



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:25 AM GMT

PDB ID : 2WSS  
Title : THE STRUCTURE OF THE MEMBRANE EXTRINSIC REGION OF BOVINE ATP SYNTHASE  
Authors : Rees, D.M.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2009-09-09  
Resolution : 3.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

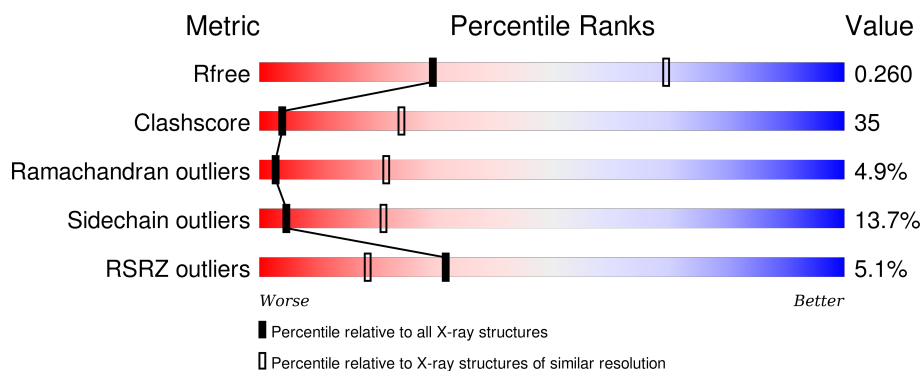
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	510	<div> <div>49%</div> <div>42%</div> <div>8%</div> <div>.</div> </div>
1	B	510	<div> <div>46%</div> <div>43%</div> <div>6%</div> <div>6%</div> </div>
1	C	510	<div> <div>3%</div> <div>36%</div> <div>48%</div> <div>10%</div> <div>5%</div> </div>
1	J	510	<div> <div>%</div> <div>43%</div> <div>44%</div> <div>8%</div> <div>5%</div> </div>
1	K	510	<div> <div>43%</div> <div>44%</div> <div>7%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	L	510	
2	D	482	
2	E	482	
2	F	482	
2	M	482	
2	N	482	
2	O	482	
3	G	272	
3	P	272	
4	H	146	
4	Q	146	
5	I	50	
5	R	50	
6	S	190	
6	W	190	
7	T	116	
7	X	116	
8	U	118	
9	V	76	
9	Z	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	ANP	B	600	X	-	-	-
10	ANP	F	600	-	-	X	-
11	MG	D	601	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	MG	F	601	-	-	-	X
11	MG	M	601	-	-	-	X
11	MG	O	601	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 54949 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, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			3882	2442	684	744	12			
1	B	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	484	Total	C	N	O	S	0	0	0
			3684	2323	653	696	12			
1	J	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	K	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	L	481	Total	C	N	O	S	0	0	0
			3670	2315	650	693	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483
B	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483
C	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483
J	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483
K	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483
L	481	GLY	SER	CONFLICT SEE REMARK 9	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	1	0
			3534	2242	600	681	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	N	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	O	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	260	Total	C	N	O	S	0	0	0
			2027	1273	351	395	8			
3	P	260	Total	C	N	O	S	0	0	0
			2027	1273	351	395	8			

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	131	Total	C	N	O	S	0	0	0
			970	609	164	195	2			
4	Q	131	Total	C	N	O	S	0	0	0
			970	609	164	195	2			

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	47	Total	C	N	O	S	0	0	0
			369	237	66	64	2			
5	R	47	Total	C	N	O	S	0	0	0
			369	237	66	64	2			

- Molecule 6 is a protein called ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	S	167	Total	C	N	O	S	Se	0	0	0
			1292	820	223	242	1	6			
6	W	146	Total	C	N	O	S	Se	0	0	0
			1120	712	191	212	1	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	129	THR	ALA	CONFLICT	UNP P13621
W	129	THR	ALA	CONFLICT	UNP P13621

- Molecule 7 is a protein called ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	T	86	Total	C	N	O	S	Se	0	0	0
			733	459	139	130	1	4			
7	X	41	Total	C	N	O	S	Se	0	0	0
			336	211	62	59	1	3			

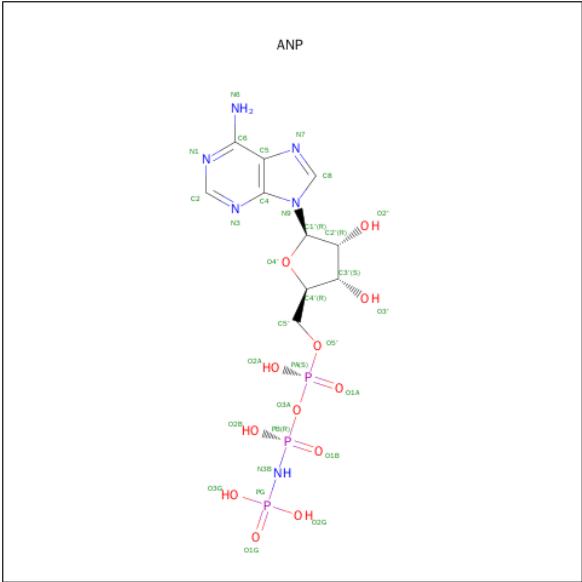
- Molecule 8 is a protein called ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	U	28	Total	C	N	O	0	0	0
			234	149	38	47			

- Molecule 9 is a protein called ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	V	66	Total	C	N	O	Se	0	0	0
			551	352	92	105	2			
9	Z	17	Total	C	N	O		0	0	0
			160	101	33	26				

- Molecule 10 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



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

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total	Mg	0	0
			1	1		
11	D	1	Total	Mg	0	0
			1	1		
11	K	1	Total	Mg	0	0
			1	1		
11	B	1	Total	Mg	0	0
			1	1		

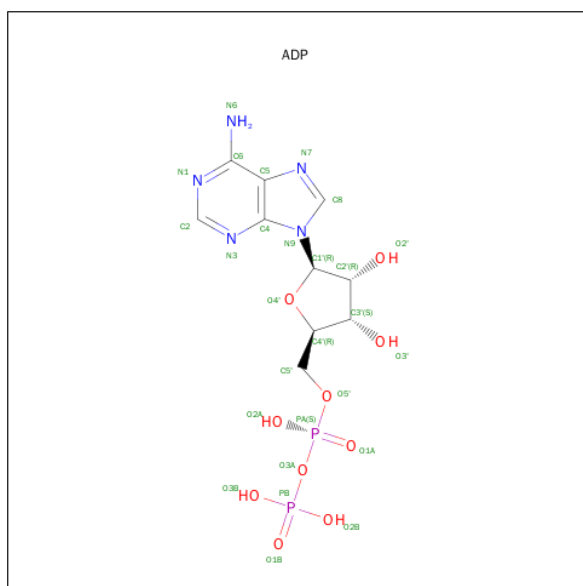
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	1	Total	Mg	0	0
			1	1		
11	A	1	Total	Mg	0	0
			1	1		
11	O	1	Total	Mg	0	0
			1	1		
11	L	1	Total	Mg	0	0
			1	1		
11	F	1	Total	Mg	0	0
			1	1		
11	M	1	Total	Mg	0	0
			1	1		

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

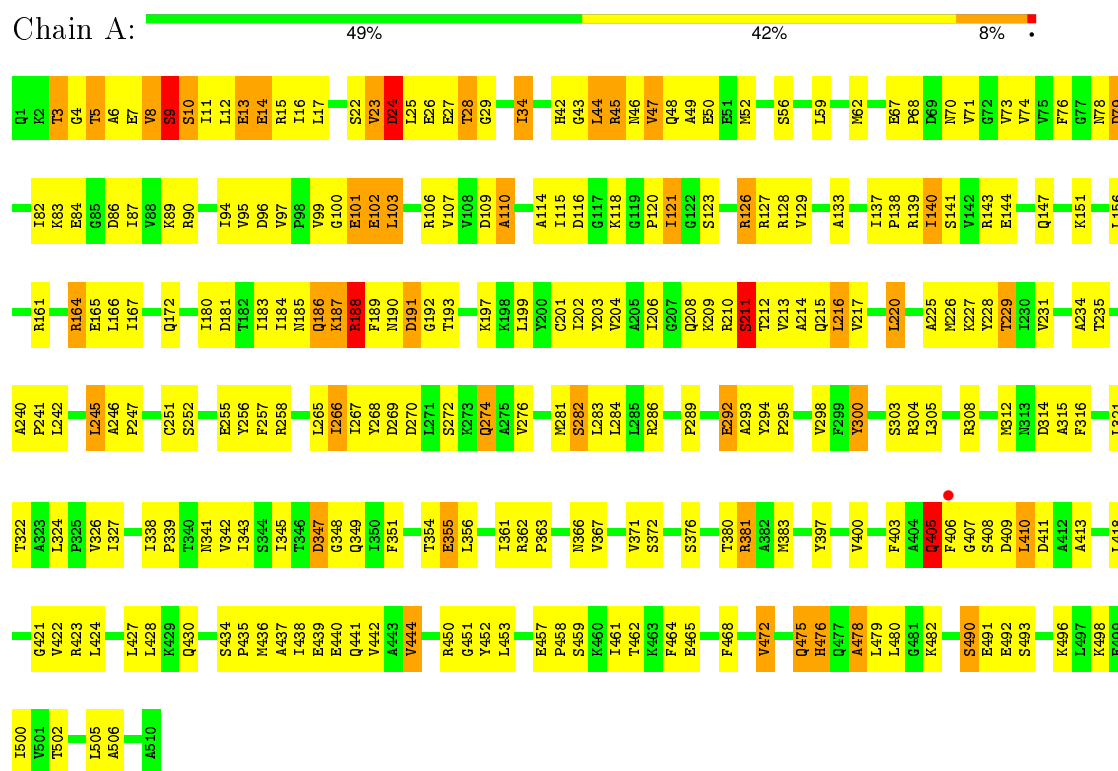


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
12	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

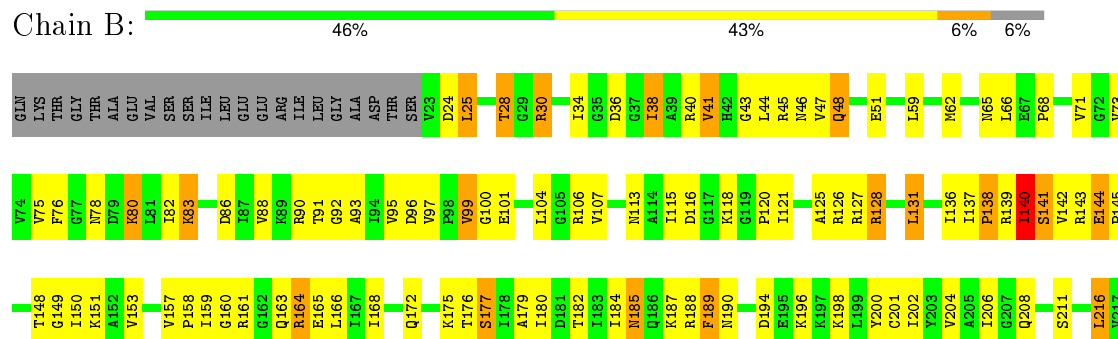
### 3 Residue-property plots

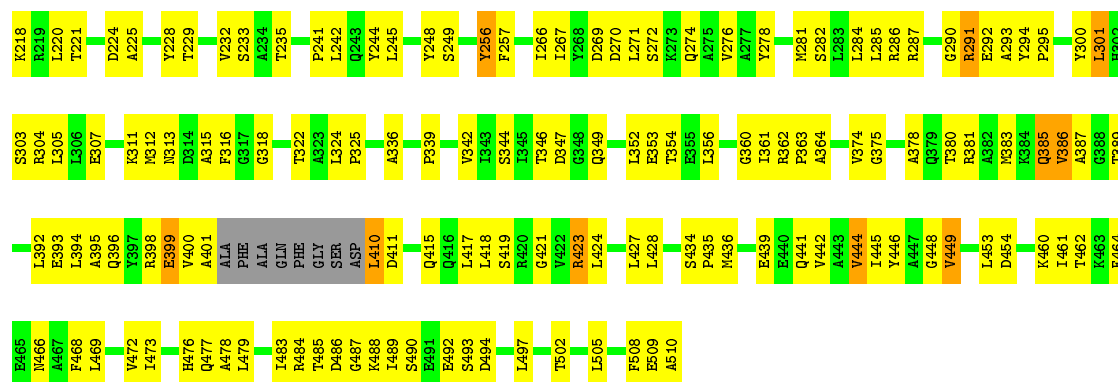
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

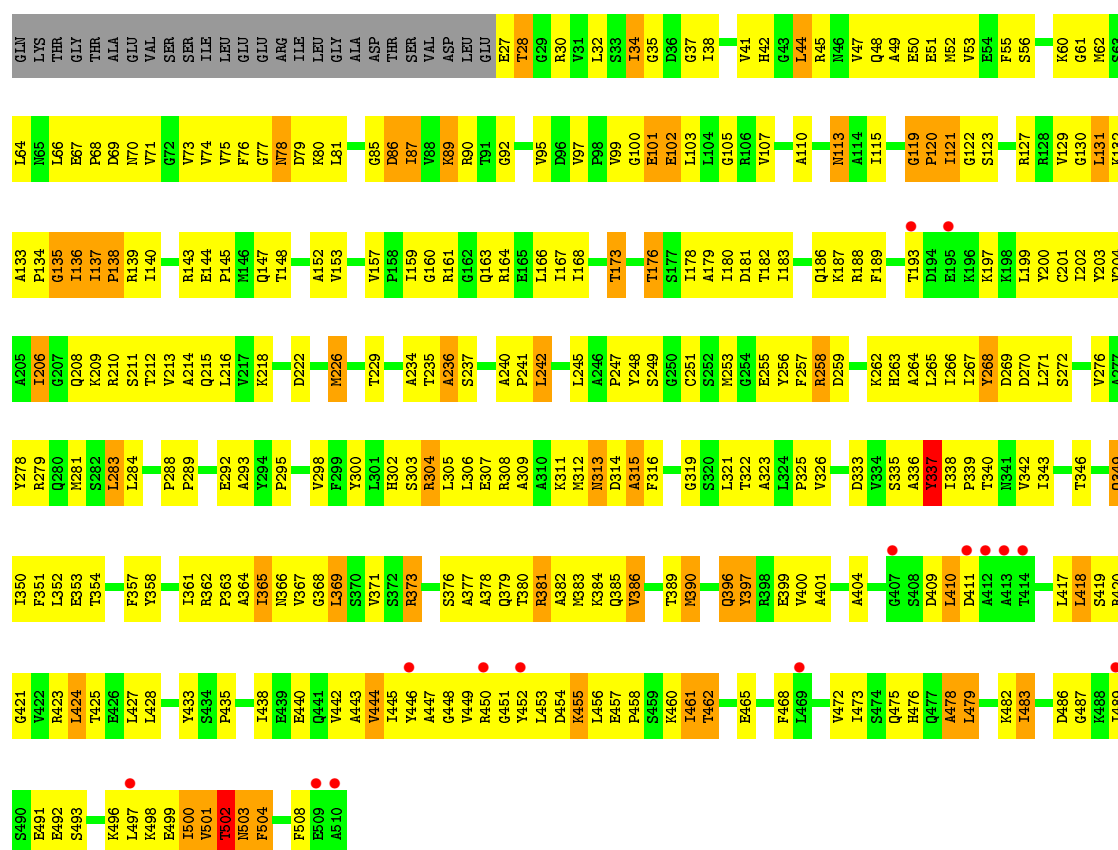


#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

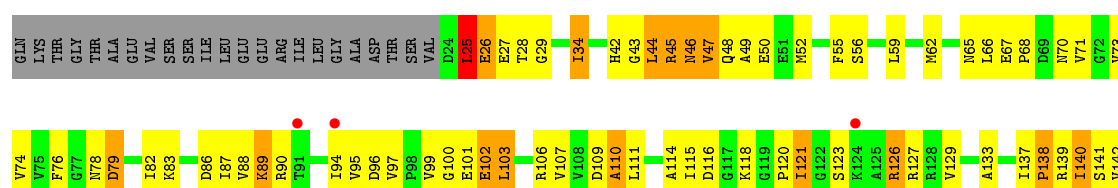
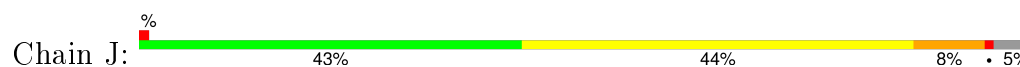


