:218:LEU:O	1:Y:218:LEU:HD22	2.03	0.58
1:Z:402:GLU:HG3	1:Z:403:LEU:H	1.68	0.58
2:c:89:ASN:HD21	2:c:93:GLU:H	1.50	0.58
3:e:86:LEU:HB3	3:e:246:MET:HE2	1.84	0.58
1:A:137:ILE:CD1	1:A:138:GLU:HA	2.14	0.58
1:C:136:VAL:O	1:C:137:ILE:HG12	2.02	0.58
1:J:401:ARG:HB2	1:J:401:ARG:HH11	1.68	0.58
1:K:385:ILE:HB	1:K:492:TYR:HB3	1.85	0.58
1:K:480:ALA:N	1:K:481:PRO:CD	2.66	0.58
2:M:22:VAL:HG13	2:M:45:GLN:HE22	1.68	0.58
2:N:243:ASN:ND2	2:N:297:TYR:HB2	2.19	0.58
1:R:113:ALA:O	1:R:115:ILE:HG23	2.03	0.58
1:S:106:ARG:CZ	1:S:118:LYS:HB3	2.33	0.58
2:V:457:LYS:HA	2:V:457:LYS:HE3	1.86	0.58
2:b:89:ASN:HD21	2:b:93:GLU:HG3	1.67	0.58
1:A:365:ARG:HB3	1:A:366:PRO:HD3	1.86	0.58
2:D:85:GLY:C	2:D:199:ILE:HD11	2.29	0.58
2:F:46:LEU:HD22	2:F:50:ILE:HD11	1.86	0.58
1:J:240:TYR:OH	1:J:293:LEU:HD12	2.02	0.58
1:K:240:TYR:HD1	1:K:300:ARG:NH2	2.01	0.58
1:K:385:ILE:HD12	1:K:492:TYR:HB2	1.86	0.58
2:M:276:GLY:O	2:M:280:GLU:HB2	2.04	0.58
1:R:456:LEU:HB2	1:R:460:GLU:CD	2.29	0.58
2:c:144:LYS:HE2	2:c:282:ILE:HG13	1.86	0.58
4:f:9:VAL:HG12	4:f:14:GLN:HG2	1.85	0.58
1:I:172:GLN:NE2	2:L:342:ARG:HH21	2.02	0.58
2:L:157:VAL:HG11	7:L:600:ADP:C8	2.39	0.58
2:M:367:TYR:CE2	2:M:390:VAL:HG13	2.39	0.58
1:Q:195:TYR:CD1	1:Q:259:ILE:HD11	2.38	0.58
1:Q:218:LEU:O	1:Q:218:LEU:HD22	2.03	0.58
1:Q:475:VAL:HG11	1:Q:507:PHE:HD2	1.69	0.58
1:R:365:ARG:HG2	5:R:600:ANP:C2	2.33	0.58
1:R:401:ARG:HB2	1:R:401:ARG:HH11	1.68	0.58
1:S:262:ASP:HB3	1:S:265:LYS:HG3	1.85	0.58
1:S:385:ILE:HD12	1:S:492:TYR:HB2	1.86	0.58
3:W:16:THR:HG22	4:X:124:ALA:HB1	1.85	0.58
1:Z:453:ARG:HH11	1:Z:453:ARG:CG	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:456:LEU:HB2	1:Z:460:GLU:CD	2.29	0.58
3:e:208:GLU:HB2	3:e:209:PRO:CD	2.33	0.58
1:B:231:SER:HB3	1:B:234:LEU:HB2	1.86	0.58
1:B:299:GLU:HG2	2:F:209:MET:HE3	1.86	0.58
2:D:144:LYS:HD3	2:D:279:GLN:HE21	1.68	0.58
2:E:380:ASP:CB	2:U:437:HIS:HA	2.34	0.58
1:I:109:ASN:HD21	1:I:113:ALA:H	1.49	0.58
1:J:231:SER:HB3	1:J:234:LEU:HB2	1.86	0.58
2:M:71:LEU:N	2:M:71:LEU:HD23	2.19	0.58
2:M:131:LYS:H	2:M:402:GLN:NE2	1.97	0.58
1:Q:318:LYS:H	1:Q:318:LYS:HD2	1.68	0.58
1:Q:463:LYS:HD2	1:Q:464:ILE:N	2.18	0.58
1:S:95:LEU:HD12	1:S:129:VAL:HG11	1.86	0.58
1:S:492:TYR:CE1	1:S:497:GLU:HB2	2.39	0.58
4:X:9:VAL:HG12	4:X:14:GLN:HG2	1.84	0.58
1:Y:475:VAL:HG11	1:Y:507:PHE:HD2	1.69	0.58
1:B:343:THR:HG22	2:F:297:TYR:OH	2.04	0.58
2:D:397:GLN:O	2:D:400:LEU:HD23	2.03	0.58
2:E:109:ILE:HG21	2:E:222:THR:HG22	1.85	0.58
2:F:243:ASN:ND2	2:F:297:TYR:HB2	2.18	0.58
1:I:195:TYR:CD1	1:I:259:ILE:HD11	2.38	0.58
1:K:492:TYR:CE1	1:K:497:GLU:HB2	2.39	0.58
2:L:311:THR:HG22	2:L:315:LEU:CD2	2.33	0.58
2:N:458:LYS:O	2:N:459:LEU:HB2	2.04	0.58
1:Q:76:MET:HE3	1:Q:233:ALA:HB1	1.86	0.58
1:R:402:GLU:HG3	1:R:403:LEU:H	1.68	0.58
1:S:333:GLN:HB3	2:V:304:THR:HG23	1.85	0.58
3:W:167:LEU:HD23	3:W:188:LEU:HD12	1.86	0.58
1:Y:55:LEU:HB3	1:Y:56:PRO:HD2	1.85	0.58
1:Y:195:TYR:CD1	1:Y:259:ILE:HD11	2.38	0.58
1:Y:198:ILE:HD11	1:Y:239:PRO:HG3	1.86	0.58
1:Z:140:GLN:HA	1:Z:140:GLN:NE2	2.14	0.58
1:Z:309:VAL:CG1	1:Z:317:VAL:HG11	2.33	0.58
1:Z:401:ARG:HB2	1:Z:401:ARG:HH11	1.68	0.58
2:b:392:ARG:O	2:b:396:ILE:HG23	2.04	0.58
2:b:397:GLN:O	2:b:400:LEU:HD23	2.04	0.58
2:c:71:LEU:N	2:c:71:LEU:HD23	2.19	0.58
2:d:94:PRO:HG3	2:d:100:GLU:HB3	1.85	0.58
2:d:126:LEU:HD23	2:d:139:PHE:O	2.04	0.58
2:d:243:ASN:ND2	2:d:297:TYR:HB2	2.18	0.58
1:A:76:MET:HE3	1:A:233:ALA:HB1	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:LEU:HD13	1:C:448:LEU:CB	2.34	0.58
2:D:111:ARG:NH1	2:D:221:LEU:HD22	2.18	0.58
2:D:202:VAL:HG23	2:D:202:VAL:O	2.04	0.58
2:E:111:ARG:HB3	2:E:111:ARG:CZ	2.34	0.58
1:K:95:LEU:HD12	1:K:129:VAL:HG11	1.86	0.58
2:M:109:ILE:HG21	2:M:222:THR:HG22	1.85	0.58
2:V:141:LYS:HA	2:V:291:THR:HG23	1.86	0.58
2:V:243:ASN:ND2	2:V:297:TYR:HB2	2.19	0.58
1:Z:48:MET:HG2	1:Z:51:GLU:OE1	2.03	0.58
2:E:285:THR:HG23	2:E:288:GLY:H	1.67	0.57
2:F:17:PHE:O	2:F:18:PRO:O	2.22	0.57
1:J:97:VAL:CG1	1:J:112:GLY:HA3	2.34	0.57
1:K:66:LEU:HB2	2:L:64:ARG:HD2	1.84	0.57
1:K:151:LYS:HE2	1:K:439:MET:SD	2.44	0.57
2:L:85:GLY:C	2:L:199:ILE:HD11	2.29	0.57
2:L:174:SER:HB2	2:L:202:VAL:HG12	1.85	0.57
2:M:144:LYS:HE2	2:M:282:ILE:HG13	1.86	0.57
1:Z:390:SER:HA	1:Z:393:ILE:HD13	1.86	0.57
1:a:385:ILE:HB	1:a:492:TYR:HB3	1.85	0.57
2:d:279:GLN:NE2	2:d:294:GLN:HE22	2.01	0.57
1:A:198:ILE:HD11	1:A:239:PRO:HG3	1.86	0.57
1:A:475:VAL:HG11	1:A:507:PHE:HD2	1.69	0.57
1:C:106:ARG:CZ	1:C:118:LYS:HB3	2.33	0.57
1:I:475:VAL:HG11	1:I:507:PHE:HD2	1.69	0.57
2:L:157:VAL:HG12	7:L:600:ADP:O1A	2.04	0.57
1:Q:198:ILE:HD11	1:Q:239:PRO:HG3	1.86	0.57
1:S:151:LYS:HE2	1:S:439:MET:SD	2.44	0.57
2:T:279:GLN:HG2	2:T:314:HIS:CG	2.39	0.57
2:U:111:ARG:HB3	2:U:111:ARG:CZ	2.34	0.57
2:U:237:VAL:HG23	2:U:290:ILE:HG23	1.86	0.57
1:a:222:ILE:HD12	1:a:245:MET:HE2	1.86	0.57
1:a:333:GLN:HB3	2:d:304:THR:HG23	1.87	0.57
2:b:85:GLY:C	2:b:199:ILE:HD11	2.29	0.57
2:b:432:GLU:N	2:b:433:GLY:HA2	2.19	0.57
2:d:12:VAL:HG11	2:d:257:LEU:HB3	1.85	0.57
2:d:116:TYR:C	2:d:116:TYR:CD2	2.82	0.57
2:d:257:LEU:H	2:d:257:LEU:HD22	1.69	0.57
2:d:332:PRO:CG	2:d:401:SER:HA	2.34	0.57
3:e:82:THR:O	3:e:120:LYS:HB2	2.04	0.57
1:C:241:ALA:O	1:C:245:MET:HG3	2.04	0.57
2:F:84:LEU:HD21	2:F:230:PHE:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:352:GLU:H	2:F:352:GLU:CD	2.12	0.57
4:H:9:VAL:HG12	4:H:14:GLN:HG2	1.85	0.57
1:I:198:ILE:HD11	1:I:239:PRO:HG3	1.86	0.57
2:L:237:VAL:HG13	2:L:290:ILE:HD13	1.86	0.57
2:L:279:GLN:HG2	2:L:314:HIS:CG	2.39	0.57
2:N:17:PHE:O	2:N:18:PRO:O	2.22	0.57
2:N:116:TYR:C	2:N:116:TYR:CD2	2.82	0.57
2:N:193:MET:HE3	2:N:202:VAL:HG11	1.86	0.57
3:O:208:GLU:HB2	3:O:209:PRO:CD	2.33	0.57
1:Q:106:ARG:HH21	1:Q:114:PRO:HB3	1.68	0.57
2:T:85:GLY:C	2:T:199:ILE:HD11	2.29	0.57
2:T:131:LYS:HG3	2:T:402:GLN:OE1	2.04	0.57
2:U:109:ILE:HG21	2:U:222:THR:HG22	1.85	0.57
2:U:285:THR:HG23	2:U:288:GLY:H	1.70	0.57
2:V:84:LEU:HD21	2:V:230:PHE:HE2	1.70	0.57
3:W:82:THR:HG22	3:W:91:ASN:OD1	2.05	0.57
3:W:186:GLN:CG	3:W:189:PRO:HD2	2.34	0.57
1:a:492:TYR:CE1	1:a:497:GLU:HB2	2.39	0.57
1:A:55:LEU:HB3	1:A:56:PRO:HD2	1.85	0.57
1:B:113:ALA:O	1:B:115:ILE:HG23	2.03	0.57
2:D:242:ASP:O	2:D:295:ALA:HB3	2.04	0.57
2:E:204:LEU:HD23	2:E:204:LEU:H	1.69	0.57
2:F:9:ILE:O	2:F:12:VAL:HG12	2.05	0.57
2:F:116:TYR:CD2	2:F:116:TYR:C	2.82	0.57
1:K:222:ILE:HD12	1:K:245:MET:HE2	1.86	0.57
1:K:241:ALA:O	1:K:245:MET:HG3	2.03	0.57
2:L:432:GLU:N	2:L:433:GLY:HA2	2.17	0.57
2:N:257:LEU:HD22	2:N:257:LEU:H	1.69	0.57
3:O:48:MET:HE3	4:P:79:LEU:HD12	1.86	0.57
1:S:241:ALA:O	1:S:245:MET:HG3	2.04	0.57
1:S:389:LEU:HD13	1:S:448:LEU:CB	2.34	0.57
2:U:22:VAL:HG13	2:U:45:GLN:HE22	1.68	0.57
2:V:126:LEU:HD23	2:V:139:PHE:O	2.04	0.57
1:Y:106:ARG:HH21	1:Y:114:PRO:HB3	1.68	0.57
1:a:193:CYS:HB2	1:a:221:THR:HB	1.85	0.57
1:a:389:LEU:HD13	1:a:448:LEU:CB	2.34	0.57
2:b:202:VAL:O	2:b:202:VAL:HG23	2.04	0.57
2:c:111:ARG:HB3	2:c:111:ARG:CZ	2.34	0.57
2:c:224:LEU:HD12	2:c:278:LEU:HD22	1.87	0.57
2:d:46:LEU:HD22	2:d:50:ILE:HD11	1.86	0.57
1:B:507:PHE:C	1:B:509:ALA:H	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:379:MET:HE1	2:D:390:VAL:CG1	2.32	0.57
2:E:71:LEU:N	2:E:71:LEU:HD23	2.19	0.57
2:E:297:TYR:C	2:E:297:TYR:HD2	2.13	0.57
2:F:126:LEU:HD23	2:F:139:PHE:O	2.04	0.57
3:G:16:THR:HG22	4:H:124:ALA:CB	2.32	0.57
1:I:137:ILE:C	1:I:137:ILE:CD1	2.56	0.57
1:I:233:ALA:HA	1:I:273:ILE:HD11	1.84	0.57
2:M:111:ARG:HB3	2:M:111:ARG:NH1	2.19	0.57
2:M:175:VAL:HG22	2:M:203:SER:HB2	1.86	0.57
2:N:126:LEU:HD23	2:N:139:PHE:O	2.04	0.57
1:S:110:THR:HG23	1:S:238:ALA:HA	1.87	0.57
2:V:46:LEU:HD22	2:V:50:ILE:HD11	1.86	0.57
1:Z:138:GLU:C	1:Z:138:GLU:CD	2.71	0.57
1:Z:430:LEU:CD2	1:Z:446:LEU:HD21	2.32	0.57
3:e:82:THR:HG22	3:e:91:ASN:OD1	2.05	0.57
3:e:189:PRO:O	3:e:190:LEU:C	2.45	0.57
1:A:233:ALA:HA	1:A:273:ILE:HD11	1.84	0.57
2:D:136:MET:HE3	2:D:336:PRO:HB3	1.86	0.57
2:E:111:ARG:HB3	2:E:111:ARG:NH1	2.19	0.57
1:I:400:TYR:CD1	1:I:424:GLY:HA3	2.40	0.57
1:J:456:LEU:HB2	1:J:460:GLU:CD	2.29	0.57
3:O:82:THR:O	3:O:120:LYS:HB2	2.04	0.57
2:T:174:SER:HB2	2:T:202:VAL:HG12	1.85	0.57
2:U:71:LEU:N	2:U:71:LEU:HD23	2.19	0.57
2:V:17:PHE:O	2:V:18:PRO:O	2.22	0.57
2:V:161:GLU:HG3	2:V:404:PHE:CB	2.33	0.57
2:V:257:LEU:HD22	2:V:257:LEU:H	1.69	0.57
3:W:82:THR:O	3:W:120:LYS:HB2	2.04	0.57
1:Y:76:MET:HE3	1:Y:233:ALA:HB1	1.86	0.57
1:Z:201:LYS:O	1:Z:205:ILE:HG13	2.05	0.57
1:a:95:LEU:HD12	1:a:129:VAL:HG11	1.86	0.57
1:a:110:THR:HG23	1:a:238:ALA:HA	1.87	0.57
1:a:241:ALA:O	1:a:245:MET:HG3	2.04	0.57
2:c:148:PHE:HZ	2:c:312:PHE:HE1	1.52	0.57
2:d:9:ILE:O	2:d:12:VAL:HG12	2.05	0.57
1:B:456:LEU:HB2	1:B:460:GLU:CD	2.29	0.57
1:C:110:THR:HG23	1:C:238:ALA:HA	1.87	0.57
1:C:151:LYS:HE2	1:C:439:MET:SD	2.44	0.57
1:C:449:PHE:HB3	1:C:504:LEU:CD1	2.35	0.57
1:I:365:ARG:HB3	1:I:366:PRO:HD3	1.86	0.57
1:J:390:SER:HA	1:J:393:ILE:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:46:LEU:HD22	2:N:50:ILE:HD11	1.86	0.57
2:N:84:LEU:HD21	2:N:230:PHE:HE2	1.70	0.57
2:N:323:ARG:HG3	2:N:323:ARG:NH1	2.11	0.57
3:O:82:THR:HG22	3:O:91:ASN:OD1	2.04	0.57
1:R:201:LYS:O	1:R:205:ILE:HG13	2.05	0.57
2:T:432:GLU:N	2:T:433:GLY:CA	2.67	0.57
1:Y:365:ARG:HB3	1:Y:366:PRO:HD3	1.86	0.57
2:b:364:LEU:HD23	2:b:396:ILE:HD11	1.86	0.57
2:d:17:PHE:O	2:d:18:PRO:O	2.22	0.57
1:A:136:VAL:HG12	1:A:137:ILE:N	2.20	0.57
1:C:240:TYR:HD1	1:C:300:ARG:NH2	2.01	0.57
1:I:93:ARG:HB2	1:I:96:GLU:HG2	1.87	0.57
1:I:175:LYS:O	1:I:176:THR:C	2.46	0.57
1:J:201:LYS:O	1:J:205:ILE:HG13	2.05	0.57
2:L:370:LEU:O	2:L:374:ILE:HG13	2.05	0.57
2:M:111:ARG:HB3	2:M:111:ARG:CZ	2.34	0.57
2:N:224:LEU:HD21	2:N:278:LEU:HD12	1.86	0.57
1:S:211:LYS:HE2	1:S:214:GLU:OE2	2.05	0.57
2:U:78:PRO:CB	2:U:103:GLU:HG2	2.30	0.57
1:Z:299:GLU:HG2	2:d:209:MET:HE3	1.87	0.57
2:c:145:VAL:HG13	2:c:293:VAL:HA	1.87	0.57
3:e:260:LEU:HD23	4:f:134:THR:HG23	1.86	0.57
1:B:113:ALA:N	1:B:114:PRO:HD2	2.20	0.57
1:C:222:ILE:HD12	1:C:245:MET:HE2	1.86	0.57
2:F:323:ARG:HG3	2:F:323:ARG:NH1	2.05	0.57
1:J:140:GLN:O	1:J:303:ARG:HG2	2.05	0.57
1:J:402:GLU:HG3	1:J:403:LEU:H	1.68	0.57
2:L:36:GLU:HG2	2:L:37:ARG:N	2.20	0.57
2:M:362:SER:O	2:M:365:GLN:HG3	2.05	0.57
1:Q:365:ARG:HB3	1:Q:366:PRO:HD3	1.86	0.57
1:S:222:ILE:HD12	1:S:245:MET:HE2	1.86	0.57
2:U:175:VAL:HG22	2:U:203:SER:HB2	1.86	0.57
2:V:116:TYR:C	2:V:116:TYR:CD2	2.82	0.57
3:W:66:TYR:CB	3:W:188:LEU:HD23	2.28	0.57
1:Y:318:LYS:H	1:Y:318:LYS:HD2	1.68	0.57
1:Z:99:VAL:HG12	1:Z:245:MET:HA	1.87	0.57
1:a:151:LYS:HE2	1:a:439:MET:SD	2.44	0.57
1:a:152:ALA:HB1	1:a:368:VAL:HG11	1.87	0.57
1:a:480:ALA:N	1:a:481:PRO:CD	2.66	0.57
2:b:311:THR:HG22	2:b:315:LEU:CD2	2.35	0.57
2:c:174:SER:HB3	2:c:238:LEU:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:84:LEU:HD21	2:d:230:PHE:HE2	1.69	0.57
2:E:224:LEU:HD12	2:E:278:LEU:HD22	1.87	0.57
2:E:279:GLN:O	2:E:282:ILE:HG12	2.04	0.57
2:E:349:VAL:HG21	2:E:353:HIS:CB	2.34	0.57
3:G:82:THR:HG22	3:G:91:ASN:OD1	2.05	0.57
1:J:99:VAL:HG12	1:J:245:MET:HA	1.87	0.57
1:J:389:LEU:HG	1:J:448:LEU:CB	2.35	0.57
2:M:204:LEU:HD23	2:M:204:LEU:H	1.69	0.57
2:U:111:ARG:HB3	2:U:111:ARG:NH1	2.19	0.57
1:Y:400:TYR:CD1	1:Y:424:GLY:HA3	2.40	0.57
1:Z:98:PRO:HB3	1:Z:123:HIS:CD2	2.40	0.57
1:Z:231:SER:HB3	1:Z:234:LEU:HB2	1.86	0.57
1:a:385:ILE:HD12	1:a:492:TYR:HB2	1.86	0.57
2:b:279:GLN:HG2	2:b:314:HIS:HB3	1.87	0.57
2:b:435:TYR:CZ	2:b:449:ILE:HG13	2.40	0.57
1:B:98:PRO:HB3	1:B:123:HIS:CD2	2.40	0.56
1:B:140:GLN:O	1:B:303:ARG:HG2	2.05	0.56
1:B:430:LEU:CD2	1:B:446:LEU:HD21	2.32	0.56
1:C:95:LEU:HD12	1:C:129:VAL:HG11	1.86	0.56
2:D:180:GLY:O	2:D:209:MET:HG2	2.05	0.56
3:G:82:THR:O	3:G:120:LYS:HB2	2.04	0.56
1:I:281:PRO:HG3	3:O:279:ILE:HG21	1.86	0.56
1:J:467:PHE:HD1	1:J:471:LEU:HD21	1.67	0.56
1:Q:243:CYS:SG	1:Q:300:ARG:HG2	2.45	0.56
1:R:98:PRO:HB3	1:R:123:HIS:CD2	2.40	0.56
1:S:152:ALA:HB1	1:S:368:VAL:HG11	1.87	0.56
2:U:174:SER:HB3	2:U:238:LEU:HB2	1.87	0.56
3:W:23:MET:SD	3:W:246:MET:HE3	2.45	0.56
1:Y:430:LEU:HD21	1:Y:446:LEU:HD23	1.87	0.56
1:Z:451:ALA:HA	1:Z:456:LEU:HD11	1.87	0.56
2:b:180:GLY:O	2:b:209:MET:HG2	2.05	0.56
2:c:175:VAL:HG22	2:c:203:SER:HB2	1.86	0.56
2:c:265:VAL:HG13	2:c:267:TYR:CD2	2.40	0.56
2:d:131:LYS:H	2:d:402:GLN:HE22	1.52	0.56
2:d:193:MET:HE3	2:d:202:VAL:HG11	1.86	0.56
2:d:457:LYS:HA	2:d:457:LYS:HE3	1.86	0.56
1:A:138:GLU:CB	1:A:305:ASN:ND2	2.67	0.56
1:A:290:VAL:HG11	1:A:340:PHE:HE1	1.71	0.56
2:D:174:SER:HB2	2:D:202:VAL:HG12	1.85	0.56
3:G:23:MET:SD	3:G:246:MET:HE3	2.45	0.56
1:I:430:LEU:HD21	1:I:446:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:389:LEU:HD13	1:K:448:LEU:CB	2.34	0.56
2:L:352:GLU:O	2:L:356:THR:HG23	2.05	0.56
2:N:279:GLN:HG2	2:N:314:HIS:HB3	1.87	0.56
3:O:23:MET:SD	3:O:246:MET:HE3	2.46	0.56
1:Q:93:ARG:HB2	1:Q:96:GLU:CG	2.36	0.56
1:R:95:LEU:CD2	1:R:129:VAL:HG21	2.27	0.56
1:R:389:LEU:HG	1:R:448:LEU:CB	2.35	0.56
2:V:9:ILE:O	2:V:12:VAL:HG12	2.05	0.56
1:Z:441:VAL:O	1:Z:444:GLN:HB3	2.05	0.56
1:A:94:ILE:HD13	1:A:94:ILE:H	1.70	0.56
1:A:110:THR:HG23	1:A:238:ALA:HA	1.88	0.56
1:A:400:TYR:CD1	1:A:424:GLY:HA3	2.40	0.56
1:B:183:ILE:HD11	1:B:259:ILE:HD12	1.87	0.56
1:B:390:SER:HA	1:B:393:ILE:HD13	1.87	0.56
1:B:401:ARG:HB2	1:B:401:ARG:HH11	1.68	0.56
1:B:441:VAL:O	1:B:444:GLN:HB3	2.05	0.56
2:D:36:GLU:HG2	2:D:37:ARG:N	2.20	0.56
2:E:175:VAL:HG22	2:E:203:SER:HB2	1.86	0.56
2:F:193:MET:HE3	2:F:202:VAL:HG11	1.86	0.56
2:F:353:HIS:HA	2:F:424:ILE:HD12	1.87	0.56
2:F:400:LEU:HD12	2:F:427:PHE:CZ	2.40	0.56
1:I:76:MET:HE3	1:I:233:ALA:HB1	1.86	0.56
1:I:93:ARG:HB2	1:I:96:GLU:CG	2.35	0.56
1:I:94:ILE:HD13	1:I:94:ILE:H	1.70	0.56
1:J:98:PRO:HB3	1:J:123:HIS:CD2	2.40	0.56
1:J:343:THR:HG22	2:N:297:TYR:OH	2.06	0.56
1:J:507:PHE:C	1:J:509:ALA:H	2.13	0.56
1:K:110:THR:HG23	1:K:238:ALA:HA	1.87	0.56
2:N:279:GLN:HG2	2:N:314:HIS:CB	2.36	0.56
1:R:113:ALA:N	1:R:114:PRO:HD2	2.20	0.56
1:R:138:GLU:HG2	1:R:308:TYR:CD2	2.40	0.56
1:R:198:ILE:CD1	1:R:239:PRO:HG3	2.36	0.56
1:R:390:SER:HA	1:R:393:ILE:HD13	1.87	0.56
1:S:193:CYS:HB2	1:S:221:THR:HB	1.85	0.56
2:T:29:LEU:HB2	2:T:40:LEU:HB2	1.88	0.56
2:T:180:GLY:O	2:T:209:MET:HG2	2.05	0.56
2:T:239:LEU:HB2	2:T:290:ILE:HD11	1.86	0.56
2:T:311:THR:HG22	2:T:315:LEU:CD2	2.35	0.56
2:U:265:VAL:O	2:U:265:VAL:HG22	2.05	0.56
2:U:395:LYS:HD3	2:U:443:PHE:CZ	2.41	0.56
2:V:417:TYR:C	2:V:417:TYR:CD2	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:94:ILE:HD13	1:Y:94:ILE:H	1.70	0.56
1:Z:389:LEU:HG	1:Z:448:LEU:CB	2.35	0.56
1:Z:507:PHE:C	1:Z:509:ALA:H	2.13	0.56
1:a:211:LYS:HE2	1:a:214:GLU:OE2	2.05	0.56
1:a:262:ASP:HB3	1:a:265:LYS:HG3	1.85	0.56
2:c:111:ARG:HB3	2:c:111:ARG:NH1	2.19	0.56
2:d:161:GLU:HG3	2:d:404:PHE:CB	2.33	0.56
3:e:23:MET:SD	3:e:246:MET:HE3	2.45	0.56
1:B:164:ARG:HA	1:B:326:ALA:O	2.06	0.56
1:C:152:ALA:HB1	1:C:368:VAL:HG11	1.87	0.56
2:D:364:LEU:HD23	2:D:396:ILE:HD11	1.86	0.56
1:I:176:THR:O	1:I:179:ALA:HB3	2.06	0.56
1:J:441:VAL:O	1:J:444:GLN:HB3	2.05	0.56
2:L:180:GLY:O	2:L:209:MET:HG2	2.05	0.56
2:L:432:GLU:N	2:L:433:GLY:CA	2.68	0.56
1:Q:430:LEU:HD21	1:Q:446:LEU:HD23	1.87	0.56
1:R:451:ALA:HA	1:R:456:LEU:HD11	1.87	0.56
3:W:194:ASP:OD2	3:W:194:ASP:N	2.38	0.56
2:b:332:PRO:HG2	2:b:402:GLN:H	1.70	0.56
2:b:336:PRO:HG3	2:b:400:LEU:HD11	1.88	0.56
2:c:395:LYS:HD3	2:c:443:PHE:CZ	2.40	0.56
3:e:16:THR:HG22	4:f:124:ALA:HB1	1.86	0.56
1:C:211:LYS:HE2	1:C:214:GLU:OE2	2.05	0.56
2:E:78:PRO:CB	2:E:103:GLU:HG2	2.30	0.56
2:E:387:LYS:HE3	2:E:390:VAL:HG11	1.88	0.56
2:E:402:GLN:N	2:E:445:MET:HE1	2.21	0.56
2:E:442:ALA:HB3	2:E:443:PHE:HD2	1.65	0.56
2:E:442:ALA:CB	2:E:443:PHE:HE2	2.07	0.56
2:F:139:PHE:N	2:F:139:PHE:CD2	2.74	0.56
1:J:108:VAL:HG13	1:J:112:GLY:O	2.06	0.56
1:K:152:ALA:HB1	1:K:368:VAL:HG11	1.87	0.56
1:K:456:LEU:N	1:K:456:LEU:CD2	2.69	0.56
2:L:29:LEU:HB2	2:L:40:LEU:HB2	1.88	0.56
2:L:438:LEU:N	2:L:438:LEU:HD23	2.19	0.56
2:N:139:PHE:HD2	2:N:139:PHE:N	2.03	0.56
1:Q:93:ARG:HB2	1:Q:96:GLU:HG2	1.87	0.56
1:Q:96:GLU:HB3	1:Q:126:PHE:CD2	2.41	0.56
1:Q:399:GLN:O	1:Q:402:GLU:HG2	2.06	0.56
1:R:108:VAL:HG13	1:R:112:GLY:O	2.06	0.56
1:R:183:ILE:HD11	1:R:259:ILE:HD12	1.87	0.56
1:R:385:ILE:HB	1:R:490:GLY:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:441:VAL:O	1:R:444:GLN:HB3	2.05	0.56
1:R:507:PHE:C	1:R:509:ALA:H	2.13	0.56
1:S:456:LEU:N	1:S:456:LEU:CD2	2.69	0.56
2:U:116:TYR:C	2:U:118:GLU:H	2.14	0.56
2:V:193:MET:HE3	2:V:202:VAL:HG11	1.86	0.56
1:Y:96:GLU:HB3	1:Y:126:PHE:CD2	2.41	0.56
1:Z:108:VAL:HG13	1:Z:112:GLY:O	2.06	0.56
1:a:35:SER:HB2	2:d:44:GLN:HG2	1.88	0.56
2:c:367:TYR:CE2	2:c:390:VAL:HG13	2.39	0.56
2:d:139:PHE:HD2	2:d:139:PHE:N	2.03	0.56
1:A:399:GLN:O	1:A:402:GLU:HG2	2.06	0.56
1:A:430:LEU:HD21	1:A:446:LEU:HD23	1.87	0.56
1:B:106:ARG:HH21	1:B:118:LYS:HB2	1.70	0.56
1:B:201:LYS:O	1:B:205:ILE:HG13	2.05	0.56
1:C:186:GLN:HG3	1:C:191:ILE:HB	1.88	0.56
2:D:29:LEU:HB2	2:D:40:LEU:HB2	1.88	0.56
2:F:417:TYR:CD2	2:F:417:TYR:C	2.83	0.56
1:I:366:PRO:HD2	1:I:432:LYS:HB3	1.88	0.56
1:K:156:MET:C	1:K:158:PRO:HD3	2.31	0.56
2:M:428:LYS:O	2:M:432:GLU:HG2	2.06	0.56
2:N:9:ILE:O	2:N:12:VAL:HG12	2.05	0.56
1:Q:400:TYR:CD1	1:Q:424:GLY:HA3	2.40	0.56
1:R:106:ARG:HH21	1:R:118:LYS:HB2	1.70	0.56
1:R:164:ARG:HA	1:R:326:ALA:O	2.06	0.56
1:R:231:SER:HB3	1:R:234:LEU:HB2	1.86	0.56
1:S:449:PHE:HB3	1:S:504:LEU:CD1	2.35	0.56
2:T:115:SER:C	2:T:117:GLU:H	2.14	0.56
2:T:388:LEU:HD11	2:T:392:ARG:NH2	2.20	0.56
1:Y:243:CYS:SG	1:Y:300:ARG:HG2	2.45	0.56
1:a:156:MET:C	1:a:158:PRO:HD3	2.31	0.56
2:c:116:TYR:C	2:c:118:GLU:H	2.14	0.56
1:A:93:ARG:HB2	1:A:96:GLU:HG2	1.87	0.56
1:A:243:CYS:SG	1:A:300:ARG:HG2	2.45	0.56
1:B:467:PHE:HD1	1:B:471:LEU:HD21	1.67	0.56
2:D:388:LEU:HD11	2:D:392:ARG:NH2	2.21	0.56
2:E:116:TYR:C	2:E:118:GLU:H	2.14	0.56
2:E:118:GLU:O	2:E:286:LYS:HG2	2.06	0.56
1:J:106:ARG:HH21	1:J:118:LYS:HB2	1.71	0.56
1:J:385:ILE:HB	1:J:490:GLY:O	2.06	0.56
1:K:449:PHE:HB3	1:K:504:LEU:CD1	2.35	0.56
2:L:157:VAL:HG11	7:L:600:ADP:H8	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:366:ARG:O	2:L:370:LEU:HD23	2.05	0.56
1:Q:94:ILE:HD13	1:Q:94:ILE:H	1.70	0.56
2:T:36:GLU:HG2	2:T:37:ARG:N	2.20	0.56
2:U:204:LEU:HD23	2:U:204:LEU:H	1.69	0.56
1:Y:110:THR:HG23	1:Y:238:ALA:HA	1.87	0.56
1:Y:299:GLU:OE1	2:c:209:MET:HE2	2.06	0.56
1:Y:399:GLN:O	1:Y:402:GLU:HG2	2.06	0.56
1:Z:140:GLN:O	1:Z:303:ARG:HG2	2.05	0.56
1:Z:164:ARG:HA	1:Z:326:ALA:O	2.06	0.56
1:a:186:GLN:HG3	1:a:191:ILE:HB	1.88	0.56
2:b:29:LEU:HB2	2:b:40:LEU:HB2	1.88	0.56
3:e:193:SER:HB2	3:e:196:ASP:H	1.70	0.56
1:A:93:ARG:HB2	1:A:96:GLU:CG	2.35	0.56
1:B:198:ILE:CD1	1:B:239:PRO:HG3	2.36	0.56
2:D:114:PRO:HD3	2:D:281:ARG:HG2	1.87	0.56
2:D:432:GLU:N	2:D:433:GLY:CA	2.67	0.56
2:E:380:ASP:HB2	2:U:437:HIS:CB	2.35	0.56
2:E:402:GLN:N	2:E:445:MET:CE	2.69	0.56
1:I:96:GLU:HB3	1:I:126:PHE:CD2	2.41	0.56
1:J:138:GLU:HG2	1:J:308:TYR:CD2	2.40	0.56
1:K:211:LYS:HE2	1:K:214:GLU:OE2	2.05	0.56
1:R:96:GLU:HB2	1:R:128:ALA:CA	2.31	0.56
1:R:140:GLN:O	1:R:303:ARG:HG2	2.05	0.56
1:S:66:LEU:HB2	2:T:64:ARG:HD2	1.88	0.56
2:T:202:VAL:HG23	2:T:202:VAL:O	2.04	0.56
2:U:394:ARG:O	2:U:398:ARG:HG3	2.06	0.56
1:Y:290:VAL:HG11	1:Y:340:PHE:HE1	1.70	0.56
2:b:89:ASN:ND2	2:b:93:GLU:HG3	2.21	0.56
2:b:320:VAL:HG21	2:b:338:ASP:HB2	1.86	0.56
2:c:337:LEU:O	2:c:338:ASP:HB2	2.05	0.56
1:A:138:GLU:HG3	1:A:305:ASN:CG	2.24	0.56
1:A:210:ARG:NH1	2:D:120:SER:O	2.39	0.56
1:B:385:ILE:O	1:B:389:LEU:HD23	2.06	0.56
2:D:408:GLU:HG3	2:D:413:SER:O	2.05	0.56
2:D:438:LEU:N	2:D:438:LEU:HD23	2.21	0.56
2:E:428:LYS:O	2:E:432:GLU:HG2	2.06	0.56
4:P:41:LEU:N	4:P:71:VAL:HG23	2.20	0.56
1:S:317:VAL:HA	1:S:318:LYS:CB	2.20	0.56
2:T:366:ARG:O	2:T:370:LEU:HD23	2.06	0.56
2:T:370:LEU:O	2:T:374:ILE:HG13	2.05	0.56
2:U:161:GLU:HG2	2:U:406:VAL:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:139:PHE:HD2	2:V:139:PHE:N	2.03	0.56
2:V:139:PHE:N	2:V:139:PHE:CD2	2.74	0.56
1:Z:183:ILE:HD11	1:Z:259:ILE:HD12	1.87	0.56
2:b:36:GLU:HG2	2:b:37:ARG:N	2.20	0.56
2:b:239:LEU:HB2	2:b:290:ILE:HD11	1.88	0.56
2:c:428:LYS:O	2:c:432:GLU:HG2	2.05	0.56
2:d:417:TYR:C	2:d:417:TYR:CD2	2.83	0.56
1:A:96:GLU:HB3	1:A:126:PHE:CD2	2.41	0.56
1:B:385:ILE:HB	1:B:490:GLY:O	2.06	0.56
1:C:156:MET:C	1:C:158:PRO:HD3	2.31	0.56
1:C:450:ALA:HA	1:C:456:LEU:CD2	2.36	0.56
2:F:183:THR:HG22	2:F:208:GLN:HG3	1.88	0.56
1:I:87:LYS:HE3	1:I:89:LYS:CE	2.36	0.56
1:J:113:ALA:N	1:J:114:PRO:HD2	2.20	0.56
1:K:47:CYS:O	2:L:63:ARG:HB2	2.04	0.56
1:K:137:ILE:HD13	2:L:96:ASP:HA	1.88	0.56
1:K:493:ASN:H	1:K:496:ILE:HG13	1.70	0.56
1:R:283:ARG:NH1	2:V:300:ALA:HB3	2.22	0.56
1:S:186:GLN:HG3	1:S:191:ILE:HB	1.88	0.56
2:T:367:TYR:CE1	2:T:390:VAL:HG23	2.41	0.56
2:U:387:LYS:HD2	2:U:390:VAL:HB	1.88	0.56
1:Y:87:LYS:HE3	1:Y:89:LYS:CE	2.36	0.56
2:c:204:LEU:H	2:c:204:LEU:HD23	1.69	0.56
2:c:446:VAL:HG21	2:c:452:ALA:HB2	1.88	0.56
1:B:451:ALA:HA	1:B:456:LEU:HD11	1.87	0.55
2:E:140:ALA:HB2	2:E:343:GLN:CD	2.31	0.55
1:J:183:ILE:HD11	1:J:259:ILE:HD12	1.87	0.55
1:K:385:ILE:HG12	1:K:444:GLN:CD	2.32	0.55
2:L:24:ARG:HG3	2:L:27:ASP:CG	2.31	0.55
2:L:202:VAL:HG23	2:L:202:VAL:O	2.04	0.55
3:O:208:GLU:CD	4:P:43:THR:HA	2.31	0.55
1:R:309:VAL:CG1	1:R:317:VAL:HG11	2.33	0.55
3:W:167:LEU:O	3:W:187:LEU:O	2.23	0.55
1:Y:93:ARG:HB2	1:Y:96:GLU:HG2	1.87	0.55
1:Z:198:ILE:CD1	1:Z:239:PRO:HG3	2.36	0.55
1:a:450:ALA:HA	1:a:456:LEU:CD2	2.36	0.55
2:b:432:GLU:N	2:b:433:GLY:CA	2.69	0.55
1:A:415:ASP:HA	1:A:418:ARG:HB3	1.88	0.55
1:B:99:VAL:HG12	1:B:245:MET:HA	1.87	0.55
1:B:138:GLU:HG2	1:B:308:TYR:CD2	2.40	0.55
1:C:440:SER:C	1:C:442:ALA:N	2.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:SER:C	2:D:117:GLU:H	2.14	0.55
2:F:76:GLU:HB2	2:F:106:ARG:NH1	2.21	0.55
1:I:480:ALA:N	1:I:481:PRO:CD	2.70	0.55
1:J:198:ILE:CD1	1:J:239:PRO:HG3	2.36	0.55
1:J:385:ILE:O	1:J:389:LEU:HD23	2.06	0.55
1:K:186:GLN:HG3	1:K:191:ILE:HB	1.88	0.55
2:L:89:ASN:ND2	2:L:93:GLU:HG3	2.21	0.55
2:M:362:SER:HA	2:M:365:GLN:HG3	1.88	0.55
1:Q:415:ASP:HA	1:Q:418:ARG:HB3	1.88	0.55
1:R:430:LEU:CD2	1:R:446:LEU:HD21	2.32	0.55
2:U:392:ARG:O	2:U:396:ILE:HG23	2.05	0.55
1:Y:411:SER:OG	4:f:113:ASP:OD1	2.20	0.55
1:Z:385:ILE:HB	1:Z:490:GLY:O	2.06	0.55
2:c:356:THR:O	2:c:360:VAL:HG23	2.06	0.55
3:e:65:PRO:O	3:e:66:TYR:CD2	2.60	0.55
2:D:89:ASN:ND2	2:D:93:GLU:HG3	2.21	0.55
2:E:337:LEU:O	2:E:338:ASP:HB2	2.04	0.55
2:F:139:PHE:N	2:F:139:PHE:HD2	2.03	0.55
1:J:451:ALA:HA	1:J:456:LEU:HD11	1.87	0.55
2:L:115:SER:C	2:L:117:GLU:H	2.14	0.55
2:M:89:ASN:ND2	2:M:93:GLU:H	2.04	0.55
2:M:445:MET:C	2:M:446:VAL:CG1	2.79	0.55
2:N:76:GLU:HB2	2:N:106:ARG:NH1	2.21	0.55
2:T:136:MET:HE3	2:T:336:PRO:HB3	1.88	0.55
2:V:183:THR:HG22	2:V:208:GLN:CG	2.36	0.55
1:a:449:PHE:HB3	1:a:504:LEU:CD1	2.35	0.55
2:d:139:PHE:N	2:d:139:PHE:CD2	2.74	0.55
1:A:480:ALA:N	1:A:481:PRO:CD	2.70	0.55
1:B:108:VAL:HG13	1:B:112:GLY:O	2.06	0.55
1:B:389:LEU:HG	1:B:448:LEU:CB	2.35	0.55
2:D:157:VAL:HG12	7:D:600:ADP:O1A	2.07	0.55
2:E:362:SER:O	2:E:365:GLN:HG3	2.06	0.55
3:G:187:LEU:HD12	3:G:188:LEU:HB3	1.88	0.55
1:I:110:THR:HG23	1:I:238:ALA:HA	1.88	0.55
1:I:243:CYS:SG	1:I:300:ARG:HG2	2.45	0.55
1:J:430:LEU:CD2	1:J:446:LEU:HD21	2.32	0.55
2:M:116:TYR:C	2:M:118:GLU:H	2.14	0.55
2:N:161:GLU:HG3	2:N:404:PHE:CB	2.36	0.55
3:O:65:PRO:O	3:O:66:TYR:CD2	2.59	0.55
1:R:385:ILE:O	1:R:389:LEU:HD23	2.06	0.55
1:S:156:MET:C	1:S:158:PRO:HD3	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:297:TYR:C	2:U:297:TYR:CD2	2.85	0.55
2:V:31:VAL:HG22	2:V:68:VAL:CG1	2.37	0.55
3:W:65:PRO:O	3:W:66:TYR:CD2	2.60	0.55
1:C:456:LEU:N	1:C:456:LEU:CD2	2.69	0.55
1:I:137:ILE:O	1:I:137:ILE:CG1	2.52	0.55
1:J:34:VAL:HG12	2:M:45:GLN:HB2	1.88	0.55
2:N:159:MET:HE2	2:N:295:ALA:HB2	1.88	0.55
2:T:89:ASN:ND2	2:T:93:GLU:HG3	2.21	0.55
2:U:349:VAL:HG21	2:U:353:HIS:ND1	2.22	0.55
1:Y:406:PHE:HE1	3:e:25:MET:HB2	1.71	0.55
1:Z:52:MET:CE	1:Z:95:LEU:CA	2.73	0.55
1:Z:157:ILE:HD12	1:Z:353:ILE:HG12	1.89	0.55
1:C:461:LEU:N	1:C:461:LEU:CD2	2.65	0.55
2:D:24:ARG:HG3	2:D:27:ASP:CG	2.31	0.55
1:I:66:LEU:HB2	2:M:8:VAL:HB	1.87	0.55
1:I:290:VAL:HG11	1:I:340:PHE:HE1	1.71	0.55
1:I:426:LYS:HZ2	1:I:457:ALA:HB2	1.70	0.55
1:I:453:ARG:HB3	1:I:455:TYR:CE2	2.42	0.55
2:N:31:VAL:HG22	2:N:68:VAL:CG1	2.37	0.55
3:O:12:SER:O	3:O:16:THR:HG23	2.07	0.55
1:S:450:ALA:HA	1:S:456:LEU:CD2	2.36	0.55
2:T:432:GLU:H	2:T:433:GLY:HA2	1.72	0.55
3:W:186:GLN:HG2	3:W:189:PRO:HD2	1.88	0.55
1:Z:138:GLU:HG2	1:Z:308:TYR:CD2	2.40	0.55
1:A:453:ARG:HB3	1:A:455:TYR:CE2	2.42	0.55
2:E:174:SER:HB3	2:E:238:LEU:HB2	1.87	0.55
1:K:107:VAL:HA	1:K:223:VAL:HG13	1.89	0.55
2:M:66:LEU:HD23	2:M:67:ASP:H	1.72	0.55
2:U:181:GLU:HB2	2:U:242:ASP:OD2	2.07	0.55
1:Y:365:ARG:HG2	5:Y:600:ANP:C2	2.37	0.55
1:Z:313:THR:HG21	1:Z:317:VAL:H	1.71	0.55
1:Z:467:PHE:HD1	1:Z:471:LEU:HD21	1.67	0.55
1:a:385:ILE:HG12	1:a:444:GLN:CD	2.32	0.55
2:c:66:LEU:HD23	2:c:67:ASP:H	1.72	0.55
2:c:89:ASN:ND2	2:c:93:GLU:H	2.04	0.55
1:A:44:LEU:HD22	1:A:90:CYS:SG	2.47	0.55
1:C:107:VAL:HA	1:C:223:VAL:HG13	1.89	0.55
2:F:257:LEU:HD22	2:F:257:LEU:H	1.69	0.55
1:J:164:ARG:HA	1:J:326:ALA:O	2.06	0.55
2:M:174:SER:HB3	2:M:238:LEU:HB2	1.87	0.55
2:M:237:VAL:HG23	2:M:290:ILE:HG23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:297:TYR:C	2:M:297:TYR:CD2	2.85	0.55
2:N:352:GLU:H	2:N:352:GLU:CD	2.15	0.55
1:R:99:VAL:HG12	1:R:245:MET:HA	1.87	0.55
1:S:384:LYS:HE2	1:S:493:ASN:HD21	1.71	0.55
2:T:24:ARG:HG3	2:T:27:ASP:CG	2.31	0.55
2:T:239:LEU:CB	2:T:290:ILE:HD11	2.36	0.55
2:V:183:THR:HG22	2:V:208:GLN:HG3	1.88	0.55
3:W:190:LEU:CD1	3:W:191:PRO:CD	2.85	0.55
1:Z:106:ARG:HH21	1:Z:118:LYS:HB2	1.70	0.55
1:Z:113:ALA:N	1:Z:114:PRO:HD2	2.20	0.55
2:b:19:GLN:CD	2:b:19:GLN:N	2.63	0.55
1:A:320:LYS:N	1:A:320:LYS:HD2	2.22	0.55
1:B:414:ASP:CA	1:B:418:ARG:CB	2.85	0.55
2:F:457:LYS:HA	2:F:457:LYS:CE	2.36	0.55
3:G:12:SER:O	3:G:16:THR:HG23	2.07	0.55
3:G:65:PRO:O	3:G:66:TYR:CD2	2.60	0.55
1:I:399:GLN:O	1:I:402:GLU:HG2	2.06	0.55
2:M:181:GLU:HB2	2:M:242:ASP:OD2	2.07	0.55
2:N:183:THR:HG22	2:N:208:GLN:CG	2.36	0.55
4:P:63:TYR:C	4:P:63:TYR:CD2	2.85	0.55
1:R:95:LEU:O	1:R:95:LEU:CG	2.53	0.55
1:R:259:ILE:HG22	1:R:327:LEU:CD2	2.37	0.55
1:S:107:VAL:HA	1:S:223:VAL:HG13	1.89	0.55
1:S:458:ASP:O	1:S:459:VAL:C	2.49	0.55
2:T:231:ARG:NH1	2:T:281:ARG:HH11	2.05	0.55
4:X:63:TYR:C	4:X:63:TYR:CD2	2.85	0.55
1:Y:93:ARG:HB2	1:Y:96:GLU:CG	2.36	0.55
1:Y:364:ILE:HG13	1:Y:432:LYS:CG	2.35	0.55
2:b:379:MET:HE1	2:b:390:VAL:CG1	2.34	0.55
2:d:183:THR:HG22	2:d:208:GLN:CG	2.36	0.55
3:e:229:GLN:HA	3:e:232:VAL:HG12	1.89	0.55
1:C:47:CYS:O	2:D:63:ARG:HB2	2.07	0.55
2:D:336:PRO:HG3	2:D:400:LEU:HD11	1.88	0.55
2:E:66:LEU:HD23	2:E:67:ASP:H	1.72	0.55
2:E:144:LYS:HZ3	2:E:279:GLN:HB3	1.72	0.55
2:F:297:TYR:HE2	2:F:299:PRO:HA	1.72	0.55
3:G:229:GLN:HA	3:G:232:VAL:HG12	1.89	0.55
1:J:259:ILE:HG22	1:J:327:LEU:CD2	2.37	0.55
1:Q:290:VAL:HG11	1:Q:340:PHE:HE1	1.71	0.55
1:R:41:ILE:HD12	1:R:53:ILE:HD13	1.90	0.55
1:R:467:PHE:HD1	1:R:471:LEU:HD21	1.67	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:163:ILE:CG2	2:U:201:LYS:HE3	2.37	0.55
2:V:240:PHE:CD2	2:V:293:VAL:HG22	2.41	0.55
3:W:12:SER:O	3:W:16:THR:HG23	2.07	0.55
2:b:242:ASP:O	2:b:295:ALA:HB3	2.07	0.55
2:b:370:LEU:O	2:b:374:ILE:HG13	2.07	0.55
1:B:259:ILE:HG22	1:B:327:LEU:CD2	2.37	0.54
1:C:446:LEU:HD23	1:C:447:VAL:N	2.23	0.54
2:E:89:ASN:ND2	2:E:93:GLU:H	2.04	0.54
2:E:148:PHE:HZ	2:E:312:PHE:CE1	2.25	0.54
2:E:275:MET:HG2	2:E:310:THR:HG22	1.89	0.54
2:F:221:LEU:O	2:F:225:THR:HG23	2.08	0.54
1:I:415:ASP:HA	1:I:418:ARG:HB3	1.88	0.54
1:K:450:ALA:HA	1:K:456:LEU:CD2	2.36	0.54
1:S:198:ILE:CD1	1:S:239:PRO:HG3	2.37	0.54
1:S:507:PHE:C	1:S:507:PHE:CD2	2.85	0.54
2:T:305:ASP:O	2:T:308:PRO:HD2	2.06	0.54
2:V:332:PRO:CG	2:V:401:SER:HA	2.37	0.54
1:Y:480:ALA:N	1:Y:481:PRO:CD	2.70	0.54
1:a:304:VAL:HG21	1:a:308:TYR:CG	2.43	0.54
1:a:446:LEU:HD23	1:a:447:VAL:N	2.23	0.54
2:c:360:VAL:O	2:c:364:LEU:HB2	2.08	0.54
2:d:76:GLU:HB2	2:d:106:ARG:NH1	2.21	0.54
1:A:172:GLN:NE2	2:D:342:ARG:HH21	2.04	0.54
1:B:49:GLN:HE22	2:F:10:GLY:H	1.55	0.54
1:C:335:GLY:O	1:C:337:VAL:HG23	2.07	0.54
1:C:385:ILE:HG12	1:C:444:GLN:CD	2.31	0.54
2:F:31:VAL:HG22	2:F:68:VAL:CG1	2.37	0.54
2:F:183:THR:HG22	2:F:208:GLN:CG	2.36	0.54
1:J:57:GLY:N	1:J:58:ASN:HA	2.21	0.54
1:K:55:LEU:HD21	1:K:61:ALA:HB2	1.89	0.54
1:K:335:GLY:O	1:K:337:VAL:HG23	2.07	0.54
1:K:337:VAL:O	1:K:337:VAL:HG12	2.07	0.54
1:K:356:GLU:HB2	1:K:359:LEU:HD23	1.89	0.54
1:S:337:VAL:O	1:S:337:VAL:HG12	2.07	0.54
1:S:409:PHE:O	1:S:412:ASP:HB2	2.08	0.54
2:T:336:PRO:HG3	2:T:400:LEU:HD11	1.89	0.54
2:U:265:VAL:CG2	3:W:272:ILE:HD13	2.38	0.54
2:V:279:GLN:HG2	2:V:314:HIS:CB	2.38	0.54
2:V:353:HIS:HA	2:V:424:ILE:HD12	1.90	0.54
3:W:66:TYR:CD2	3:W:188:LEU:HD21	2.42	0.54
3:W:229:GLN:HA	3:W:232:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:41:ILE:HD12	1:Z:53:ILE:HD13	1.89	0.54
1:A:34:VAL:HG12	2:D:45:GLN:HB3	1.88	0.54
1:A:365:ARG:HG2	5:A:600:ANP:C2	2.37	0.54
1:C:458:ASP:O	1:C:459:VAL:C	2.50	0.54
1:C:504:LEU:O	1:C:507:PHE:HB3	2.07	0.54
2:D:279:GLN:HG2	2:D:314:HIS:CG	2.43	0.54
2:E:163:ILE:CG2	2:E:201:LYS:HE3	2.37	0.54
2:E:174:SER:HB3	2:E:238:LEU:CB	2.38	0.54
1:I:180:ILE:O	1:I:183:ILE:N	2.40	0.54
1:J:313:THR:HG21	1:J:317:VAL:H	1.72	0.54
1:J:450:ALA:HA	1:J:455:TYR:HB2	1.90	0.54
2:M:445:MET:HA	2:M:445:MET:CE	2.30	0.54
2:N:183:THR:HG22	2:N:208:GLN:HG3	1.88	0.54
2:N:221:LEU:O	2:N:225:THR:HG23	2.08	0.54
1:Q:172:GLN:HA	5:Q:600:ANP:HNB1	1.71	0.54
1:Q:453:ARG:HB3	1:Q:455:TYR:CE2	2.42	0.54
1:R:209:VAL:HA	1:R:212:LEU:HB2	1.89	0.54
1:S:385:ILE:HG12	1:S:444:GLN:CD	2.32	0.54
2:U:107:TRP:HB3	2:U:111:ARG:HH22	1.73	0.54
4:X:41:LEU:N	4:X:71:VAL:HG23	2.20	0.54
1:Y:44:LEU:HD22	1:Y:90:CYS:SG	2.47	0.54
1:Z:57:GLY:N	1:Z:58:ASN:HA	2.21	0.54
1:Z:259:ILE:HG22	1:Z:327:LEU:CD2	2.37	0.54
2:b:408:GLU:HG3	2:b:413:SER:O	2.07	0.54
4:f:72:GLN:HB2	4:f:73:PRO:HD2	1.90	0.54
2:D:90:VAL:HG11	2:D:215:ASN:ND2	2.22	0.54
2:D:231:ARG:HD2	2:D:281:ARG:HH12	1.71	0.54
2:E:181:GLU:HB2	2:E:242:ASP:OD2	2.07	0.54
2:E:380:ASP:HB2	2:U:437:HIS:HB3	1.88	0.54
3:G:14:GLN:HA	3:G:257:ILE:HD11	1.90	0.54
4:H:41:LEU:N	4:H:71:VAL:HG23	2.20	0.54
4:H:63:TYR:C	4:H:63:TYR:CD2	2.85	0.54
1:K:144:GLN:HG3	1:K:161:ARG:HD3	1.90	0.54
1:Q:320:LYS:HD2	1:Q:320:LYS:N	2.22	0.54
1:Q:388:LYS:HD3	1:Q:492:TYR:CE1	2.42	0.54
1:R:313:THR:HG21	1:R:317:VAL:H	1.72	0.54
1:Y:388:LYS:HD3	1:Y:492:TYR:CE1	2.42	0.54
1:a:458:ASP:O	1:a:459:VAL:C	2.50	0.54
2:b:90:VAL:HG11	2:b:215:ASN:ND2	2.22	0.54
2:b:432:GLU:H	2:b:433:GLY:HA2	1.73	0.54
2:c:174:SER:HB3	2:c:238:LEU:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:31:VAL:HG22	2:d:68:VAL:CG1	2.37	0.54
1:B:209:VAL:HA	1:B:212:LEU:HB2	1.89	0.54
2:D:231:ARG:NH1	2:D:281:ARG:HH11	2.04	0.54
1:I:218:LEU:HA	1:I:221:THR:HG23	1.90	0.54
1:Q:44:LEU:HD22	1:Q:90:CYS:SG	2.47	0.54
1:Q:348:ILE:HG23	2:U:209:MET:CE	2.35	0.54
1:R:157:ILE:HD12	1:R:353:ILE:HG12	1.89	0.54
2:V:76:GLU:HB2	2:V:106:ARG:NH1	2.21	0.54
4:X:72:GLN:HB2	4:X:73:PRO:HD2	1.90	0.54
1:Y:453:ARG:HB3	1:Y:455:TYR:CE2	2.42	0.54
1:a:107:VAL:HA	1:a:223:VAL:HG13	1.89	0.54
1:a:335:GLY:O	1:a:337:VAL:HG23	2.07	0.54
2:b:24:ARG:HG3	2:b:27:ASP:CG	2.31	0.54
2:c:181:GLU:HB2	2:c:242:ASP:OD2	2.07	0.54
2:d:221:LEU:O	2:d:225:THR:HG23	2.08	0.54
4:f:63:TYR:C	4:f:63:TYR:CD2	2.85	0.54
1:A:388:LYS:HD3	1:A:492:TYR:CE1	2.42	0.54
1:B:414:ASP:HA	1:B:418:ARG:CB	2.38	0.54
1:C:256:ALA:HB3	1:C:324:LEU:HD23	1.90	0.54
2:D:432:GLU:H	2:D:433:GLY:HA2	1.72	0.54
2:E:437:HIS:CD2	2:E:438:LEU:HD12	2.42	0.54
2:F:371:LYS:HB3	4:H:131:ILE:HG21	1.88	0.54
4:H:72:GLN:HB2	4:H:73:PRO:HD2	1.90	0.54
1:I:458:ASP:OD1	1:I:508:LYS:NZ	2.40	0.54
1:J:157:ILE:HD12	1:J:353:ILE:HG12	1.89	0.54
1:K:198:ILE:CD1	1:K:239:PRO:HG3	2.37	0.54
1:K:256:ALA:HB3	1:K:324:LEU:HD23	1.90	0.54
2:M:163:ILE:CG2	2:M:201:LYS:HE3	2.37	0.54
2:M:370:LEU:HD13	2:M:382:LEU:HD11	1.89	0.54
2:M:433:GLY:O	2:M:434:GLU:HB2	2.06	0.54
3:O:14:GLN:HA	3:O:257:ILE:HD11	1.90	0.54
3:O:66:TYR:HB3	3:O:188:LEU:CD1	2.38	0.54
1:Q:110:THR:HG23	1:Q:238:ALA:HA	1.88	0.54
1:S:304:VAL:HG21	1:S:308:TYR:CG	2.43	0.54
1:S:496:ILE:H	1:S:496:ILE:HD13	1.73	0.54
1:Z:209:VAL:HA	1:Z:212:LEU:HB2	1.89	0.54
2:b:131:LYS:HG3	2:b:402:GLN:OE1	2.08	0.54
2:b:136:MET:HE3	2:b:336:PRO:HB3	1.89	0.54
3:e:9:LYS:HD3	4:f:129:ARG:HG2	1.90	0.54
1:B:157:ILE:HD12	1:B:353:ILE:HG12	1.89	0.54
1:C:151:LYS:HE3	1:C:433:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:VAL:HG21	1:C:308:TYR:CG	2.43	0.54
1:K:365:ARG:HG3	5:K:600:ANP:N1	2.21	0.54
2:L:360:VAL:HG13	2:L:396:ILE:HD12	1.89	0.54
1:Q:480:ALA:N	1:Q:481:PRO:CD	2.70	0.54
1:S:413:LEU:H	1:S:413:LEU:HD12	1.73	0.54
2:T:90:VAL:HG11	2:T:215:ASN:ND2	2.22	0.54
2:T:352:GLU:O	2:T:356:THR:HG23	2.08	0.54
1:Y:320:LYS:HD2	1:Y:320:LYS:N	2.22	0.54
1:Y:450:ALA:HB1	1:Y:456:LEU:HD21	1.90	0.54
1:a:55:LEU:HD21	1:a:61:ALA:HB2	1.89	0.54
1:a:409:PHE:O	1:a:412:ASP:HB2	2.08	0.54
1:a:504:LEU:O	1:a:507:PHE:HB3	2.07	0.54
2:c:265:VAL:CG2	3:e:272:ILE:HD13	2.37	0.54
2:d:319:VAL:HA	2:d:339:SER:OG	2.06	0.54
4:f:41:LEU:N	4:f:71:VAL:HG23	2.20	0.54
1:B:450:ALA:HA	1:B:455:TYR:HB2	1.90	0.54
1:C:413:LEU:H	1:C:413:LEU:HD12	1.73	0.54
2:F:5:ILE:HG21	2:F:64:ARG:HA	1.89	0.54
2:F:162:LEU:O	2:F:166:ILE:HG13	2.08	0.54
1:I:320:LYS:HD2	1:I:320:LYS:N	2.22	0.54
2:M:89:ASN:HD22	2:M:89:ASN:N	2.06	0.54
1:R:95:LEU:O	1:R:95:LEU:CD1	2.46	0.54
2:U:131:LYS:HG3	2:U:418:VAL:CG1	2.37	0.54
2:V:118:GLU:O	2:V:286:LYS:HG2	2.08	0.54
2:V:162:LEU:O	2:V:166:ILE:HG13	2.08	0.54
1:Z:385:ILE:O	1:Z:389:LEU:HD23	2.06	0.54
1:a:55:LEU:HD13	1:a:88:VAL:HG13	1.90	0.54
1:B:57:GLY:N	1:B:58:ASN:HA	2.21	0.54
2:E:166:ILE:HA	2:E:170:HIS:HB2	1.90	0.54
1:I:44:LEU:HD22	1:I:90:CYS:SG	2.47	0.54
2:M:360:VAL:O	2:M:364:LEU:HB2	2.06	0.54
2:U:174:SER:HB3	2:U:238:LEU:CB	2.38	0.54
1:a:144:GLN:HG3	1:a:161:ARG:HD3	1.90	0.54
1:a:198:ILE:CD1	1:a:239:PRO:HG3	2.37	0.54
2:d:118:GLU:O	2:d:286:LYS:HG2	2.07	0.54
2:d:183:THR:HG22	2:d:208:GLN:HG3	1.88	0.54
1:A:318:LYS:HD2	1:A:319:GLY:H	1.73	0.54
1:B:56:PRO:C	1:B:58:ASN:HA	2.33	0.54
1:B:313:THR:HG21	1:B:317:VAL:H	1.71	0.54
1:C:144:GLN:HG3	1:C:161:ARG:HD3	1.89	0.54
1:C:507:PHE:CD2	1:C:507:PHE:C	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:405:PHE:CZ	2:E:416:LYS:HA	2.42	0.54
2:L:90:VAL:HG11	2:L:215:ASN:ND2	2.22	0.54
2:N:5:ILE:HG21	2:N:64:ARG:HA	1.89	0.54
2:N:161:GLU:HG3	2:N:404:PHE:CG	2.43	0.54
3:O:229:GLN:HA	3:O:232:VAL:HG12	1.89	0.54
1:R:57:GLY:N	1:R:58:ASN:HA	2.21	0.54
1:S:446:LEU:HD23	1:S:447:VAL:N	2.23	0.54
1:S:504:LEU:O	1:S:507:PHE:HB3	2.07	0.54
2:T:3:GLY:HA3	2:T:17:PHE:CD2	2.42	0.54
2:V:221:LEU:O	2:V:225:THR:HG23	2.08	0.54
3:W:186:GLN:CG	3:W:189:PRO:CD	2.86	0.54
1:Y:84:GLU:OE2	2:b:48:GLY:HA2	2.08	0.54
1:Y:361:ASN:HD22	1:Y:361:ASN:N	2.06	0.54
1:a:265:LYS:O	1:a:268:VAL:HG12	2.08	0.54
1:a:493:ASN:H	1:a:496:ILE:HG13	1.70	0.54
2:b:3:GLY:HA3	2:b:17:PHE:CD2	2.43	0.54
2:c:332:PRO:HD2	2:c:401:SER:HA	1.89	0.54
2:d:162:LEU:O	2:d:166:ILE:HG13	2.08	0.54
1:A:361:ASN:HD22	1:A:361:ASN:N	2.06	0.53
2:D:224:LEU:O	2:D:228:GLU:HB2	2.08	0.53
2:E:194:THR:HG22	2:E:199:ILE:HG21	1.90	0.53
1:J:158:PRO:HB3	1:J:382:GLN:HE21	1.73	0.53
1:J:309:VAL:CG1	1:J:317:VAL:HG11	2.33	0.53
1:K:55:LEU:HD13	1:K:88:VAL:HG13	1.90	0.53
1:Q:135:GLY:N	1:Q:138:GLU:HG3	2.24	0.53
1:S:265:LYS:O	1:S:268:VAL:HG12	2.08	0.53
1:S:335:GLY:O	1:S:337:VAL:HG23	2.07	0.53
2:U:166:ILE:HA	2:U:170:HIS:HB2	1.90	0.53
1:Y:415:ASP:HA	1:Y:418:ARG:HB3	1.88	0.53
1:a:507:PHE:C	1:a:507:PHE:CD2	2.85	0.53
2:c:112:ALA:CA	2:c:114:PRO:HD2	2.37	0.53
2:c:387:LYS:HE3	2:c:390:VAL:HG11	1.90	0.53
1:A:218:LEU:HA	1:A:221:THR:HG23	1.90	0.53
1:A:413:LEU:HD22	1:A:413:LEU:N	2.23	0.53
1:B:158:PRO:HB3	1:B:382:GLN:HE21	1.73	0.53
1:B:210:ARG:HA	1:B:210:ARG:HE	1.73	0.53
1:C:55:LEU:HD13	1:C:88:VAL:HG13	1.90	0.53
1:C:198:ILE:CD1	1:C:239:PRO:HG3	2.37	0.53
1:C:243:CYS:SG	1:C:300:ARG:HG2	2.49	0.53
2:D:392:ARG:O	2:D:396:ILE:HG23	2.07	0.53
2:E:135:LEU:HD21	2:E:357:ALA:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:LEU:HD23	2:F:47:GLY:N	2.23	0.53
2:F:410:PHE:CD2	2:F:410:PHE:N	2.76	0.53
1:K:304:VAL:HG21	1:K:308:TYR:CG	2.43	0.53
1:K:409:PHE:O	1:K:412:ASP:HB2	2.07	0.53
2:M:166:ILE:HA	2:M:170:HIS:HB2	1.90	0.53
1:Q:87:LYS:HE3	1:Q:89:LYS:CE	2.36	0.53
1:Q:157:ILE:HG21	1:Q:353:ILE:HG12	1.91	0.53
1:Q:361:ASN:HD22	1:Q:361:ASN:N	2.06	0.53
1:R:210:ARG:HA	1:R:210:ARG:HE	1.73	0.53
1:S:250:ARG:HG3	1:S:251:ASP:N	2.23	0.53
2:U:66:LEU:HD23	2:U:67:ASP:H	1.72	0.53
1:a:151:LYS:HE3	1:a:433:GLN:HG2	1.90	0.53
2:c:370:LEU:HD13	2:c:382:LEU:HD11	1.89	0.53
1:A:304:VAL:HG21	1:A:308:TYR:CD1	2.44	0.53
1:C:356:GLU:HB2	1:C:359:LEU:HD23	1.89	0.53
2:E:112:ALA:CA	2:E:114:PRO:HD2	2.37	0.53
2:E:337:LEU:HD12	2:E:338:ASP:N	2.20	0.53
2:F:145:VAL:HG22	2:F:317:ALA:HB3	1.89	0.53
2:F:161:GLU:HG3	2:F:404:PHE:CB	2.36	0.53
3:G:188:LEU:O	3:G:188:LEU:CG	2.42	0.53
1:K:265:LYS:O	1:K:268:VAL:HG12	2.08	0.53
2:L:242:ASP:O	2:L:295:ALA:HB3	2.09	0.53
2:T:224:LEU:O	2:T:228:GLU:HB2	2.08	0.53
2:T:278:LEU:HD13	2:T:278:LEU:C	2.34	0.53
2:T:450:GLU:O	2:T:453:VAL:HG22	2.08	0.53
2:U:89:ASN:ND2	2:U:93:GLU:H	2.04	0.53
2:V:5:ILE:HG21	2:V:64:ARG:HA	1.89	0.53
2:V:145:VAL:HG22	2:V:317:ALA:HB3	1.90	0.53
3:W:14:GLN:HA	3:W:257:ILE:HD11	1.90	0.53
3:W:187:LEU:HD13	3:W:223:VAL:HG22	1.90	0.53
1:a:250:ARG:HG3	1:a:251:ASP:N	2.23	0.53
1:a:337:VAL:HG12	1:a:337:VAL:O	2.07	0.53
2:b:416:LYS:HD2	2:b:451:GLU:OE2	2.08	0.53
2:c:107:TRP:HB3	2:c:111:ARG:HH22	1.73	0.53
2:c:382:LEU:HD12	2:c:387:LYS:HD3	1.89	0.53
3:e:12:SER:O	3:e:16:THR:HG23	2.07	0.53
3:e:14:GLN:HA	3:e:257:ILE:HD11	1.90	0.53
1:A:364:ILE:HG13	1:A:432:LYS:CG	2.36	0.53
1:C:409:PHE:O	1:C:412:ASP:HB2	2.08	0.53
2:D:239:LEU:HB2	2:D:290:ILE:HD11	1.90	0.53
1:I:388:LYS:HD3	1:I:492:TYR:CE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:209:VAL:HA	1:J:212:LEU:HB2	1.89	0.53
1:K:296:ARG:HA	2:L:210:ASN:HB3	1.91	0.53
2:L:3:GLY:HA3	2:L:17:PHE:CD2	2.43	0.53
2:L:429:GLY:O	2:L:433:GLY:HA2	2.08	0.53
2:M:112:ALA:CA	2:M:114:PRO:HD2	2.37	0.53
2:M:135:LEU:HD21	2:M:357:ALA:HA	1.89	0.53
2:M:337:LEU:HD12	2:M:338:ASP:N	2.18	0.53
3:O:7:ARG:HG3	3:O:264:TYR:CE1	2.44	0.53
4:P:72:GLN:HB2	4:P:73:PRO:HD2	1.89	0.53
1:S:243:CYS:O	1:S:247:GLU:HG3	2.09	0.53
1:S:440:SER:C	1:S:442:ALA:N	2.64	0.53
1:Z:102:GLY:HA3	1:Z:122:ASP:HB2	1.91	0.53
2:d:141:LYS:HA	2:d:291:THR:HG23	1.89	0.53
4:H:2:MET:HE1	2:U:197:ASN:HA	1.90	0.53
1:K:151:LYS:HE3	1:K:433:GLN:HG2	1.90	0.53
1:K:507:PHE:C	1:K:507:PHE:CD2	2.85	0.53
2:N:46:LEU:HD23	2:N:47:GLY:N	2.23	0.53
1:S:55:LEU:HD13	1:S:88:VAL:HG13	1.90	0.53
2:T:428:LYS:O	2:T:432:GLU:HG3	2.09	0.53
2:V:352:GLU:H	2:V:352:GLU:CD	2.16	0.53
1:Y:304:VAL:HG21	1:Y:308:TYR:CD1	2.44	0.53
1:Y:330:ILE:HG13	1:Y:345:VAL:HG11	1.90	0.53
1:a:454:GLY:HA3	1:a:457:ALA:HB2	1.91	0.53
2:c:337:LEU:HD12	2:c:338:ASP:N	2.19	0.53
1:C:243:CYS:O	1:C:247:GLU:HG3	2.09	0.53
1:C:454:GLY:HA3	1:C:457:ALA:HB2	1.91	0.53
2:D:366:ARG:O	2:D:370:LEU:HD23	2.09	0.53
3:G:7:ARG:HG3	3:G:264:TYR:CE1	2.44	0.53
1:I:180:ILE:CD1	1:I:211:LYS:HE2	2.38	0.53
1:J:56:PRO:C	1:J:58:ASN:HA	2.33	0.53
2:L:397:GLN:O	2:L:400:LEU:HD23	2.09	0.53
2:M:394:ARG:O	2:M:398:ARG:HG3	2.08	0.53
2:N:139:PHE:N	2:N:139:PHE:CD2	2.74	0.53
1:R:158:PRO:HB3	1:R:382:GLN:HE21	1.73	0.53
1:R:450:ALA:HA	1:R:455:TYR:HB2	1.90	0.53
1:Z:450:ALA:HA	1:Z:455:TYR:HB2	1.90	0.53
1:a:356:GLU:HB2	1:a:359:LEU:HD23	1.89	0.53
2:b:224:LEU:O	2:b:228:GLU:HB2	2.08	0.53
3:e:62:TYR:N	3:e:62:TYR:CD1	2.75	0.53
1:B:41:ILE:HD12	1:B:53:ILE:HD13	1.90	0.53
1:B:104:LEU:HB2	1:B:219:ALA:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:GLU:OE2	2:F:183:THR:HG23	2.09	0.53
1:J:210:ARG:HA	1:J:210:ARG:HE	1.73	0.53
1:K:504:LEU:O	1:K:507:PHE:HB3	2.07	0.53
2:L:231:ARG:NH1	2:L:281:ARG:HH11	2.06	0.53
2:L:279:GLN:HG2	2:L:314:HIS:HB3	1.90	0.53
2:N:162:LEU:O	2:N:166:ILE:HG13	2.08	0.53
1:S:144:GLN:HG3	1:S:161:ARG:HD3	1.90	0.53
1:S:454:GLY:HA3	1:S:457:ALA:HB2	1.91	0.53
2:U:446:VAL:HG21	2:U:452:ALA:HB2	1.91	0.53
1:Y:318:LYS:HD2	1:Y:319:GLY:H	1.73	0.53
1:Y:424:GLY:O	1:Y:428:THR:HG23	2.08	0.53
1:Z:104:LEU:HB2	1:Z:219:ALA:O	2.09	0.53
1:a:243:CYS:O	1:a:247:GLU:HG3	2.09	0.53
1:a:369:ASN:O	1:a:372:ILE:HG22	2.09	0.53
2:c:163:ILE:CG2	2:c:201:LYS:HE3	2.37	0.53
2:c:166:ILE:HA	2:c:170:HIS:HB2	1.90	0.53
2:d:5:ILE:HG21	2:d:64:ARG:HA	1.89	0.53
3:e:7:ARG:HG3	3:e:264:TYR:CE1	2.44	0.53
1:C:55:LEU:HD21	1:C:61:ALA:HB2	1.89	0.53
1:C:250:ARG:HG3	1:C:251:ASP:N	2.23	0.53
1:C:337:VAL:O	1:C:337:VAL:HG12	2.07	0.53
2:E:89:ASN:HD22	2:E:89:ASN:N	2.06	0.53
2:E:398:ARG:O	2:E:443:PHE:O	2.27	0.53
1:I:318:LYS:HD2	1:I:319:GLY:H	1.73	0.53
1:I:450:ALA:HB1	1:I:456:LEU:HD21	1.90	0.53
1:J:41:ILE:HD12	1:J:53:ILE:HD13	1.90	0.53
1:K:413:LEU:H	1:K:413:LEU:HD12	1.73	0.53
1:K:454:GLY:HA3	1:K:457:ALA:HB2	1.91	0.53
2:M:174:SER:HB3	2:M:238:LEU:CB	2.38	0.53
2:M:197:ASN:CB	4:f:2:MET:SD	2.97	0.53
3:O:201:LYS:HZ1	2:c:171:SER:HA	1.73	0.53
1:S:243:CYS:SG	1:S:300:ARG:HG2	2.49	0.53
2:T:144:LYS:HD3	2:T:279:GLN:HE21	1.73	0.53
2:T:226:MET:O	2:T:230:PHE:HD1	1.92	0.53
2:U:231:ARG:HD2	2:U:285:THR:HG22	1.91	0.53
3:W:7:ARG:HG3	3:W:264:TYR:CE1	2.44	0.53
3:W:52:ILE:HD13	3:W:219:LEU:HD12	1.91	0.53
1:Y:172:GLN:HA	5:Y:600:ANP:HNB1	1.73	0.53
1:a:456:LEU:N	1:a:456:LEU:CD2	2.69	0.53
2:c:276:GLY:O	2:c:280:GLU:HB2	2.09	0.53
2:d:353:HIS:CE1	2:d:420:LEU:HD11	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLN:HA	5:A:600:ANP:HNB1	1.74	0.53
1:A:424:GLY:O	1:A:428:THR:HG23	2.08	0.53
1:C:265:LYS:O	1:C:268:VAL:HG12	2.08	0.53
2:E:107:TRP:HB3	2:E:111:ARG:HH22	1.73	0.53
2:E:161:GLU:CG	2:E:404:PHE:HB3	2.38	0.53
2:E:163:ILE:HG22	2:E:201:LYS:HE3	1.91	0.53
1:I:304:VAL:HG21	1:I:308:TYR:CD1	2.44	0.53
1:I:361:ASN:HD22	1:I:361:ASN:N	2.06	0.53
1:J:158:PRO:CB	1:J:382:GLN:HG2	2.38	0.53
1:K:446:LEU:HD23	1:K:447:VAL:N	2.23	0.53
1:K:458:ASP:O	1:K:459:VAL:C	2.50	0.53
2:L:19:GLN:O	2:L:20:ASP:C	2.51	0.53
2:M:107:TRP:HB3	2:M:111:ARG:HH22	1.73	0.53
1:Q:56:PRO:HG3	1:Q:86:MET:HE2	1.91	0.53
1:R:102:GLY:HA3	1:R:122:ASP:HB2	1.91	0.53
1:R:140:GLN:HA	1:R:140:GLN:NE2	2.14	0.53
1:S:55:LEU:HD21	1:S:61:ALA:HB2	1.89	0.53
1:S:356:GLU:HB2	1:S:359:LEU:HD23	1.89	0.53
2:T:429:GLY:O	2:T:433:GLY:HA2	2.09	0.53
2:U:89:ASN:HD22	2:U:89:ASN:N	2.06	0.53
1:Y:138:GLU:HG3	1:Y:305:ASN:HB3	1.91	0.53
1:Y:211:LYS:HD2	1:Y:436:TYR:CZ	2.44	0.53
1:Y:218:LEU:HA	1:Y:221:THR:HG23	1.90	0.53
1:a:256:ALA:HB3	1:a:324:LEU:HD23	1.90	0.53
1:a:365:ARG:HG3	5:a:600:ANP:N1	2.23	0.53
2:b:134:ASP:HB3	2:b:420:LEU:HD23	1.90	0.53
2:b:169:GLU:O	2:b:170:HIS:HD2	1.92	0.53
2:b:428:LYS:O	2:b:432:GLU:HG3	2.09	0.53
2:c:131:LYS:H	2:c:402:GLN:NE2	1.95	0.53
1:A:87:LYS:HE3	1:A:89:LYS:CE	2.36	0.53
2:D:3:GLY:HA3	2:D:17:PHE:HE2	1.74	0.53
2:E:144:LYS:NZ	2:E:279:GLN:HB3	2.24	0.53
1:I:365:ARG:HG2	5:I:600:ANP:C2	2.39	0.53
1:I:413:LEU:HD22	1:I:413:LEU:N	2.23	0.53
2:M:402:GLN:C	2:M:445:MET:CE	2.82	0.53
1:Q:450:ALA:HB1	1:Q:456:LEU:HD21	1.90	0.53
2:U:194:THR:HG22	2:U:199:ILE:HG21	1.90	0.53
2:c:304:THR:HG22	3:e:269:GLN:OE1	2.09	0.53
1:A:450:ALA:HB1	1:A:456:LEU:HD21	1.90	0.52
1:B:140:GLN:HA	1:B:140:GLN:NE2	2.14	0.52
1:C:494:ASP:O	1:C:495:GLU:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:VAL:HG22	2:D:23:PRO:N	2.23	0.52
3:G:52:ILE:HD13	3:G:219:LEU:HD12	1.91	0.52
3:G:187:LEU:O	3:G:188:LEU:HB3	2.09	0.52
1:J:354:PHE:CE2	1:J:372:ILE:HG12	2.44	0.52
1:K:250:ARG:HG3	1:K:251:ASP:N	2.23	0.52
1:K:309:VAL:HG23	1:K:318:LYS:HB3	1.92	0.52
2:M:194:THR:HG22	2:M:199:ILE:HG21	1.90	0.52
2:N:225:THR:HG22	2:N:281:ARG:HH12	1.74	0.52
1:Q:211:LYS:HD2	1:Q:436:TYR:CZ	2.44	0.52
1:Q:304:VAL:HG21	1:Q:308:TYR:CD1	2.44	0.52
1:S:66:LEU:HD12	2:T:8:VAL:HB	1.91	0.52
1:S:123:HIS:NE2	1:S:126:PHE:HE1	2.07	0.52
1:S:180:ILE:O	1:S:184:ILE:HG13	2.09	0.52
2:U:336:PRO:HG3	2:U:400:LEU:HD11	1.90	0.52
1:a:123:HIS:NE2	1:a:126:PHE:HE1	2.07	0.52
2:c:297:TYR:C	2:c:297:TYR:CD2	2.87	0.52
1:B:354:PHE:CE2	1:B:372:ILE:HG12	2.44	0.52
1:I:180:ILE:HD12	1:I:211:LYS:CE	2.36	0.52
1:K:495:GLU:HG2	1:K:496:ILE:HD13	1.92	0.52
2:L:169:GLU:O	2:L:170:HIS:HD2	1.92	0.52
2:L:226:MET:O	2:L:230:PHE:HD1	1.92	0.52
2:L:428:LYS:O	2:L:432:GLU:HG3	2.09	0.52
2:M:172:GLY:HA2	2:M:235:ARG:HD3	1.91	0.52
1:Q:218:LEU:HA	1:Q:221:THR:HG23	1.90	0.52
1:S:256:ALA:HB3	1:S:324:LEU:HD23	1.90	0.52
1:S:369:ASN:O	1:S:372:ILE:HG22	2.09	0.52
1:Z:56:PRO:C	1:Z:58:ASN:HA	2.33	0.52
1:a:413:LEU:HD12	1:a:413:LEU:H	1.73	0.52
2:b:104:GLU:HG3	2:b:106:ARG:HH11	1.75	0.52
2:c:161:GLU:CG	2:c:404:PHE:HB3	2.38	0.52
1:A:218:LEU:HD13	1:A:219:ALA:N	2.25	0.52
1:B:95:LEU:CG	1:B:129:VAL:HG22	2.39	0.52
1:C:123:HIS:NE2	1:C:126:PHE:HE1	2.07	0.52
1:C:369:ASN:O	1:C:372:ILE:HG22	2.09	0.52
1:I:56:PRO:HG3	1:I:86:MET:HE2	1.91	0.52
1:I:157:ILE:HG21	1:I:353:ILE:HG12	1.91	0.52
2:L:104:GLU:HG3	2:L:106:ARG:HH11	1.75	0.52
2:M:401:SER:HB2	2:M:445:MET:HE3	1.92	0.52
1:Q:424:GLY:O	1:Q:428:THR:HG23	2.08	0.52
1:R:354:PHE:CE2	1:R:372:ILE:HG12	2.44	0.52
1:S:151:LYS:HE3	1:S:433:GLN:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:362:SER:O	2:U:365:GLN:HG3	2.10	0.52
2:U:382:LEU:HD12	2:U:387:LYS:HD3	1.91	0.52
3:W:187:LEU:HD12	3:W:188:LEU:HB3	1.62	0.52
4:X:2:MET:O	4:X:3:THR:CG2	2.57	0.52
4:X:50:ILE:HG22	4:X:62:ILE:O	2.10	0.52
1:Z:158:PRO:CB	1:Z:382:GLN:HG2	2.38	0.52
2:d:46:LEU:HD23	2:d:47:GLY:N	2.23	0.52
2:d:240:PHE:CD2	2:d:293:VAL:HG22	2.44	0.52
1:A:56:PRO:HG3	1:A:86:MET:HE2	1.91	0.52
1:B:205:ILE:HD13	1:B:225:VAL:HG23	1.92	0.52
2:D:120:SER:HA	2:D:121:ASN:C	2.35	0.52
2:D:217:LEU:HD12	2:D:254:VAL:HG21	1.92	0.52
2:D:226:MET:O	2:D:230:PHE:HD1	1.92	0.52
2:E:442:ALA:C	2:E:443:PHE:CD2	2.82	0.52
1:I:211:LYS:HD2	1:I:436:TYR:CZ	2.44	0.52
1:I:218:LEU:HD13	1:I:219:ALA:N	2.25	0.52
1:J:102:GLY:HA3	1:J:122:ASP:HB2	1.91	0.52
1:J:460:GLU:OE1	1:J:468:GLU:HG2	2.10	0.52
2:L:239:LEU:HB2	2:L:290:ILE:HD11	1.92	0.52
2:M:356:THR:O	2:M:360:VAL:HG23	2.09	0.52
2:N:147:LEU:HD23	2:N:319:VAL:HG22	1.91	0.52
3:O:208:GLU:OE2	3:O:209:PRO:HD2	2.09	0.52
2:T:279:GLN:HG2	2:T:314:HIS:HB3	1.91	0.52
2:U:112:ALA:CA	2:U:114:PRO:HD2	2.37	0.52
2:U:140:ALA:HB2	2:U:343:GLN:HG2	1.91	0.52
2:V:46:LEU:HD23	2:V:47:GLY:N	2.23	0.52
3:W:201:LYS:HD3	3:W:202:SER:N	2.18	0.52
1:Y:56:PRO:HG3	1:Y:86:MET:HE2	1.91	0.52
1:Y:157:ILE:HG21	1:Y:353:ILE:HG12	1.91	0.52
1:Z:210:ARG:HA	1:Z:210:ARG:HE	1.73	0.52
1:a:94:ILE:HD13	1:a:94:ILE:H	1.75	0.52
1:a:180:ILE:O	1:a:184:ILE:HG13	2.09	0.52
1:a:217:ALA:O	1:a:221:THR:HG22	2.09	0.52
1:a:495:GLU:HG2	1:a:496:ILE:HD13	1.92	0.52
2:c:135:LEU:HD21	2:c:357:ALA:HA	1.92	0.52
2:c:163:ILE:HG22	2:c:201:LYS:HE3	1.91	0.52
1:B:172:GLN:HA	5:B:600:ANP:N3B	2.21	0.52
1:B:283:ARG:NH1	2:F:300:ALA:HB3	2.22	0.52
1:C:341:VAL:HB	1:C:342:PRO:HD3	1.92	0.52
1:C:454:GLY:HA3	1:C:457:ALA:CB	2.40	0.52
2:F:3:GLY:HA3	2:F:17:PHE:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:96:ASP:OD1	2:F:98:LYS:HG2	2.10	0.52
2:F:225:THR:HG22	2:F:281:ARG:HH12	1.74	0.52
1:J:104:LEU:HB2	1:J:219:ALA:O	2.09	0.52
1:K:94:ILE:HD13	1:K:94:ILE:H	1.75	0.52
2:L:224:LEU:O	2:L:228:GLU:HB2	2.08	0.52
2:M:148:PHE:HZ	2:M:312:PHE:CE1	2.26	0.52
2:N:111:ARG:HG3	2:N:111:ARG:NH1	2.21	0.52
1:Q:231:SER:HB3	1:Q:234:LEU:CD2	2.40	0.52
1:Q:330:ILE:HG13	1:Q:345:VAL:HG11	1.90	0.52
1:Q:364:ILE:HG13	1:Q:432:LYS:CG	2.36	0.52
1:R:434:LYS:HA	1:R:434:LYS:HE3	1.92	0.52
1:S:309:VAL:HG23	1:S:318:LYS:HB3	1.92	0.52
2:V:279:GLN:NE2	2:V:294:GLN:HE22	2.06	0.52
1:Z:205:ILE:HD13	1:Z:225:VAL:HG23	1.92	0.52
1:a:243:CYS:SG	1:a:300:ARG:HG2	2.49	0.52
1:a:309:VAL:HG23	1:a:318:LYS:HB3	1.92	0.52
2:c:89:ASN:HD22	2:c:89:ASN:N	2.06	0.52
2:c:144:LYS:NZ	2:c:279:GLN:HB3	2.25	0.52
2:c:194:THR:HG22	2:c:199:ILE:HG21	1.90	0.52
2:c:265:VAL:HG23	3:e:272:ILE:HG21	1.90	0.52
2:c:362:SER:HA	2:c:365:GLN:HG3	1.91	0.52
2:d:96:ASP:OD1	2:d:98:LYS:HG2	2.10	0.52
1:A:211:LYS:HD2	1:A:436:TYR:CZ	2.44	0.52
1:B:348:ILE:HG23	2:F:209:MET:HE1	1.91	0.52
1:C:217:ALA:O	1:C:221:THR:HG22	2.09	0.52
2:E:172:GLY:HA2	2:E:235:ARG:HD3	1.91	0.52
2:E:360:VAL:O	2:E:364:LEU:HB2	2.09	0.52
1:I:424:GLY:O	1:I:428:THR:HG23	2.08	0.52
1:K:243:CYS:SG	1:K:300:ARG:HG2	2.49	0.52
2:L:42:VAL:HG13	2:L:51:VAL:HG13	1.92	0.52
2:L:120:SER:HA	2:L:121:ASN:C	2.35	0.52
1:Q:218:LEU:HD13	1:Q:219:ALA:N	2.24	0.52
1:Q:413:LEU:HD22	1:Q:413:LEU:N	2.23	0.52
1:R:56:PRO:C	1:R:58:ASN:HA	2.33	0.52
2:T:120:SER:HA	2:T:121:ASN:C	2.35	0.52
3:W:187:LEU:HD11	3:W:223:VAL:HG22	1.91	0.52
1:a:54:SER:HA	1:a:60:TYR:HD1	1.75	0.52
1:a:66:LEU:HB2	2:b:64:ARG:HD2	1.92	0.52
2:b:217:LEU:HD12	2:b:254:VAL:HG21	1.92	0.52
2:d:105:GLU:CG	2:d:106:ARG:H	2.23	0.52
3:e:52:ILE:HD13	3:e:219:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:GLY:HA3	1:B:122:ASP:HB2	1.91	0.52
2:D:265:VAL:O	2:D:265:VAL:HG12	2.10	0.52
3:G:201:LYS:CE	2:U:171:SER:HA	2.39	0.52
1:K:243:CYS:O	1:K:247:GLU:HG3	2.09	0.52
1:K:369:ASN:O	1:K:372:ILE:HG22	2.09	0.52
1:K:454:GLY:HA3	1:K:457:ALA:CB	2.40	0.52
2:M:332:PRO:HD3	2:M:402:GLN:H	1.73	0.52
2:N:285:THR:HG22	2:N:286:LYS:N	2.24	0.52
2:N:353:HIS:HA	2:N:424:ILE:HD12	1.91	0.52
1:Q:295:SER:HA	1:Q:348:ILE:HD13	1.92	0.52
1:Q:318:LYS:HD2	1:Q:319:GLY:H	1.73	0.52
1:R:104:LEU:HB2	1:R:219:ALA:O	2.09	0.52
1:R:192:LYS:HD2	1:R:192:LYS:N	2.25	0.52
1:S:217:ALA:O	1:S:221:THR:HG22	2.09	0.52
2:T:169:GLU:O	2:T:170:HIS:HD2	1.92	0.52
1:Z:95:LEU:HD11	1:Z:129:VAL:CG1	2.40	0.52
1:Z:283:ARG:NH1	2:d:300:ALA:HB3	2.24	0.52
2:b:128:THR:N	2:b:129:GLY:HA2	2.24	0.52
2:b:227:ALA:HB1	2:b:290:ILE:HD13	1.92	0.52
2:d:3:GLY:HA3	2:d:17:PHE:CD2	2.45	0.52
1:A:157:ILE:HG21	1:A:353:ILE:HG12	1.91	0.52
1:C:385:ILE:HB	1:C:492:TYR:HB3	1.91	0.52
2:D:169:GLU:O	2:D:170:HIS:HD2	1.92	0.52
1:I:330:ILE:HG13	1:I:345:VAL:HG11	1.90	0.52
1:J:192:LYS:HD2	1:J:192:LYS:N	2.25	0.52
2:N:19:GLN:O	2:N:20:ASP:C	2.53	0.52
1:Q:439:MET:HG2	1:Q:443:GLN:HB3	1.92	0.52
1:R:98:PRO:HD3	1:R:126:PHE:CE2	2.45	0.52
1:R:460:GLU:OE1	1:R:468:GLU:HG2	2.10	0.52
1:S:459:VAL:O	1:S:459:VAL:CG1	2.57	0.52
2:T:379:MET:HE1	2:T:390:VAL:CG1	2.35	0.52
2:U:141:LYS:HD2	2:U:236:ASP:OD2	2.10	0.52
2:V:3:GLY:HA3	2:V:17:PHE:CD2	2.45	0.52