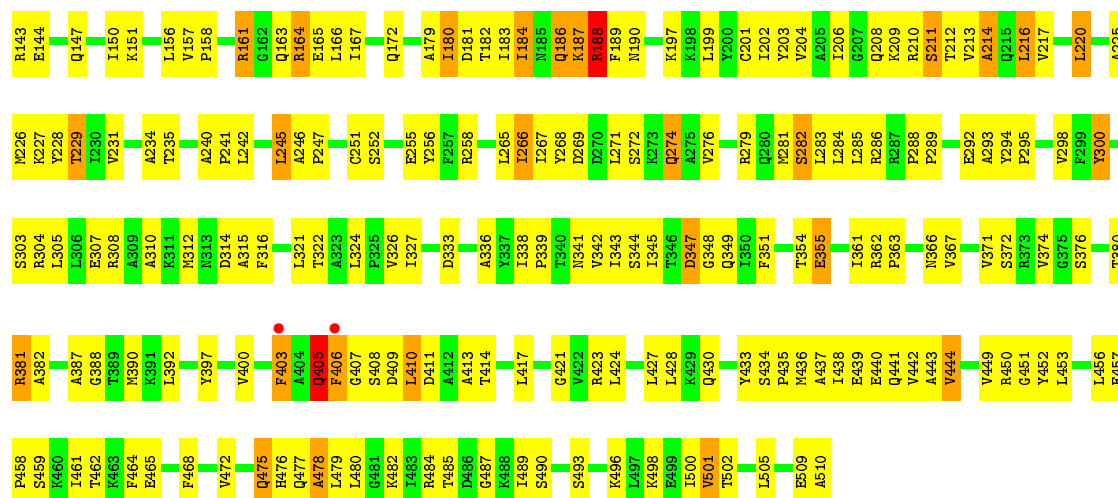


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



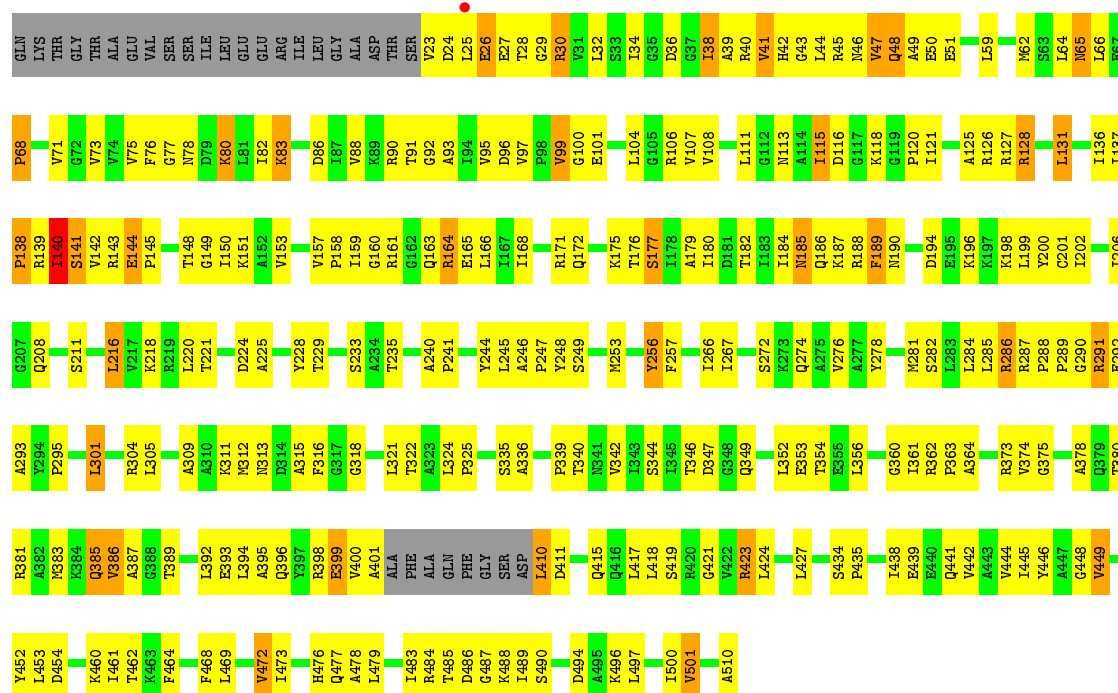
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL





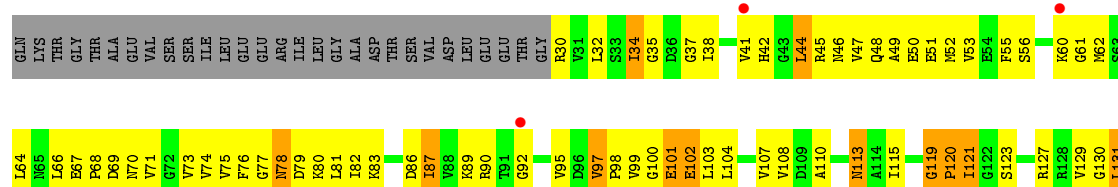
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

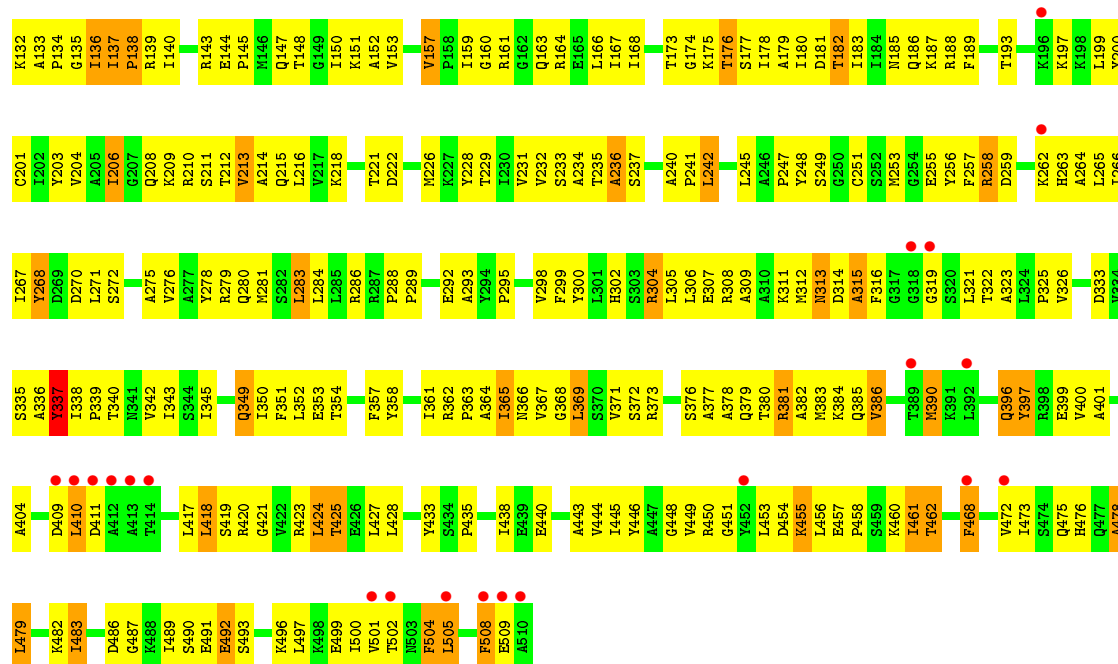
Chain K: 43% 44% 7% 6%



• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL

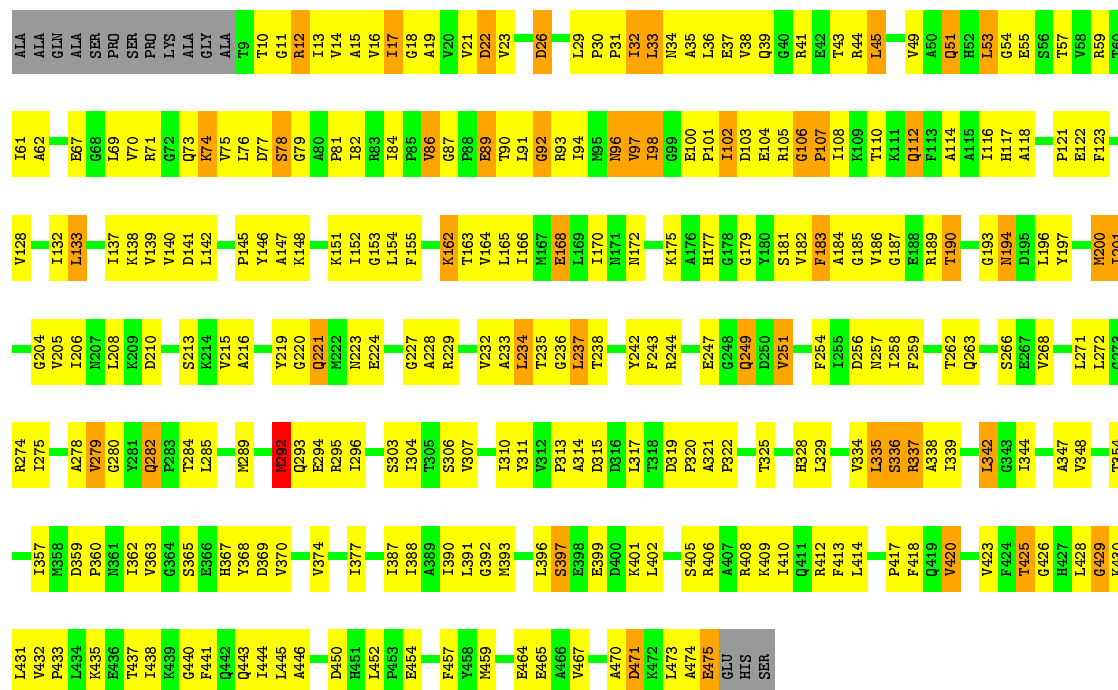
Chain L: 5% 34% 50% 10% 6%





• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

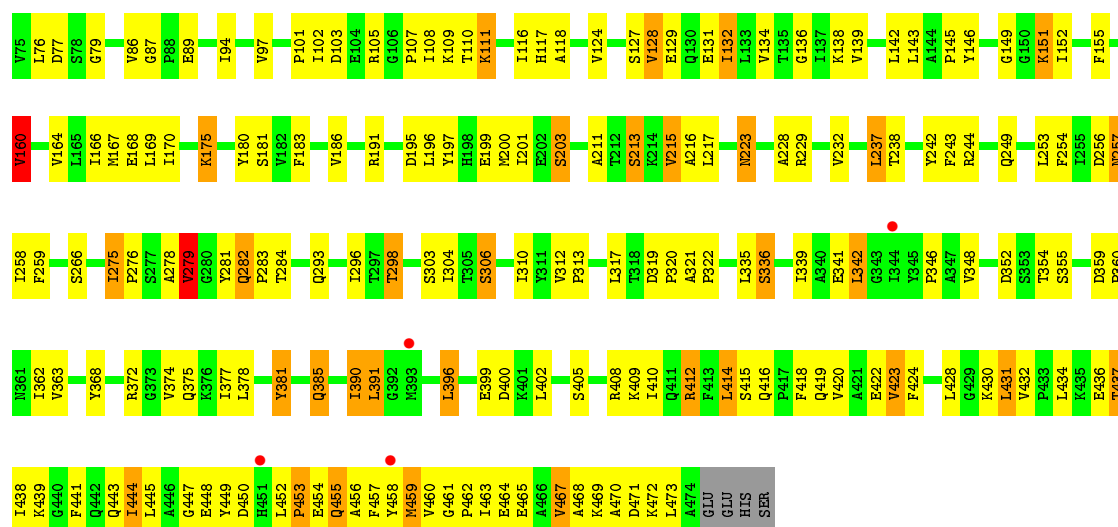
Chain D: 40% 47% 10%



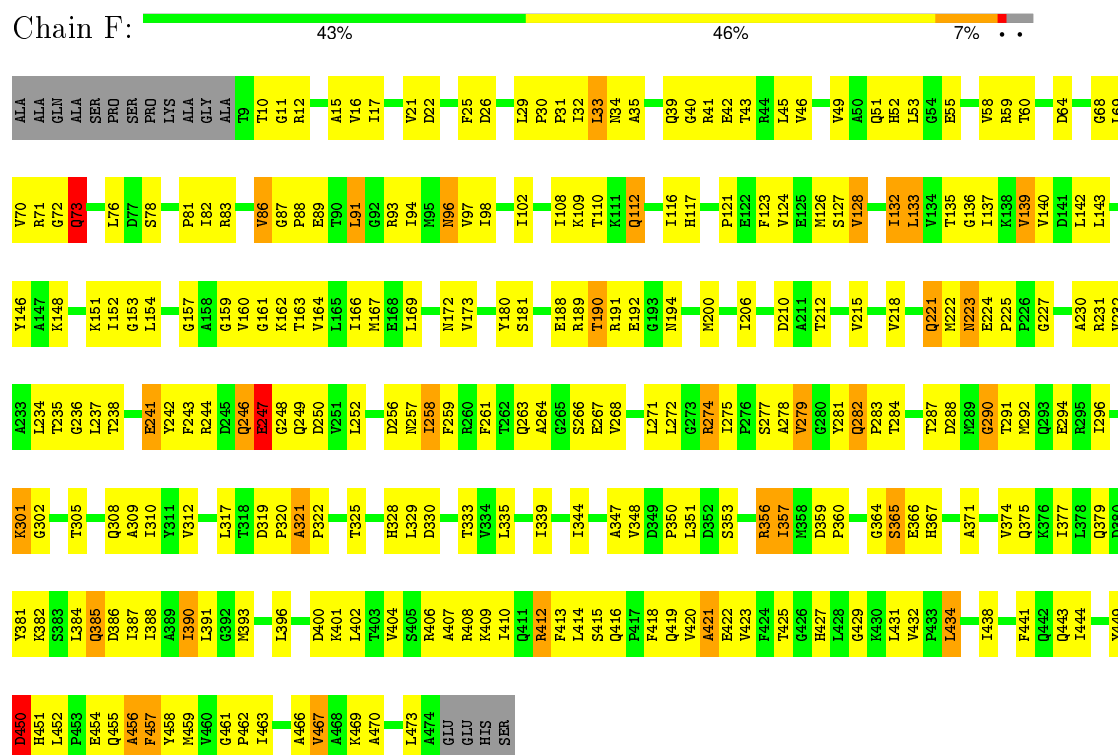
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain E: 53% 37% 7%

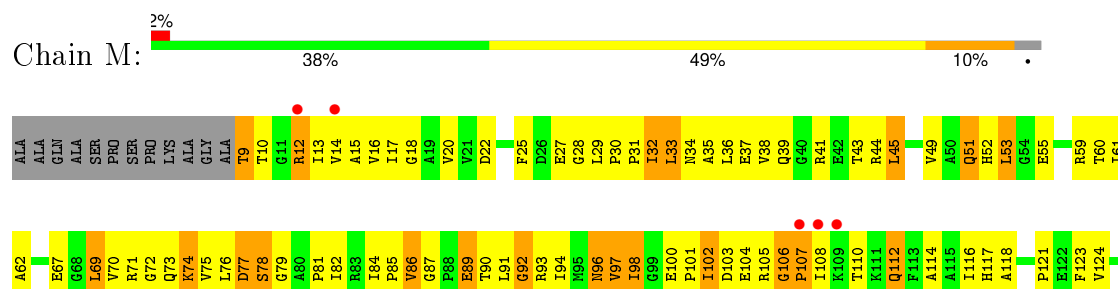


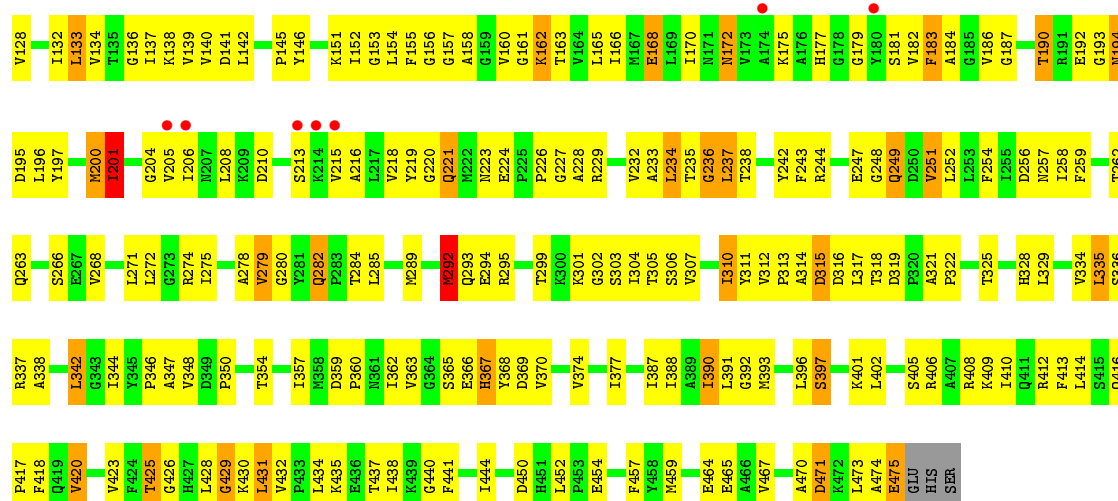


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



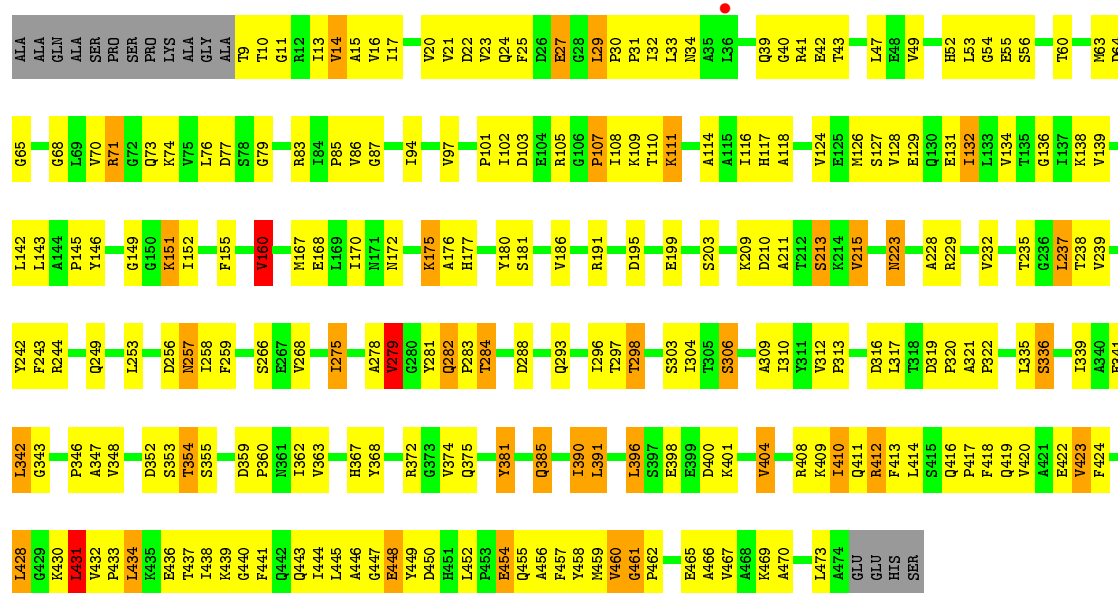
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL





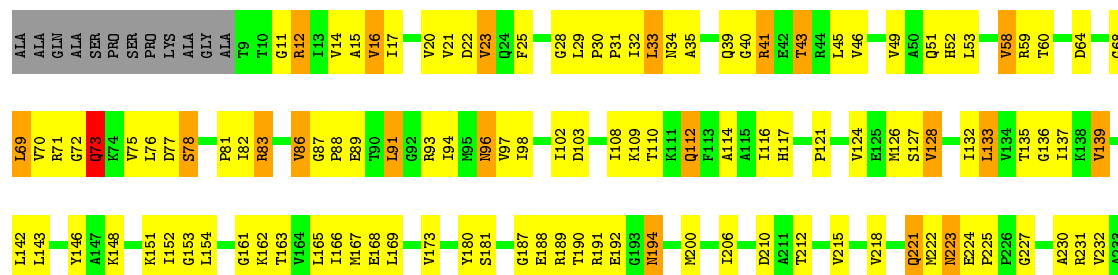
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

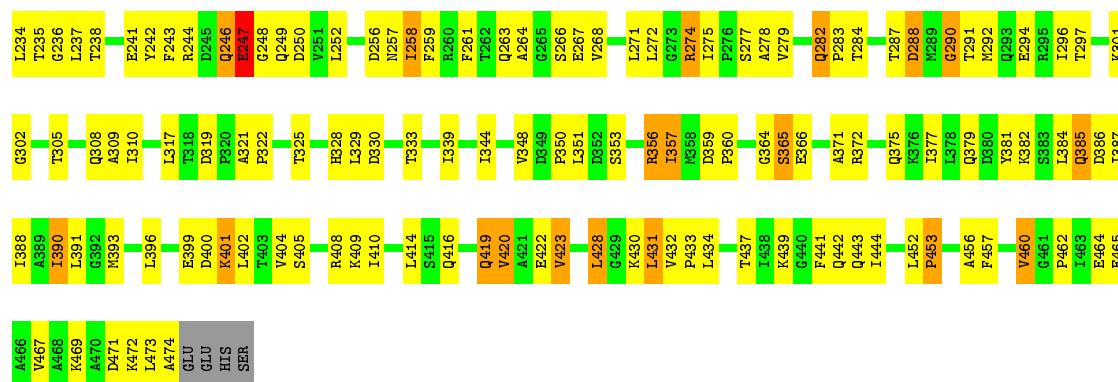
Chain N: 49% 39% 8%



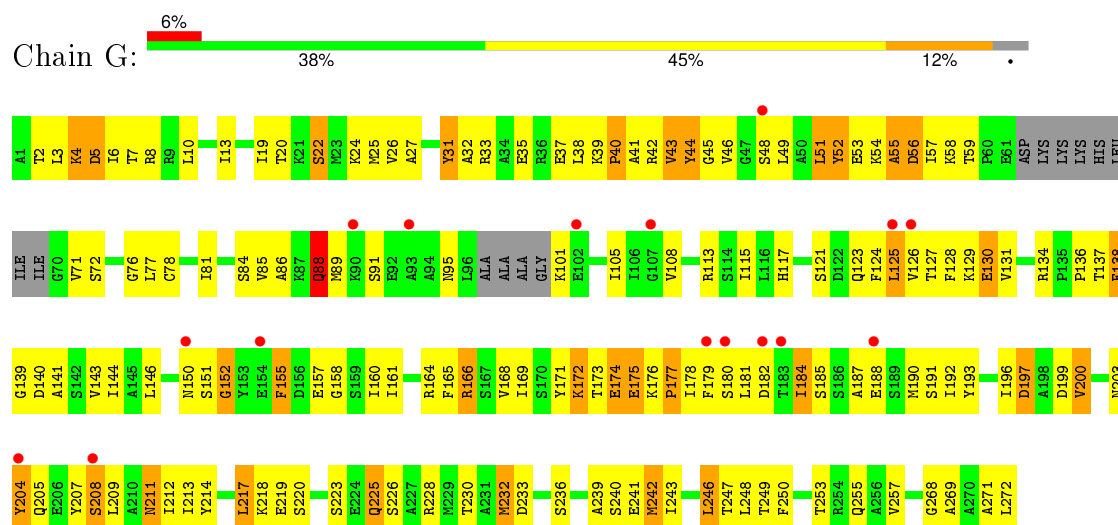
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

Chain O: 46% 42% 8%

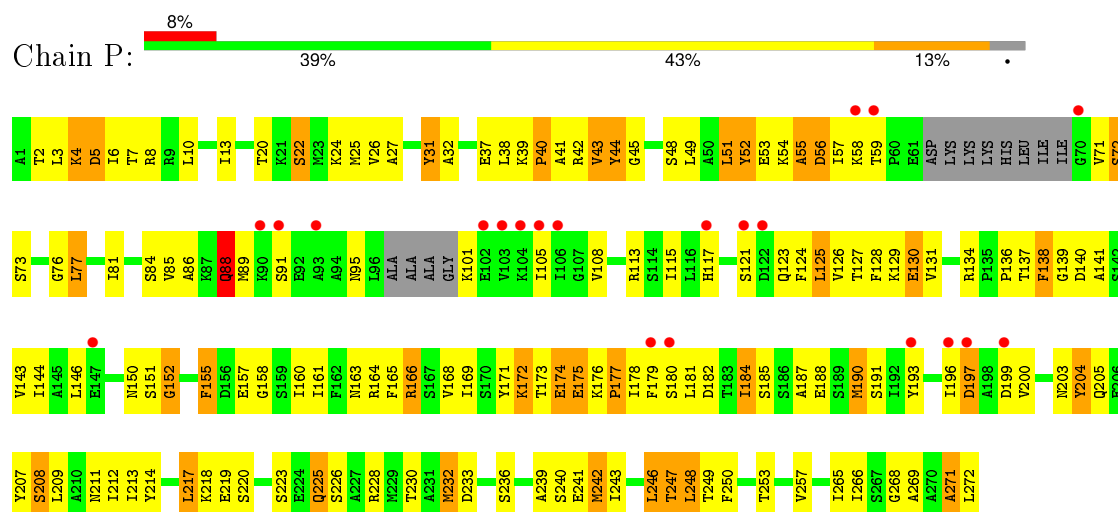




• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



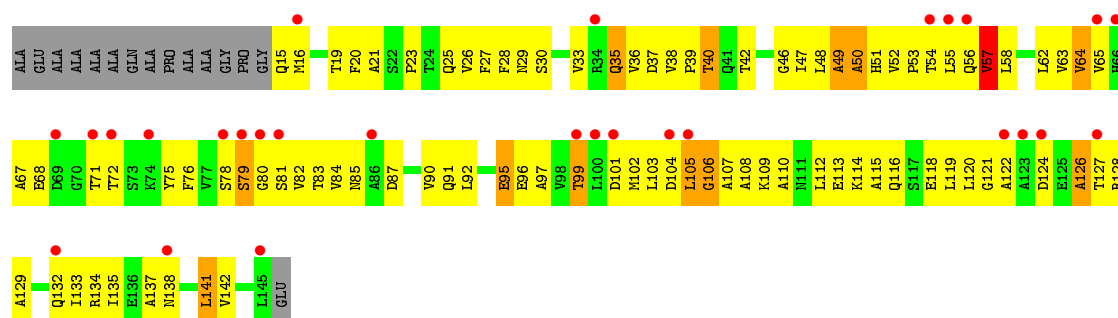
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL



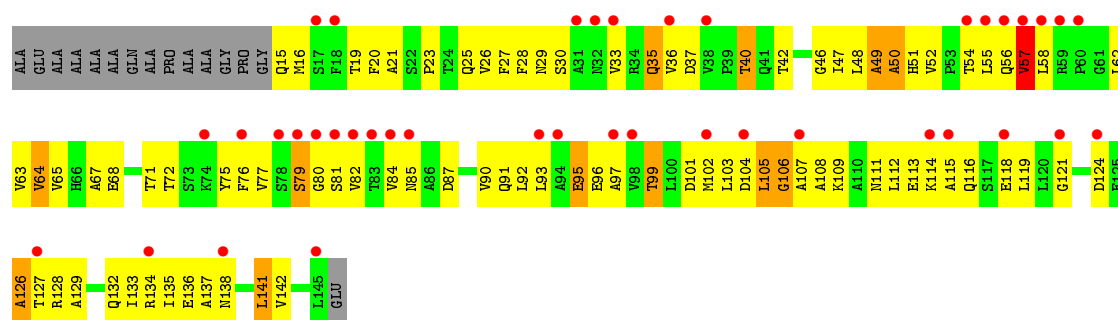
• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



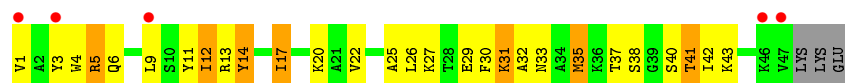
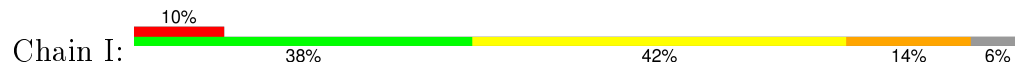




• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



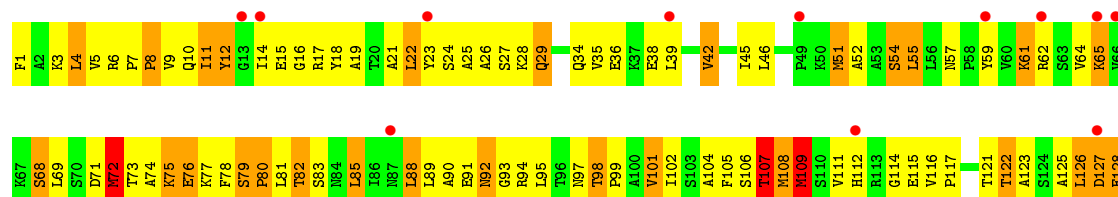
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

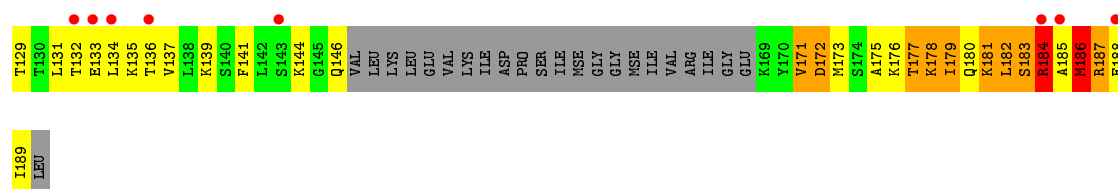


• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

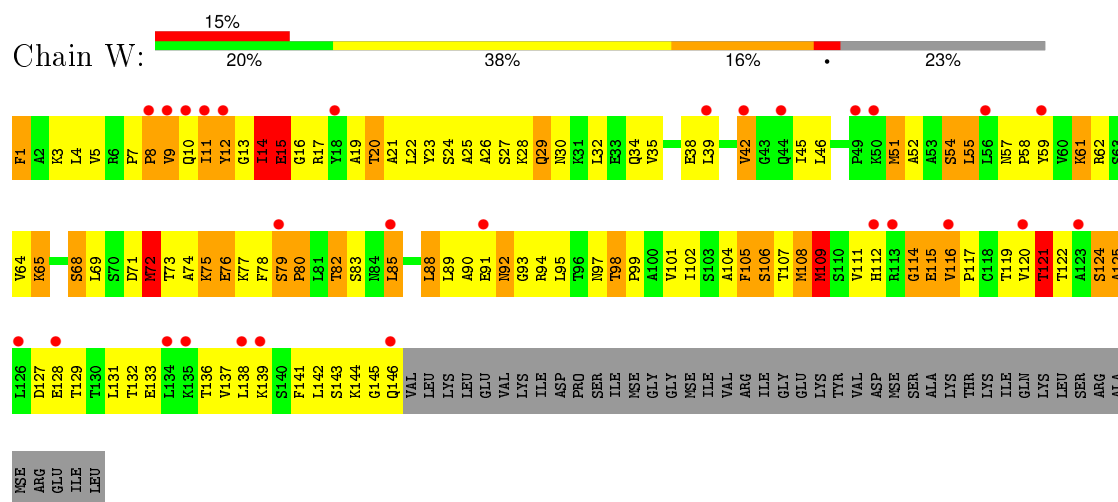


• Molecule 6: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

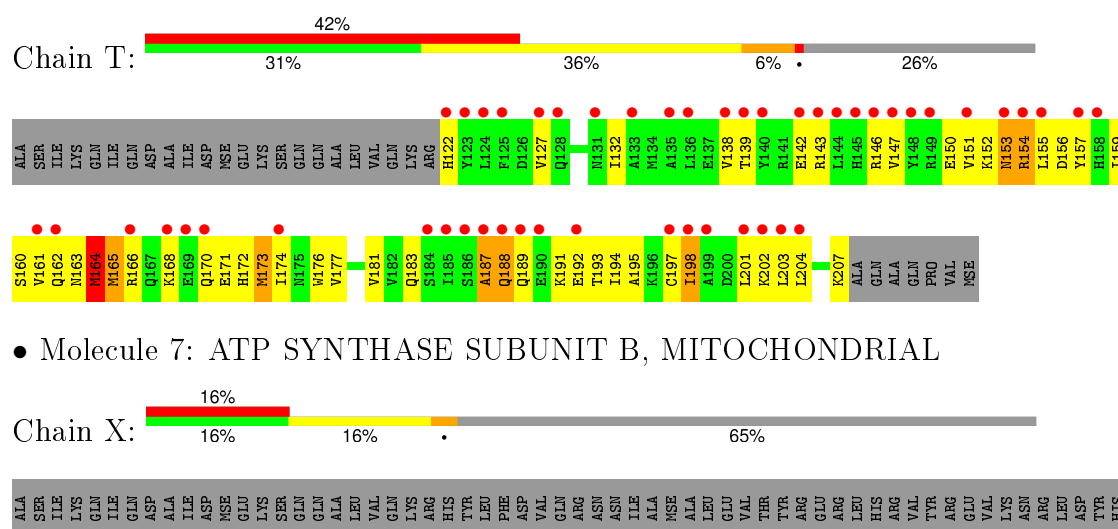




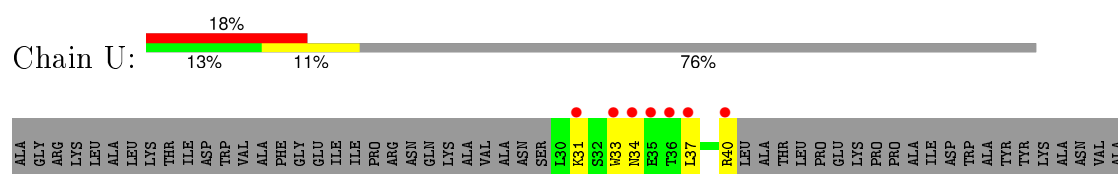
• Molecule 6: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL

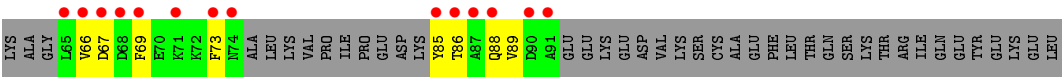


• Molecule 7: ATP SYNTHASE SUBUNIT B, MITOCHONDRIAL

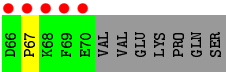
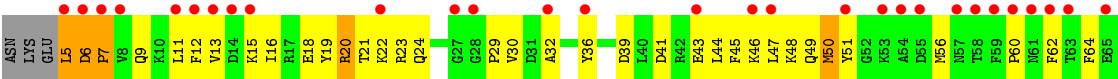


• Molecule 8: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL

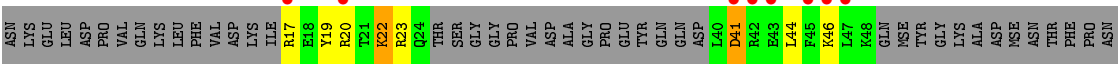




● Molecule 9: ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL



● Molecule 9: ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	158.24Å 231.25Å 286.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.77 – 3.20 41.77 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.1 (41.77-3.20) 93.1 (41.77-3.20)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.5_2)	Depositor
R, $R_{free}$	0.217 , 0.271 0.203 , 0.260	Depositor DCC
$R_{free}$ test set	8034 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.0	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 68.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 161021 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	54949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ANP, ADP

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	0.80	1/3933 (0.0%)	0.75	2/5306 (0.0%)
1	B	0.55	0/3711	0.71	0/5005
1	C	0.46	0/3735	0.64	0/5038
1	J	0.58	0/3766	0.75	1/5080 (0.0%)
1	K	0.56	0/3711	0.73	0/5005
1	L	0.45	0/3721	0.65	0/5019
2	D	0.48	0/3596	0.65	0/4879
2	E	0.54	0/3587	0.70	1/4867 (0.0%)
2	F	0.51	0/3594	0.68	0/4877
2	M	0.47	0/3596	0.66	0/4879
2	N	0.52	0/3587	0.71	2/4867 (0.0%)
2	O	0.50	0/3587	0.70	0/4867
3	G	0.44	0/2050	0.61	0/2752
3	P	0.46	0/2050	0.61	0/2752
4	H	0.29	0/982	0.48	0/1337
4	Q	0.28	0/982	0.48	0/1337
5	I	0.29	0/374	0.46	0/501
5	R	0.28	0/374	0.45	0/501
6	S	0.39	0/1301	0.76	4/1740 (0.2%)
6	W	0.39	0/1131	0.74	3/1521 (0.2%)
7	T	0.31	0/739	0.61	3/982 (0.3%)
7	X	0.37	0/334	0.71	3/437 (0.7%)
8	U	0.27	0/236	0.47	0/315
9	V	0.34	0/562	0.61	2/751 (0.3%)
9	Z	0.28	0/160	0.46	0/207
All	All	0.51	1/55399 (0.0%)	0.68	21/74822 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	J	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ASP	C-N	33.82	1.94	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ASP	C-N-CA	-10.48	100.28	122.30
6	S	72	MSE	CG-SE-CE	6.24	112.64	98.90
6	W	109	MSE	CG-SE-CE	6.17	112.47	98.90
7	T	165	MSE	CG-SE-CE	6.17	112.47	98.90
6	S	109	MSE	CG-SE-CE	5.97	112.04	98.90
2	N	215	VAL	CB-CA-C	-5.91	100.17	111.40
2	N	431	LEU	CA-CB-CG	5.74	128.51	115.30
9	V	50	MSE	CG-SE-CE	5.72	111.49	98.90
7	X	173	MSE	CG-SE-CE	5.69	111.42	98.90
7	T	173	MSE	CG-SE-CE	5.53	111.06	98.90
7	X	165	MSE	CG-SE-CE	5.52	111.05	98.90
6	W	72	MSE	CG-SE-CE	5.43	110.86	98.90
1	J	25	LEU	CA-CB-CG	5.42	127.77	115.30
6	W	51	MSE	CG-SE-CE	5.42	110.82	98.90
6	S	22	LEU	CA-CB-CG	-5.38	102.92	115.30
2	E	215	VAL	CB-CA-C	-5.31	101.31	111.40
6	S	51	MSE	CG-SE-CE	5.27	110.50	98.90
1	A	270	ASP	N-CA-CB	-5.25	101.14	110.60
9	V	56	MSE	CG-SE-CE	5.24	110.43	98.90
7	X	164	MSE	CG-SE-CE	5.22	110.38	98.90
7	T	164	MSE	CG-SE-CE	5.17	110.28	98.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ASP	Peptide
1	J	269	ASP	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	3882	0	3986	260	0
1	B	3663	0	3774	206	0
1	C	3684	0	3785	301	0
1	J	3715	0	3814	252	0
1	K	3663	0	3774	229	0
1	L	3670	0	3778	319	0
2	D	3539	0	3592	250	0
2	E	3530	0	3587	200	0
2	F	3534	0	3595	251	0
2	M	3539	0	3592	280	0
2	N	3530	0	3587	208	0
2	O	3530	0	3586	258	0
3	G	2027	0	2082	167	0
3	P	2027	0	2082	167	0
4	H	970	0	972	98	0
4	Q	970	0	972	93	0
5	I	369	0	395	32	0
5	R	369	0	395	37	0
6	S	1292	0	1382	171	0
6	W	1120	0	1191	149	0
7	T	733	0	751	81	0
7	X	336	0	362	20	0
8	U	234	0	222	15	0
9	V	551	0	534	62	0
9	Z	160	0	171	11	0
10	A	31	0	13	2	0
10	B	31	0	12	1	0
10	C	31	0	13	0	0
10	F	31	0	13	9	0
10	J	31	0	13	2	0
10	K	31	0	13	4	0
10	L	31	0	13	2	0
10	O	31	0	13	6	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	F	1	0	0	0	0
11	J	1	0	0	0	0
11	K	1	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
11	O	1	0	0	0	0
12	D	27	0	12	3	0
12	M	27	0	12	4	0
All	All	54949	0	56088	3856	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 35.