2:V:225:THR:HG22	2:V:281:ARG:HH12	1.75	0.52
4:X:84:ILE:H	4:X:84:ILE:HD12	1.75	0.52
1:Y:231:SER:HB3	1:Y:234:LEU:CD2	2.40	0.52
1:Y:313:THR:OG1	1:Y:316:GLU:HB3	2.10	0.52
1:Y:439:MET:HG2	1:Y:443:GLN:HB3	1.92	0.52
1:Z:98:PRO:HD3	1:Z:126:PHE:CE2	2.45	0.52
1:Z:158:PRO:HB3	1:Z:382:GLN:HE21	1.73	0.52
1:a:341:VAL:HB	1:a:342:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:46:LEU:HB3	2:d:50:ILE:HG13	1.92	0.52
2:d:145:VAL:HG22	2:d:317:ALA:HB3	1.91	0.52
1:A:231:SER:HB3	1:A:234:LEU:CD2	2.40	0.52
1:A:313:THR:HG21	1:A:317:VAL:HG22	1.92	0.52
1:A:423:HIS:CD2	1:A:426:LYS:HE2	2.45	0.52
1:A:439:MET:HG2	1:A:443:GLN:HB3	1.92	0.52
1:B:139:ARG:HH21	2:F:183:THR:HG1	1.58	0.52
1:B:158:PRO:CB	1:B:382:GLN:HG2	2.38	0.52
1:B:309:VAL:CG1	1:B:317:VAL:HG11	2.33	0.52
1:B:460:GLU:OE1	1:B:468:GLU:HG2	2.10	0.52
2:D:42:VAL:HG13	2:D:51:VAL:HG13	1.92	0.52
2:D:441:GLN:CD	2:D:441:GLN:H	2.18	0.52
2:E:141:LYS:HD2	2:E:236:ASP:OD2	2.10	0.52
2:F:19:GLN:O	2:F:20:ASP:C	2.53	0.52
2:F:111:ARG:HG3	2:F:111:ARG:NH1	2.21	0.52
2:L:134:ASP:HB3	2:L:420:LEU:HD23	1.91	0.52
2:L:323:ARG:CD	2:L:323:ARG:N	2.69	0.52
2:N:105:GLU:CG	2:N:106:ARG:H	2.23	0.52
1:Q:313:THR:HG21	1:Q:317:VAL:HG22	1.92	0.52
1:Q:431:LEU:C	1:Q:432:LYS:HD2	2.35	0.52
1:S:454:GLY:HA3	1:S:457:ALA:CB	2.40	0.52
2:T:42:VAL:HG13	2:T:51:VAL:HG13	1.92	0.52
2:T:104:GLU:HG3	2:T:106:ARG:HH11	1.75	0.52
2:T:242:ASP:O	2:T:295:ALA:HB3	2.10	0.52
2:U:107:TRP:HB3	2:U:111:ARG:NH2	2.25	0.52
2:U:265:VAL:N	3:W:273:THR:HG22	2.13	0.52
2:U:312:PHE:HD1	2:U:315:LEU:HD12	1.75	0.52
2:V:417:TYR:C	2:V:417:TYR:HD2	2.18	0.52
1:Y:218:LEU:HD13	1:Y:219:ALA:N	2.25	0.52
1:Y:428:THR:O	1:Y:432:LYS:HD3	2.09	0.52
2:c:172:GLY:HA2	2:c:235:ARG:HD3	1.91	0.52
2:c:279:GLN:O	2:c:282:ILE:HG12	2.09	0.52
2:d:198:VAL:O	2:d:198:VAL:HG12	2.10	0.52
1:B:192:LYS:HD2	1:B:192:LYS:N	2.25	0.52
2:D:239:LEU:CB	2:D:290:ILE:HD11	2.40	0.52
1:I:231:SER:HB3	1:I:234:LEU:CD2	2.40	0.52
1:I:264:SER:HB3	1:I:330:ILE:HD13	1.91	0.52
1:J:97:VAL:CG2	1:J:111:LEU:O	2.49	0.52
1:J:434:LYS:HA	1:J:434:LYS:HE3	1.92	0.52
2:L:144:LYS:HE2	2:L:279:GLN:O	2.10	0.52
2:M:144:LYS:N	2:M:144:LYS:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:3:GLY:HA3	2:N:17:PHE:CD2	2.45	0.52
4:P:2:MET:HE2	4:P:3:THR:H	1.75	0.52
1:Q:164:ARG:HB3	1:Q:326:ALA:HB3	1.92	0.52
1:Q:428:THR:O	1:Q:432:LYS:HD3	2.09	0.52
1:S:80:ALA:HA	2:V:25:VAL:CG1	2.36	0.52
2:V:46:LEU:HB3	2:V:50:ILE:HG13	1.92	0.52
1:Z:192:LYS:HD2	1:Z:192:LYS:N	2.25	0.52
1:Z:460:GLU:OE1	1:Z:468:GLU:HG2	2.10	0.52
2:b:120:SER:HA	2:b:121:ASN:C	2.35	0.52
2:b:360:VAL:HG13	2:b:396:ILE:HD12	1.91	0.52
2:b:388:LEU:HD11	2:b:392:ARG:NH2	2.24	0.52
2:c:141:LYS:HD2	2:c:236:ASP:OD2	2.10	0.52
2:d:111:ARG:HG3	2:d:111:ARG:NH1	2.22	0.52
1:B:98:PRO:HD3	1:B:126:PHE:CE2	2.45	0.51
1:C:180:ILE:O	1:C:184:ILE:HG13	2.09	0.51
1:C:495:GLU:CG	1:C:496:ILE:N	2.73	0.51
2:D:104:GLU:HG3	2:D:106:ARG:HH11	1.75	0.51
2:E:332:PRO:HD2	2:E:401:SER:HA	1.92	0.51
2:E:347:LEU:HD12	2:E:348:VAL:CA	2.39	0.51
2:E:362:SER:HA	2:E:365:GLN:HG3	1.91	0.51
3:G:201:LYS:NZ	2:U:171:SER:HA	2.25	0.51
1:J:95:LEU:HD12	1:J:95:LEU:C	2.34	0.51
1:J:98:PRO:HD3	1:J:126:PHE:CE2	2.45	0.51
1:K:492:TYR:HE1	1:K:497:GLU:HB2	1.75	0.51
2:M:396:ILE:C	2:M:396:ILE:HD12	2.35	0.51
2:N:176:PHE:HD1	2:N:240:PHE:HB2	1.74	0.51
2:N:417:TYR:C	2:N:417:TYR:HD2	2.17	0.51
1:Q:305:ASN:O	1:Q:309:VAL:HG23	2.10	0.51
2:T:392:ARG:HD3	2:T:431:MET:HA	1.92	0.51
2:T:397:GLN:O	2:T:400:LEU:HD23	2.10	0.51
2:U:262:PRO:HG3	3:W:276:LEU:HD12	1.92	0.51
2:U:392:ARG:NH2	2:U:433:GLY:HA2	2.25	0.51
1:Y:431:LEU:C	1:Y:432:LYS:HD2	2.35	0.51
1:Z:354:PHE:CE2	1:Z:372:ILE:HG12	2.44	0.51
2:d:173:TYR:CD1	2:d:173:TYR:N	2.79	0.51
3:e:201:LYS:HD3	3:e:202:SER:N	2.18	0.51
4:f:50:ILE:HG22	4:f:62:ILE:O	2.10	0.51
1:A:110:THR:HB	1:A:234:LEU:HD12	1.93	0.51
1:A:330:ILE:HG13	1:A:345:VAL:HG11	1.90	0.51
1:C:365:ARG:HG3	5:C:600:ANP:C2	2.40	0.51
2:E:144:LYS:N	2:E:144:LYS:HD2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:50:ILE:HG22	4:H:62:ILE:O	2.10	0.51
1:I:305:ASN:O	1:I:309:VAL:HG23	2.10	0.51
1:I:385:ILE:HG23	1:I:386:MET:N	2.25	0.51
1:I:449:PHE:HB3	1:I:504:LEU:CD1	2.40	0.51
1:K:217:ALA:O	1:K:221:THR:HG22	2.09	0.51
2:M:107:TRP:HB3	2:M:111:ARG:NH2	2.25	0.51
2:M:141:LYS:HD2	2:M:236:ASP:OD2	2.10	0.51
2:N:173:TYR:CD1	2:N:173:TYR:N	2.79	0.51
1:Q:313:THR:OG1	1:Q:316:GLU:HB3	2.10	0.51
1:S:161:ARG:HB3	1:S:323:SER:OG	2.11	0.51
2:T:101:ILE:HD13	2:T:101:ILE:N	2.26	0.51
2:U:144:LYS:N	2:U:144:LYS:HD2	2.25	0.51
2:U:353:HIS:HE1	2:U:420:LEU:HD11	1.75	0.51
3:W:64:HIS:CE1	3:W:66:TYR:HA	2.46	0.51
1:Y:385:ILE:HG23	1:Y:386:MET:N	2.25	0.51
1:Y:413:LEU:HD22	1:Y:413:LEU:N	2.23	0.51
1:Y:499:LYS:O	1:Y:503:ILE:HG13	2.11	0.51
1:a:66:LEU:CD1	2:b:8:VAL:HB	2.39	0.51
1:a:454:GLY:HA3	1:a:457:ALA:CB	2.40	0.51
2:b:323:ARG:CD	2:b:323:ARG:N	2.73	0.51
2:c:322:SER:HB3	2:c:325:ILE:HB	1.91	0.51
2:c:362:SER:O	2:c:365:GLN:HG3	2.10	0.51
2:c:392:ARG:O	2:c:396:ILE:HG23	2.11	0.51
1:A:295:SER:HA	1:A:348:ILE:HD13	1.92	0.51
2:D:128:THR:N	2:D:129:GLY:HA2	2.24	0.51
2:D:279:GLN:HE22	2:D:294:GLN:NE2	2.07	0.51
2:D:392:ARG:HD3	2:D:431:MET:HA	1.92	0.51
2:F:105:GLU:CG	2:F:106:ARG:H	2.23	0.51
3:G:214:LEU:HD13	4:H:42:LEU:HG	1.92	0.51
1:I:423:HIS:CD2	1:I:426:LYS:HE2	2.45	0.51
1:J:205:ILE:HD13	1:J:225:VAL:HG23	1.92	0.51
1:K:123:HIS:NE2	1:K:126:PHE:HE1	2.07	0.51
2:L:367:TYR:CE1	2:L:371:LYS:HG3	2.46	0.51
2:M:437:HIS:CD2	2:M:438:LEU:HD12	2.44	0.51
2:N:131:LYS:H	2:N:402:GLN:NE2	2.04	0.51
2:N:155:LYS:HB2	8:N:530:SO4:O3	2.11	0.51
2:N:198:VAL:O	2:N:198:VAL:HG12	2.10	0.51
2:N:235:ARG:HH21	1:R:479:HIS:CD2	2.28	0.51
3:O:52:ILE:HD13	3:O:219:LEU:HD12	1.91	0.51
3:O:64:HIS:CE1	3:O:66:TYR:HA	2.45	0.51
1:R:146:VAL:CG2	1:R:161:ARG:HD3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:401:ARG:HG2	1:S:401:ARG:HH11	1.75	0.51
2:T:128:THR:N	2:T:129:GLY:HA2	2.24	0.51
2:U:163:ILE:HG22	2:U:201:LYS:HE3	1.91	0.51
2:V:19:GLN:O	2:V:20:ASP:C	2.53	0.51
2:V:197:ASN:O	2:V:197:ASN:CG	2.54	0.51
1:a:400:TYR:HB2	1:a:424:GLY:HA3	1.93	0.51
1:a:492:TYR:HE1	1:a:497:GLU:HB2	1.75	0.51
2:b:42:VAL:HG13	2:b:51:VAL:HG13	1.92	0.51
2:b:226:MET:O	2:b:230:PHE:HD1	1.92	0.51
2:c:395:LYS:HD3	2:c:443:PHE:CE2	2.45	0.51
1:A:138:GLU:HB3	1:A:305:ASN:HD22	1.75	0.51
1:B:434:LYS:HA	1:B:434:LYS:HE3	1.91	0.51
1:C:94:ILE:HD13	1:C:94:ILE:H	1.75	0.51
1:C:95:LEU:HB3	1:C:129:VAL:CG2	2.41	0.51
2:E:131:LYS:H	2:E:402:GLN:NE2	2.01	0.51
2:F:198:VAL:O	2:F:198:VAL:HG12	2.10	0.51
1:I:499:LYS:O	1:I:503:ILE:HG13	2.11	0.51
1:K:180:ILE:O	1:K:184:ILE:HG13	2.09	0.51
2:M:163:ILE:HG22	2:M:201:LYS:HE3	1.91	0.51
2:N:46:LEU:HB3	2:N:50:ILE:HG13	1.92	0.51
4:P:84:ILE:HD12	4:P:84:ILE:H	1.75	0.51
1:Q:385:ILE:HG23	1:Q:386:MET:N	2.25	0.51
1:Q:423:HIS:CD2	1:Q:426:LYS:HE2	2.45	0.51
1:S:492:TYR:HE1	1:S:497:GLU:HB2	1.75	0.51
2:T:231:ARG:HD2	2:T:281:ARG:HH12	1.76	0.51
2:U:172:GLY:HA2	2:U:235:ARG:HD3	1.91	0.51
2:U:447:GLY:H	2:U:451:GLU:HG2	1.76	0.51
2:V:198:VAL:O	2:V:198:VAL:HG12	2.10	0.51
1:Y:423:HIS:CD2	1:Y:426:LYS:HE2	2.45	0.51
2:d:175:VAL:O	2:d:239:LEU:HD23	2.10	0.51
4:f:84:ILE:HD12	4:f:84:ILE:H	1.75	0.51
1:A:428:THR:O	1:A:432:LYS:HD3	2.10	0.51
1:B:384:LYS:HE2	1:B:384:LYS:N	2.24	0.51
1:C:309:VAL:HG23	1:C:318:LYS:HB3	1.92	0.51
2:E:107:TRP:HB3	2:E:111:ARG:NH2	2.25	0.51
2:F:458:LYS:O	2:F:459:LEU:HB2	2.10	0.51
3:G:62:TYR:N	3:G:62:TYR:CD1	2.75	0.51
1:I:164:ARG:HB3	1:I:326:ALA:HB3	1.92	0.51
1:I:213:GLU:HB3	1:I:218:LEU:HB3	1.93	0.51
1:K:161:ARG:HB3	1:K:323:SER:OG	2.11	0.51
1:K:262:ASP:HB3	1:K:265:LYS:CG	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:341:VAL:HB	1:K:342:PRO:HD3	1.92	0.51
4:P:50:ILE:HG22	4:P:62:ILE:O	2.10	0.51
4:P:55:GLN:O	4:P:56:HIS:HB2	2.11	0.51
1:Q:499:LYS:O	1:Q:503:ILE:HG13	2.11	0.51
2:T:360:VAL:HG13	2:T:396:ILE:HD12	1.93	0.51
2:U:148:PHE:HZ	2:U:312:PHE:CE1	2.27	0.51
2:U:224:LEU:HD12	2:U:278:LEU:HD22	1.92	0.51
2:V:105:GLU:CG	2:V:106:ARG:H	2.23	0.51
2:V:176:PHE:HD1	2:V:240:PHE:HB2	1.74	0.51
1:Y:137:ILE:HD12	2:c:97:MET:H	1.76	0.51
3:e:64:HIS:CE1	3:e:66:TYR:HA	2.45	0.51
1:A:59:ARG:NH2	1:A:81:ASP:OD2	2.44	0.51
1:A:313:THR:OG1	1:A:316:GLU:HB3	2.10	0.51
1:B:341:VAL:HB	1:B:342:PRO:HD3	1.93	0.51
1:C:66:LEU:CD1	2:D:8:VAL:HB	2.40	0.51
1:C:262:ASP:HB3	1:C:265:LYS:CG	2.41	0.51
2:D:17:PHE:HD1	2:D:23:PRO:HD2	1.73	0.51
2:D:144:LYS:HE2	2:D:279:GLN:O	2.10	0.51
1:K:136:VAL:HG12	1:K:137:ILE:N	2.25	0.51
2:M:336:PRO:HG3	2:M:400:LEU:HD11	1.92	0.51
2:M:349:VAL:HG21	2:M:353:HIS:CG	2.46	0.51
1:S:54:SER:HA	1:S:60:TYR:HD1	1.75	0.51
1:S:94:ILE:HD13	1:S:94:ILE:H	1.75	0.51
2:U:322:SER:HB3	2:U:325:ILE:HB	1.93	0.51
1:Y:110:THR:HB	1:Y:234:LEU:HD12	1.93	0.51
1:Y:449:PHE:HB3	1:Y:504:LEU:CD1	2.40	0.51
1:Z:434:LYS:HA	1:Z:434:LYS:HE3	1.92	0.51
2:c:144:LYS:N	2:c:144:LYS:HD2	2.25	0.51
2:c:399:PHE:HA	2:c:443:PHE:O	2.10	0.51
3:e:208:GLU:OE2	3:e:209:PRO:HD2	2.09	0.51
1:A:264:SER:HB3	1:A:330:ILE:HD13	1.91	0.51
1:C:54:SER:HA	1:C:60:TYR:HD1	1.75	0.51
1:C:400:TYR:HB2	1:C:424:GLY:HA3	1.93	0.51
2:E:231:ARG:HD3	2:E:290:ILE:CG1	2.41	0.51
2:E:332:PRO:O	2:E:334:VAL:N	2.43	0.51
2:E:346:PRO:CB	2:E:348:VAL:HG12	2.40	0.51
2:F:176:PHE:HD1	2:F:240:PHE:HB2	1.74	0.51
2:F:182:ARG:O	2:F:185:GLU:HG3	2.11	0.51
3:G:64:HIS:CE1	3:G:66:TYR:HA	2.45	0.51
1:I:313:THR:HG21	1:I:317:VAL:HG22	1.92	0.51
1:K:95:LEU:HB3	1:K:129:VAL:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:217:LEU:HD12	2:L:254:VAL:HG21	1.92	0.51
2:N:197:ASN:CG	2:N:197:ASN:O	2.54	0.51
2:N:264:ALA:C	2:N:265:VAL:HG23	2.35	0.51
1:Q:59:ARG:NH2	1:Q:81:ASP:OD2	2.44	0.51
1:Q:94:ILE:O	1:Q:94:ILE:HG12	2.11	0.51
1:Q:186:GLN:HG3	1:Q:191:ILE:HB	1.92	0.51
2:T:111:ARG:HD3	2:T:281:ARG:CB	2.37	0.51
2:V:76:GLU:O	2:V:76:GLU:HG2	2.11	0.51
2:V:96:ASP:OD1	2:V:98:LYS:HG2	2.10	0.51
1:Z:146:VAL:CG2	1:Z:161:ARG:HD3	2.40	0.51
1:a:303:ARG:NH2	1:a:321:THR:HG21	2.26	0.51
2:b:279:GLN:HG2	2:b:314:HIS:CG	2.45	0.51
2:c:231:ARG:HD2	2:c:285:THR:HG22	1.91	0.51
2:d:176:PHE:HD1	2:d:240:PHE:HB2	1.74	0.51
1:A:186:GLN:HG3	1:A:191:ILE:HB	1.92	0.51
1:A:213:GLU:HB3	1:A:218:LEU:HB3	1.93	0.51
1:A:236:TYR:CE2	1:A:237:LEU:HD13	2.46	0.51
1:A:341:VAL:O	1:A:345:VAL:HG12	2.11	0.51
1:A:431:LEU:C	1:A:432:LYS:HD2	2.35	0.51
2:D:435:TYR:CZ	2:D:449:ILE:HG13	2.46	0.51
2:F:111:ARG:HH11	2:F:111:ARG:CG	2.21	0.51
2:F:175:VAL:O	2:F:239:LEU:HD23	2.10	0.51
4:H:84:ILE:HD12	4:H:84:ILE:H	1.75	0.51
1:I:110:THR:HB	1:I:234:LEU:HD12	1.93	0.51
1:I:295:SER:HA	1:I:348:ILE:HD13	1.92	0.51
1:J:146:VAL:CG2	1:J:161:ARG:HD3	2.40	0.51
2:L:128:THR:N	2:L:129:GLY:HA2	2.24	0.51
2:L:279:GLN:HE22	2:L:294:GLN:HE22	1.59	0.51
2:N:182:ARG:O	2:N:185:GLU:HG3	2.11	0.51
1:S:303:ARG:NH2	1:S:321:THR:HG21	2.26	0.51
1:S:341:VAL:HB	1:S:342:PRO:HD3	1.92	0.51
1:S:472:LEU:HD23	1:S:507:PHE:CD1	2.46	0.51
2:U:140:ALA:HB2	2:U:343:GLN:CD	2.35	0.51
2:U:275:MET:HG2	2:U:310:THR:HG22	1.92	0.51
2:U:297:TYR:C	2:U:297:TYR:HD2	2.18	0.51
3:W:208:GLU:OE2	3:W:209:PRO:HD2	2.09	0.51
4:X:2:MET:C	4:X:3:THR:CG2	2.79	0.51
1:Y:264:SER:HB3	1:Y:330:ILE:HD13	1.91	0.51
1:Y:295:SER:HA	1:Y:348:ILE:HD13	1.92	0.51
1:Y:423:HIS:O	1:Y:427:VAL:HG12	2.11	0.51
1:a:161:ARG:HB3	1:a:323:SER:OG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:296:ARG:HA	2:b:210:ASN:HB3	1.93	0.51
2:b:332:PRO:CG	2:b:402:GLN:H	2.23	0.51
2:c:89:ASN:HD22	2:c:89:ASN:H	1.59	0.51
1:C:161:ARG:HB3	1:C:323:SER:OG	2.11	0.51
1:I:236:TYR:CE2	1:I:237:LEU:HD13	2.46	0.51
2:L:101:ILE:HD13	2:L:101:ILE:N	2.26	0.51
1:R:205:ILE:HD13	1:R:225:VAL:HG23	1.92	0.51
1:S:365:ARG:HG3	5:S:600:ANP:C2	2.40	0.51
2:U:118:GLU:O	2:U:286:LYS:HG2	2.10	0.51
2:U:353:HIS:C	2:U:353:HIS:CD2	2.88	0.51
2:U:392:ARG:HH21	2:U:433:GLY:HA2	1.76	0.51
2:V:173:TYR:CD1	2:V:173:TYR:N	2.79	0.51
2:V:175:VAL:O	2:V:239:LEU:HD23	2.10	0.51
4:X:32:LEU:HD12	4:X:33:GLY:H	1.76	0.51
1:Y:59:ARG:NH2	1:Y:81:ASP:OD2	2.44	0.51
1:a:41:ILE:HB	1:a:71:VAL:HG13	1.93	0.51
2:c:273:GLU:O	2:c:277:VAL:HG23	2.10	0.51
2:c:448:SER:O	2:c:451:GLU:HB3	2.10	0.51
1:A:385:ILE:HG23	1:A:386:MET:N	2.25	0.51
1:C:247:GLU:HG2	1:C:250:ARG:HH12	1.76	0.51
2:D:101:ILE:HD13	2:D:101:ILE:N	2.26	0.51
4:H:32:LEU:HD12	4:H:33:GLY:H	1.76	0.51
1:J:292:TYR:CE1	1:J:296:ARG:HD3	2.46	0.51
1:K:54:SER:HA	1:K:60:TYR:HD1	1.75	0.51
1:K:303:ARG:NH2	1:K:321:THR:HG21	2.26	0.51
1:K:400:TYR:HB2	1:K:424:GLY:HA3	1.93	0.51
1:K:401:ARG:HG2	1:K:401:ARG:HH11	1.75	0.51
2:L:136:MET:HE3	2:L:336:PRO:HB3	1.92	0.51
2:L:278:LEU:HD13	2:L:278:LEU:C	2.35	0.51
2:L:427:PHE:O	2:L:431:MET:HG2	2.11	0.51
2:N:323:ARG:CG	2:N:323:ARG:NH1	2.72	0.51
1:Q:264:SER:HB3	1:Q:330:ILE:HD13	1.91	0.51
1:S:401:ARG:HH12	2:T:324:GLN:HE22	1.59	0.51
2:T:441:GLN:CD	2:T:441:GLN:H	2.18	0.51
2:U:78:PRO:HG2	2:U:88:MET:HE3	1.93	0.51
2:U:348:VAL:HG13	2:U:349:VAL:H	1.76	0.51
2:V:161:GLU:CG	2:V:404:PHE:HB3	2.37	0.51
3:W:66:TYR:CB	3:W:188:LEU:HD21	2.38	0.51
1:Z:34:VAL:HG23	1:Z:39:ILE:HG13	1.93	0.51
1:a:247:GLU:HG2	1:a:250:ARG:HH12	1.76	0.51
1:a:401:ARG:HH11	1:a:401:ARG:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:101:ILE:HD13	2:b:101:ILE:N	2.26	0.51
2:b:183:THR:HA	2:b:208:GLN:HE22	1.76	0.51
2:d:19:GLN:O	2:d:20:ASP:C	2.53	0.51
4:f:55:GLN:O	4:f:56:HIS:HB2	2.11	0.51
1:A:499:LYS:O	1:A:503:ILE:HG13	2.11	0.50
1:B:146:VAL:CG2	1:B:161:ARG:HD3	2.40	0.50
1:B:292:TYR:CE1	1:B:296:ARG:HD3	2.46	0.50
1:C:303:ARG:NH2	1:C:321:THR:HG21	2.26	0.50
1:C:472:LEU:HD23	1:C:507:PHE:CD1	2.46	0.50
2:D:134:ASP:HB3	2:D:420:LEU:HD23	1.92	0.50
2:D:341:SER:C	2:D:343:GLN:H	2.18	0.50
4:H:2:MET:CE	2:U:197:ASN:HA	2.41	0.50
1:I:313:THR:OG1	1:I:316:GLU:HB3	2.10	0.50
1:K:475:VAL:O	1:K:478:ASP:HB3	2.12	0.50
2:M:265:VAL:O	2:M:265:VAL:HG22	2.11	0.50
2:N:76:GLU:O	2:N:76:GLU:HG2	2.11	0.50
2:N:96:ASP:OD1	2:N:98:LYS:HG2	2.10	0.50
2:N:126:LEU:HD23	2:N:126:LEU:H	1.77	0.50
1:Q:295:SER:OG	2:U:209:MET:HB3	2.11	0.50
1:S:95:LEU:HB3	1:S:129:VAL:CG2	2.41	0.50
1:S:262:ASP:HB3	1:S:265:LYS:CG	2.41	0.50
1:S:400:TYR:HB2	1:S:424:GLY:HA3	1.93	0.50
2:T:134:ASP:HB3	2:T:420:LEU:HD23	1.93	0.50
2:V:279:GLN:HG2	2:V:314:HIS:HB3	1.92	0.50
2:V:285:THR:HG22	2:V:286:LYS:N	2.27	0.50
1:Y:305:ASN:O	1:Y:309:VAL:HG23	2.10	0.50
1:Z:384:LYS:HE2	1:Z:384:LYS:N	2.24	0.50
2:b:352:GLU:O	2:b:356:THR:HG23	2.10	0.50
2:c:78:PRO:HG2	2:c:88:MET:HE3	1.93	0.50
2:c:348:VAL:HG13	2:c:349:VAL:H	1.75	0.50
2:c:353:HIS:C	2:c:353:HIS:CD2	2.89	0.50
2:c:432:GLU:O	2:c:432:GLU:HG3	2.11	0.50
2:d:182:ARG:O	2:d:185:GLU:HG3	2.11	0.50
2:d:225:THR:HG22	2:d:281:ARG:HH12	1.75	0.50
1:A:423:HIS:O	1:A:427:VAL:HG12	2.11	0.50
1:A:484:GLN:O	1:A:488:GLN:HG2	2.11	0.50
1:C:166:LEU:HB2	1:C:349:THR:HG21	1.94	0.50
2:D:183:THR:HA	2:D:208:GLN:HE22	1.76	0.50
2:D:278:LEU:HD13	2:D:278:LEU:C	2.37	0.50
2:E:265:VAL:H	3:G:273:THR:CG2	2.16	0.50
2:F:76:GLU:O	2:F:76:GLU:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:197:ASN:O	2:F:197:ASN:CG	2.54	0.50
2:F:417:TYR:C	2:F:417:TYR:HD2	2.18	0.50
3:G:208:GLU:OE2	3:G:209:PRO:HD2	2.09	0.50
1:I:94:ILE:O	1:I:94:ILE:HG12	2.11	0.50
2:M:89:ASN:HD22	2:M:89:ASN:H	1.59	0.50
1:R:341:VAL:HB	1:R:342:PRO:HD3	1.93	0.50
1:S:166:LEU:HB2	1:S:349:THR:HG21	1.93	0.50
2:T:392:ARG:O	2:T:396:ILE:HG23	2.11	0.50
2:U:135:LEU:HD21	2:U:357:ALA:HA	1.93	0.50
2:U:360:VAL:O	2:U:364:LEU:HB2	2.11	0.50
3:W:62:TYR:N	3:W:62:TYR:CD1	2.75	0.50
1:Y:186:GLN:HG3	1:Y:191:ILE:HB	1.92	0.50
1:a:475:VAL:O	1:a:478:ASP:HB3	2.11	0.50
2:b:126:LEU:HD11	2:b:141:LYS:HG2	1.93	0.50
1:A:41:ILE:HD13	1:A:88:VAL:HG21	1.94	0.50
1:C:475:VAL:O	1:C:478:ASP:HB3	2.12	0.50
1:C:492:TYR:O	1:C:493:ASN:CG	2.54	0.50
2:D:379:MET:HE3	2:D:387:LYS:HB2	1.94	0.50
2:E:89:ASN:HD22	2:E:89:ASN:H	1.59	0.50
2:E:401:SER:HB2	2:E:445:MET:HE1	1.93	0.50
2:F:46:LEU:HB3	2:F:50:ILE:HG13	1.92	0.50
1:I:59:ARG:NH2	1:I:81:ASP:OD2	2.44	0.50
1:K:472:LEU:HD23	1:K:507:PHE:CD1	2.46	0.50
2:N:175:VAL:O	2:N:239:LEU:HD23	2.11	0.50
1:Q:284:GLU:HB2	1:Q:286:PHE:HD2	1.76	0.50
1:R:384:LYS:HE2	1:R:384:LYS:N	2.24	0.50
1:Y:164:ARG:HB3	1:Y:326:ALA:HB3	1.92	0.50
1:Y:236:TYR:CE2	1:Y:237:LEU:HD13	2.46	0.50
1:Z:341:VAL:HB	1:Z:342:PRO:HD3	1.93	0.50
2:b:239:LEU:CB	2:b:290:ILE:HD11	2.42	0.50
2:c:25:VAL:O	2:c:42:VAL:HB	2.12	0.50
2:c:86:ARG:HH22	2:c:99:GLY:H	1.60	0.50
2:d:161:GLU:CG	2:d:404:PHE:HB3	2.38	0.50
1:C:401:ARG:HG2	1:C:401:ARG:HH11	1.75	0.50
1:C:401:ARG:HH12	2:D:324:GLN:HE22	1.58	0.50
2:D:126:LEU:HD11	2:D:141:LYS:HG2	1.93	0.50
2:F:125:LEU:HA	2:F:140:ALA:HA	1.93	0.50
1:I:240:TYR:HH	1:I:293:LEU:HD12	1.72	0.50
1:I:284:GLU:HB2	1:I:286:PHE:HD2	1.76	0.50
1:J:104:LEU:CA	1:J:222:ILE:HG22	2.41	0.50
2:L:114:PRO:HD3	2:L:281:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:155:LYS:HA	2:M:158:ASN:HD22	1.77	0.50
1:Q:341:VAL:O	1:Q:345:VAL:HG12	2.11	0.50
1:R:34:VAL:HG23	1:R:39:ILE:HG13	1.93	0.50
1:R:453:ARG:CG	1:R:453:ARG:NH1	2.75	0.50
2:T:217:LEU:HD12	2:T:254:VAL:HG21	1.92	0.50
2:T:356:THR:O	2:T:360:VAL:HG23	2.12	0.50
2:T:438:LEU:N	2:T:438:LEU:HD23	2.26	0.50
2:T:438:LEU:HD23	2:T:438:LEU:H	1.76	0.50
2:U:155:LYS:HA	2:U:158:ASN:HD22	1.77	0.50
1:a:166:LEU:HG	1:a:345:VAL:HG12	1.94	0.50
1:A:107:VAL:HB	1:A:223:VAL:HG13	1.94	0.50
1:A:284:GLU:HB2	1:A:286:PHE:HD2	1.76	0.50
1:B:449:PHE:CE2	1:B:500:LEU:HB2	2.47	0.50
1:C:151:LYS:HG3	1:C:433:GLN:CD	2.37	0.50
1:C:166:LEU:HG	1:C:345:VAL:HG12	1.94	0.50
2:E:25:VAL:O	2:E:42:VAL:HB	2.12	0.50
2:E:130:ILE:HD12	2:E:404:PHE:CZ	2.47	0.50
2:E:379:MET:HB2	2:E:387:LYS:HZ3	1.75	0.50
1:I:341:VAL:O	1:I:345:VAL:HG12	2.11	0.50
1:I:423:HIS:O	1:I:427:VAL:HG12	2.11	0.50
1:J:384:LYS:HE2	1:J:384:LYS:N	2.24	0.50
1:K:41:ILE:HB	1:K:71:VAL:HG13	1.93	0.50
1:K:415:ASP:HA	1:K:418:ARG:HB3	1.94	0.50
2:L:341:SER:C	2:L:343:GLN:H	2.19	0.50
2:L:367:TYR:CE1	2:L:390:VAL:HG23	2.46	0.50
2:M:402:GLN:O	2:M:445:MET:HE1	2.10	0.50
1:Q:110:THR:HB	1:Q:234:LEU:HD12	1.93	0.50
1:R:104:LEU:HA	1:R:222:ILE:HG22	1.94	0.50
1:S:151:LYS:HG3	1:S:433:GLN:CD	2.37	0.50
1:Y:41:ILE:HD13	1:Y:88:VAL:HG21	1.94	0.50
1:Y:94:ILE:O	1:Y:94:ILE:HG12	2.11	0.50
2:b:118:GLU:OE1	2:b:118:GLU:O	2.30	0.50
2:d:76:GLU:O	2:d:76:GLU:HG2	2.11	0.50
2:d:323:ARG:CG	2:d:323:ARG:NH1	2.70	0.50
2:d:345:ASP:OD1	2:d:347:LEU:HG	2.11	0.50
1:A:305:ASN:O	1:A:309:VAL:HG23	2.10	0.50
2:E:353:HIS:C	2:E:353:HIS:CD2	2.88	0.50
2:E:394:ARG:O	2:E:398:ARG:HG3	2.10	0.50
2:F:6:VAL:HG23	2:F:14:ASP:O	2.12	0.50
3:G:31:MET:HE1	3:G:243:MET:HE3	1.93	0.50
3:G:86:LEU:HD22	3:G:246:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:295:SER:OG	2:M:209:MET:HB3	2.12	0.50
1:K:386:MET:O	1:K:390:SER:HB3	2.12	0.50
2:M:200:ASP:OD2	2:M:200:ASP:O	2.30	0.50
3:O:62:TYR:N	3:O:62:TYR:CD1	2.74	0.50
3:O:86:LEU:HD22	3:O:246:MET:HE1	1.94	0.50
1:R:104:LEU:CA	1:R:222:ILE:HG22	2.41	0.50
2:U:145:VAL:HG13	2:U:293:VAL:HA	1.93	0.50
3:W:187:LEU:CD1	3:W:188:LEU:N	2.54	0.50
4:X:38:HIS:CE1	4:X:41:LEU:HD23	2.46	0.50
1:Y:341:VAL:O	1:Y:345:VAL:HG12	2.11	0.50
1:Z:292:TYR:CE1	1:Z:296:ARG:HD3	2.46	0.50
1:a:95:LEU:HB3	1:a:129:VAL:CG2	2.41	0.50
1:a:151:LYS:HG3	1:a:433:GLN:CD	2.37	0.50
1:a:166:LEU:HB2	1:a:349:THR:HG21	1.94	0.50
1:a:262:ASP:HB3	1:a:265:LYS:CG	2.41	0.50
2:c:107:TRP:HB3	2:c:111:ARG:NH2	2.25	0.50
1:A:100:GLY:HA2	1:A:248:TYR:CE2	2.47	0.50
1:A:164:ARG:HB3	1:A:326:ALA:HB3	1.92	0.50
1:A:449:PHE:HB3	1:A:504:LEU:CD1	2.40	0.50
1:B:461:LEU:C	1:B:461:LEU:HD13	2.37	0.50
2:F:159:MET:HE2	2:F:295:ALA:HB2	1.94	0.50
4:H:38:HIS:CE1	4:H:41:LEU:HD23	2.46	0.50
1:I:138:GLU:HG2	1:I:305:ASN:CG	2.37	0.50
1:I:186:GLN:HG3	1:I:191:ILE:HB	1.92	0.50
1:I:439:MET:HG2	1:I:443:GLN:HB3	1.92	0.50
1:K:151:LYS:HG3	1:K:433:GLN:CD	2.37	0.50
1:K:166:LEU:HB2	1:K:349:THR:HG21	1.94	0.50
7:L:600:ADP:O2B	8:L:630:SO4:O3	2.30	0.50
2:M:367:TYR:HE2	2:M:390:VAL:HG13	1.76	0.50
2:M:442:ALA:HA	2:M:455:LYS:HG2	1.93	0.50
2:M:447:GLY:H	2:M:451:GLU:HG2	1.77	0.50
1:R:292:TYR:CE1	1:R:296:ARG:HD3	2.46	0.50
1:S:166:LEU:HG	1:S:345:VAL:HG12	1.94	0.50
1:S:247:GLU:HG2	1:S:250:ARG:HH12	1.76	0.50
1:a:472:LEU:HD23	1:a:507:PHE:CD1	2.46	0.50
2:b:7:GLN:HB2	2:b:14:ASP:OD1	2.12	0.50
2:c:222:THR:O	2:c:226:MET:HG3	2.12	0.50
2:c:285:THR:HG23	2:c:288:GLY:H	1.77	0.50
2:c:297:TYR:C	2:c:297:TYR:HD2	2.20	0.50
2:d:105:GLU:HG2	2:d:106:ARG:H	1.77	0.50
2:d:197:ASN:CG	2:d:197:ASN:O	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:38:HIS:CE1	4:f:41:LEU:HD23	2.46	0.50
1:C:41:ILE:HB	1:C:71:VAL:HG13	1.93	0.50
2:E:222:THR:O	2:E:226:MET:HG3	2.12	0.50
2:F:126:LEU:HD23	2:F:126:LEU:H	1.77	0.50
1:I:484:GLN:O	1:I:488:GLN:HG2	2.11	0.50
1:J:51:GLU:CA	1:J:94:ILE:HG22	2.42	0.50
2:L:231:ARG:HD2	2:L:281:ARG:HH12	1.77	0.50
2:N:6:VAL:HG23	2:N:14:ASP:O	2.12	0.50
3:O:31:MET:HE1	3:O:243:MET:HE3	1.93	0.50
1:Q:299:GLU:OE1	2:U:209:MET:HE2	2.12	0.50
2:U:25:VAL:O	2:U:42:VAL:HB	2.12	0.50
2:V:161:GLU:HG3	2:V:404:PHE:CG	2.46	0.50
2:V:345:ASP:OD1	2:V:347:LEU:HG	2.11	0.50
4:X:55:GLN:O	4:X:56:HIS:HB2	2.11	0.50
1:Y:313:THR:HG21	1:Y:317:VAL:HG22	1.92	0.50
1:Z:104:LEU:HA	1:Z:222:ILE:HG22	1.94	0.50
2:d:161:GLU:HG3	2:d:404:PHE:CG	2.47	0.50
4:f:32:LEU:HD12	4:f:33:GLY:H	1.77	0.50
2:E:142:GLY:HA2	2:E:290:ILE:O	2.11	0.50
4:H:55:GLN:O	4:H:56:HIS:HB2	2.10	0.50
1:J:34:VAL:HG23	1:J:39:ILE:HG13	1.93	0.50
1:J:104:LEU:HA	1:J:222:ILE:HG22	1.94	0.50
2:L:7:GLN:HB2	2:L:14:ASP:OD1	2.12	0.50
2:L:183:THR:HA	2:L:208:GLN:HE22	1.76	0.50
2:L:408:GLU:HG3	2:L:413:SER:O	2.12	0.50
2:M:161:GLU:CG	2:M:404:PHE:HB3	2.39	0.50
4:P:38:HIS:CE1	4:P:41:LEU:HD23	2.46	0.50
1:Q:236:TYR:CE2	1:Q:237:LEU:HD13	2.46	0.50
1:R:449:PHE:CE2	1:R:500:LEU:HB2	2.47	0.50
1:S:386:MET:O	1:S:390:SER:HB3	2.12	0.50
2:T:169:GLU:HG2	2:T:417:TYR:CZ	2.47	0.50
2:T:449:ILE:O	2:T:453:VAL:HG13	2.11	0.50
2:V:182:ARG:O	2:V:185:GLU:HG3	2.11	0.50
3:W:86:LEU:HD22	3:W:246:MET:HE1	1.94	0.50
1:Y:138:GLU:HB3	1:Y:305:ASN:ND2	2.27	0.50
1:Z:449:PHE:CE2	1:Z:500:LEU:HB2	2.47	0.50
1:Z:461:LEU:C	1:Z:461:LEU:HD13	2.37	0.50
2:c:379:MET:HB2	2:c:387:LYS:HZ3	1.73	0.50
2:E:441:GLN:HG3	2:E:441:GLN:O	2.12	0.49
1:I:107:VAL:HB	1:I:223:VAL:HG13	1.94	0.49
1:I:138:GLU:CG	1:I:305:ASN:CG	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:22:VAL:O	2:L:22:VAL:HG13	2.12	0.49
2:L:144:LYS:HD3	2:L:279:GLN:HE21	1.76	0.49
2:M:353:HIS:C	2:M:353:HIS:CD2	2.90	0.49
2:M:392:ARG:O	2:M:396:ILE:HG23	2.12	0.49
4:P:32:LEU:HD12	4:P:33:GLY:H	1.76	0.49
1:Q:100:GLY:HA2	1:Q:248:TYR:CE2	2.47	0.49
1:Q:213:GLU:HB3	1:Q:218:LEU:HB3	1.93	0.49
1:Q:423:HIS:O	1:Q:427:VAL:HG12	2.11	0.49
1:Q:484:GLN:O	1:Q:488:GLN:HG2	2.11	0.49
1:S:41:ILE:HB	1:S:71:VAL:HG13	1.93	0.49
1:S:48:MET:HB3	2:T:61:GLY:HA2	1.94	0.49
2:T:126:LEU:HD11	2:T:141:LYS:HG2	1.93	0.49
2:T:183:THR:HA	2:T:208:GLN:HE22	1.77	0.49
2:T:241:VAL:CG1	2:T:294:GLN:HB3	2.29	0.49
2:U:15:VAL:HG12	2:U:51:VAL:HG12	1.94	0.49
1:Y:484:GLN:O	1:Y:488:GLN:HG2	2.11	0.49
1:a:454:GLY:C	1:a:457:ALA:H	2.20	0.49
2:b:241:VAL:CG1	2:b:294:GLN:HB3	2.34	0.49
2:b:384:GLU:OE2	2:b:387:LYS:HD3	2.12	0.49
2:c:131:LYS:HG3	2:c:418:VAL:CG1	2.41	0.49
2:d:126:LEU:HD23	2:d:126:LEU:H	1.77	0.49
1:C:493:ASN:H	1:C:496:ILE:CG1	2.24	0.49
2:D:237:VAL:HG13	2:D:290:ILE:HD13	1.94	0.49
1:I:100:GLY:HA2	1:I:248:TYR:CE2	2.47	0.49
1:I:172:GLN:HA	5:I:600:ANP:HNB1	1.77	0.49
1:J:449:PHE:CE2	1:J:500:LEU:HB2	2.47	0.49
1:J:461:LEU:C	1:J:461:LEU:HD13	2.37	0.49
2:L:239:LEU:CB	2:L:290:ILE:HD11	2.42	0.49
2:M:222:THR:O	2:M:226:MET:HG3	2.12	0.49
2:M:279:GLN:O	2:M:282:ILE:HG12	2.12	0.49
2:M:297:TYR:HE2	2:M:299:PRO:HA	1.77	0.49
1:Q:107:VAL:HB	1:Q:223:VAL:HG13	1.94	0.49
1:Q:449:PHE:HB3	1:Q:504:LEU:CD1	2.40	0.49
1:S:366:PRO:C	1:S:368:VAL:H	2.21	0.49
1:S:477:ARG:HA	1:S:480:ALA:HB2	1.94	0.49
2:U:86:ARG:HH22	2:U:99:GLY:H	1.60	0.49
2:V:284:SER:HA	2:V:289:SER:HA	1.93	0.49
1:Y:107:VAL:HB	1:Y:223:VAL:HG13	1.94	0.49
1:Y:213:GLU:HB3	1:Y:218:LEU:HB3	1.93	0.49
2:b:36:GLU:HG2	2:b:37:ARG:H	1.77	0.49
2:b:438:LEU:HD23	2:b:438:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:125:LEU:HA	2:d:140:ALA:HA	1.93	0.49
3:e:31:MET:HE1	3:e:243:MET:HE3	1.93	0.49
1:A:94:ILE:O	1:A:94:ILE:HG12	2.10	0.49
1:C:386:MET:O	1:C:390:SER:HB3	2.12	0.49
2:E:244:ILE:HD11	2:E:275:MET:HE1	1.94	0.49
2:F:285:THR:HG22	2:F:286:LYS:N	2.26	0.49
1:J:341:VAL:HB	1:J:342:PRO:HD3	1.93	0.49
2:L:132:VAL:HG23	2:L:400:LEU:HD12	1.94	0.49
2:L:392:ARG:O	2:L:396:ILE:HG23	2.13	0.49
2:M:86:ARG:HH22	2:M:99:GLY:H	1.60	0.49
3:O:203:TRP:CD1	4:P:73:PRO:HG2	2.47	0.49
1:R:158:PRO:CB	1:R:382:GLN:HG2	2.38	0.49
1:R:330:ILE:HD11	1:R:345:VAL:HG21	1.94	0.49
1:R:461:LEU:C	1:R:461:LEU:HD13	2.37	0.49
2:U:356:THR:O	2:U:360:VAL:HG23	2.13	0.49
2:V:125:LEU:HA	2:V:140:ALA:HA	1.93	0.49
3:W:31:MET:HE1	3:W:243:MET:HE3	1.93	0.49
2:c:155:LYS:HA	2:c:158:ASN:HD22	1.77	0.49
2:d:6:VAL:HG23	2:d:14:ASP:O	2.12	0.49
1:A:272:GLN:NE2	2:D:270:THR:HA	2.28	0.49
1:B:104:LEU:CA	1:B:222:ILE:HG22	2.41	0.49
1:B:109:ASN:OD1	1:B:111:LEU:HG	2.13	0.49
1:C:76:MET:CE	1:C:111:LEU:HD11	2.43	0.49
1:C:366:PRO:C	1:C:368:VAL:H	2.20	0.49
2:F:105:GLU:HG2	2:F:106:ARG:H	1.77	0.49
1:J:53:ILE:CG2	1:J:88:VAL:HG13	2.42	0.49
1:J:109:ASN:OD1	1:J:111:LEU:HG	2.13	0.49
1:K:166:LEU:HG	1:K:345:VAL:HG12	1.94	0.49
2:M:25:VAL:O	2:M:42:VAL:HB	2.12	0.49
2:N:125:LEU:HA	2:N:140:ALA:HA	1.93	0.49
1:Q:41:ILE:HD13	1:Q:88:VAL:HG21	1.94	0.49
2:T:404:PHE:O	2:T:408:GLU:OE1	2.31	0.49
2:U:31:VAL:HG12	2:U:32:GLN:N	2.28	0.49
2:U:89:ASN:HD22	2:U:89:ASN:H	1.59	0.49
2:V:126:LEU:HD23	2:V:126:LEU:H	1.76	0.49
1:Y:281:PRO:HG3	3:e:279:ILE:HG21	1.93	0.49
1:Y:284:GLU:HB2	1:Y:286:PHE:HD2	1.76	0.49
1:Z:53:ILE:CG2	1:Z:88:VAL:HG13	2.42	0.49
1:Z:104:LEU:CA	1:Z:222:ILE:HG22	2.42	0.49
2:b:103:GLU:CD	2:b:104:GLU:N	2.71	0.49
1:B:95:LEU:HG	1:B:129:VAL:HG21	1.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:HA	1:B:222:ILE:HG22	1.94	0.49
1:C:472:LEU:HA	1:C:507:PHE:HE1	1.78	0.49
2:D:7:GLN:HB2	2:D:14:ASP:OD1	2.12	0.49
2:D:241:VAL:CG1	2:D:294:GLN:HB3	2.32	0.49
2:D:279:GLN:HG2	2:D:314:HIS:HB3	1.94	0.49
2:D:332:PRO:CG	2:D:402:GLN:H	2.26	0.49
2:E:78:PRO:HG2	2:E:88:MET:HE3	1.93	0.49
2:M:31:VAL:HG12	2:M:32:GLN:N	2.28	0.49
2:N:105:GLU:HG2	2:N:106:ARG:H	1.77	0.49
2:T:103:GLU:CD	2:T:104:GLU:N	2.71	0.49
2:V:105:GLU:HG2	2:V:106:ARG:H	1.77	0.49
1:Z:394:ARG:HG3	1:Z:394:ARG:HH11	1.78	0.49
2:b:132:VAL:CG2	2:b:400:LEU:HD12	2.43	0.49
2:b:215:ASN:O	2:b:219:VAL:HG23	2.12	0.49
2:b:331:TYR:C	2:b:333:ALA:N	2.71	0.49
2:b:332:PRO:HG2	2:b:402:GLN:N	2.27	0.49
2:c:15:VAL:HG12	2:c:51:VAL:HG12	1.95	0.49
3:e:66:TYR:HB3	3:e:188:LEU:CD1	2.40	0.49
2:E:132:VAL:HG11	2:E:334:VAL:HB	1.94	0.49
2:F:322:SER:OG	2:F:325:ILE:HG13	2.13	0.49
3:G:208:GLU:CD	4:H:43:THR:HA	2.38	0.49
1:J:49:GLN:HE22	2:N:10:GLY:H	1.60	0.49
1:K:440:SER:C	1:K:442:ALA:N	2.65	0.49
1:K:461:LEU:N	1:K:461:LEU:CD2	2.65	0.49
2:M:78:PRO:HG2	2:M:88:MET:HE3	1.93	0.49
1:S:415:ASP:HA	1:S:418:ARG:HB3	1.94	0.49
1:S:496:ILE:CD1	1:S:496:ILE:H	2.25	0.49
2:T:7:GLN:HB2	2:T:14:ASP:OD1	2.12	0.49
1:a:415:ASP:HA	1:a:418:ARG:HB3	1.94	0.49
2:b:132:VAL:HG23	2:b:400:LEU:HD12	1.94	0.49
2:c:31:VAL:HG12	2:c:32:GLN:N	2.28	0.49
2:D:103:GLU:CD	2:D:104:GLU:N	2.71	0.49
2:E:332:PRO:C	2:E:334:VAL:H	2.20	0.49
1:I:41:ILE:HD13	1:I:88:VAL:HG21	1.94	0.49
1:K:247:GLU:HG2	1:K:250:ARG:HH12	1.76	0.49
2:L:103:GLU:CD	2:L:104:GLU:N	2.71	0.49
2:M:278:LEU:HD13	2:M:278:LEU:C	2.38	0.49
2:T:215:ASN:O	2:T:219:VAL:HG23	2.12	0.49
2:T:384:GLU:OE2	2:T:387:LYS:HD3	2.12	0.49
2:U:222:THR:O	2:U:226:MET:HG3	2.12	0.49
2:U:442:ALA:HA	2:U:455:LYS:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5:ILE:HG22	2:b:64:ARG:HA	1.95	0.49
2:b:173:TYR:HD1	2:b:201:LYS:HD2	1.78	0.49
1:A:284:GLU:HB2	1:A:286:PHE:CD2	2.48	0.49
1:B:34:VAL:HG23	1:B:39:ILE:HG13	1.93	0.49
2:E:322:SER:HB3	2:E:325:ILE:HB	1.94	0.49
1:J:330:ILE:HD11	1:J:345:VAL:HG21	1.94	0.49
1:K:365:ARG:HG3	5:K:600:ANP:C2	2.43	0.49
1:K:472:LEU:HA	1:K:507:PHE:HE1	1.78	0.49
2:L:126:LEU:HD11	2:L:141:LYS:HG2	1.93	0.49
2:L:215:ASN:O	2:L:219:VAL:HG23	2.12	0.49
2:N:141:LYS:HA	2:N:291:THR:HG23	1.93	0.49
1:R:52:MET:HE3	1:R:95:LEU:HA	1.95	0.49
2:T:5:ILE:HG22	2:T:64:ARG:HA	1.95	0.49
2:T:323:ARG:CD	2:T:323:ARG:N	2.75	0.49
2:T:416:LYS:HD2	2:T:451:GLU:OE2	2.13	0.49
2:U:302:ASP:C	2:U:304:THR:H	2.21	0.49
2:V:6:VAL:HG23	2:V:14:ASP:O	2.12	0.49
3:W:224:GLU:OE2	4:X:85:ARG:NH2	2.46	0.49
1:Y:100:GLY:HA2	1:Y:248:TYR:CE2	2.47	0.49
2:d:285:THR:HG22	2:d:286:LYS:N	2.27	0.49
2:d:353:HIS:HA	2:d:424:ILE:HD12	1.94	0.49
1:C:109:ASN:HB2	1:C:113:ALA:O	2.12	0.49
1:C:453:ARG:HG2	1:C:454:GLY:N	2.28	0.49
1:C:477:ARG:HA	1:C:480:ALA:HB2	1.94	0.49
2:D:323:ARG:CD	2:D:323:ARG:N	2.73	0.49
2:D:367:TYR:CE1	2:D:390:VAL:HG23	2.47	0.49
1:I:385:ILE:HG13	1:I:492:TYR:HB2	1.95	0.49
1:S:472:LEU:HA	1:S:507:PHE:HE1	1.78	0.49
2:T:36:GLU:HG2	2:T:37:ARG:H	1.77	0.49
2:T:430:ILE:O	2:T:430:ILE:HG12	2.13	0.49
2:U:432:GLU:HG3	2:U:432:GLU:O	2.12	0.49
2:V:360:VAL:O	2:V:364:LEU:HB2	2.13	0.49
3:W:48:MET:HE3	4:X:79:LEU:HD12	1.95	0.49
1:Z:327:LEU:HD23	1:Z:327:LEU:N	2.28	0.49
2:D:137:CYS:SG	2:D:319:VAL:HG22	2.53	0.49
2:D:215:ASN:O	2:D:219:VAL:HG23	2.12	0.49
2:E:86:ARG:HH22	2:E:99:GLY:H	1.60	0.49
1:K:109:ASN:HB2	1:K:113:ALA:O	2.12	0.49
2:L:36:GLU:HG2	2:L:37:ARG:H	1.77	0.49
2:M:297:TYR:C	2:M:297:TYR:HD2	2.20	0.49
2:M:348:VAL:HG13	2:M:349:VAL:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:78:PRO:HB3	2:N:103:GLU:HB3	1.95	0.49
1:R:109:ASN:OD1	1:R:111:LEU:HG	2.13	0.49
1:R:365:ARG:O	1:R:367:ALA:N	2.46	0.49
1:R:402:GLU:CG	1:R:403:LEU:HD23	2.41	0.49
2:U:174:SER:O	2:U:202:VAL:HA	2.13	0.49
2:U:448:SER:O	2:U:451:GLU:HB3	2.13	0.49
1:Y:284:GLU:C	1:Y:286:PHE:H	2.21	0.49
1:Z:34:VAL:HG12	2:c:45:GLN:CB	2.42	0.49
1:Z:51:GLU:CA	1:Z:94:ILE:HG22	2.42	0.49
1:Z:109:ASN:OD1	1:Z:111:LEU:HG	2.13	0.49
1:Z:198:ILE:HD13	1:Z:239:PRO:HG3	1.95	0.49
1:Z:330:ILE:HD11	1:Z:345:VAL:HG21	1.94	0.49
1:Z:365:ARG:O	1:Z:367:ALA:N	2.46	0.49
1:a:366:PRO:C	1:a:368:VAL:H	2.20	0.49
1:B:53:ILE:CG2	1:B:88:VAL:HG13	2.42	0.48
1:B:198:ILE:HD13	1:B:239:PRO:HG3	1.95	0.48
2:D:438:LEU:HD23	2:D:438:LEU:H	1.76	0.48
2:E:31:VAL:HG12	2:E:32:GLN:N	2.28	0.48
2:E:380:ASP:HB2	2:U:437:HIS:HA	1.95	0.48
2:F:25:VAL:HG13	2:F:26:TYR:H	1.78	0.48
2:F:307:SER:HB2	2:F:308:PRO:CD	2.37	0.48
3:G:48:MET:HE3	4:H:79:LEU:CD1	2.43	0.48
1:I:236:TYR:CZ	1:I:237:LEU:HD13	2.48	0.48
1:J:52:MET:HE1	1:J:95:LEU:HD13	1.95	0.48
1:K:68:ARG:N	2:L:7:GLN:HG2	2.28	0.48
2:N:324:GLN:O	2:N:328:LEU:HD23	2.12	0.48
1:Q:236:TYR:CZ	1:Q:237:LEU:HD13	2.48	0.48
1:R:216:GLY:HA2	1:R:217:ALA:HA	1.46	0.48
1:R:394:ARG:HG3	1:R:394:ARG:HH11	1.78	0.48
1:S:34:VAL:HG13	2:V:45:GLN:HB2	1.96	0.48
2:T:137:CYS:SG	2:T:319:VAL:HG22	2.53	0.48
2:T:332:PRO:HG2	2:T:402:GLN:H	1.77	0.48
1:Y:385:ILE:HG13	1:Y:492:TYR:HB2	1.95	0.48
1:Z:461:LEU:HD13	1:Z:463:LYS:N	2.28	0.48
1:a:93:ARG:HA	1:a:93:ARG:HD2	1.61	0.48
1:a:386:MET:O	1:a:390:SER:HB3	2.12	0.48
2:d:118:GLU:O	2:d:118:GLU:HG2	2.13	0.48
1:B:365:ARG:O	1:B:367:ALA:N	2.46	0.48
2:D:227:ALA:HB1	2:D:290:ILE:HD13	1.94	0.48
2:E:155:LYS:HA	2:E:158:ASN:HD22	1.77	0.48
2:E:336:PRO:HG3	2:E:400:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:137:ILE:O	1:I:138:GLU:OE1	2.31	0.48
1:I:284:GLU:HB2	1:I:286:PHE:CD2	2.48	0.48
1:J:44:LEU:HD22	1:J:90:CYS:HB3	1.96	0.48
1:J:299:GLU:HG2	2:N:209:MET:HE3	1.95	0.48
1:K:68:ARG:H	2:L:7:GLN:HG2	1.78	0.48
2:L:173:TYR:HD1	2:L:201:LYS:HD2	1.78	0.48
2:M:119:LEU:HA	2:M:285:THR:HA	1.95	0.48
2:N:82:ALA:HB1	2:N:102:GLY:HA2	1.96	0.48
1:S:109:ASN:HB2	1:S:113:ALA:O	2.12	0.48
1:S:475:VAL:O	1:S:478:ASP:HB3	2.11	0.48
2:T:265:VAL:O	2:T:265:VAL:HG12	2.14	0.48
1:Z:104:LEU:HD13	1:Z:104:LEU:H	1.78	0.48
2:b:118:GLU:N	2:b:118:GLU:CD	2.72	0.48
2:b:413:SER:OG	2:b:414:PRO:HD2	2.13	0.48
2:c:140:ALA:HB2	2:c:343:GLN:HG2	1.95	0.48
1:B:330:ILE:HD11	1:B:345:VAL:HG21	1.94	0.48
1:C:454:GLY:C	1:C:457:ALA:H	2.20	0.48
2:D:307:SER:HB3	2:D:308:PRO:HD3	1.94	0.48
2:D:404:PHE:O	2:D:408:GLU:OE1	2.31	0.48
2:E:174:SER:O	2:E:202:VAL:HA	2.13	0.48
2:F:199:ILE:HA	2:F:202:VAL:HG12	1.96	0.48
2:F:332:PRO:O	2:F:334:VAL:N	2.36	0.48
2:F:453:VAL:HG12	2:F:454:GLU:N	2.29	0.48
1:I:62:ILE:O	1:I:73:ALA:HA	2.14	0.48
1:K:366:PRO:C	1:K:368:VAL:H	2.21	0.48
1:K:477:ARG:HA	1:K:480:ALA:HB2	1.94	0.48
1:Q:139:ARG:HB2	1:Q:303:ARG:O	2.14	0.48
1:Q:385:ILE:HG13	1:Q:492:TYR:HB2	1.95	0.48
1:R:44:LEU:HD22	1:R:90:CYS:HB3	1.96	0.48
1:R:388:LYS:HG2	1:R:492:TYR:CE1	2.48	0.48
3:W:9:LYS:NZ	4:X:128:LEU:HD22	2.28	0.48
1:Y:62:ILE:O	1:Y:73:ALA:HA	2.13	0.48
1:Y:139:ARG:HB2	1:Y:303:ARG:O	2.13	0.48
1:Y:151:LYS:HE2	1:Y:439:MET:SD	2.53	0.48
1:Y:213:GLU:CA	1:Y:218:LEU:HB3	2.44	0.48
1:Z:453:ARG:CG	1:Z:453:ARG:NH1	2.75	0.48
1:a:109:ASN:HB2	1:a:113:ALA:O	2.12	0.48
2:b:113:ALA:HA	2:b:281:ARG:CG	2.39	0.48
2:b:278:LEU:HD13	2:b:278:LEU:C	2.38	0.48
2:c:3:GLY:HA3	2:c:17:PHE:HE2	1.76	0.48
1:A:213:GLU:CA	1:A:218:LEU:HB3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ARG:HG3	1:B:394:ARG:HH11	1.78	0.48
1:C:296:ARG:HA	2:D:210:ASN:HB3	1.94	0.48
2:E:231:ARG:HD2	2:E:285:THR:HG22	1.93	0.48
2:E:396:ILE:C	2:E:396:ILE:HD12	2.39	0.48
2:F:323:ARG:CG	2:F:323:ARG:NH1	2.66	0.48
1:I:121:LEU:HD23	1:I:123:HIS:HB3	1.96	0.48
1:J:97:VAL:HG12	1:J:98:PRO:CG	2.43	0.48
2:L:408:GLU:OE2	2:L:413:SER:O	2.31	0.48
2:M:145:VAL:HG13	2:M:293:VAL:HA	1.96	0.48
2:M:174:SER:O	2:M:202:VAL:HA	2.13	0.48
1:R:53:ILE:CG2	1:R:88:VAL:HG13	2.42	0.48
2:T:279:GLN:HE22	2:T:294:GLN:HE22	1.61	0.48
2:T:377:LEU:HD21	4:X:115:ALA:CB	2.36	0.48
3:W:173:LYS:HE3	3:W:233:GLU:OE2	2.14	0.48
1:Y:236:TYR:CZ	1:Y:237:LEU:HD13	2.49	0.48
1:Z:138:GLU:OE2	1:Z:304:VAL:HG12	2.14	0.48
1:a:80:ALA:HA	2:d:25:VAL:CG1	2.40	0.48
2:d:78:PRO:HB3	2:d:103:GLU:HB3	1.95	0.48
1:B:44:LEU:HD22	1:B:90:CYS:HB3	1.96	0.48
1:B:388:LYS:HG2	1:B:492:TYR:CE1	2.48	0.48
1:B:453:ARG:CG	1:B:453:ARG:NH1	2.75	0.48
2:D:332:PRO:HG2	2:D:402:GLN:H	1.79	0.48
2:D:374:ILE:HD11	2:D:382:LEU:HD21	1.95	0.48
2:D:384:GLU:OE2	2:D:387:LYS:HD3	2.13	0.48
1:K:76:MET:CE	1:K:111:LEU:HD11	2.43	0.48
1:K:454:GLY:C	1:K:457:ALA:H	2.21	0.48
2:N:199:ILE:HA	2:N:202:VAL:HG12	1.96	0.48
2:N:330:ILE:HD12	2:N:330:ILE:N	2.29	0.48
1:R:461:LEU:HD13	1:R:463:LYS:H	1.79	0.48
1:R:461:LEU:HD13	1:R:463:LYS:N	2.28	0.48
1:S:107:VAL:HG11	2:V:116:TYR:CE1	2.36	0.48
1:S:454:GLY:C	1:S:457:ALA:H	2.20	0.48
2:T:132:VAL:HG23	2:T:400:LEU:HD12	1.96	0.48
2:V:82:ALA:HB1	2:V:102:GLY:HA2	1.96	0.48
1:Y:295:SER:OG	2:c:209:MET:HB3	2.13	0.48
1:a:76:MET:CE	1:a:111:LEU:HD11	2.43	0.48
1:a:472:LEU:HA	1:a:507:PHE:HE1	1.78	0.48
1:a:477:ARG:HA	1:a:480:ALA:HB2	1.94	0.48
2:c:349:VAL:HG21	2:c:353:HIS:CG	2.49	0.48
2:d:330:ILE:HD12	2:d:330:ILE:N	2.28	0.48
1:B:386:MET:SD	1:B:444:GLN:HG3	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:496:ILE:HD13	1:C:496:ILE:H	1.79	0.48
2:D:5:ILE:HG22	2:D:64:ARG:HA	1.95	0.48
1:I:151:LYS:HE2	1:I:439:MET:SD	2.53	0.48
1:J:104:LEU:HD13	1:J:104:LEU:H	1.78	0.48
1:J:365:ARG:O	1:J:367:ALA:N	2.46	0.48
1:J:394:ARG:HG3	1:J:394:ARG:HH11	1.78	0.48
1:K:261:ASP:O	1:K:262:ASP:HB2	2.14	0.48
1:K:474:TYR:C	1:K:474:TYR:CD1	2.92	0.48
2:M:197:ASN:HB3	4:f:2:MET:SD	2.54	0.48
2:T:132:VAL:CG2	2:T:400:LEU:HD12	2.43	0.48
2:U:40:LEU:HD23	2:U:55:ALA:HA	1.96	0.48
1:Y:284:GLU:HB2	1:Y:286:PHE:CD2	2.48	0.48
2:b:307:SER:HB3	2:b:308:PRO:HD3	1.95	0.48
2:c:392:ARG:NH2	2:c:433:GLY:HA2	2.29	0.48
2:d:82:ALA:HB1	2:d:102:GLY:HA2	1.96	0.48
1:B:402:GLU:CG	1:B:403:LEU:HD23	2.41	0.48
1:J:94:ILE:O	1:J:95:LEU:C	2.57	0.48
1:J:138:GLU:OE2	1:J:304:VAL:HG12	2.14	0.48
1:K:218:LEU:C	1:K:220:ASN:H	2.21	0.48
2:L:5:ILE:HG22	2:L:64:ARG:HA	1.95	0.48
2:M:15:VAL:HG12	2:M:51:VAL:HG12	1.94	0.48
2:M:347:LEU:HG	2:M:347:LEU:O	2.12	0.48
2:M:400:LEU:HB3	2:M:427:PHE:CZ	2.49	0.48
1:Q:136:VAL:O	1:Q:137:ILE:HB	2.14	0.48
1:Q:213:GLU:CA	1:Q:218:LEU:HB3	2.44	0.48
1:R:327:LEU:HD23	1:R:327:LEU:N	2.28	0.48
1:R:403:LEU:HD21	1:R:420:GLN:NE2	2.27	0.48
1:S:76:MET:CE	1:S:111:LEU:HD11	2.43	0.48
1:S:453:ARG:HG2	1:S:454:GLY:N	2.28	0.48
2:T:237:VAL:HG13	2:T:290:ILE:HD13	1.95	0.48
2:c:312:PHE:HD1	2:c:315:LEU:HD12	1.79	0.48
2:d:199:ILE:HA	2:d:202:VAL:HG12	1.96	0.48
1:A:121:LEU:HD23	1:A:123:HIS:HB3	1.96	0.48
1:A:176:THR:O	1:A:179:ALA:HB3	2.14	0.48
1:A:205:ILE:HD13	1:A:225:VAL:HG13	1.96	0.48
1:A:236:TYR:CZ	1:A:237:LEU:HD13	2.48	0.48
1:C:218:LEU:C	1:C:220:ASN:H	2.21	0.48
1:C:261:ASP:O	1:C:262:ASP:HB2	2.13	0.48
1:C:467:PHE:CZ	1:C:511:GLN:CD	2.90	0.48
2:D:3:GLY:HA3	2:D:17:PHE:CD2	2.49	0.48
2:D:36:GLU:HG2	2:D:37:ARG:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:155:LYS:HB2	8:F:530:SO4:O3	2.14	0.48
1:I:102:GLY:HA3	1:I:122:ASP:O	2.14	0.48
1:I:213:GLU:CA	1:I:218:LEU:HB3	2.44	0.48
1:J:490:GLY:O	1:J:492:TYR:N	2.47	0.48
1:K:459:VAL:O	1:K:459:VAL:CG1	2.57	0.48
2:M:179:VAL:H	2:M:242:ASP:HB3	1.78	0.48
2:T:173:TYR:HD1	2:T:201:LYS:HD2	1.78	0.48
1:Y:262:ASP:H	1:Y:329:ILE:HB	1.79	0.48
1:Z:36:ASP:OD2	2:c:260:ARG:HD3	2.13	0.48
1:a:34:VAL:HG13	2:d:45:GLN:HB2	1.95	0.48
1:a:467:PHE:CZ	1:a:511:GLN:CD	2.90	0.48
1:a:496:ILE:HD13	1:a:496:ILE:H	1.79	0.48
2:c:238:LEU:HD23	2:c:240:PHE:CE1	2.49	0.48
1:B:461:LEU:HD13	1:B:463:LYS:N	2.28	0.48
2:E:15:VAL:HG12	2:E:51:VAL:HG12	1.94	0.48
2:E:40:LEU:HD23	2:E:55:ALA:HA	1.96	0.48
2:E:392:ARG:NH2	2:E:433:GLY:HA2	2.29	0.48
2:F:284:SER:HA	2:F:289:SER:HA	1.94	0.48
1:J:394:ARG:HG3	1:J:394:ARG:NH1	2.29	0.48
2:L:18:PRO:O	2:L:19:GLN:C	2.54	0.48
3:O:173:LYS:HE3	3:O:233:GLU:OE2	2.14	0.48
1:Q:102:GLY:HA3	1:Q:122:ASP:O	2.14	0.48
1:Q:151:LYS:HE2	1:Q:439:MET:SD	2.53	0.48
1:S:205:ILE:O	1:S:209:VAL:HG12	2.14	0.48
1:S:218:LEU:C	1:S:220:ASN:H	2.21	0.48
2:V:199:ILE:HA	2:V:202:VAL:HG12	1.96	0.48
1:Y:64:LEU:HD12	1:Y:277:LEU:HD21	1.96	0.48
1:Y:205:ILE:HD13	1:Y:225:VAL:HG13	1.96	0.48
1:Z:402:GLU:CG	1:Z:403:LEU:HD23	2.41	0.48
1:Z:472:LEU:HD12	1:Z:472:LEU:O	2.14	0.48
1:a:150:TYR:HA	1:a:433:GLN:NE2	2.28	0.48
1:C:195:TYR:HD1	1:C:259:ILE:HD11	1.79	0.48
1:C:415:ASP:HA	1:C:418:ARG:HB3	1.94	0.48
2:E:94:PRO:HG3	2:E:101:ILE:CG2	2.44	0.48
3:G:14:GLN:HG2	3:G:257:ILE:HD13	1.96	0.48
1:I:205:ILE:HD13	1:I:225:VAL:HG13	1.96	0.48
1:J:145:PRO:HB3	1:J:381:ALA:O	2.14	0.48
1:J:368:VAL:O	1:J:370:PRO:HD3	2.14	0.48
1:J:388:LYS:HG2	1:J:492:TYR:CE1	2.48	0.48
1:J:472:LEU:HD12	1:J:472:LEU:O	2.14	0.48
2:L:398:ARG:HB2	2:L:444:TYR:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:238:LEU:HD23	2:M:240:PHE:CE1	2.49	0.48
2:V:74:PRO:O	2:V:75:ILE:HG12	2.14	0.48
2:V:458:LYS:O	2:V:459:LEU:HB2	2.14	0.48
3:W:180:GLN:HG2	3:W:237:SER:HB3	1.95	0.48
1:a:453:ARG:HG2	1:a:454:GLY:N	2.28	0.48
2:b:356:THR:O	2:b:360:VAL:HG23	2.14	0.48
2:d:74:PRO:O	2:d:75:ILE:HG12	2.14	0.48
1:A:64:LEU:HD12	1:A:277:LEU:HD21	1.96	0.47
1:B:472:LEU:HD12	1:B:472:LEU:O	2.14	0.47
2:F:279:GLN:HG2	2:F:314:HIS:CB	2.43	0.47
3:G:173:LYS:HE3	3:G:233:GLU:OE2	2.14	0.47
1:J:461:LEU:HD13	1:J:463:LYS:N	2.28	0.47
1:K:496:ILE:HD13	1:K:496:ILE:H	1.79	0.47
2:M:94:PRO:HG3	2:M:101:ILE:CG2	2.44	0.47
1:Q:284:GLU:HB2	1:Q:286:PHE:CD2	2.48	0.47
1:Q:358:ASN:HA	1:Q:361:ASN:HD21	1.79	0.47
1:R:145:PRO:HB3	1:R:381:ALA:O	2.14	0.47
2:U:349:VAL:HG21	2:U:353:HIS:CG	2.49	0.47
2:V:25:VAL:CG1	2:V:26:TYR:N	2.77	0.47
2:V:276:GLY:O	2:V:280:GLU:HB2	2.13	0.47
1:a:218:LEU:C	1:a:220:ASN:H	2.21	0.47
1:a:454:GLY:C	1:a:456:LEU:N	2.70	0.47
2:b:144:LYS:CD	2:b:279:GLN:HE21	2.25	0.47
2:b:305:ASP:O	2:b:308:PRO:HD2	2.14	0.47
2:c:94:PRO:HG3	2:c:101:ILE:CG2	2.44	0.47
3:e:86:LEU:HD22	3:e:246:MET:HE1	1.94	0.47
1:A:102:GLY:HA3	1:A:122:ASP:O	2.14	0.47
1:B:490:GLY:O	1:B:492:TYR:N	2.47	0.47
2:D:17:PHE:CE1	2:D:23:PRO:HD3	2.48	0.47
2:D:173:TYR:HD1	2:D:201:LYS:HD2	1.78	0.47
3:G:180:GLN:HG2	3:G:237:SER:HB3	1.95	0.47
1:I:178:LEU:HD12	1:I:179:ALA:CA	2.43	0.47
1:J:327:LEU:HD23	1:J:327:LEU:N	2.28	0.47
2:M:402:GLN:H	2:M:445:MET:CE	2.14	0.47
2:N:284:SER:HA	2:N:289:SER:HA	1.96	0.47
1:R:472:LEU:HD12	1:R:472:LEU:O	2.14	0.47
1:S:56:PRO:HG2	1:S:86:MET:HB3	1.95	0.47
2:U:179:VAL:H	2:U:242:ASP:HB3	1.78	0.47
2:U:183:THR:HA	2:U:208:GLN:HG2	1.96	0.47
2:U:231:ARG:HD3	2:U:290:ILE:CG1	2.41	0.47
1:Y:385:ILE:HG23	1:Y:386:MET:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:261:ASP:O	1:a:262:ASP:HB2	2.13	0.47
1:a:440:SER:C	1:a:442:ALA:N	2.65	0.47
1:a:474:TYR:C	1:a:474:TYR:CD1	2.92	0.47
2:c:174:SER:O	2:c:202:VAL:HA	2.13	0.47
2:d:284:SER:HA	2:d:289:SER:HA	1.95	0.47
1:A:139:ARG:HA	1:A:305:ASN:H	1.79	0.47
1:A:151:LYS:HE2	1:A:439:MET:SD	2.53	0.47
1:A:385:ILE:HG13	1:A:492:TYR:HB2	1.95	0.47
1:B:327:LEU:HD23	1:B:327:LEU:N	2.28	0.47
1:B:368:VAL:O	1:B:370:PRO:HD3	2.14	0.47
2:D:332:PRO:HG2	2:D:402:GLN:N	2.29	0.47
2:E:131:LYS:HG3	2:E:418:VAL:CG1	2.43	0.47
2:E:179:VAL:H	2:E:242:ASP:HB3	1.78	0.47
2:E:448:SER:O	2:E:451:GLU:HB3	2.13	0.47
2:F:74:PRO:O	2:F:75:ILE:HG12	2.14	0.47
1:J:386:MET:SD	1:J:444:GLN:HG3	2.54	0.47
1:J:453:ARG:CG	1:J:453:ARG:NH1	2.75	0.47
1:J:456:LEU:HD12	1:J:457:ALA:N	2.30	0.47
1:J:461:LEU:O	1:J:465:GLY:N	2.48	0.47
1:K:39:ILE:HD11	1:K:82:LEU:CD1	2.44	0.47
1:K:56:PRO:HG2	1:K:86:MET:HB3	1.95	0.47
1:K:259:ILE:HG13	1:K:259:ILE:O	2.15	0.47
3:O:201:LYS:HD3	3:O:202:SER:N	2.18	0.47
1:Q:262:ASP:H	1:Q:329:ILE:HB	1.79	0.47
1:R:386:MET:SD	1:R:444:GLN:HG3	2.54	0.47
1:S:95:LEU:HB3	1:S:129:VAL:HG22	1.97	0.47
1:S:150:TYR:HA	1:S:433:GLN:NE2	2.28	0.47
1:S:493:ASN:O	1:S:495:GLU:N	2.46	0.47
2:U:348:VAL:HG13	2:U:349:VAL:N	2.29	0.47
3:W:16:THR:HG22	4:X:124:ALA:CB	2.44	0.47
1:Y:137:ILE:HA	1:Y:138:GLU:HA	1.47	0.47
1:Z:313:THR:O	1:Z:314:LYS:HB2	2.14	0.47
1:Z:386:MET:SD	1:Z:444:GLN:HG3	2.54	0.47
1:Z:456:LEU:HD12	1:Z:457:ALA:N	2.30	0.47
1:a:103:LEU:C	1:a:222:ILE:HG22	2.38	0.47
2:d:417:TYR:C	2:d:417:TYR:HD2	2.19	0.47
1:A:139:ARG:HB2	1:A:303:ARG:O	2.14	0.47
1:A:218:LEU:HD13	1:A:218:LEU:C	2.40	0.47
1:B:138:GLU:OE2	1:B:304:VAL:HG12	2.14	0.47
1:B:216:GLY:HA2	1:B:217:ALA:HA	1.46	0.47
1:B:419:LYS:HD2	1:B:419:LYS:C	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:78:PRO:HB3	2:F:103:GLU:HB3	1.95	0.47
1:J:313:THR:O	1:J:314:LYS:HB2	2.14	0.47
1:K:453:ARG:HG2	1:K:454:GLY:N	2.28	0.47
2:M:348:VAL:HG13	2:M:349:VAL:N	2.29	0.47
2:N:319:VAL:HA	2:N:339:SER:OG	2.14	0.47
3:O:66:TYR:CD2	3:O:188:LEU:HD11	2.49	0.47
1:Q:64:LEU:HD12	1:Q:277:LEU:HD21	1.96	0.47
1:Q:121:LEU:HD23	1:Q:123:HIS:HB3	1.96	0.47
1:R:461:LEU:O	1:R:465:GLY:N	2.48	0.47
1:Y:102:GLY:HA3	1:Y:122:ASP:O	2.13	0.47
1:Z:394:ARG:HG3	1:Z:394:ARG:NH1	2.29	0.47
2:b:24:ARG:O	2:b:27:ASP:HB2	2.15	0.47
2:c:179:VAL:H	2:c:242:ASP:HB3	1.78	0.47
2:d:25:VAL:CG1	2:d:26:TYR:N	2.77	0.47
3:e:180:GLN:HG2	3:e:237:SER:HB3	1.95	0.47
1:B:399:GLN:O	1:B:402:GLU:HG2	2.15	0.47
1:C:107:VAL:HG22	1:C:223:VAL:CG1	2.45	0.47
2:D:17:PHE:HD1	2:D:22:VAL:HG23	1.79	0.47
2:D:24:ARG:O	2:D:27:ASP:HB2	2.15	0.47
1:J:374:VAL:HG12	1:J:375:SER:N	2.30	0.47
1:K:103:LEU:C	1:K:222:ILE:HG22	2.39	0.47
1:K:107:VAL:HG22	1:K:223:VAL:CG1	2.45	0.47
1:K:205:ILE:O	1:K:209:VAL:HG12	2.14	0.47
2:N:166:ILE:HD12	2:N:167:ALA:N	2.30	0.47
1:S:132:ILE:H	1:S:132:ILE:CD1	2.21	0.47
2:T:24:ARG:O	2:T:27:ASP:HB2	2.15	0.47
2:U:55:ALA:C	2:U:57:GLY:H	2.23	0.47
2:U:204:LEU:HD23	2:U:204:LEU:N	2.29	0.47
2:U:238:LEU:HD23	2:U:240:PHE:CE1	2.49	0.47
2:U:395:LYS:HG3	2:U:443:PHE:CD2	2.49	0.47
1:Z:368:VAL:O	1:Z:370:PRO:HD3	2.14	0.47
1:Z:388:LYS:HG2	1:Z:492:TYR:CE1	2.48	0.47
1:a:107:VAL:HG22	1:a:223:VAL:CG1	2.45	0.47
2:c:231:ARG:HD3	2:c:290:ILE:CG1	2.44	0.47
3:e:173:LYS:HE3	3:e:233:GLU:OE2	2.14	0.47
1:A:62:ILE:O	1:A:73:ALA:HA	2.14	0.47
1:B:104:LEU:HD13	1:B:104:LEU:H	1.78	0.47
1:B:145:PRO:HB3	1:B:381:ALA:O	2.14	0.47
1:B:374:VAL:HG12	1:B:375:SER:N	2.30	0.47
1:C:205:ILE:O	1:C:209:VAL:HG12	2.14	0.47
2:E:297:TYR:HE2	2:E:299:PRO:HA	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:349:VAL:CG2	2:E:353:HIS:CG	2.84	0.47
3:G:48:MET:HE3	4:H:79:LEU:HD12	1.96	0.47
1:I:262:ASP:H	1:I:329:ILE:HB	1.79	0.47
1:J:403:LEU:HD21	1:J:420:GLN:NE2	2.27	0.47
1:K:467:PHE:CZ	1:K:511:GLN:CD	2.90	0.47
2:M:429:GLY:O	2:M:434:GLU:HB3	2.14	0.47
1:R:442:ALA:C	1:R:444:GLN:H	2.22	0.47
1:R:490:GLY:O	1:R:492:TYR:N	2.47	0.47
1:S:93:ARG:HD2	1:S:93:ARG:HA	1.61	0.47
1:S:103:LEU:C	1:S:222:ILE:HG22	2.39	0.47
1:S:259:ILE:HG13	1:S:259:ILE:O	2.15	0.47
2:V:111:ARG:HG3	2:V:111:ARG:NH1	2.22	0.47
1:Y:218:LEU:HD13	1:Y:218:LEU:C	2.40	0.47
1:Z:44:LEU:HD22	1:Z:90:CYS:HB3	1.96	0.47
1:Z:95:LEU:CD1	1:Z:129:VAL:CG2	2.63	0.47
1:Z:419:LYS:HD2	1:Z:419:LYS:C	2.40	0.47
1:a:95:LEU:HB3	1:a:129:VAL:HG22	1.97	0.47
2:b:101:ILE:HD13	2:b:101:ILE:H	1.80	0.47
2:b:404:PHE:O	2:b:408:GLU:OE1	2.32	0.47
2:c:27:ASP:HA	2:c:74:PRO:HA	1.97	0.47
2:c:55:ALA:C	2:c:57:GLY:H	2.23	0.47
2:c:337:LEU:O	2:c:338:ASP:CB	2.63	0.47
2:d:81:GLU:H	2:d:81:GLU:CD	2.22	0.47
2:d:166:ILE:HD12	2:d:167:ALA:N	2.30	0.47
1:A:240:TYR:HH	1:A:293:LEU:HD12	1.76	0.47
1:A:262:ASP:H	1:A:329:ILE:HB	1.79	0.47
1:A:284:GLU:C	1:A:286:PHE:H	2.21	0.47
1:A:290:VAL:HG11	1:A:340:PHE:CE1	2.50	0.47
1:C:103:LEU:C	1:C:222:ILE:HG22	2.39	0.47
2:D:449:ILE:O	2:D:453:VAL:HG13	2.15	0.47
2:E:140:ALA:HB2	2:E:343:GLN:HG2	1.95	0.47
2:E:163:ILE:HG13	2:E:240:PHE:CE1	2.49	0.47
2:F:25:VAL:CG1	2:F:26:TYR:N	2.77	0.47
2:F:126:LEU:HD12	2:F:166:ILE:CG2	2.45	0.47
2:F:221:LEU:CD2	2:F:278:LEU:HD13	2.39	0.47
1:I:282:GLY:HA2	3:O:276:LEU:HD21	1.96	0.47
1:I:358:ASN:HA	1:I:361:ASN:HD21	1.79	0.47
1:J:476:ASP:OD2	1:J:477:ARG:N	2.48	0.47
1:J:510:THR:HG22	1:J:511:GLN:H	1.79	0.47
1:K:508:LYS:HA	1:K:508:LYS:HD2	1.69	0.47
2:L:101:ILE:HD13	2:L:101:ILE:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:356:THR:O	2:L:360:VAL:HG23	2.15	0.47
2:L:435:TYR:CZ	2:L:449:ILE:HG13	2.50	0.47
2:L:441:GLN:CD	2:L:441:GLN:H	2.21	0.47
2:M:55:ALA:C	2:M:57:GLY:H	2.23	0.47
2:M:402:GLN:CA	2:M:445:MET:CE	2.92	0.47
2:N:25:VAL:HG13	2:N:26:TYR:H	1.79	0.47
2:N:25:VAL:CG1	2:N:26:TYR:N	2.77	0.47
2:N:118:GLU:HG2	2:N:118:GLU:O	2.14	0.47
3:O:180:GLN:HG2	3:O:237:SER:HB3	1.95	0.47
1:Q:218:LEU:HD13	1:Q:218:LEU:C	2.40	0.47
1:R:49:GLN:HE22	2:V:10:GLY:H	1.62	0.47
1:R:368:VAL:O	1:R:370:PRO:HD3	2.14	0.47
2:T:101:ILE:HD13	2:T:101:ILE:H	1.80	0.47
2:U:94:PRO:HG3	2:U:101:ILE:CG2	2.44	0.47
2:U:396:ILE:HD12	2:U:396:ILE:C	2.39	0.47
2:V:78:PRO:HB3	2:V:103:GLU:HB3	1.95	0.47
2:V:323:ARG:CG	2:V:323:ARG:NH1	2.68	0.47
3:W:189:PRO:CG	3:W:189:PRO:O	2.63	0.47
3:W:191:PRO:CB	3:W:192:ALA:HB3	2.44	0.47
1:Z:145:PRO:HB3	1:Z:381:ALA:O	2.14	0.47
1:Z:461:LEU:HD13	1:Z:463:LYS:H	1.78	0.47
1:a:56:PRO:HG2	1:a:86:MET:HB3	1.95	0.47
2:b:379:MET:HE3	2:b:387:LYS:HB2	1.96	0.47
2:c:40:LEU:HD23	2:c:55:ALA:HA	1.96	0.47
2:c:78:PRO:HD2	2:c:92:GLY:HA3	1.97	0.47
2:c:148:PHE:HZ	2:c:312:PHE:CE1	2.32	0.47
2:c:163:ILE:HG13	2:c:240:PHE:CE1	2.49	0.47
2:c:303:LEU:H	2:c:303:LEU:CD2	2.23	0.47
2:c:446:VAL:HB	2:c:451:GLU:HG3	1.97	0.47
2:d:458:LYS:O	2:d:459:LEU:HB2	2.14	0.47
1:A:179:ALA:HB1	1:A:259:ILE:CD1	2.42	0.47
1:B:394:ARG:HG3	1:B:394:ARG:NH1	2.29	0.47
1:B:461:LEU:HD13	1:B:463:LYS:H	1.78	0.47
1:B:510:THR:HG22	1:B:511:GLN:H	1.79	0.47
1:C:454:GLY:C	1:C:456:LEU:N	2.70	0.47
2:E:113:ALA:HB3	2:E:281:ARG:CG	2.44	0.47
2:F:82:ALA:HB1	2:F:102:GLY:HA2	1.96	0.47
2:F:118:GLU:O	2:F:118:GLU:HG2	2.13	0.47
1:I:218:LEU:HD13	1:I:218:LEU:C	2.40	0.47
1:J:51:GLU:OE2	1:J:90:CYS:HB2	2.15	0.47
2:L:353:HIS:CE1	2:L:420:LEU:HD21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:379:MET:HE1	2:L:390:VAL:CG1	2.45	0.47
1:Q:139:ARG:HA	1:Q:305:ASN:H	1.79	0.47
1:Q:313:THR:HG21	1:Q:317:VAL:H	1.80	0.47
1:R:104:LEU:HD13	1:R:104:LEU:H	1.79	0.47
1:S:393:ILE:CD1	1:S:451:ALA:HB2	2.45	0.47
1:S:474:TYR:C	1:S:474:TYR:CD1	2.92	0.47
2:U:332:PRO:O	2:U:334:VAL:N	2.47	0.47
2:V:81:GLU:CD	2:V:81:GLU:H	2.23	0.47
2:V:118:GLU:O	2:V:118:GLU:HG2	2.13	0.47
3:W:186:GLN:HG3	3:W:189:PRO:CG	2.44	0.47
1:Y:313:THR:HG21	1:Y:317:VAL:H	1.80	0.47
1:A:179:ALA:CB	1:A:259:ILE:HD12	2.41	0.47
1:A:313:THR:HG21	1:A:317:VAL:H	1.80	0.47
1:B:476:ASP:OD2	1:B:477:ARG:N	2.48	0.47
1:C:56:PRO:HG2	1:C:86:MET:HB3	1.95	0.47
2:F:81:GLU:CD	2:F:81:GLU:H	2.22	0.47
1:I:139:ARG:HB2	1:I:303:ARG:O	2.14	0.47
1:I:176:THR:HB	5:I:600:ANP:O2B	2.13	0.47
1:I:186:GLN:HA	1:I:189:SER:HB3	1.97	0.47
1:J:399:GLN:O	1:J:402:GLU:HG2	2.14	0.47
1:K:195:TYR:HD1	1:K:259:ILE:HD11	1.79	0.47
2:L:24:ARG:O	2:L:27:ASP:HB2	2.15	0.47
2:L:135:LEU:HD11	2:L:357:ALA:HA	1.97	0.47
2:L:449:ILE:HD13	2:L:449:ILE:N	2.29	0.47
2:M:40:LEU:HD23	2:M:55:ALA:HA	1.96	0.47
2:M:113:ALA:HB3	2:M:281:ARG:CG	2.43	0.47
2:M:163:ILE:HG13	2:M:240:PHE:CE1	2.49	0.47
2:N:81:GLU:CD	2:N:81:GLU:H	2.23	0.47
2:N:145:VAL:HG22	2:N:317:ALA:HB3	1.96	0.47
2:N:181:GLU:HB3	2:N:242:ASP:OD2	2.15	0.47
1:Q:385:ILE:HG23	1:Q:386:MET:H	1.80	0.47
1:Q:474:TYR:HD2	1:Q:474:TYR:O	1.98	0.47
1:R:138:GLU:OE2	1:R:304:VAL:HG12	2.14	0.47
1:R:198:ILE:HD13	1:R:239:PRO:HG3	1.95	0.47
1:S:362:ALA:HA	2:V:365:GLN:HG2	1.97	0.47
2:T:115:SER:O	2:T:117:GLU:N	2.48	0.47
2:T:332:PRO:CG	2:T:402:GLN:H	2.28	0.47
2:U:27:ASP:HA	2:U:74:PRO:HA	1.97	0.47
2:U:144:LYS:NZ	2:U:279:GLN:HB3	2.30	0.47
2:V:330:ILE:HD12	2:V:330:ILE:N	2.30	0.47
3:W:14:GLN:HG2	3:W:257:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:358:ASN:HA	1:Y:361:ASN:HD21	1.79	0.47
1:Z:399:GLN:O	1:Z:402:GLU:HG2	2.15	0.47
1:Z:490:GLY:O	1:Z:492:TYR:N	2.47	0.47
1:a:205:ILE:O	1:a:209:VAL:HG12	2.14	0.47
2:d:426:GLY:O	2:d:430:ILE:HG13	2.15	0.47
3:e:14:GLN:HG2	3:e:257:ILE:HD13	1.96	0.47
1:B:456:LEU:HD12	1:B:457:ALA:N	2.30	0.47
2:D:17:PHE:HE1	2:D:23:PRO:HG3	1.75	0.47
2:E:238:LEU:HD23	2:E:240:PHE:CE1	2.49	0.47
2:E:445:MET:HE3	2:E:445:MET:H	1.79	0.47
1:I:210:ARG:NH1	2:L:120:SER:O	2.45	0.47
1:J:198:ILE:HD13	1:J:239:PRO:HG3	1.95	0.47
2:L:400:LEU:CB	2:L:427:PHE:HZ	2.21	0.47
2:L:404:PHE:O	2:L:408:GLU:OE1	2.33	0.47
2:M:183:THR:HA	2:M:208:GLN:HG2	1.97	0.47
2:M:400:LEU:HB3	2:M:427:PHE:HZ	1.80	0.47
2:M:445:MET:C	2:M:446:VAL:HG13	2.40	0.47
2:N:74:PRO:O	2:N:75:ILE:HG12	2.14	0.47
3:O:14:GLN:HG2	3:O:257:ILE:HD13	1.96	0.47
3:O:16:THR:HG22	4:P:124:ALA:CB	2.45	0.47
1:S:107:VAL:HG22	1:S:223:VAL:CG1	2.45	0.47
1:S:261:ASP:O	1:S:262:ASP:HB2	2.14	0.47
2:T:14:ASP:HB3	2:T:52:ARG:HA	1.97	0.47
2:U:230:PHE:HB2	2:U:237:VAL:HG11	1.97	0.47
2:U:362:SER:HA	2:U:365:GLN:HG3	1.97	0.47
1:Y:180:ILE:CD1	1:Y:211:LYS:HZ3	2.28	0.47
1:Y:186:GLN:HA	1:Y:189:SER:HB3	1.97	0.47
2:b:320:VAL:HG23	2:b:320:VAL:O	2.15	0.47
2:b:337:LEU:HD22	2:b:365:GLN:HG2	1.97	0.47
2:c:437:HIS:CD2	2:c:438:LEU:HD12	2.50	0.47
1:A:358:ASN:HA	1:A:361:ASN:HD21	1.79	0.46
1:B:35:SER:HB2	2:E:44:GLN:HG2	1.97	0.46
1:B:51:GLU:OE2	1:B:90:CYS:HB2	2.15	0.46
1:B:313:THR:O	1:B:314:LYS:HB2	2.14	0.46
1:C:472:LEU:HA	1:C:507:PHE:CE1	2.50	0.46
2:E:27:ASP:HA	2:E:74:PRO:HA	1.97	0.46
2:E:101:ILE:HG23	2:E:101:ILE:O	2.15	0.46
2:E:346:PRO:HB2	2:E:347:LEU:O	2.15	0.46
2:F:161:GLU:HG3	2:F:404:PHE:CG	2.50	0.46
2:F:166:ILE:HD12	2:F:167:ALA:N	2.30	0.46
2:M:204:LEU:HD23	2:M:204:LEU:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:307:SER:HB2	2:N:308:PRO:CD	2.37	0.46
1:Q:59:ARG:HH22	1:Q:81:ASP:CG	2.23	0.46
1:Q:62:ILE:O	1:Q:73:ALA:HA	2.14	0.46
1:Q:357:THR:HG23	1:Q:358:ASN:N	2.30	0.46
1:S:472:LEU:HA	1:S:507:PHE:CE1	2.51	0.46
2:T:227:ALA:HB1	2:T:290:ILE:HD13	1.97	0.46
2:U:364:LEU:HD23	2:U:396:ILE:HD11	1.97	0.46
2:V:111:ARG:HH11	2:V:111:ARG:CG	2.21	0.46
1:Y:198:ILE:CD1	1:Y:239:PRO:HG3	2.45	0.46
1:Y:318:LYS:HD2	1:Y:318:LYS:N	2.31	0.46
1:Y:417:THR:O	1:Y:421:LEU:HD23	2.15	0.46
1:Y:426:LYS:HE3	1:Y:456:LEU:CD1	2.46	0.46
1:a:472:LEU:HA	1:a:507:PHE:CE1	2.50	0.46
2:c:387:LYS:HD2	2:c:387:LYS:HA	1.59	0.46
1:A:59:ARG:HH22	1:A:81:ASP:CG	2.23	0.46
1:A:318:LYS:HD2	1:A:318:LYS:N	2.30	0.46
1:C:359:LEU:HD13	1:C:364:ILE:HD12	1.97	0.46
2:D:19:GLN:CA	2:D:20:ASP:OD2	2.62	0.46
2:E:135:LEU:HD23	2:E:135:LEU:C	2.41	0.46
2:E:273:GLU:O	2:E:277:VAL:HG23	2.16	0.46
2:E:346:PRO:C	2:E:348:VAL:HG12	2.40	0.46
2:E:432:GLU:HG3	2:E:432:GLU:O	2.15	0.46
3:G:167:LEU:O	3:G:187:LEU:O	2.32	0.46
1:I:59:ARG:HH22	1:I:81:ASP:CG	2.23	0.46
1:I:313:THR:HG21	1:I:317:VAL:H	1.80	0.46
1:I:385:ILE:HG23	1:I:386:MET:H	1.80	0.46
1:J:116:ASP:HA	1:J:117:GLY:HA2	1.57	0.46
1:J:461:LEU:HD13	1:J:463:LYS:H	1.79	0.46
1:K:385:ILE:HG23	1:K:444:GLN:OE1	2.16	0.46
2:L:14:ASP:HB3	2:L:52:ARG:HA	1.97	0.46
2:M:50:ILE:HG22	2:M:51:VAL:N	2.31	0.46
2:M:101:ILE:HG23	2:M:101:ILE:O	2.15	0.46
1:Q:137:ILE:HD12	2:U:97:MET:H	1.80	0.46
1:Q:426:LYS:HE3	1:Q:456:LEU:CD1	2.46	0.46
1:R:399:GLN:O	1:R:402:GLU:HG2	2.14	0.46
2:U:332:PRO:C	2:U:334:VAL:H	2.24	0.46
2:U:377:LEU:HD23	2:U:377:LEU:HA	1.79	0.46
1:Y:59:ARG:HH22	1:Y:81:ASP:CG	2.23	0.46
1:Z:461:LEU:O	1:Z:465:GLY:N	2.48	0.46
2:b:441:GLN:CD	2:b:441:GLN:H	2.22	0.46
2:c:15:VAL:HG21	2:c:68:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:348:VAL:HG13	2:c:349:VAL:HG12	1.97	0.46
1:A:198:ILE:CD1	1:A:239:PRO:HG3	2.45	0.46
1:B:138:GLU:O	1:B:139:ARG:CG	2.61	0.46
2:E:3:GLY:HA3	2:E:17:PHE:HE2	1.76	0.46
2:E:15:VAL:HG21	2:E:68:VAL:CG1	2.45	0.46
2:E:50:ILE:HG22	2:E:51:VAL:N	2.31	0.46
3:G:219:LEU:HD12	3:G:219:LEU:HA	1.76	0.46
1:I:139:ARG:HA	1:I:305:ASN:H	1.79	0.46
1:J:434:LYS:N	1:J:434:LYS:HD2	2.30	0.46
1:K:166:LEU:HB3	1:K:352:GLN:HB3	1.97	0.46
2:L:87:ILE:HA	2:L:204:LEU:HB2	1.97	0.46
2:M:15:VAL:HG21	2:M:68:VAL:CG1	2.45	0.46
2:M:322:SER:HB3	2:M:325:ILE:HB	1.96	0.46
2:M:382:LEU:HD12	2:M:387:LYS:HD3	1.97	0.46
1:R:397:LEU:HD22	1:R:397:LEU:HA	1.75	0.46
1:R:419:LYS:HD2	1:R:419:LYS:C	2.40	0.46
1:R:510:THR:HG22	1:R:511:GLN:H	1.79	0.46
1:S:467:PHE:CZ	1:S:511:GLN:CD	2.90	0.46
2:U:50:ILE:HG22	2:U:51:VAL:N	2.31	0.46
2:U:78:PRO:HD2	2:U:92:GLY:HA3	1.97	0.46
2:U:135:LEU:HD23	2:U:135:LEU:C	2.41	0.46
2:U:437:HIS:CD2	2:U:438:LEU:HD12	2.50	0.46
2:V:166:ILE:HD12	2:V:167:ALA:N	2.30	0.46
1:Z:51:GLU:OE2	1:Z:90:CYS:HB2	2.15	0.46
1:Z:374:VAL:HG12	1:Z:375:SER:N	2.30	0.46
1:a:47:CYS:O	2:b:63:ARG:HB2	2.14	0.46
2:b:87:ILE:HA	2:b:204:LEU:HB2	1.97	0.46
2:b:429:GLY:O	2:b:433:GLY:HA2	2.16	0.46
2:d:390:VAL:O	2:d:394:ARG:HG3	2.15	0.46
3:e:16:THR:HG22	4:f:124:ALA:CB	2.44	0.46
1:C:95:LEU:HB3	1:C:129:VAL:HG22	1.97	0.46
2:D:89:ASN:HD21	2:D:93:GLU:CG	2.29	0.46
2:E:392:ARG:O	2:E:396:ILE:HG23	2.15	0.46
2:F:28:ALA:O	2:F:29:LEU:HB3	2.16	0.46
1:I:198:ILE:CD1	1:I:239:PRO:HG3	2.45	0.46
1:I:229:SER:OG	2:L:113:ALA:HB2	2.15	0.46
1:I:426:LYS:HE3	1:I:456:LEU:CD1	2.46	0.46
1:K:95:LEU:HB3	1:K:129:VAL:HG22	1.97	0.46
1:K:507:PHE:C	1:K:509:ALA:H	2.24	0.46
2:L:128:THR:O	2:L:165:ASN:HB3	2.16	0.46
2:L:367:TYR:CZ	2:L:371:LYS:HE3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:135:LEU:HD23	2:M:135:LEU:C	2.41	0.46
2:N:370:LEU:O	2:N:374:ILE:HG13	2.15	0.46
1:Q:135:GLY:H	1:Q:138:GLU:CD	2.19	0.46
1:Q:417:THR:O	1:Q:421:LEU:HD23	2.15	0.46
1:S:359:LEU:HD13	1:S:364:ILE:HD12	1.97	0.46
2:U:15:VAL:HG21	2:U:68:VAL:CG1	2.45	0.46
2:U:244:ILE:O	2:U:248:THR:HG22	2.16	0.46
2:U:387:LYS:HE3	2:U:390:VAL:HG11	1.96	0.46
2:V:126:LEU:HB3	2:V:141:LYS:CD	2.42	0.46
1:Y:186:GLN:HE21	1:Y:191:ILE:HD12	1.81	0.46
1:Z:48:MET:HE3	1:Z:94:ILE:HG23	1.97	0.46
1:Z:237:LEU:HD12	1:Z:237:LEU:HA	1.82	0.46
1:Z:442:ALA:C	1:Z:444:GLN:H	2.22	0.46
1:Z:476:ASP:OD2	1:Z:477:ARG:N	2.48	0.46
1:a:393:ILE:CD1	1:a:451:ALA:HB2	2.45	0.46
1:a:492:TYR:CD2	1:a:492:TYR:O	2.69	0.46
2:b:128:THR:O	2:b:165:ASN:HB3	2.16	0.46
2:c:135:LEU:C	2:c:135:LEU:HD23	2.41	0.46
2:d:25:VAL:HG13	2:d:26:TYR:H	1.78	0.46
1:A:186:GLN:HA	1:A:189:SER:HB3	1.97	0.46
1:B:95:LEU:CG	1:B:129:VAL:CG2	2.91	0.46
1:B:461:LEU:O	1:B:465:GLY:N	2.48	0.46
1:C:62:ILE:HG22	1:C:64:LEU:HG	1.98	0.46
2:D:14:ASP:HB3	2:D:52:ARG:HA	1.97	0.46
2:D:84:LEU:HD13	2:D:201:LYS:HG2	1.98	0.46
2:E:115:SER:CB	2:E:118:GLU:HB2	2.46	0.46
2:E:244:ILE:O	2:E:248:THR:HG22	2.16	0.46
2:F:330:ILE:HD12	2:F:330:ILE:N	2.29	0.46
2:F:332:PRO:CG	2:F:401:SER:HA	2.45	0.46
1:I:137:ILE:HD11	2:M:97:MET:HB2	1.98	0.46
1:I:284:GLU:C	1:I:286:PHE:H	2.21	0.46
1:J:419:LYS:HD2	1:J:419:LYS:C	2.40	0.46
1:K:359:LEU:HD13	1:K:364:ILE:HD12	1.97	0.46
1:K:393:ILE:CD1	1:K:451:ALA:HB2	2.45	0.46
1:K:496:ILE:H	1:K:496:ILE:CD1	2.28	0.46
2:M:244:ILE:O	2:M:248:THR:HG22	2.16	0.46
2:N:28:ALA:O	2:N:29:LEU:HB3	2.16	0.46
2:N:202:VAL:HG22	2:N:203:SER:N	2.30	0.46
1:Q:449:PHE:HE2	1:Q:501:LYS:N	2.14	0.46
1:S:39:ILE:HD11	1:S:82:LEU:CD1	2.44	0.46
2:T:87:ILE:HA	2:T:204:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:124:GLU:HB3	2:T:141:LYS:HE3	1.97	0.46
2:T:126:LEU:H	2:T:126:LEU:CD2	2.26	0.46
2:U:132:VAL:HG11	2:U:334:VAL:HB	1.97	0.46
4:X:41:LEU:C	4:X:41:LEU:HD12	2.41	0.46
1:Z:510:THR:HG22	1:Z:511:GLN:H	1.79	0.46
1:a:166:LEU:HB3	1:a:352:GLN:HB3	1.97	0.46
1:a:500:LEU:HA	1:a:503:ILE:HD12	1.98	0.46
2:b:111:ARG:HB2	2:b:111:ARG:CZ	2.46	0.46
2:c:364:LEU:HD23	2:c:396:ILE:HD11	1.98	0.46
2:d:353:HIS:HE1	2:d:420:LEU:HD11	1.78	0.46
3:e:268:ARG:O	3:e:272:ILE:HG22	2.15	0.46
1:A:426:LYS:HE3	1:A:456:LEU:CD1	2.45	0.46
1:B:313:THR:CG2	1:B:317:VAL:H	2.29	0.46
1:C:150:TYR:HA	1:C:433:GLN:NE2	2.28	0.46
1:C:166:LEU:HB3	1:C:352:GLN:HB3	1.97	0.46
2:D:132:VAL:HG21	2:D:334:VAL:CG2	2.46	0.46
2:E:278:LEU:C	2:E:278:LEU:HD13	2.41	0.46
2:F:202:VAL:HG22	2:F:203:SER:N	2.30	0.46
2:F:229:LYS:HE3	2:F:233:GLU:OE2	2.15	0.46
3:G:63:LYS:CD	3:G:212:LYS:HE2	2.46	0.46
4:H:41:LEU:C	4:H:41:LEU:HD12	2.41	0.46
1:K:62:ILE:HG22	1:K:64:LEU:HG	1.98	0.46
1:K:492:TYR:O	1:K:492:TYR:CD2	2.69	0.46
2:L:115:SER:O	2:L:117:GLU:N	2.48	0.46
2:L:265:VAL:O	2:L:265:VAL:HG12	2.16	0.46
2:M:27:ASP:HA	2:M:74:PRO:HA	1.97	0.46
2:M:275:MET:HG2	2:M:310:THR:HG22	1.96	0.46
2:M:332:PRO:C	2:M:334:VAL:H	2.24	0.46
1:R:374:VAL:HG12	1:R:375:SER:N	2.30	0.46
1:S:410:ALA:HA	1:S:413:LEU:HD11	1.98	0.46
2:T:128:THR:O	2:T:165:ASN:HB3	2.16	0.46
2:U:101:ILE:HG23	2:U:101:ILE:O	2.15	0.46
1:Z:339:ALA:HB3	1:Z:342:PRO:HG2	1.98	0.46
1:Z:444:GLN:O	1:Z:447:VAL:HG13	2.16	0.46
1:a:410:ALA:HA	1:a:413:LEU:HD11	1.98	0.46
2:b:199:ILE:C	2:b:202:VAL:HG22	2.41	0.46
2:c:204:LEU:HD23	2:c:204:LEU:N	2.29	0.46
2:c:244:ILE:O	2:c:248:THR:HG22	2.16	0.46
2:d:126:LEU:HD12	2:d:166:ILE:CG2	2.45	0.46
2:d:229:LYS:HE3	2:d:233:GLU:OE2	2.15	0.46
3:e:187:LEU:O	3:e:188:LEU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:GLN:O	1:B:447:VAL:HG13	2.16	0.46
1:C:132:ILE:H	1:C:132:ILE:CD1	2.21	0.46
2:D:353:HIS:CE1	2:D:420:LEU:HD21	2.50	0.46
2:D:430:ILE:O	2:D:430:ILE:HG12	2.16	0.46
2:E:111:ARG:HH12	2:E:225:THR:HG22	1.81	0.46
2:E:204:LEU:HD23	2:E:204:LEU:N	2.29	0.46
1:I:474:TYR:HD2	1:I:474:TYR:O	1.98	0.46
1:K:454:GLY:C	1:K:456:LEU:N	2.70	0.46
1:K:472:LEU:HA	1:K:507:PHE:CE1	2.51	0.46
2:L:84:LEU:HD13	2:L:201:LYS:HG2	1.98	0.46
2:L:124:GLU:HB3	2:L:141:LYS:HE3	1.97	0.46
2:L:435:TYR:HB3	2:L:438:LEU:HD21	1.96	0.46
2:N:118:GLU:O	2:N:286:LYS:HG2	2.16	0.46
1:Q:284:GLU:C	1:Q:286:PHE:H	2.21	0.46
1:R:394:ARG:HG3	1:R:394:ARG:NH1	2.29	0.46
1:S:507:PHE:C	1:S:509:ALA:H	2.24	0.46
2:U:225:THR:HG22	2:U:281:ARG:NH2	2.30	0.46
1:Z:434:LYS:N	1:Z:434:LYS:HD2	2.30	0.46
1:a:39:ILE:HD11	1:a:82:LEU:CD1	2.44	0.46
1:a:365:ARG:HG3	5:a:600:ANP:C2	2.45	0.46
2:b:89:ASN:HD21	2:b:93:GLU:CG	2.29	0.46
2:d:181:GLU:HB3	2:d:242:ASP:OD2	2.15	0.46
1:A:186:GLN:HE21	1:A:191:ILE:HD12	1.81	0.46
1:A:211:LYS:NZ	1:A:436:TYR:CE2	2.82	0.46
1:A:417:THR:O	1:A:421:LEU:HD23	2.15	0.46
1:B:397:LEU:HD22	1:B:397:LEU:HA	1.75	0.46
1:C:259:ILE:O	1:C:259:ILE:HG13	2.15	0.46
1:C:385:ILE:HG23	1:C:444:GLN:OE1	2.16	0.46
2:E:183:THR:HA	2:E:208:GLN:HG2	1.97	0.46
1:I:95:LEU:HA	1:I:95:LEU:HD13	1.80	0.46
1:I:211:LYS:NZ	1:I:436:TYR:CE2	2.82	0.46
2:L:137:CYS:SG	2:L:319:VAL:HG22	2.55	0.46
2:M:297:TYR:O	2:M:299:PRO:HD3	2.16	0.46
1:Q:186:GLN:HE21	1:Q:191:ILE:HD12	1.81	0.46
1:Q:198:ILE:CD1	1:Q:239:PRO:HG3	2.45	0.46
1:Q:290:VAL:HG11	1:Q:340:PHE:CE1	2.50	0.46
1:R:198:ILE:HD11	1:R:239:PRO:HG3	1.98	0.46
1:R:313:THR:O	1:R:314:LYS:HB2	2.14	0.46
1:R:476:ASP:OD2	1:R:477:ARG:N	2.48	0.46
1:S:492:TYR:O	1:S:492:TYR:CD2	2.69	0.46
2:T:111:ARG:CG	2:T:112:ALA:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:420:LEU:HD13	2:T:420:LEU:O	2.16	0.46
2:U:163:ILE:HG13	2:U:240:PHE:CE1	2.49	0.46
2:U:276:GLY:O	2:U:280:GLU:HB2	2.16	0.46
2:U:348:VAL:HG13	2:U:349:VAL:HG12	1.96	0.46
2:V:229:LYS:HE3	2:V:233:GLU:OE2	2.15	0.46
3:W:63:LYS:CD	3:W:212:LYS:HE2	2.46	0.46
1:Y:121:LEU:HD23	1:Y:123:HIS:HB3	1.96	0.46
1:Y:176:THR:OG1	5:Y:600:ANP:O2B	2.33	0.46
1:Y:449:PHE:HE2	1:Y:501:LYS:N	2.14	0.46
1:a:359:LEU:HD13	1:a:364:ILE:HD12	1.97	0.46
1:a:507:PHE:C	1:a:509:ALA:H	2.24	0.46
2:b:14:ASP:HB3	2:b:52:ARG:HA	1.97	0.46
2:b:430:ILE:HG12	2:b:430:ILE:O	2.16	0.46
2:c:377:LEU:HD23	2:c:377:LEU:HA	1.78	0.46
2:d:126:LEU:HB3	2:d:141:LYS:CD	2.43	0.46
4:f:41:LEU:C	4:f:41:LEU:HD12	2.41	0.46
1:A:449:PHE:HE2	1:A:501:LYS:N	2.14	0.46
1:C:97:VAL:HG22	1:C:98:PRO:HD2	1.98	0.46
1:C:393:ILE:CD1	1:C:451:ALA:HB2	2.45	0.46
1:C:410:ALA:HA	1:C:413:LEU:HD11	1.98	0.46
2:D:124:GLU:HB3	2:D:141:LYS:HE3	1.97	0.46
2:D:128:THR:O	2:D:165:ASN:HB3	2.16	0.46
2:D:337:LEU:HD21	2:D:364:LEU:HB3	1.98	0.46
2:D:387:LYS:HA	2:D:390:VAL:CG1	2.45	0.46
2:E:337:LEU:O	2:E:338:ASP:CB	2.63	0.46
2:F:237:VAL:CG2	2:F:290:ILE:HG12	2.45	0.46
1:I:35:SER:HB2	2:L:44:GLN:HG2	1.98	0.46
1:I:417:THR:O	1:I:421:LEU:HD23	2.15	0.46
2:L:331:TYR:C	2:L:333:ALA:N	2.73	0.46
2:L:347:LEU:H	2:L:347:LEU:HG	1.52	0.46
2:L:449:ILE:HD13	2:L:449:ILE:H	1.80	0.46
2:M:392:ARG:NH2	2:M:433:GLY:HA2	2.31	0.46
1:R:107:VAL:CG2	1:R:116:ASP:HB2	2.42	0.46
1:R:456:LEU:HD12	1:R:457:ALA:N	2.30	0.46
1:S:35:SER:HB2	2:V:44:GLN:HG2	1.98	0.46
2:T:128:THR:HG23	2:T:129:GLY:HA2	1.98	0.46
2:T:255:SER:OG	2:T:260:ARG:HB2	2.16	0.46
2:V:131:LYS:H	2:V:402:GLN:NE2	2.11	0.46
1:Y:474:TYR:HD2	1:Y:474:TYR:O	1.98	0.46
1:a:62:ILE:HG22	1:a:64:LEU:HG	1.98	0.46
2:b:93:GLU:HA	2:b:94:PRO:HD3	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:348:VAL:HG13	2:c:349:VAL:N	2.31	0.46
1:A:229:SER:OG	2:D:113:ALA:HB2	2.16	0.46
1:B:510:THR:HG22	1:B:511:GLN:N	2.31	0.46
1:C:508:LYS:HD2	1:C:508:LYS:HA	1.69	0.46
2:D:132:VAL:HG23	2:D:400:LEU:HD12	1.97	0.46
2:E:78:PRO:HD2	2:E:92:GLY:HA3	1.97	0.46
2:F:181:GLU:HB3	2:F:242:ASP:OD2	2.15	0.46
1:I:109:ASN:HD21	1:I:113:ALA:N	2.14	0.46
2:L:85:GLY:O	2:L:199:ILE:HD11	2.16	0.46
2:L:124:GLU:HG2	2:L:141:LYS:NZ	2.31	0.46
2:L:128:THR:HG23	2:L:129:GLY:HA2	1.98	0.46
2:N:229:LYS:HE3	2:N:233:GLU:OE2	2.15	0.46
1:S:138:GLU:O	1:S:304:VAL:HG23	2.16	0.46
2:T:84:LEU:HD13	2:T:201:LYS:HG2	1.98	0.46
2:T:156:THR:HA	2:T:159:MET:HE2	1.98	0.46
2:T:347:LEU:H	2:T:347:LEU:HG	1.55	0.46
2:V:148:PHE:CZ	2:V:296:VAL:HG11	2.51	0.46
2:V:181:GLU:O	2:V:209:MET:HG2	2.16	0.46
1:Y:139:ARG:HA	1:Y:305:ASN:H	1.79	0.46
1:Z:426:LYS:HD3	1:Z:426:LYS:HA	1.50	0.46
1:a:365:ARG:HA	1:a:365:ARG:HD2	1.59	0.46
1:a:385:ILE:HG23	1:a:444:GLN:OE1	2.15	0.46
2:b:85:GLY:O	2:b:199:ILE:HD11	2.16	0.46
2:b:156:THR:HA	2:b:159:MET:HE2	1.98	0.46
2:b:374:ILE:HD11	2:b:382:LEU:HD21	1.98	0.46
2:c:132:VAL:HG11	2:c:334:VAL:HB	1.98	0.46
2:c:230:PHE:HB2	2:c:237:VAL:HG11	1.98	0.46
2:c:396:ILE:C	2:c:396:ILE:HD12	2.41	0.46
3:e:63:LYS:CD	3:e:212:LYS:HE2	2.46	0.46
1:A:341:VAL:HB	1:A:342:PRO:HD3	1.98	0.45
1:A:474:TYR:HD2	1:A:474:TYR:O	1.98	0.45
1:B:96:GLU:O	1:B:97:VAL:HG23	2.17	0.45
1:B:198:ILE:HD11	1:B:239:PRO:HG3	1.98	0.45
1:C:39:ILE:HD11	1:C:82:LEU:CD1	2.44	0.45
1:C:496:ILE:CD1	1:C:496:ILE:H	2.28	0.45
2:D:101:ILE:HD13	2:D:101:ILE:H	1.80	0.45
2:E:312:PHE:HD1	2:E:315:LEU:HD12	1.81	0.45
2:E:332:PRO:HD3	2:E:402:GLN:H	1.81	0.45
2:E:429:GLY:O	2:E:434:GLU:HB3	2.16	0.45
1:J:140:GLN:HA	1:J:140:GLN:NE2	2.14	0.45
1:J:158:PRO:CG	1:J:382:GLN:HG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:313:THR:CG2	1:J:317:VAL:H	2.29	0.45
1:J:510:THR:HG22	1:J:511:GLN:N	2.31	0.45
1:K:138:GLU:O	1:K:304:VAL:HG23	2.16	0.45
1:K:198:ILE:HD11	1:K:239:PRO:HG3	1.98	0.45
1:K:305:ASN:OD1	1:K:307:GLU:HB2	2.17	0.45
1:K:500:LEU:HA	1:K:503:ILE:HD12	1.98	0.45
2:L:413:SER:OG	2:L:414:PRO:HD2	2.16	0.45
2:M:78:PRO:HD2	2:M:92:GLY:HA3	1.97	0.45
3:O:63:LYS:CD	3:O:212:LYS:HE2	2.46	0.45
1:Q:186:GLN:HA	1:Q:189:SER:HB3	1.97	0.45
1:Q:205:ILE:HD13	1:Q:225:VAL:HG13	1.96	0.45
1:R:434:LYS:N	1:R:434:LYS:HD2	2.30	0.45
1:R:510:THR:HG22	1:R:511:GLN:N	2.31	0.45
2:U:111:ARG:HH12	2:U:225:THR:HG22	1.81	0.45
2:V:106:ARG:C	2:V:107:TRP:CD1	2.91	0.45
1:Z:313:THR:CG2	1:Z:317:VAL:H	2.29	0.45
1:a:198:ILE:HD11	1:a:239:PRO:HG3	1.98	0.45
2:d:181:GLU:O	2:d:209:MET:HG2	2.16	0.45
2:d:324:GLN:O	2:d:328:LEU:HD23	2.16	0.45
4:f:129:ARG:HG2	4:f:129:ARG:H	1.62	0.45
1:B:453:ARG:CZ	1:B:453:ARG:HB2	2.47	0.45
1:C:139:ARG:NH1	2:D:183:THR:HB	2.31	0.45
2:D:124:GLU:HG2	2:D:141:LYS:NZ	2.31	0.45
2:D:128:THR:HG23	2:D:129:GLY:HA2	1.98	0.45
2:E:55:ALA:C	2:E:57:GLY:H	2.23	0.45
1:J:48:MET:HE3	1:J:94:ILE:HG23	1.97	0.45
2:M:111:ARG:CZ	2:M:111:ARG:CB	2.95	0.45
2:M:337:LEU:O	2:M:338:ASP:CB	2.63	0.45
2:N:332:PRO:O	2:N:334:VAL:N	2.42	0.45
1:Q:446:LEU:HD22	1:Q:446:LEU:C	2.42	0.45
1:S:198:ILE:HD11	1:S:239:PRO:HG3	1.98	0.45
1:S:385:ILE:HG23	1:S:444:GLN:OE1	2.16	0.45
2:T:124:GLU:O	2:T:125:LEU:C	2.59	0.45
2:U:119:LEU:HA	2:U:285:THR:HA	1.98	0.45
2:V:25:VAL:HG13	2:V:26:TYR:H	1.79	0.45
2:b:265:VAL:O	2:b:265:VAL:HG12	2.15	0.45
2:c:183:THR:HA	2:c:208:GLN:HG2	1.96	0.45
2:d:28:ALA:O	2:d:29:LEU:HB3	2.16	0.45
2:d:106:ARG:C	2:d:107:TRP:CD1	2.91	0.45
3:e:190:LEU:HD13	3:e:191:PRO:N	2.22	0.45
1:A:29:GLY:HA3	1:A:44:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:HG2	1:A:305:ASN:ND2	2.28	0.45
2:D:124:GLU:O	2:D:125:LEU:C	2.59	0.45
2:D:198:VAL:O	2:D:200:ASP:N	2.50	0.45
2:E:446:VAL:HB	2:E:451:GLU:CG	2.46	0.45
1:J:402:GLU:CG	1:J:403:LEU:HD23	2.41	0.45
1:J:444:GLN:O	1:J:447:VAL:HG13	2.16	0.45
1:K:342:PRO:O	1:K:346:ILE:HG13	2.17	0.45
2:L:147:LEU:HD13	2:L:293:VAL:HG23	1.98	0.45
2:L:198:VAL:O	2:L:200:ASP:N	2.50	0.45
2:N:126:LEU:HB3	2:N:141:LYS:CD	2.42	0.45
1:Q:109:ASN:HD21	1:Q:113:ALA:N	2.14	0.45
2:T:73:HIS:HB2	2:T:74:PRO:HD2	1.99	0.45
2:T:85:GLY:O	2:T:199:ILE:HD11	2.17	0.45
2:V:180:GLY:O	2:V:209:MET:HB3	2.16	0.45
1:a:74:VAL:CG1	1:a:233:ALA:HB2	2.47	0.45
1:a:195:TYR:HD1	1:a:259:ILE:HD11	1.79	0.45
1:a:305:ASN:OD1	1:a:307:GLU:HB2	2.17	0.45
2:b:84:LEU:HD13	2:b:201:LYS:HG2	1.98	0.45
2:b:90:VAL:HG13	2:b:91:LEU:HG	1.99	0.45
2:b:124:GLU:HB3	2:b:141:LYS:HE3	1.97	0.45
2:b:128:THR:HG23	2:b:129:GLY:HA2	1.98	0.45
2:c:332:PRO:HD3	2:c:402:GLN:H	1.81	0.45
3:e:25:MET:O	3:e:28:ALA:HB3	2.17	0.45
1:A:385:ILE:HG23	1:A:386:MET:H	1.80	0.45
1:A:449:PHE:HA	1:A:452:GLU:CB	2.47	0.45
1:C:304:VAL:HG21	1:C:308:TYR:CD1	2.52	0.45
1:C:507:PHE:C	1:C:509:ALA:H	2.24	0.45
2:D:90:VAL:HG13	2:D:91:LEU:HG	1.99	0.45
2:D:115:SER:O	2:D:117:GLU:N	2.48	0.45
2:D:305:ASP:O	2:D:308:PRO:HD2	2.16	0.45
2:D:398:ARG:HB2	2:D:444:TYR:HA	1.98	0.45
2:E:145:VAL:HG13	2:E:293:VAL:HA	1.98	0.45
2:E:166:ILE:HG12	2:E:238:LEU:HD22	1.98	0.45
2:E:230:PHE:HB2	2:E:237:VAL:HG11	1.98	0.45
1:I:341:VAL:HB	1:I:342:PRO:HD3	1.98	0.45
1:I:446:LEU:HD22	1:I:446:LEU:C	2.42	0.45
1:J:453:ARG:CZ	1:J:453:ARG:HB2	2.47	0.45
1:K:304:VAL:HG21	1:K:308:TYR:CD1	2.52	0.45
2:L:90:VAL:HG13	2:L:91:LEU:HG	1.99	0.45
2:L:111:ARG:CG	2:L:112:ALA:N	2.78	0.45
2:L:199:ILE:C	2:L:202:VAL:HG22	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:332:PRO:CG	2:L:402:GLN:H	2.29	0.45
2:N:243:ASN:HB3	2:N:246:ARG:HG2	1.99	0.45
4:P:41:LEU:C	4:P:41:LEU:HD12	2.41	0.45
1:S:62:ILE:HG22	1:S:64:LEU:HG	1.98	0.45
3:W:206:LEU:HG	3:W:206:LEU:O	2.17	0.45
1:Y:446:LEU:HD22	1:Y:446:LEU:C	2.42	0.45
1:Y:449:PHE:HA	1:Y:452:GLU:CB	2.47	0.45
1:Z:138:GLU:O	1:Z:139:ARG:CG	2.61	0.45
1:Z:453:ARG:CZ	1:Z:453:ARG:HB2	2.47	0.45
1:a:164:ARG:HA	1:a:326:ALA:O	2.17	0.45
1:a:442:ALA:C	1:a:444:GLN:N	2.72	0.45
2:b:244:ILE:HG23	2:b:275:MET:HE1	1.98	0.45
2:b:435:TYR:HB3	2:b:438:LEU:HD21	1.99	0.45
2:c:50:ILE:HG22	2:c:51:VAL:N	2.31	0.45
2:c:331:TYR:HD2	2:c:331:TYR:HA	1.65	0.45
2:d:202:VAL:HG22	2:d:203:SER:N	2.30	0.45
1:B:158:PRO:CG	1:B:382:GLN:HG2	2.47	0.45
1:C:198:ILE:HD13	1:C:239:PRO:HG3	1.99	0.45
1:C:333:GLN:HB3	2:F:304:THR:HG23	1.99	0.45
2:D:87:ILE:HA	2:D:204:LEU:HB2	1.97	0.45
7:D:600:ADP:O2B	8:D:630:SO4:O3	2.34	0.45
2:E:377:LEU:HD23	2:E:377:LEU:HA	1.83	0.45
1:I:67:GLU:HB2	1:I:70:SER:O	2.17	0.45
1:I:449:PHE:HE2	1:I:501:LYS:N	2.14	0.45
2:L:374:ILE:HD11	2:L:382:LEU:HD21	1.98	0.45
2:L:387:LYS:HA	2:L:390:VAL:CG1	2.46	0.45
2:M:111:ARG:HH12	2:M:225:THR:HG22	1.81	0.45
2:M:166:ILE:HG12	2:M:238:LEU:HD22	1.98	0.45
2:M:188:ASP:O	2:M:192:GLU:HG3	2.17	0.45
3:O:206:LEU:HG	3:O:206:LEU:O	2.17	0.45
1:Q:341:VAL:HB	1:Q:342:PRO:HD3	1.98	0.45
1:R:51:GLU:OE2	1:R:90:CYS:HB2	2.15	0.45
1:R:158:PRO:CG	1:R:382:GLN:HG2	2.46	0.45
1:R:430:LEU:HD23	1:R:430:LEU:HA	1.79	0.45
1:S:500:LEU:HA	1:S:503:ILE:HD12	1.98	0.45
2:T:199:ILE:C	2:T:202:VAL:HG22	2.41	0.45
2:T:400:LEU:CB	2:T:427:PHE:HZ	2.23	0.45
2:U:111:ARG:CZ	2:U:111:ARG:CB	2.95	0.45
2:V:410:PHE:CD2	2:V:410:PHE:N	2.78	0.45
4:X:137:ALA:O	4:X:138:MET:HB3	2.17	0.45
1:Y:29:GLY:HA3	1:Y:44:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:139:ARG:NH1	2:b:183:THR:HB	2.31	0.45
1:a:401:ARG:HH12	2:b:324:GLN:HE22	1.64	0.45
2:b:198:VAL:O	2:b:200:ASP:N	2.50	0.45
2:c:90:VAL:HG21	2:c:215:ASN:HB3	1.99	0.45
2:d:237:VAL:CG2	2:d:290:ILE:HG12	2.47	0.45
1:C:500:LEU:HA	1:C:503:ILE:HD12	1.98	0.45
2:E:90:VAL:HG21	2:E:215:ASN:HB3	1.99	0.45
2:E:119:LEU:HA	2:E:285:THR:HA	1.98	0.45
1:I:463:LYS:HD2	1:I:463:LYS:C	2.42	0.45
1:J:442:ALA:C	1:J:444:GLN:H	2.22	0.45
1:K:492:TYR:CD2	1:K:492:TYR:C	2.95	0.45
1:K:493:ASN:H	1:K:496:ILE:HG12	1.82	0.45
2:L:156:THR:HA	2:L:159:MET:HE2	1.98	0.45
2:L:244:ILE:HG23	2:L:275:MET:HE1	1.97	0.45
2:N:181:GLU:O	2:N:209:MET:HG2	2.16	0.45
1:Q:463:LYS:HD2	1:Q:463:LYS:C	2.42	0.45
1:Q:507:PHE:C	1:Q:509:ALA:H	2.25	0.45
1:R:339:ALA:HB3	1:R:342:PRO:HG2	1.98	0.45
1:S:166:LEU:HB3	1:S:352:GLN:HB3	1.98	0.45
1:S:305:ASN:OD1	1:S:307:GLU:HB2	2.17	0.45
1:S:454:GLY:C	1:S:456:LEU:N	2.70	0.45
2:T:229:LYS:HE2	2:T:229:LYS:HB2	1.81	0.45
2:U:161:GLU:CG	2:U:404:PHE:HB3	2.42	0.45
2:V:353:HIS:CE1	2:V:420:LEU:HD11	2.51	0.45
3:W:268:ARG:O	3:W:272:ILE:HG22	2.15	0.45
1:Z:94:ILE:H	1:Z:94:ILE:HG12	1.67	0.45
1:Z:510:THR:HG22	1:Z:511:GLN:N	2.31	0.45
1:a:496:ILE:H	1:a:496:ILE:CD1	2.28	0.45
2:b:332:PRO:HG2	2:b:401:SER:HA	1.98	0.45
2:b:377:LEU:O	4:f:108:SER:HB2	2.17	0.45
2:c:101:ILE:HG23	2:c:101:ILE:O	2.15	0.45
2:c:118:GLU:O	2:c:286:LYS:HG2	2.16	0.45
2:d:243:ASN:HB3	2:d:246:ARG:HG2	1.99	0.45
1:A:91:THR:HB	1:A:93:ARG:HG2	1.99	0.45
1:B:369:ASN:HD22	1:B:369:ASN:C	2.25	0.45
1:B:434:LYS:N	1:B:434:LYS:HD2	2.30	0.45
1:B:442:ALA:C	1:B:444:GLN:H	2.22	0.45
1:C:198:ILE:HD11	1:C:239:PRO:HG3	1.98	0.45
1:C:474:TYR:C	1:C:474:TYR:CD1	2.92	0.45
2:D:347:LEU:H	2:D:347:LEU:HG	1.52	0.45
2:E:116:TYR:C	2:E:118:GLU:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:188:ASP:O	2:E:192:GLU:HG3	2.17	0.45
2:F:183:THR:HG22	2:F:208:GLN:NE2	2.31	0.45
3:G:206:LEU:HG	3:G:206:LEU:O	2.17	0.45
3:G:268:ARG:O	3:G:272:ILE:HG22	2.15	0.45
1:I:64:LEU:HD12	1:I:277:LEU:HD21	1.96	0.45
1:I:449:PHE:HA	1:I:452:GLU:CB	2.47	0.45
2:M:101:ILE:O	2:M:101:ILE:HG12	2.17	0.45
2:M:230:PHE:HB2	2:M:237:VAL:HG11	1.97	0.45
2:M:263:SER:OG	2:M:264:ALA:N	2.48	0.45
2:N:33:ASN:HB3	2:N:62:LEU:HD23	1.98	0.45
2:N:77:VAL:HG11	2:N:222:THR:OG1	2.17	0.45
3:O:25:MET:O	3:O:28:ALA:HB3	2.17	0.45
3:O:48:MET:HE3	4:P:79:LEU:HD13	1.97	0.45
3:O:268:ARG:O	3:O:272:ILE:HG22	2.16	0.45
1:Q:67:GLU:HB2	1:Q:70:SER:O	2.17	0.45
1:R:103:LEU:HG	1:R:245:MET:HE2	1.99	0.45
1:R:416:ALA:O	1:R:420:GLN:HG2	2.17	0.45
1:S:97:VAL:HG22	1:S:98:PRO:HD2	1.98	0.45
1:S:342:PRO:O	1:S:346:ILE:HG13	2.17	0.45
2:U:455:LYS:O	2:U:455:LYS:HG3	2.17	0.45
2:V:28:ALA:O	2:V:29:LEU:HB3	2.16	0.45
2:V:181:GLU:HB3	2:V:242:ASP:OD2	2.15	0.45
3:W:218:LEU:HD11	4:X:68:ILE:HG13	1.98	0.45
1:Y:67:GLU:HB2	1:Y:70:SER:O	2.17	0.45
1:Y:74:VAL:CG1	1:Y:233:ALA:HB2	2.47	0.45
1:Y:262:ASP:HB3	1:Y:265:LYS:HG3	1.99	0.45
1:Y:333:GLN:HG2	2:b:304:THR:OG1	2.17	0.45
1:Z:369:ASN:C	1:Z:369:ASN:HD22	2.25	0.45
1:Z:370:PRO:C	1:Z:372:ILE:H	2.25	0.45
1:a:259:ILE:HG13	1:a:259:ILE:O	2.15	0.45
2:b:124:GLU:HG2	2:b:141:LYS:NZ	2.31	0.45
2:c:166:ILE:HG12	2:c:238:LEU:HD22	1.98	0.45
2:d:279:GLN:HG2	2:d:314:HIS:CB	2.47	0.45
3:e:190:LEU:CD1	3:e:191:PRO:O	2.65	0.45
1:A:74:VAL:CG1	1:A:233:ALA:HB2	2.47	0.45
1:B:416:ALA:O	1:B:420:GLN:HG2	2.17	0.45
1:C:74:VAL:CG1	1:C:233:ALA:HB2	2.46	0.45
1:C:102:GLY:HA3	1:C:122:ASP:O	2.17	0.45
2:D:420:LEU:HD13	2:D:420:LEU:O	2.17	0.45
2:F:33:ASN:HB3	2:F:62:LEU:HD23	1.98	0.45
1:I:68:ARG:N	2:M:7:GLN:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:186:GLN:HE21	1:I:191:ILE:HD12	1.81	0.45
1:I:290:VAL:HG11	1:I:340:PHE:CE1	2.50	0.45
1:I:318:LYS:HD2	1:I:318:LYS:N	2.31	0.45
1:I:370:PRO:HB2	1:I:398:ALA:HB2	1.99	0.45
1:J:96:GLU:C	1:J:97:VAL:HG23	2.41	0.45
1:J:134:PRO:HB2	1:J:139:ARG:NH1	2.32	0.45
1:K:97:VAL:HG22	1:K:98:PRO:HD2	1.98	0.45
1:K:164:ARG:HA	1:K:326:ALA:O	2.17	0.45
2:L:332:PRO:HG2	2:L:402:GLN:N	2.32	0.45
2:M:167:ALA:CB	2:M:201:LYS:HG3	2.47	0.45
2:N:126:LEU:HD12	2:N:166:ILE:CG2	2.45	0.45
2:N:180:GLY:O	2:N:209:MET:HB3	2.16	0.45
1:R:483:MET:O	1:R:486:ILE:HG23	2.17	0.45
2:T:124:GLU:HG2	2:T:141:LYS:NZ	2.31	0.45
2:U:193:MET:HE1	2:U:202:VAL:HG21	1.99	0.45
2:U:225:THR:HG22	2:U:281:ARG:HH22	1.80	0.45
2:V:243:ASN:HB3	2:V:246:ARG:HG2	1.99	0.45
2:V:307:SER:HB2	2:V:308:PRO:CD	2.38	0.45
1:Z:66:LEU:HB3	2:d:64:ARG:HD3	1.99	0.45
2:c:111:ARG:CZ	2:c:111:ARG:CB	2.95	0.45
2:d:183:THR:HG22	2:d:208:GLN:NE2	2.31	0.45
1:B:483:MET:O	1:B:486:ILE:HG23	2.17	0.45
2:D:17:PHE:CE1	2:D:23:PRO:HG3	2.51	0.45
1:I:262:ASP:HB3	1:I:265:LYS:HG3	1.99	0.45
1:J:426:LYS:N	1:J:426:LYS:HE3	2.32	0.45
1:K:74:VAL:CG1	1:K:233:ALA:HB2	2.46	0.45
1:K:401:ARG:HH12	2:L:324:GLN:HE22	1.65	0.45
2:L:124:GLU:O	2:L:125:LEU:C	2.59	0.45
2:L:419:SER:OG	2:L:422:ASP:HB2	2.17	0.45
2:M:244:ILE:HD11	2:M:275:MET:CE	2.44	0.45
2:N:183:THR:HG22	2:N:208:GLN:NE2	2.31	0.45
2:T:337:LEU:HD21	2:T:364:LEU:HB3	1.99	0.45
2:U:101:ILE:O	2:U:101:ILE:HG12	2.17	0.45
2:U:216:ARG:O	2:U:219:VAL:HG12	2.17	0.45
1:Y:507:PHE:C	1:Y:509:ALA:H	2.25	0.45
1:a:304:VAL:HG21	1:a:308:TYR:CD1	2.52	0.45
2:c:116:TYR:C	2:c:118:GLU:N	2.75	0.45
2:c:188:ASP:O	2:c:192:GLU:HG3	2.17	0.45
2:c:367:TYR:CE1	2:c:371:LYS:HE3	2.52	0.45
2:c:446:VAL:HB	2:c:451:GLU:CG	2.47	0.45
1:B:103:LEU:HG	1:B:245:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:GLY:O	2:D:199:ILE:HD11	2.17	0.45
2:D:199:ILE:C	2:D:202:VAL:HG22	2.41	0.45
2:D:408:GLU:OE2	2:D:413:SER:O	2.35	0.45
2:E:111:ARG:CZ	2:E:111:ARG:CB	2.95	0.45
2:F:181:GLU:O	2:F:209:MET:HG2	2.16	0.45
2:F:231:ARG:C	2:F:233:GLU:H	2.25	0.45
1:J:66:LEU:HB3	2:N:64:ARG:HD3	1.98	0.45
1:J:198:ILE:HD11	1:J:239:PRO:HG3	1.98	0.45
1:K:99:VAL:HG11	1:K:127:SER:HB3	1.99	0.45
1:K:442:ALA:C	1:K:444:GLN:N	2.72	0.45
2:L:161:GLU:HG3	2:L:404:PHE:HB3	1.99	0.45
2:L:332:PRO:HG2	2:L:401:SER:HA	1.98	0.45
2:M:132:VAL:HG11	2:M:334:VAL:HB	1.99	0.45
2:N:231:ARG:C	2:N:233:GLU:H	2.25	0.45
2:N:237:VAL:CG2	2:N:290:ILE:HG12	2.47	0.45
2:N:325:ILE:CD1	2:N:335:ASP:HA	2.47	0.45
1:Q:262:ASP:HB3	1:Q:265:LYS:HG3	1.99	0.45
2:T:332:PRO:HG2	2:T:402:GLN:N	2.32	0.45
2:U:221:LEU:O	2:U:225:THR:HG23	2.17	0.45
1:Z:426:LYS:N	1:Z:426:LYS:HE3	2.32	0.45
1:a:97:VAL:HG22	1:a:98:PRO:HD2	1.98	0.45
1:a:102:GLY:HA3	1:a:122:ASP:O	2.17	0.45
2:b:124:GLU:O	2:b:125:LEU:C	2.59	0.45
2:c:111:ARG:HH12	2:c:225:THR:HG22	1.81	0.45
2:c:116:TYR:C	2:c:117:GLU:HG2	2.41	0.45
2:c:125:LEU:HD21	2:c:349:VAL:HB	1.99	0.45
2:c:237:VAL:HG23	2:c:290:ILE:HG23	1.98	0.45
2:c:353:HIS:HE1	2:c:420:LEU:HD11	1.77	0.45
3:e:48:MET:HE3	4:f:79:LEU:HD12	1.99	0.45
1:A:370:PRO:HB2	1:A:398:ALA:HB2	1.99	0.44
1:A:446:LEU:HD22	1:A:446:LEU:C	2.41	0.44
1:B:339:ALA:HB3	1:B:342:PRO:HG2	1.98	0.44
1:C:164:ARG:HA	1:C:326:ALA:O	2.17	0.44
2:D:199:ILE:O	2:D:199:ILE:HD12	2.17	0.44
2:E:221:LEU:O	2:E:225:THR:HG23	2.17	0.44
2:F:180:GLY:O	2:F:209:MET:HB3	2.16	0.44
2:F:243:ASN:HB3	2:F:246:ARG:HG2	1.99	0.44
1:I:74:VAL:CG1	1:I:233:ALA:HB2	2.47	0.44
1:I:299:GLU:OE1	2:M:209:MET:HE2	2.17	0.44
1:Q:91:THR:HB	1:Q:93:ARG:HG2	1.99	0.44
1:R:158:PRO:HB2	1:R:381:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:99:VAL:HG11	1:S:127:SER:HB3	1.99	0.44
1:S:104:LEU:HA	1:S:222:ILE:CG2	2.47	0.44
2:T:147:LEU:HD13	2:T:293:VAL:HG23	1.99	0.44
2:U:167:ALA:CB	2:U:201:LYS:HG3	2.47	0.44
2:V:33:ASN:HB3	2:V:62:LEU:HD23	1.98	0.44
2:V:183:THR:HG22	2:V:208:GLN:NE2	2.31	0.44
2:V:321:LEU:HA	2:V:333:ALA:O	2.17	0.44
1:Y:91:THR:HB	1:Y:93:ARG:HG2	1.99	0.44
1:Y:290:VAL:HG11	1:Y:340:PHE:CE1	2.50	0.44
1:Z:103:LEU:HG	1:Z:245:MET:HE2	1.99	0.44
1:Z:129:VAL:O	1:Z:240:TYR:HB3	2.17	0.44
1:Z:158:PRO:CG	1:Z:382:GLN:HG2	2.47	0.44
1:a:104:LEU:HA	1:a:222:ILE:CG2	2.47	0.44
1:a:198:ILE:HD13	1:a:239:PRO:HG3	1.99	0.44
1:a:342:PRO:O	1:a:346:ILE:HG13	2.17	0.44
1:a:458:ASP:O	1:a:460:GLU:N	2.50	0.44
2:b:35:ASN:HD22	2:b:35:ASN:HA	1.59	0.44
2:c:101:ILE:O	2:c:101:ILE:HG12	2.17	0.44
4:f:137:ALA:O	4:f:138:MET:HB3	2.17	0.44
2:F:106:ARG:O	2:F:107:TRP:HD1	2.00	0.44
3:G:201:LYS:HD3	3:G:202:SER:N	2.18	0.44
1:I:176:THR:OG1	1:I:261:ASP:OD2	2.35	0.44
1:J:369:ASN:C	1:J:369:ASN:HD22	2.25	0.44
1:K:410:ALA:HA	1:K:413:LEU:HD11	1.98	0.44
2:L:332:PRO:HG2	2:L:402:GLN:H	1.83	0.44
2:L:438:LEU:HD23	2:L:438:LEU:H	1.83	0.44
2:M:115:SER:CB	2:M:118:GLU:HB2	2.46	0.44
2:M:382:LEU:HD23	2:M:382:LEU:HA	1.73	0.44
1:Q:29:GLY:HA3	1:Q:44:LEU:HG	1.99	0.44
1:Q:136:VAL:HG23	2:U:183:THR:HG23	1.99	0.44
1:S:494:ASP:O	1:S:497:GLU:HB3	2.16	0.44
2:U:379:MET:HB2	2:U:387:LYS:HZ2	1.78	0.44
2:V:324:GLN:O	2:V:328:LEU:HD23	2.16	0.44
1:Y:211:LYS:NZ	1:Y:436:TYR:CE2	2.82	0.44
1:Z:343:THR:HG22	2:d:297:TYR:OH	2.16	0.44
1:a:492:TYR:CD2	1:a:492:TYR:C	2.95	0.44
2:c:221:LEU:O	2:c:225:THR:HG23	2.17	0.44
2:d:180:GLY:O	2:d:209:MET:HB3	2.16	0.44
2:d:231:ARG:C	2:d:233:GLU:H	2.25	0.44
1:A:55:LEU:HD11	1:A:61:ALA:HB2	2.00	0.44
1:A:463:LYS:HD2	1:A:463:LYS:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:VAL:CG2	1:B:116:ASP:HB2	2.42	0.44
1:B:129:VAL:O	1:B:240:TYR:HB3	2.17	0.44
1:B:158:PRO:HB2	1:B:381:ALA:HB3	1.99	0.44
1:C:138:GLU:O	1:C:304:VAL:HG23	2.16	0.44
2:D:449:ILE:HD13	2:D:449:ILE:H	1.82	0.44
2:E:167:ALA:CB	2:E:201:LYS:HG3	2.47	0.44
2:E:201:LYS:O	2:E:201:LYS:CG	2.65	0.44
1:I:178:LEU:HD12	1:I:179:ALA:HA	1.98	0.44
1:J:339:ALA:HB3	1:J:342:PRO:HG2	1.98	0.44
1:K:102:GLY:HA3	1:K:122:ASP:O	2.17	0.44
2:M:390:VAL:O	2:M:394:ARG:HB2	2.18	0.44
2:N:240:PHE:CD2	2:N:293:VAL:HG22	2.48	0.44
1:R:370:PRO:C	1:R:372:ILE:H	2.25	0.44
1:R:384:LYS:H	1:R:384:LYS:CE	2.28	0.44
1:S:74:VAL:CG1	1:S:233:ALA:HB2	2.47	0.44
2:T:90:VAL:HG13	2:T:91:LEU:HG	1.99	0.44
2:T:199:ILE:O	2:T:199:ILE:HD12	2.17	0.44
2:T:200:ASP:HA	2:T:201:LYS:HA	1.69	0.44
2:T:302:ASP:OD1	2:T:304:THR:HG22	2.18	0.44
2:T:331:TYR:C	2:T:333:ALA:N	2.75	0.44
3:W:66:TYR:CG	3:W:188:LEU:CD2	2.97	0.44
1:Z:134:PRO:HB2	1:Z:139:ARG:NH1	2.32	0.44
1:B:150:TYR:HE1	1:B:181:ASP:HB2	1.82	0.44
1:C:458:ASP:O	1:C:460:GLU:N	2.50	0.44
2:D:147:LEU:HD13	2:D:293:VAL:HG23	1.98	0.44
2:D:416:LYS:HD2	2:D:451:GLU:OE2	2.18	0.44
2:E:101:ILE:O	2:E:101:ILE:HG12	2.17	0.44
2:E:193:MET:HE1	2:E:202:VAL:HG21	1.99	0.44
2:E:402:GLN:CA	2:E:445:MET:HE2	2.47	0.44
2:F:77:VAL:HG11	2:F:222:THR:OG1	2.17	0.44
4:H:137:ALA:O	4:H:138:MET:HB3	2.17	0.44
2:M:140:ALA:HB2	2:M:343:GLN:HG2	1.99	0.44
2:N:225:THR:CG2	2:N:281:ARG:HH12	2.29	0.44
2:N:324:GLN:CD	2:N:324:GLN:H	2.25	0.44
1:Q:135:GLY:N	1:Q:138:GLU:CG	2.81	0.44
1:Q:318:LYS:HD2	1:Q:318:LYS:N	2.30	0.44
1:R:62:ILE:O	1:R:73:ALA:HA	2.17	0.44
1:S:304:VAL:HG21	1:S:308:TYR:CD1	2.52	0.44
1:S:492:TYR:C	1:S:492:TYR:CD2	2.95	0.44
2:T:198:VAL:O	2:T:200:ASP:N	2.50	0.44
2:T:398:ARG:H	2:T:398:ARG:HG2	1.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:390:VAL:O	2:U:394:ARG:HB2	2.18	0.44
2:U:435:TYR:HA	2:U:438:LEU:HD13	2.00	0.44
2:V:231:ARG:C	2:V:233:GLU:H	2.25	0.44
4:X:129:ARG:H	4:X:129:ARG:HG2	1.62	0.44
1:Z:39:ILE:HG22	1:Z:73:ALA:HB3	2.00	0.44
1:Z:198:ILE:HD11	1:Z:239:PRO:HG3	1.98	0.44
1:a:99:VAL:HG11	1:a:127:SER:HB3	1.99	0.44
2:b:73:HIS:HB2	2:b:74:PRO:HD2	1.99	0.44
2:c:216:ARG:O	2:c:219:VAL:HG12	2.18	0.44
2:d:33:ASN:HB3	2:d:62:LEU:HD23	1.98	0.44
3:e:206:LEU:O	3:e:206:LEU:HG	2.17	0.44
1:B:384:LYS:H	1:B:384:LYS:CE	2.28	0.44
1:B:426:LYS:N	1:B:426:LYS:HE3	2.32	0.44
2:D:12:VAL:HG12	2:D:52:ARG:HD2	2.00	0.44
2:D:156:THR:HA	2:D:159:MET:HE2	1.98	0.44
2:E:94:PRO:HG3	2:E:101:ILE:HG22	1.99	0.44
2:F:155:LYS:HZ1	2:F:297:TYR:N	2.15	0.44
2:F:345:ASP:OD1	2:F:347:LEU:HG	2.17	0.44
1:I:29:GLY:HA3	1:I:44:LEU:HG	1.99	0.44
1:J:96:GLU:C	1:J:97:VAL:CG2	2.91	0.44
2:L:132:VAL:HG21	2:L:334:VAL:CG2	2.47	0.44
2:L:360:VAL:HA	2:L:431:MET:HE1	2.00	0.44
2:M:231:ARG:HD2	2:M:285:THR:HG22	2.00	0.44
2:M:312:PHE:HD1	2:M:315:LEU:HD12	1.83	0.44
2:M:325:ILE:HG23	2:M:330:ILE:HG12	1.98	0.44
2:M:395:LYS:HB2	2:M:395:LYS:HE3	1.76	0.44
2:N:407:ALA:HA	2:N:410:PHE:HE2	1.82	0.44
1:Q:55:LEU:HD11	1:Q:61:ALA:HB2	2.00	0.44
1:R:444:GLN:O	1:R:447:VAL:HG13	2.16	0.44
2:U:94:PRO:HG3	2:U:101:ILE:HG22	2.00	0.44
2:U:113:ALA:HB3	2:U:281:ARG:CG	2.47	0.44
2:U:166:ILE:HG12	2:U:238:LEU:HD22	1.98	0.44
2:U:297:TYR:O	2:U:299:PRO:HD3	2.18	0.44
1:Z:352:GLN:HG3	1:Z:354:PHE:CZ	2.53	0.44
7:b:600:ADP:O2B	8:b:630:SO4:O3	2.35	0.44
3:e:190:LEU:HD11	3:e:191:PRO:O	2.17	0.44
3:e:191:PRO:CB	3:e:192:ALA:HB2	2.46	0.44
1:A:109:ASN:HD21	1:A:113:ALA:N	2.14	0.44
1:B:352:GLN:HG3	1:B:354:PHE:CZ	2.53	0.44
1:C:157:ILE:N	1:C:158:PRO:HD3	2.33	0.44
1:C:342:PRO:O	1:C:346:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:HIS:HB2	2:D:74:PRO:HD2	1.98	0.44
2:D:438:LEU:HA	2:D:439:PRO:HD3	1.82	0.44
2:F:117:GLU:H	2:F:117:GLU:HG3	1.55	0.44
1:I:507:PHE:C	1:I:509:ALA:H	2.25	0.44
1:J:370:PRO:C	1:J:372:ILE:H	2.25	0.44
1:K:274:SER:CB	1:K:287:PRO:HG3	2.48	0.44
2:L:89:ASN:HD21	2:L:93:GLU:CG	2.29	0.44
2:L:199:ILE:O	2:L:199:ILE:HD12	2.17	0.44
2:M:221:LEU:O	2:M:225:THR:HG23	2.17	0.44
2:M:377:LEU:HD23	2:M:377:LEU:HA	1.80	0.44
4:P:137:ALA:O	4:P:138:MET:HB3	2.17	0.44
1:Q:180:ILE:HD11	1:Q:211:LYS:HZ3	1.83	0.44
1:Q:449:PHE:HA	1:Q:452:GLU:CB	2.47	0.44
1:R:259:ILE:HG22	1:R:327:LEU:HD23	2.00	0.44
1:R:313:THR:CG2	1:R:317:VAL:H	2.29	0.44
1:R:453:ARG:CZ	1:R:453:ARG:HB2	2.47	0.44
2:T:144:LYS:HE2	2:T:279:GLN:O	2.17	0.44
2:U:125:LEU:HD21	2:U:349:VAL:HB	1.99	0.44
2:U:443:PHE:HE1	2:U:449:ILE:HD11	1.83	0.44
3:W:113:ASP:C	3:W:114:LEU:HD12	2.43	0.44
1:Y:341:VAL:HB	1:Y:342:PRO:HD3	1.98	0.44
1:Y:370:PRO:HB2	1:Y:398:ALA:HB2	1.99	0.44
1:Z:394:ARG:O	1:Z:394:ARG:HD2	2.18	0.44
1:Z:416:ALA:O	1:Z:420:GLN:HG2	2.17	0.44
1:a:140:GLN:HB3	1:a:303:ARG:HD3	2.00	0.44
2:b:54:ILE:N	2:b:54:ILE:HD12	2.33	0.44
2:b:199:ILE:O	2:b:199:ILE:HD12	2.17	0.44
2:c:201:LYS:O	2:c:201:LYS:CG	2.65	0.44
1:A:34:VAL:CG1	2:D:45:GLN:HB3	2.47	0.44
1:A:507:PHE:C	1:A:509:ALA:H	2.25	0.44
1:C:305:ASN:OD1	1:C:307:GLU:HB2	2.17	0.44
2:D:87:ILE:H	2:D:87:ILE:HG13	1.62	0.44
2:D:331:TYR:C	2:D:333:ALA:N	2.76	0.44
2:D:341:SER:C	2:D:343:GLN:N	2.76	0.44
2:D:345:ASP:HB2	2:D:346:PRO:HD2	1.99	0.44
2:D:449:ILE:HD13	2:D:449:ILE:N	2.32	0.44
2:E:216:ARG:O	2:E:219:VAL:HG12	2.17	0.44
3:G:25:MET:O	3:G:28:ALA:HB3	2.17	0.44
1:I:91:THR:HB	1:I:93:ARG:HG2	1.99	0.44
1:I:427:VAL:O	1:I:431:LEU:HB2	2.18	0.44
1:J:27:ASN:HD21	1:J:46:ASP:CB	2.12	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:129:VAL:O	1:J:240:TYR:HB3	2.18	0.44
1:J:352:GLN:HG3	1:J:354:PHE:CZ	2.53	0.44
2:L:54:ILE:N	2:L:54:ILE:HD12	2.33	0.44
2:M:116:TYR:C	2:M:117:GLU:HG2	2.41	0.44
2:N:106:ARG:O	2:N:107:TRP:HD1	2.00	0.44
1:Q:370:PRO:HB2	1:Q:398:ALA:HB2	1.99	0.44
1:R:129:VAL:O	1:R:240:TYR:HB3	2.17	0.44
1:R:394:ARG:O	1:R:394:ARG:HD2	2.18	0.44
1:S:157:ILE:N	1:S:158:PRO:HD3	2.33	0.44
1:S:164:ARG:HA	1:S:326:ALA:O	2.17	0.44
2:T:11:ALA:O	2:T:54:ILE:HA	2.18	0.44
2:U:119:LEU:O	2:U:119:LEU:HD23	2.18	0.44
2:U:367:TYR:HE2	2:U:390:VAL:HG13	1.77	0.44
1:Y:238:ALA:HB3	1:Y:239:PRO:HD3	2.00	0.44
1:a:32:VAL:O	2:d:47:GLY:HA2	2.17	0.44
2:c:99:GLY:O	2:c:100:GLU:HB2	2.18	0.44
2:d:410:PHE:CD2	2:d:410:PHE:N	2.79	0.44
1:B:134:PRO:HB2	1:B:139:ARG:NH1	2.32	0.44
1:C:439:MET:HB2	1:C:443:GLN:NE2	2.33	0.44
2:F:12:VAL:CG1	2:F:257:LEU:HB3	2.48	0.44
2:F:111:ARG:NH1	2:F:111:ARG:CG	2.80	0.44
1:J:62:ILE:O	1:J:73:ALA:HA	2.17	0.44
1:J:97:VAL:CG1	1:J:98:PRO:N	2.77	0.44
1:J:150:TYR:HE1	1:J:181:ASP:HB2	1.82	0.44
1:J:446:LEU:HD23	1:J:446:LEU:C	2.43	0.44
1:J:483:MET:O	1:J:486:ILE:HG23	2.17	0.44
1:K:136:VAL:C	1:K:138:GLU:N	2.67	0.44
1:K:157:ILE:N	1:K:158:PRO:HD3	2.33	0.44
1:K:277:LEU:HD12	1:K:277:LEU:HA	1.77	0.44
2:M:405:PHE:CZ	2:M:416:LYS:HA	2.53	0.44
1:Q:74:VAL:CG1	1:Q:233:ALA:HB2	2.47	0.44
1:R:134:PRO:HB2	1:R:139:ARG:NH1	2.32	0.44
2:U:188:ASP:O	2:U:192:GLU:HG3	2.17	0.44
2:U:337:LEU:O	2:U:338:ASP:CB	2.65	0.44
2:V:126:LEU:HD12	2:V:166:ILE:CG2	2.45	0.44
2:V:407:ALA:HA	2:V:410:PHE:HE2	1.81	0.44
2:b:17:PHE:CD1	2:b:23:PRO:CD	3.01	0.44
2:b:200:ASP:HA	2:b:201:LYS:HA	1.68	0.44
2:c:119:LEU:HD23	2:c:119:LEU:O	2.18	0.44
2:d:111:ARG:NH1	2:d:111:ARG:CG	2.80	0.44
2:d:349:VAL:O	2:d:349:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:113:ASP:C	3:e:114:LEU:HD12	2.43	0.44
1:A:67:GLU:HB2	1:A:70:SER:O	2.17	0.44
1:B:62:ILE:O	1:B:73:ALA:HA	2.17	0.44
1:B:113:ALA:N	1:B:114:PRO:CD	2.81	0.44
1:B:230:GLU:HB3	1:B:234:LEU:HD23	2.00	0.44
3:G:190:LEU:HD13	3:G:191:PRO:HD2	2.00	0.44
1:I:282:GLY:CA	3:O:276:LEU:HD21	2.48	0.44
1:J:259:ILE:HG22	1:J:327:LEU:HD23	2.00	0.44
2:L:11:ALA:O	2:L:54:ILE:HA	2.18	0.44
2:L:87:ILE:H	2:L:87:ILE:HG13	1.62	0.44
2:L:119:LEU:HB2	2:L:286:LYS:HD2	1.99	0.44
2:L:382:LEU:HD12	2:L:382:LEU:H	1.83	0.44
2:L:450:GLU:O	2:L:453:VAL:HG22	2.17	0.44
2:N:322:SER:OG	2:N:325:ILE:HG13	2.18	0.44
1:R:352:GLN:HG3	1:R:354:PHE:CZ	2.53	0.44
1:R:426:LYS:N	1:R:426:LYS:HE3	2.32	0.44
1:R:446:LEU:HD23	1:R:446:LEU:C	2.43	0.44
1:R:446:LEU:HD23	1:R:447:VAL:N	2.33	0.44
2:T:446:VAL:HG21	2:T:452:ALA:HB2	1.99	0.44
2:U:90:VAL:HG21	2:U:215:ASN:HB3	1.99	0.44
1:Z:62:ILE:O	1:Z:73:ALA:HA	2.17	0.44
1:Z:116:ASP:HA	1:Z:117:GLY:HA2	1.57	0.44
1:Z:158:PRO:HB2	1:Z:381:ALA:HB3	1.99	0.44
1:Z:259:ILE:HG22	1:Z:327:LEU:HD23	2.00	0.44
1:a:138:GLU:O	1:a:304:VAL:HG23	2.16	0.44
1:a:439:MET:HB2	1:a:443:GLN:NE2	2.33	0.44
1:a:459:VAL:O	1:a:459:VAL:CG1	2.57	0.44
2:b:155:LYS:HB2	2:b:155:LYS:NZ	2.33	0.44
2:c:167:ALA:CB	2:c:201:LYS:HG3	2.47	0.44
2:c:193:MET:HE1	2:c:202:VAL:HG21	1.99	0.44
1:A:357:THR:HG23	1:A:358:ASN:N	2.30	0.43
1:B:446:LEU:HD23	1:B:447:VAL:N	2.33	0.43
1:B:476:ASP:OD2	1:B:476:ASP:C	2.61	0.43
2:D:16:GLU:HG3	2:D:17:PHE:N	2.33	0.43
2:E:285:THR:HG23	2:E:288:GLY:N	2.33	0.43
3:G:113:ASP:C	3:G:114:LEU:HD12	2.43	0.43
1:I:68:ARG:HG3	2:M:6:VAL:HG12	2.00	0.43
1:J:103:LEU:HG	1:J:245:MET:HE2	1.99	0.43
1:J:384:LYS:H	1:J:384:LYS:CE	2.28	0.43
1:K:458:ASP:O	1:K:460:GLU:N	2.50	0.43
2:L:155:LYS:N	7:L:600:ADP:O1B	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:229:LYS:O	2:L:232:ASP:HB3	2.18	0.43
2:M:216:ARG:O	2:M:219:VAL:HG12	2.17	0.43
3:O:167:LEU:O	3:O:187:LEU:O	2.36	0.43
1:Q:238:ALA:HB3	1:Q:239:PRO:HD3	2.00	0.43
1:Q:480:ALA:HB1	1:Q:483:MET:HE2	2.00	0.43
1:R:423:HIS:CD2	1:R:423:HIS:C	2.96	0.43
1:S:393:ILE:HD13	1:S:451:ALA:HB2	2.01	0.43
2:T:427:PHE:O	2:T:431:MET:HG2	2.18	0.43
2:U:115:SER:CB	2:U:118:GLU:HB2	2.46	0.43
2:U:201:LYS:O	2:U:201:LYS:CG	2.65	0.43
2:V:77:VAL:HG11	2:V:222:THR:OG1	2.17	0.43
3:W:63:LYS:HD2	3:W:212:LYS:HE2	2.00	0.43
3:W:74:ARG:HE	3:W:111:GLN:HB2	1.83	0.43
1:Y:463:LYS:HD2	1:Y:463:LYS:C	2.42	0.43
1:Z:113:ALA:N	1:Z:114:PRO:CD	2.81	0.43
1:Z:186:GLN:NE2	1:Z:189:SER:OG	2.51	0.43
1:Z:230:GLU:HB3	1:Z:234:LEU:HD23	2.00	0.43
1:Z:423:HIS:C	1:Z:423:HIS:CD2	2.96	0.43
1:Z:446:LEU:HD23	1:Z:446:LEU:C	2.43	0.43
1:a:151:LYS:HE3	1:a:433:GLN:CG	2.48	0.43
1:a:209:VAL:HA	1:a:212:LEU:HB2	2.00	0.43
2:c:135:LEU:HD22	2:c:136:MET:SD	2.58	0.43
2:c:382:LEU:HD23	2:c:382:LEU:HA	1.76	0.43
2:d:77:VAL:HG11	2:d:222:THR:OG1	2.17	0.43
2:d:219:VAL:O	2:d:222:THR:HG22	2.18	0.43
3:e:63:LYS:HD2	3:e:212:LYS:HE2	2.00	0.43
1:A:74:VAL:HG12	1:A:233:ALA:HB2	2.01	0.43
1:A:163:GLN:HG2	1:A:164:ARG:H	1.83	0.43
1:A:180:ILE:CD1	1:A:211:LYS:HZ3	2.29	0.43
1:B:348:ILE:HG23	2:F:209:MET:CE	2.47	0.43
1:C:209:VAL:HA	1:C:212:LEU:HB2	2.00	0.43
2:E:325:ILE:HG23	2:E:330:ILE:HG12	2.00	0.43
1:I:55:LEU:HD11	1:I:61:ALA:HB2	2.00	0.43
1:I:138:GLU:CG	1:I:305:ASN:ND2	2.81	0.43
1:J:113:ALA:N	1:J:114:PRO:CD	2.81	0.43
1:J:259:ILE:O	1:J:259:ILE:CG1	2.65	0.43
1:J:442:ALA:C	1:J:444:GLN:N	2.76	0.43
2:L:227:ALA:HB1	2:L:290:ILE:HD13	2.00	0.43
2:M:94:PRO:HG3	2:M:101:ILE:HG22	1.99	0.43
2:M:388:LEU:HD21	2:M:392:ARG:NH1	2.33	0.43
2:N:42:VAL:HG13	2:N:51:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:219:VAL:O	2:N:222:THR:HG22	2.18	0.43
3:O:113:ASP:C	3:O:114:LEU:HD12	2.43	0.43
1:S:220:ASN:O	1:S:220:ASN:CG	2.62	0.43
1:S:350:ASP:HB3	2:T:184:ARG:HH21	1.83	0.43
2:T:12:VAL:HG12	2:T:52:ARG:HD2	2.00	0.43
2:V:101:ILE:HG22	2:V:102:GLY:N	2.33	0.43
3:W:25:MET:O	3:W:28:ALA:HB3	2.17	0.43
1:Y:55:LEU:HD11	1:Y:61:ALA:HB2	2.00	0.43
1:Y:163:GLN:HG2	1:Y:164:ARG:H	1.83	0.43
1:a:166:LEU:HD22	1:a:166:LEU:C	2.43	0.43
2:b:337:LEU:HD21	2:b:364:LEU:HB3	2.00	0.43
2:b:345:ASP:HB2	2:b:346:PRO:HD2	2.00	0.43
2:c:225:THR:HG22	2:c:281:ARG:NH2	2.34	0.43
2:d:321:LEU:HA	2:d:333:ALA:O	2.18	0.43
1:A:111:LEU:HD13	1:A:111:LEU:HA	1.87	0.43
1:B:446:LEU:HD23	1:B:446:LEU:C	2.43	0.43
1:C:159:ILE:HA	1:C:163:GLN:OE1	2.19	0.43
1:C:220:ASN:O	1:C:220:ASN:CG	2.62	0.43
2:D:421:LYS:O	2:D:425:ARG:HB2	2.17	0.43
2:E:119:LEU:O	2:E:119:LEU:HD23	2.18	0.43
1:I:238:ALA:HB3	1:I:239:PRO:HD3	2.00	0.43
1:I:357:THR:HG23	1:I:358:ASN:N	2.30	0.43
1:K:100:GLY:HA2	1:K:248:TYR:CE2	2.54	0.43
1:K:166:LEU:HD22	1:K:166:LEU:C	2.43	0.43
1:K:220:ASN:O	1:K:220:ASN:CG	2.61	0.43
1:K:385:ILE:CD1	1:K:444:GLN:HG2	2.49	0.43
1:K:439:MET:HB2	1:K:443:GLN:NE2	2.33	0.43
2:L:128:THR:OG1	2:L:130:ILE:HG13	2.18	0.43
2:M:46:LEU:HD23	2:M:47:GLY:H	1.83	0.43
2:M:302:ASP:C	2:M:304:THR:H	2.27	0.43
1:R:150:TYR:HE1	1:R:181:ASP:HB2	1.83	0.43
1:R:237:LEU:HD12	1:R:237:LEU:HA	1.82	0.43
1:R:259:ILE:O	1:R:259:ILE:CG1	2.65	0.43
1:R:387:LYS:HA	1:R:387:LYS:HD2	1.79	0.43
1:S:458:ASP:O	1:S:460:GLU:N	2.50	0.43
2:T:408:GLU:OE2	2:T:413:SER:O	2.36	0.43
2:U:387:LYS:HD2	2:U:387:LYS:HA	1.59	0.43
2:V:370:LEU:O	2:V:374:ILE:HG13	2.17	0.43
3:W:253:GLY:O	3:W:257:ILE:HG13	2.18	0.43
1:Z:442:ALA:C	1:Z:444:GLN:N	2.76	0.43
1:Z:446:LEU:HD23	1:Z:447:VAL:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:341:SER:C	2:b:343:GLN:H	2.26	0.43
2:d:28:ALA:HB3	2:d:71:LEU:HD21	2.01	0.43
2:d:42:VAL:HG13	2:d:51:VAL:HG13	2.00	0.43
1:A:446:LEU:HD13	1:A:446:LEU:H	1.84	0.43
1:B:186:GLN:NE2	1:B:189:SER:OG	2.51	0.43
1:C:99:VAL:HG11	1:C:127:SER:HB3	1.99	0.43
2:E:399:PHE:C	2:E:401:SER:H	2.25	0.43
2:F:28:ALA:HB3	2:F:71:LEU:HD21	2.01	0.43
1:I:84:GLU:OE2	2:L:48:GLY:HA2	2.18	0.43
1:I:91:THR:HG21	1:I:93:ARG:HD3	2.01	0.43
1:I:138:GLU:HB3	1:I:305:ASN:ND2	2.34	0.43
1:J:138:GLU:O	1:J:139:ARG:CG	2.61	0.43
1:J:416:ALA:O	1:J:420:GLN:HG2	2.17	0.43
1:K:150:TYR:HA	1:K:433:GLN:NE2	2.28	0.43
1:K:159:ILE:HA	1:K:163:GLN:OE1	2.19	0.43
1:K:198:ILE:HD13	1:K:239:PRO:HG3	1.99	0.43
1:K:460:GLU:H	1:K:460:GLU:HG3	1.52	0.43
2:L:73:HIS:HB2	2:L:74:PRO:HD2	1.99	0.43
2:L:161:GLU:HG3	2:L:404:PHE:CB	2.48	0.43
2:L:387:LYS:CA	2:L:390:VAL:HG12	2.48	0.43
2:M:99:GLY:O	2:M:100:GLU:HB2	2.18	0.43
2:M:402:GLN:N	2:M:445:MET:HE2	2.33	0.43
2:N:106:ARG:C	2:N:107:TRP:CD1	2.91	0.43
2:N:453:VAL:HG12	2:N:454:GLU:N	2.33	0.43
3:O:66:TYR:CG	3:O:188:LEU:HD13	2.53	0.43
1:Q:138:GLU:O	1:Q:305:ASN:CG	2.62	0.43
1:Q:397:LEU:O	1:Q:397:LEU:HD23	2.18	0.43
1:R:453:ARG:NH1	1:R:453:ARG:HB2	2.34	0.43
1:S:140:GLN:HB3	1:S:303:ARG:HD3	2.00	0.43
1:S:159:ILE:HA	1:S:163:GLN:OE1	2.19	0.43
1:S:441:VAL:O	1:S:441:VAL:HG12	2.19	0.43
2:T:17:PHE:CD1	2:T:23:PRO:CD	3.01	0.43
2:T:84:LEU:HD13	2:T:201:LYS:CG	2.49	0.43
2:T:210:ASN:OD1	2:T:210:ASN:N	2.51	0.43
2:T:279:GLN:HE22	2:T:294:GLN:NE2	2.16	0.43
2:U:135:LEU:HD22	2:U:136:MET:SD	2.58	0.43
3:W:173:LYS:HG2	3:W:233:GLU:OE2	2.19	0.43
1:Y:480:ALA:HB1	1:Y:483:MET:HE2	2.00	0.43
1:Z:150:TYR:HE1	1:Z:181:ASP:HB2	1.83	0.43
1:a:100:GLY:HA2	1:a:248:TYR:CE2	2.54	0.43
1:a:274:SER:CB	1:a:287:PRO:HG3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:279:GLN:NE2	2:b:294:GLN:HE22	2.13	0.43
2:c:442:ALA:HA	2:c:455:LYS:HG2	1.99	0.43
2:d:116:TYR:C	2:d:116:TYR:HD2	2.26	0.43
1:B:370:PRO:C	1:B:372:ILE:H	2.25	0.43
1:B:453:ARG:NH1	1:B:453:ARG:HB2	2.34	0.43
1:C:441:VAL:O	1:C:441:VAL:HG12	2.19	0.43
2:D:128:THR:OG1	2:D:130:ILE:HG13	2.18	0.43
2:D:360:VAL:HG13	2:D:396:ILE:HD12	2.00	0.43
2:E:446:VAL:HB	2:E:451:GLU:HG2	2.00	0.43
2:F:116:TYR:C	2:F:116:TYR:HD2	2.26	0.43
2:F:376:ILE:HG21	4:H:125:ILE:HD11	2.00	0.43
1:I:74:VAL:HG12	1:I:233:ALA:HB2	2.01	0.43
1:J:186:GLN:NE2	1:J:189:SER:OG	2.51	0.43
1:J:348:ILE:HG23	2:N:209:MET:HE1	1.99	0.43
1:J:430:LEU:HD23	1:J:430:LEU:HA	1.79	0.43
1:K:140:GLN:HB3	1:K:303:ARG:HD3	2.00	0.43
2:L:22:VAL:O	2:L:22:VAL:CG1	2.65	0.43
2:M:119:LEU:O	2:M:119:LEU:HD23	2.18	0.43
2:M:201:LYS:O	2:M:201:LYS:CG	2.65	0.43
2:M:282:ILE:HG13	2:M:282:ILE:O	2.18	0.43
2:M:388:LEU:O	2:M:392:ARG:HG3	2.18	0.43
4:P:2:MET:CE	2:c:197:ASN:CB	2.42	0.43
2:T:155:LYS:HB2	2:T:155:LYS:NZ	2.33	0.43
2:U:46:LEU:HD23	2:U:47:GLY:N	2.34	0.43
2:U:116:TYR:C	2:U:117:GLU:HG2	2.41	0.43
2:V:28:ALA:HB3	2:V:71:LEU:HD21	2.01	0.43
2:V:173:TYR:CD1	2:V:236:ASP:O	2.72	0.43
2:V:202:VAL:HG22	2:V:203:SER:N	2.30	0.43
3:W:27:ALA:HB2	3:W:242:ARG:HG2	2.01	0.43
1:Z:95:LEU:CD1	1:Z:129:VAL:CG1	2.96	0.43
1:Z:453:ARG:NH1	1:Z:453:ARG:HB2	2.34	0.43
1:a:365:ARG:O	1:a:367:ALA:N	2.52	0.43
1:a:441:VAL:O	1:a:441:VAL:HG12	2.19	0.43
1:a:474:TYR:HD1	1:a:475:VAL:N	2.17	0.43
2:b:126:LEU:H	2:b:126:LEU:CD2	2.26	0.43
2:c:140:ALA:HB2	2:c:343:GLN:CD	2.43	0.43
2:d:25:VAL:CG1	2:d:26:TYR:H	2.31	0.43
2:d:135:LEU:HB2	2:d:423:THR:HG21	1.99	0.43
3:e:224:GLU:OE2	4:f:85:ARG:NH2	2.52	0.43
1:A:262:ASP:HB3	1:A:265:LYS:HG3	1.99	0.43
1:A:474:TYR:O	1:A:477:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:GLN:O	2:D:20:ASP:C	2.61	0.43
2:D:126:LEU:H	2:D:126:LEU:CD2	2.26	0.43
2:D:254:VAL:O	2:D:258:LEU:HB2	2.18	0.43
2:D:302:ASP:OD1	2:D:304:THR:HG22	2.18	0.43
2:E:135:LEU:HD22	2:E:136:MET:SD	2.58	0.43
2:E:242:ASP:O	2:E:295:ALA:HB3	2.19	0.43
1:I:446:LEU:HD13	1:I:446:LEU:H	1.84	0.43
1:J:107:VAL:CG2	1:J:116:ASP:HB2	2.42	0.43
1:J:230:GLU:HB3	1:J:234:LEU:HD23	2.00	0.43
1:J:439:MET:HG3	1:J:443:GLN:HB2	2.01	0.43
1:K:333:GLN:HB3	2:N:304:THR:HG23	2.01	0.43
2:L:335:ASP:HA	2:L:336:PRO:HD3	1.88	0.43
2:M:46:LEU:HD23	2:M:47:GLY:N	2.34	0.43
2:M:242:ASP:O	2:M:295:ALA:HB3	2.19	0.43
2:M:411:THR:HB	2:M:412:GLY:H	1.62	0.43
2:N:161:GLU:CG	2:N:404:PHE:HB3	2.43	0.43
3:O:27:ALA:HB2	3:O:242:ARG:HG2	2.01	0.43
3:O:173:LYS:HG2	3:O:233:GLU:OE2	2.19	0.43
1:Q:74:VAL:HG12	1:Q:233:ALA:HB2	2.00	0.43
1:R:39:ILE:HG22	1:R:73:ALA:HB3	2.00	0.43
1:S:100:GLY:HA2	1:S:248:TYR:CE2	2.54	0.43
2:T:54:ILE:HD12	2:T:54:ILE:N	2.33	0.43
2:T:135:LEU:HD11	2:T:357:ALA:HA	2.01	0.43
2:T:413:SER:OG	2:T:414:PRO:HD2	2.19	0.43
2:V:42:VAL:HG13	2:V:51:VAL:HG13	2.01	0.43
2:V:73:HIS:CD2	2:V:74:PRO:HD2	2.49	0.43
2:V:225:THR:CG2	2:V:281:ARG:HH12	2.32	0.43
2:V:233:GLU:HG3	2:V:234:GLY:N	2.26	0.43
1:Y:268:VAL:HG23	1:Y:271:ARG:NH2	2.34	0.43
1:Y:427:VAL:O	1:Y:431:LEU:HB2	2.18	0.43
1:Z:49:GLN:HE22	2:d:10:GLY:H	1.67	0.43
1:Z:483:MET:O	1:Z:486:ILE:HG23	2.17	0.43
2:b:128:THR:OG1	2:b:130:ILE:HG13	2.18	0.43
2:c:332:PRO:O	2:c:334:VAL:N	2.52	0.43
2:d:173:TYR:CD1	2:d:236:ASP:O	2.72	0.43
3:e:191:PRO:CA	3:e:192:ALA:HB3	2.34	0.43
3:e:253:GLY:O	3:e:257:ILE:HG13	2.18	0.43
1:A:238:ALA:HB3	1:A:239:PRO:HD3	2.00	0.43
1:A:427:VAL:O	1:A:431:LEU:HB2	2.18	0.43
1:C:100:GLY:HA2	1:C:248:TYR:CE2	2.54	0.43
1:C:151:LYS:HE3	1:C:433:GLN:CG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:LEU:HD22	1:C:166:LEU:C	2.43	0.43
1:C:471:LEU:HD13	1:C:474:TYR:HE1	1.83	0.43
2:D:35:ASN:HD22	2:D:35:ASN:HA	1.59	0.43
2:D:54:ILE:N	2:D:54:ILE:HD12	2.33	0.43
2:D:161:GLU:HG3	2:D:404:PHE:CB	2.49	0.43
2:D:255:SER:OG	2:D:260:ARG:HD2	2.18	0.43
2:F:132:VAL:HG11	2:F:334:VAL:CB	2.46	0.43
2:F:173:TYR:CD1	2:F:236:ASP:O	2.72	0.43
3:G:173:LYS:HG2	3:G:233:GLU:OE2	2.19	0.43
1:J:39:ILE:HG22	1:J:73:ALA:HB3	2.00	0.43
1:J:453:ARG:NH1	1:J:453:ARG:HB2	2.34	0.43
1:K:209:VAL:HA	1:K:212:LEU:HB2	2.00	0.43
1:K:259:ILE:O	1:K:259:ILE:CG1	2.66	0.43
1:K:457:ALA:O	1:K:460:GLU:HG2	2.19	0.43
1:K:471:LEU:HD13	1:K:474:TYR:HE1	1.83	0.43
2:L:12:VAL:HG12	2:L:52:ARG:HD2	2.00	0.43
2:L:341:SER:C	2:L:343:GLN:N	2.77	0.43
2:M:118:GLU:O	2:M:286:LYS:HG2	2.18	0.43
2:N:28:ALA:HB3	2:N:71:LEU:HD21	2.01	0.43
1:Q:136:VAL:CG1	1:Q:137:ILE:N	2.78	0.43
1:Q:427:VAL:O	1:Q:431:LEU:HB2	2.18	0.43
1:R:51:GLU:CA	1:R:94:ILE:HG22	2.40	0.43
1:S:102:GLY:HA3	1:S:122:ASP:O	2.17	0.43
1:S:166:LEU:HD22	1:S:166:LEU:C	2.43	0.43
1:S:263:LEU:HD12	1:S:328:PRO:HB2	2.01	0.43
2:T:89:ASN:HD21	2:T:93:GLU:CG	2.29	0.43
2:T:132:VAL:HG21	2:T:334:VAL:CG2	2.49	0.43
2:T:229:LYS:O	2:T:232:ASP:HB3	2.18	0.43
2:T:353:HIS:CE1	2:T:420:LEU:HD21	2.54	0.43
2:U:86:ARG:NH2	2:U:99:GLY:H	2.17	0.43
2:V:119:LEU:HD22	2:V:283:THR:HG21	2.00	0.43
2:V:124:GLU:HG2	2:V:141:LYS:HE2	2.01	0.43
2:b:254:VAL:O	2:b:258:LEU:HB2	2.19	0.43
2:d:332:PRO:O	2:d:334:VAL:N	2.41	0.43
1:A:91:THR:HG21	1:A:93:ARG:HD3	2.01	0.43
1:A:268:VAL:HG23	1:A:271:ARG:NH2	2.34	0.43
1:B:439:MET:HG3	1:B:443:GLN:HB2	2.01	0.43
2:D:84:LEU:HD13	2:D:201:LYS:CG	2.49	0.43
2:D:229:LYS:O	2:D:232:ASP:HB3	2.18	0.43
2:D:279:GLN:NE2	2:D:294:GLN:HE22	2.13	0.43
2:D:413:SER:OG	2:D:414:PRO:HD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:265:VAL:CA	3:G:273:THR:HG22	2.48	0.43
2:E:437:HIS:HB2	2:U:381:GLU:HG3	1.99	0.43
2:F:42:VAL:HG13	2:F:51:VAL:HG13	2.00	0.43
2:F:325:ILE:CD1	2:F:335:ASP:HA	2.48	0.43
3:G:9:LYS:HD3	4:H:129:ARG:HG2	2.01	0.43
3:G:63:LYS:HD2	3:G:212:LYS:HE2	2.00	0.43
3:G:190:LEU:HD22	3:G:190:LEU:HA	1.83	0.43
4:H:131:ILE:HD12	4:H:131:ILE:HA	1.92	0.43
1:I:205:ILE:HD13	1:I:225:VAL:CG1	2.49	0.43
1:J:446:LEU:HD23	1:J:447:VAL:N	2.33	0.43
1:K:151:LYS:HE3	1:K:433:GLN:CG	2.48	0.43
1:K:236:TYR:CE1	1:K:293:LEU:HD11	2.52	0.43
1:K:365:ARG:O	1:K:367:ALA:N	2.52	0.43
2:M:193:MET:HE1	2:M:202:VAL:HG21	1.99	0.43
2:N:25:VAL:CG1	2:N:26:TYR:H	2.31	0.43
3:O:253:GLY:O	3:O:257:ILE:HG13	2.18	0.43
1:Q:368:VAL:O	1:Q:370:PRO:HD3	2.19	0.43
1:R:186:GLN:NE2	1:R:189:SER:OG	2.52	0.43
1:R:369:ASN:C	1:R:369:ASN:HD22	2.25	0.43
1:R:474:TYR:CD2	1:R:474:TYR:C	2.97	0.43
1:S:198:ILE:HD13	1:S:239:PRO:HG3	1.99	0.43
1:S:366:PRO:HD2	1:S:432:LYS:HA	2.01	0.43
2:V:392:ARG:NH1	2:V:436:ASP:OD2	2.52	0.43
1:a:220:ASN:CG	1:a:220:ASN:O	2.62	0.43
1:a:471:LEU:HD13	1:a:474:TYR:HE1	1.83	0.43
2:b:426:GLY:CA	2:b:449:ILE:HD12	2.44	0.43
2:c:115:SER:CB	2:c:118:GLU:HB2	2.46	0.43
2:d:101:ILE:HG22	2:d:102:GLY:N	2.33	0.43
1:C:393:ILE:HD13	1:C:451:ALA:HB2	2.01	0.43
1:C:474:TYR:HD1	1:C:475:VAL:N	2.17	0.43
2:D:450:GLU:O	2:D:453:VAL:HG22	2.17	0.43
2:D:456:ALA:O	2:D:459:LEU:HB3	2.19	0.43
2:E:116:TYR:C	2:E:117:GLU:HG2	2.41	0.43
2:E:217:LEU:O	2:E:217:LEU:HD22	2.19	0.43
2:E:238:LEU:HD23	2:E:240:PHE:CZ	2.54	0.43
2:F:135:LEU:HB2	2:F:423:THR:HG21	2.01	0.43
3:G:74:ARG:HE	3:G:111:GLN:HB2	1.83	0.43
1:J:150:TYR:HE1	1:J:181:ASP:CB	2.32	0.43
2:L:17:PHE:CD1	2:L:23:PRO:CD	3.01	0.43
2:L:155:LYS:HB2	2:L:155:LYS:NZ	2.33	0.43
2:L:241:VAL:CG1	2:L:294:GLN:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:254:VAL:O	2:L:258:LEU:HB2	2.18	0.43
2:L:408:GLU:OE1	2:L:408:GLU:N	2.51	0.43
2:M:90:VAL:HG21	2:M:215:ASN:HB3	1.99	0.43
2:M:225:THR:HG22	2:M:281:ARG:HH22	1.84	0.43
2:N:173:TYR:CD1	2:N:236:ASP:O	2.72	0.43
3:O:102:MET:O	3:O:106:THR:HG23	2.19	0.43
1:S:32:VAL:O	2:V:47:GLY:HA2	2.19	0.43
1:S:195:TYR:HD1	1:S:259:ILE:HD11	1.79	0.43
2:V:77:VAL:HA	2:V:78:PRO:HD3	1.82	0.43
2:V:219:VAL:O	2:V:222:THR:HG22	2.18	0.43
1:Y:357:THR:HG23	1:Y:358:ASN:N	2.30	0.43
1:Y:368:VAL:O	1:Y:370:PRO:HD3	2.19	0.43
1:a:144:GLN:HE21	1:a:144:GLN:HB3	1.56	0.43
2:c:46:LEU:HD23	2:c:47:GLY:H	1.84	0.43
1:B:99:VAL:HG11	1:B:127:SER:HB3	2.01	0.43
1:B:104:LEU:HB3	1:B:222:ILE:HG22	2.01	0.43
2:D:11:ALA:O	2:D:54:ILE:HA	2.18	0.43
2:D:427:PHE:HA	2:D:430:ILE:CG2	2.46	0.43
2:F:25:VAL:CG1	2:F:26:TYR:H	2.31	0.43
2:F:324:GLN:CD	2:F:324:GLN:H	2.27	0.43