All (3856) 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:191:ASP:C	1:A:192:GLY:N	1.93	1.20
1:L:179:ALA:HB1	1:L:267:ILE:HD13	1.23	1.15
1:C:212:THR:HG23	2:F:356:ARG:HH21	1.07	1.15
1:L:212:THR:HG23	2:O:356:ARG:HH21	1.10	1.14
1:A:16:ILE:HD13	6:S:22:LEU:HD21	1.29	1.14
1:C:179:ALA:HB1	1:C:267:ILE:HD13	1.23	1.12
6:S:22:LEU:HD13	6:S:85:LEU:HD13	1.32	1.10
6:W:22:LEU:HD13	6:W:85:LEU:HD13	1.27	1.10
2:O:274:ARG:HH11	2:O:274:ARG:HG2	1.16	1.09
1:C:501:VAL:HG23	1:C:502:THR:H	1.18	1.08
2:D:105:ARG:HH12	2:D:208:LEU:HD22	1.14	1.08
1:L:137:ILE:HG12	1:L:138:PRO:HD3	1.36	1.07
2:E:412:ARG:HG2	2:E:458:TYR:HB2	1.38	1.06
6:S:175:ALA:HA	6:S:178:LYS:HE2	1.33	1.05
2:F:274:ARG:HG2	2:F:274:ARG:HH11	1.17	1.03
2:M:105:ARG:HH12	2:M:208:LEU:HD22	1.21	1.03
2:O:237:LEU:HD11	2:O:296:ILE:HG13	1.39	1.02
2:F:301:LYS:HD3	9:V:46:LYS:HD2	1.40	1.02
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.38	1.02
1:C:137:ILE:HG12	1:C:138:PRO:HD3	1.39	1.01
1:C:137:ILE:H	1:C:137:ILE:HD13	1.25	1.01
2:N:13:ILE:HD12	2:N:73:GLN:HB3	1.43	1.00
1:K:179:ALA:HB1	1:K:267:ILE:HD13	1.38	1.00
2:N:412:ARG:HH11	2:N:455:GLN:NE2	1.60	1.00
2:O:409:LYS:HD3	2:O:457:PHE:HE1	1.21	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:282:GLN:NE2	2:N:282:GLN:H	1.59	0.99
2:F:159:GLY:H	10:F:600:ANP:HNB1	1.07	0.98
2:O:112:GLN:H	2:O:112:GLN:HE21	1.11	0.98
1:L:152:ALA:HA	1:L:428:LEU:HD23	1.46	0.97
2:E:434:LEU:HG	2:E:438:ILE:HD11	1.47	0.97
2:F:237:LEU:HD11	2:F:296:ILE:HG13	1.44	0.97
2:O:137:ILE:HA	2:O:416:GLN:HE22	1.26	0.97
3:G:138:PHE:HD1	4:H:23:PRO:HG2	1.28	0.96
1:B:385:GLN:HE22	1:B:489:ILE:H	1.13	0.96
2:F:112:GLN:H	2:F:112:GLN:HE21	1.12	0.96
1:A:151:LYS:H	1:A:430:GLN:NE2	1.63	0.96
1:K:385:GLN:HE22	1:K:489:ILE:H	1.08	0.96
6:W:116:VAL:H	6:W:117:PRO:HD3	1.29	0.95
1:L:306:LEU:HD21	1:L:325:PRO:HG3	1.48	0.95
1:C:248:TYR:HE2	1:C:305:LEU:HB2	1.32	0.95
1:A:151:LYS:N	1:A:430:GLN:HE22	1.65	0.95
1:C:28:THR:CB	1:C:89:LYS:HA	1.96	0.95
3:G:138:PHE:HD1	4:H:23:PRO:CG	1.80	0.95
2:E:412:ARG:HD3	2:E:455:GLN:NE2	1.82	0.95
1:L:248:TYR:HE2	1:L:305:LEU:HB2	1.31	0.95
2:M:96:ASN:ND2	2:M:98:ILE:H	1.64	0.95
1:J:206:ILE:HD11	1:J:247:PRO:HG3	1.46	0.94
1:J:151:LYS:H	1:J:430:GLN:NE2	1.66	0.94
1:C:306:LEU:HD21	1:C:325:PRO:HG3	1.46	0.94
1:C:152:ALA:HA	1:C:428:LEU:HD23	1.47	0.93
2:D:96:ASN:ND2	2:D:98:ILE:H	1.66	0.93
2:E:282:GLN:HE21	2:E:282:GLN:H	0.97	0.93
6:W:116:VAL:H	6:W:117:PRO:CD	1.81	0.93
6:S:9:VAL:HB	6:S:108:MSE:HG2	1.50	0.93
2:F:96:ASN:HD22	2:F:96:ASN:C	1.73	0.93
1:J:403:PHE:CE1	3:P:22:SER:HB2	2.04	0.93
1:A:23:VAL:HG11	1:A:28:THR:HG23	1.51	0.92
10:F:600:ANP:O2B	10:F:600:ANP:O2G	1.85	0.92
2:M:96:ASN:C	2:M:96:ASN:HD22	1.71	0.92
1:J:151:LYS:N	1:J:430:GLN:HE22	1.67	0.92
2:E:282:GLN:NE2	2:E:282:GLN:H	1.67	0.92
3:P:138:PHE:HD1	4:Q:23:PRO:HG2	1.34	0.92
2:O:387:ILE:H	2:O:387:ILE:HD12	1.34	0.92
1:L:300:TYR:CE1	1:L:304:ARG:HD2	2.05	0.92
2:M:417:PRO:HG3	2:M:459:MET:HG3	1.52	0.92
2:E:138:LYS:HG2	2:E:437:THR:HG23	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLN:HG3	1:A:199:LEU:HB3	1.52	0.91
2:E:458:TYR:CE1	2:E:459:MET:HG2	2.06	0.91
2:D:96:ASN:C	2:D:96:ASN:HD22	1.72	0.91
2:N:282:GLN:N	2:N:282:GLN:HE21	1.68	0.91
2:E:139:VAL:HA	2:E:414:LEU:HD23	1.53	0.91
2:D:31:PRO:HD2	2:D:34:ASN:ND2	1.86	0.90
2:D:105:ARG:NH1	2:D:208:LEU:HD22	1.86	0.90
2:M:31:PRO:HD2	2:M:34:ASN:ND2	1.87	0.90
1:K:241:PRO:HG3	1:K:281:MET:HE3	1.54	0.90
1:B:180:ILE:HD11	1:B:216:LEU:HD11	1.54	0.90
2:M:282:GLN:NE2	2:M:282:GLN:H	1.68	0.89
2:O:32:ILE:HA	2:O:49:VAL:HG12	1.55	0.89
1:K:385:GLN:NE2	1:K:489:ILE:H	1.68	0.89
2:N:390:ILE:HG12	3:P:25:MET:HG2	1.53	0.89
2:M:247:GLU:HB3	2:M:249:GLN:HB2	1.55	0.89
1:B:385:GLN:NE2	1:B:489:ILE:H	1.69	0.88
2:M:9:THR:HG21	2:M:28:GLY:HA3	1.54	0.88
1:L:137:ILE:HD13	1:L:137:ILE:H	1.39	0.88
2:F:387:ILE:H	2:F:387:ILE:HD12	1.39	0.88
1:B:106:ARG:HH11	1:B:106:ARG:HG3	1.39	0.88
2:E:49:VAL:HA	2:E:60:THR:HG22	1.55	0.88
1:A:8:VAL:HG22	2:D:55:GLU:OE1	1.74	0.88
1:C:160:GLY:H	1:C:163:GLN:HE21	1.19	0.88
2:N:412:ARG:HH11	2:N:455:GLN:HE21	0.89	0.88
1:K:106:ARG:HH11	1:K:106:ARG:HG3	1.39	0.88
2:O:96:ASN:HD22	2:O:96:ASN:C	1.77	0.88
2:N:49:VAL:HA	2:N:60:THR:HG22	1.56	0.87
2:D:247:GLU:HB3	2:D:249:GLN:HB2	1.56	0.87
1:A:206:ILE:HD11	1:A:247:PRO:HG3	1.56	0.87
2:F:32:ILE:O	2:F:33:LEU:HB2	1.74	0.87
2:O:409:LYS:HD3	2:O:457:PHE:CE1	2.08	0.86
2:D:417:PRO:HG3	2:D:459:MET:HG3	1.55	0.86
1:L:288:PRO:HG3	3:P:271:ALA:O	1.74	0.86
2:O:218:VAL:HG21	2:O:236:GLY:HA2	1.58	0.86
2:O:32:ILE:O	2:O:33:LEU:HB2	1.74	0.86
1:J:266:ILE:HG22	1:J:321:LEU:HD11	1.57	0.86
1:L:160:GLY:H	1:L:163:GLN:HE21	1.22	0.85
1:A:156:LEU:HD13	1:A:367:VAL:HG11	1.58	0.85
6:W:133:GLU:HA	6:W:136:THR:HG23	1.58	0.85
1:K:172:GLN:HA	10:K:600:ANP:HNB1	1.40	0.85
2:E:223:ASN:H	2:E:223:ASN:HD22	1.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:319:ASP:O	2:N:322:PRO:HD2	1.76	0.85
6:S:133:GLU:HG2	7:T:207:LYS:HE2	1.59	0.85
6:W:28:LYS:O	6:W:29:GLN:HB2	1.76	0.85
2:N:136:GLY:HA3	2:N:431:LEU:HD13	1.57	0.85
3:G:253:THR:O	3:G:257:VAL:HG23	1.77	0.85
2:N:412:ARG:NH1	2:N:455:GLN:HE21	1.72	0.84
2:E:31:PRO:HD2	2:E:34:ASN:ND2	1.92	0.84
1:J:186:GLN:HG3	1:J:199:LEU:HB3	1.58	0.84
1:B:218:LYS:HD3	2:E:128:VAL:HG21	1.58	0.84
6:S:133:GLU:HA	6:S:136:THR:CG2	2.07	0.84
2:M:221:GLN:HE21	2:M:221:GLN:HA	1.42	0.84
2:N:381:TYR:HE1	2:N:385:GLN:HG3	1.41	0.84
2:F:274:ARG:HG2	2:F:274:ARG:NH1	1.92	0.84
1:K:218:LYS:HD3	2:N:128:VAL:HG21	1.58	0.84
1:C:137:ILE:HD13	1:C:137:ILE:N	1.91	0.84
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.59	0.84
2:N:223:ASN:HD22	2:N:223:ASN:H	1.26	0.84
2:O:31:PRO:HD2	2:O:34:ASN:ND2	1.93	0.84
1:B:127:ARG:HH21	1:B:131:LEU:CD2	1.91	0.84
1:K:180:ILE:HD11	1:K:216:LEU:HD11	1.58	0.83
2:F:32:ILE:HA	2:F:49:VAL:HG12	1.61	0.83
1:B:395:ALA:HA	1:B:398:ARG:NH1	1.94	0.83
1:L:110:ALA:HB3	1:L:242:LEU:HD23	1.59	0.83
6:S:78:PHE:C	6:S:80:PRO:HD3	1.98	0.83
2:E:319:ASP:O	2:E:322:PRO:HD2	1.79	0.83
7:T:146:ARG:HH12	9:V:64:PHE:HA	1.44	0.83
2:M:310:ILE:HG12	2:M:325:THR:HG21	1.60	0.83
3:G:31:TYR:HB2	3:G:225:GLN:HB3	1.61	0.83
1:C:212:THR:HG23	2:F:356:ARG:NH2	1.92	0.83
1:A:9:SER:HB2	2:D:55:GLU:OE1	1.79	0.83
2:O:200:MET:HB3	2:O:206:ILE:HD12	1.61	0.83
3:P:203:ASN:HD21	5:R:4:TRP:HH2	1.25	0.83
2:M:154:LEU:HD13	2:M:165:LEU:HD23	1.59	0.82
6:S:28:LYS:O	6:S:29:GLN:HB2	1.77	0.82
1:K:127:ARG:HH21	1:K:131:LEU:CD2	1.92	0.82
1:J:107:VAL:HG11	2:M:123:PHE:CE2	2.14	0.82
2:O:274:ARG:NH1	2:O:274:ARG:HG2	1.89	0.82
3:P:138:PHE:HD1	4:Q:23:PRO:CG	1.92	0.82
2:O:136:GLY:HA3	2:O:431:LEU:HD22	1.62	0.82
2:D:282:GLN:H	2:D:282:GLN:NE2	1.76	0.82
6:W:7:PRO:HB3	6:W:108:MSE:SE	2.29	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:105:ARG:NH1	2:M:208:LEU:HD22	1.93	0.82
2:F:218:VAL:HG21	2:F:236:GLY:HA2	1.61	0.82
2:M:39:GLN:NE2	2:M:76:LEU:HD12	1.95	0.81
2:N:31:PRO:HD2	2:N:34:ASN:ND2	1.95	0.81
1:C:48:GLN:HB2	1:C:51:GLU:HB2	1.63	0.81
6:S:133:GLU:HA	6:S:136:THR:HG23	1.61	0.81
2:O:223:ASN:H	2:O:223:ASN:HD22	1.25	0.81
2:F:223:ASN:H	2:F:223:ASN:HD22	1.25	0.81
1:C:255:GLU:HG2	1:C:258:ARG:HH12	1.45	0.81
1:L:357:PHE:CE2	1:L:362:ARG:HD3	2.14	0.81
2:D:92:GLY:HA2	2:D:206:ILE:HD12	1.63	0.81
2:E:381:TYR:HE1	2:E:385:GLN:HG3	1.44	0.81
2:M:118:ALA:H	2:M:295:ARG:NH1	1.76	0.81
2:M:92:GLY:HA2	2:M:206:ILE:HD12	1.61	0.81
2:O:11:GLY:HA3	2:O:25:PHE:CD2	2.16	0.81
2:O:15:ALA:HB3	2:O:22:ASP:HB2	1.63	0.81
2:D:118:ALA:H	2:D:295:ARG:NH1	1.78	0.81
2:D:221:GLN:HA	2:D:221:GLN:HE21	1.47	0.80
1:L:255:GLU:HG2	1:L:258:ARG:HH12	1.47	0.80
6:W:78:PHE:C	6:W:80:PRO:HD3	2.01	0.80
2:E:412:ARG:HD3	2:E:455:GLN:HE21	1.45	0.80
1:L:268:TYR:CE2	1:L:305:LEU:HD21	2.16	0.80
6:S:5:VAL:O	6:S:7:PRO:HD3	1.82	0.80
2:F:31:PRO:HD2	2:F:34:ASN:ND2	1.95	0.80
2:M:32:ILE:O	2:M:33:LEU:HB2	1.81	0.80
3:G:138:PHE:CD1	4:H:23:PRO:HG2	2.15	0.80
1:B:180:ILE:HG13	1:B:216:LEU:HD21	1.64	0.80
1:K:107:VAL:HB	1:K:116:ASP:HB3	1.64	0.80
1:K:180:ILE:HG13	1:K:216:LEU:HD21	1.62	0.80
2:D:162:LYS:HB2	12:D:600:ADP:O1B	1.80	0.80
2:N:446:ALA:HB3	2:N:448:GLU:HB2	1.63	0.80
6:S:137:VAL:HG22	7:T:203:LEU:HD13	1.64	0.80
1:C:110:ALA:HB3	1:C:242:LEU:HD23	1.62	0.80
1:L:48:GLN:HB2	1:L:51:GLU:HB2	1.62	0.80
2:M:282:GLN:HE21	2:M:282:GLN:N	1.79	0.80
2:O:25:PHE:CD1	2:O:30:PRO:HD3	2.16	0.80
1:C:300:TYR:CE1	1:C:304:ARG:HD2	2.17	0.80
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.64	0.80
1:C:160:GLY:H	1:C:163:GLN:NE2	1.81	0.79
1:B:241:PRO:HG3	1:B:281:MET:HE3	1.63	0.79
2:D:32:ILE:O	2:D:33:LEU:HB2	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:247:GLU:CB	2:M:249:GLN:HB2	2.11	0.79
2:E:180:TYR:H	2:E:249:GLN:NE2	1.80	0.79
2:D:146:TYR:HB3	2:D:152:ILE:HD11	1.63	0.79
2:O:25:PHE:HB2	2:O:29:LEU:HD12	1.64	0.79
2:O:321:ALA:HB3	2:O:322:PRO:HD3	1.64	0.79
3:G:138:PHE:CD1	4:H:23:PRO:CG	2.67	0.78
1:J:407:GLY:HA3	1:J:410:LEU:HD21	1.63	0.78
2:D:186:VAL:HG21	2:D:233:ALA:HB2	1.64	0.78
6:W:5:VAL:HB	6:W:24:SER:HA	1.65	0.78
4:Q:58:LEU:HD11	4:Q:92:LEU:HD11	1.63	0.78
2:N:439:LYS:O	2:N:443:GLN:HG3	1.81	0.78
1:L:479:LEU:HD22	1:L:483:ILE:HD11	1.65	0.78
1:L:365:ILE:HD12	1:L:366:ASN:H	1.48	0.78
6:W:114:GLY:O	6:W:115:GLU:HB2	1.81	0.78
1:C:479:LEU:HD22	1:C:483:ILE:HD11	1.66	0.78
3:P:31:TYR:HB2	3:P:225:GLN:HB3	1.63	0.78
4:H:57:VAL:HG11	5:I:11:TYR:CE1	2.19	0.78
1:K:385:GLN:HE22	1:K:489:ILE:N	1.80	0.78
2:F:200:MET:HB3	2:F:206:ILE:HD12	1.65	0.78
7:T:143:ARG:CZ	9:V:64:PHE:HB3	2.14	0.77
1:L:136:ILE:HD11	2:M:219:TYR:CD2	2.19	0.77
1:B:78:ASN:HD21	1:B:80:LYS:HE3	1.48	0.77
1:A:193:THR:HB	2:N:42:GLU:HG2	1.65	0.77
1:B:83:LYS:HB2	1:B:83:LYS:NZ	2.00	0.77
2:F:455:GLN:HE21	2:F:473:LEU:HD22	1.50	0.77
2:O:310:ILE:HD13	2:O:325:THR:HG21	1.66	0.77
1:C:357:PHE:CE2	1:C:362:ARG:HD3	2.19	0.77
1:B:312:MET:O	1:B:318:GLY:HA2	1.83	0.77
1:J:156:LEU:HD13	1:J:367:VAL:HG11	1.64	0.77
2:O:11:GLY:HA3	2:O:25:PHE:CE2	2.20	0.77
1:B:99:VAL:HG21	1:B:127:ARG:HG3	1.65	0.77
3:G:2:THR:HB	3:G:5:ASP:OD1	1.85	0.77
2:D:39:GLN:NE2	2:D:76:LEU:HD12	1.99	0.77
1:C:365:ILE:HD12	1:C:366:ASN:H	1.48	0.77
2:N:282:GLN:H	2:N:282:GLN:HE21	0.84	0.77
1:A:151:LYS:H	1:A:430:GLN:HE22	0.82	0.77
1:B:107:VAL:HB	1:B:116:ASP:HB3	1.67	0.77
1:A:407:GLY:HA3	1:A:410:LEU:HD21	1.67	0.77
6:W:133:GLU:HB3	7:X:207:LYS:HD3	1.67	0.77
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.65	0.77
1:K:83:LYS:NZ	1:K:83:LYS:HB2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:HD11	1:B:143:ARG:HH21	1.49	0.77
1:L:137:ILE:HD13	1:L:137:ILE:N	1.99	0.76
1:C:366:ASN:OD1	1:C:369:LEU:HB2	1.84	0.76
3:G:20:THR:HG22	3:G:236:SER:HB3	1.66	0.76
2:O:46:VAL:HG21	2:O:98:ILE:HG21	1.67	0.76
2:D:247:GLU:CB	2:D:249:GLN:HB2	2.14	0.76
1:J:47:VAL:O	2:N:70:VAL:HG13	1.84	0.76
1:K:106:ARG:HG3	1:K:106:ARG:NH1	1.98	0.76
2:O:23:VAL:HG23	2:O:58:VAL:HG23	1.67	0.76
6:W:7:PRO:HB3	6:W:108:MSE:HE1	1.67	0.76
1:L:160:GLY:H	1:L:163:GLN:NE2	1.82	0.76
4:H:58:LEU:HD11	4:H:92:LEU:HD11	1.66	0.76
1:L:289:PRO:HD2	3:P:268:GLY:HA2	1.66	0.76
2:E:282:GLN:N	2:E:282:GLN:HE21	1.80	0.76
6:S:79:SER:N	6:S:80:PRO:HD3	2.01	0.76
1:A:423:ARG:HG2	1:A:461:ILE:HD11	1.67	0.76
6:S:51:MSE:HE2	6:S:72:MSE:HG3	1.68	0.76
1:L:366:ASN:OD1	1:L:369:LEU:HB2	1.84	0.76
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.21	0.76
1:B:78:ASN:ND2	1:B:80:LYS:HE3	1.99	0.76
2:D:310:ILE:HG12	2:D:325:THR:HG21	1.68	0.76
2:N:449:TYR:HD2	2:N:452:LEU:HD12	1.51	0.75
2:E:139:VAL:HA	2:E:414:LEU:CD2	2.16	0.75
3:P:2:THR:HB	3:P:5:ASP:OD1	1.86	0.75
1:B:385:GLN:HE22	1:B:489:ILE:N	1.84	0.75
2:E:14:VAL:HG11	2:E:24:GLN:HB2	1.68	0.75
4:H:109:LYS:HG2	4:H:142:VAL:HG22	1.66	0.75