2:F:407:ALA:HA	2:F:410:PHE:HE2	1.84	0.43
1:J:158:PRO:HB2	1:J:381:ALA:HB3	1.99	0.43
1:K:263:LEU:HD12	1:K:328:PRO:HB2	2.01	0.43
1:K:474:TYR:HD1	1:K:475:VAL:N	2.17	0.43
2:M:131:LYS:HG3	2:M:418:VAL:CG1	2.45	0.43
3:O:63:LYS:HD2	3:O:212:LYS:HE2	2.00	0.43
3:O:74:ARG:HE	3:O:111:GLN:HB2	1.83	0.43
3:O:187:LEU:O	3:O:188:LEU:C	2.61	0.43
1:Q:98:PRO:HD2	1:Q:112:GLY:HA3	2.01	0.43
1:Q:268:VAL:HG23	1:Q:271:ARG:NH2	2.34	0.43
1:R:96:GLU:CG	1:R:97:VAL:N	2.80	0.43
1:S:259:ILE:O	1:S:259:ILE:CG1	2.66	0.43
2:T:128:THR:OG1	2:T:130:ILE:HG13	2.18	0.43
2:T:382:LEU:HD12	2:T:382:LEU:H	1.83	0.43
2:U:217:LEU:O	2:U:217:LEU:HD22	2.19	0.43
2:V:168:ILE:C	2:V:170:HIS:H	2.27	0.43
1:Y:397:LEU:O	1:Y:397:LEU:HD23	2.18	0.43
1:Y:446:LEU:HD13	1:Y:446:LEU:H	1.84	0.43
1:Z:150:TYR:HE1	1:Z:181:ASP:CB	2.32	0.43
1:a:159:ILE:HA	1:a:163:GLN:OE1	2.19	0.43
2:b:135:LEU:HD11	2:b:357:ALA:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:c:225:THR:HG22	2:c:281:ARG:HH22	1.84	0.43
2:c:238:LEU:HD23	2:c:240:PHE:CZ	2.54	0.43
2:d:73:HIS:CD2	2:d:74:PRO:HD2	2.49	0.43
2:d:106:ARG:O	2:d:107:TRP:HD1	2.00	0.43
2:d:368:GLN:HE22	2:d:371:LYS:NZ	2.17	0.43
2:d:398:ARG:HD2	2:d:440:GLU:HB3	2.01	0.43
1:A:205:ILE:HD13	1:A:225:VAL:CG1	2.49	0.42
1:B:394:ARG:O	1:B:394:ARG:HD2	2.18	0.42
1:C:104:LEU:HA	1:C:222:ILE:CG2	2.47	0.42
1:C:440:SER:OG	1:C:442:ALA:HB3	2.19	0.42
2:F:219:VAL:O	2:F:222:THR:HG22	2.18	0.42
3:G:27:ALA:HB2	3:G:242:ARG:HG2	2.01	0.42
3:G:102:MET:O	3:G:106:THR:HG23	2.19	0.42
1:I:268:VAL:HG23	1:I:271:ARG:NH2	2.34	0.42
1:I:282:GLY:O	3:O:276:LEU:CD2	2.67	0.42
1:J:99:VAL:HG11	1:J:127:SER:HB3	2.01	0.42
1:J:104:LEU:HD22	1:J:104:LEU:N	2.34	0.42
1:J:476:ASP:OD2	1:J:476:ASP:C	2.61	0.42
2:L:84:LEU:HD13	2:L:201:LYS:CG	2.49	0.42
2:L:126:LEU:H	2:L:126:LEU:CD2	2.26	0.42
2:M:135:LEU:HD22	2:M:136:MET:SD	2.58	0.42
2:M:238:LEU:HD23	2:M:240:PHE:CZ	2.54	0.42
2:M:285:THR:HG23	2:M:288:GLY:N	2.34	0.42
2:N:135:LEU:C	2:N:135:LEU:HD13	2.44	0.42
2:N:136:MET:HA	2:N:136:MET:HE3	2.01	0.42
2:N:437:HIS:CD2	2:N:437:HIS:H	2.37	0.42
3:O:283:ALA:O	3:O:284:ALA:C	2.62	0.42
1:S:209:VAL:HA	1:S:212:LEU:HB2	2.00	0.42
1:S:439:MET:HB2	1:S:443:GLN:NE2	2.33	0.42
2:T:254:VAL:O	2:T:258:LEU:HB2	2.18	0.42
2:V:106:ARG:O	2:V:107:TRP:HD1	2.00	0.42
2:V:116:TYR:C	2:V:116:TYR:HD2	2.26	0.42
3:W:188:LEU:HB2	3:W:223:VAL:CG2	2.49	0.42
3:W:260:LEU:HD23	4:X:134:THR:HG23	2.01	0.42
4:X:84:ILE:HD12	4:X:84:ILE:N	2.34	0.42
1:Y:138:GLU:HG3	1:Y:305:ASN:CB	2.48	0.42
1:a:136:VAL:C	1:a:138:GLU:N	2.77	0.42
1:a:440:SER:OG	1:a:442:ALA:HB3	2.19	0.42
2:b:84:LEU:HD13	2:b:201:LYS:CG	2.49	0.42
2:b:229:LYS:O	2:b:232:ASP:HB3	2.18	0.42
2:b:403:PRO:CD	2:b:445:MET:HG3	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:420:LEU:O	2:b:420:LEU:HD13	2.19	0.42
2:c:46:LEU:HD23	2:c:47:GLY:N	2.34	0.42
2:c:86:ARG:NH2	2:c:99:GLY:H	2.17	0.42
2:c:94:PRO:HG3	2:c:101:ILE:HG22	2.00	0.42
3:e:102:MET:O	3:e:106:THR:HG23	2.19	0.42
1:A:109:ASN:ND2	1:A:113:ALA:N	2.68	0.42
1:B:387:LYS:HA	1:B:387:LYS:HD2	1.79	0.42
2:D:42:VAL:HG22	2:D:51:VAL:HG11	2.01	0.42
2:D:155:LYS:HB2	2:D:155:LYS:NZ	2.33	0.42
2:E:86:ARG:NH2	2:E:99:GLY:H	2.17	0.42
2:E:99:GLY:O	2:E:100:GLU:HB2	2.18	0.42
2:E:193:MET:HE2	2:E:198:VAL:HG23	2.01	0.42
2:E:238:LEU:HA	2:E:291:THR:O	2.19	0.42
2:F:101:ILE:HG22	2:F:102:GLY:N	2.33	0.42
3:G:253:GLY:O	3:G:257:ILE:HG13	2.18	0.42
1:I:137:ILE:HD12	2:M:97:MET:H	1.84	0.42
1:I:480:ALA:HB1	1:I:483:MET:HE2	2.00	0.42
1:K:87:LYS:HE3	1:K:87:LYS:N	2.34	0.42
1:K:123:HIS:ND1	1:K:123:HIS:C	2.77	0.42
1:K:441:VAL:O	1:K:441:VAL:HG12	2.19	0.42
2:L:383:SER:O	2:L:387:LYS:HG2	2.19	0.42
2:M:142:GLY:HA3	2:M:284:SER:HB2	2.01	0.42
2:N:155:LYS:HZ1	2:N:297:TYR:N	2.17	0.42
1:Q:48:MET:HG3	1:Q:51:GLU:HB2	2.01	0.42
1:Q:136:VAL:CG2	2:U:183:THR:HG23	2.49	0.42
1:R:66:LEU:HB3	2:V:64:ARG:HD3	2.01	0.42
1:R:113:ALA:N	1:R:114:PRO:CD	2.81	0.42
1:R:442:ALA:C	1:R:444:GLN:N	2.76	0.42
1:R:476:ASP:OD2	1:R:476:ASP:C	2.61	0.42
1:S:365:ARG:O	1:S:367:ALA:N	2.52	0.42
2:T:161:GLU:HG3	2:T:404:PHE:CB	2.49	0.42
2:U:140:ALA:HB2	2:U:343:GLN:CG	2.49	0.42
2:U:238:LEU:HD23	2:U:240:PHE:CZ	2.54	0.42
2:V:199:ILE:O	2:V:202:VAL:HG12	2.19	0.42
1:Y:40:ARG:NH1	1:Y:40:ARG:HB2	2.35	0.42
1:Z:474:TYR:CD2	1:Z:474:TYR:C	2.97	0.42
1:a:104:LEU:CA	1:a:222:ILE:HG22	2.47	0.42
1:a:236:TYR:CE1	1:a:293:LEU:HD11	2.52	0.42
2:d:124:GLU:HG2	2:d:141:LYS:HE2	2.01	0.42
2:d:136:MET:HA	2:d:136:MET:HE3	2.01	0.42
2:d:177:ALA:HA	2:d:205:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:74:ARG:HE	3:e:111:GLN:HB2	1.83	0.42
4:f:84:ILE:HD12	4:f:84:ILE:N	2.34	0.42
1:B:39:ILE:HG22	1:B:73:ALA:HB3	2.00	0.42
1:B:103:LEU:HG	1:B:245:MET:CE	2.50	0.42
1:B:150:TYR:HE1	1:B:181:ASP:CB	2.32	0.42
1:C:365:ARG:O	1:C:367:ALA:N	2.52	0.42
2:D:111:ARG:CG	2:D:112:ALA:N	2.78	0.42
2:D:144:LYS:HA	2:D:292:SER:O	2.20	0.42
2:D:200:ASP:HA	2:D:201:LYS:HA	1.68	0.42
2:E:46:LEU:HD23	2:E:47:GLY:H	1.83	0.42
2:F:334:VAL:O	2:F:336:PRO:HD3	2.19	0.42
1:J:279:ARG:HA	1:J:280:PRO:HD3	1.90	0.42
1:K:136:VAL:O	1:K:137:ILE:CB	2.66	0.42
1:K:393:ILE:HD13	1:K:451:ALA:HB2	2.00	0.42
2:M:3:GLY:O	2:M:67:ASP:HA	2.20	0.42
2:M:402:GLN:CA	2:M:445:MET:HE2	2.48	0.42
1:R:193:CYS:HA	1:R:257:LEU:O	2.19	0.42
2:T:345:ASP:HB2	2:T:346:PRO:HD2	1.99	0.42
2:V:25:VAL:CG1	2:V:26:TYR:H	2.31	0.42
2:V:177:ALA:HA	2:V:205:VAL:HG13	2.01	0.42
1:a:263:LEU:HD12	1:a:328:PRO:HB2	2.01	0.42
2:b:11:ALA:O	2:b:54:ILE:HA	2.18	0.42
2:b:81:GLU:H	2:b:81:GLU:CD	2.27	0.42
2:b:243:ASN:HD22	2:b:243:ASN:HA	1.64	0.42
2:c:193:MET:HE2	2:c:198:VAL:HG23	2.02	0.42
1:A:40:ARG:NH1	1:A:40:ARG:HB2	2.35	0.42
1:B:193:CYS:HA	1:B:257:LEU:O	2.19	0.42
1:B:231:SER:HB3	1:B:234:LEU:HD22	2.01	0.42
1:C:104:LEU:CA	1:C:222:ILE:HG22	2.47	0.42
1:C:140:GLN:HB3	1:C:303:ARG:HD3	2.00	0.42
1:C:385:ILE:CD1	1:C:444:GLN:HG2	2.49	0.42
2:E:73:HIS:HB3	2:E:76:GLU:HG2	2.01	0.42
2:F:297:TYR:CE2	2:F:299:PRO:HA	2.53	0.42
2:F:359:GLY:HA3	2:F:431:MET:HE1	2.01	0.42
1:I:137:ILE:CD1	2:M:97:MET:H	2.32	0.42
1:I:256:ALA:O	1:I:324:LEU:HD12	2.20	0.42
1:I:284:GLU:O	1:I:285:ALA:HB3	2.19	0.42
1:I:308:TYR:CD1	1:I:308:TYR:C	2.98	0.42
1:I:397:LEU:O	1:I:397:LEU:HD23	2.18	0.42
1:J:231:SER:HB3	1:J:234:LEU:HD22	2.01	0.42
1:J:365:ARG:HA	1:J:365:ARG:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:394:ARG:O	1:J:394:ARG:HD2	2.18	0.42
1:K:93:ARG:HA	1:K:93:ARG:HD2	1.61	0.42
1:K:144:GLN:HE21	1:K:144:GLN:HB3	1.56	0.42
1:K:440:SER:OG	1:K:442:ALA:HB3	2.19	0.42
2:L:81:GLU:CD	2:L:81:GLU:H	2.27	0.42
2:M:432:GLU:HG3	2:M:432:GLU:O	2.19	0.42
4:P:10:SER:OG	4:P:82:THR:HG22	2.19	0.42
1:S:151:LYS:HE3	1:S:433:GLN:CG	2.48	0.42
1:S:175:LYS:HE3	1:S:175:LYS:HB2	1.86	0.42
2:U:139:PHE:CE2	2:U:162:LEU:HD21	2.49	0.42
2:U:282:ILE:HG13	2:U:282:ILE:O	2.19	0.42
3:W:34:SER:HB3	3:W:236:ALA:HA	2.01	0.42
3:W:283:ALA:O	3:W:284:ALA:C	2.62	0.42
1:Y:233:ALA:CA	1:Y:273:ILE:HD11	2.49	0.42
1:Y:256:ALA:O	1:Y:324:LEU:HD12	2.20	0.42
1:Z:104:LEU:HB3	1:Z:222:ILE:HG22	2.01	0.42
1:Z:231:SER:HB3	1:Z:234:LEU:HD22	2.01	0.42
1:Z:397:LEU:HD22	1:Z:397:LEU:HA	1.75	0.42
1:a:259:ILE:O	1:a:259:ILE:CG1	2.66	0.42
1:a:426:LYS:CD	1:a:460:GLU:HB3	2.47	0.42
2:b:132:VAL:HG21	2:b:334:VAL:CG2	2.49	0.42
2:b:331:TYR:C	2:b:333:ALA:H	2.28	0.42
2:c:217:LEU:O	2:c:217:LEU:HD22	2.19	0.42
2:c:325:ILE:HG23	2:c:330:ILE:HG12	2.02	0.42
2:c:353:HIS:HD2	2:c:353:HIS:O	2.03	0.42
3:e:173:LYS:HG2	3:e:233:GLU:OE2	2.19	0.42
1:A:104:LEU:HA	1:A:222:ILE:HG12	2.02	0.42
1:A:480:ALA:HB1	1:A:483:MET:HE2	2.00	0.42
1:B:49:GLN:NE2	2:F:10:GLY:H	2.16	0.42
1:B:259:ILE:O	1:B:259:ILE:CG1	2.65	0.42
1:C:510:THR:O	1:C:511:GLN:CB	2.68	0.42
2:D:356:THR:O	2:D:360:VAL:HG23	2.20	0.42
2:D:387:LYS:CA	2:D:390:VAL:HG12	2.48	0.42
2:E:147:LEU:HD23	2:E:319:VAL:HB	2.02	0.42
2:E:167:ALA:HB1	2:E:201:LYS:HG3	2.02	0.42
2:F:194:THR:HA	2:F:199:ILE:HG13	2.02	0.42
2:F:264:ALA:C	2:F:265:VAL:HG23	2.43	0.42
4:H:31:GLU:O	4:H:31:GLU:HG3	2.20	0.42
1:I:40:ARG:NH1	1:I:40:ARG:HB2	2.35	0.42
1:I:98:PRO:HD2	1:I:112:GLY:HA3	2.01	0.42
1:J:140:GLN:HB2	1:J:305:ASN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:144:LYS:HA	2:L:292:SER:O	2.18	0.42
2:M:443:PHE:HD2	2:M:443:PHE:H	1.65	0.42
1:Q:84:GLU:OE1	2:T:22:VAL:HG11	2.20	0.42
1:Q:103:LEU:HD22	1:Q:121:LEU:HD21	2.02	0.42
1:Q:205:ILE:HD13	1:Q:225:VAL:CG1	2.49	0.42
1:Q:233:ALA:O	1:Q:237:LEU:HB2	2.20	0.42
1:R:230:GLU:HB3	1:R:234:LEU:HD23	2.00	0.42
1:S:186:GLN:CG	1:S:191:ILE:HB	2.49	0.42
1:S:291:PHE:HZ	2:T:209:MET:CE	2.33	0.42
2:U:46:LEU:HD23	2:U:47:GLY:H	1.84	0.42
2:U:242:ASP:O	2:U:295:ALA:HB3	2.19	0.42
3:W:224:GLU:OE1	4:X:85:ARG:NH2	2.49	0.42
1:Y:104:LEU:HA	1:Y:222:ILE:HG12	2.02	0.42
1:a:157:ILE:N	1:a:158:PRO:HD3	2.33	0.42
2:b:115:SER:C	2:b:117:GLU:OE1	2.62	0.42
2:b:302:ASP:OD1	2:b:304:THR:HG22	2.20	0.42
2:b:398:ARG:HB2	2:b:444:TYR:HA	2.02	0.42
2:c:332:PRO:C	2:c:334:VAL:H	2.28	0.42
2:d:70:ASP:C	2:d:70:ASP:OD1	2.63	0.42
1:A:98:PRO:HD2	1:A:112:GLY:HA3	2.01	0.42
1:A:175:LYS:O	1:A:176:THR:C	2.58	0.42
1:A:308:TYR:CD1	1:A:308:TYR:C	2.98	0.42
1:A:368:VAL:O	1:A:370:PRO:HD3	2.19	0.42
1:B:151:LYS:HD2	1:B:430:LEU:O	2.20	0.42
1:B:430:LEU:HA	1:B:430:LEU:HD23	1.79	0.42
1:C:44:LEU:HD11	1:C:90:CYS:HB2	2.01	0.42
1:C:87:LYS:N	1:C:87:LYS:HE3	2.34	0.42
2:E:140:ALA:HB2	2:E:343:GLN:CG	2.50	0.42
2:F:106:ARG:C	2:F:107:TRP:CD1	2.91	0.42
2:F:360:VAL:O	2:F:364:LEU:HB2	2.19	0.42
3:G:283:ALA:O	3:G:284:ALA:C	2.62	0.42
4:H:10:SER:OG	4:H:82:THR:HG22	2.19	0.42
1:J:193:CYS:HA	1:J:257:LEU:O	2.19	0.42
1:J:211:LYS:HG3	1:J:215:HIS:HD2	1.85	0.42
1:J:233:ALA:HA	1:J:236:TYR:HD2	1.84	0.42
1:K:104:LEU:CA	1:K:222:ILE:HG22	2.47	0.42
1:K:366:PRO:HD2	1:K:432:LYS:HA	2.01	0.42
2:L:229:LYS:HE2	2:L:229:LYS:HB2	1.81	0.42
2:L:337:LEU:HD22	2:L:365:GLN:HG2	2.01	0.42
2:M:86:ARG:NH2	2:M:99:GLY:H	2.17	0.42
1:Q:136:VAL:HG12	1:Q:137:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:233:ALA:CA	1:Q:273:ILE:HD11	2.49	0.42
1:R:211:LYS:HG3	1:R:215:HIS:HD2	1.85	0.42
1:R:365:ARG:HA	1:R:365:ARG:HD2	1.82	0.42
1:S:474:TYR:HD1	1:S:475:VAL:N	2.17	0.42
2:T:155:LYS:N	7:T:600:ADP:O1B	2.53	0.42
2:U:3:GLY:O	2:U:67:ASP:HA	2.20	0.42
2:U:93:GLU:HA	2:U:94:PRO:HD3	1.92	0.42
2:U:330:ILE:O	2:U:330:ILE:HG13	2.20	0.42
2:V:148:PHE:CE1	2:V:296:VAL:HG11	2.55	0.42
2:V:332:PRO:O	2:V:334:VAL:N	2.42	0.42
3:W:224:GLU:CD	4:X:85:ARG:NH2	2.77	0.42
4:X:31:GLU:O	4:X:31:GLU:HG3	2.20	0.42
1:Y:74:VAL:HG12	1:Y:233:ALA:HB2	2.00	0.42
1:Y:98:PRO:HD2	1:Y:112:GLY:HA3	2.01	0.42
1:Y:109:ASN:HD21	1:Y:113:ALA:N	2.14	0.42
1:Z:233:ALA:HA	1:Z:236:TYR:HD2	1.84	0.42
1:Z:439:MET:HG3	1:Z:443:GLN:HB2	2.01	0.42
1:Z:476:ASP:OD2	1:Z:476:ASP:C	2.61	0.42
2:b:255:SER:OG	2:b:260:ARG:HB2	2.19	0.42
2:c:302:ASP:C	2:c:304:THR:H	2.27	0.42
2:d:168:ILE:C	2:d:170:HIS:H	2.27	0.42
2:d:376:ILE:HG21	4:f:125:ILE:HD11	2.00	0.42
1:B:365:ARG:HD2	1:B:365:ARG:HA	1.82	0.42
1:B:442:ALA:C	1:B:444:GLN:N	2.76	0.42
1:B:474:TYR:CD2	1:B:474:TYR:C	2.97	0.42
1:C:259:ILE:O	1:C:259:ILE:CG1	2.66	0.42
1:C:274:SER:CB	1:C:287:PRO:HG3	2.48	0.42
1:I:48:MET:HG3	1:I:51:GLU:HB2	2.01	0.42
1:I:93:ARG:HB2	1:I:96:GLU:HG3	2.01	0.42
1:I:163:GLN:HG2	1:I:164:ARG:H	1.83	0.42
1:J:104:LEU:HB3	1:J:222:ILE:HG22	2.01	0.42
1:J:259:ILE:HG22	1:J:327:LEU:HD21	2.01	0.42
1:J:283:ARG:NH1	2:N:300:ALA:HB3	2.31	0.42
1:K:238:ALA:HB3	1:K:239:PRO:HD3	2.02	0.42
2:L:133:ILE:HG22	2:L:133:ILE:O	2.20	0.42
2:L:224:LEU:C	2:L:224:LEU:HD13	2.45	0.42
2:M:144:LYS:NZ	2:M:279:GLN:HB3	2.35	0.42
2:N:16:GLU:CG	2:N:18:PRO:HD3	2.47	0.42
2:N:70:ASP:C	2:N:70:ASP:OD1	2.62	0.42
2:N:124:GLU:HG2	2:N:141:LYS:HE2	2.01	0.42
2:N:199:ILE:O	2:N:202:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:219:LEU:HD12	3:O:219:LEU:HA	1.76	0.42
1:Q:40:ARG:NH1	1:Q:40:ARG:HB2	2.35	0.42
1:Q:237:LEU:HD12	1:Q:237:LEU:HA	1.82	0.42
1:R:231:SER:HB3	1:R:234:LEU:HD22	2.02	0.42
1:R:259:ILE:HG22	1:R:327:LEU:HD21	2.01	0.42
1:R:484:GLN:HA	1:R:487:ASN:OD1	2.20	0.42
1:S:129:VAL:HG23	1:S:130:GLU:N	2.35	0.42
2:T:161:GLU:HG3	2:T:404:PHE:HB3	2.01	0.42
2:T:255:SER:OG	2:T:260:ARG:HD2	2.19	0.42
2:U:15:VAL:HG21	2:U:68:VAL:HG11	2.02	0.42
2:U:73:HIS:HB3	2:U:76:GLU:HG2	2.01	0.42
2:U:402:GLN:HA	2:U:403:PRO:HD3	1.92	0.42
2:V:3:GLY:O	2:V:67:ASP:HA	2.20	0.42
2:V:111:ARG:NH1	2:V:111:ARG:CG	2.80	0.42
2:V:136:MET:HA	2:V:136:MET:HE3	2.01	0.42
2:V:257:LEU:HD22	2:V:257:LEU:N	2.34	0.42
3:W:201:LYS:HD2	3:W:203:TRP:HD1	1.85	0.42
2:b:4:LYS:HA	2:b:66:LEU:O	2.20	0.42
2:b:224:LEU:HD13	2:b:224:LEU:C	2.45	0.42
2:b:449:ILE:O	2:b:453:VAL:HG13	2.20	0.42
2:c:392:ARG:HH21	2:c:433:GLY:HA2	1.84	0.42
2:d:298:VAL:HA	2:d:299:PRO:HD3	1.79	0.42
1:A:397:LEU:O	1:A:397:LEU:HD23	2.18	0.42
1:A:479:HIS:HE2	1:A:503:ILE:HG23	1.85	0.42
1:B:104:LEU:HD22	1:B:104:LEU:N	2.34	0.42
1:B:233:ALA:HA	1:B:236:TYR:HD2	1.84	0.42
1:B:238:ALA:N	1:B:239:PRO:CD	2.83	0.42
2:D:244:ILE:HG23	2:D:275:MET:HE1	2.01	0.42
2:E:353:HIS:HD2	2:E:353:HIS:O	2.03	0.42
2:F:124:GLU:HG2	2:F:141:LYS:HE2	2.01	0.42
2:F:168:ILE:C	2:F:170:HIS:H	2.27	0.42
2:F:177:ALA:HA	2:F:205:VAL:HG13	2.02	0.42
3:G:7:ARG:HG3	3:G:264:TYR:HE1	1.84	0.42
1:I:282:GLY:C	3:O:276:LEU:HD21	2.45	0.42
1:J:151:LYS:HD2	1:J:430:LEU:O	2.20	0.42
1:J:474:TYR:CD2	1:J:474:TYR:C	2.97	0.42
2:M:167:ALA:HB1	2:M:201:LYS:HG3	2.02	0.42
2:N:276:GLY:O	2:N:280:GLU:HB2	2.19	0.42
3:O:187:LEU:HD13	3:O:223:VAL:HG13	2.01	0.42
4:P:31:GLU:O	4:P:31:GLU:HG3	2.20	0.42
4:P:84:ILE:HD12	4:P:84:ILE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:116:ASP:HA	1:R:117:GLY:HA2	1.57	0.42
1:R:238:ALA:N	1:R:239:PRO:CD	2.83	0.42
1:S:87:LYS:N	1:S:87:LYS:HE3	2.34	0.42
1:S:104:LEU:CA	1:S:222:ILE:HG22	2.47	0.42
1:S:510:THR:O	1:S:511:GLN:CB	2.68	0.42
2:T:398:ARG:HB2	2:T:444:TYR:HA	2.01	0.42
2:V:12:VAL:CG1	2:V:257:LEU:HB3	2.48	0.42
2:V:117:GLU:H	2:V:117:GLU:HG3	1.55	0.42
4:X:10:SER:OG	4:X:82:THR:HG22	2.19	0.42
1:Z:107:VAL:CG2	1:Z:116:ASP:HB2	2.42	0.42
1:a:53:ILE:HD11	1:a:63:ALA:HB2	2.02	0.42
1:a:493:ASN:H	1:a:496:ILE:HG12	1.81	0.42
2:b:12:VAL:HG12	2:b:52:ARG:HD2	2.00	0.42
2:b:427:PHE:O	2:b:431:MET:HG2	2.20	0.42
2:c:15:VAL:HG21	2:c:68:VAL:HG11	2.02	0.42
2:c:367:TYR:HE2	2:c:390:VAL:HG13	1.79	0.42
2:d:12:VAL:CG1	2:d:257:LEU:HB3	2.48	0.42
2:d:233:GLU:HG3	2:d:234:GLY:N	2.25	0.42
4:f:10:SER:OG	4:f:82:THR:HG22	2.19	0.42
1:B:259:ILE:HG22	1:B:327:LEU:HD23	2.00	0.42
1:B:484:GLN:HA	1:B:487:ASN:OD1	2.20	0.42
1:C:263:LEU:HD12	1:C:328:PRO:HB2	2.01	0.42
1:C:366:PRO:HD2	1:C:432:LYS:HA	2.01	0.42
2:E:46:LEU:HD23	2:E:47:GLY:N	2.34	0.42
2:E:130:ILE:HD12	2:E:404:PHE:CE2	2.55	0.42
2:E:166:ILE:C	2:E:166:ILE:HD12	2.45	0.42
2:E:282:ILE:HG13	2:E:282:ILE:O	2.20	0.42
2:E:384:GLU:HG3	2:E:385:GLU:H	1.85	0.42
3:G:42:ARG:N	3:G:43:PRO:CD	2.83	0.42
1:I:368:VAL:O	1:I:370:PRO:HD3	2.19	0.42
1:I:448:LEU:O	1:I:452:GLU:N	2.53	0.42
1:I:479:HIS:HE2	1:I:503:ILE:HG23	1.85	0.42
1:J:84:GLU:OE1	2:M:49:GLY:HA2	2.20	0.42
1:K:510:THR:O	1:K:511:GLN:CB	2.68	0.42
2:L:32:GLN:HE21	2:L:32:GLN:HB3	1.74	0.42
2:L:42:VAL:HG22	2:L:51:VAL:HG11	2.01	0.42
2:L:200:ASP:HA	2:L:201:LYS:HA	1.68	0.42
2:M:101:ILE:O	2:M:103:GLU:HG3	2.20	0.42
2:N:101:ILE:HG22	2:N:102:GLY:N	2.33	0.42
2:N:448:SER:OG	2:N:450:GLU:HG2	2.20	0.42
3:O:7:ARG:HG3	3:O:264:TYR:HE1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:91:THR:HG21	1:Q:93:ARG:HD3	2.01	0.42
1:Q:109:ASN:ND2	1:Q:113:ALA:N	2.67	0.42
1:Q:210:ARG:HH12	2:T:120:SER:C	2.28	0.42
1:Q:446:LEU:HD13	1:Q:446:LEU:H	1.84	0.42
1:R:104:LEU:HB3	1:R:222:ILE:HG22	2.01	0.42
1:S:238:ALA:HB3	1:S:239:PRO:HD3	2.02	0.42
2:U:3:GLY:HA3	2:U:17:PHE:HE2	1.76	0.42
2:U:299:PRO:HD2	2:U:308:PRO:CG	2.50	0.42
2:V:135:LEU:C	2:V:135:LEU:HD13	2.44	0.42
2:V:319:VAL:HA	2:V:339:SER:HG	1.83	0.42
2:V:349:VAL:HG22	2:V:349:VAL:O	2.19	0.42
3:W:189:PRO:HG2	3:W:189:PRO:O	2.19	0.42
1:Y:204:THR:O	1:Y:208:VAL:HG12	2.20	0.42
1:Z:99:VAL:HG11	1:Z:127:SER:HB3	2.00	0.42
1:Z:259:ILE:O	1:Z:259:ILE:CG1	2.65	0.42
1:a:44:LEU:HD11	1:a:90:CYS:HB2	2.01	0.42
2:b:347:LEU:H	2:b:347:LEU:HG	1.51	0.42
2:c:101:ILE:O	2:c:103:GLU:HG3	2.20	0.42
2:c:119:LEU:HA	2:c:285:THR:HA	2.02	0.42
2:c:161:GLU:HG2	2:c:406:VAL:HG13	2.01	0.42
2:d:131:LYS:H	2:d:402:GLN:NE2	2.17	0.42
3:e:201:LYS:HD2	3:e:203:TRP:HD1	1.85	0.42
3:e:283:ALA:O	3:e:284:ALA:C	2.62	0.42
4:f:64:LEU:C	4:f:66:GLY:H	2.28	0.42
1:A:66:LEU:HB2	2:E:8:VAL:HB	2.01	0.42
1:A:95:LEU:HA	1:A:95:LEU:HD13	1.80	0.42
1:A:204:THR:O	1:A:208:VAL:HG12	2.20	0.42
1:A:223:VAL:O	1:A:223:VAL:HG22	2.20	0.42
1:A:256:ALA:O	1:A:324:LEU:HD12	2.20	0.42
1:B:250:ARG:HG3	1:B:251:ASP:N	2.34	0.42
1:C:31:ILE:HG23	1:C:39:ILE:HG23	2.02	0.42
1:C:398:ALA:HA	1:C:401:ARG:NH2	2.35	0.42
2:E:286:LYS:HG2	2:E:286:LYS:H	1.72	0.42
2:E:435:TYR:HA	2:E:438:LEU:HD13	2.00	0.42
2:F:43:GLN:HG3	2:F:54:ILE:HG13	2.01	0.42
2:F:135:LEU:C	2:F:135:LEU:HD13	2.44	0.42
2:F:298:VAL:HA	2:F:299:PRO:HD3	1.82	0.42
4:H:24:GLN:NE2	4:H:51:ARG:HH11	2.18	0.42
4:H:129:ARG:HG2	4:H:129:ARG:H	1.62	0.42
1:I:223:VAL:O	1:I:223:VAL:HG22	2.20	0.42
1:J:62:ILE:CD1	1:J:95:LEU:CD2	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:484:GLN:HA	1:J:487:ASN:OD1	2.20	0.42
1:K:129:VAL:HG23	1:K:130:GLU:N	2.35	0.42
1:K:186:GLN:CG	1:K:191:ILE:HB	2.49	0.42
1:K:453:ARG:CG	1:K:454:GLY:N	2.83	0.42
2:M:445:MET:O	2:M:446:VAL:HG12	2.19	0.42
2:N:46:LEU:HD23	2:N:47:GLY:H	1.84	0.42
2:N:116:TYR:C	2:N:116:TYR:HD2	2.26	0.42
2:N:257:LEU:HD22	2:N:257:LEU:N	2.34	0.42
2:N:354:TYR:CZ	2:N:358:ARG:HD3	2.55	0.42
3:O:49:ARG:HA	3:O:49:ARG:HD2	1.90	0.42
4:P:24:GLN:NE2	4:P:51:ARG:HH11	2.18	0.42
1:R:99:VAL:HG11	1:R:127:SER:HB3	2.01	0.42
1:R:150:TYR:HE1	1:R:181:ASP:CB	2.32	0.42
1:R:233:ALA:HA	1:R:236:TYR:HD2	1.84	0.42
1:R:439:MET:HG3	1:R:443:GLN:HB2	2.01	0.42
2:T:133:ILE:O	2:T:133:ILE:HG22	2.20	0.42
2:T:427:PHE:O	2:T:430:ILE:HG22	2.20	0.42
2:U:99:GLY:O	2:U:100:GLU:HB2	2.18	0.42
2:V:275:MET:HE2	2:V:311:THR:OG1	2.20	0.42
1:Y:205:ILE:HD13	1:Y:225:VAL:CG1	2.49	0.42
1:Z:103:LEU:HG	1:Z:245:MET:CE	2.50	0.42
1:a:87:LYS:N	1:a:87:LYS:HE3	2.34	0.42
1:a:106:ARG:NH2	1:a:118:LYS:HB3	2.35	0.42
1:a:393:ILE:HD13	1:a:451:ALA:HB2	2.01	0.42
2:b:449:ILE:HD13	2:b:449:ILE:N	2.35	0.42
2:c:131:LYS:NZ	2:c:446:VAL:O	2.52	0.42
2:c:444:TYR:O	2:c:445:MET:HB2	2.19	0.42
2:d:264:ALA:C	2:d:265:VAL:HG23	2.45	0.42
1:A:233:ALA:O	1:A:237:LEU:HB2	2.20	0.41
1:A:459:VAL:O	1:A:459:VAL:HG22	2.20	0.41
1:C:213:GLU:OE1	1:C:218:LEU:HD23	2.20	0.41
1:C:272:GLN:HE22	2:F:273:GLU:HG3	1.84	0.41
1:C:442:ALA:C	1:C:444:GLN:N	2.72	0.41
1:C:457:ALA:O	1:C:460:GLU:HG2	2.19	0.41
2:D:4:LYS:HA	2:D:66:LEU:O	2.20	0.41
2:D:133:ILE:HG22	2:D:133:ILE:O	2.20	0.41
2:E:113:ALA:HB3	2:E:281:ARG:CB	2.50	0.41
2:F:70:ASP:OD1	2:F:70:ASP:C	2.63	0.41
2:F:116:TYR:HD2	2:F:116:TYR:O	2.03	0.41
1:I:95:LEU:HB3	1:I:129:VAL:HB	2.02	0.41
1:K:384:LYS:CE	1:K:493:ASN:HD21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:109:ILE:HA	2:L:225:THR:OG1	2.20	0.41
2:L:396:ILE:O	2:L:400:LEU:HD22	2.20	0.41
2:M:166:ILE:C	2:M:166:ILE:HD12	2.45	0.41
2:M:217:LEU:O	2:M:217:LEU:HD22	2.19	0.41
2:M:332:PRO:O	2:M:334:VAL:N	2.53	0.41
2:N:177:ALA:HA	2:N:205:VAL:HG13	2.02	0.41
2:N:233:GLU:HG3	2:N:234:GLY:N	2.25	0.41
1:R:176:THR:CB	5:R:600:ANP:O2B	2.67	0.41
1:R:446:LEU:HD11	1:R:469:ALA:HB1	2.02	0.41
1:S:44:LEU:HD11	1:S:90:CYS:HB2	2.01	0.41
1:S:385:ILE:CD1	1:S:444:GLN:HG2	2.49	0.41
1:S:457:ALA:O	1:S:460:GLU:HG2	2.19	0.41
2:T:109:ILE:HA	2:T:225:THR:OG1	2.20	0.41
2:T:213:PRO:HB3	2:T:253:GLU:HB2	2.02	0.41
2:V:70:ASP:OD1	2:V:70:ASP:C	2.63	0.41
3:W:102:MET:O	3:W:106:THR:HG23	2.19	0.41
4:X:64:LEU:C	4:X:66:GLY:H	2.28	0.41
1:Y:103:LEU:HD22	1:Y:121:LEU:HD21	2.02	0.41
1:Y:284:GLU:O	1:Y:285:ALA:HB3	2.19	0.41
1:Z:104:LEU:N	1:Z:104:LEU:HD22	2.34	0.41
2:b:42:VAL:HG22	2:b:51:VAL:HG11	2.01	0.41
2:b:137:CYS:SG	2:b:319:VAL:HG22	2.60	0.41
2:b:161:GLU:HG3	2:b:404:PHE:CB	2.50	0.41
2:b:237:VAL:HG22	2:b:238:LEU:N	2.35	0.41
2:b:456:ALA:O	2:b:459:LEU:HB3	2.20	0.41
2:d:116:TYR:HD2	2:d:116:TYR:O	2.03	0.41
3:e:27:ALA:HB2	3:e:242:ARG:HG2	2.01	0.41
1:B:211:LYS:HG3	1:B:215:HIS:HD2	1.85	0.41
1:B:482:LEU:C	1:B:484:GLN:N	2.78	0.41
1:C:89:LYS:HD3	1:C:89:LYS:N	2.35	0.41
1:C:453:ARG:CG	1:C:454:GLY:N	2.83	0.41
2:D:109:ILE:HA	2:D:225:THR:OG1	2.21	0.41
2:E:387:LYS:HD2	2:E:387:LYS:HA	1.56	0.41
2:F:29:LEU:HD13	2:F:40:LEU:O	2.20	0.41
2:F:398:ARG:HD2	2:F:440:GLU:HB3	2.02	0.41
4:H:84:ILE:HD12	4:H:84:ILE:N	2.34	0.41
1:J:238:ALA:N	1:J:239:PRO:CD	2.83	0.41
1:J:297:LEU:O	1:J:300:ARG:HB2	2.21	0.41
1:J:299:GLU:OE2	2:N:183:THR:HG23	2.19	0.41
1:K:89:LYS:HD3	1:K:89:LYS:N	2.36	0.41
1:K:398:ALA:HA	1:K:401:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:73:HIS:HB3	2:M:76:GLU:HG2	2.01	0.41
2:M:448:SER:O	2:M:451:GLU:HB3	2.20	0.41
1:Q:40:ARG:HB2	1:Q:40:ARG:HH11	1.85	0.41
1:Q:256:ALA:O	1:Q:324:LEU:HD12	2.20	0.41
1:Q:284:GLU:O	1:Q:285:ALA:HB3	2.19	0.41
1:R:104:LEU:N	1:R:104:LEU:HD22	2.34	0.41
1:S:274:SER:CB	1:S:287:PRO:HG3	2.48	0.41
1:S:398:ALA:HA	1:S:401:ARG:NH2	2.35	0.41
1:S:442:ALA:C	1:S:444:GLN:N	2.72	0.41
2:T:81:GLU:CD	2:T:81:GLU:H	2.27	0.41
2:T:224:LEU:C	2:T:224:LEU:HD13	2.45	0.41
2:V:29:LEU:HD13	2:V:40:LEU:O	2.20	0.41
2:V:194:THR:HA	2:V:199:ILE:HG13	2.02	0.41
1:Y:272:GLN:NE2	2:b:270:THR:HA	2.35	0.41
1:Y:308:TYR:CD1	1:Y:308:TYR:C	2.98	0.41
1:Y:364:ILE:CG1	1:Y:432:LYS:HE2	2.51	0.41
1:Y:413:LEU:HD21	1:Y:418:ARG:HD3	2.02	0.41
1:Z:95:LEU:O	1:Z:95:LEU:CG	2.64	0.41
1:Z:151:LYS:HD2	1:Z:430:LEU:O	2.20	0.41
1:a:95:LEU:HD12	1:a:129:VAL:CG1	2.49	0.41
1:a:366:PRO:HD2	1:a:432:LYS:HA	2.01	0.41
1:a:457:ALA:O	1:a:460:GLU:HG2	2.19	0.41
2:c:3:GLY:O	2:c:67:ASP:HA	2.20	0.41
2:d:3:GLY:O	2:d:67:ASP:HA	2.20	0.41
2:d:135:LEU:C	2:d:135:LEU:HD13	2.44	0.41
2:d:360:VAL:O	2:d:364:LEU:HB2	2.20	0.41
4:f:31:GLU:O	4:f:31:GLU:HG3	2.20	0.41
1:A:48:MET:HG3	1:A:51:GLU:HB2	2.01	0.41
1:B:292:TYR:CD2	2:F:216:ARG:NH1	2.85	0.41
1:C:53:ILE:HD11	1:C:63:ALA:HB2	2.02	0.41
1:C:129:VAL:HG23	1:C:130:GLU:N	2.35	0.41
2:D:111:ARG:HG3	2:D:112:ALA:H	1.85	0.41
2:E:388:LEU:O	2:E:392:ARG:HG3	2.20	0.41
2:F:199:ILE:O	2:F:202:VAL:HG12	2.19	0.41
1:I:104:LEU:HA	1:I:222:ILE:HG12	2.02	0.41
1:I:204:THR:O	1:I:208:VAL:HG12	2.20	0.41
1:K:53:ILE:HD11	1:K:63:ALA:HB2	2.02	0.41
1:K:344:ASN:O	1:K:348:ILE:HG13	2.20	0.41
2:L:123:GLN:HG3	2:L:123:GLN:O	2.20	0.41
2:L:132:VAL:CG2	2:L:400:LEU:HD12	2.50	0.41
2:M:353:HIS:HD2	2:M:353:HIS:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:29:LEU:HD13	2:N:40:LEU:O	2.20	0.41
1:R:151:LYS:HD2	1:R:430:LEU:O	2.20	0.41
1:R:257:LEU:HD11	1:R:327:LEU:HD22	2.03	0.41
1:R:297:LEU:O	1:R:300:ARG:HB2	2.20	0.41
1:S:106:ARG:NH2	1:S:118:LYS:HB3	2.35	0.41
2:T:93:GLU:HA	2:T:94:PRO:HD3	1.76	0.41
2:V:43:GLN:HG3	2:V:54:ILE:HG13	2.02	0.41
2:V:116:TYR:HD2	2:V:116:TYR:O	2.03	0.41
2:V:324:GLN:CD	2:V:324:GLN:H	2.26	0.41
3:W:48:MET:HE3	4:X:79:LEU:CD1	2.50	0.41
1:Y:48:MET:HG3	1:Y:51:GLU:HB2	2.01	0.41
1:Y:91:THR:HG21	1:Y:93:ARG:HD3	2.01	0.41
1:Y:109:ASN:ND2	1:Y:113:ALA:N	2.68	0.41
1:Y:348:ILE:HG23	2:c:209:MET:CE	2.39	0.41
1:Z:484:GLN:HA	1:Z:487:ASN:OD1	2.20	0.41
2:b:123:GLN:HG3	2:b:123:GLN:O	2.20	0.41
2:d:43:GLN:HG3	2:d:54:ILE:HG13	2.01	0.41
2:d:180:GLY:C	2:d:209:MET:HB3	2.45	0.41
3:e:7:ARG:HG3	3:e:264:TYR:HE1	1.84	0.41
1:A:210:ARG:HH12	2:D:120:SER:C	2.29	0.41
1:A:284:GLU:O	1:A:285:ALA:HB3	2.19	0.41
1:A:364:ILE:CG1	1:A:432:LYS:HE2	2.51	0.41
1:C:106:ARG:NH2	1:C:118:LYS:HB3	2.35	0.41
1:C:365:ARG:HG3	5:C:600:ANP:C6	2.50	0.41
1:C:365:ARG:HA	1:C:365:ARG:HD2	1.59	0.41
2:E:3:GLY:O	2:E:67:ASP:HA	2.20	0.41
2:E:28:ALA:HB2	2:E:75:ILE:HB	2.02	0.41
2:E:171:SER:HA	3:W:201:LYS:HE2	2.03	0.41
2:F:257:LEU:HD22	2:F:257:LEU:N	2.34	0.41
2:F:349:VAL:O	2:F:349:VAL:HG22	2.20	0.41
1:I:40:ARG:HB2	1:I:40:ARG:HH11	1.86	0.41
1:J:436:TYR:C	1:J:438:PRO:HD3	2.46	0.41
1:K:44:LEU:HD11	1:K:90:CYS:HB2	2.01	0.41
1:K:365:ARG:HB3	1:K:366:PRO:HD3	2.03	0.41
2:L:398:ARG:H	2:L:398:ARG:HG2	1.50	0.41
2:L:438:LEU:HA	2:L:439:PRO:HD3	1.84	0.41
2:M:193:MET:HE2	2:M:198:VAL:HG23	2.02	0.41
2:M:265:VAL:HG23	3:O:272:ILE:CG2	2.50	0.41
2:N:43:GLN:HG3	2:N:54:ILE:HG13	2.01	0.41
2:N:180:GLY:C	2:N:209:MET:HB3	2.45	0.41
2:N:306:PRO:O	2:N:310:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:410:PHE:CD2	2:N:410:PHE:N	2.75	0.41
3:O:9:LYS:HD3	4:P:129:ARG:HG2	2.02	0.41
3:O:18:LYS:O	3:O:18:LYS:HG2	2.21	0.41
3:O:42:ARG:N	3:O:43:PRO:CD	2.83	0.41
4:P:129:ARG:HG2	4:P:129:ARG:H	1.62	0.41
1:Q:163:GLN:HG2	1:Q:164:ARG:H	1.83	0.41
1:Q:308:TYR:CD1	1:Q:308:TYR:C	2.98	0.41
1:R:96:GLU:HA	1:R:129:VAL:HG13	2.02	0.41
1:R:449:PHE:HD1	1:R:453:ARG:NH1	2.19	0.41
1:S:440:SER:OG	1:S:442:ALA:HB3	2.19	0.41
2:T:4:LYS:HA	2:T:66:LEU:O	2.20	0.41
2:T:42:VAL:HG22	2:T:51:VAL:HG11	2.01	0.41
2:U:411:THR:HB	2:U:412:GLY:H	1.70	0.41
2:V:180:GLY:C	2:V:209:MET:HB3	2.45	0.41
1:Y:459:VAL:O	1:Y:459:VAL:HG22	2.20	0.41
1:Z:140:GLN:HB2	1:Z:305:ASN:HB3	2.02	0.41
1:Z:250:ARG:HG3	1:Z:251:ASP:N	2.34	0.41
1:Z:384:LYS:H	1:Z:384:LYS:CE	2.28	0.41
1:Z:430:LEU:CD1	1:Z:451:ALA:HB2	2.50	0.41
1:a:31:ILE:HG23	1:a:39:ILE:HG23	2.02	0.41
2:b:231:ARG:HD2	2:b:281:ARG:NH1	2.33	0.41
2:b:408:GLU:OE1	2:b:408:GLU:N	2.53	0.41
2:c:166:ILE:C	2:c:166:ILE:HD12	2.45	0.41
2:c:167:ALA:HB1	2:c:201:LYS:HG3	2.02	0.41
2:c:405:PHE:CZ	2:c:416:LYS:HA	2.56	0.41
2:d:162:LEU:HD13	2:d:162:LEU:HA	1.89	0.41
2:d:199:ILE:O	2:d:202:VAL:HG12	2.19	0.41
1:B:27:ASN:HD21	1:B:46:ASP:CB	2.11	0.41
1:B:116:ASP:HA	1:B:117:GLY:HA2	1.57	0.41
1:B:403:LEU:HD21	1:B:420:GLN:NE2	2.27	0.41
1:B:436:TYR:C	1:B:438:PRO:HD3	2.46	0.41
2:D:50:ILE:H	2:D:50:ILE:HG13	1.64	0.41
2:D:81:GLU:H	2:D:81:GLU:CD	2.27	0.41
2:F:161:GLU:CG	2:F:404:PHE:HB3	2.41	0.41
2:F:180:GLY:C	2:F:209:MET:HB3	2.45	0.41
3:G:201:LYS:HD2	3:G:203:TRP:HD1	1.85	0.41
1:K:213:GLU:OE1	1:K:218:LEU:HD23	2.20	0.41
1:K:263:LEU:HD22	1:K:294:HIS:CD2	2.56	0.41
1:K:474:TYR:CD1	1:K:475:VAL:N	2.89	0.41
2:L:377:LEU:CD1	2:L:381:GLU:HG2	2.50	0.41
2:N:3:GLY:O	2:N:67:ASP:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:17:PHE:CZ	2:N:70:ASP:HB2	2.56	0.41
2:N:116:TYR:HD2	2:N:116:TYR:O	2.03	0.41
2:N:159:MET:HE2	2:N:295:ALA:CB	2.50	0.41
3:O:201:LYS:HD2	3:O:203:TRP:HD1	1.85	0.41
4:P:64:LEU:C	4:P:66:GLY:H	2.28	0.41
1:Q:413:LEU:HD21	1:Q:418:ARG:HD3	2.02	0.41
1:R:103:LEU:HG	1:R:245:MET:CE	2.50	0.41
1:R:430:LEU:CD1	1:R:451:ALA:HB2	2.50	0.41
1:S:53:ILE:HD11	1:S:63:ALA:HB2	2.02	0.41
1:S:164:ARG:O	1:S:349:THR:HB	2.21	0.41
1:S:263:LEU:HD22	1:S:294:HIS:CD2	2.55	0.41
2:U:166:ILE:C	2:U:166:ILE:HD12	2.45	0.41
2:V:9:ILE:HB	2:V:12:VAL:HG12	2.03	0.41
2:V:12:VAL:O	2:V:12:VAL:HG13	2.21	0.41
2:V:448:SER:OG	2:V:450:GLU:HG2	2.20	0.41
1:Y:431:LEU:HD12	1:Y:431:LEU:HA	1.84	0.41
1:Z:103:LEU:HD22	1:Z:103:LEU:N	2.36	0.41
1:Z:257:LEU:HD11	1:Z:327:LEU:HD22	2.03	0.41
1:Z:397:LEU:HD11	1:Z:428:THR:HG22	2.03	0.41
1:a:263:LEU:HD22	1:a:294:HIS:CD2	2.55	0.41
1:a:453:ARG:CG	1:a:454:GLY:N	2.83	0.41
2:b:89:ASN:N	2:b:89:ASN:HD22	2.18	0.41
2:c:198:VAL:O	2:c:201:LYS:HE2	2.21	0.41
1:A:132:ILE:HD12	1:A:132:ILE:HA	1.95	0.41
1:B:62:ILE:HD13	1:B:62:ILE:N	2.35	0.41
1:B:257:LEU:HD11	1:B:327:LEU:HD22	2.03	0.41
1:B:297:LEU:O	1:B:300:ARG:HB2	2.20	0.41
2:D:64:ARG:HD3	2:D:64:ARG:H	1.86	0.41
2:D:332:PRO:HG2	2:D:401:SER:HA	2.02	0.41
2:D:419:SER:OG	2:D:422:ASP:HB2	2.21	0.41
2:E:399:PHE:HA	2:E:443:PHE:O	2.21	0.41
2:F:9:ILE:HB	2:F:12:VAL:HG12	2.03	0.41
1:I:34:VAL:HG12	2:L:45:GLN:HB3	2.01	0.41
1:I:177:ALA:HB2	5:I:600:ANP:O1A	2.21	0.41
1:J:366:PRO:C	1:J:368:VAL:H	2.29	0.41
1:K:106:ARG:NH2	1:K:118:LYS:HB3	2.35	0.41
2:L:3:GLY:HA3	2:L:17:PHE:HE2	1.79	0.41
2:L:4:LYS:HA	2:L:66:LEU:O	2.20	0.41
2:L:237:VAL:HG22	2:L:238:LEU:N	2.35	0.41
2:M:15:VAL:HG21	2:M:68:VAL:HG11	2.02	0.41
1:Q:364:ILE:CG1	1:Q:432:LYS:HE2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:266:GLN:HE21	1:R:266:GLN:HB3	1.62	0.41
1:S:493:ASN:O	1:S:496:ILE:HD11	2.19	0.41
2:T:442:ALA:HB1	2:T:452:ALA:O	2.21	0.41
2:T:449:ILE:HD13	2:T:449:ILE:N	2.35	0.41
2:U:167:ALA:HB1	2:U:201:LYS:HG3	2.02	0.41
2:V:221:LEU:HD22	2:V:281:ARG:NH2	2.36	0.41
3:W:7:ARG:HG3	3:W:264:TYR:HE1	1.84	0.41
1:Y:40:ARG:HB2	1:Y:40:ARG:HH11	1.86	0.41
1:Z:238:ALA:N	1:Z:239:PRO:CD	2.83	0.41
1:Z:449:PHE:HD1	1:Z:453:ARG:NH1	2.19	0.41
1:a:213:GLU:OE1	1:a:218:LEU:HD23	2.20	0.41
2:c:142:GLY:HA2	2:c:290:ILE:O	2.20	0.41
2:d:5:ILE:CG2	2:d:64:ARG:HA	2.51	0.41
2:d:257:LEU:HD22	2:d:257:LEU:N	2.34	0.41
1:A:237:LEU:HA	1:A:237:LEU:HD12	1.82	0.41
1:B:103:LEU:HD22	1:B:103:LEU:N	2.36	0.41
1:B:397:LEU:HD11	1:B:428:THR:HG22	2.03	0.41
1:B:423:HIS:CD2	1:B:423:HIS:C	2.96	0.41
1:C:263:LEU:HD22	1:C:294:HIS:CD2	2.56	0.41
1:C:344:ASN:O	1:C:348:ILE:HG13	2.20	0.41
1:C:424:GLY:HA2	1:C:427:VAL:HG12	2.03	0.41
2:D:89:ASN:N	2:D:89:ASN:HD22	2.18	0.41
2:D:135:LEU:HD11	2:D:357:ALA:HA	2.02	0.41
2:D:213:PRO:HB3	2:D:253:GLU:HB2	2.02	0.41
2:E:402:GLN:HA	2:E:403:PRO:HD3	1.92	0.41
1:I:176:THR:O	1:I:177:ALA:C	2.63	0.41
1:I:233:ALA:CA	1:I:273:ILE:HD11	2.49	0.41
1:J:103:LEU:HG	1:J:245:MET:CE	2.50	0.41
1:J:103:LEU:HD22	1:J:103:LEU:N	2.36	0.41
1:J:176:THR:CB	5:J:600:ANP:O2B	2.68	0.41
1:J:397:LEU:HD11	1:J:428:THR:HG22	2.03	0.41
1:J:423:HIS:CD2	1:J:423:HIS:C	2.96	0.41
2:L:345:ASP:HB2	2:L:346:PRO:HD2	2.02	0.41
2:M:3:GLY:HA3	2:M:17:PHE:HE2	1.76	0.41
2:M:125:LEU:HD21	2:M:349:VAL:HB	2.03	0.41
2:M:230:PHE:CB	2:M:237:VAL:HG11	2.51	0.41
2:M:231:ARG:HD3	2:M:290:ILE:CG1	2.48	0.41
2:M:273:GLU:O	2:M:277:VAL:HG23	2.21	0.41
2:N:33:ASN:HB3	2:N:62:LEU:CD2	2.51	0.41
2:N:168:ILE:C	2:N:170:HIS:H	2.27	0.41
1:R:449:PHE:CD1	1:R:453:ARG:NH1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:144:LYS:HA	2:T:292:SER:O	2.20	0.41
2:U:22:VAL:HA	2:U:23:PRO:HD3	1.90	0.41
2:U:193:MET:HE2	2:U:198:VAL:HG23	2.01	0.41
2:V:100:GLU:HG2	2:V:102:GLY:N	2.36	0.41
1:Y:95:LEU:HA	1:Y:95:LEU:HD13	1.80	0.41
1:Y:95:LEU:HB3	1:Y:129:VAL:HB	2.02	0.41
1:Y:231:SER:HB3	1:Y:234:LEU:HD22	2.03	0.41
1:Y:233:ALA:O	1:Y:237:LEU:HB2	2.20	0.41
1:Y:262:ASP:CG	1:Y:265:LYS:HG3	2.46	0.41
1:Z:84:GLU:HB2	2:c:22:VAL:HG11	2.03	0.41
1:Z:193:CYS:HA	1:Z:257:LEU:O	2.19	0.41
1:Z:297:LEU:O	1:Z:300:ARG:HB2	2.20	0.41
1:Z:403:LEU:HD21	1:Z:420:GLN:NE2	2.27	0.41
1:a:238:ALA:HB3	1:a:239:PRO:HD3	2.02	0.41
1:a:275:LEU:HD23	2:d:269:PRO:HG3	2.02	0.41
1:a:474:TYR:CD1	1:a:475:VAL:N	2.89	0.41
2:b:109:ILE:HA	2:b:225:THR:OG1	2.21	0.41
2:b:133:ILE:HG22	2:b:133:ILE:O	2.20	0.41
2:b:190:TYR:O	2:b:194:THR:HG23	2.21	0.41
2:b:229:LYS:HE2	2:b:229:LYS:HB2	1.81	0.41
2:c:77:VAL:HB	2:c:78:PRO:HD2	2.03	0.41
2:c:139:PHE:CE2	2:c:162:LEU:HD21	2.49	0.41
2:c:155:LYS:HB3	8:c:530:SO4:O2	2.21	0.41
2:d:194:THR:HA	2:d:199:ILE:HG13	2.02	0.41
4:f:24:GLN:NE2	4:f:51:ARG:HH11	2.18	0.41
1:A:304:VAL:HG21	1:A:308:TYR:CG	2.56	0.41
1:A:344:ASN:O	1:A:348:ILE:HG13	2.21	0.41
1:B:66:LEU:HB3	2:F:64:ARG:HD3	2.03	0.41
1:B:426:LYS:HD3	1:B:426:LYS:HA	1.50	0.41
1:B:449:PHE:CD1	1:B:453:ARG:NH1	2.89	0.41
1:B:449:PHE:HD1	1:B:453:ARG:NH1	2.19	0.41
1:C:140:GLN:HG2	1:C:305:ASN:CB	2.51	0.41
1:C:164:ARG:O	1:C:349:THR:HB	2.21	0.41
2:D:101:ILE:O	2:D:101:ILE:HG12	2.21	0.41
2:D:123:GLN:HG3	2:D:123:GLN:O	2.20	0.41
2:D:190:TYR:O	2:D:194:THR:HG23	2.21	0.41
2:D:231:ARG:HD2	2:D:281:ARG:NH1	2.36	0.41
2:E:101:ILE:O	2:E:103:GLU:HG3	2.20	0.41
2:F:33:ASN:HB3	2:F:62:LEU:CD2	2.51	0.41
2:F:126:LEU:HB3	2:F:141:LYS:CD	2.42	0.41
2:F:231:ARG:HD3	2:F:290:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:233:GLU:HG3	2:F:234:GLY:N	2.25	0.41
2:F:392:ARG:NH1	2:F:436:ASP:OD2	2.50	0.41
3:G:18:LYS:O	3:G:18:LYS:HG2	2.21	0.41
1:I:233:ALA:O	1:I:237:LEU:HB2	2.20	0.41
1:I:456:LEU:H	1:I:456:LEU:HD12	1.86	0.41
1:J:449:PHE:CD1	1:J:453:ARG:NH1	2.89	0.41
2:L:180:GLY:HA2	2:L:207:GLY:O	2.21	0.41
2:M:239:LEU:HD23	2:M:282:ILE:HG21	2.02	0.41
2:M:321:LEU:HD12	2:M:321:LEU:N	2.36	0.41
2:M:387:LYS:HD2	2:M:387:LYS:HA	1.62	0.41
2:M:402:GLN:HA	2:M:403:PRO:HD3	1.91	0.41
2:N:12:VAL:CG1	2:N:257:LEU:HB3	2.48	0.41
2:N:144:LYS:CE	2:N:282:ILE:HB	2.51	0.41
1:Q:151:LYS:HG3	1:Q:433:GLN:OE1	2.20	0.41
1:Q:262:ASP:CG	1:Q:265:LYS:HG3	2.46	0.41
1:R:96:GLU:CG	1:R:126:PHE:HB3	2.51	0.41
1:S:213:GLU:OE1	1:S:218:LEU:HD23	2.20	0.41
1:S:424:GLY:HA2	1:S:427:VAL:HG12	2.03	0.41
2:T:166:ILE:HG21	2:T:238:LEU:HD22	2.03	0.41
2:T:180:GLY:HA2	2:T:207:GLY:O	2.21	0.41
2:U:72:GLU:O	2:U:74:PRO:HD3	2.21	0.41
2:U:230:PHE:CB	2:U:237:VAL:HG11	2.51	0.41
2:U:399:PHE:HA	2:U:443:PHE:O	2.20	0.41
2:V:5:ILE:CG2	2:V:64:ARG:HA	2.51	0.41
2:V:237:VAL:CG2	2:V:290:ILE:HG12	2.50	0.41
2:V:395:LYS:HG3	2:V:443:PHE:CD2	2.56	0.41
3:W:42:ARG:N	3:W:43:PRO:CD	2.83	0.41
1:Y:406:PHE:CE1	3:e:25:MET:HB2	2.53	0.41
1:Z:216:GLY:HA2	1:Z:217:ALA:HA	1.46	0.41
1:Z:259:ILE:HG22	1:Z:327:LEU:HD21	2.01	0.41
1:Z:313:THR:HG21	1:Z:317:VAL:HG12	2.03	0.41
1:a:93:ARG:HB3	1:a:94:ILE:H	1.75	0.41
1:a:136:VAL:O	1:a:138:GLU:N	2.54	0.41
1:a:232:ALA:N	2:d:273:GLU:OE1	2.54	0.41
2:d:100:GLU:HG2	2:d:102:GLY:N	2.36	0.41
2:d:105:GLU:O	2:d:106:ARG:HG3	2.21	0.41
3:e:18:LYS:O	3:e:18:LYS:HG2	2.21	0.41
1:A:151:LYS:HG3	1:A:433:GLN:OE1	2.20	0.41
1:B:140:GLN:HB2	1:B:305:ASN:HB3	2.02	0.41
1:B:266:GLN:HE21	1:B:266:GLN:HB3	1.62	0.41
1:C:95:LEU:HD12	1:C:129:VAL:CG1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:GLY:O	1:C:428:THR:HG23	2.21	0.41
2:D:132:VAL:CG2	2:D:400:LEU:HD12	2.49	0.41
2:D:155:LYS:N	7:D:600:ADP:O1B	2.52	0.41
2:D:224:LEU:C	2:D:224:LEU:HD13	2.45	0.41
2:D:237:VAL:HG22	2:D:238:LEU:N	2.35	0.41
2:E:77:VAL:HB	2:E:78:PRO:HD2	2.03	0.41
2:E:146:GLY:N	2:E:315:LEU:HD22	2.35	0.41
2:E:198:VAL:O	2:E:201:LYS:HE2	2.21	0.41
2:E:325:ILE:HG23	2:E:330:ILE:CG1	2.51	0.41
2:E:349:VAL:HG21	2:E:353:HIS:HB3	1.93	0.41
2:E:382:LEU:HD23	2:E:382:LEU:HA	1.78	0.41
2:E:402:GLN:H	2:E:445:MET:HE1	1.84	0.41
2:F:3:GLY:O	2:F:67:ASP:HA	2.20	0.41
2:F:5:ILE:CG2	2:F:64:ARG:HA	2.51	0.41
2:F:136:MET:HA	2:F:136:MET:HE3	2.01	0.41
3:G:34:SER:HB3	3:G:236:ALA:HA	2.01	0.41
1:I:151:LYS:HG3	1:I:433:GLN:OE1	2.20	0.41
1:K:31:ILE:HG23	1:K:39:ILE:HG23	2.02	0.41
1:K:32:VAL:O	2:N:47:GLY:HA2	2.21	0.41
1:K:295:SER:HA	1:K:348:ILE:HD13	2.03	0.41
1:K:385:ILE:CB	1:K:492:TYR:HB3	2.49	0.41
2:L:93:GLU:HA	2:L:94:PRO:HD3	1.76	0.41
2:L:199:ILE:HA	2:L:202:VAL:HG22	2.03	0.41
2:L:243:ASN:HD22	2:L:243:ASN:HA	1.64	0.41
2:L:255:SER:OG	2:L:260:ARG:HB2	2.21	0.41
2:M:140:ALA:HB2	2:M:343:GLN:CG	2.51	0.41
2:M:225:THR:HG22	2:M:281:ARG:NH2	2.35	0.41
2:M:331:TYR:HD2	2:M:331:TYR:HA	1.63	0.41
2:M:409:VAL:HG23	4:f:55:GLN:HE22	1.86	0.41
2:N:111:ARG:NH1	2:N:111:ARG:CG	2.80	0.41
2:N:141:LYS:HE3	2:N:141:LYS:HB2	1.94	0.41
2:N:194:THR:HA	2:N:199:ILE:HG13	2.02	0.41
1:Q:204:THR:O	1:Q:208:VAL:HG12	2.20	0.41
1:Q:223:VAL:O	1:Q:223:VAL:HG22	2.20	0.41
1:Q:231:SER:HB3	1:Q:234:LEU:HD22	2.03	0.41
1:Q:344:ASN:O	1:Q:348:ILE:HG13	2.21	0.41
1:R:27:ASN:HD21	1:R:46:ASP:CB	2.12	0.41
1:R:97:VAL:HG11	1:R:111:LEU:O	2.21	0.41
1:R:279:ARG:HA	1:R:280:PRO:HD3	1.90	0.41
1:R:366:PRO:C	1:R:368:VAL:H	2.29	0.41
1:S:95:LEU:HD12	1:S:129:VAL:CG1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:277:LEU:HD12	1:S:277:LEU:HA	1.77	0.41
1:S:344:ASN:O	1:S:348:ILE:HG13	2.20	0.41
1:S:453:ARG:CG	1:S:454:GLY:N	2.83	0.41
1:S:464:ILE:C	1:S:466:SER:H	2.29	0.41
2:T:101:ILE:O	2:T:101:ILE:HG12	2.21	0.41
2:U:101:ILE:O	2:U:103:GLU:HG3	2.20	0.41
2:V:46:LEU:HD23	2:V:47:GLY:H	1.84	0.41
2:V:100:GLU:OE2	2:V:102:GLY:HA3	2.21	0.41
2:V:105:GLU:O	2:V:106:ARG:HG3	2.21	0.41
2:V:275:MET:O	2:V:279:GLN:HB2	2.21	0.41
2:V:298:VAL:HA	2:V:299:PRO:HD3	1.77	0.41
1:Y:137:ILE:CD1	2:c:97:MET:HB2	2.51	0.41
1:Y:456:LEU:H	1:Y:456:LEU:HD12	1.86	0.41
1:Z:172:GLN:HA	5:Z:600:ANP:N3B	2.32	0.41
1:Z:449:PHE:CD1	1:Z:453:ARG:NH1	2.89	0.41
1:Z:482:LEU:C	1:Z:484:GLN:N	2.78	0.41
1:a:129:VAL:HG23	1:a:130:GLU:N	2.35	0.41
1:a:191:ILE:HD12	1:a:191:ILE:H	1.86	0.41
1:a:385:ILE:CD1	1:a:444:GLN:HG2	2.49	0.41
1:a:398:ALA:HA	1:a:401:ARG:NH2	2.35	0.41
1:a:481:PRO:C	1:a:483:MET:H	2.29	0.41
2:b:161:GLU:HG3	2:b:404:PHE:CD2	2.56	0.41
2:b:244:ILE:CG2	2:b:275:MET:HE1	2.51	0.41
2:b:398:ARG:H	2:b:398:ARG:HG2	1.49	0.41
2:c:28:ALA:HB2	2:c:75:ILE:HB	2.02	0.41
2:c:73:HIS:HB3	2:c:76:GLU:HG2	2.01	0.41
2:d:100:GLU:OE2	2:d:102:GLY:HA3	2.21	0.41
3:e:42:ARG:N	3:e:43:PRO:CD	2.83	0.41
1:B:97:VAL:HG11	1:B:111:LEU:O	2.21	0.41
1:B:109:ASN:OD1	1:B:114:PRO:HG2	2.21	0.41
1:B:471:LEU:HD13	1:B:471:LEU:N	2.36	0.41
1:C:238:ALA:HB3	1:C:239:PRO:HD3	2.02	0.41
2:D:111:ARG:HH12	2:D:221:LEU:HD22	1.86	0.41
2:D:180:GLY:HA2	2:D:207:GLY:O	2.21	0.41
2:F:12:VAL:O	2:F:12:VAL:HG13	2.21	0.41
2:F:46:LEU:HD23	2:F:47:GLY:H	1.84	0.41
2:F:233:GLU:CG	2:F:234:GLY:H	2.26	0.41
3:G:49:ARG:HA	3:G:49:ARG:HD2	1.90	0.41
1:I:48:MET:HB2	2:M:61:GLY:C	2.46	0.41
1:I:109:ASN:ND2	1:I:113:ALA:N	2.68	0.41
1:I:231:SER:HB3	1:I:234:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:262:ASP:CG	1:I:265:LYS:HG3	2.46	0.41
1:J:426:LYS:HD3	1:J:426:LYS:HA	1.50	0.41
1:J:471:LEU:N	1:J:471:LEU:HD13	2.36	0.41
1:K:140:GLN:HG2	1:K:305:ASN:CB	2.51	0.41
2:L:64:ARG:H	2:L:64:ARG:HD3	1.86	0.41
2:L:377:LEU:HD12	2:L:381:GLU:HG2	2.03	0.41
2:M:72:GLU:O	2:M:74:PRO:HD3	2.21	0.41
2:N:100:GLU:OE2	2:N:102:GLY:HA3	2.21	0.41
2:N:100:GLU:HG2	2:N:102:GLY:N	2.36	0.41
2:N:221:LEU:CD2	2:N:278:LEU:HD13	2.44	0.41
2:N:351:GLN:HE21	2:N:355:ASP:CG	2.29	0.41
3:O:34:SER:HB3	3:O:236:ALA:HA	2.01	0.41
1:Q:456:LEU:H	1:Q:456:LEU:HD12	1.86	0.41
1:R:250:ARG:HG3	1:R:251:ASP:N	2.34	0.41
1:S:89:LYS:HD3	1:S:89:LYS:N	2.36	0.41
1:S:393:ILE:O	1:S:397:LEU:HB2	2.21	0.41
1:S:461:LEU:N	1:S:461:LEU:CD2	2.65	0.41
1:S:474:TYR:CD1	1:S:475:VAL:N	2.89	0.41
2:T:64:ARG:H	2:T:64:ARG:HD3	1.86	0.41
2:U:28:ALA:HB2	2:U:75:ILE:HB	2.02	0.41
2:V:279:GLN:CG	2:V:314:HIS:HB3	2.51	0.41
3:W:18:LYS:O	3:W:18:LYS:HG2	2.21	0.41
1:Y:94:ILE:O	1:Y:95:LEU:C	2.63	0.41
1:Y:103:LEU:CD1	1:Y:245:MET:HE3	2.50	0.41
1:Y:137:ILE:CD1	1:Y:137:ILE:C	2.52	0.41
1:a:151:LYS:HE2	1:a:439:MET:CE	2.51	0.41
1:a:344:ASN:O	1:a:348:ILE:HG13	2.20	0.41
1:a:365:ARG:HB3	1:a:366:PRO:HD3	2.03	0.41
2:b:118:GLU:O	2:b:120:SER:N	2.52	0.41
2:c:435:TYR:HA	2:c:438:LEU:HD13	2.03	0.41
2:d:12:VAL:O	2:d:12:VAL:HG13	2.21	0.41
2:d:17:PHE:CZ	2:d:70:ASP:HB2	2.56	0.41
2:d:82:ALA:HB1	2:d:102:GLY:CA	2.51	0.41
1:B:257:LEU:HD11	1:B:327:LEU:CD2	2.51	0.40
1:B:259:ILE:HG22	1:B:327:LEU:HD21	2.01	0.40
1:C:93:ARG:HA	1:C:93:ARG:HD2	1.61	0.40
1:C:295:SER:HA	1:C:348:ILE:HD13	2.03	0.40
1:C:382:GLN:HG2	1:C:386:MET:HB2	2.03	0.40
1:C:385:ILE:HG12	1:C:444:GLN:NE2	2.37	0.40
1:C:495:GLU:HG3	1:C:496:ILE:N	2.31	0.40
1:C:507:PHE:O	1:C:509:ALA:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:ILE:HA	2:D:202:VAL:HG22	2.03	0.40
2:D:324:GLN:O	2:D:328:LEU:HD23	2.21	0.40
2:E:72:GLU:O	2:E:74:PRO:HD3	2.21	0.40
2:E:237:VAL:CG2	2:E:290:ILE:HG23	2.47	0.40
2:E:353:HIS:HE1	2:E:420:LEU:HD11	1.83	0.40
2:F:82:ALA:HB1	2:F:102:GLY:CA	2.51	0.40
2:F:100:GLU:HG2	2:F:102:GLY:N	2.36	0.40
1:I:304:VAL:HG21	1:I:308:TYR:CG	2.56	0.40
1:I:364:ILE:HG13	1:I:432:LYS:HE3	2.00	0.40
1:J:62:ILE:N	1:J:62:ILE:HD13	2.35	0.40
1:K:80:ALA:HA	2:N:25:VAL:CG1	2.46	0.40
1:K:140:GLN:CG	1:K:305:ASN:HA	2.52	0.40
2:M:28:ALA:HB2	2:M:75:ILE:HB	2.02	0.40
2:M:365:GLN:CD	2:M:366:ARG:N	2.79	0.40
2:N:105:GLU:O	2:N:106:ARG:HG3	2.21	0.40
2:N:164:ARG:O	2:N:168:ILE:HG12	2.22	0.40
2:N:298:VAL:HA	2:N:299:PRO:HD3	1.77	0.40
3:O:66:TYR:CG	3:O:188:LEU:CD1	3.05	0.40
1:Q:95:LEU:HA	1:Q:95:LEU:HD13	1.80	0.40
1:R:313:THR:HG21	1:R:317:VAL:HG12	2.03	0.40
1:R:471:LEU:HD13	1:R:471:LEU:N	2.36	0.40
1:S:139:ARG:NH1	2:T:183:THR:HB	2.36	0.40
1:S:151:LYS:HE2	1:S:439:MET:CE	2.51	0.40
1:S:295:SER:HA	1:S:348:ILE:HD13	2.03	0.40
2:U:38:LEU:HD11	2:U:55:ALA:HB1	2.03	0.40
2:U:77:VAL:HB	2:U:78:PRO:HD2	2.03	0.40
2:V:386:ASP:O	2:V:390:VAL:HG13	2.21	0.40
4:X:41:LEU:HD12	4:X:42:LEU:N	2.37	0.40
1:Y:223:VAL:O	1:Y:223:VAL:HG22	2.20	0.40
1:Y:344:ASN:O	1:Y:348:ILE:HG13	2.21	0.40
1:Z:430:LEU:HA	1:Z:430:LEU:HD23	1.79	0.40
1:a:89:LYS:HD3	1:a:89:LYS:N	2.36	0.40
1:a:258:ILE:O	1:a:326:ALA:HA	2.21	0.40
1:a:393:ILE:O	1:a:397:LEU:HB2	2.21	0.40
2:b:438:LEU:HD23	2:b:438:LEU:H	1.85	0.40
2:c:72:GLU:O	2:c:74:PRO:HD3	2.21	0.40
2:d:9:ILE:HB	2:d:12:VAL:HG12	2.03	0.40
2:d:16:GLU:CG	2:d:18:PRO:HD3	2.47	0.40
2:d:29:LEU:HD13	2:d:40:LEU:O	2.20	0.40
3:e:34:SER:HB3	3:e:236:ALA:HA	2.01	0.40
3:e:118:GLY:O	3:e:122:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:O	1:A:95:LEU:C	2.63	0.40
1:A:95:LEU:HB3	1:A:129:VAL:HB	2.02	0.40
1:A:103:LEU:HD22	1:A:121:LEU:HD21	2.02	0.40
1:A:231:SER:HB3	1:A:234:LEU:HD22	2.03	0.40
1:A:504:LEU:HD23	1:A:504:LEU:HA	1.85	0.40
1:B:376:ARG:HA	2:F:410:PHE:CD1	2.56	0.40
2:D:229:LYS:HB2	2:D:229:LYS:HE2	1.81	0.40
2:D:428:LYS:O	2:D:432:GLU:HG3	2.21	0.40
2:E:379:MET:HB2	2:E:387:LYS:HZ1	1.81	0.40
2:E:418:VAL:HG23	2:E:422:ASP:HB2	2.02	0.40
1:I:440:SER:C	1:I:442:ALA:N	2.79	0.40
1:J:109:ASN:OD1	1:J:114:PRO:HG2	2.21	0.40
1:J:387:LYS:HA	1:J:387:LYS:HD2	1.79	0.40
1:J:397:LEU:HD22	1:J:397:LEU:HA	1.75	0.40
1:J:430:LEU:CD1	1:J:451:ALA:HB2	2.50	0.40
1:K:35:SER:HB2	2:N:44:GLN:HG2	2.04	0.40
2:L:89:ASN:N	2:L:89:ASN:HD22	2.18	0.40
2:L:305:ASP:O	2:L:308:PRO:HD2	2.21	0.40
2:L:426:GLY:CA	2:L:449:ILE:HD12	2.47	0.40
2:M:238:LEU:HA	2:M:291:THR:O	2.21	0.40
2:M:374:ILE:O	2:M:377:LEU:O	2.39	0.40
2:N:332:PRO:CG	2:N:401:SER:HA	2.51	0.40
3:O:64:HIS:CD2	3:O:64:HIS:C	2.98	0.40
1:Q:104:LEU:HA	1:Q:222:ILE:HG12	2.02	0.40
1:Q:304:VAL:HG21	1:Q:308:TYR:CG	2.56	0.40
1:Q:423:HIS:HA	1:Q:426:LYS:HD3	2.03	0.40
1:R:183:ILE:HD11	1:R:259:ILE:CD1	2.51	0.40
1:R:295:SER:HA	1:R:348:ILE:HD13	2.04	0.40
1:S:247:GLU:HG2	1:S:250:ARG:NH1	2.37	0.40
1:S:397:LEU:HD22	1:S:427:VAL:HG13	2.03	0.40
2:T:32:GLN:HE21	2:T:32:GLN:HB3	1.73	0.40
2:T:89:ASN:N	2:T:89:ASN:HD22	2.18	0.40
2:T:123:GLN:HG3	2:T:123:GLN:O	2.20	0.40
2:U:132:VAL:HG22	2:U:400:LEU:O	2.21	0.40
2:U:198:VAL:O	2:U:201:LYS:HE2	2.21	0.40
2:U:364:LEU:HD23	2:U:396:ILE:CG1	2.51	0.40
2:V:164:ARG:O	2:V:168:ILE:HG12	2.22	0.40
2:V:180:GLY:O	2:V:246:ARG:HD2	2.22	0.40
1:Y:139:ARG:O	1:Y:139:ARG:HG3	2.21	0.40
1:Y:304:VAL:HG21	1:Y:308:TYR:CG	2.56	0.40
1:a:295:SER:HA	1:a:348:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:144:LYS:HA	2:b:292:SER:O	2.22	0.40
2:b:166:ILE:HG21	2:b:238:LEU:HD22	2.03	0.40
2:b:180:GLY:HA2	2:b:207:GLY:O	2.21	0.40
2:b:384:GLU:O	2:b:388:LEU:HB2	2.21	0.40
2:c:38:LEU:HD11	2:c:55:ALA:HB1	2.03	0.40
1:A:40:ARG:HB2	1:A:40:ARG:HH11	1.86	0.40
1:A:139:ARG:O	1:A:139:ARG:HG3	2.21	0.40
1:B:136:VAL:HG11	2:F:206:TYR:CD1	2.56	0.40
1:B:313:THR:HG21	1:B:317:VAL:HG12	2.03	0.40
1:B:507:PHE:C	1:B:509:ALA:N	2.78	0.40
1:C:140:GLN:CG	1:C:305:ASN:HA	2.52	0.40
1:C:186:GLN:CG	1:C:191:ILE:HB	2.49	0.40
1:C:191:ILE:HD12	1:C:191:ILE:H	1.86	0.40
1:C:247:GLU:HG2	1:C:250:ARG:NH1	2.37	0.40
1:C:492:TYR:CE1	1:C:497:GLU:HB2	2.55	0.40
2:D:384:GLU:OE2	2:D:384:GLU:HA	2.21	0.40
2:E:385:GLU:O	2:E:389:VAL:HG23	2.21	0.40
1:I:103:LEU:HD22	1:I:121:LEU:HD21	2.02	0.40
1:J:482:LEU:C	1:J:484:GLN:N	2.78	0.40
1:K:66:LEU:HD12	2:L:8:VAL:HB	2.03	0.40
1:K:258:ILE:O	1:K:326:ALA:HA	2.21	0.40
1:K:385:ILE:HG12	1:K:444:GLN:NE2	2.37	0.40
1:K:424:GLY:O	1:K:428:THR:HG23	2.21	0.40
1:K:426:LYS:CD	1:K:460:GLU:HB3	2.47	0.40
2:L:166:ILE:HG21	2:L:238:LEU:HD22	2.03	0.40
2:L:190:TYR:O	2:L:194:THR:HG23	2.21	0.40
2:L:213:PRO:HB3	2:L:253:GLU:HB2	2.02	0.40
2:M:353:HIS:HE1	2:M:420:LEU:HD11	1.77	0.40
2:N:180:GLY:O	2:N:246:ARG:HD2	2.22	0.40
1:Q:139:ARG:HG3	1:Q:139:ARG:O	2.21	0.40
1:Q:211:LYS:NZ	1:Q:436:TYR:CE2	2.82	0.40
1:Q:459:VAL:O	1:Q:459:VAL:HG22	2.20	0.40
1:S:136:VAL:C	1:S:138:GLU:N	2.77	0.40
1:S:140:GLN:CG	1:S:305:ASN:HA	2.52	0.40
1:S:144:GLN:HE21	1:S:144:GLN:HB3	1.56	0.40
1:S:385:ILE:CB	1:S:492:TYR:HB3	2.49	0.40
2:T:123:GLN:O	2:T:123:GLN:CG	2.70	0.40
2:V:156:THR:HG22	2:V:157:VAL:N	2.32	0.40
3:W:190:LEU:HA	3:W:191:PRO:HD3	1.09	0.40
3:W:224:GLU:CD	4:X:85:ARG:HH21	2.29	0.40
4:X:24:GLN:NE2	4:X:51:ARG:HH11	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:151:LYS:HG3	1:Y:433:GLN:OE1	2.20	0.40
1:a:140:GLN:CG	1:a:305:ASN:HA	2.52	0.40
1:a:385:ILE:HG12	1:a:444:GLN:NE2	2.37	0.40
1:a:385:ILE:CB	1:a:492:TYR:HB3	2.49	0.40
1:a:507:PHE:O	1:a:509:ALA:N	2.55	0.40
2:b:64:ARG:HD3	2:b:64:ARG:H	1.86	0.40
2:b:268:GLN:C	2:b:270:THR:H	2.30	0.40
2:b:450:GLU:O	2:b:453:VAL:HG22	2.21	0.40
2:d:75:ILE:HB	2:d:109:ILE:HG12	2.03	0.40
2:d:221:LEU:CD2	2:d:278:LEU:HD13	2.43	0.40
1:B:137:ILE:HG21	2:F:96:ASP:HA	2.02	0.40
1:C:39:ILE:O	1:C:72:GLY:HA2	2.22	0.40
2:D:164:ARG:NH2	2:D:168:ILE:HD11	2.37	0.40
2:D:444:TYR:C	2:D:444:TYR:CD1	2.98	0.40
2:E:131:LYS:HB2	2:E:402:GLN:NE2	2.37	0.40
2:E:331:TYR:HD2	2:E:331:TYR:HA	1.66	0.40
2:E:356:THR:O	2:E:360:VAL:HG23	2.21	0.40
2:E:367:TYR:CE1	2:E:371:LYS:HE3	2.57	0.40
1:J:61:ALA:C	1:J:62:ILE:HD13	2.47	0.40
1:J:250:ARG:HG3	1:J:251:ASP:N	2.34	0.40
1:J:257:LEU:HD11	1:J:327:LEU:CD2	2.51	0.40
1:J:350:ASP:HA	1:J:376:ARG:NH2	2.37	0.40
1:J:467:PHE:O	1:J:471:LEU:HD22	2.22	0.40
1:K:382:GLN:HG2	1:K:386:MET:HB2	2.03	0.40
2:L:144:LYS:HE3	2:L:282:ILE:O	2.21	0.40
2:L:430:ILE:HG12	2:L:430:ILE:O	2.22	0.40
2:M:38:LEU:HD11	2:M:55:ALA:HB1	2.03	0.40
2:N:131:LYS:HE3	2:N:399:PHE:O	2.21	0.40
2:N:231:ARG:HG3	2:N:288:GLY:O	2.21	0.40
4:P:41:LEU:HD12	4:P:42:LEU:N	2.37	0.40
1:Q:95:LEU:HB3	1:Q:129:VAL:HB	2.02	0.40
2:T:307:SER:HB3	2:T:308:PRO:HD3	2.04	0.40
2:T:332:PRO:HG2	2:T:401:SER:HA	2.03	0.40
2:U:111:ARG:HH12	2:U:225:THR:CG2	2.35	0.40
2:U:384:GLU:HG3	2:U:385:GLU:H	1.86	0.40
3:W:64:HIS:CD2	3:W:64:HIS:C	2.98	0.40
1:Y:93:ARG:HG2	1:Y:93:ARG:H	1.74	0.40
1:Z:436:TYR:C	1:Z:438:PRO:HD3	2.46	0.40
1:Z:480:ALA:N	1:Z:481:PRO:CD	2.85	0.40
1:a:175:LYS:HE3	1:a:175:LYS:HB2	1.86	0.40
1:a:186:GLN:CG	1:a:191:ILE:HB	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:307:GLU:C	1:a:309:VAL:H	2.30	0.40
1:a:510:THR:O	1:a:511:GLN:CB	2.68	0.40
2:b:50:ILE:H	2:b:50:ILE:HG13	1.64	0.40
2:b:255:SER:OG	2:b:260:ARG:HD2	2.21	0.40
2:c:262:PRO:HD2	3:e:280:VAL:HG11	2.02	0.40
2:d:231:ARG:HG3	2:d:288:GLY:O	2.22	0.40
2:d:453:VAL:HG12	2:d:454:GLU:N	2.36	0.40
4:f:41:LEU:HD12	4:f:42:LEU:N	2.37	0.40
1:A:413:LEU:HD21	1:A:418:ARG:HD3	2.02	0.40
1:C:307:GLU:C	1:C:309:VAL:H	2.30	0.40
1:C:365:ARG:HB3	1:C:366:PRO:HD3	2.03	0.40
1:C:446:LEU:HD23	1:C:447:VAL:HG23	2.04	0.40
1:C:474:TYR:CD1	1:C:475:VAL:N	2.89	0.40
1:C:492:TYR:CA	1:C:496:ILE:HG13	2.50	0.40
2:D:73:HIS:ND1	2:D:73:HIS:N	2.70	0.40
2:D:128:THR:HG23	2:D:134:ASP:OD1	2.22	0.40
2:E:230:PHE:CB	2:E:237:VAL:HG11	2.51	0.40
2:E:305:ASP:C	2:E:308:PRO:HD2	2.47	0.40
2:F:214:GLY:O	2:F:217:LEU:HD23	2.22	0.40
4:H:75:ASN:HD22	4:H:75:ASN:C	2.29	0.40
1:I:413:LEU:HD21	1:I:418:ARG:HD3	2.02	0.40
1:K:481:PRO:C	1:K:483:MET:H	2.29	0.40
2:L:101:ILE:HG12	2:L:101:ILE:O	2.21	0.40
2:L:161:GLU:CG	2:L:404:PHE:HB3	2.51	0.40
2:M:198:VAL:O	2:M:201:LYS:HE2	2.21	0.40
2:M:325:ILE:HG23	2:M:330:ILE:CG1	2.52	0.40
2:N:73:HIS:CD2	2:N:74:PRO:HD2	2.49	0.40
3:O:72:VAL:CG1	3:O:166:LYS:HG3	2.52	0.40
3:O:118:GLY:O	3:O:122:VAL:HG23	2.21	0.40
1:Q:172:GLN:NE2	2:T:342:ARG:HH21	2.19	0.40
1:R:138:GLU:O	1:R:139:ARG:CG	2.61	0.40
1:R:138:GLU:OE1	1:R:305:ASN:ND2	2.55	0.40
1:R:343:THR:HG22	2:V:297:TYR:OH	2.21	0.40
1:S:31:ILE:HG23	1:S:39:ILE:HG23	2.02	0.40
1:S:258:ILE:O	1:S:326:ALA:HA	2.21	0.40
2:T:164:ARG:NH2	2:T:168:ILE:HD11	2.36	0.40
2:T:190:TYR:O	2:T:194:THR:HG23	2.21	0.40
2:T:379:MET:HE3	2:T:387:LYS:HB2	2.02	0.40
2:V:82:ALA:HB1	2:V:102:GLY:CA	2.51	0.40
2:V:216:ARG:O	2:V:219:VAL:HG12	2.22	0.40
3:W:191:PRO:HB3	3:W:192:ALA:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:410:ALA:HB2	3:e:26:VAL:HG22	2.04	0.40
1:Y:423:HIS:HA	1:Y:426:LYS:HD3	2.03	0.40
1:Y:495:GLU:O	1:Y:499:LYS:HG3	2.22	0.40
1:Z:266:GLN:HE21	1:Z:266:GLN:HB3	1.62	0.40
1:Z:295:SER:HA	1:Z:348:ILE:HD13	2.03	0.40
1:Z:366:PRO:C	1:Z:368:VAL:H	2.29	0.40
1:a:272:GLN:HE22	2:d:273:GLU:HG3	1.86	0.40
1:a:276:LEU:HD12	1:a:276:LEU:HA	1.84	0.40
1:a:384:LYS:CE	1:a:493:ASN:HD21	2.33	0.40
1:a:424:GLY:HA2	1:a:427:VAL:HG12	2.03	0.40
2:b:101:ILE:O	2:b:101:ILE:HG12	2.21	0.40
2:b:147:LEU:HD13	2:b:293:VAL:HG23	2.02	0.40
2:c:111:ARG:HH12	2:c:225:THR:CG2	2.35	0.40
2:c:230:PHE:CB	2:c:237:VAL:HG11	2.51	0.40
2:d:33:ASN:HB3	2:d:62:LEU:CD2	2.51	0.40
2:d:307:SER:HB2	2:d:308:PRO:CD	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	486/513 (95%)	433 (89%)	48 (10%)	5 (1%)	12	40
1	B	484/513 (94%)	421 (87%)	54 (11%)	9 (2%)	6	28
1	C	485/513 (94%)	429 (88%)	48 (10%)	8 (2%)	7	30
1	I	486/513 (95%)	433 (89%)	49 (10%)	4 (1%)	16	44
1	J	484/513 (94%)	419 (87%)	56 (12%)	9 (2%)	6	28
1	K	485/513 (94%)	428 (88%)	49 (10%)	8 (2%)	7	30
1	Q	486/513 (95%)	433 (89%)	47 (10%)	6 (1%)	10	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	484/513 (94%)	417 (86%)	58 (12%)	9 (2%)	6	28
1	S	485/513 (94%)	429 (88%)	48 (10%)	8 (2%)	7	30
1	Y	486/513 (95%)	431 (89%)	49 (10%)	6 (1%)	10	36
1	Z	484/513 (94%)	418 (86%)	57 (12%)	9 (2%)	6	28
1	a	485/513 (94%)	427 (88%)	50 (10%)	8 (2%)	7	30
2	D	456/459 (99%)	397 (87%)	54 (12%)	5 (1%)	11	38
2	E	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	4	21
2	F	456/459 (99%)	411 (90%)	40 (9%)	5 (1%)	11	38
2	L	456/459 (99%)	398 (87%)	53 (12%)	5 (1%)	11	38
2	M	456/459 (99%)	405 (89%)	41 (9%)	10 (2%)	5	25
2	N	456/459 (99%)	413 (91%)	37 (8%)	6 (1%)	9	34
2	T	456/459 (99%)	402 (88%)	48 (10%)	6 (1%)	9	34
2	U	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	4	21
2	V	456/459 (99%)	410 (90%)	40 (9%)	6 (1%)	9	34
2	b	456/459 (99%)	398 (87%)	51 (11%)	7 (2%)	8	32
2	c	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	4	21
2	d	456/459 (99%)	411 (90%)	39 (9%)	6 (1%)	9	34
3	G	282/286 (99%)	265 (94%)	17 (6%)	0	100	100
3	O	282/286 (99%)	266 (94%)	15 (5%)	1 (0%)	30	59
3	W	282/286 (99%)	264 (94%)	16 (6%)	2 (1%)	18	48
3	e	282/286 (99%)	265 (94%)	15 (5%)	2 (1%)	18	48
4	H	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	32
4	P	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	32
4	X	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	32
4	f	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	32
All	All	12964/13360 (97%)	11533 (89%)	1237 (10%)	194 (2%)	8	32

All (194) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	455	TYR
1	B	491	GLY
1	C	137	ILE

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Mol	Chain	Res	Type
2	E	333	ALA
2	E	348	VAL
2	F	18	PRO
1	I	137	ILE
1	J	455	TYR
1	J	491	GLY
1	K	137	ILE
2	M	348	VAL
2	N	18	PRO
1	Q	137	ILE
1	R	455	TYR
1	R	491	GLY
1	S	137	ILE
2	U	348	VAL
2	V	18	PRO
1	Y	137	ILE
1	Z	455	TYR
1	Z	491	GLY
1	a	137	ILE
2	c	348	VAL
2	d	18	PRO
1	A	458	ASP
1	B	216	GLY
1	B	410	ALA
1	C	441	VAL
2	E	102	GLY
2	F	333	ALA
1	J	216	GLY
1	J	410	ALA
1	K	441	VAL
2	M	102	GLY
2	M	333	ALA
2	N	333	ALA
1	Q	458	ASP
1	R	216	GLY
1	R	410	ALA
1	S	441	VAL
2	U	102	GLY
2	U	333	ALA
2	V	333	ALA
1	Y	458	ASP
1	Z	216	GLY

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Mol	Chain	Res	Type
1	Z	410	ALA
1	a	441	VAL
2	b	111	ARG
2	b	333	ALA
2	c	102	GLY
2	c	333	ALA
2	d	333	ALA
1	A	459	VAL
1	C	316	GLU
1	C	508	LYS
2	E	117	GLU
1	K	316	GLU
1	K	508	LYS
2	L	333	ALA
2	M	117	GLU
1	Q	459	VAL
1	S	316	GLU
1	S	508	LYS
2	T	333	ALA
2	U	117	GLU
1	Y	459	VAL
1	a	316	GLU
1	a	508	LYS
2	c	117	GLU
2	c	434	GLU
1	A	316	GLU
1	B	98	PRO
1	B	114	PRO
1	C	367	ALA
2	D	116	TYR
2	D	199	ILE
2	E	64	ARG
1	I	316	GLU
1	J	98	PRO
1	J	114	PRO
1	K	367	ALA
2	L	116	TYR
2	L	199	ILE
2	M	64	ARG
1	Q	316	GLU
1	R	98	PRO
1	R	114	PRO