1:K:389:THR:O	1:K:393:GLU:HG3	1.85	0.75
1:A:83:LYS:HD3	2:D:31:PRO:HG3	1.67	0.75
1:B:389:THR:O	1:B:393:GLU:HG3	1.86	0.75
5:I:4:TRP:CZ3	5:I:5:ARG:HG2	2.21	0.75
1:J:225:ALA:HA	1:J:228:TYR:CE2	2.22	0.75
1:A:172:GLN:HA	10:A:600:ANP:HNB1	1.52	0.75
2:F:94:ILE:HG22	2:F:102:ILE:HG13	1.69	0.75
9:V:62:PHE:HB3	9:V:64:PHE:CZ	2.22	0.75
2:F:221:GLN:HA	2:F:221:GLN:HE21	1.52	0.75
1:C:289:PRO:HD2	3:G:268:GLY:HA2	1.68	0.75
1:K:140:ILE:HD11	1:K:143:ARG:HH21	1.51	0.75
3:G:128:PHE:CZ	3:G:144:ILE:HG23	2.22	0.75
1:K:66:LEU:HB2	2:O:16:VAL:HG23	1.69	0.75
1:A:8:VAL:HG23	6:S:17:ARG:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.67	0.75
1:L:62:MET:H	1:L:73:VAL:HG13	1.52	0.75
2:O:282:GLN:H	2:O:282:GLN:NE2	1.83	0.75
2:D:12:ARG:HH21	6:S:10:GLN:NE2	1.85	0.75
6:W:138:LEU:O	6:W:141:PHE:HB2	1.87	0.74
6:W:51:MSE:HE2	6:W:72:MSE:HG3	1.68	0.74
1:B:106:ARG:NH1	1:B:106:ARG:HG3	1.98	0.74
2:D:282:GLN:HE21	2:D:282:GLN:N	1.84	0.74
6:W:4:LEU:HB3	6:W:24:SER:OG	1.86	0.74
6:W:79:SER:N	6:W:80:PRO:HD3	2.03	0.74
6:W:133:GLU:OE1	7:X:207:LYS:HG2	1.86	0.74
3:P:253:THR:O	3:P:257:VAL:HG23	1.86	0.74
2:M:39:GLN:HE21	2:M:76:LEU:HD12	1.51	0.74
6:S:42:VAL:HA	6:S:45:ILE:HG13	1.70	0.74
2:N:381:TYR:CE1	2:N:385:GLN:HG3	2.23	0.74
1:B:469:LEU:O	1:B:473:ILE:HG13	1.88	0.74
7:T:173:MSE:HG3	9:V:22:LYS:CG	2.18	0.74
1:A:496:LYS:O	1:A:500:ILE:HG13	1.87	0.74
2:D:452:LEU:HD22	2:D:470:ALA:HB1	1.70	0.73
6:W:42:VAL:HA	6:W:45:ILE:HG13	1.69	0.73
2:O:274:ARG:HH11	2:O:274:ARG:CG	1.99	0.73
1:K:184:ILE:HG22	1:K:435:PRO:HG2	1.70	0.73
1:L:48:GLN:HA	2:M:70:VAL:HG22	1.68	0.73
1:L:457:GLU:O	1:L:460:LYS:HE2	1.88	0.73
1:K:395:ALA:HA	1:K:398:ARG:NH1	2.02	0.73
4:Q:109:LYS:HG2	4:Q:142:VAL:HG22	1.70	0.73
1:L:212:THR:HG23	2:O:356:ARG:NH2	1.96	0.73
1:L:206:ILE:H	1:L:206:ILE:HD12	1.52	0.73
1:K:99:VAL:HG21	1:K:127:ARG:HG3	1.70	0.73
2:N:449:TYR:CD2	2:N:452:LEU:HD12	2.24	0.73
2:M:96:ASN:ND2	2:M:96:ASN:C	2.39	0.73
1:L:159:ILE:HA	1:L:163:GLN:NE2	2.03	0.73
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.69	0.73
2:F:282:GLN:H	2:F:282:GLN:NE2	1.86	0.73
2:E:399:GLU:O	2:E:402:LEU:HB3	1.87	0.73
2:M:183:PHE:CD2	2:M:183:PHE:C	2.62	0.73
2:M:183:PHE:HD2	2:M:183:PHE:C	1.91	0.73
2:F:274:ARG:CG	2:F:274:ARG:HH11	2.01	0.73
2:D:39:GLN:HE21	2:D:76:LEU:HD12	1.54	0.73
3:G:239:ALA:O	3:G:243:ILE:HG12	1.88	0.73
2:M:452:LEU:HD22	2:M:470:ALA:HB1	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:328:HIS:O	2:D:329:LEU:HD23	1.87	0.73
2:F:139:VAL:HG13	2:F:414:LEU:HB3	1.69	0.73
2:M:146:TYR:HB3	2:M:152:ILE:HD11	1.70	0.73
1:K:48:GLN:NE2	2:O:68:GLY:HA2	2.02	0.73
1:A:403:PHE:CD1	3:G:22:SER:HB2	2.24	0.73
1:B:34:ILE:HG21	1:B:82:ILE:O	1.89	0.73
6:S:137:VAL:HG23	7:T:207:LYS:HZ1	1.53	0.73
1:C:386:VAL:HG12	1:C:449:VAL:HG11	1.71	0.73
2:N:180:TYR:H	2:N:249:GLN:NE2	1.86	0.73
2:E:139:VAL:HG11	2:E:348:VAL:HB	1.71	0.73
2:E:346:PRO:HG3	2:E:418:PHE:HZ	1.54	0.73
1:K:312:MET:O	1:K:318:GLY:HA2	1.88	0.73
1:J:190:ASN:ND2	1:J:228:TYR:CD1	2.57	0.72
2:O:94:ILE:HG22	2:O:102:ILE:HG13	1.71	0.72
3:P:128:PHE:CZ	3:P:144:ILE:HG23	2.24	0.72
6:S:182:LEU:HD21	7:T:202:LYS:NZ	2.03	0.72
2:M:15:ALA:HB3	2:M:22:ASP:HB2	1.70	0.72
1:L:159:ILE:HA	1:L:163:GLN:HE22	1.54	0.72
2:E:381:TYR:CE1	2:E:385:GLN:HG3	2.24	0.72
7:T:176:TRP:CE3	9:V:22:LYS:HD3	2.24	0.72
1:L:386:VAL:HG12	1:L:449:VAL:HG11	1.70	0.72
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.71	0.72
7:T:198:ILE:HD13	9:V:11:LEU:HD21	1.72	0.72
3:G:20:THR:CG2	3:G:236:SER:HB3	2.18	0.72
5:R:4:TRP:CZ3	5:R:5:ARG:HG2	2.25	0.72
2:D:183:PHE:C	2:D:183:PHE:HD2	1.92	0.72
7:X:170:GLN:HG2	7:X:173:MSE:HE2	1.70	0.72
2:M:367:HIS:HA	2:M:438:ILE:HD13	1.72	0.72
2:F:35:ALA:HB2	2:F:82:ILE:HG13	1.69	0.72
2:O:32:ILE:HA	2:O:49:VAL:CG1	2.18	0.72
3:G:134:ARG:HB2	5:I:41:THR:HG21	1.72	0.72
2:F:244:ARG:HG3	2:F:302:GLY:HA3	1.70	0.72
2:O:360:PRO:HB3	2:O:365:SER:HB3	1.70	0.72
2:M:96:ASN:HB3	2:M:102:ILE:HD11	1.70	0.72
2:M:275:ILE:HG23	3:P:269:ALA:HB2	1.72	0.72
1:J:407:GLY:O	1:J:410:LEU:HD11	1.90	0.72
6:S:39:LEU:HB3	6:S:102:ILE:HG23	1.71	0.72
2:O:282:GLN:H	2:O:282:GLN:HE21	1.37	0.72
1:C:309:ALA:HB1	1:C:321:LEU:O	1.90	0.72
1:L:110:ALA:HB3	1:L:242:LEU:CD2	2.19	0.72
2:M:328:HIS:O	2:M:329:LEU:HD23	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:HD13	1:A:496:LYS:NZ	2.05	0.72
1:K:336:ALA:HB3	1:K:339:PRO:HD2	1.72	0.72
7:T:132:ILE:HG13	8:U:88:GLN:HE22	1.54	0.72
1:C:159:ILE:HA	1:C:163:GLN:NE2	2.04	0.71
1:A:52:MET:HG3	1:A:95:VAL:HG22	1.72	0.71
6:S:74:ALA:HA	6:S:79:SER:HB3	1.71	0.71
1:A:225:ALA:HA	1:A:228:TYR:CE2	2.25	0.71
2:N:139:VAL:HG11	2:N:348:VAL:HB	1.72	0.71
2:E:390:ILE:HG12	3:G:25:MET:HG2	1.72	0.71
1:C:457:GLU:O	1:C:460:LYS:HE2	1.89	0.71
2:F:360:PRO:HB3	2:F:365:SER:HB3	1.71	0.71
2:M:9:THR:HG21	2:M:28:GLY:CA	2.20	0.71
1:C:159:ILE:HA	1:C:163:GLN:HE22	1.55	0.71
1:C:47:VAL:HG23	1:C:51:GLU:OE1	1.90	0.71
9:V:22:LYS:HZ2	9:V:30:VAL:HG22	1.55	0.71
1:J:468:PHE:CE1	1:J:501:VAL:HG23	2.25	0.71
2:M:13:ILE:HD13	2:M:69:LEU:HD13	1.72	0.71
6:W:51:MSE:HE1	6:W:69:LEU:HD21	1.73	0.71
1:C:247:PRO:HB3	1:C:268:TYR:HD2	1.55	0.71
1:A:23:VAL:C	1:A:25:LEU:H	1.93	0.71
2:M:266:SER:HA	2:M:282:GLN:HE22	1.55	0.71
1:K:99:VAL:HG13	1:K:100:GLY:N	2.06	0.71
1:C:62:MET:H	1:C:73:VAL:HG13	1.54	0.71
1:C:30:ARG:O	1:C:41:VAL:HG13	1.90	0.71
2:M:38:VAL:HG21	2:M:45:LEU:HD23	1.72	0.71
2:D:183:PHE:CD2	2:D:183:PHE:C	2.62	0.71
2:F:25:PHE:HB2	2:F:29:LEU:HD12	1.71	0.71
1:J:216:LEU:HD13	1:J:220:LEU:HD12	1.72	0.71
2:O:387:ILE:N	2:O:387:ILE:HD12	2.05	0.71
2:O:284:THR:O	2:O:288:ASP:HB2	1.90	0.71
5:R:13:ARG:O	5:R:17:ILE:HG12	1.90	0.71
3:G:125:LEU:HD12	3:G:126:VAL:HG22	1.73	0.71
6:W:68:SER:O	6:W:69:LEU:HD23	1.90	0.71
7:T:170:GLN:HG2	7:T:173:MSE:HE2	1.72	0.71
2:O:434:LEU:HD23	2:O:434:LEU:O	1.89	0.71
2:O:35:ALA:HB2	2:O:82:ILE:HG13	1.73	0.71
6:S:51:MSE:HE1	6:S:69:LEU:HD21	1.73	0.71
1:L:69:ASP:O	1:L:70:ASN:HB3	1.90	0.71
2:N:430:LYS:HD2	2:N:465:GLU:OE1	1.90	0.71
6:W:74:ALA:HA	6:W:79:SER:HB3	1.71	0.71
3:G:115:ILE:O	3:G:115:ILE:HG22	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:27:LYS:HE3	5:R:29:GLU:HB3	1.73	0.71
1:K:194:ASP:OD1	1:K:196:LYS:HE2	1.89	0.71
2:D:154:LEU:HD13	2:D:165:LEU:HD23	1.72	0.71
2:E:412:ARG:HH11	2:E:455:GLN:NE2	1.89	0.70
2:E:396:LEU:HB3	2:E:400:ASP:HB2	1.71	0.70
2:D:266:SER:HA	2:D:282:GLN:HE22	1.56	0.70
2:N:396:LEU:HB3	2:N:400:ASP:HB2	1.72	0.70
1:C:49:ALA:O	1:C:50:GLU:HB2	1.91	0.70
1:L:248:TYR:CE2	1:L:305:LEU:HB2	2.21	0.70
2:M:162:LYS:HB2	12:M:600:ADP:O1B	1.91	0.70
1:C:501:VAL:HG23	1:C:502:THR:N	2.01	0.70
2:O:456:ALA:HA	2:O:469:LYS:HD3	1.72	0.70
6:W:46:LEU:CD2	6:W:51:MSE:HE3	2.21	0.70
1:C:248:TYR:CD2	1:C:305:LEU:HD12	2.26	0.70
1:A:403:PHE:CE1	3:G:22:SER:HB2	2.25	0.70
1:K:469:LEU:O	1:K:473:ILE:HG13	1.91	0.70
1:L:265:LEU:HD12	1:L:322:THR:HB	1.73	0.70
2:M:186:VAL:HG21	2:M:233:ALA:HB2	1.72	0.70
3:G:44:TYR:CE2	4:H:23:PRO:HD3	2.27	0.70
1:L:247:PRO:HB3	1:L:268:TYR:HD2	1.57	0.70
2:O:319:ASP:O	2:O:322:PRO:HD2	1.91	0.70
2:D:39:GLN:HB2	2:D:74:LYS:HB2	1.73	0.70
1:A:209:LYS:HZ2	1:A:211:SER:HB2	1.56	0.70
2:D:38:VAL:HG21	2:D:45:LEU:HD23	1.72	0.70
2:N:63:MET:CE	2:N:228:ALA:HA	2.20	0.70
3:P:20:THR:HG22	3:P:236:SER:HB3	1.73	0.70
9:V:46:LYS:HA	9:V:49:GLN:HG3	1.72	0.70
1:A:47:VAL:O	2:E:70:VAL:HG13	1.91	0.70
1:L:183:ILE:HG23	1:L:201:CYS:SG	2.32	0.70
3:P:125:LEU:HD12	3:P:126:VAL:HG22	1.73	0.70
5:I:13:ARG:O	5:I:17:ILE:HG12	1.92	0.70
1:A:23:VAL:O	1:A:25:LEU:N	2.20	0.69
3:P:239:ALA:O	3:P:243:ILE:HG12	1.91	0.69
6:S:7:PRO:HB3	6:S:112:HIS:NE2	2.07	0.69
2:N:101:PRO:HG3	2:N:108:ILE:HG13	1.74	0.69
1:K:38:ILE:HG12	1:K:285:LEU:HD23	1.74	0.69
1:L:271:LEU:HB3	1:L:302:HIS:NE2	2.08	0.69
2:M:282:GLN:NE2	2:M:282:GLN:N	2.37	0.69
2:M:153:GLY:HA3	2:M:329:LEU:CD1	2.21	0.69
1:A:191:ASP:C	1:A:192:GLY:CA	2.61	0.69
1:L:136:ILE:HG23	2:M:194:ASN:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:468:PHE:CE1	1:K:501:VAL:HG23	2.27	0.69
1:C:248:TYR:CE2	1:C:305:LEU:HB2	2.22	0.69
3:P:20:THR:CG2	3:P:236:SER:HB3	2.23	0.69
1:L:67:GLU:HB3	1:L:68:PRO:HD2	1.74	0.69
1:J:496:LYS:O	1:J:500:ILE:HG13	1.92	0.69
2:D:91:LEU:HD13	2:D:213:SER:O	1.91	0.69
2:D:96:ASN:HB3	2:D:102:ILE:HD11	1.74	0.69
1:B:25:LEU:O	1:B:45:ARG:HG2	1.92	0.69
2:M:39:GLN:HB2	2:M:74:LYS:HB2	1.73	0.69
6:W:14:ILE:O	6:W:15:GLU:HB2	1.93	0.69
2:E:186:VAL:HG22	2:E:232:VAL:HG13	1.74	0.69
2:N:412:ARG:C	2:N:414:LEU:H	1.94	0.69
6:S:46:LEU:CD2	6:S:51:MSE:HE3	2.22	0.69
2:D:92:GLY:HA2	2:D:206:ILE:HG23	1.75	0.69
2:D:367:HIS:HA	2:D:438:ILE:HD13	1.72	0.69
2:F:137:ILE:HA	2:F:416:GLN:HE22	1.57	0.69
2:D:93:ARG:NH1	2:D:108:ILE:HD13	2.08	0.69
1:L:49:ALA:O	1:L:50:GLU:HB2	1.93	0.69
1:C:453:LEU:HA	1:C:456:LEU:HD13	1.75	0.69
1:B:399:GLU:H	1:B:399:GLU:CD	1.96	0.69
1:L:453:LEU:HA	1:L:456:LEU:HD13	1.75	0.69
1:J:114:ALA:HB2	1:J:121:ILE:HD11	1.75	0.69
3:G:139:GLY:O	3:G:143:VAL:HG23	1.93	0.69
3:P:271:ALA:O	3:P:272:LEU:HD23	1.92	0.69
1:B:127:ARG:HH21	1:B:131:LEU:HD21	1.56	0.69
3:P:115:ILE:HG22	3:P:115:ILE:O	1.92	0.69
2:E:63:MET:CE	2:E:228:ALA:HA	2.22	0.69
6:W:120:VAL:HG12	6:W:121:THR:HG23	1.73	0.69
1:C:265:LEU:HD12	1:C:322:THR:HB	1.75	0.69
2:D:96:ASN:C	2:D:96:ASN:ND2	2.40	0.68
1:J:199:LEU:HD21	1:J:265:LEU:HB2	1.75	0.68
1:L:358:TYR:HE2	2:O:375:GLN:NE2	1.90	0.68
1:J:423:ARG:HG2	1:J:461:ILE:HD11	1.73	0.68
2:F:12:ARG:CZ	2:F:12:ARG:HB2	2.22	0.68
6:W:22:LEU:CD1	6:W:85:LEU:HD13	2.15	0.68
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.75	0.68
1:C:183:ILE:HG23	1:C:201:CYS:SG	2.33	0.68
3:P:139:GLY:O	3:P:143:VAL:HG23	1.93	0.68
1:J:44:LEU:O	1:J:47:VAL:HG22	1.94	0.68
7:T:173:MSE:HG3	9:V:22:LYS:HG2	1.73	0.68
6:W:7:PRO:HB3	6:W:108:MSE:CE	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:7:PRO:HB2	6:S:108:MSE:SE	2.44	0.68
2:D:266:SER:HA	2:D:282:GLN:NE2	2.08	0.68
1:C:255:GLU:HG2	1:C:258:ARG:NH1	2.07	0.68
2:M:92:GLY:HA2	2:M:206:ILE:HG23	1.76	0.68
1:C:69:ASP:O	1:C:70:ASN:HB3	1.92	0.68
3:P:212:ILE:HG23	3:P:213:ILE:N	2.09	0.68
1:K:78:ASN:HD21	1:K:80:LYS:HE3	1.58	0.68
2:O:25:PHE:HD1	2:O:30:PRO:HD3	1.58	0.68
9:V:22:LYS:NZ	9:V:30:VAL:HG22	2.09	0.68
2:O:439:LYS:O	2:O:443:GLN:HG3	1.94	0.68
6:W:35:VAL:HA	6:W:38:GLU:HB2	1.75	0.68
1:A:114:ALA:HB2	1:A:121:ILE:HD11	1.75	0.68
2:M:91:LEU:HD13	2:M:213:SER:O	1.94	0.68
7:T:189:GLN:HA	7:T:192:GLU:CD	2.14	0.68
2:N:34:ASN:O	2:N:49:VAL:HG23	1.93	0.68
1:C:110:ALA:HB3	1:C:242:LEU:CD2	2.23	0.68
1:J:71:VAL:HG23	2:N:71:ARG:NH2	2.08	0.68
1:K:78:ASN:ND2	1:K:80:LYS:HE3	2.09	0.68
1:K:160:GLY:H	1:K:163:GLN:NE2	1.91	0.68
1:J:217:VAL:HB	1:J:226:MET:HE3	1.76	0.68
2:F:142:LEU:HD22	2:F:441:PHE:CD1	2.29	0.68
6:W:133:GLU:HA	6:W:136:THR:CG2	2.23	0.68
2:O:223:ASN:HD22	2:O:223:ASN:N	1.92	0.68
2:O:244:ARG:HG3	2:O:302:GLY:HA3	1.76	0.68
2:M:170:ILE:HG13	2:M:254:PHE:CE2	2.29	0.68
1:C:136:ILE:HD11	2:D:219:TYR:CD2	2.27	0.68
2:M:13:ILE:CD1	2:M:69:LEU:HD13	2.24	0.68
2:E:374:VAL:HG13	2:E:410:ILE:HG21	1.76	0.68
2:M:27:GLU:HA	6:W:3:LYS:HD2	1.76	0.68
5:I:27:LYS:HE3	5:I:29:GLU:HB3	1.74	0.68
2:O:25:PHE:HE1	2:O:30:PRO:CG	2.07	0.67
6:W:116:VAL:N	6:W:117:PRO:CD	2.56	0.67
1:J:151:LYS:H	1:J:430:GLN:HE22	0.83	0.67
1:B:166:LEU:HD22	1:B:342:VAL:HG12	1.75	0.67
3:G:181:LEU:O	3:G:184:ILE:HG22	1.95	0.67
2:F:96:ASN:C	2:F:96:ASN:ND2	2.45	0.67
2:F:387:ILE:N	2:F:387:ILE:HD12	2.08	0.67
1:K:48:GLN:HE21	2:O:68:GLY:HA2	1.59	0.67
3:P:181:LEU:O	3:P:184:ILE:HG22	1.94	0.67
1:B:194:ASP:OD1	1:B:196:LYS:HE2	1.94	0.67
3:P:10:LEU:HD23	3:P:246:LEU:HD13	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:240:ALA:HB3	1:L:241:PRO:HD3	1.77	0.67