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Mol	Chain	Res	Type
1	S	367	ALA
2	T	116	TYR
2	T	199	ILE
2	U	64	ARG
2	U	75	ILE
3	W	191	PRO
1	Y	316	GLU
1	Z	98	PRO
1	Z	114	PRO
1	a	367	ALA
2	b	199	ILE
2	c	64	ARG
2	D	172	GLY
2	E	75	ILE
2	E	434	GLU
2	F	17	PHE
4	H	31	GLU
2	L	172	GLY
2	M	75	ILE
2	N	17	PHE
4	P	31	GLU
2	T	172	GLY
2	V	17	PHE
3	W	189	PRO
4	X	31	GLU
2	b	172	GLY
2	c	75	ILE
2	d	17	PHE
3	e	192	ALA
4	f	31	GLU
2	E	149	GLY
2	M	149	GLY
2	U	149	GLY
2	U	383	SER
2	U	434	GLU
2	c	149	GLY
1	B	364	ILE
1	B	454	GLY
1	J	364	ILE
1	J	454	GLY
1	R	364	ILE
1	R	454	GLY

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Mol	Chain	Res	Type
1	Z	364	ILE
1	Z	454	GLY
2	b	114	PRO
2	c	433	GLY
3	e	189	PRO
1	A	364	ILE
2	D	74	PRO
2	D	265	VAL
2	F	74	PRO
2	F	331	TYR
1	I	364	ILE
2	L	74	PRO
2	N	74	PRO
3	O	189	PRO
1	Q	364	ILE
2	T	74	PRO
2	V	74	PRO
1	Y	364	ILE
2	b	74	PRO
2	b	265	VAL
2	d	74	PRO
2	d	331	TYR
2	E	113	ALA
2	E	308	PRO
2	M	113	ALA
2	N	331	TYR
2	T	265	VAL
2	U	113	ALA
2	U	433	GLY
2	V	265	VAL
2	V	331	TYR
2	c	113	ALA
2	c	331	TYR
1	A	366	PRO
1	B	99	VAL
2	E	331	TYR
4	H	73	PRO
1	I	366	PRO
1	J	99	VAL
1	K	317	VAL
2	M	308	PRO
2	M	331	TYR

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Mol	Chain	Res	Type
4	P	73	PRO
1	Q	366	PRO
1	R	99	VAL
2	U	331	TYR
4	X	73	PRO
1	Y	366	PRO
1	Z	99	VAL
2	c	415	GLY
2	d	265	VAL
4	f	73	PRO
1	C	317	VAL
1	C	364	ILE
1	C	480	ALA
2	E	433	GLY
1	K	364	ILE
1	K	480	ALA
2	N	265	VAL
1	S	317	VAL
1	S	364	ILE
1	S	480	ALA
1	a	317	VAL
1	a	364	ILE
1	a	480	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	A	380/407 (93%)	316 (83%)	64 (17%)	2	10
1	B	371/407 (91%)	302 (81%)	69 (19%)	1	7
1	C	375/407 (92%)	299 (80%)	76 (20%)	1	5
1	I	380/407 (93%)	314 (83%)	66 (17%)	2	8
1	J	371/407 (91%)	302 (81%)	69 (19%)	1	7
1	K	375/407 (92%)	303 (81%)	72 (19%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	380/407 (93%)	317 (83%)	63 (17%)	2	10
1	R	371/407 (91%)	301 (81%)	70 (19%)	1	6
1	S	375/407 (92%)	300 (80%)	75 (20%)	1	5
1	Y	380/407 (93%)	318 (84%)	62 (16%)	2	10
1	Z	371/407 (91%)	301 (81%)	70 (19%)	1	6
1	a	375/407 (92%)	302 (80%)	73 (20%)	1	6
2	D	380/380 (100%)	317 (83%)	63 (17%)	2	10
2	E	380/380 (100%)	297 (78%)	83 (22%)	1	4
2	F	380/380 (100%)	307 (81%)	73 (19%)	1	6
2	L	380/380 (100%)	320 (84%)	60 (16%)	2	11
2	M	380/380 (100%)	302 (80%)	78 (20%)	1	5
2	N	380/380 (100%)	305 (80%)	75 (20%)	1	6
2	T	380/380 (100%)	320 (84%)	60 (16%)	2	11
2	U	380/380 (100%)	303 (80%)	77 (20%)	1	5
2	V	380/380 (100%)	307 (81%)	73 (19%)	1	6
2	b	380/380 (100%)	321 (84%)	59 (16%)	2	12
2	c	380/380 (100%)	303 (80%)	77 (20%)	1	5
2	d	380/380 (100%)	307 (81%)	73 (19%)	1	6
3	G	236/239 (99%)	202 (86%)	34 (14%)	3	14
3	O	236/239 (99%)	202 (86%)	34 (14%)	3	14
3	W	236/239 (99%)	199 (84%)	37 (16%)	2	11
3	e	236/239 (99%)	200 (85%)	36 (15%)	3	12
4	H	109/109 (100%)	96 (88%)	13 (12%)	5	20
4	P	109/109 (100%)	96 (88%)	13 (12%)	5	20
4	X	109/109 (100%)	97 (89%)	12 (11%)	6	23
4	f	109/109 (100%)	96 (88%)	13 (12%)	5	20
All	All	10444/10836 (96%)	8572 (82%)	1872 (18%)	2	7

All (1872) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	51	GLU

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Mol	Chain	Res	Type
1	A	76	MET
1	A	87	LYS
1	A	89	LYS
1	A	91	THR
1	A	94	ILE
1	A	95	LEU
1	A	103	LEU
1	A	107	VAL
1	A	109	ASN
1	A	111	LEU
1	A	122	ASP
1	A	127	SER
1	A	136	VAL
1	A	137	ILE
1	A	142	VAL
1	A	146	VAL
1	A	147	GLN
1	A	164	ARG
1	A	166	LEU
1	A	178	LEU
1	A	181	ASP
1	A	186	GLN
1	A	209	VAL
1	A	212	LEU
1	A	218	LEU
1	A	221	THR
1	A	223	VAL
1	A	234	LEU
1	A	236	TYR
1	A	262	ASP
1	A	263	LEU
1	A	277	LEU
1	A	283	ARG
1	A	305	ASN
1	A	313	THR
1	A	318	LYS
1	A	333	GLN
1	A	337	VAL
1	A	345	VAL
1	A	350	ASP
1	A	356	GLU
1	A	358	ASN

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Mol	Chain	Res	Type
1	A	361	ASN
1	A	383	THR
1	A	386	MET
1	A	389	LEU
1	A	412	ASP
1	A	413	LEU
1	A	415	ASP
1	A	422	ASP
1	A	434	LYS
1	A	446	LEU
1	A	456	LEU
1	A	461	LEU
1	A	463	LYS
1	A	468	GLU
1	A	475	VAL
1	A	486	ILE
1	A	487	ASN
1	A	497	GLU
1	A	504	LEU
1	A	508	LYS
1	B	39	ILE
1	B	40	ARG
1	B	76	MET
1	B	94	ILE
1	B	95	LEU
1	B	97	VAL
1	B	104	LEU
1	B	106	ARG
1	B	107	VAL
1	B	108	VAL
1	B	109	ASN
1	B	110	THR
1	B	115	ILE
1	B	121	LEU
1	B	138	GLU
1	B	140	GLN
1	B	142	VAL
1	B	157	ILE
1	B	161	ARG
1	B	166	LEU
1	B	188	ASP
1	B	200	GLN

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Mol	Chain	Res	Type
1	B	221	THR
1	B	222	ILE
1	B	223	VAL
1	B	225	VAL
1	B	227	THR
1	B	234	LEU
1	B	236	TYR
1	B	237	LEU
1	B	252	ARG
1	B	259	ILE
1	B	262	ASP
1	B	274	SER
1	B	277	LEU
1	B	300	ARG
1	B	303	ARG
1	B	317	VAL
1	B	327	LEU
1	B	350	ASP
1	B	383	THR
1	B	384	LYS
1	B	395	THR
1	B	397	LEU
1	B	401	ARG
1	B	403	LEU
1	B	419	LYS
1	B	420	GLN
1	B	426	LYS
1	B	434	LYS
1	B	439	MET
1	B	443	GLN
1	B	444	GLN
1	B	447	VAL
1	B	453	ARG
1	B	456	LEU
1	B	458	ASP
1	B	461	LEU
1	B	468	GLU
1	B	471	LEU
1	B	472	LEU
1	B	482	LEU
1	B	483	MET
1	B	485	GLU

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Mol	Chain	Res	Type
1	B	486	ILE
1	B	488	GLN
1	B	494	ASP
1	B	495	GLU
1	B	503	ILE
1	C	34	VAL
1	C	38	VAL
1	C	52	MET
1	C	58	ASN
1	C	59	ARG
1	C	65	ASN
1	C	66	LEU
1	C	71	VAL
1	C	87	LYS
1	C	91	THR
1	C	94	ILE
1	C	95	LEU
1	C	96	GLU
1	C	97	VAL
1	C	99	VAL
1	C	103	LEU
1	C	106	ARG
1	C	111	LEU
1	C	115	ILE
1	C	121	LEU
1	C	123	HIS
1	C	124	ASP
1	C	136	VAL
1	C	137	ILE
1	C	142	VAL
1	C	144	GLN
1	C	147	GLN
1	C	164	ARG
1	C	166	LEU
1	C	172	GLN
1	C	178	LEU
1	C	180	ILE
1	C	187	ARG
1	C	200	GLN
1	C	201	LYS
1	C	209	VAL
1	C	223	VAL

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Mol	Chain	Res	Type
1	C	227	THR
1	C	236	TYR
1	C	252	ARG
1	C	266	GLN
1	C	276	LEU
1	C	277	LEU
1	C	305	ASN
1	C	308	TYR
1	C	327	LEU
1	C	350	ASP
1	C	357	THR
1	C	365	ARG
1	C	383	THR
1	C	387	LYS
1	C	390	SER
1	C	397	LEU
1	C	401	ARG
1	C	402	GLU
1	C	413	LEU
1	C	430	LEU
1	C	439	MET
1	C	446	LEU
1	C	456	LEU
1	C	460	GLU
1	C	461	LEU
1	C	467	PHE
1	C	468	GLU
1	C	471	LEU
1	C	474	TYR
1	C	483	MET
1	C	485	GLU
1	C	487	ASN
1	C	492	TYR
1	C	493	ASN
1	C	494	ASP
1	C	495	GLU
1	C	496	ILE
1	C	497	GLU
1	C	511	GLN
2	D	5	ILE
2	D	9	ILE
2	D	13	VAL

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Mol	Chain	Res	Type
2	D	20	ASP
2	D	27	ASP
2	D	32	GLN
2	D	35	ASN
2	D	50	ILE
2	D	63	ARG
2	D	66	LEU
2	D	73	HIS
2	D	81	GLU
2	D	89	ASN
2	D	90	VAL
2	D	91	LEU
2	D	95	VAL
2	D	98	LYS
2	D	101	ILE
2	D	103	GLU
2	D	111	ARG
2	D	117	GLU
2	D	118	GLU
2	D	128	THR
2	D	157	VAL
2	D	198	VAL
2	D	199	ILE
2	D	203	SER
2	D	229	LYS
2	D	231	ARG
2	D	241	VAL
2	D	243	ASN
2	D	249	LEU
2	D	257	LEU
2	D	277	VAL
2	D	283	THR
2	D	287	THR
2	D	290	ILE
2	D	291	THR
2	D	293	VAL
2	D	304	THR
2	D	310	THR
2	D	323	ARG
2	D	331	TYR
2	D	340	THR
2	D	344	LEU

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Mol	Chain	Res	Type
2	D	345	ASP
2	D	347	LEU
2	D	364	LEU
2	D	368	GLN
2	D	373	ILE
2	D	377	LEU
2	D	388	LEU
2	D	396	ILE
2	D	398	ARG
2	D	406	VAL
2	D	408	GLU
2	D	409	VAL
2	D	438	LEU
2	D	441	GLN
2	D	445	MET
2	D	449	ILE
2	D	454	GLU
2	D	459	LEU
2	E	6	VAL
2	E	13	VAL
2	E	15	VAL
2	E	16	GLU
2	E	24	ARG
2	E	32	GLN
2	E	38	LEU
2	E	41	GLU
2	E	46	LEU
2	E	51	VAL
2	E	56	MET
2	E	62	LEU
2	E	64	ARG
2	E	66	LEU
2	E	68	VAL
2	E	71	LEU
2	E	76	GLU
2	E	84	LEU
2	E	89	ASN
2	E	97	MET
2	E	111	ARG
2	E	115	SER
2	E	117	GLU
2	E	119	LEU

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Mol	Chain	Res	Type
2	E	121	ASN
2	E	132	VAL
2	E	144	LYS
2	E	157	VAL
2	E	163	ILE
2	E	164	ARG
2	E	174	SER
2	E	179	VAL
2	E	181	GLU
2	E	200	ASP
2	E	201	LYS
2	E	204	LEU
2	E	217	LEU
2	E	238	LEU
2	E	244	ILE
2	E	246	ARG
2	E	248	THR
2	E	249	LEU
2	E	268	GLN
2	E	271	LEU
2	E	290	ILE
2	E	293	VAL
2	E	297	TYR
2	E	303	LEU
2	E	304	THR
2	E	330	ILE
2	E	331	TYR
2	E	337	LEU
2	E	340	THR
2	E	343	GLN
2	E	344	LEU
2	E	345	ASP
2	E	347	LEU
2	E	348	VAL
2	E	349	VAL
2	E	352	GLU
2	E	358	ARG
2	E	364	LEU
2	E	366	ARG
2	E	371	LYS
2	E	373	ILE
2	E	377	LEU

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Mol	Chain	Res	Type
2	E	380	ASP
2	E	382	LEU
2	E	388	LEU
2	E	394	ARG
2	E	396	ILE
2	E	400	LEU
2	E	409	VAL
2	E	410	PHE
2	E	416	LYS
2	E	418	VAL
2	E	431	MET
2	E	443	PHE
2	E	445	MET
2	E	446	VAL
2	E	449	ILE
2	E	454	GLU
2	E	457	LYS
2	F	5	ILE
2	F	6	VAL
2	F	14	ASP
2	F	16	GLU
2	F	17	PHE
2	F	22	VAL
2	F	29	LEU
2	F	36	GLU
2	F	51	VAL
2	F	66	LEU
2	F	68	VAL
2	F	86	ARG
2	F	97	MET
2	F	98	LYS
2	F	100	GLU
2	F	101	ILE
2	F	103	GLU
2	F	104	GLU
2	F	117	GLU
2	F	121	ASN
2	F	131	LYS
2	F	136	MET
2	F	139	PHE
2	F	141	LYS
2	F	144	LYS

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Mol	Chain	Res	Type
2	F	145	VAL
2	F	157	VAL
2	F	162	LEU
2	F	164	ARG
2	F	169	GLU
2	F	173	TYR
2	F	179	VAL
2	F	181	GLU
2	F	185	GLU
2	F	194	THR
2	F	197	ASN
2	F	201	LYS
2	F	205	VAL
2	F	210	ASN
2	F	224	LEU
2	F	239	LEU
2	F	260	ARG
2	F	265	VAL
2	F	268	GLN
2	F	271	LEU
2	F	283	THR
2	F	291	THR
2	F	293	VAL
2	F	296	VAL
2	F	298	VAL
2	F	319	VAL
2	F	320	VAL
2	F	323	ARG
2	F	324	GLN
2	F	338	ASP
2	F	344	LEU
2	F	347	LEU
2	F	364	LEU
2	F	372	ASP
2	F	385	GLU
2	F	387	LYS
2	F	390	VAL
2	F	392	ARG
2	F	400	LEU
2	F	402	GLN
2	F	410	PHE
2	F	417	TYR

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Mol	Chain	Res	Type
2	F	419	SER
2	F	441	GLN
2	F	450	GLU
2	F	453	VAL
2	F	457	LYS
2	F	459	LEU
3	G	4	LYS
3	G	5	GLU
3	G	9	LYS
3	G	16	THR
3	G	47	THR
3	G	49	ARG
3	G	55	LEU
3	G	62	TYR
3	G	64	HIS
3	G	67	LEU
3	G	72	VAL
3	G	110	VAL
3	G	120	LYS
3	G	137	THR
3	G	145	LEU
3	G	173	LYS
3	G	190	LEU
3	G	193	SER
3	G	195	ASP
3	G	199	LYS
3	G	200	HIS
3	G	206	LEU
3	G	208	GLU
3	G	218	LEU
3	G	219	LEU
3	G	232	VAL
3	G	242	ARG
3	G	246	MET
3	G	255	SER
3	G	258	LYS
3	G	272	ILE
3	G	276	LEU
3	G	277	THR
3	G	280	VAL
4	H	2	MET
4	H	41	LEU

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Mol	Chain	Res	Type
4	H	49	MET
4	H	50	ILE
4	H	60	GLU
4	H	75	ASN
4	H	76	VAL
4	H	85	ARG
4	H	91	GLU
4	H	103	GLU
4	H	121	LEU
4	H	129	ARG
4	H	131	ILE
1	I	27	ASN
1	I	51	GLU
1	I	76	MET
1	I	87	LYS
1	I	89	LYS
1	I	91	THR
1	I	94	ILE
1	I	95	LEU
1	I	103	LEU
1	I	107	VAL
1	I	109	ASN
1	I	111	LEU
1	I	122	ASP
1	I	127	SER
1	I	137	ILE
1	I	142	VAL
1	I	146	VAL
1	I	147	GLN
1	I	164	ARG
1	I	166	LEU
1	I	176	THR
1	I	178	LEU
1	I	181	ASP
1	I	186	GLN
1	I	209	VAL
1	I	212	LEU
1	I	218	LEU
1	I	221	THR
1	I	223	VAL
1	I	234	LEU
1	I	236	TYR

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Mol	Chain	Res	Type
1	I	262	ASP
1	I	263	LEU
1	I	277	LEU
1	I	283	ARG
1	I	305	ASN
1	I	313	THR
1	I	318	LYS
1	I	333	GLN
1	I	337	VAL
1	I	345	VAL
1	I	350	ASP
1	I	356	GLU
1	I	358	ASN
1	I	361	ASN
1	I	383	THR
1	I	386	MET
1	I	389	LEU
1	I	412	ASP
1	I	413	LEU
1	I	415	ASP
1	I	422	ASP
1	I	434	LYS
1	I	446	LEU
1	I	456	LEU
1	I	458	ASP
1	I	459	VAL
1	I	461	LEU
1	I	463	LYS
1	I	468	GLU
1	I	475	VAL
1	I	486	ILE
1	I	487	ASN
1	I	497	GLU
1	I	504	LEU
1	I	508	LYS
1	J	39	ILE
1	J	40	ARG
1	J	76	MET
1	J	94	ILE
1	J	95	LEU
1	J	96	GLU
1	J	104	LEU

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Mol	Chain	Res	Type
1	J	106	ARG
1	J	107	VAL
1	J	108	VAL
1	J	109	ASN
1	J	110	THR
1	J	115	ILE
1	J	121	LEU
1	J	138	GLU
1	J	140	GLN
1	J	142	VAL
1	J	157	ILE
1	J	161	ARG
1	J	166	LEU
1	J	188	ASP
1	J	200	GLN
1	J	221	THR
1	J	222	ILE
1	J	223	VAL
1	J	225	VAL
1	J	227	THR
1	J	234	LEU
1	J	236	TYR
1	J	237	LEU
1	J	252	ARG
1	J	259	ILE
1	J	262	ASP
1	J	274	SER
1	J	277	LEU
1	J	300	ARG
1	J	303	ARG
1	J	317	VAL
1	J	327	LEU
1	J	350	ASP
1	J	383	THR
1	J	384	LYS
1	J	395	THR
1	J	397	LEU
1	J	401	ARG
1	J	403	LEU
1	J	419	LYS
1	J	420	GLN
1	J	426	LYS

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Mol	Chain	Res	Type
1	J	434	LYS
1	J	439	MET
1	J	443	GLN
1	J	444	GLN
1	J	447	VAL
1	J	453	ARG
1	J	456	LEU
1	J	458	ASP
1	J	461	LEU
1	J	468	GLU
1	J	471	LEU
1	J	472	LEU
1	J	482	LEU
1	J	483	MET
1	J	485	GLU
1	J	486	ILE
1	J	488	GLN
1	J	494	ASP
1	J	495	GLU
1	J	503	ILE
1	K	34	VAL
1	K	38	VAL
1	K	52	MET
1	K	58	ASN
1	K	59	ARG
1	K	65	ASN
1	K	66	LEU
1	K	71	VAL
1	K	87	LYS
1	K	91	THR
1	K	94	ILE
1	K	95	LEU
1	K	96	GLU
1	K	97	VAL
1	K	99	VAL
1	K	103	LEU
1	K	106	ARG
1	K	111	LEU
1	K	115	ILE
1	K	121	LEU
1	K	123	HIS
1	K	124	ASP

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Mol	Chain	Res	Type
1	K	137	ILE
1	K	142	VAL
1	K	144	GLN
1	K	147	GLN
1	K	164	ARG
1	K	166	LEU
1	K	172	GLN
1	K	178	LEU
1	K	180	ILE
1	K	187	ARG
1	K	200	GLN
1	K	201	LYS
1	K	209	VAL
1	K	223	VAL
1	K	227	THR
1	K	236	TYR
1	K	252	ARG
1	K	266	GLN
1	K	276	LEU
1	K	277	LEU
1	K	305	ASN
1	K	308	TYR
1	K	327	LEU
1	K	350	ASP
1	K	357	THR
1	K	365	ARG
1	K	383	THR
1	K	387	LYS
1	K	390	SER
1	K	397	LEU
1	K	401	ARG
1	K	402	GLU
1	K	413	LEU
1	K	430	LEU
1	K	439	MET
1	K	446	LEU
1	K	456	LEU
1	K	460	GLU
1	K	461	LEU
1	K	467	PHE
1	K	468	GLU
1	K	471	LEU

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Mol	Chain	Res	Type
1	K	474	TYR
1	K	483	MET
1	K	485	GLU
1	K	487	ASN
1	K	492	TYR
1	K	496	ILE
1	K	497	GLU
1	K	511	GLN
2	L	5	ILE
2	L	9	ILE
2	L	13	VAL
2	L	20	ASP
2	L	27	ASP
2	L	32	GLN
2	L	35	ASN
2	L	50	ILE
2	L	63	ARG
2	L	66	LEU
2	L	73	HIS
2	L	81	GLU
2	L	89	ASN
2	L	90	VAL
2	L	91	LEU
2	L	95	VAL
2	L	98	LYS
2	L	101	ILE
2	L	103	GLU
2	L	111	ARG
2	L	117	GLU
2	L	118	GLU
2	L	128	THR
2	L	157	VAL
2	L	198	VAL
2	L	199	ILE
2	L	203	SER
2	L	229	LYS
2	L	231	ARG
2	L	241	VAL
2	L	243	ASN
2	L	249	LEU
2	L	257	LEU
2	L	283	THR

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Mol	Chain	Res	Type
2	L	287	THR
2	L	290	ILE
2	L	291	THR
2	L	293	VAL
2	L	304	THR
2	L	310	THR
2	L	323	ARG
2	L	331	TYR
2	L	340	THR
2	L	344	LEU
2	L	345	ASP
2	L	347	LEU
2	L	364	LEU
2	L	373	ILE
2	L	377	LEU
2	L	388	LEU
2	L	396	ILE
2	L	398	ARG
2	L	406	VAL
2	L	408	GLU
2	L	409	VAL
2	L	438	LEU
2	L	445	MET
2	L	449	ILE
2	L	454	GLU
2	L	459	LEU
2	M	6	VAL
2	M	13	VAL
2	M	15	VAL
2	M	16	GLU
2	M	24	ARG
2	M	32	GLN
2	M	38	LEU
2	M	41	GLU
2	M	46	LEU
2	M	51	VAL
2	M	56	MET
2	M	62	LEU
2	M	64	ARG
2	M	66	LEU
2	M	68	VAL
2	M	71	LEU

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Mol	Chain	Res	Type
2	M	76	GLU
2	M	84	LEU
2	M	89	ASN
2	M	97	MET
2	M	111	ARG
2	M	115	SER
2	M	117	GLU
2	M	119	LEU
2	M	121	ASN
2	M	132	VAL
2	M	144	LYS
2	M	157	VAL
2	M	163	ILE
2	M	164	ARG
2	M	174	SER
2	M	179	VAL
2	M	181	GLU
2	M	201	LYS
2	M	204	LEU
2	M	217	LEU
2	M	238	LEU
2	M	244	ILE
2	M	246	ARG
2	M	248	THR
2	M	249	LEU
2	M	268	GLN
2	M	271	LEU
2	M	293	VAL
2	M	297	TYR
2	M	303	LEU
2	M	304	THR
2	M	331	TYR
2	M	337	LEU
2	M	340	THR
2	M	343	GLN
2	M	344	LEU
2	M	345	ASP
2	M	348	VAL
2	M	349	VAL
2	M	358	ARG
2	M	364	LEU
2	M	366	ARG

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Mol	Chain	Res	Type
2	M	371	LYS
2	M	373	ILE
2	M	377	LEU
2	M	380	ASP
2	M	382	LEU
2	M	388	LEU
2	M	389	VAL
2	M	394	ARG
2	M	396	ILE
2	M	400	LEU
2	M	406	VAL
2	M	410	PHE
2	M	416	LYS
2	M	418	VAL
2	M	431	MET
2	M	443	PHE
2	M	446	VAL
2	M	449	ILE
2	M	454	GLU
2	M	457	LYS
2	N	5	ILE
2	N	6	VAL
2	N	14	ASP
2	N	16	GLU
2	N	17	PHE
2	N	22	VAL
2	N	29	LEU
2	N	36	GLU
2	N	51	VAL
2	N	66	LEU
2	N	68	VAL
2	N	86	ARG
2	N	97	MET
2	N	98	LYS
2	N	100	GLU
2	N	101	ILE
2	N	103	GLU
2	N	104	GLU
2	N	117	GLU
2	N	121	ASN
2	N	131	LYS
2	N	136	MET

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Mol	Chain	Res	Type
2	N	139	PHE
2	N	141	LYS
2	N	144	LYS
2	N	145	VAL
2	N	157	VAL
2	N	162	LEU
2	N	164	ARG
2	N	169	GLU
2	N	173	TYR
2	N	179	VAL
2	N	181	GLU
2	N	185	GLU
2	N	194	THR
2	N	197	ASN
2	N	201	LYS
2	N	205	VAL
2	N	210	ASN
2	N	224	LEU
2	N	239	LEU
2	N	260	ARG
2	N	265	VAL
2	N	268	GLN
2	N	271	LEU
2	N	283	THR
2	N	291	THR
2	N	293	VAL
2	N	296	VAL
2	N	298	VAL
2	N	319	VAL
2	N	320	VAL
2	N	323	ARG
2	N	324	GLN
2	N	338	ASP
2	N	344	LEU
2	N	347	LEU
2	N	363	ILE
2	N	364	LEU
2	N	372	ASP
2	N	385	GLU
2	N	387	LYS
2	N	390	VAL
2	N	392	ARG

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Mol	Chain	Res	Type
2	N	396	ILE
2	N	400	LEU
2	N	402	GLN
2	N	410	PHE
2	N	417	TYR
2	N	419	SER
2	N	441	GLN
2	N	450	GLU
2	N	453	VAL
2	N	457	LYS
2	N	459	LEU
3	O	4	LYS
3	O	5	GLU
3	O	9	LYS
3	O	16	THR
3	O	47	THR
3	O	49	ARG
3	O	55	LEU
3	O	62	TYR
3	O	64	HIS
3	O	67	LEU
3	O	72	VAL
3	O	110	VAL
3	O	120	LYS
3	O	137	THR
3	O	145	LEU
3	O	173	LYS
3	O	187	LEU
3	O	190	LEU
3	O	195	ASP
3	O	199	LYS
3	O	200	HIS
3	O	206	LEU
3	O	208	GLU
3	O	218	LEU
3	O	219	LEU
3	O	232	VAL
3	O	242	ARG
3	O	246	MET
3	O	255	SER
3	O	258	LYS
3	O	272	ILE

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Mol	Chain	Res	Type
3	O	276	LEU
3	O	277	THR
3	O	280	VAL
4	P	2	MET
4	P	41	LEU
4	P	49	MET
4	P	50	ILE
4	P	60	GLU
4	P	75	ASN
4	P	76	VAL
4	P	85	ARG
4	P	91	GLU
4	P	103	GLU
4	P	121	LEU
4	P	129	ARG
4	P	131	ILE
1	Q	27	ASN
1	Q	51	GLU
1	Q	76	MET
1	Q	87	LYS
1	Q	89	LYS
1	Q	91	THR
1	Q	94	ILE
1	Q	95	LEU
1	Q	103	LEU
1	Q	107	VAL
1	Q	109	ASN
1	Q	111	LEU
1	Q	122	ASP
1	Q	127	SER
1	Q	137	ILE
1	Q	138	GLU
1	Q	142	VAL
1	Q	146	VAL
1	Q	147	GLN
1	Q	164	ARG
1	Q	166	LEU
1	Q	181	ASP
1	Q	186	GLN
1	Q	209	VAL
1	Q	212	LEU
1	Q	218	LEU

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Mol	Chain	Res	Type
1	Q	221	THR
1	Q	223	VAL
1	Q	234	LEU
1	Q	236	TYR
1	Q	262	ASP
1	Q	263	LEU
1	Q	277	LEU
1	Q	283	ARG
1	Q	305	ASN
1	Q	313	THR
1	Q	318	LYS
1	Q	333	GLN
1	Q	337	VAL
1	Q	345	VAL
1	Q	350	ASP
1	Q	356	GLU
1	Q	358	ASN
1	Q	361	ASN
1	Q	383	THR
1	Q	386	MET
1	Q	389	LEU
1	Q	412	ASP
1	Q	413	LEU
1	Q	415	ASP
1	Q	422	ASP
1	Q	434	LYS
1	Q	446	LEU
1	Q	456	LEU
1	Q	461	LEU
1	Q	463	LYS
1	Q	468	GLU
1	Q	475	VAL
1	Q	486	ILE
1	Q	487	ASN
1	Q	497	GLU
1	Q	504	LEU
1	Q	508	LYS
1	R	39	ILE
1	R	40	ARG
1	R	76	MET
1	R	94	ILE
1	R	95	LEU

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Mol	Chain	Res	Type
1	R	96	GLU
1	R	97	VAL
1	R	104	LEU
1	R	106	ARG
1	R	107	VAL
1	R	108	VAL
1	R	109	ASN
1	R	110	THR
1	R	115	ILE
1	R	121	LEU
1	R	138	GLU
1	R	140	GLN
1	R	142	VAL
1	R	157	ILE
1	R	161	ARG
1	R	166	LEU
1	R	188	ASP
1	R	200	GLN
1	R	221	THR
1	R	222	ILE
1	R	223	VAL
1	R	225	VAL
1	R	227	THR
1	R	234	LEU
1	R	236	TYR
1	R	237	LEU
1	R	252	ARG
1	R	259	ILE
1	R	262	ASP
1	R	274	SER
1	R	277	LEU
1	R	300	ARG
1	R	303	ARG
1	R	317	VAL
1	R	327	LEU
1	R	350	ASP
1	R	383	THR
1	R	384	LYS
1	R	395	THR
1	R	397	LEU
1	R	401	ARG
1	R	403	LEU

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Mol	Chain	Res	Type
1	R	419	LYS
1	R	420	GLN
1	R	426	LYS
1	R	434	LYS
1	R	439	MET
1	R	443	GLN
1	R	444	GLN
1	R	447	VAL
1	R	453	ARG
1	R	456	LEU
1	R	458	ASP
1	R	461	LEU
1	R	468	GLU
1	R	471	LEU
1	R	472	LEU
1	R	482	LEU
1	R	483	MET
1	R	485	GLU
1	R	486	ILE
1	R	488	GLN
1	R	494	ASP
1	R	495	GLU
1	R	503	ILE
1	S	34	VAL
1	S	38	VAL
1	S	52	MET
1	S	58	ASN
1	S	59	ARG
1	S	65	ASN
1	S	66	LEU
1	S	71	VAL
1	S	87	LYS
1	S	91	THR
1	S	94	ILE
1	S	95	LEU
1	S	96	GLU
1	S	97	VAL
1	S	99	VAL
1	S	103	LEU
1	S	106	ARG
1	S	111	LEU
1	S	115	ILE

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Mol	Chain	Res	Type
1	S	121	LEU
1	S	123	HIS
1	S	124	ASP
1	S	136	VAL
1	S	137	ILE
1	S	142	VAL
1	S	144	GLN
1	S	147	GLN
1	S	164	ARG
1	S	166	LEU
1	S	172	GLN
1	S	178	LEU
1	S	180	ILE
1	S	187	ARG
1	S	200	GLN
1	S	201	LYS
1	S	209	VAL
1	S	223	VAL
1	S	227	THR
1	S	236	TYR
1	S	252	ARG
1	S	266	GLN
1	S	276	LEU
1	S	277	LEU
1	S	305	ASN
1	S	308	TYR
1	S	327	LEU
1	S	350	ASP
1	S	357	THR
1	S	365	ARG
1	S	383	THR
1	S	387	LYS
1	S	390	SER
1	S	397	LEU
1	S	401	ARG
1	S	402	GLU
1	S	413	LEU
1	S	430	LEU
1	S	439	MET
1	S	446	LEU
1	S	456	LEU
1	S	460	GLU

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Mol	Chain	Res	Type
1	S	461	LEU
1	S	467	PHE
1	S	468	GLU
1	S	471	LEU
1	S	474	TYR
1	S	483	MET
1	S	485	GLU
1	S	487	ASN
1	S	492	TYR
1	S	493	ASN
1	S	494	ASP
1	S	496	ILE
1	S	497	GLU
1	S	511	GLN
2	T	5	ILE
2	T	9	ILE
2	T	13	VAL
2	T	27	ASP
2	T	32	GLN
2	T	35	ASN
2	T	50	ILE
2	T	63	ARG
2	T	66	LEU
2	T	73	HIS
2	T	81	GLU
2	T	89	ASN
2	T	90	VAL
2	T	91	LEU
2	T	95	VAL
2	T	98	LYS
2	T	101	ILE
2	T	103	GLU
2	T	111	ARG
2	T	117	GLU
2	T	118	GLU
2	T	128	THR
2	T	157	VAL
2	T	198	VAL
2	T	199	ILE
2	T	203	SER
2	T	229	LYS
2	T	231	ARG

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Mol	Chain	Res	Type
2	T	241	VAL
2	T	243	ASN
2	T	249	LEU
2	T	257	LEU
2	T	283	THR
2	T	287	THR
2	T	290	ILE
2	T	291	THR
2	T	293	VAL
2	T	304	THR
2	T	310	THR
2	T	323	ARG
2	T	331	TYR
2	T	340	THR
2	T	344	LEU
2	T	345	ASP
2	T	347	LEU
2	T	364	LEU
2	T	368	GLN
2	T	373	ILE
2	T	377	LEU
2	T	388	LEU
2	T	396	ILE
2	T	398	ARG
2	T	406	VAL
2	T	408	GLU
2	T	409	VAL
2	T	438	LEU
2	T	445	MET
2	T	449	ILE
2	T	454	GLU
2	T	459	LEU
2	U	6	VAL
2	U	13	VAL
2	U	15	VAL
2	U	16	GLU
2	U	24	ARG
2	U	32	GLN
2	U	38	LEU
2	U	41	GLU
2	U	46	LEU
2	U	51	VAL

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Mol	Chain	Res	Type
2	U	56	MET
2	U	62	LEU
2	U	64	ARG
2	U	66	LEU
2	U	68	VAL
2	U	71	LEU
2	U	76	GLU
2	U	84	LEU
2	U	89	ASN
2	U	97	MET
2	U	111	ARG
2	U	115	SER
2	U	117	GLU
2	U	119	LEU
2	U	121	ASN
2	U	132	VAL
2	U	144	LYS
2	U	157	VAL
2	U	163	ILE
2	U	164	ARG
2	U	174	SER
2	U	179	VAL
2	U	181	GLU
2	U	200	ASP
2	U	201	LYS
2	U	204	LEU
2	U	217	LEU
2	U	238	LEU
2	U	244	ILE
2	U	246	ARG
2	U	248	THR
2	U	249	LEU
2	U	268	GLN
2	U	271	LEU
2	U	293	VAL
2	U	297	TYR
2	U	303	LEU
2	U	304	THR
2	U	331	TYR
2	U	337	LEU
2	U	340	THR
2	U	343	GLN

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Mol	Chain	Res	Type
2	U	344	LEU
2	U	345	ASP
2	U	348	VAL
2	U	349	VAL
2	U	358	ARG
2	U	364	LEU
2	U	366	ARG
2	U	371	LYS
2	U	373	ILE
2	U	377	LEU
2	U	380	ASP
2	U	382	LEU
2	U	388	LEU
2	U	394	ARG
2	U	396	ILE
2	U	400	LEU
2	U	406	VAL
2	U	409	VAL
2	U	410	PHE
2	U	416	LYS
2	U	418	VAL
2	U	446	VAL
2	U	449	ILE
2	U	454	GLU
2	U	457	LYS
2	V	5	ILE
2	V	6	VAL
2	V	14	ASP
2	V	16	GLU
2	V	17	PHE
2	V	22	VAL
2	V	29	LEU
2	V	36	GLU
2	V	51	VAL
2	V	66	LEU
2	V	68	VAL
2	V	86	ARG
2	V	97	MET
2	V	98	LYS
2	V	100	GLU
2	V	101	ILE
2	V	103	GLU

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Mol	Chain	Res	Type
2	V	104	GLU
2	V	117	GLU
2	V	121	ASN
2	V	131	LYS
2	V	136	MET
2	V	139	PHE
2	V	141	LYS
2	V	144	LYS
2	V	145	VAL
2	V	157	VAL
2	V	162	LEU
2	V	164	ARG
2	V	169	GLU
2	V	173	TYR
2	V	179	VAL
2	V	181	GLU
2	V	185	GLU
2	V	194	THR
2	V	197	ASN
2	V	201	LYS
2	V	205	VAL
2	V	210	ASN
2	V	224	LEU
2	V	239	LEU
2	V	260	ARG
2	V	265	VAL
2	V	268	GLN
2	V	271	LEU
2	V	283	THR
2	V	291	THR
2	V	293	VAL
2	V	296	VAL
2	V	298	VAL
2	V	319	VAL
2	V	320	VAL
2	V	323	ARG
2	V	324	GLN
2	V	338	ASP
2	V	344	LEU
2	V	347	LEU
2	V	364	LEU
2	V	372	ASP

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Mol	Chain	Res	Type
2	V	385	GLU
2	V	387	LYS
2	V	390	VAL
2	V	392	ARG
2	V	396	ILE
2	V	400	LEU
2	V	410	PHE
2	V	417	TYR
2	V	419	SER
2	V	441	GLN
2	V	450	GLU
2	V	453	VAL
2	V	457	LYS
2	V	459	LEU
3	W	4	LYS
3	W	5	GLU
3	W	9	LYS
3	W	16	THR
3	W	47	THR
3	W	49	ARG
3	W	55	LEU
3	W	62	TYR
3	W	64	HIS
3	W	67	LEU
3	W	72	VAL
3	W	110	VAL
3	W	120	LYS
3	W	137	THR
3	W	145	LEU
3	W	173	LYS
3	W	187	LEU
3	W	188	LEU
3	W	190	LEU
3	W	193	SER
3	W	194	ASP
3	W	195	ASP
3	W	199	LYS
3	W	200	HIS
3	W	206	LEU
3	W	208	GLU
3	W	218	LEU
3	W	219	LEU

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Mol	Chain	Res	Type
3	W	232	VAL
3	W	242	ARG
3	W	246	MET
3	W	255	SER
3	W	258	LYS
3	W	272	ILE
3	W	276	LEU
3	W	277	THR
3	W	280	VAL
4	X	41	LEU
4	X	49	MET
4	X	50	ILE
4	X	60	GLU
4	X	75	ASN
4	X	76	VAL
4	X	85	ARG
4	X	91	GLU
4	X	103	GLU
4	X	121	LEU
4	X	129	ARG
4	X	131	ILE
1	Y	27	ASN
1	Y	51	GLU
1	Y	76	MET
1	Y	87	LYS
1	Y	89	LYS
1	Y	91	THR
1	Y	94	ILE
1	Y	95	LEU
1	Y	103	LEU
1	Y	107	VAL
1	Y	109	ASN
1	Y	111	LEU
1	Y	122	ASP
1	Y	127	SER
1	Y	137	ILE
1	Y	142	VAL
1	Y	146	VAL
1	Y	147	GLN
1	Y	164	ARG
1	Y	166	LEU
1	Y	181	ASP

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Mol	Chain	Res	Type
1	Y	186	GLN
1	Y	209	VAL
1	Y	212	LEU
1	Y	218	LEU
1	Y	221	THR
1	Y	223	VAL
1	Y	234	LEU
1	Y	236	TYR
1	Y	262	ASP
1	Y	263	LEU
1	Y	277	LEU
1	Y	283	ARG
1	Y	305	ASN
1	Y	313	THR
1	Y	318	LYS
1	Y	333	GLN
1	Y	337	VAL
1	Y	345	VAL
1	Y	350	ASP
1	Y	356	GLU
1	Y	358	ASN
1	Y	361	ASN
1	Y	383	THR
1	Y	386	MET
1	Y	389	LEU
1	Y	412	ASP
1	Y	413	LEU
1	Y	415	ASP
1	Y	422	ASP
1	Y	434	LYS
1	Y	446	LEU
1	Y	456	LEU
1	Y	461	LEU
1	Y	463	LYS
1	Y	468	GLU
1	Y	475	VAL
1	Y	486	ILE
1	Y	487	ASN
1	Y	497	GLU
1	Y	504	LEU
1	Y	508	LYS
1	Z	39	ILE

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Mol	Chain	Res	Type
1	Z	40	ARG
1	Z	52	MET
1	Z	76	MET
1	Z	94	ILE
1	Z	95	LEU
1	Z	97	VAL
1	Z	104	LEU
1	Z	106	ARG
1	Z	107	VAL
1	Z	108	VAL
1	Z	109	ASN
1	Z	110	THR
1	Z	115	ILE
1	Z	121	LEU
1	Z	138	GLU
1	Z	140	GLN
1	Z	142	VAL
1	Z	157	ILE
1	Z	161	ARG
1	Z	166	LEU
1	Z	188	ASP
1	Z	200	GLN
1	Z	221	THR
1	Z	222	ILE
1	Z	223	VAL
1	Z	225	VAL
1	Z	227	THR
1	Z	234	LEU
1	Z	236	TYR
1	Z	237	LEU
1	Z	252	ARG
1	Z	259	ILE
1	Z	262	ASP
1	Z	274	SER
1	Z	277	LEU
1	Z	300	ARG
1	Z	303	ARG
1	Z	317	VAL
1	Z	327	LEU
1	Z	350	ASP
1	Z	383	THR
1	Z	384	LYS

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Mol	Chain	Res	Type
1	Z	395	THR
1	Z	397	LEU
1	Z	401	ARG
1	Z	403	LEU
1	Z	419	LYS
1	Z	420	GLN
1	Z	426	LYS
1	Z	434	LYS
1	Z	439	MET
1	Z	443	GLN
1	Z	444	GLN
1	Z	447	VAL
1	Z	453	ARG
1	Z	456	LEU
1	Z	458	ASP
1	Z	461	LEU
1	Z	468	GLU
1	Z	471	LEU
1	Z	472	LEU
1	Z	482	LEU
1	Z	483	MET
1	Z	485	GLU
1	Z	486	ILE
1	Z	488	GLN
1	Z	494	ASP
1	Z	495	GLU
1	Z	503	ILE
1	a	34	VAL
1	a	38	VAL
1	a	52	MET
1	a	58	ASN
1	a	59	ARG
1	a	65	ASN
1	a	66	LEU
1	a	71	VAL
1	a	87	LYS
1	a	91	THR
1	a	94	ILE
1	a	95	LEU
1	a	96	GLU
1	a	97	VAL
1	a	99	VAL

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Mol	Chain	Res	Type
1	a	103	LEU
1	a	106	ARG
1	a	111	LEU
1	a	115	ILE
1	a	121	LEU
1	a	123	HIS
1	a	124	ASP
1	a	136	VAL
1	a	137	ILE
1	a	142	VAL
1	a	144	GLN
1	a	147	GLN
1	a	164	ARG
1	a	166	LEU
1	a	172	GLN
1	a	178	LEU
1	a	180	ILE
1	a	187	ARG
1	a	200	GLN
1	a	201	LYS
1	a	209	VAL
1	a	223	VAL
1	a	227	THR
1	a	236	TYR
1	a	252	ARG
1	a	266	GLN
1	a	276	LEU
1	a	277	LEU
1	a	305	ASN
1	a	308	TYR
1	a	327	LEU
1	a	350	ASP
1	a	357	THR
1	a	365	ARG
1	a	383	THR
1	a	387	LYS
1	a	390	SER
1	a	397	LEU
1	a	401	ARG
1	a	402	GLU
1	a	413	LEU
1	a	430	LEU

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Mol	Chain	Res	Type
1	a	439	MET
1	a	446	LEU
1	a	456	LEU
1	a	460	GLU
1	a	461	LEU
1	a	467	PHE
1	a	468	GLU
1	a	471	LEU
1	a	474	TYR
1	a	483	MET
1	a	485	GLU
1	a	487	ASN
1	a	492	TYR
1	a	496	ILE
1	a	497	GLU
1	a	511	GLN
2	b	5	ILE
2	b	9	ILE
2	b	13	VAL
2	b	27	ASP
2	b	32	GLN
2	b	35	ASN
2	b	50	ILE
2	b	63	ARG
2	b	66	LEU
2	b	73	HIS
2	b	81	GLU
2	b	89	ASN
2	b	90	VAL
2	b	91	LEU
2	b	95	VAL
2	b	98	LYS
2	b	101	ILE
2	b	103	GLU
2	b	111	ARG
2	b	117	GLU
2	b	118	GLU
2	b	128	THR
2	b	157	VAL
2	b	198	VAL
2	b	199	ILE
2	b	203	SER

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Mol	Chain	Res	Type
2	b	229	LYS
2	b	231	ARG
2	b	241	VAL
2	b	243	ASN
2	b	249	LEU
2	b	257	LEU
2	b	283	THR
2	b	287	THR
2	b	290	ILE
2	b	291	THR
2	b	293	VAL
2	b	304	THR
2	b	310	THR
2	b	323	ARG
2	b	331	TYR
2	b	340	THR
2	b	344	LEU
2	b	345	ASP
2	b	347	LEU
2	b	364	LEU
2	b	366	ARG
2	b	373	ILE
2	b	377	LEU
2	b	396	ILE
2	b	398	ARG
2	b	406	VAL
2	b	408	GLU
2	b	409	VAL
2	b	438	LEU
2	b	445	MET
2	b	449	ILE
2	b	454	GLU
2	b	459	LEU
2	c	6	VAL
2	c	13	VAL
2	c	15	VAL
2	c	16	GLU
2	c	24	ARG
2	c	32	GLN
2	c	38	LEU
2	c	41	GLU
2	c	46	LEU

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Mol	Chain	Res	Type
2	c	51	VAL
2	c	56	MET
2	c	62	LEU
2	c	64	ARG
2	c	66	LEU
2	c	68	VAL
2	c	71	LEU
2	c	76	GLU
2	c	84	LEU
2	c	89	ASN
2	c	97	MET
2	c	111	ARG
2	c	115	SER
2	c	117	GLU
2	c	119	LEU
2	c	121	ASN
2	c	132	VAL
2	c	144	LYS
2	c	157	VAL
2	c	163	ILE
2	c	164	ARG
2	c	174	SER
2	c	179	VAL
2	c	181	GLU
2	c	200	ASP
2	c	201	LYS
2	c	204	LEU
2	c	217	LEU
2	c	238	LEU
2	c	244	ILE
2	c	246	ARG
2	c	248	THR
2	c	249	LEU
2	c	268	GLN
2	c	271	LEU
2	c	293	VAL
2	c	297	TYR
2	c	303	LEU
2	c	304	THR
2	c	331	TYR
2	c	337	LEU
2	c	340	THR

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Mol	Chain	Res	Type
2	c	343	GLN
2	c	344	LEU
2	c	345	ASP
2	c	348	VAL
2	c	349	VAL
2	c	352	GLU
2	c	358	ARG
2	c	364	LEU
2	c	366	ARG
2	c	371	LYS
2	c	377	LEU
2	c	380	ASP
2	c	382	LEU
2	c	388	LEU
2	c	394	ARG
2	c	396	ILE
2	c	400	LEU
2	c	406	VAL
2	c	409	VAL
2	c	410	PHE
2	c	416	LYS
2	c	418	VAL
2	c	431	MET
2	c	449	ILE
2	c	454	GLU
2	c	457	LYS
2	d	5	ILE
2	d	6	VAL
2	d	14	ASP
2	d	16	GLU
2	d	17	PHE
2	d	22	VAL
2	d	29	LEU
2	d	36	GLU
2	d	51	VAL
2	d	66	LEU
2	d	68	VAL
2	d	86	ARG
2	d	97	MET
2	d	98	LYS
2	d	100	GLU
2	d	101	ILE

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Mol	Chain	Res	Type
2	d	103	GLU
2	d	104	GLU
2	d	117	GLU
2	d	121	ASN
2	d	131	LYS
2	d	136	MET
2	d	139	PHE
2	d	141	LYS
2	d	144	LYS
2	d	145	VAL
2	d	157	VAL
2	d	162	LEU
2	d	164	ARG
2	d	169	GLU
2	d	173	TYR
2	d	179	VAL
2	d	181	GLU
2	d	185	GLU
2	d	194	THR
2	d	197	ASN
2	d	201	LYS
2	d	205	VAL
2	d	210	ASN
2	d	224	LEU
2	d	239	LEU
2	d	260	ARG
2	d	265	VAL
2	d	268	GLN
2	d	271	LEU
2	d	283	THR
2	d	291	THR
2	d	293	VAL
2	d	296	VAL
2	d	298	VAL
2	d	319	VAL
2	d	320	VAL
2	d	323	ARG
2	d	324	GLN
2	d	338	ASP
2	d	344	LEU
2	d	347	LEU
2	d	364	LEU