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.77	0.67
1:K:399:GLU:CD	1:K:399:GLU:H	1.98	0.67
1:B:137:ILE:HB	1:B:138:PRO:HD3	1.76	0.67
2:F:210:ASP:HB2	2:F:212:THR:H	1.59	0.67
2:F:223:ASN:HD22	2:F:223:ASN:N	1.92	0.67
4:Q:36:VAL:HG12	4:Q:37:ASP:H	1.59	0.67
4:Q:15:GLN:N	4:Q:49:ALA:HB1	2.09	0.67
1:C:399:GLU:HG3	2:D:342:LEU:HD12	1.75	0.67
1:L:137:ILE:CD1	1:L:137:ILE:H	2.03	0.67
2:M:266:SER:HA	2:M:282:GLN:NE2	2.09	0.67
2:M:33:LEU:HD22	2:M:117:HIS:CG	2.29	0.67
1:B:38:ILE:HG12	1:B:285:LEU:HD23	1.76	0.67
6:S:22:LEU:CD1	6:S:85:LEU:HD13	2.19	0.67
1:L:248:TYR:CD2	1:L:305:LEU:HD12	2.29	0.67
6:S:89:LEU:HD13	6:S:98:THR:HG22	1.76	0.67
1:J:180:ILE:HD11	1:J:216:LEU:HD21	1.76	0.67
3:P:49:LEU:HD21	3:P:212:ILE:HD13	1.77	0.67
1:A:87:ILE:H	1:A:87:ILE:HD12	1.59	0.67
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.77	0.67
2:F:11:GLY:HA3	2:F:25:PHE:CD2	2.30	0.67
4:Q:21:ALA:CB	4:Q:26:VAL:HA	2.25	0.67
2:E:94:ILE:HG22	2:E:102:ILE:HG12	1.77	0.67
2:M:263:GLN:O	2:M:266:SER:HB3	1.95	0.66
6:S:35:VAL:HA	6:S:38:GLU:HB2	1.76	0.66
2:M:310:ILE:N	2:M:310:ILE:HD12	2.11	0.66
1:A:71:VAL:HG23	2:E:71:ARG:NH2	2.10	0.66
4:H:113:GLU:C	4:H:115:ALA:H	1.98	0.66
1:B:336:ALA:HB3	1:B:339:PRO:HD2	1.77	0.66
2:N:25:PHE:O	2:N:56:SER:HB3	1.95	0.66
3:P:117:HIS:O	3:P:121:SER:HB2	1.96	0.66
2:F:456:ALA:HA	2:F:469:LYS:HD3	1.77	0.66
2:F:32:ILE:HA	2:F:49:VAL:CG1	2.25	0.66
2:O:221:GLN:HA	2:O:221:GLN:HE21	1.59	0.66
1:B:160:GLY:H	1:B:163:GLN:NE2	1.93	0.66
2:N:132:ILE:HD13	2:N:145:PRO:HB3	1.77	0.66
2:F:284:THR:O	2:F:288:ASP:HB2	1.95	0.66
2:N:32:ILE:O	2:N:33:LEU:HB2	1.93	0.66
4:H:15:GLN:N	4:H:49:ALA:HB1	2.10	0.66
1:L:309:ALA:HB1	1:L:321:LEU:O	1.95	0.66
3:G:212:ILE:HG23	3:G:213:ILE:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:438:ILE:O	1:J:442:VAL:HG23	1.95	0.66
1:J:71:VAL:HG12	1:J:73:VAL:HG23	1.78	0.66
2:E:142:LEU:HD21	2:E:374:VAL:HG21	1.78	0.66
3:G:40:PRO:O	3:G:42:ARG:N	2.29	0.66
2:N:170:ILE:HG21	2:N:215:VAL:HG22	1.77	0.66
9:V:43:GLU:HG2	9:V:46:LYS:HE2	1.77	0.66
1:K:179:ALA:CB	1:K:267:ILE:HD13	2.22	0.66
2:E:32:ILE:O	2:E:33:LEU:HB2	1.94	0.66
2:M:151:LYS:HA	2:M:306:SER:OG	1.96	0.66
2:O:387:ILE:H	2:O:387:ILE:CD1	2.07	0.66
1:L:255:GLU:HG2	1:L:258:ARG:NH1	2.11	0.66
1:L:47:VAL:HG23	1:L:51:GLU:OE1	1.95	0.66
1:A:44:LEU:O	1:A:47:VAL:HG22	1.95	0.66
3:G:117:HIS:O	3:G:121:SER:HB2	1.96	0.66
4:H:36:VAL:HG12	4:H:37:ASP:H	1.61	0.66
1:C:501:VAL:CG2	1:C:502:THR:H	1.99	0.66
6:S:68:SER:O	6:S:69:LEU:HD23	1.96	0.66
1:L:339:PRO:O	1:L:343:ILE:HG13	1.96	0.66
2:M:41:ARG:HH11	2:M:69:LEU:HD23	1.61	0.66
1:K:453:LEU:HD13	1:K:461:ILE:HD12	1.77	0.66
7:T:154:ARG:CZ	9:V:60:PRO:HG3	2.26	0.66
1:L:167:ILE:HB	1:L:326:VAL:HG22	1.78	0.66
1:J:151:LYS:HE3	1:J:427:LEU:O	1.96	0.66
2:O:218:VAL:HG21	2:O:236:GLY:CA	2.26	0.66
2:F:319:ASP:O	2:F:322:PRO:HD2	1.94	0.66
1:C:339:PRO:O	1:C:343:ILE:HG13	1.96	0.66
2:O:32:ILE:O	2:O:33:LEU:CB	2.44	0.65
1:C:268:TYR:CE2	1:C:305:LEU:HD21	2.31	0.65
2:F:282:GLN:H	2:F:282:GLN:HE21	1.42	0.65
2:N:63:MET:HE3	2:N:228:ALA:HA	1.78	0.65
3:P:53:GLU:O	3:P:54:LYS:HG3	1.96	0.65
2:E:456:ALA:HA	2:E:469:LYS:HD3	1.77	0.65
1:C:74:VAL:HG11	1:C:281:MET:HE3	1.77	0.65
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.31	0.65
1:B:445:ILE:O	1:B:449:VAL:HG23	1.95	0.65
2:O:12:ARG:HB2	2:O:12:ARG:NH1	2.10	0.65
1:L:30:ARG:O	1:L:41:VAL:HG13	1.96	0.65
6:W:89:LEU:HD13	6:W:98:THR:HG22	1.76	0.65
2:N:266:SER:HB2	2:N:282:GLN:HE22	1.62	0.65
6:S:173:MSE:HG2	7:T:174:ILE:HB	1.78	0.65
3:P:161:ILE:HG22	3:P:174:GLU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:CD1	1:B:143:ARG:HH21	2.09	0.65
1:L:144:GLU:HG3	1:L:311:LYS:HE2	1.79	0.65
2:D:13:ILE:CD1	2:D:69:LEU:HD13	2.25	0.65
1:J:87:ILE:H	1:J:87:ILE:HD12	1.62	0.65
4:H:21:ALA:CB	4:H:26:VAL:HA	2.27	0.65
9:V:45:PHE:O	9:V:49:GLN:HG2	1.96	0.65
1:A:151:LYS:HE3	1:A:427:LEU:O	1.97	0.65
2:M:96:ASN:HD21	2:M:98:ILE:H	1.43	0.65
2:F:393:MET:O	2:F:396:LEU:HB2	1.97	0.65
1:C:389:THR:HG22	2:D:425:THR:O	1.96	0.65
2:N:87:GLY:HA2	2:N:242:TYR:CE2	2.32	0.65
2:O:49:VAL:HA	2:O:60:THR:HG22	1.79	0.65
1:L:396:GLN:O	1:L:400:VAL:HG23	1.97	0.65
1:A:9:SER:N	1:A:12:LEU:HB2	2.11	0.65
1:J:267:ILE:HD13	1:J:324:LEU:HB2	1.78	0.65
7:T:143:ARG:HG2	7:T:146:ARG:CZ	2.26	0.65
2:E:168:GLU:HG2	2:E:418:PHE:CD2	2.31	0.65
1:B:113:ASN:H	1:B:113:ASN:HD22	1.45	0.65
1:L:99:VAL:HG12	1:L:100:GLY:N	2.11	0.65
2:N:142:LEU:HD22	2:N:441:PHE:CD1	2.31	0.65
1:J:339:PRO:O	1:J:343:ILE:HG13	1.97	0.65
3:G:105:ILE:HB	3:G:124:PHE:HA	1.78	0.65
4:H:51:HIS:CE1	4:H:52:VAL:HG22	2.31	0.65
2:F:32:ILE:O	2:F:33:LEU:CB	2.44	0.65
2:E:12:ARG:HH11	2:E:72:GLY:HA2	1.62	0.65
3:G:49:LEU:HD21	3:G:212:ILE:HD13	1.79	0.65
4:H:48:LEU:HB2	4:H:51:HIS:HD2	1.61	0.65
2:O:112:GLN:H	2:O:112:GLN:NE2	1.89	0.65
2:O:96:ASN:ND2	2:O:96:ASN:C	2.50	0.65
3:G:53:GLU:O	3:G:54:LYS:HG3	1.96	0.65
2:O:210:ASP:HB2	2:O:212:THR:H	1.63	0.64
4:Q:48:LEU:HB2	4:Q:51:HIS:HD2	1.61	0.64
4:Q:51:HIS:CE1	4:Q:52:VAL:HG22	2.32	0.64
1:L:461:ILE:O	1:L:461:ILE:HG22	1.97	0.64
3:P:76:GLY:O	3:P:228:ARG:NH1	2.30	0.64
1:C:461:ILE:HG22	1:C:461:ILE:O	1.97	0.64
2:N:186:VAL:HG22	2:N:232:VAL:HG13	1.79	0.64
6:W:104:ALA:O	6:W:108:MSE:HB2	1.97	0.64
2:D:92:GLY:HA2	2:D:206:ILE:CD1	2.27	0.64
1:A:403:PHE:CZ	3:G:25:MET:HE1	2.32	0.64
9:V:5:LEU:HD23	9:V:9:GLN:HE21	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:181:SER:HB2	2:O:215:VAL:HG22	1.79	0.64
2:F:227:GLY:O	2:F:230:ALA:HB3	1.97	0.64
2:F:274:ARG:HB3	2:F:283:PRO:HG2	1.80	0.64
7:T:147:VAL:HA	9:V:62:PHE:HZ	1.63	0.64
1:A:266:ILE:HG22	1:A:321:LEU:HD11	1.77	0.64
1:C:206:ILE:H	1:C:206:ILE:HD12	1.62	0.64
1:B:78:ASN:HD21	1:B:80:LYS:CE	2.10	0.64
7:X:170:GLN:O	7:X:174:ILE:HG12	1.98	0.64
2:F:82:ILE:HB	2:F:116:ILE:HD11	1.77	0.64
3:P:26:VAL:HG12	3:P:27:ALA:N	2.12	0.64
1:J:355:GLU:H	1:J:355:GLU:CD	2.01	0.64
1:A:438:ILE:O	1:A:442:VAL:HG23	1.98	0.64
10:F:600:ANP:C5'	10:F:600:ANP:H8	2.26	0.64
1:B:392:LEU:CD1	1:B:396:GLN:HE21	2.11	0.64
2:M:13:ILE:O	2:M:72:GLY:N	2.31	0.64
2:F:172:ASN:ND2	2:F:431:LEU:HD12	2.12	0.64
2:N:381:TYR:O	2:N:381:TYR:HD1	1.81	0.64
1:K:137:ILE:HB	1:K:138:PRO:HD3	1.79	0.64
1:C:397:TYR:HB2	1:C:417:LEU:HG	1.80	0.64
3:G:164:ARG:HH22	3:G:166:ARG:NH1	1.96	0.64
1:A:217:VAL:HB	1:A:226:MET:CE	2.27	0.64
4:Q:113:GLU:C	4:Q:115:ALA:H	2.00	0.64
2:M:93:ARG:NH1	2:M:108:ILE:HD13	2.13	0.64
2:F:88:PRO:O	2:F:91:LEU:HD12	1.97	0.64
2:F:157:GLY:O	2:F:160[B]:VAL:HG23	1.97	0.64
1:C:240:ALA:HB3	1:C:241:PRO:HD3	1.80	0.64
1:B:48:GLN:NE2	2:F:68:GLY:HA2	2.13	0.64
2:O:274:ARG:HB3	2:O:283:PRO:HG2	1.77	0.64
2:O:404:VAL:O	2:O:408:ARG:HG3	1.97	0.64
2:E:94:ILE:HG22	2:E:102:ILE:CG1	2.28	0.64
2:D:258:ILE:HD11	2:D:292:MET:CE	2.28	0.64
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.12	0.64
1:B:399:GLU:C	1:B:401:ALA:H	2.01	0.64
3:P:212:ILE:CG2	3:P:213:ILE:H	2.10	0.64
2:N:447:GLY:HA2	2:N:450:ASP:OD1	1.98	0.64
6:W:119:THR:HG23	6:W:125:ALA:HB2	1.78	0.64
1:K:34:ILE:HG21	1:K:82:ILE:O	1.97	0.64
1:C:48:GLN:HA	2:D:70:VAL:HG22	1.80	0.63
1:A:476:HIS:HD2	1:A:496:LYS:HE2	1.63	0.63
2:E:431:LEU:C	2:E:431:LEU:HD12	2.18	0.63
1:L:147:GLN:OE1	1:L:438:ILE:HD13	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:ARG:HA	1:K:86:ASP:O	1.97	0.63
2:M:142:LEU:HD22	2:M:441:PHE:CD1	2.34	0.63
1:J:164:ARG:HD3	1:J:164:ARG:N	2.13	0.63
2:E:381:TYR:HD1	2:E:381:TYR:O	1.79	0.63
7:T:154:ARG:NE	9:V:60:PRO:HG3	2.13	0.63
1:C:396:GLN:O	1:C:400:VAL:HG23	1.98	0.63
2:E:253:LEU:HB3	2:E:306:SER:HB2	1.81	0.63
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.33	0.63
6:W:14:ILE:N	6:W:14:ILE:HD12	2.12	0.63
1:A:355:GLU:CD	1:A:355:GLU:H	2.02	0.63
2:O:88:PRO:O	2:O:91:LEU:HD12	1.99	0.63
4:Q:67:ALA:HB3	4:Q:71:THR:H	1.63	0.63
1:C:271:LEU:HB3	1:C:302:HIS:NE2	2.13	0.63
3:P:138:PHE:CD1	4:Q:23:PRO:HG2	2.26	0.63
2:N:381:TYR:C	2:N:381:TYR:HD1	2.01	0.63
1:A:407:GLY:O	1:A:410:LEU:HD11	1.97	0.63
1:A:209:LYS:NZ	1:A:211:SER:HB2	2.13	0.63
1:L:74:VAL:HG11	1:L:281:MET:HE3	1.80	0.63
6:W:125:ALA:O	6:W:127:ASP:OD1	2.17	0.63
2:F:348:VAL:O	2:F:350:PRO:HD3	1.99	0.63
2:M:430:LYS:HE2	2:M:465:GLU:OE1	1.98	0.63
2:N:9:THR:HB	2:N:27:GLU:HG3	1.80	0.63
2:E:138:LYS:HG2	2:E:437:THR:CG2	2.25	0.63
2:D:263:GLN:O	2:D:266:SER:HB3	1.99	0.63
1:L:62:MET:H	1:L:73:VAL:CG1	2.12	0.63
2:F:139:VAL:HG12	2:F:414:LEU:HD22	1.81	0.63
2:F:377:ILE:HG21	2:F:410:ILE:HD12	1.81	0.63
6:W:23:TYR:CE2	6:W:108:MSE:SE	3.01	0.63
1:L:300:TYR:CZ	1:L:304:ARG:HD2	2.34	0.63
7:T:176:TRP:CZ3	9:V:22:LYS:HB2	2.33	0.63
2:D:258:ILE:HD11	2:D:292:MET:HE3	1.80	0.63
2:F:181:SER:HB2	2:F:215:VAL:HG22	1.81	0.63
3:P:212:ILE:CG2	3:P:213:ILE:N	2.61	0.63
2:F:128:VAL:O	2:F:128:VAL:HG23	1.98	0.63
1:J:240:ALA:HB3	1:J:241:PRO:HD3	1.79	0.63
2:M:258:ILE:HD11	2:M:292:MET:HE3	1.81	0.63
2:N:372:ARG:HH11	2:N:375:GLN:HE22	1.47	0.63
1:L:179:ALA:HB1	1:L:267:ILE:CD1	2.16	0.63
1:C:137:ILE:CD1	1:C:137:ILE:H	1.95	0.63
1:L:206:ILE:HD12	1:L:206:ILE:N	2.13	0.63
6:S:106:SER:O	6:S:109:MSE:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:218:VAL:HG21	2:F:236:GLY:CA	2.29	0.63
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.29	0.63
1:J:451:GLY:O	1:J:453:LEU:N	2.31	0.63
6:W:139:LYS:HG2	6:W:142:LEU:HD12	1.80	0.63
2:E:434:LEU:CG	2:E:438:ILE:HD11	2.26	0.63
1:K:225:ALA:HA	1:K:228:TYR:CE2	2.33	0.63
2:O:223:ASN:H	2:O:223:ASN:ND2	1.96	0.63
2:O:266:SER:HB2	2:O:282:GLN:HE22	1.63	0.63
7:T:127:VAL:HG13	8:U:34:ASN:HD22	1.63	0.63
3:P:105:ILE:HB	3:P:124:PHE:HA	1.79	0.63
1:C:376:SER:C	1:C:378:ALA:H	2.01	0.63
2:N:440:GLY:O	2:N:444:ILE:HG13	1.98	0.63
1:C:424:LEU:O	1:C:427:LEU:HB2	1.98	0.63
2:D:26:ASP:HA	6:S:6:ARG:HH12	1.64	0.63
1:C:358:TYR:HE2	2:F:375:GLN:NE2	1.97	0.63
2:O:287:THR:O	2:O:291:THR:HG23	1.98	0.62
2:N:428:LEU:HD21	2:N:430:LYS:HE3	1.79	0.62
1:L:75:VAL:HG12	1:L:77:GLY:H	1.64	0.62
1:C:479:LEU:O	1:C:483:ILE:HG13	1.99	0.62
3:G:13:ILE:HG22	3:G:243:ILE:HD11	1.80	0.62
1:C:307:GLU:HG3	2:D:223:ASN:HB3	1.80	0.62
2:M:82:ILE:HD13	2:M:98:ILE:HG22	1.81	0.62
1:K:127:ARG:HH21	1:K:131:LEU:HD21	1.62	0.62
2:D:146:TYR:CG	2:D:152:ILE:HD13	2.35	0.62
1:A:62:MET:HB2	1:A:76:PHE:HE1	1.64	0.62
1:L:397:TYR:HB2	1:L:417:LEU:HG	1.79	0.62
2:F:272:LEU:HD12	2:F:274:ARG:HE	1.65	0.62
3:G:138:PHE:CD1	4:H:23:PRO:HG3	2.34	0.62
2:F:49:VAL:HA	2:F:60:THR:HG22	1.81	0.62
2:D:33:LEU:HD22	2:D:117:HIS:CG	2.34	0.62
1:J:367:VAL:HG12	1:J:367:VAL:O	1.98	0.62
2:M:16:VAL:O	2:M:16:VAL:HG12	1.99	0.62
1:J:209:LYS:NZ	1:J:211:SER:HB2	2.15	0.62
1:C:180:ILE:HG12	1:C:216:LEU:HD21	1.82	0.62
1:K:166:LEU:HD22	1:K:342:VAL:HG12	1.80	0.62
1:K:140:ILE:CD1	1:K:143:ARG:HH21	2.12	0.62
9:V:16:ILE:HA	9:V:19:TYR:HB3	1.80	0.62
3:G:193:TYR:HA	4:H:53:PRO:HB2	1.81	0.62
3:G:158:GLY:HA3	3:G:178:ILE:O	2.00	0.62
1:C:99:VAL:HG12	1:C:100:GLY:N	2.13	0.62
2:O:168:GLU:OE1	2:O:420:VAL:HB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:600:ANP:O5'	10:F:600:ANP:H8	1.99	0.62
2:N:381:TYR:C	2:N:381:TYR:CD1	2.72	0.62
1:K:127:ARG:HH21	1:K:131:LEU:HD22	1.61	0.62
2:F:223:ASN:ND2	2:F:223:ASN:H	1.97	0.62
1:K:148:THR:HG21	1:K:153:VAL:HG11	1.80	0.62
1:L:161:ARG:HA	1:L:322:THR:OG1	1.99	0.62
1:J:217:VAL:HB	1:J:226:MET:CE	2.29	0.62
3:G:212:ILE:CG2	3:G:213:ILE:N	2.63	0.62
3:G:161:ILE:HG22	3:G:174:GLU:O	1.99	0.62
3:P:164:ARG:HH22	3:P:166:ARG:NH1	1.98	0.62
6:W:109:MSE:HE3	6:W:112:HIS:HB2	1.81	0.62
2:F:159:GLY:N	10:F:600:ANP:HNB1	1.89	0.62
6:S:65:LYS:O	6:S:69:LEU:HG	2.00	0.62
4:Q:35:GLN:HG2	4:Q:36:VAL:N	2.15	0.62
7:X:162:GLN:HE21	7:X:166:ARG:HH21	1.47	0.62
1:L:376:SER:C	1:L:378:ALA:H	2.01	0.62
7:T:162:GLN:HE21	7:T:166:ARG:HH21	1.46	0.62
1:J:505:LEU:O	1:J:505:LEU:HG	1.99	0.62