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Mol	Chain	Res	Type
2	d	372	ASP
2	d	385	GLU
2	d	387	LYS
2	d	390	VAL
2	d	392	ARG
2	d	396	ILE
2	d	400	LEU
2	d	410	PHE
2	d	417	TYR
2	d	419	SER
2	d	441	GLN
2	d	450	GLU
2	d	453	VAL
2	d	457	LYS
2	d	459	LEU
3	e	4	LYS
3	e	5	GLU
3	e	9	LYS
3	e	16	THR
3	e	47	THR
3	e	49	ARG
3	e	55	LEU
3	e	62	TYR
3	e	64	HIS
3	e	67	LEU
3	e	72	VAL
3	e	110	VAL
3	e	120	LYS
3	e	137	THR
3	e	145	LEU
3	e	173	LYS
3	e	187	LEU
3	e	188	LEU
3	e	190	LEU
3	e	193	SER
3	e	195	ASP
3	e	199	LYS
3	e	200	HIS
3	e	206	LEU
3	e	208	GLU
3	e	218	LEU
3	e	219	LEU

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Mol	Chain	Res	Type
3	e	232	VAL
3	e	242	ARG
3	e	246	MET
3	e	255	SER
3	e	258	LYS
3	e	272	ILE
3	e	276	LEU
3	e	277	THR
3	e	280	VAL
4	f	2	MET
4	f	41	LEU
4	f	49	MET
4	f	50	ILE
4	f	60	GLU
4	f	75	ASN
4	f	76	VAL
4	f	85	ARG
4	f	91	GLU
4	f	103	GLU
4	f	121	LEU
4	f	129	ARG
4	f	131	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (390) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	144	GLN
1	A	172	GLN
1	A	185	ASN
1	A	186	GLN
1	A	215	HIS
1	A	266	GLN
1	A	272	GLN
1	A	344	ASN
1	A	361	ASN
1	A	382	GLN
1	A	408	GLN
1	A	423	HIS
1	A	435	GLN
1	B	27	ASN
1	B	140	GLN

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Mol	Chain	Res	Type
1	B	144	GLN
1	B	147	GLN
1	B	185	ASN
1	B	186	GLN
1	B	200	GLN
1	B	215	HIS
1	B	266	GLN
1	B	272	GLN
1	B	294	HIS
1	B	344	ASN
1	B	369	ASN
1	B	382	GLN
1	B	399	GLN
1	B	420	GLN
1	B	423	HIS
1	B	443	GLN
1	B	444	GLN
1	B	488	GLN
1	B	511	GLN
1	C	26	HIS
1	C	42	HIS
1	C	144	GLN
1	C	172	GLN
1	C	185	ASN
1	C	186	GLN
1	C	200	GLN
1	C	215	HIS
1	C	272	GLN
1	C	305	ASN
1	C	344	ASN
1	C	382	GLN
1	C	423	HIS
1	C	443	GLN
2	D	35	ASN
2	D	89	ASN
2	D	170	HIS
2	D	208	GLN
2	D	215	ASN
2	D	279	GLN
2	D	324	GLN
2	D	397	GLN
2	E	32	GLN

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Mol	Chain	Res	Type
2	E	89	ASN
2	E	121	ASN
2	E	158	ASN
2	E	197	ASN
2	E	208	GLN
2	E	268	GLN
2	E	314	HIS
2	E	343	GLN
2	E	351	GLN
2	E	353	HIS
2	E	368	GLN
2	E	397	GLN
2	E	402	GLN
2	F	7	GLN
2	F	19	GLN
2	F	32	GLN
2	F	73	HIS
2	F	123	GLN
2	F	197	ASN
2	F	208	GLN
2	F	243	ASN
2	F	268	GLN
2	F	279	GLN
2	F	368	GLN
2	F	397	GLN
2	F	402	GLN
2	F	437	HIS
2	F	441	GLN
3	G	54	HIS
3	G	59	ASN
3	G	111	GLN
3	G	157	GLN
3	G	265	ASN
4	H	55	GLN
4	H	56	HIS
4	H	75	ASN
4	H	87	GLN
4	H	116	GLN
1	I	109	ASN
1	I	144	GLN
1	I	147	GLN
1	I	172	GLN

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Mol	Chain	Res	Type
1	I	185	ASN
1	I	186	GLN
1	I	215	HIS
1	I	266	GLN
1	I	272	GLN
1	I	344	ASN
1	I	361	ASN
1	I	382	GLN
1	I	408	GLN
1	I	423	HIS
1	I	435	GLN
1	J	27	ASN
1	J	140	GLN
1	J	144	GLN
1	J	147	GLN
1	J	185	ASN
1	J	186	GLN
1	J	200	GLN
1	J	207	ASN
1	J	215	HIS
1	J	266	GLN
1	J	272	GLN
1	J	344	ASN
1	J	369	ASN
1	J	382	GLN
1	J	420	GLN
1	J	423	HIS
1	J	443	GLN
1	J	444	GLN
1	J	511	GLN
1	K	26	HIS
1	K	42	HIS
1	K	144	GLN
1	K	172	GLN
1	K	185	ASN
1	K	186	GLN
1	K	200	GLN
1	K	215	HIS
1	K	272	GLN
1	K	305	ASN
1	K	344	ASN
1	K	382	GLN

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Mol	Chain	Res	Type
1	K	423	HIS
1	K	443	GLN
1	K	493	ASN
2	L	35	ASN
2	L	89	ASN
2	L	170	HIS
2	L	187	ASN
2	L	208	GLN
2	L	215	ASN
2	L	279	GLN
2	L	324	GLN
2	L	397	GLN
2	M	32	GLN
2	M	89	ASN
2	M	121	ASN
2	M	158	ASN
2	M	208	GLN
2	M	268	GLN
2	M	343	GLN
2	M	351	GLN
2	M	368	GLN
2	M	397	GLN
2	M	402	GLN
2	N	7	GLN
2	N	19	GLN
2	N	32	GLN
2	N	73	HIS
2	N	123	GLN
2	N	197	ASN
2	N	208	GLN
2	N	243	ASN
2	N	268	GLN
2	N	279	GLN
2	N	351	GLN
2	N	353	HIS
2	N	368	GLN
2	N	402	GLN
2	N	437	HIS
3	O	54	HIS
3	O	59	ASN
3	O	111	GLN
3	O	131	ASN

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Mol	Chain	Res	Type
3	O	157	GLN
3	O	172	ASN
3	O	265	ASN
4	P	55	GLN
4	P	56	HIS
4	P	75	ASN
4	P	87	GLN
4	P	116	GLN
1	Q	109	ASN
1	Q	144	GLN
1	Q	147	GLN
1	Q	172	GLN
1	Q	185	ASN
1	Q	186	GLN
1	Q	215	HIS
1	Q	266	GLN
1	Q	272	GLN
1	Q	344	ASN
1	Q	361	ASN
1	Q	382	GLN
1	Q	408	GLN
1	Q	435	GLN
1	R	27	ASN
1	R	140	GLN
1	R	147	GLN
1	R	185	ASN
1	R	186	GLN
1	R	200	GLN
1	R	207	ASN
1	R	215	HIS
1	R	266	GLN
1	R	272	GLN
1	R	294	HIS
1	R	344	ASN
1	R	369	ASN
1	R	382	GLN
1	R	420	GLN
1	R	423	HIS
1	R	443	GLN
1	R	444	GLN
1	R	488	GLN
1	R	511	GLN

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Mol	Chain	Res	Type
1	S	26	HIS
1	S	42	HIS
1	S	144	GLN
1	S	172	GLN
1	S	185	ASN
1	S	186	GLN
1	S	200	GLN
1	S	215	HIS
1	S	272	GLN
1	S	305	ASN
1	S	333	GLN
1	S	344	ASN
1	S	382	GLN
1	S	423	HIS
1	S	443	GLN
1	S	493	ASN
2	T	35	ASN
2	T	89	ASN
2	T	170	HIS
2	T	208	GLN
2	T	215	ASN
2	T	279	GLN
2	T	314	HIS
2	T	324	GLN
2	T	397	GLN
2	U	32	GLN
2	U	89	ASN
2	U	121	ASN
2	U	123	GLN
2	U	158	ASN
2	U	208	GLN
2	U	268	GLN
2	U	314	HIS
2	U	343	GLN
2	U	351	GLN
2	U	353	HIS
2	U	361	GLN
2	U	368	GLN
2	U	397	GLN
2	U	402	GLN
2	V	7	GLN
2	V	19	GLN

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Mol	Chain	Res	Type
2	V	32	GLN
2	V	73	HIS
2	V	123	GLN
2	V	197	ASN
2	V	208	GLN
2	V	268	GLN
2	V	279	GLN
2	V	353	HIS
2	V	368	GLN
2	V	397	GLN
2	V	402	GLN
2	V	437	HIS
3	W	54	HIS
3	W	59	ASN
3	W	111	GLN
3	W	126	ASN
3	W	131	ASN
3	W	157	GLN
3	W	172	ASN
3	W	234	ASN
3	W	265	ASN
4	X	55	GLN
4	X	56	HIS
4	X	87	GLN
4	X	116	GLN
4	X	127	GLN
1	Y	109	ASN
1	Y	144	GLN
1	Y	172	GLN
1	Y	185	ASN
1	Y	186	GLN
1	Y	215	HIS
1	Y	266	GLN
1	Y	272	GLN
1	Y	344	ASN
1	Y	361	ASN
1	Y	382	GLN
1	Y	408	GLN
1	Y	423	HIS
1	Y	435	GLN
1	Z	27	ASN
1	Z	140	GLN

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Mol	Chain	Res	Type
1	Z	147	GLN
1	Z	185	ASN
1	Z	186	GLN
1	Z	200	GLN
1	Z	207	ASN
1	Z	215	HIS
1	Z	266	GLN
1	Z	272	GLN
1	Z	294	HIS
1	Z	344	ASN
1	Z	369	ASN
1	Z	382	GLN
1	Z	420	GLN
1	Z	423	HIS
1	Z	443	GLN
1	Z	444	GLN
1	Z	488	GLN
1	Z	511	GLN
1	a	26	HIS
1	a	144	GLN
1	a	172	GLN
1	a	185	ASN
1	a	186	GLN
1	a	200	GLN
1	a	215	HIS
1	a	272	GLN
1	a	333	GLN
1	a	344	ASN
1	a	382	GLN
1	a	423	HIS
1	a	443	GLN
1	a	493	ASN
2	b	35	ASN
2	b	89	ASN
2	b	170	HIS
2	b	208	GLN
2	b	215	ASN
2	b	279	GLN
2	b	324	GLN
2	b	397	GLN
2	c	32	GLN
2	c	45	GLN

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Mol	Chain	Res	Type
2	c	89	ASN
2	c	121	ASN
2	c	158	ASN
2	c	268	GLN
2	c	314	HIS
2	c	343	GLN
2	c	351	GLN
2	c	368	GLN
2	c	397	GLN
2	c	402	GLN
2	d	7	GLN
2	d	19	GLN
2	d	32	GLN
2	d	73	HIS
2	d	123	GLN
2	d	197	ASN
2	d	208	GLN
2	d	243	ASN
2	d	268	GLN
2	d	279	GLN
2	d	353	HIS
2	d	368	GLN
2	d	397	GLN
2	d	402	GLN
2	d	437	HIS
3	e	54	HIS
3	e	59	ASN
3	e	111	GLN
3	e	126	ASN
3	e	131	ASN
3	e	157	GLN
3	e	172	ASN
3	e	186	GLN
4	f	55	GLN
4	f	56	HIS
4	f	75	ASN
4	f	87	GLN
4	f	116	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 49 ligands modelled in this entry, 16 are monoatomic - leaving 33 for Mogul analysis.

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	$\# Z > 2$
8	SO4	P	200	-	4,4,4	0.37	0	6,6,6	0.49	0
5	ANP	Y	600	6	33,33,33	2.94	11 (33%)	45,52,52	2.82	14 (31%)
5	ANP	I	600	6	33,33,33	2.93	12 (36%)	45,52,52	2.82	14 (31%)
5	ANP	C	600	6	33,33,33	2.93	12 (36%)	45,52,52	2.81	14 (31%)
5	ANP	B	600	6	33,33,33	2.57	11 (33%)	45,52,52	2.90	17 (37%)
8	SO4	N	530	-	4,4,4	0.24	0	6,6,6	0.10	0
8	SO4	T	630	6	4,4,4	0.22	0	6,6,6	0.11	0
8	SO4	U	530	-	4,4,4	0.23	0	6,6,6	0.08	0
5	ANP	R	600	6	33,33,33	2.56	11 (33%)	45,52,52	2.91	17 (37%)
5	ANP	Z	600	6	33,33,33	2.57	11 (33%)	45,52,52	2.94	17 (37%)
8	SO4	E	530	-	4,4,4	0.22	0	6,6,6	0.10	0
7	ADP	L	600	6	28,29,29	2.12	8 (28%)	43,45,45	1.94	12 (27%)
5	ANP	A	600	6	33,33,33	2.94	12 (36%)	45,52,52	2.82	14 (31%)
8	SO4	b	630	6	4,4,4	0.25	0	6,6,6	0.10	0
8	SO4	d	530	-	4,4,4	0.22	0	6,6,6	0.13	0
5	ANP	J	600	6	33,33,33	2.56	11 (33%)	45,52,52	2.91	17 (37%)
7	ADP	b	600	6	28,29,29	2.09	8 (28%)	43,45,45	1.97	12 (27%)
8	SO4	W	300	-	4,4,4	0.22	0	6,6,6	0.28	0
7	ADP	T	600	6	28,29,29	2.09	9 (32%)	43,45,45	1.94	11 (25%)
8	SO4	G	300	-	4,4,4	0.47	0	6,6,6	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ADP	D	600	6	28,29,29	2.13	8 (28%)	43,45,45	1.94	12 (27%)
5	ANP	K	600	6	33,33,33	2.94	12 (36%)	45,52,52	2.85	14 (31%)
5	ANP	a	600	6	33,33,33	2.96	12 (36%)	45,52,52	2.81	13 (28%)
8	SO4	O	300	-	4,4,4	0.43	0	6,6,6	0.60	0
5	ANP	Q	600	6	33,33,33	2.93	12 (36%)	45,52,52	2.82	14 (31%)
8	SO4	D	630	6	4,4,4	0.22	0	6,6,6	0.09	0
8	SO4	F	530	-	4,4,4	0.22	0	6,6,6	0.10	0
8	SO4	V	530	-	4,4,4	0.21	0	6,6,6	0.12	0
8	SO4	c	530	-	4,4,4	0.21	0	6,6,6	0.08	0
8	SO4	M	530	-	4,4,4	0.22	0	6,6,6	0.10	0
8	SO4	L	630	6	4,4,4	0.22	0	6,6,6	0.10	0
8	SO4	H	200	-	4,4,4	0.40	0	6,6,6	0.35	0
5	ANP	S	600	6	33,33,33	2.95	11 (33%)	45,52,52	2.83	13 (28%)

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
5	ANP	J	600	6	-	6/18/38/38	0/3/3/3
7	ADP	b	600	6	-	4/16/32/32	0/3/3/3
5	ANP	R	600	6	-	6/18/38/38	0/3/3/3
7	ADP	L	600	6	-	4/16/32/32	0/3/3/3
5	ANP	Y	600	6	-	2/18/38/38	0/3/3/3
7	ADP	T	600	6	-	4/16/32/32	0/3/3/3
5	ANP	Z	600	6	-	6/18/38/38	0/3/3/3
7	ADP	D	600	6	-	4/16/32/32	0/3/3/3
5	ANP	I	600	6	-	2/18/38/38	0/3/3/3
5	ANP	K	600	6	-	2/18/38/38	0/3/3/3
5	ANP	C	600	6	-	2/18/38/38	0/3/3/3
5	ANP	B	600	6	-	6/18/38/38	0/3/3/3
5	ANP	A	600	6	-	2/18/38/38	0/3/3/3
5	ANP	a	600	6	-	2/18/38/38	0/3/3/3
5	ANP	S	600	6	-	2/18/38/38	0/3/3/3
5	ANP	Q	600	6	-	2/18/38/38	0/3/3/3

All (171) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	a	600	ANP	PB-O1B	9.13	1.60	1.46
5	S	600	ANP	PB-O1B	8.96	1.59	1.46
5	A	600	ANP	PB-O1B	8.94	1.59	1.46
5	C	600	ANP	PB-O1B	8.94	1.59	1.46
5	Y	600	ANP	PB-O1B	8.94	1.59	1.46
5	Q	600	ANP	PB-O1B	8.94	1.59	1.46
5	I	600	ANP	PB-O1B	8.93	1.59	1.46
5	K	600	ANP	PB-O1B	8.90	1.59	1.46
5	B	600	ANP	PB-O1B	7.77	1.57	1.46
5	Z	600	ANP	PB-O1B	7.66	1.57	1.46
5	R	600	ANP	PB-O1B	7.55	1.57	1.46
5	J	600	ANP	PB-O1B	7.49	1.57	1.46
5	C	600	ANP	PG-O1G	6.62	1.56	1.46
5	Y	600	ANP	PG-O1G	6.60	1.56	1.46
5	a	600	ANP	PG-O1G	6.60	1.56	1.46
5	A	600	ANP	PG-O1G	6.59	1.56	1.46
5	S	600	ANP	PG-O1G	6.57	1.56	1.46
5	Q	600	ANP	PG-O1G	6.57	1.56	1.46
5	K	600	ANP	PG-O1G	6.55	1.56	1.46
5	I	600	ANP	PG-O1G	6.52	1.56	1.46
7	D	600	ADP	C6-N6	6.32	1.50	1.34
7	L	600	ADP	C6-N6	6.32	1.50	1.34
7	T	600	ADP	C6-N6	6.31	1.50	1.34
7	b	600	ADP	C6-N6	6.31	1.50	1.34
7	D	600	ADP	PA-O3A	-5.60	1.53	1.59
7	L	600	ADP	PA-O3A	-5.45	1.53	1.59
7	b	600	ADP	PA-O3A	-5.39	1.53	1.59
7	T	600	ADP	PA-O3A	-5.22	1.53	1.59
5	Z	600	ANP	PB-N3B	5.02	1.76	1.63
5	J	600	ANP	PB-N3B	4.93	1.76	1.63
5	B	600	ANP	PB-N3B	4.93	1.76	1.63
5	R	600	ANP	PB-N3B	4.91	1.76	1.63
5	Q	600	ANP	O2'-C2'	-4.88	1.30	1.43
5	K	600	ANP	O2'-C2'	-4.88	1.30	1.43
5	Y	600	ANP	O2'-C2'	-4.88	1.30	1.43
5	A	600	ANP	O2'-C2'	-4.85	1.30	1.43
5	I	600	ANP	O2'-C2'	-4.84	1.31	1.43
5	S	600	ANP	C5'-C4'	-4.84	1.37	1.51
5	C	600	ANP	O2'-C2'	-4.82	1.31	1.43
5	S	600	ANP	O2'-C2'	-4.82	1.31	1.43
5	a	600	ANP	C5'-C4'	-4.82	1.37	1.51
5	I	600	ANP	C5'-C4'	-4.77	1.37	1.51
5	A	600	ANP	C5'-C4'	-4.76	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	600	ANP	C5'-C4'	-4.76	1.37	1.51
5	Y	600	ANP	C5'-C4'	-4.76	1.37	1.51
5	Q	600	ANP	C5'-C4'	-4.75	1.37	1.51
5	a	600	ANP	O2'-C2'	-4.74	1.31	1.43
5	K	600	ANP	C5'-C4'	-4.73	1.37	1.51
5	R	600	ANP	PG-O1G	4.72	1.53	1.46
5	S	600	ANP	PB-N3B	4.69	1.75	1.63
5	K	600	ANP	PB-N3B	4.61	1.75	1.63
5	a	600	ANP	PB-N3B	4.61	1.75	1.63
5	Z	600	ANP	PG-O1G	4.57	1.53	1.46
5	A	600	ANP	PB-N3B	4.54	1.75	1.63
5	Y	600	ANP	PB-N3B	4.53	1.75	1.63
5	C	600	ANP	PB-N3B	4.53	1.75	1.63
5	I	600	ANP	PB-N3B	4.53	1.75	1.63
5	Q	600	ANP	PB-N3B	4.51	1.75	1.63
5	J	600	ANP	O2'-C2'	-4.51	1.31	1.43
5	R	600	ANP	O2'-C2'	-4.51	1.31	1.43
5	B	600	ANP	O2'-C2'	-4.51	1.31	1.43
5	B	600	ANP	PG-O1G	4.50	1.53	1.46
5	J	600	ANP	PG-O1G	4.46	1.52	1.46
5	Z	600	ANP	O2'-C2'	-4.43	1.32	1.43
5	a	600	ANP	PA-O3A	-4.42	1.54	1.59
5	J	600	ANP	C5'-C4'	-4.37	1.38	1.51
5	B	600	ANP	C5'-C4'	-4.37	1.38	1.51
5	Z	600	ANP	C5'-C4'	-4.36	1.38	1.51
5	K	600	ANP	PA-O3A	-4.34	1.54	1.59
5	R	600	ANP	C5'-C4'	-4.32	1.38	1.51
5	S	600	ANP	C6-N6	4.31	1.45	1.34
5	a	600	ANP	C6-N6	4.30	1.45	1.34
5	K	600	ANP	C6-N6	4.29	1.45	1.34
5	S	600	ANP	PA-O3A	-4.28	1.54	1.59
5	I	600	ANP	C6-N6	4.26	1.45	1.34
5	Q	600	ANP	C6-N6	4.26	1.45	1.34
5	A	600	ANP	C6-N6	4.25	1.45	1.34
5	C	600	ANP	C6-N6	4.24	1.45	1.34
5	Y	600	ANP	C6-N6	4.23	1.45	1.34
5	Z	600	ANP	PG-N3B	4.21	1.74	1.63
5	A	600	ANP	PA-O3A	-4.17	1.55	1.59
5	C	600	ANP	PA-O3A	-4.15	1.55	1.59
5	K	600	ANP	PG-N3B	4.13	1.74	1.63
5	I	600	ANP	PA-O3A	-4.12	1.55	1.59
5	Y	600	ANP	PA-O3A	-4.11	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	600	ANP	PA-O3A	-4.10	1.55	1.59
5	R	600	ANP	PG-N3B	4.10	1.74	1.63
5	S	600	ANP	PG-N3B	4.09	1.74	1.63
5	J	600	ANP	PG-N3B	4.08	1.74	1.63
5	B	600	ANP	PG-N3B	4.06	1.74	1.63
5	Q	600	ANP	PG-N3B	4.06	1.74	1.63
5	I	600	ANP	PG-N3B	4.05	1.74	1.63
5	Y	600	ANP	PG-N3B	4.05	1.73	1.63
5	A	600	ANP	PG-N3B	4.04	1.73	1.63
5	C	600	ANP	PG-N3B	4.02	1.73	1.63
5	a	600	ANP	PG-N3B	3.96	1.73	1.63
5	R	600	ANP	C6-N6	3.50	1.43	1.34
5	Z	600	ANP	C6-N6	3.46	1.43	1.34
5	J	600	ANP	C6-N6	3.43	1.43	1.34
5	B	600	ANP	C6-N6	3.42	1.42	1.34
7	b	600	ADP	O2'-C2'	-2.84	1.35	1.43
7	T	600	ADP	O2'-C2'	-2.81	1.36	1.43
7	L	600	ADP	O2'-C2'	-2.81	1.36	1.43
7	D	600	ADP	O2'-C2'	-2.79	1.36	1.43
5	J	600	ANP	PA-O3A	-2.75	1.56	1.59
5	B	600	ANP	PA-O3A	-2.56	1.56	1.59
5	R	600	ANP	PA-O3A	-2.50	1.56	1.59
5	Z	600	ANP	PA-O3A	-2.47	1.56	1.59
7	D	600	ADP	C5'-C4'	-2.45	1.44	1.51
7	L	600	ADP	C5'-C4'	-2.43	1.44	1.51
7	b	600	ADP	C5'-C4'	-2.43	1.44	1.51
7	T	600	ADP	C5'-C4'	-2.42	1.44	1.51
5	I	600	ANP	C3'-C4'	-2.41	1.46	1.53
5	Y	600	ANP	C3'-C4'	-2.39	1.46	1.53
5	A	600	ANP	C3'-C4'	-2.39	1.46	1.53
5	C	600	ANP	C3'-C4'	-2.38	1.46	1.53
5	Q	600	ANP	C3'-C4'	-2.37	1.47	1.53
5	a	600	ANP	C3'-C4'	-2.37	1.47	1.53
7	L	600	ADP	C5-N7	-2.35	1.34	1.39
7	L	600	ADP	O3'-C3'	-2.35	1.37	1.43
7	T	600	ADP	O3'-C3'	-2.35	1.37	1.43
5	K	600	ANP	C3'-C4'	-2.32	1.47	1.53
5	S	600	ANP	C3'-C4'	-2.32	1.47	1.53
7	D	600	ADP	C5-N7	-2.30	1.34	1.39
7	L	600	ADP	C2'-C3'	-2.28	1.47	1.53
5	J	600	ANP	C5-N7	-2.28	1.34	1.39
7	T	600	ADP	C2'-C3'	-2.27	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	600	ADP	C5-N7	-2.27	1.34	1.39
7	D	600	ADP	O3'-C3'	-2.27	1.37	1.43
7	b	600	ADP	C5-N7	-2.25	1.35	1.39
5	B	600	ANP	C5-N7	-2.25	1.35	1.39
7	b	600	ADP	O3'-C3'	-2.24	1.37	1.43
7	D	600	ADP	C2'-C3'	-2.22	1.47	1.53
7	D	600	ADP	C3'-C4'	-2.22	1.47	1.53
5	Z	600	ANP	C5-N7	-2.21	1.35	1.39
5	B	600	ANP	C3'-C4'	-2.20	1.47	1.53
7	L	600	ADP	C3'-C4'	-2.20	1.47	1.53
5	R	600	ANP	C5-N7	-2.18	1.35	1.39
5	Z	600	ANP	C3'-C4'	-2.18	1.47	1.53
7	b	600	ADP	C2'-C3'	-2.18	1.47	1.53
5	K	600	ANP	O3'-C3'	-2.17	1.37	1.43
5	a	600	ANP	O3'-C3'	-2.17	1.37	1.43
5	J	600	ANP	C3'-C4'	-2.17	1.47	1.53
7	T	600	ADP	C3'-C4'	-2.17	1.47	1.53
5	Y	600	ANP	O3'-C3'	-2.16	1.37	1.43
5	A	600	ANP	O3'-C3'	-2.16	1.37	1.43
5	Q	600	ANP	O3'-C3'	-2.15	1.37	1.43
5	C	600	ANP	O3'-C3'	-2.14	1.37	1.43
5	I	600	ANP	O3'-C3'	-2.14	1.37	1.43
7	b	600	ADP	C3'-C4'	-2.12	1.47	1.53
5	R	600	ANP	C3'-C4'	-2.11	1.47	1.53
5	R	600	ANP	C2'-C3'	-2.10	1.47	1.53
5	Y	600	ANP	C8-N9	-2.10	1.34	1.37
5	B	600	ANP	C2'-C3'	-2.10	1.47	1.53
5	S	600	ANP	O3'-C3'	-2.10	1.37	1.43
5	I	600	ANP	C8-N9	-2.10	1.34	1.37
5	J	600	ANP	C2'-C3'	-2.09	1.47	1.53
5	C	600	ANP	C8-N9	-2.09	1.34	1.37
5	a	600	ANP	C8-N9	-2.09	1.34	1.37
5	a	600	ANP	C5-N7	-2.08	1.35	1.39
5	Z	600	ANP	C2'-C3'	-2.07	1.47	1.53
5	K	600	ANP	C8-N9	-2.07	1.34	1.37
5	A	600	ANP	C8-N9	-2.07	1.34	1.37
5	Q	600	ANP	C5-N7	-2.06	1.35	1.39
5	S	600	ANP	C8-N9	-2.04	1.34	1.37
5	C	600	ANP	C5-N7	-2.04	1.35	1.39
5	K	600	ANP	C5-N7	-2.03	1.35	1.39
5	Q	600	ANP	C8-N9	-2.03	1.34	1.37
5	I	600	ANP	C5-N7	-2.03	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	600	ANP	C5-N7	-2.02	1.35	1.39
7	T	600	ADP	C8-N7	2.01	1.35	1.31

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	600	ANP	O1B-PB-N3B	-11.49	94.85	111.77
5	C	600	ANP	O1B-PB-N3B	-11.38	95.02	111.77
5	I	600	ANP	O1B-PB-N3B	-11.37	95.03	111.77
5	A	600	ANP	O1B-PB-N3B	-11.36	95.05	111.77
5	Q	600	ANP	O1B-PB-N3B	-11.35	95.05	111.77
5	Y	600	ANP	O1B-PB-N3B	-11.35	95.05	111.77
5	S	600	ANP	O1B-PB-N3B	-11.28	95.17	111.77
5	a	600	ANP	O1B-PB-N3B	-11.27	95.18	111.77
5	Z	600	ANP	O1B-PB-N3B	-11.03	95.52	111.77
5	R	600	ANP	O1B-PB-N3B	-10.79	95.88	111.77
5	J	600	ANP	O1B-PB-N3B	-10.77	95.91	111.77
5	B	600	ANP	O1B-PB-N3B	-10.71	96.00	111.77
5	J	600	ANP	C5-C4-N3	-5.61	118.99	126.72
5	R	600	ANP	C5-C4-N3	-5.61	118.99	126.72
5	Z	600	ANP	C5-C4-N3	-5.58	119.03	126.72
5	B	600	ANP	C5-C4-N3	-5.58	119.04	126.72
7	T	600	ADP	C5-C4-N3	-5.33	119.37	126.72
7	b	600	ADP	C5-C4-N3	-5.33	119.38	126.72
7	L	600	ADP	C5-C4-N3	-5.30	119.42	126.72
7	D	600	ADP	C5-C4-N3	-5.23	119.52	126.72
5	Z	600	ANP	O3A-PB-N3B	-5.22	92.12	106.59
5	B	600	ANP	O3A-PB-N3B	-5.21	92.15	106.59
5	J	600	ANP	O3A-PB-N3B	-5.17	92.25	106.59
5	R	600	ANP	O3A-PB-N3B	-5.15	92.30	106.59
5	K	600	ANP	N3-C2-N1	-5.13	120.81	128.58
5	S	600	ANP	N3-C2-N1	-5.09	120.88	128.58
5	Z	600	ANP	O2B-PB-O1B	5.08	120.77	109.87
5	Y	600	ANP	N3-C2-N1	-5.07	120.90	128.58
5	Q	600	ANP	N3-C2-N1	-5.07	120.91	128.58
5	I	600	ANP	N3-C2-N1	-5.06	120.93	128.58
5	A	600	ANP	N3-C2-N1	-5.05	120.93	128.58
5	C	600	ANP	N3-C2-N1	-5.05	120.94	128.58
5	a	600	ANP	N3-C2-N1	-5.03	120.96	128.58
5	R	600	ANP	O2B-PB-O1B	5.03	120.66	109.87
5	J	600	ANP	O2B-PB-O1B	5.02	120.63	109.87
5	Y	600	ANP	C5-C4-N3	-5.02	119.81	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	600	ANP	C5-C4-N3	-5.01	119.82	126.72
5	I	600	ANP	C5-C4-N3	-4.99	119.85	126.72
5	A	600	ANP	C5-C4-N3	-4.98	119.85	126.72
5	Q	600	ANP	C5-C4-N3	-4.98	119.85	126.72
5	B	600	ANP	O2B-PB-O1B	4.98	120.56	109.87
5	S	600	ANP	C5-C4-N3	-4.96	119.88	126.72
5	C	600	ANP	C5-C4-N3	-4.94	119.92	126.72
5	a	600	ANP	C5-C4-N3	-4.93	119.93	126.72
5	I	600	ANP	O2B-PB-O3A	4.83	120.75	104.64
5	A	600	ANP	O2B-PB-O3A	4.82	120.73	104.64
5	Y	600	ANP	O2B-PB-O3A	4.82	120.72	104.64
5	C	600	ANP	O2B-PB-O3A	4.82	120.72	104.64
5	Q	600	ANP	O2B-PB-O3A	4.82	120.72	104.64
5	K	600	ANP	O2B-PB-O3A	4.79	120.62	104.64
5	S	600	ANP	O2B-PB-O3A	4.78	120.59	104.64
5	a	600	ANP	O2B-PB-O3A	4.75	120.49	104.64
5	Z	600	ANP	N3-C4-N9	4.74	135.24	127.17
5	J	600	ANP	N3-C4-N9	4.72	135.20	127.17
5	R	600	ANP	N3-C4-N9	4.72	135.20	127.17
7	D	600	ADP	N3-C2-N1	-4.69	121.49	128.58
7	L	600	ADP	N3-C2-N1	-4.68	121.49	128.58
5	B	600	ANP	N3-C4-N9	4.67	135.12	127.17
5	R	600	ANP	O2B-PB-O3A	4.66	120.19	104.64
7	b	600	ADP	N3-C2-N1	-4.64	121.55	128.58
5	Z	600	ANP	O2B-PB-O3A	4.63	120.10	104.64
5	J	600	ANP	O2B-PB-O3A	4.62	120.05	104.64
5	B	600	ANP	O2B-PB-O3A	4.61	120.04	104.64
7	T	600	ADP	N3-C2-N1	-4.59	121.64	128.58
5	J	600	ANP	N3-C2-N1	-4.49	121.78	128.58
5	K	600	ANP	O3A-PB-N3B	-4.44	94.28	106.59
5	B	600	ANP	N3-C2-N1	-4.42	121.89	128.58
5	Y	600	ANP	O3A-PB-N3B	-4.41	94.36	106.59
5	A	600	ANP	O3A-PB-N3B	-4.41	94.37	106.59
5	I	600	ANP	O3A-PB-N3B	-4.40	94.38	106.59
5	Q	600	ANP	O3A-PB-N3B	-4.40	94.38	106.59
5	C	600	ANP	O3A-PB-N3B	-4.40	94.38	106.59
5	Z	600	ANP	N3-C2-N1	-4.38	121.96	128.58
5	R	600	ANP	N3-C2-N1	-4.36	121.99	128.58
5	S	600	ANP	N3-C4-N9	4.34	134.55	127.17
5	S	600	ANP	N9-C8-N7	-4.34	107.78	113.94
5	a	600	ANP	N9-C8-N7	-4.33	107.79	113.94
5	a	600	ANP	N3-C4-N9	4.33	134.54	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	600	ANP	O3A-PB-N3B	-4.32	94.61	106.59
5	K	600	ANP	N3-C4-N9	4.30	134.49	127.17
5	Z	600	ANP	N9-C8-N7	-4.28	107.86	113.94
5	K	600	ANP	N9-C8-N7	-4.26	107.89	113.94
5	a	600	ANP	O3A-PB-N3B	-4.26	94.78	106.59
5	Y	600	ANP	N3-C4-N9	4.26	134.40	127.17
5	J	600	ANP	N9-C8-N7	-4.24	107.92	113.94
5	I	600	ANP	N3-C4-N9	4.24	134.37	127.17
5	R	600	ANP	N9-C8-N7	-4.23	107.93	113.94
5	C	600	ANP	N3-C4-N9	4.23	134.37	127.17
5	A	600	ANP	N3-C4-N9	4.23	134.35	127.17
5	Q	600	ANP	N3-C4-N9	4.22	134.35	127.17
5	Q	600	ANP	N9-C8-N7	-4.20	107.97	113.94
5	B	600	ANP	N9-C8-N7	-4.20	107.97	113.94
5	S	600	ANP	C4-N9-C8	4.19	110.14	105.74
5	Y	600	ANP	N9-C8-N7	-4.17	108.02	113.94
5	I	600	ANP	N9-C8-N7	-4.17	108.02	113.94
5	A	600	ANP	N9-C8-N7	-4.17	108.02	113.94
5	C	600	ANP	N9-C8-N7	-4.16	108.03	113.94
5	a	600	ANP	C4-N9-C8	4.16	110.11	105.74
5	K	600	ANP	C4-N9-C8	4.02	109.96	105.74
5	Y	600	ANP	C4-N9-C8	3.96	109.89	105.74
5	K	600	ANP	O2B-PB-O1B	3.96	118.35	109.87
5	C	600	ANP	C4-N9-C8	3.94	109.87	105.74
5	I	600	ANP	C4-N9-C8	3.93	109.86	105.74
5	Q	600	ANP	C4-N9-C8	3.92	109.85	105.74
5	A	600	ANP	C4-N9-C8	3.91	109.84	105.74
5	S	600	ANP	O2B-PB-O1B	3.86	118.14	109.87
5	Y	600	ANP	O2B-PB-O1B	3.83	118.08	109.87
5	C	600	ANP	O2B-PB-O1B	3.82	118.07	109.87
5	A	600	ANP	O2B-PB-O1B	3.81	118.05	109.87
5	a	600	ANP	O2B-PB-O1B	3.80	118.02	109.87
5	Q	600	ANP	O2B-PB-O1B	3.80	118.02	109.87
5	I	600	ANP	O2B-PB-O1B	3.79	118.00	109.87
5	Z	600	ANP	C4-N9-C8	3.79	109.72	105.74
5	R	600	ANP	C4-N9-C8	3.75	109.68	105.74
5	J	600	ANP	C4-N9-C8	3.73	109.66	105.74
5	Z	600	ANP	C5-N7-C8	3.72	109.30	103.45
5	B	600	ANP	C5-N7-C8	3.67	109.22	103.45
5	R	600	ANP	C5-N7-C8	3.66	109.20	103.45
5	J	600	ANP	C5-N7-C8	3.65	109.19	103.45
5	B	600	ANP	C4-N9-C8	3.62	109.54	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	600	ADP	N3-C4-N9	3.54	133.18	127.17
5	J	600	ANP	C2-N3-C4	3.51	120.40	111.83
7	T	600	ADP	N3-C4-N9	3.49	133.11	127.17
5	K	600	ANP	C2-N3-C4	3.49	120.36	111.83
7	D	600	ADP	N3-C4-N9	3.49	133.10	127.17
5	S	600	ANP	C2-N3-C4	3.48	120.33	111.83
5	Y	600	ANP	C2-N3-C4	3.48	120.33	111.83
5	I	600	ANP	C2-N3-C4	3.47	120.32	111.83
5	Z	600	ANP	C2-N3-C4	3.47	120.31	111.83
5	Q	600	ANP	C2-N3-C4	3.47	120.30	111.83
5	A	600	ANP	C2-N3-C4	3.46	120.29	111.83
5	B	600	ANP	C2-N3-C4	3.46	120.28	111.83
5	R	600	ANP	C2-N3-C4	3.45	120.25	111.83
7	L	600	ADP	N3-C4-N9	3.44	133.02	127.17
5	C	600	ANP	C2-N3-C4	3.44	120.23	111.83
5	a	600	ANP	C2-N3-C4	3.44	120.23	111.83
5	S	600	ANP	C5-N7-C8	3.42	108.83	103.45
5	K	600	ANP	C5-N7-C8	3.42	108.82	103.45
5	a	600	ANP	C5-N7-C8	3.42	108.82	103.45
7	b	600	ADP	C5-N7-C8	3.39	108.78	103.45
7	b	600	ADP	N9-C8-N7	-3.38	109.14	113.94
7	D	600	ADP	N9-C8-N7	-3.37	109.15	113.94
7	L	600	ADP	C2-N3-C4	3.37	120.07	111.83
7	b	600	ADP	C2-N3-C4	3.37	120.07	111.83
7	b	600	ADP	C4-C5-N7	-3.37	106.73	110.58
7	T	600	ADP	C2-N3-C4	3.37	120.05	111.83
7	D	600	ADP	C2-N3-C4	3.36	120.04	111.83
5	Q	600	ANP	C5-N7-C8	3.35	108.72	103.45
7	D	600	ADP	C5-N7-C8	3.35	108.72	103.45
5	A	600	ANP	C5-N7-C8	3.33	108.69	103.45
5	I	600	ANP	C5-N7-C8	3.33	108.68	103.45
5	C	600	ANP	C5-N7-C8	3.32	108.67	103.45
7	L	600	ADP	C4-C5-N7	-3.31	106.80	110.58
5	Y	600	ANP	C5-N7-C8	3.30	108.64	103.45
7	T	600	ADP	N9-C8-N7	-3.30	109.26	113.94
7	L	600	ADP	C5-N7-C8	3.29	108.63	103.45
7	T	600	ADP	C4-C5-N7	-3.28	106.83	110.58
7	T	600	ADP	C5-N7-C8	3.28	108.61	103.45
7	L	600	ADP	N9-C8-N7	-3.24	109.33	113.94
7	D	600	ADP	C4-C5-N7	-3.24	106.88	110.58
7	b	600	ADP	O4'-C1'-N9	3.18	114.19	108.09
7	D	600	ADP	O4'-C1'-N9	3.12	114.07	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	600	ADP	O4'-C1'-N9	3.05	113.95	108.09
5	Z	600	ANP	O1G-PG-N3B	-3.01	107.33	111.77
7	L	600	ADP	O4'-C1'-N9	3.00	113.85	108.09
5	J	600	ANP	O1G-PG-N3B	-2.91	107.48	111.77
5	R	600	ANP	C4-C5-N7	-2.80	107.38	110.58
5	Z	600	ANP	C4-C5-N7	-2.79	107.39	110.58
5	B	600	ANP	O1G-PG-N3B	-2.77	107.69	111.77
5	B	600	ANP	C4-C5-N7	-2.77	107.42	110.58
5	J	600	ANP	C4-C5-N7	-2.77	107.42	110.58
5	R	600	ANP	O1G-PG-N3B	-2.74	107.73	111.77
5	K	600	ANP	C4-C5-N7	-2.58	107.64	110.58
5	A	600	ANP	C4-C5-N7	-2.56	107.65	110.58
5	I	600	ANP	C4-C5-N7	-2.56	107.65	110.58
5	Y	600	ANP	C4-C5-N7	-2.56	107.66	110.58
5	Q	600	ANP	C4-C5-N7	-2.56	107.66	110.58
5	S	600	ANP	C4-C5-N7	-2.53	107.69	110.58
5	B	600	ANP	O2G-PG-O1G	-2.53	107.11	113.45
5	C	600	ANP	C4-C5-N7	-2.52	107.70	110.58
5	J	600	ANP	O2G-PG-O1G	-2.52	107.13	113.45
5	R	600	ANP	O2G-PG-O1G	-2.50	107.19	113.45
5	a	600	ANP	C4-C5-N7	-2.48	107.75	110.58
5	Z	600	ANP	O2G-PG-O1G	-2.44	107.33	113.45
7	T	600	ADP	O5'-C5'-C4'	2.38	117.11	108.99
5	C	600	ANP	O2G-PG-O1G	-2.38	107.48	113.45
7	D	600	ADP	O5'-C5'-C4'	2.38	117.10	108.99
5	S	600	ANP	O2G-PG-O1G	-2.38	107.49	113.45
5	Z	600	ANP	C3'-C2'-C1'	2.37	105.95	101.46
7	T	600	ADP	C3'-C2'-C1'	2.37	105.95	101.46
5	A	600	ANP	O2G-PG-O1G	-2.37	107.51	113.45
7	L	600	ADP	C3'-C2'-C1'	2.37	105.94	101.46
5	I	600	ANP	O2G-PG-O1G	-2.36	107.52	113.45
5	K	600	ANP	O2G-PG-O1G	-2.36	107.52	113.45
5	Q	600	ANP	O2G-PG-O1G	-2.36	107.53	113.45
7	b	600	ADP	O5'-C5'-C4'	2.36	117.03	108.99
5	Y	600	ANP	O2G-PG-O1G	-2.35	107.55	113.45
5	a	600	ANP	O2G-PG-O1G	-2.34	107.57	113.45
7	L	600	ADP	O5'-C5'-C4'	2.34	116.95	108.99
5	J	600	ANP	C3'-C2'-C1'	2.33	105.86	101.46
5	B	600	ANP	C3'-C2'-C1'	2.32	105.86	101.46
7	D	600	ADP	C3'-C2'-C1'	2.32	105.86	101.46
5	R	600	ANP	C3'-C2'-C1'	2.31	105.84	101.46
7	b	600	ADP	C3'-C2'-C1'	2.29	105.79	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	600	ADP	O3B-PB-O3A	2.28	112.29	104.64
7	D	600	ADP	O3B-PB-O3A	2.27	112.26	104.64
7	b	600	ADP	O3B-PB-O3A	2.26	112.22	104.64
5	B	600	ANP	C2'-C3'-C4'	2.26	106.97	102.61
5	R	600	ANP	C2'-C3'-C4'	2.25	106.96	102.61
7	T	600	ADP	O3B-PB-O3A	2.22	112.07	104.64
5	R	600	ANP	O5'-C5'-C4'	2.20	116.47	108.99
5	J	600	ANP	C2'-C3'-C4'	2.17	106.80	102.61
5	J	600	ANP	O5'-C5'-C4'	2.14	116.26	108.99
5	Z	600	ANP	C2'-C3'-C4'	2.13	106.73	102.61
5	B	600	ANP	O5'-C5'-C4'	2.09	116.11	108.99
7	b	600	ADP	C4-N9-C8	2.07	107.91	105.74
5	Z	600	ANP	O5'-C5'-C4'	2.06	116.00	108.99
5	Y	600	ANP	O1G-PG-N3B	-2.05	108.75	111.77
5	K	600	ANP	O1G-PG-N3B	-2.05	108.76	111.77
5	Q	600	ANP	O1G-PG-N3B	-2.04	108.77	111.77
5	I	600	ANP	O1G-PG-N3B	-2.04	108.77	111.77
7	L	600	ADP	C4'-O4'-C1'	-2.03	104.98	109.47
5	A	600	ANP	O1G-PG-N3B	-2.03	108.78	111.77
7	D	600	ADP	C4-N9-C8	2.03	107.86	105.74
5	C	600	ANP	O1G-PG-N3B	-2.02	108.79	111.77

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	ANP	PB-N3B-PG-O1G
5	A	600	ANP	PG-N3B-PB-O1B
5	B	600	ANP	PG-N3B-PB-O1B
5	B	600	ANP	C5'-O5'-PA-O1A
5	B	600	ANP	O4'-C4'-C5'-O5'
5	C	600	ANP	PB-N3B-PG-O1G
5	C	600	ANP	PG-N3B-PB-O1B
5	I	600	ANP	PB-N3B-PG-O1G
5	I	600	ANP	PG-N3B-PB-O1B
5	J	600	ANP	PG-N3B-PB-O1B
5	J	600	ANP	C5'-O5'-PA-O1A
5	J	600	ANP	O4'-C4'-C5'-O5'
5	K	600	ANP	PB-N3B-PG-O1G
5	K	600	ANP	PG-N3B-PB-O1B
5	Q	600	ANP	PB-N3B-PG-O1G
5	Q	600	ANP	PG-N3B-PB-O1B

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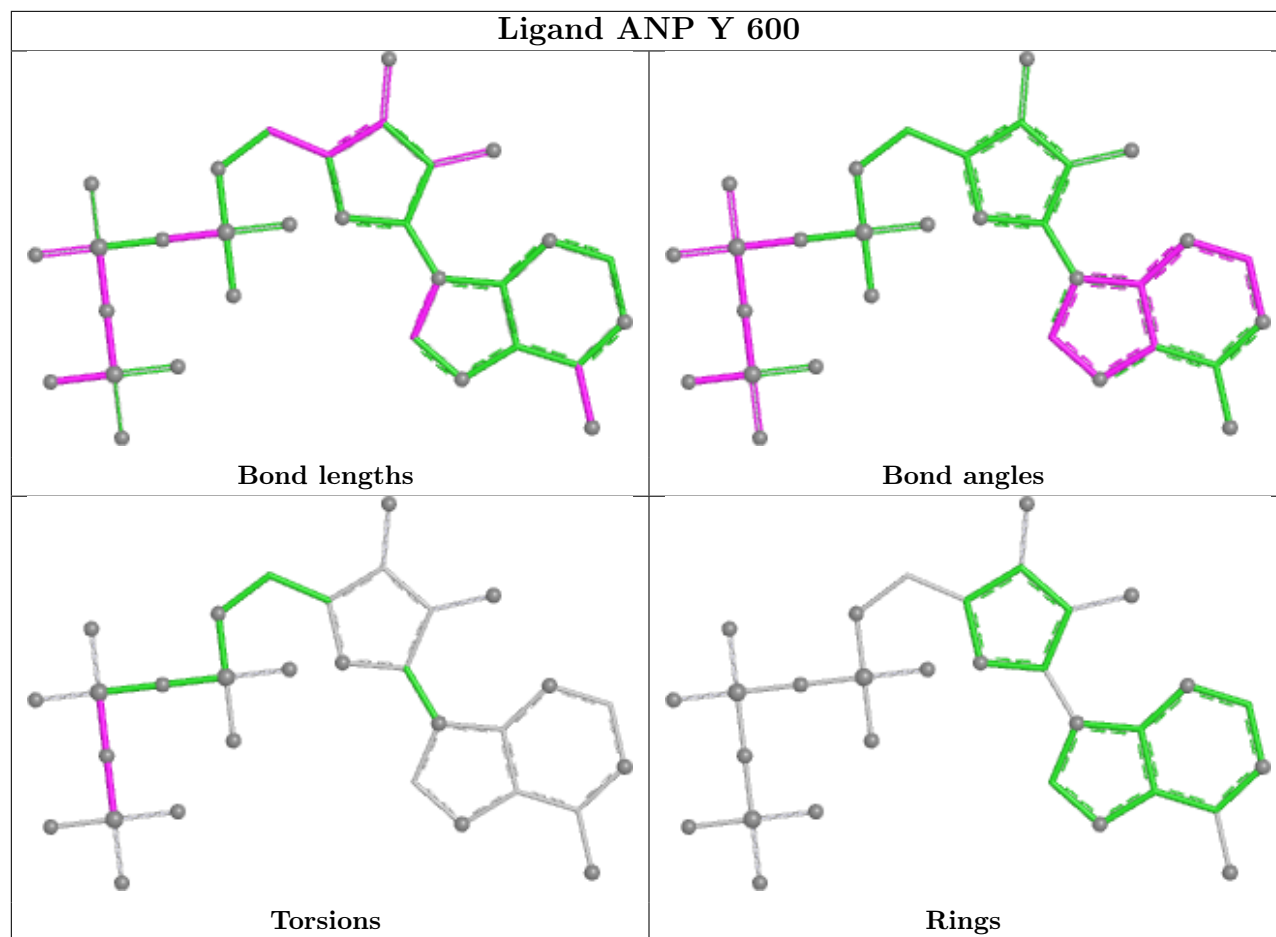
Mol	Chain	Res	Type	Atoms
5	R	600	ANP	PG-N3B-PB-O1B
5	R	600	ANP	C5'-O5'-PA-O1A
5	R	600	ANP	O4'-C4'-C5'-O5'
5	S	600	ANP	PB-N3B-PG-O1G
5	S	600	ANP	PG-N3B-PB-O1B
5	Y	600	ANP	PB-N3B-PG-O1G
5	Y	600	ANP	PG-N3B-PB-O1B
5	Z	600	ANP	PG-N3B-PB-O1B
5	Z	600	ANP	C5'-O5'-PA-O1A
5	Z	600	ANP	O4'-C4'-C5'-O5'
5	a	600	ANP	PB-N3B-PG-O1G
5	a	600	ANP	PG-N3B-PB-O1B
7	D	600	ADP	C5'-O5'-PA-O2A
7	D	600	ADP	C5'-O5'-PA-O3A
7	L	600	ADP	C5'-O5'-PA-O2A
7	L	600	ADP	C5'-O5'-PA-O3A
7	T	600	ADP	C5'-O5'-PA-O2A
7	T	600	ADP	C5'-O5'-PA-O3A
7	b	600	ADP	C5'-O5'-PA-O2A
7	b	600	ADP	C5'-O5'-PA-O3A
7	D	600	ADP	O4'-C4'-C5'-O5'
7	L	600	ADP	O4'-C4'-C5'-O5'
7	T	600	ADP	O4'-C4'-C5'-O5'
7	b	600	ADP	O4'-C4'-C5'-O5'
5	B	600	ANP	C3'-C4'-C5'-O5'
5	J	600	ANP	C3'-C4'-C5'-O5'
5	R	600	ANP	C3'-C4'-C5'-O5'
5	Z	600	ANP	C3'-C4'-C5'-O5'
7	D	600	ADP	C3'-C4'-C5'-O5'
7	L	600	ADP	C3'-C4'-C5'-O5'
7	T	600	ADP	C3'-C4'-C5'-O5'
7	b	600	ADP	C3'-C4'-C5'-O5'
5	B	600	ANP	C5'-O5'-PA-O2A
5	B	600	ANP	C5'-O5'-PA-O3A
5	J	600	ANP	C5'-O5'-PA-O2A
5	J	600	ANP	C5'-O5'-PA-O3A
5	R	600	ANP	C5'-O5'-PA-O2A
5	R	600	ANP	C5'-O5'-PA-O3A
5	Z	600	ANP	C5'-O5'-PA-O2A
5	Z	600	ANP	C5'-O5'-PA-O3A

There are no ring outliers.

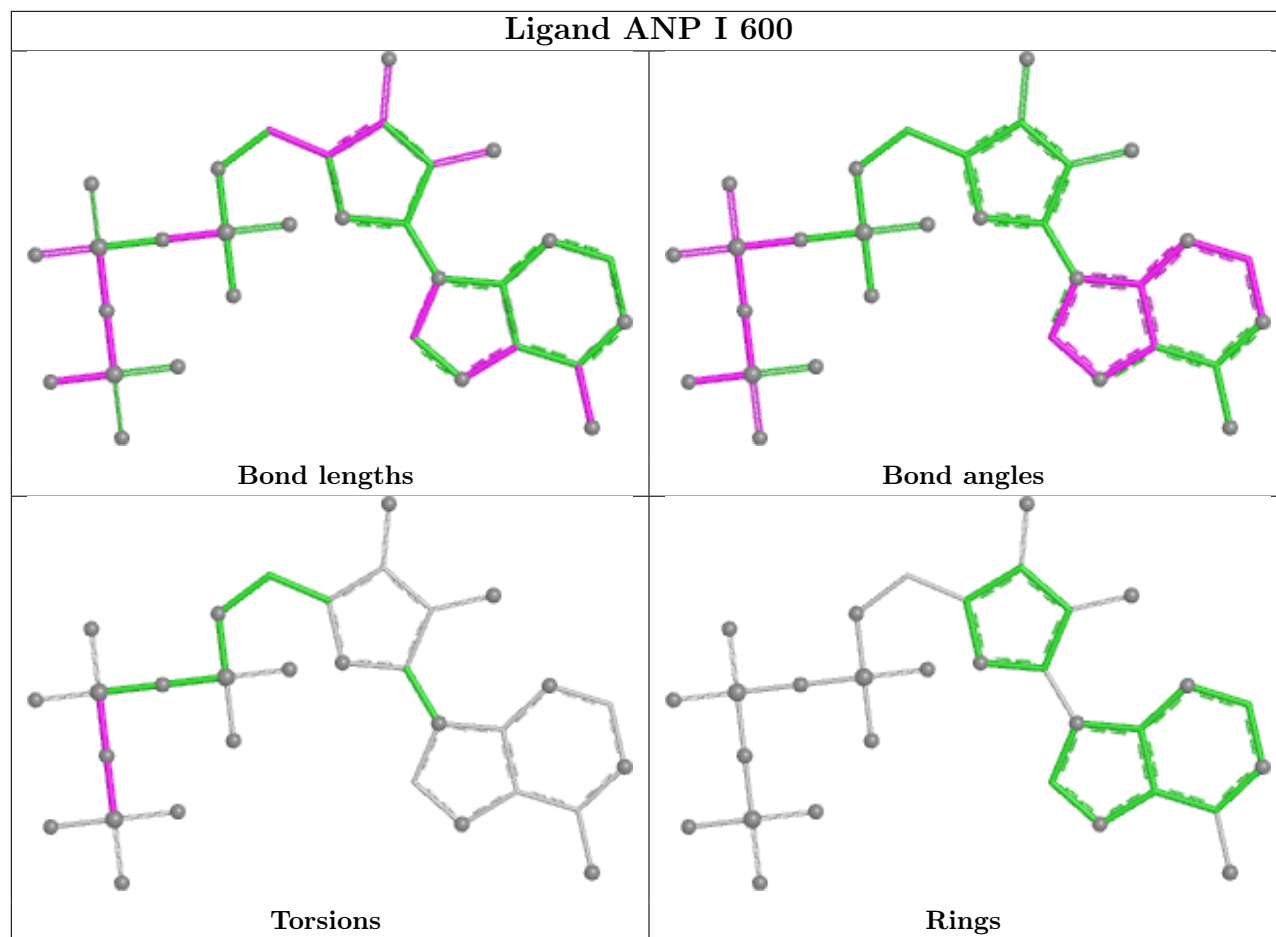
23 monomers are involved in 54 short contacts:

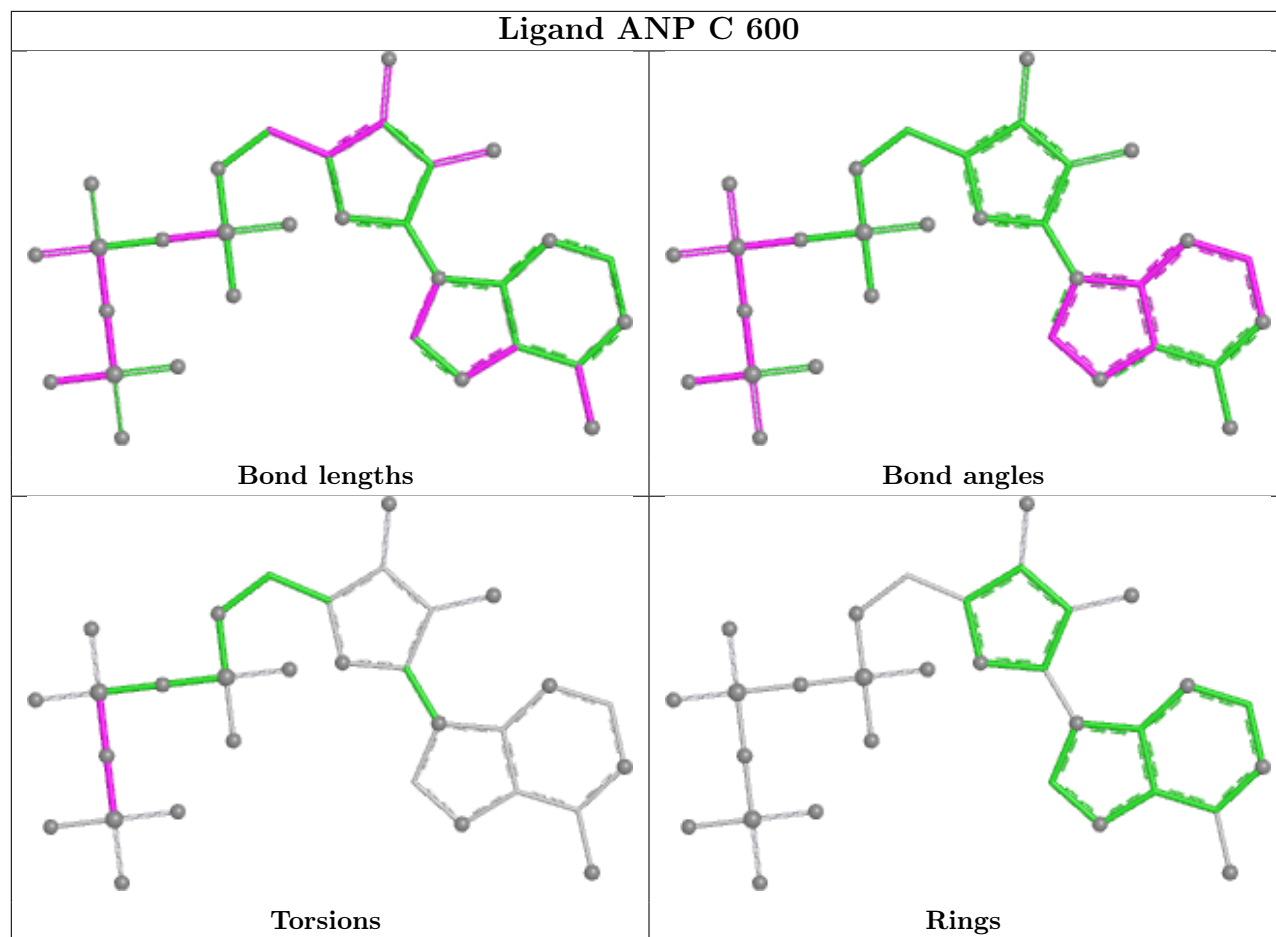
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	600	ANP	3	0
5	I	600	ANP	4	0
5	C	600	ANP	3	0
5	B	600	ANP	3	0
8	N	530	SO4	1	0
5	R	600	ANP	3	0
5	Z	600	ANP	3	0
7	L	600	ADP	5	0
5	A	600	ANP	2	0
8	b	630	SO4	1	0
5	J	600	ANP	3	0
7	b	600	ADP	4	0
8	W	300	SO4	1	0
7	T	600	ADP	4	0
7	D	600	ADP	5	0
5	K	600	ANP	2	0
5	a	600	ANP	2	0
5	Q	600	ANP	2	0
8	D	630	SO4	1	0
8	F	530	SO4	1	0
8	c	530	SO4	1	0
8	L	630	SO4	1	0
5	S	600	ANP	2	0

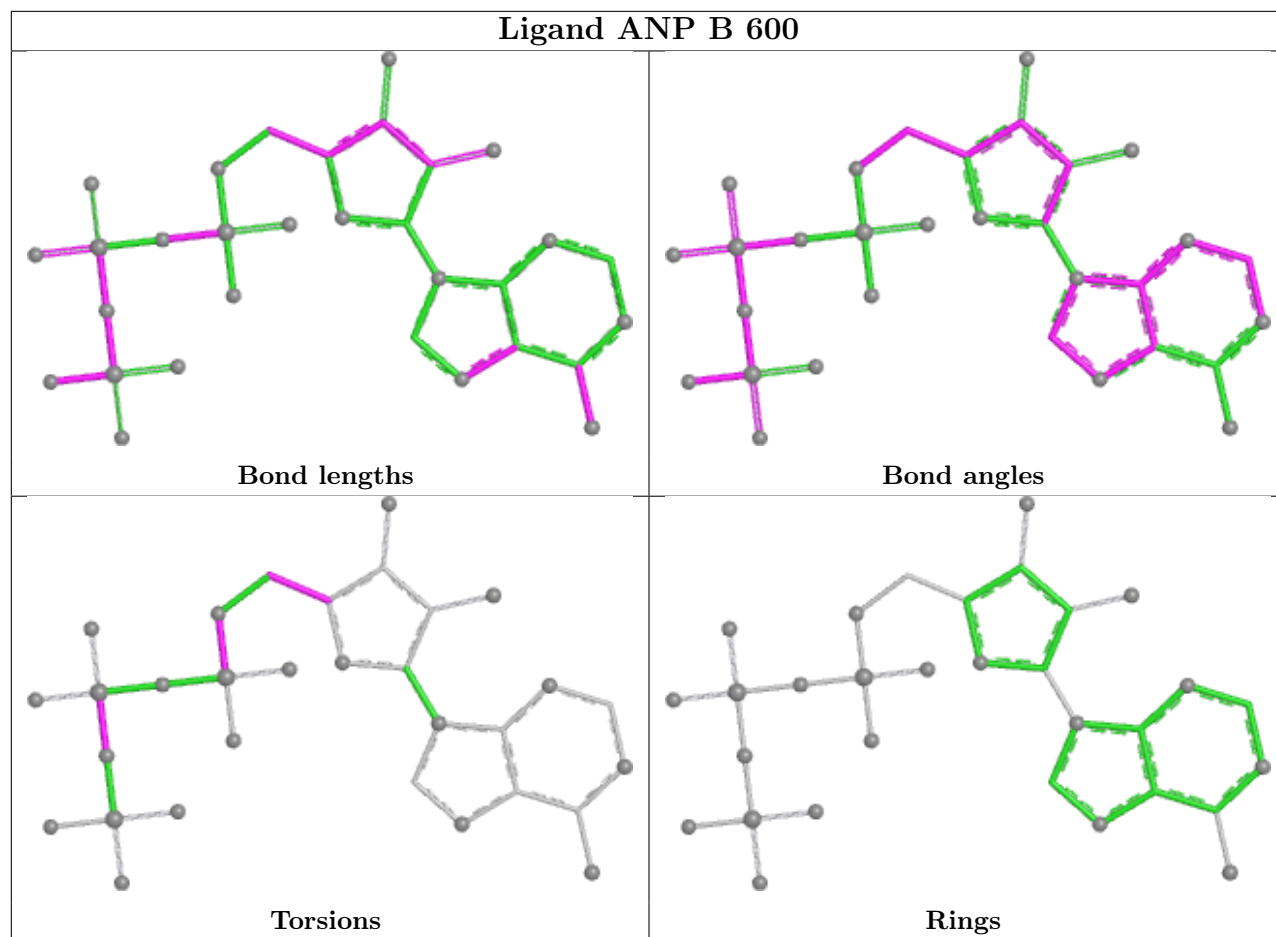
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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.

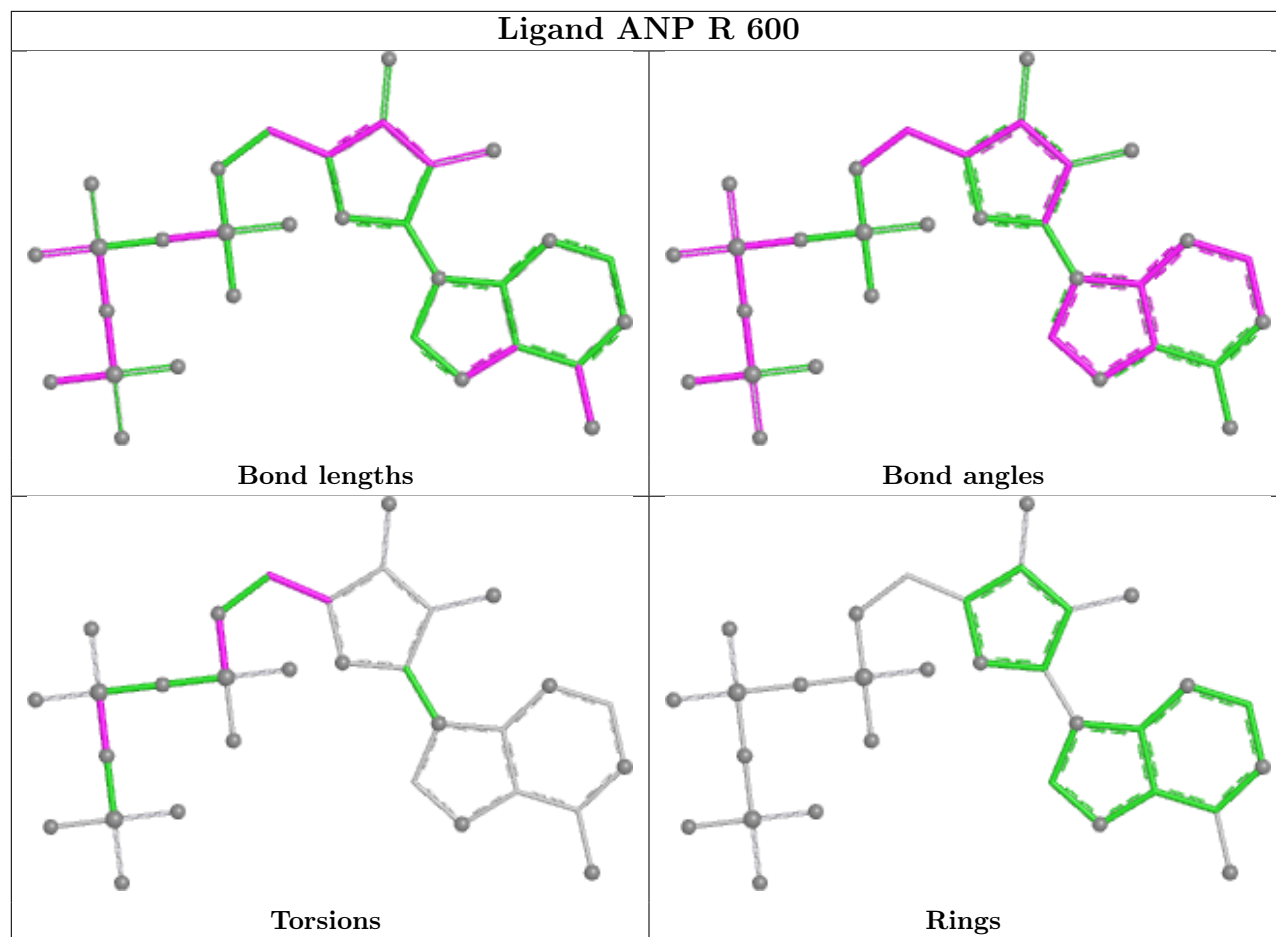


Ligand ANP I 600

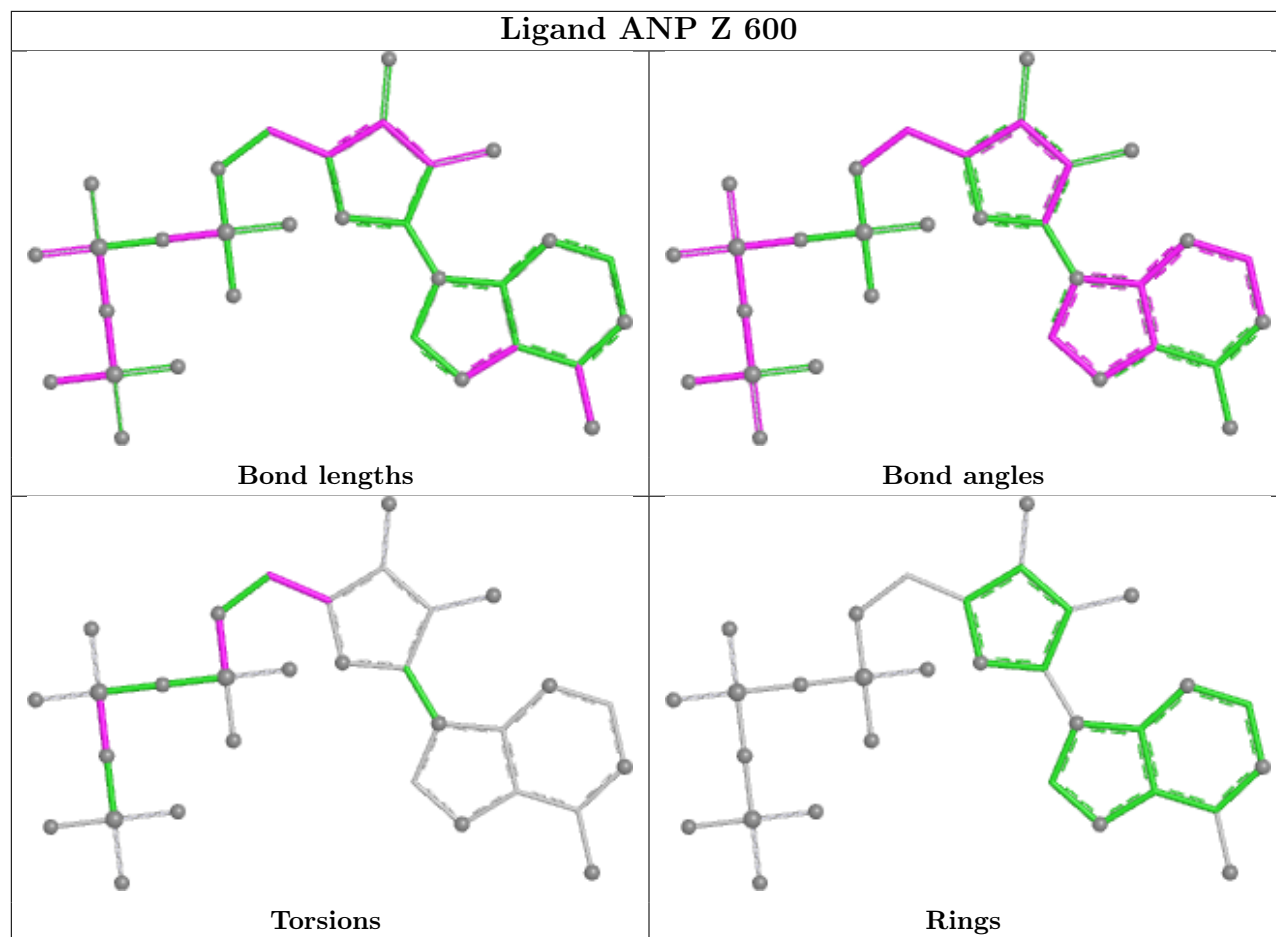




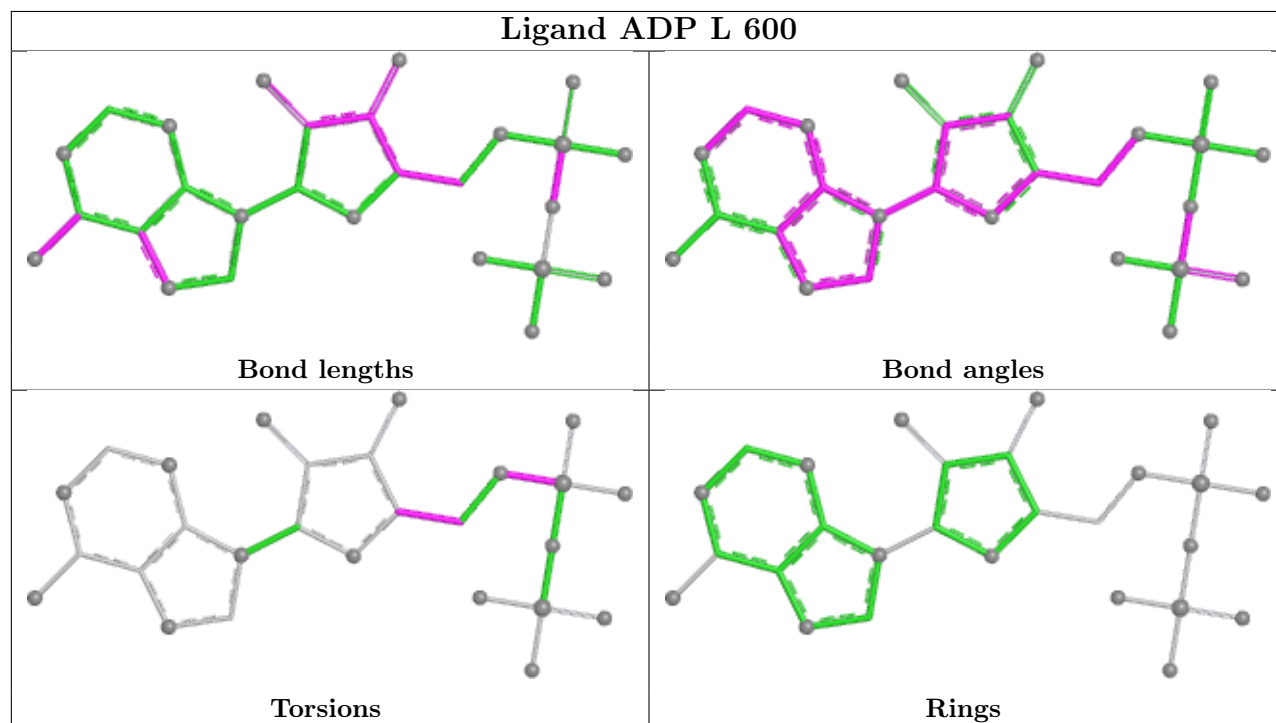


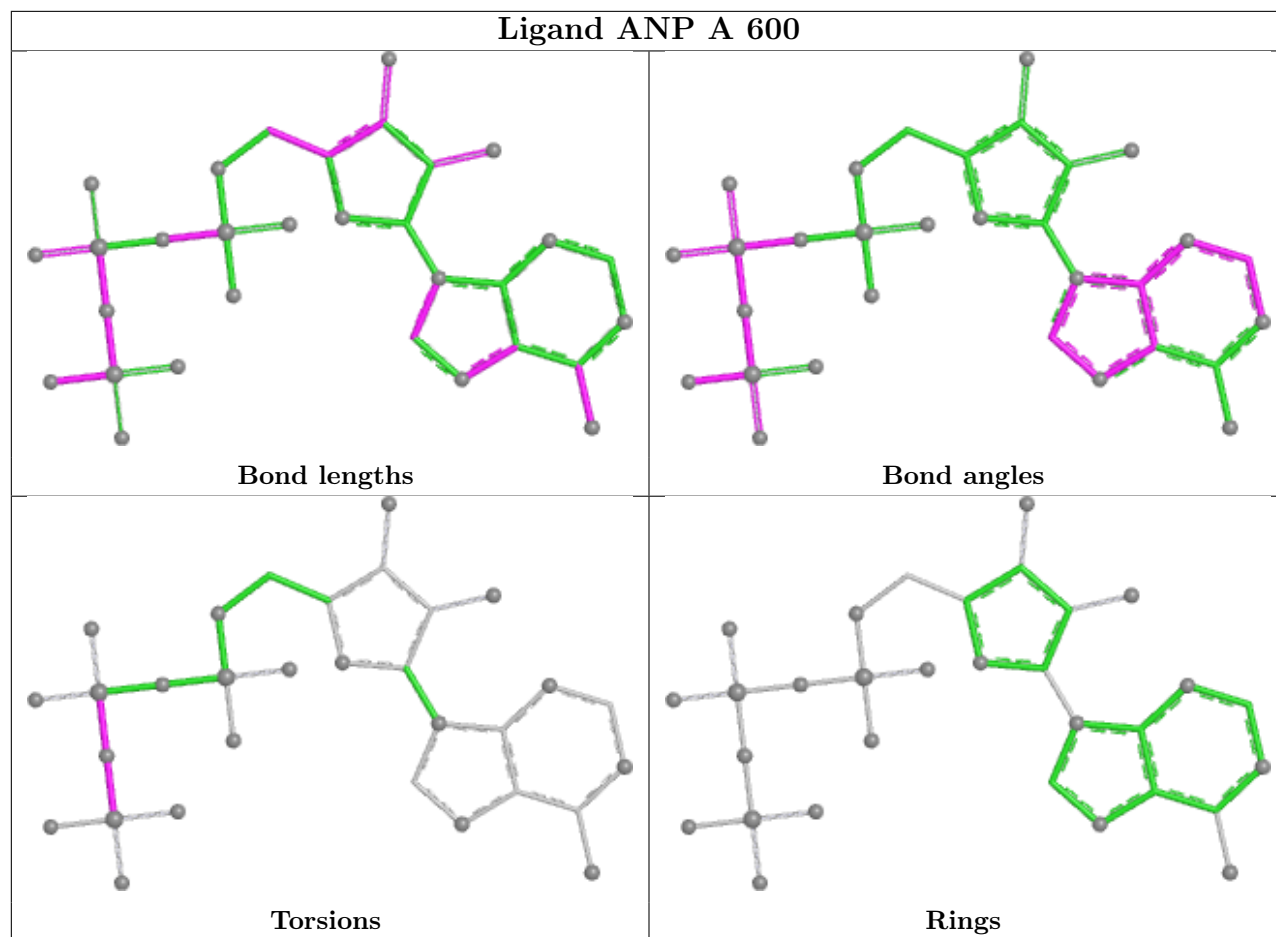


Ligand ANP Z 600

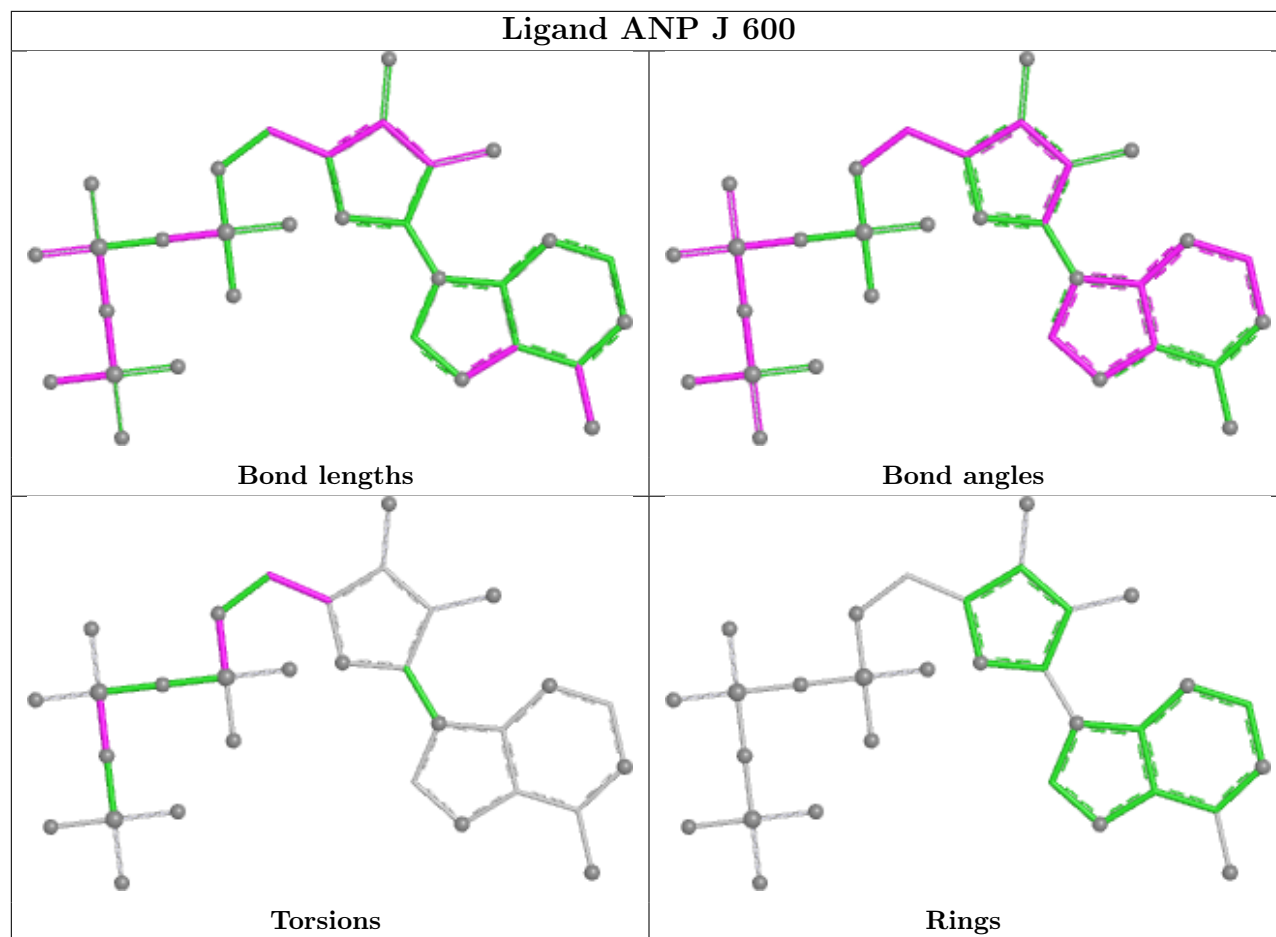


Ligand ADP L 600

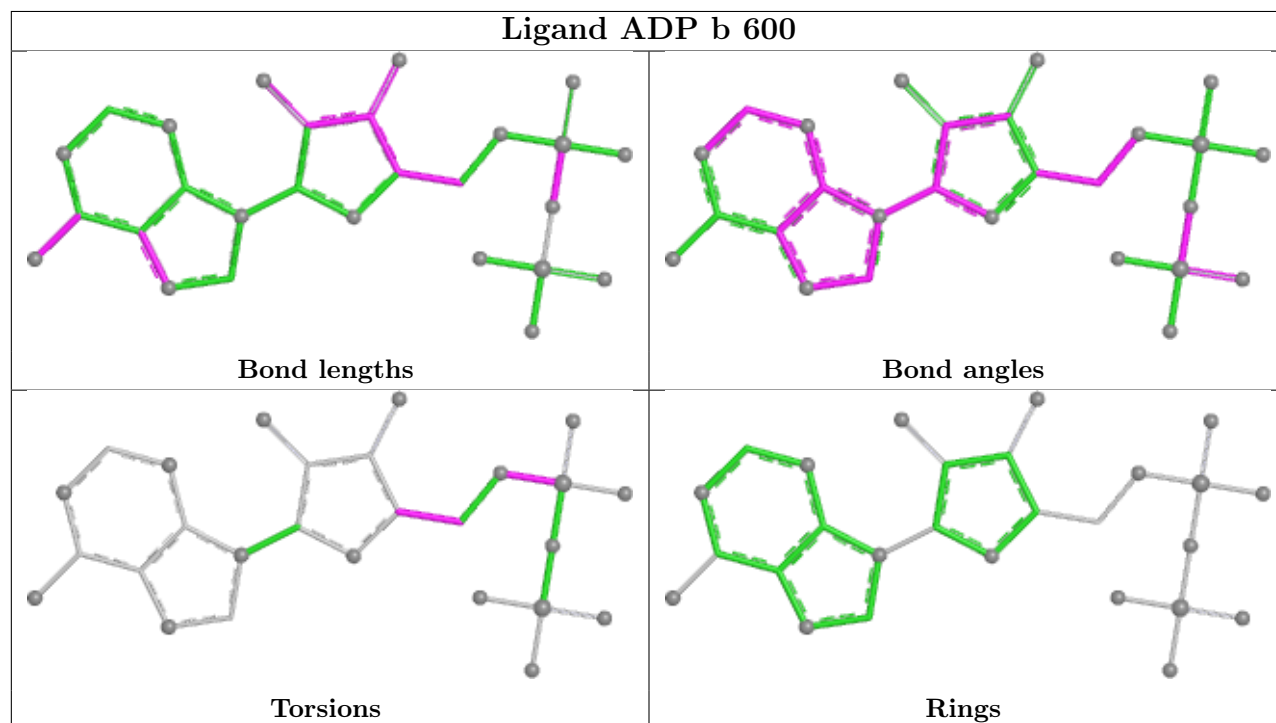


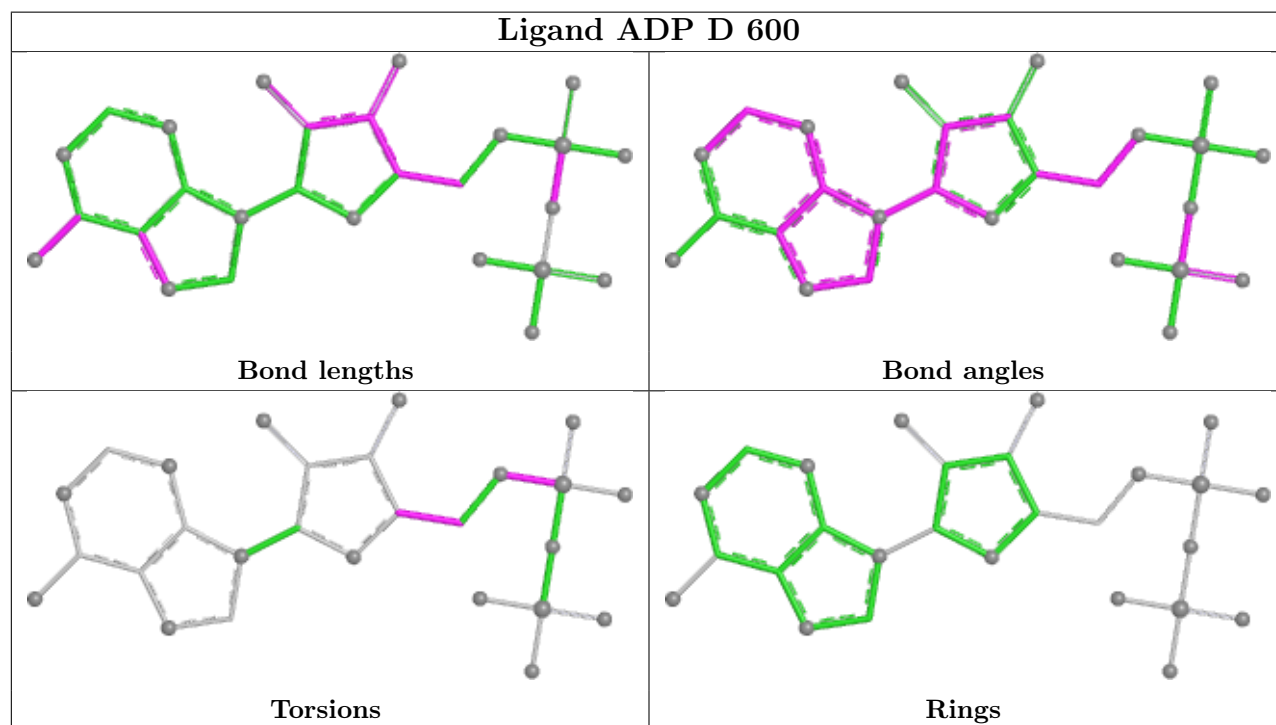
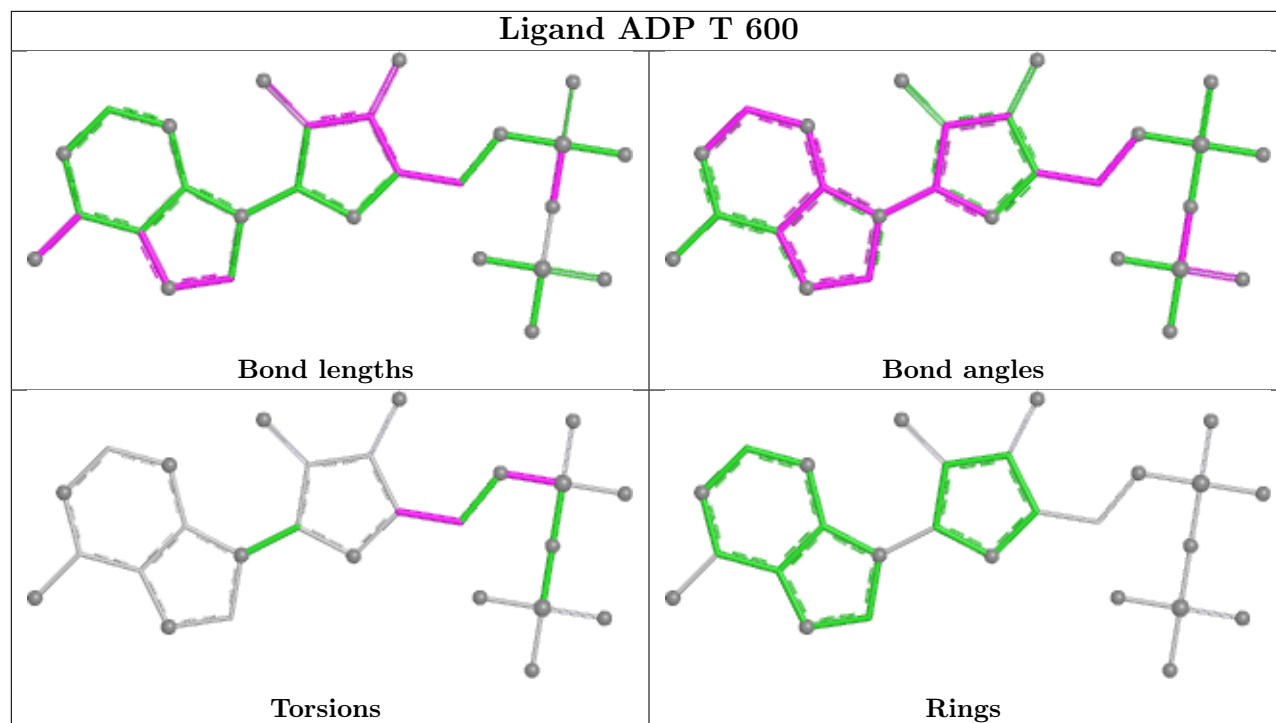


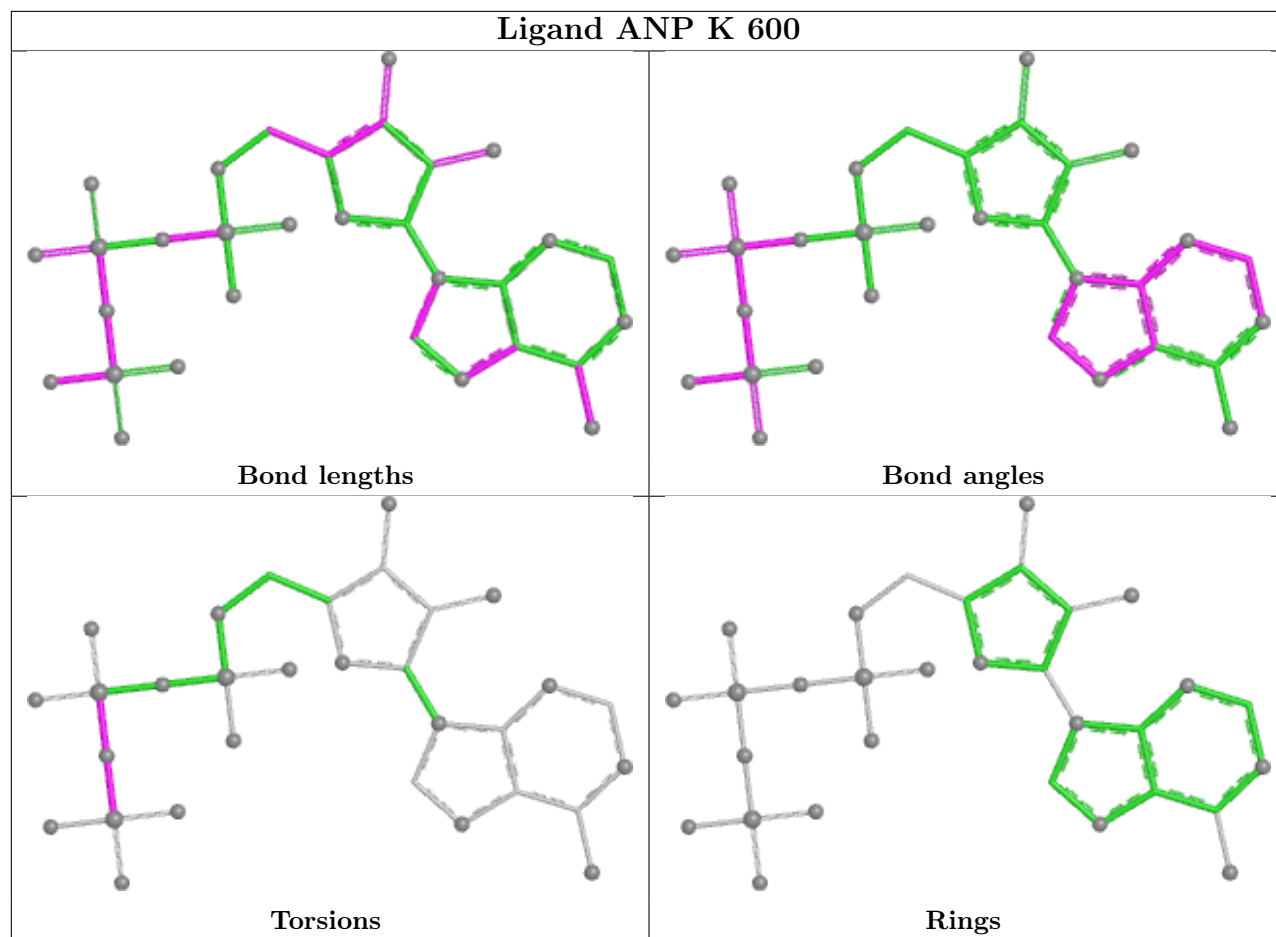
Ligand ANP J 600

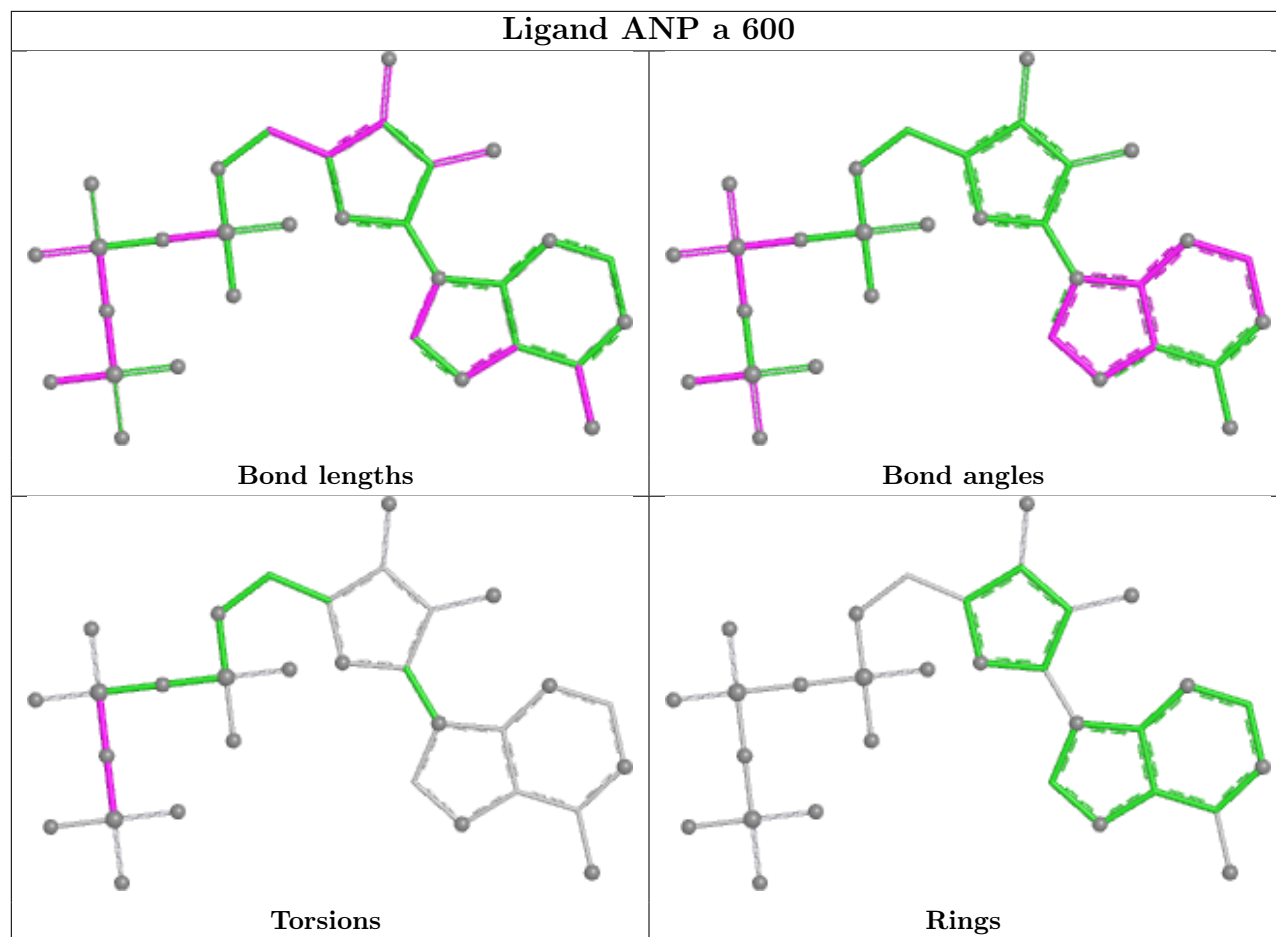


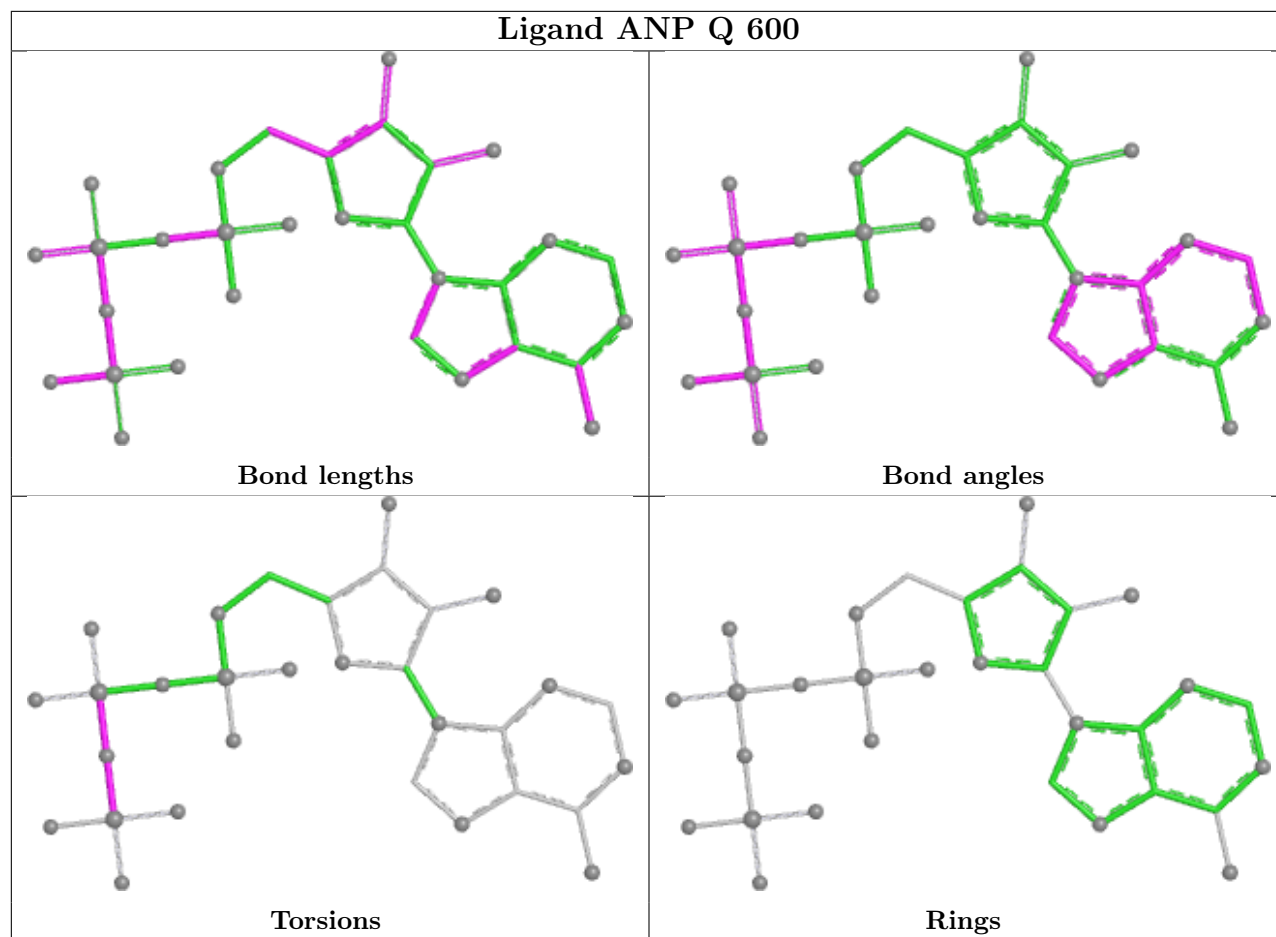
Ligand ADP b 600

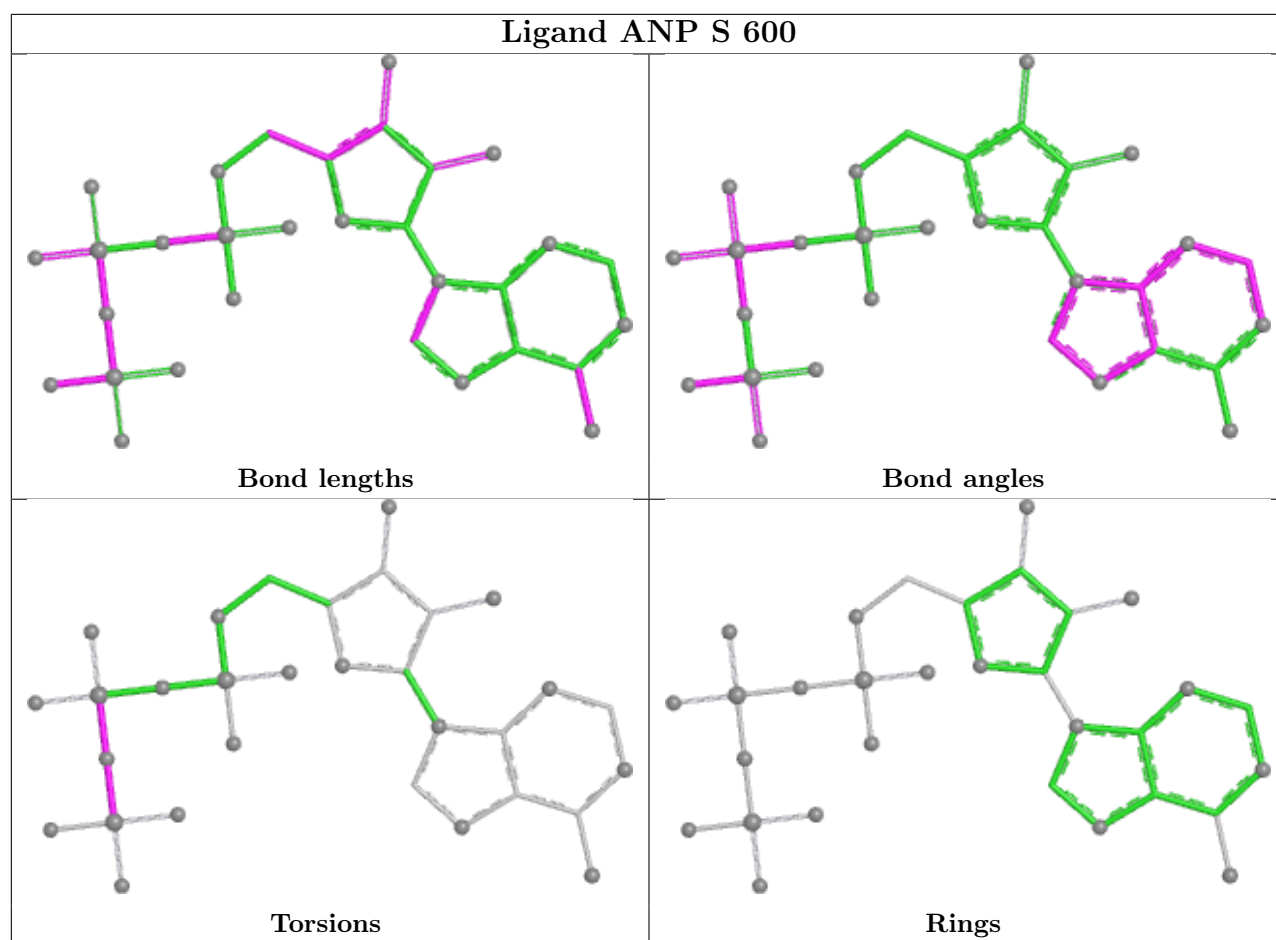












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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, 95th 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	A	488/513 (95%)	-0.31	0 100 100	49, 93, 144, 177	0
1	B	486/513 (94%)	-0.18	5 (1%) 79 62	55, 116, 181, 216	0
1	C	487/513 (94%)	-0.24	2 (0%) 88 78	51, 102, 151, 231	0
1	I	488/513 (95%)	-0.18	5 (1%) 79 62	66, 120, 167, 205	0
1	J	486/513 (94%)	-0.13	6 (1%) 76 58	47, 103, 183, 223	0
1	K	487/513 (94%)	-0.20	5 (1%) 79 62	46, 91, 149, 211	0
1	Q	488/513 (95%)	-0.25	1 (0%) 91 85	50, 104, 153, 214	0
1	R	486/513 (94%)	0.08	5 (1%) 79 62	66, 123, 195, 227	0
1	S	487/513 (94%)	-0.05	3 (0%) 85 73	78, 131, 180, 226	0
1	Y	488/513 (95%)	0.02	1 (0%) 91 85	79, 142, 184, 224	0
1	Z	486/513 (94%)	0.26	8 (1%) 70 52	76, 152, 215, 254	0
1	a	487/513 (94%)	0.11	5 (1%) 79 62	89, 146, 200, 249	0
2	D	458/459 (99%)	-0.38	1 (0%) 91 85	44, 92, 142, 186	0
2	E	458/459 (99%)	-0.39	1 (0%) 91 85	53, 102, 152, 184	0
2	F	458/459 (99%)	-0.38	1 (0%) 91 85	41, 103, 158, 216	0
2	L	458/459 (99%)	-0.17	0 100 100	46, 111, 167, 217	0
2	M	458/459 (99%)	-0.22	2 (0%) 88 78	55, 114, 161, 219	0
2	N	458/459 (99%)	-0.29	6 (1%) 75 56	33, 73, 131, 186	0
2	T	458/459 (99%)	-0.17	3 (0%) 84 70	73, 124, 181, 229	0
2	U	458/459 (99%)	-0.16	3 (0%) 84 70	54, 102, 170, 232	0
2	V	458/459 (99%)	0.01	8 (1%) 69 50	67, 124, 180, 233	0
2	b	458/459 (99%)	0.27	7 (1%) 72 53	102, 158, 204, 240	0
2	c	458/459 (99%)	-0.04	2 (0%) 88 78	68, 119, 174, 213	0
2	d	458/459 (99%)	0.12	4 (0%) 81 65	92, 151, 200, 243	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	G	284/286 (99%)	-0.49	0 100 100	29, 54, 137, 200	0
3	O	284/286 (99%)	-0.40	1 (0%) 88 78	26, 57, 140, 209	0
3	W	284/286 (99%)	-0.15	1 (0%) 88 78	51, 116, 192, 232	0
3	e	284/286 (99%)	-0.02	0 100 100	84, 142, 205, 230	0
4	H	138/138 (100%)	-0.47	0 100 100	35, 72, 120, 144	0
4	P	138/138 (100%)	-0.36	0 100 100	43, 71, 129, 156	0
4	X	138/138 (100%)	-0.14	0 100 100	77, 136, 175, 227	0
4	f	138/138 (100%)	-0.04	1 (0%) 84 70	94, 151, 198, 217	0
All	All	13028/13360 (97%)	-0.14	87 (0%) 84 70	26, 116, 183, 254	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	101	ILE	4.4
1	R	460	GLU	4.4
2	b	284	SER	4.1
2	V	101	ILE	3.7
2	d	207	GLY	3.4
2	c	22	VAL	3.4
2	V	173	TYR	3.4
1	J	460	GLU	3.2
2	c	210	ASN	3.1
1	R	111	LEU	3.1
1	R	476	ASP	3.1
2	U	316	ASP	3.1
2	b	29	LEU	3.0
1	C	312	PHE	2.9
2	V	208	GLN	2.9
2	V	11	ALA	2.9
1	R	217	ALA	2.8
1	K	460	GLU	2.8
1	S	121	LEU	2.8
2	T	119	LEU	2.8
1	I	475	VAL	2.8
1	C	313	THR	2.8
2	T	242	ASP	2.8
1	K	508	LYS	2.7
1	J	138	GLU	2.7
1	Z	217	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	137	ILE	2.6
1	B	475	VAL	2.6
1	Z	111	LEU	2.6
1	K	313	THR	2.5
2	F	101	ILE	2.5
2	V	442	ALA	2.5
2	M	345	ASP	2.5
1	S	465	GLY	2.5
1	a	172	GLN	2.4
2	d	208	GLN	2.4
1	R	412	ASP	2.4
1	Z	262	ASP	2.4
2	b	153	VAL	2.4
2	N	173	TYR	2.4
2	N	208	GLN	2.4
1	B	460	GLU	2.4
2	T	181	GLU	2.3
2	b	442	ALA	2.3
2	d	173	TYR	2.3
1	I	476	ASP	2.3
1	Z	460	GLU	2.3
1	a	460	GLU	2.3
2	E	115	SER	2.3
1	K	475	VAL	2.3
2	N	76	GLU	2.2
2	M	346	PRO	2.2
1	J	387	LYS	2.2
1	a	121	LEU	2.2
1	Y	172	GLN	2.2
2	b	185	GLU	2.2
2	N	100	GLU	2.2
1	Q	476	ASP	2.2
1	J	410	ALA	2.2
1	Z	473	ALA	2.2
1	S	313	THR	2.1
1	a	313	THR	2.1
1	J	408	GLN	2.1
2	V	234	GLY	2.1
1	Z	66	LEU	2.1
1	B	366	PRO	2.1
1	a	27	ASN	2.1
1	Z	387	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	b	281	ARG	2.1
1	B	382	GLN	2.1
2	b	177	ALA	2.1
2	V	457	LYS	2.1
2	d	459	LEU	2.1
1	J	396	ALA	2.1
1	Z	414	ASP	2.1
2	U	345	ASP	2.1
3	W	198	LEU	2.0
1	B	412	ASP	2.0
1	I	176	THR	2.0
1	K	476	ASP	2.0
3	O	65	PRO	2.0
2	N	181	GLU	2.0
2	U	115	SER	2.0
4	f	26	THR	2.0
1	I	465	GLY	2.0
2	D	123	GLN	2.0
2	V	185	GLU	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 oligosaccharides 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, 95th 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
8	SO4	c	530	5/5	0.58	0.15	113,113,115,116	0
6	MG	B	601	1/1	0.69	0.08	125,125,125,125	0
8	SO4	W	300	5/5	0.76	0.25	207,210,212,214	0
8	SO4	U	530	5/5	0.77	0.11	106,106,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	M	530	5/5	0.78	0.13	117,118,119,119	0
6	MG	Z	601	1/1	0.80	0.08	147,147,147,147	0
5	ANP	Y	600	31/31	0.82	0.10	87,93,109,129	0
8	SO4	E	530	5/5	0.82	0.14	109,109,109,110	0
6	MG	Q	601	1/1	0.83	0.12	64,64,64,64	0
5	ANP	Z	600	31/31	0.84	0.10	147,151,153,154	0
6	MG	R	601	1/1	0.84	0.08	118,118,118,118	0
6	MG	A	601	1/1	0.86	0.12	64,64,64,64	0
8	SO4	d	530	5/5	0.86	0.12	107,108,108,109	0
5	ANP	A	600	31/31	0.87	0.12	87,93,109,129	0
6	MG	I	601	1/1	0.88	0.09	64,64,64,64	0
5	ANP	Q	600	31/31	0.88	0.12	87,93,109,129	0
8	SO4	G	300	5/5	0.89	0.21	95,101,102,103	0
8	SO4	O	300	5/5	0.89	0.27	109,115,118,119	0
6	MG	Y	601	1/1	0.90	0.08	64,64,64,64	0
6	MG	J	601	1/1	0.90	0.06	122,122,122,122	0
6	MG	a	601	1/1	0.90	0.06	83,83,83,83	0
8	SO4	V	530	5/5	0.90	0.07	82,83,85,87	0
5	ANP	S	600	31/31	0.90	0.10	109,114,121,135	0
5	ANP	I	600	31/31	0.90	0.09	87,93,109,129	0
8	SO4	H	200	5/5	0.90	0.16	114,115,117,119	0
5	ANP	a	600	31/31	0.91	0.09	123,126,130,136	0
5	ANP	R	600	31/31	0.92	0.09	91,101,110,112	0
5	ANP	C	600	31/31	0.92	0.09	87,93,109,129	0
8	SO4	b	630	5/5	0.92	0.08	98,99,100,101	0
8	SO4	P	200	5/5	0.92	0.18	120,120,123,124	0
7	ADP	b	600	27/27	0.92	0.07	136,139,142,143	0
8	SO4	F	530	5/5	0.93	0.08	79,81,82,82	0
7	ADP	T	600	27/27	0.93	0.07	114,118,121,123	0
7	ADP	L	600	27/27	0.94	0.07	77,86,95,98	0
5	ANP	B	600	31/31	0.94	0.08	96,107,111,112	0
8	SO4	T	630	5/5	0.94	0.07	85,88,88,89	0
6	MG	L	601	1/1	0.95	0.04	66,66,66,66	0
6	MG	T	601	1/1	0.95	0.05	80,80,80,80	0
8	SO4	N	530	5/5	0.95	0.07	64,64,67,67	0
6	MG	b	601	1/1	0.95	0.08	127,127,127,127	0
7	ADP	D	600	27/27	0.95	0.06	75,81,87,90	0
5	ANP	J	600	31/31	0.95	0.08	83,96,100,103	0
5	ANP	K	600	31/31	0.96	0.08	63,81,109,131	0
6	MG	C	601	1/1	0.96	0.05	64,64,64,64	0
8	SO4	D	630	5/5	0.96	0.05	72,74,75,77	0
6	MG	S	601	1/1	0.97	0.04	60,60,60,60	0

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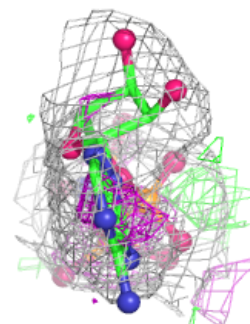
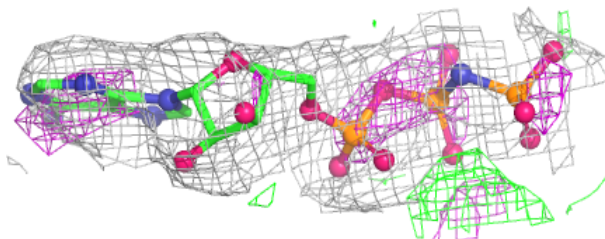
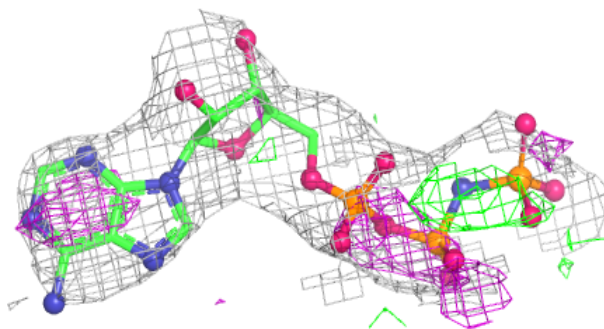
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	L	630	5/5	0.98	0.06	81,83,84,85	0
6	MG	K	601	1/1	0.98	0.05	44,44,44,44	0
6	MG	D	601	1/1	0.99	0.06	51,51,51,51	0

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.

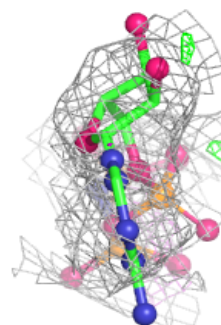
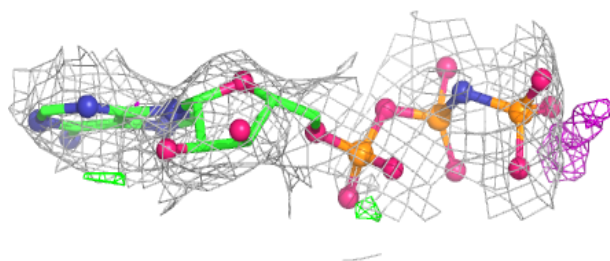
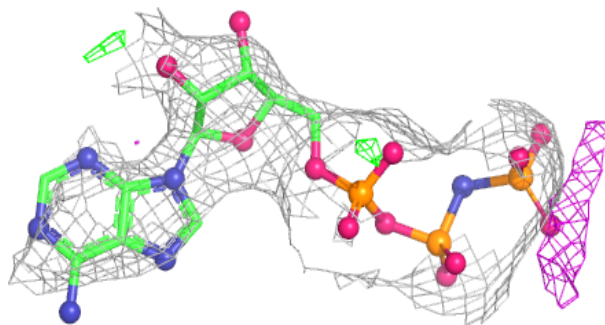
Electron density around ANP Y 600:

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

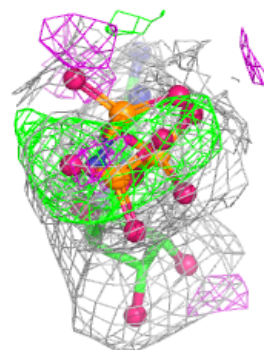
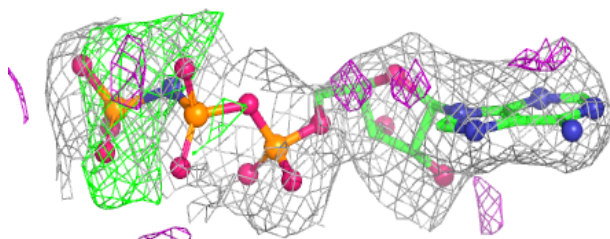
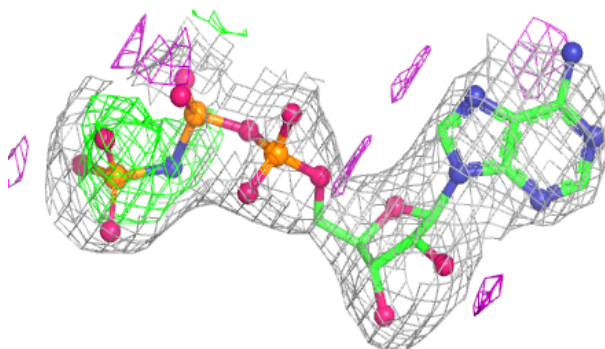


Electron density around ANP Z 600:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

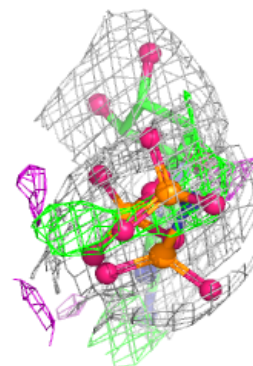
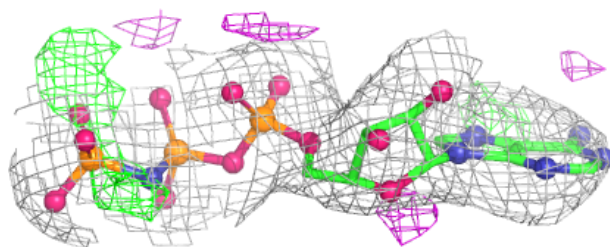
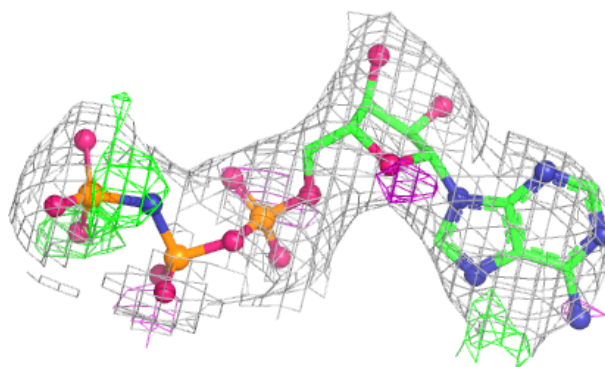
**Electron density around ANP A 600:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

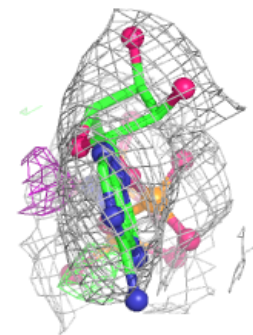
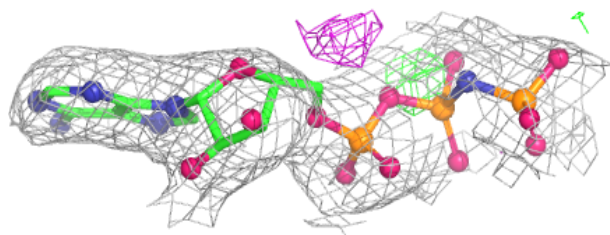
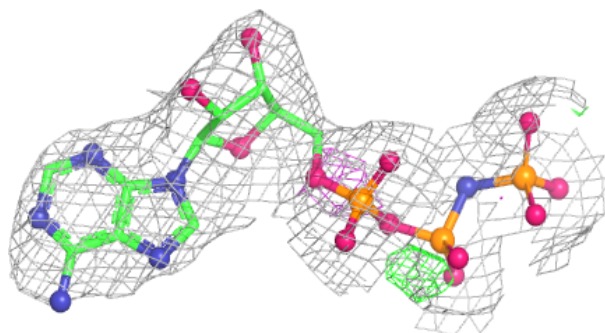


Electron density around ANP Q 600:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

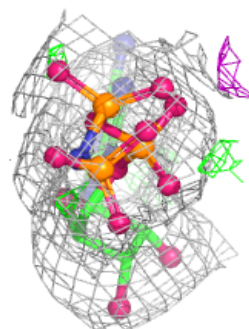
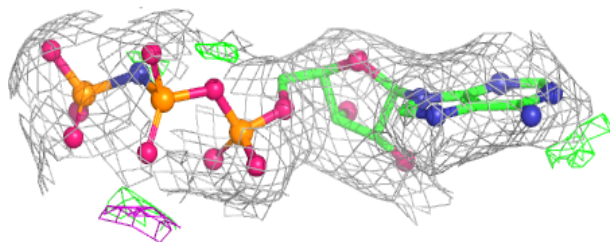
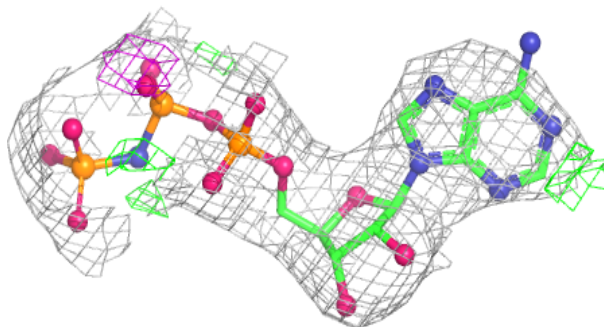
**Electron density around ANP S 600:**

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and green (positive)

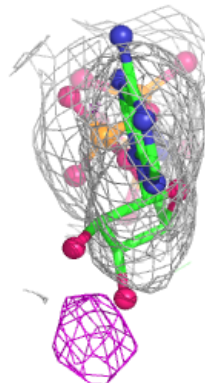
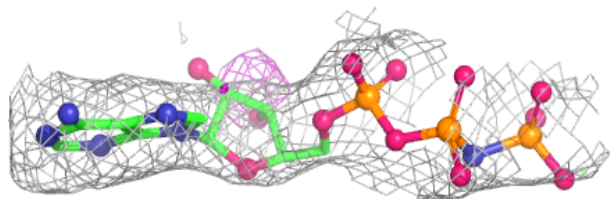
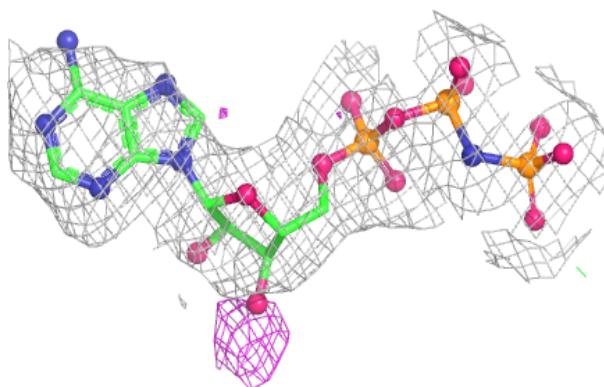


Electron density around ANP I 600:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

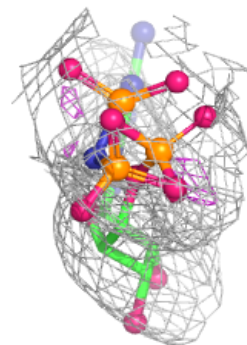
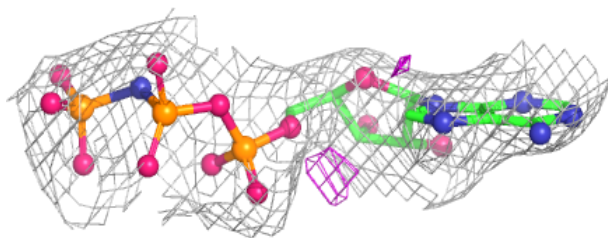
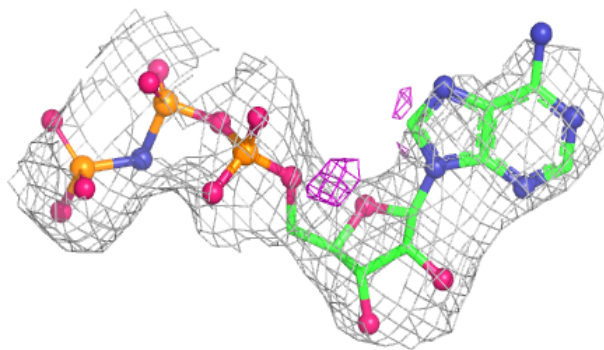
**Electron density around ANP a 600:**

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

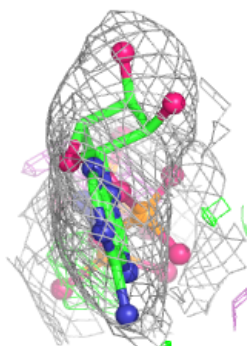
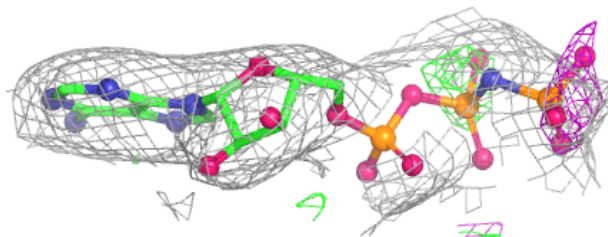
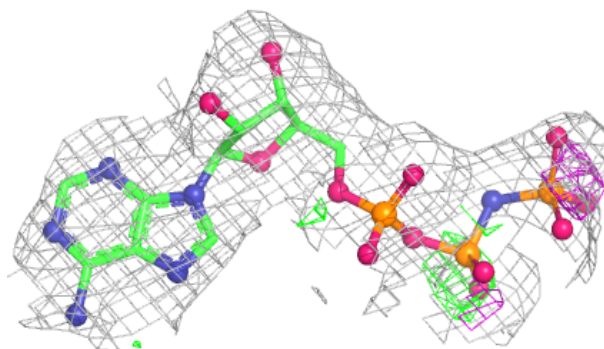


Electron density around ANP R 600:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

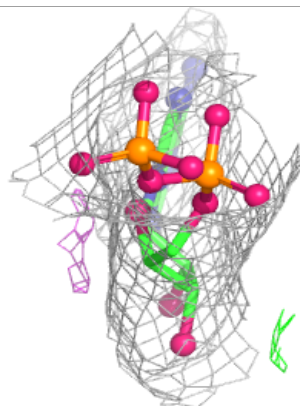
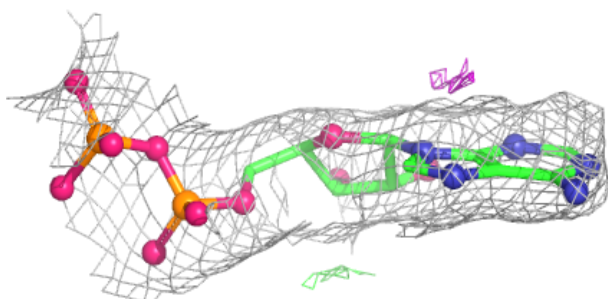
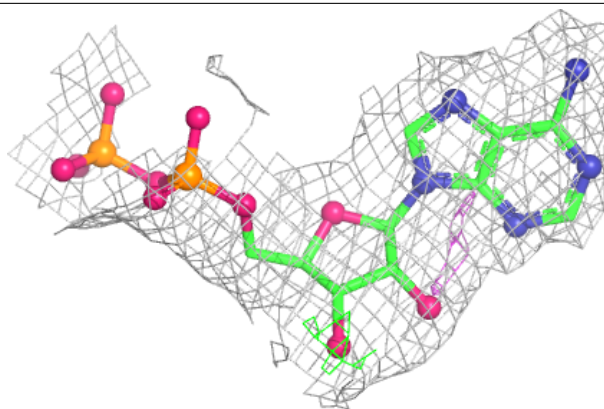
**Electron density around ANP C 600:**

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and green (positive)

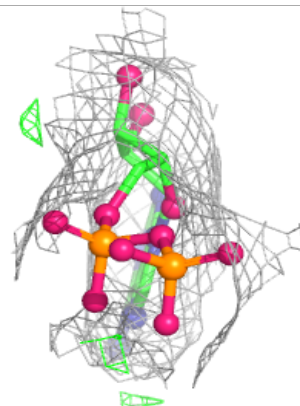
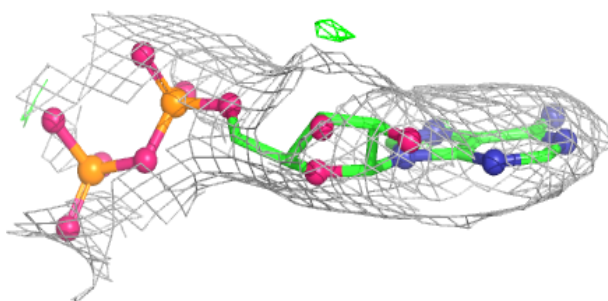
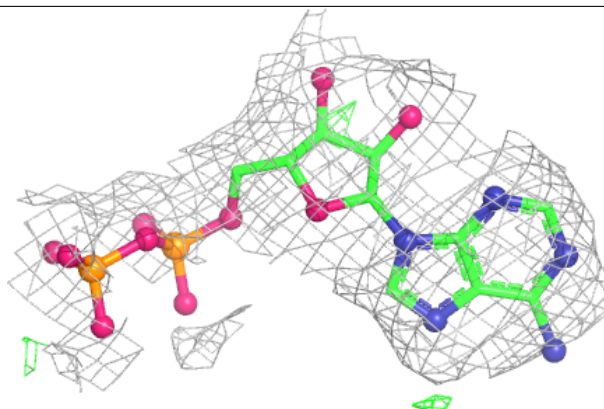


Electron density around ADP b 600:

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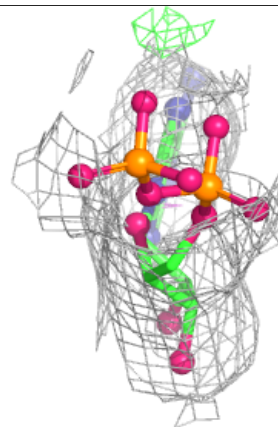
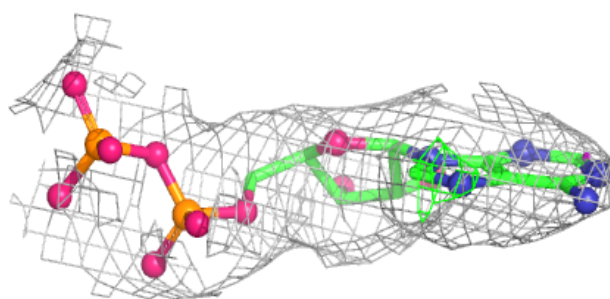
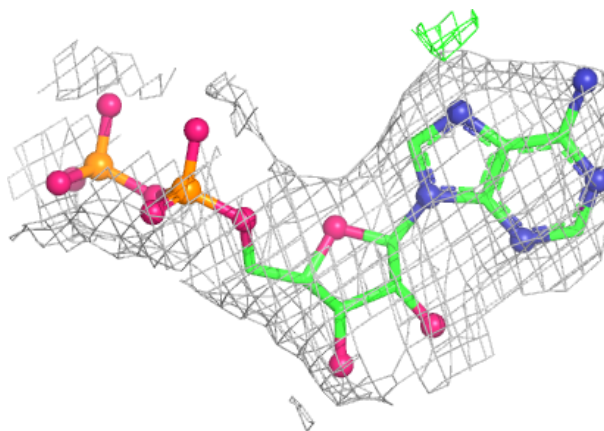
**Electron density around ADP T 600:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

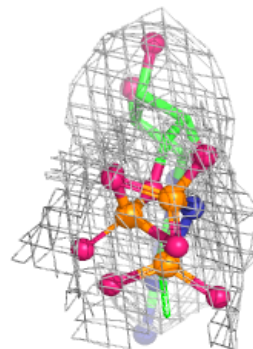
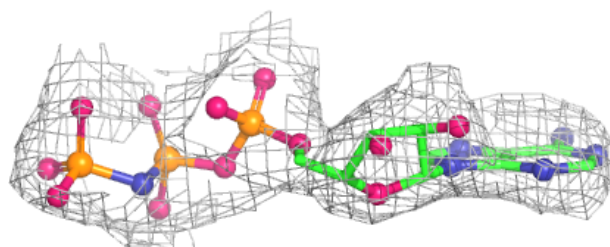
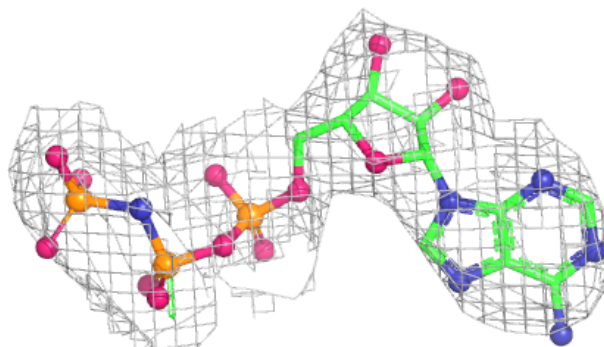


Electron density around ADP L 600:

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

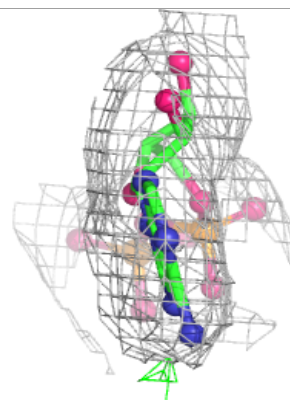
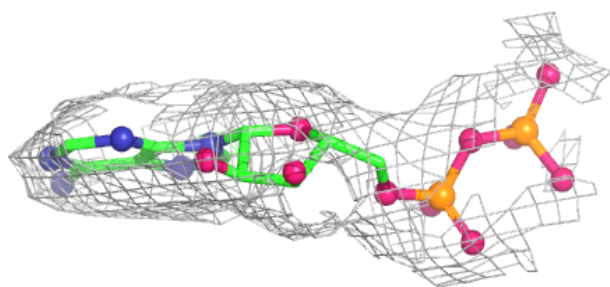
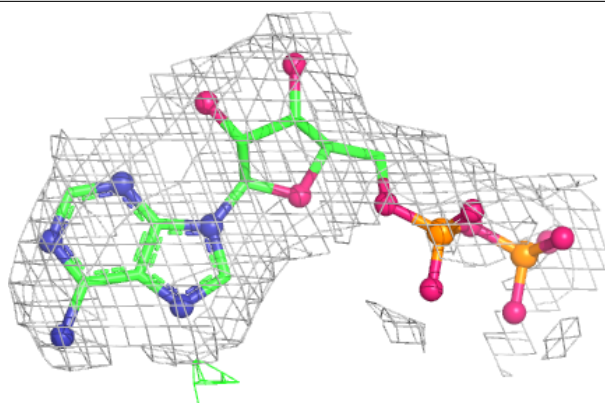
**Electron density around ANP B 600:**

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

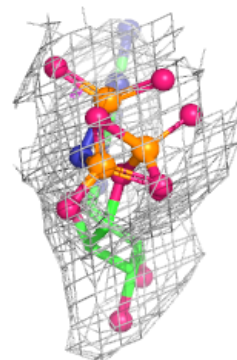
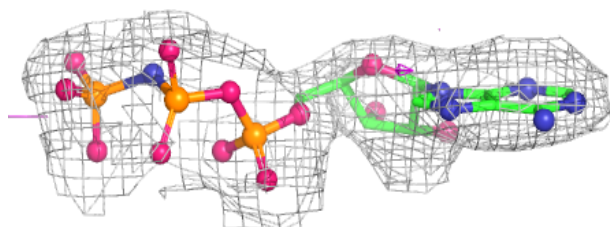
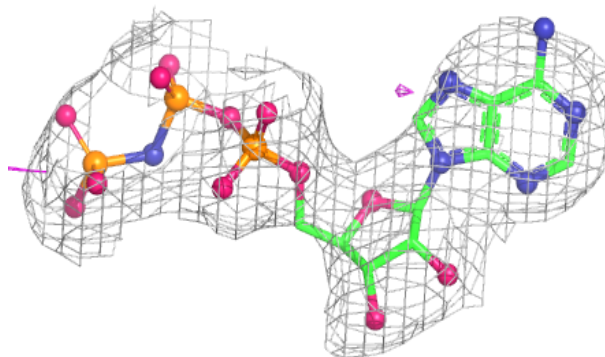


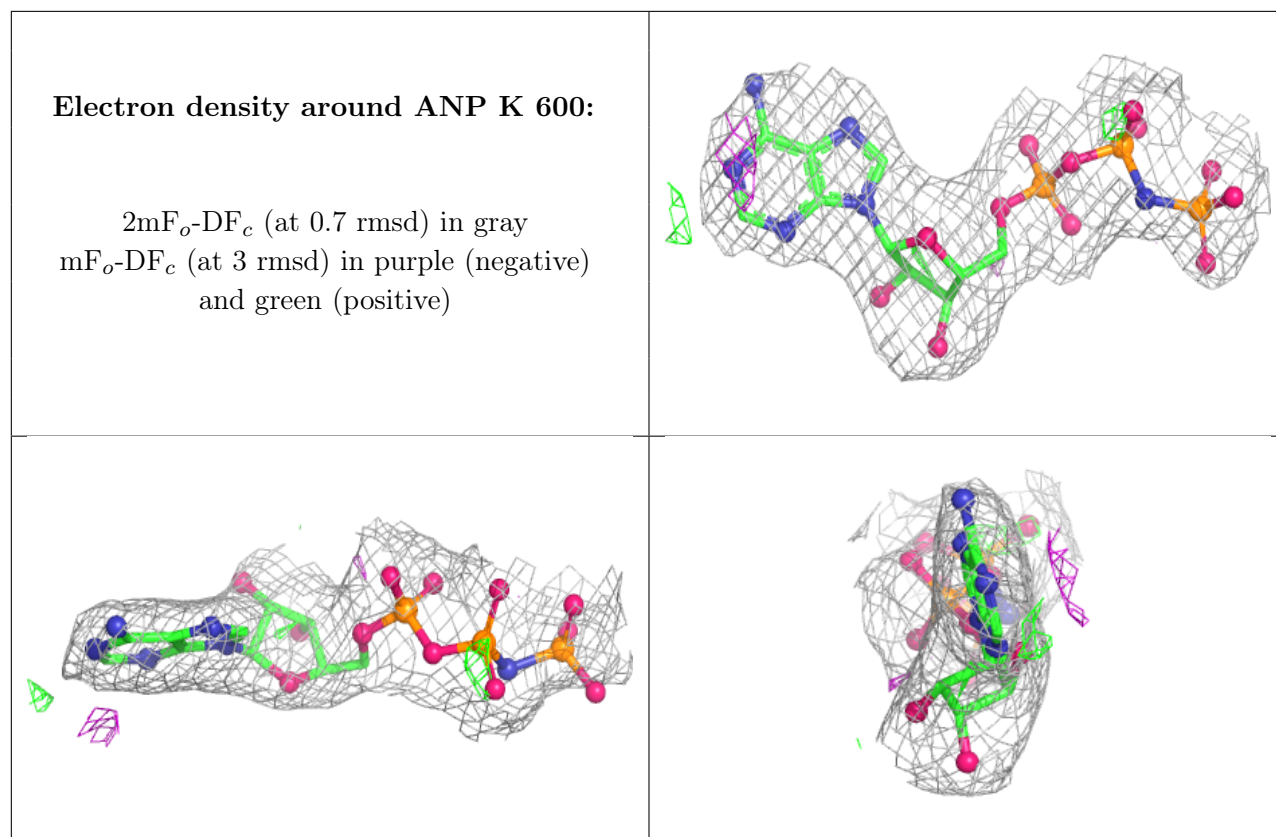
Electron density around ADP D 600:

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

**Electron density around ANP J 600:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.