2:N:412:ARG:NH1	2:N:455:GLN:NE2	2.41	0.62
2:F:112:GLN:H	2:F:112:GLN:NE2	1.91	0.62
3:G:10:LEU:HD23	3:G:246:LEU:HD13	1.81	0.62
7:X:177:VAL:O	7:X:181:VAL:HG23	1.99	0.62
2:M:258:ILE:HD11	2:M:292:MET:CE	2.29	0.62
6:W:65:LYS:O	6:W:69:LEU:HG	1.98	0.62
1:L:479:LEU:HD21	1:L:493:SER:HB3	1.82	0.62
2:D:153:GLY:HA3	2:D:329:LEU:HD13	1.82	0.62
2:D:153:GLY:HA3	2:D:329:LEU:CD1	2.30	0.62
1:C:95:VAL:O	1:C:129:VAL:HG22	2.00	0.62
2:D:16:VAL:HG22	2:D:21:VAL:HG13	1.82	0.62
2:M:139:VAL:HG21	2:M:348:VAL:HB	1.81	0.62
2:M:440:GLY:O	2:M:444:ILE:HG13	2.00	0.62
2:N:412:ARG:HD3	2:N:455:GLN:HE21	1.65	0.61
1:K:468:PHE:CZ	1:K:501:VAL:HG23	2.34	0.61
1:J:62:MET:HB2	1:J:76:PHE:HE1	1.65	0.61
2:N:359:ASP:OD2	2:N:360:PRO:HD2	1.99	0.61
1:L:218:LYS:HE2	1:L:222:ASP:OD1	1.99	0.61
1:C:496:LYS:O	1:C:500:ILE:HG13	2.00	0.61
1:K:399:GLU:C	1:K:401:ALA:H	2.01	0.61
2:F:396:LEU:HD22	2:F:400:ASP:HB3	1.80	0.61
3:P:40:PRO:O	3:P:42:ARG:N	2.32	0.61
2:D:388:ILE:HG22	2:D:396:LEU:HD21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:GLY:O	1:A:453:LEU:N	2.33	0.61
1:J:141:SER:O	1:J:143:ARG:HG3	2.00	0.61
2:D:116:ILE:HA	2:D:238:THR:OG1	2.00	0.61
3:P:158:GLY:HA3	3:P:178:ILE:O	2.00	0.61
2:F:169:LEU:O	2:F:173:VAL:HB	2.00	0.61
2:O:437:THR:O	2:O:441:PHE:HD1	1.83	0.61
6:S:115:GLU:OE1	6:S:132:THR:HG22	2.00	0.61
2:E:34:ASN:O	2:E:49:VAL:HG23	1.99	0.61
1:L:361:ILE:HG22	1:L:361:ILE:O	2.00	0.61
1:K:188:ARG:HG3	1:K:189:PHE:CD1	2.35	0.61
2:D:141:ASP:O	2:D:145:PRO:HG3	1.99	0.61
2:F:33:LEU:HD22	2:F:117:HIS:CD2	2.35	0.61
1:L:479:LEU:O	1:L:483:ILE:HG13	2.00	0.61
1:J:209:LYS:HZ2	1:J:211:SER:HB2	1.66	0.61
1:A:166:LEU:HD11	1:A:327:ILE:HG12	1.82	0.61
6:S:179:ILE:O	6:S:183:SER:HB2	2.00	0.61
2:M:31:PRO:O	2:M:34:ASN:HB2	2.00	0.61
1:C:160:GLY:N	1:C:163:GLN:NE2	2.46	0.61
2:M:193:GLY:HA3	2:M:219:TYR:HE2	1.64	0.61
7:T:201:LEU:HD13	9:V:7:PRO:HB3	1.82	0.61
1:C:161:ARG:HA	1:C:322:THR:OG1	2.00	0.61
1:J:56:SER:OG	1:J:86:ASP:HB3	2.00	0.61
1:A:367:VAL:O	1:A:367:VAL:HG12	2.01	0.61
2:M:33:LEU:HD22	2:M:117:HIS:CD2	2.35	0.61
1:A:164:ARG:HD3	1:A:164:ARG:N	2.15	0.61
7:T:153:ASN:HD21	9:V:51:TYR:HD2	1.47	0.61
2:E:359:ASP:OD2	2:E:360:PRO:HD2	2.01	0.61
4:H:27:PHE:HE2	4:H:97:ALA:HB3	1.66	0.61
2:O:169:LEU:O	2:O:173:VAL:HB	2.00	0.61
1:B:374:VAL:HG23	1:B:375:GLY:H	1.65	0.61
2:E:132:ILE:HD13	2:E:145:PRO:HB3	1.81	0.61
2:O:272:LEU:HD12	2:O:274:ARG:HE	1.64	0.61
1:A:23:VAL:HG13	1:A:27:GLU:H	1.66	0.61
2:N:321:ALA:HB3	2:N:322:PRO:HD3	1.82	0.61
2:E:381:TYR:CD1	2:E:381:TYR:C	2.74	0.61
1:J:52:MET:HG3	1:J:95:VAL:HG22	1.82	0.61
1:K:439:GLU:O	1:K:442:VAL:HG12	2.01	0.61
6:W:7:PRO:CB	6:W:108:MSE:SE	2.99	0.61
1:J:206:ILE:CD1	1:J:247:PRO:HG3	2.25	0.61
7:T:181:VAL:HG21	9:V:15:LYS:HZ3	1.65	0.61
2:N:417:PRO:HG2	2:N:430:LYS:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:26:VAL:HG12	3:G:27:ALA:N	2.16	0.61
2:M:53:LEU:HD21	2:M:59:ARG:HB2	1.83	0.61
2:F:46:VAL:HG21	2:F:98:ILE:HG21	1.81	0.61
2:O:25:PHE:HE1	2:O:30:PRO:HG2	1.66	0.61
1:L:160:GLY:N	1:L:163:GLN:NE2	2.49	0.61
1:B:166:LEU:HB2	1:B:346:THR:HG21	1.83	0.61
2:N:342:LEU:N	2:N:342:LEU:HD23	2.16	0.61
1:L:390:MET:O	1:L:390:MET:HG3	2.00	0.61
4:H:67:ALA:HB3	4:H:71:THR:H	1.64	0.61
1:J:246:ALA:HB3	1:J:247:PRO:HD3	1.83	0.60
1:A:410:LEU:HD12	1:A:410:LEU:N	2.15	0.60
1:C:307:GLU:OE2	2:D:190:THR:HB	2.01	0.60
4:Q:27:PHE:HE2	4:Q:97:ALA:HB3	1.66	0.60
2:E:39:GLN:HE21	2:E:76:LEU:CB	2.14	0.60
2:O:275:ILE:O	2:O:283:PRO:HG3	2.00	0.60
2:E:458:TYR:CD1	2:E:459:MET:HG2	2.36	0.60
2:M:221:GLN:HA	2:M:221:GLN:NE2	2.15	0.60
1:L:173:THR:HB	1:L:352:LEU:HB3	1.83	0.60
1:A:216:LEU:HD13	1:A:220:LEU:HD12	1.82	0.60
1:L:45:ARG:HH11	2:M:71:ARG:NH1	1.99	0.60
2:E:436:GLU:OE2	2:E:462:PRO:HB3	2.01	0.60
2:D:41:ARG:HH11	2:D:69:LEU:HD23	1.64	0.60
3:P:39:LYS:HB3	3:P:40:PRO:HD3	1.83	0.60
2:F:452:LEU:HD11	2:F:467:VAL:HG13	1.82	0.60
1:L:278:TYR:CE2	1:L:295:PRO:HG2	2.35	0.60
3:P:138:PHE:CD1	4:Q:23:PRO:CG	2.81	0.60
2:F:139:VAL:CG1	2:F:414:LEU:HD22	2.31	0.60
2:M:359:ASP:OD1	2:M:360:PRO:HD2	2.01	0.60
2:E:336:SER:HB3	2:E:339:ILE:H	1.67	0.60
2:N:39:GLN:HE21	2:N:76:LEU:CB	2.13	0.60
9:V:29:PRO:HG2	9:V:36:TYR:CE2	2.35	0.60
1:J:26:GLU:HG2	1:J:46:ASN:HD22	1.67	0.60
3:P:10:LEU:HD21	3:P:246:LEU:HB3	1.84	0.60
3:P:108:VAL:HG23	3:P:128:PHE:HB2	1.84	0.60
1:K:172:GLN:HA	10:K:600:ANP:N3B	2.15	0.60
1:K:180:ILE:CG1	1:K:216:LEU:HD21	2.31	0.60
1:C:52:MET:HG3	1:C:61:GLY:O	2.00	0.60
1:B:179:ALA:CB	1:B:267:ILE:HD13	2.23	0.60
2:D:282:GLN:NE2	2:D:282:GLN:N	2.43	0.60
3:G:39:LYS:HB3	3:G:40:PRO:HD3	1.83	0.60
1:B:381:ARG:O	1:B:381:ARG:HD3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:88:LEU:HD13	6:W:92:ASN:ND2	2.16	0.60
1:J:479:LEU:HD13	1:J:496:LYS:CD	2.31	0.60
4:H:35:GLN:HG2	4:H:36:VAL:N	2.16	0.60
2:N:142:LEU:HD21	2:N:374:VAL:HG21	1.82	0.60
1:C:218:LYS:HE2	1:C:222:ASP:OD1	2.01	0.60
2:M:141:ASP:O	2:M:145:PRO:HG3	2.01	0.60
2:E:409:LYS:HG2	2:E:457:PHE:HD1	1.66	0.60
1:A:341:ASN:O	1:A:345:ILE:HG13	2.01	0.60
6:W:8:PRO:HD3	6:W:112:HIS:NE2	2.17	0.60
2:D:104:GLU:O	2:D:105:ARG:HG3	2.02	0.60
1:B:83:LYS:HB2	1:B:83:LYS:HZ3	1.66	0.60
3:G:54:LYS:HD2	4:H:85:ASN:ND2	2.17	0.60
1:L:143:ARG:O	1:L:145:PRO:HD3	2.02	0.60
4:H:119:LEU:HD11	4:H:128:ARG:HH21	1.66	0.60
1:A:48:GLN:HB3	2:E:68:GLY:HA2	1.83	0.60
1:A:16:ILE:HD13	6:S:22:LEU:CD2	2.20	0.60
3:G:212:ILE:CG2	3:G:213:ILE:H	2.14	0.60
1:L:272:SER:O	1:L:276:VAL:HG23	2.02	0.60
1:B:453:LEU:HD13	1:B:461:ILE:HD12	1.83	0.60
2:E:101:PRO:HG3	2:E:108:ILE:HG13	1.84	0.60
9:Z:22:LYS:C	9:Z:22:LYS:HD2	2.22	0.60
6:W:4:LEU:HD21	6:W:28:LYS:NZ	2.17	0.60
1:J:300:TYR:HE1	2:N:223:ASN:O	1.84	0.60
1:C:365:ILE:HD12	1:C:366:ASN:N	2.17	0.60
2:O:396:LEU:HD22	2:O:400:ASP:HB3	1.83	0.60
1:C:90:ARG:HH21	1:C:92:GLY:HA2	1.66	0.60
2:O:266:SER:HA	2:O:282:GLN:NE2	2.16	0.59
1:A:71:VAL:HG12	1:A:73:VAL:HG23	1.83	0.59
2:F:89:GLU:HG3	2:F:109:LYS:O	2.02	0.59
2:N:94:ILE:HG22	2:N:102:ILE:HG12	1.84	0.59
4:Q:119:LEU:HD11	4:Q:128:ARG:HH21	1.67	0.59
4:Q:132:GLN:O	4:Q:135:ILE:HB	2.02	0.59
6:S:22:LEU:HD23	6:S:25:ALA:HB3	1.84	0.59
1:A:8:VAL:HA	1:A:12:LEU:HD12	1.84	0.59
2:F:457:PHE:CD1	2:F:457:PHE:N	2.71	0.59
2:F:266:SER:HA	2:F:282:GLN:NE2	2.17	0.59
9:Z:19:TYR:CG	9:Z:19:TYR:O	2.56	0.59
2:E:422:GLU:C	2:E:424:PHE:H	2.06	0.59
2:F:421:ALA:C	2:F:423:VAL:H	2.04	0.59
1:J:99:VAL:CG1	1:J:256:TYR:HB2	2.33	0.59
2:N:336:SER:HB3	2:N:339:ILE:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:268:TYR:CZ	1:L:305:LEU:HD21	2.37	0.59
2:O:11:GLY:HA3	2:O:25:PHE:HD2	1.67	0.59
2:D:397:SER:O	2:D:401:LYS:HG2	2.03	0.59
1:C:208:GLN:O	1:C:235:THR:HB	2.03	0.59
1:B:200:TYR:CD2	1:B:257:PHE:HE2	2.20	0.59
7:T:177:VAL:O	7:T:181:VAL:HG23	2.03	0.59
2:F:266:SER:HB2	2:F:282:GLN:HE22	1.67	0.59
1:J:140:ILE:HD12	1:J:141:SER:H	1.67	0.59
2:O:393:MET:O	2:O:396:LEU:HB2	2.02	0.59
2:N:94:ILE:HG22	2:N:102:ILE:CG1	2.32	0.59
2:N:346:PRO:HG3	2:N:418:PHE:CZ	2.38	0.59
2:M:413:PHE:HB2	2:M:457:PHE:HB3	1.83	0.59
2:M:388:ILE:HG22	2:M:396:LEU:HD21	1.83	0.59
2:O:137:ILE:HA	2:O:416:GLN:NE2	2.08	0.59
1:L:496:LYS:O	1:L:500:ILE:HG13	2.02	0.59
2:O:291:THR:OG1	2:O:292:MET:N	2.36	0.59
2:O:29:LEU:HD23	2:O:52:HIS:ND1	2.16	0.59
2:E:279:VAL:HG13	2:E:279:VAL:O	2.02	0.59
1:K:200:TYR:CD2	1:K:257:PHE:HE2	2.20	0.59
1:C:173:THR:HB	1:C:352:LEU:HB3	1.85	0.59
2:O:266:SER:CA	2:O:282:GLN:NE2	2.65	0.59
1:L:376:SER:O	1:L:378:ALA:N	2.36	0.59
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.03	0.59
1:B:30:ARG:HA	1:B:86:ASP:O	2.02	0.59
2:O:264:ALA:HA	2:O:267:GLU:HG3	1.84	0.59
1:J:183:ILE:O	1:J:186:GLN:HB2	2.02	0.59
1:C:44:LEU:O	1:C:47:VAL:HG12	2.02	0.59
2:E:381:TYR:HD1	2:E:381:TYR:C	2.05	0.59
1:A:423:ARG:HG2	1:A:461:ILE:CD1	2.31	0.59
2:O:82:ILE:HB	2:O:116:ILE:HD11	1.84	0.59
1:L:144:GLU:O	1:L:161:ARG:HG3	2.02	0.59
1:K:399:GLU:C	1:K:401:ALA:N	2.56	0.59
3:P:171:TYR:O	3:P:172:LYS:CB	2.50	0.59
3:P:81:ILE:HD11	3:P:223:SER:O	2.02	0.59
2:O:128:VAL:O	2:O:128:VAL:HG23	2.03	0.59
2:M:116:ILE:HA	2:M:238:THR:OG1	2.02	0.59
2:N:469:LYS:O	2:N:473:LEU:HG	2.02	0.59
2:E:412:ARG:HH11	2:E:455:GLN:HE22	1.51	0.59
2:E:63:MET:HE1	2:E:228:ALA:HA	1.83	0.59
1:L:501:VAL:HG23	1:L:502:THR:N	2.17	0.59
6:S:144:LYS:O	6:S:146:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:282:SER:CB	1:K:295:PRO:HG3	2.33	0.59
6:S:18:TYR:O	6:S:21:ALA:HB3	2.03	0.59
6:W:106:SER:O	6:W:108:MSE:N	2.36	0.59
6:W:46:LEU:HD23	6:W:51:MSE:HE3	1.85	0.59
1:B:99:VAL:HG13	1:B:100:GLY:N	2.16	0.59
1:B:28:THR:O	1:B:44:LEU:N	2.24	0.59
4:H:48:LEU:HB2	4:H:51:HIS:CD2	2.38	0.59
3:G:76:GLY:O	3:G:228:ARG:NH1	2.36	0.59
2:O:89:GLU:HG3	2:O:110:THR:HA	1.85	0.59
1:A:23:VAL:HG12	1:A:23:VAL:O	2.03	0.59
3:P:203:ASN:OD1	5:R:11:TYR:HB2	2.03	0.59
1:K:83:LYS:HZ3	1:K:83:LYS:HB2	1.66	0.59
2:E:170:ILE:HG21	2:E:215:VAL:CG2	2.32	0.59
1:B:410:LEU:N	1:B:410:LEU:HD12	2.18	0.59
7:T:165:MSE:HA	7:T:165:MSE:HE3	1.84	0.59
2:E:467:VAL:HG12	2:E:468:ALA:N	2.18	0.59
3:P:130:GLU:HB3	5:R:41:THR:O	2.03	0.59
3:G:155:PHE:HB3	3:G:180:SER:OG	2.03	0.59
6:W:35:VAL:HG22	6:W:82:THR:HG21	1.85	0.58
1:K:241:PRO:HA	1:K:244:TYR:HB3	1.84	0.58
4:Q:57:VAL:HG11	5:R:11:TYR:CE1	2.37	0.58
2:E:372:ARG:HH11	2:E:375:GLN:HE22	1.50	0.58
2:E:223:ASN:HD22	2:E:223:ASN:N	1.95	0.58
1:B:101:GLU:O	1:B:104:LEU:HD12	2.04	0.58
2:D:146:TYR:HB3	2:D:152:ILE:CD1	2.33	0.58
7:T:170:GLN:O	7:T:174:ILE:HG12	2.02	0.58
1:J:209:LYS:HD3	2:M:328:HIS:HA	1.85	0.58
1:J:498:LYS:O	1:J:502:THR:HG23	2.02	0.58
1:B:399:GLU:C	1:B:401:ALA:N	2.56	0.58
1:C:145:PRO:HB3	1:C:147:GLN:NE2	2.18	0.58
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.85	0.58
3:P:155:PHE:HB3	3:P:180:SER:OG	2.03	0.58
9:V:46:LYS:HA	9:V:49:GLN:CG	2.33	0.58
1:J:403:PHE:N	1:J:403:PHE:CD1	2.69	0.58
7:T:143:ARG:HA	7:T:146:ARG:HG3	1.85	0.58
2:F:244:ARG:CG	2:F:302:GLY:HA3	2.33	0.58
5:I:31:LYS:HE3	5:I:35:MET:HG2	1.85	0.58
1:K:362:ARG:HA	1:K:363:PRO:C	2.23	0.58
2:D:53:LEU:HD21	2:D:59:ARG:HB2	1.86	0.58
1:A:49:ALA:O	1:A:50:GLU:HB2	2.01	0.58
2:M:397:SER:O	2:M:401:LYS:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:229:ARG:O	2:N:232:VAL:HG12	2.02	0.58
2:O:51:GLN:HB2	2:O:59:ARG:HB3	1.84	0.58
6:W:19:ALA:C	6:W:21:ALA:H	2.07	0.58
1:L:424:LEU:O	1:L:427:LEU:HB2	2.03	0.58
1:C:32:LEU:CD1	1:C:42:HIS:HB2	2.33	0.58
2:E:298:THR:HG23	2:E:303:SER:HB3	1.86	0.58
6:W:115:GLU:O	6:W:116:VAL:HG23	2.03	0.58
2:F:96:ASN:ND2	2:F:98:ILE:H	2.02	0.58
1:K:38:ILE:HG12	1:K:285:LEU:CD2	2.33	0.58
1:J:479:LEU:HD13	1:J:496:LYS:NZ	2.18	0.58
2:E:63:MET:HE3	2:E:228:ALA:HA	1.85	0.58
3:G:39:LYS:HB3	3:G:40:PRO:CD	2.34	0.58
4:H:36:VAL:HG13	4:H:65:VAL:HG13	1.84	0.58
2:N:374:VAL:HG13	2:N:410:ILE:HD13	1.85	0.58
2:M:321:ALA:HB3	2:M:322:PRO:CD	2.33	0.58
2:F:425:THR:C	2:F:427:HIS:H	2.07	0.58
2:F:252:LEU:HD23	2:F:305:THR:HB	1.86	0.58
1:A:267:ILE:HD13	1:A:324:LEU:HB2	1.86	0.58
1:L:307:GLU:OE2	2:M:190:THR:HB	2.03	0.58
2:D:96:ASN:HD21	2:D:98:ILE:H	1.47	0.58
6:S:122:THR:OG1	6:S:123:ALA:N	2.37	0.58
2:O:72:GLY:O	2:O:73:GLN:O	2.21	0.58
1:B:248:TYR:CE2	1:B:305:LEU:HB2	2.39	0.58
1:B:202:ILE:CG2	1:B:266:ILE:HG13	2.33	0.58
7:T:191:LYS:HA	7:T:194:ILE:HG12	1.86	0.58
1:K:163:GLN:HG2	1:K:164:ARG:N	2.17	0.58
1:K:399:GLU:O	1:K:401:ALA:N	2.36	0.58
2:E:175:LYS:CD	2:E:431:LEU:HD23	2.32	0.58
2:F:287:THR:O	2:F:291:THR:HG23	2.03	0.58
4:Q:48:LEU:HB2	4:Q:51:HIS:CD2	2.39	0.58
1:C:376:SER:O	1:C:378:ALA:N	2.37	0.58
3:P:39:LYS:HB3	3:P:40:PRO:CD	2.34	0.58
1:B:374:VAL:HG23	1:B:375:GLY:N	2.19	0.58
2:D:22:ASP:N	2:D:22:ASP:OD1	2.37	0.58
2:O:351:LEU:HD13	2:O:379:GLN:HB2	1.86	0.58
6:W:106:SER:C	6:W:108:MSE:H	2.07	0.58
6:S:88:LEU:HD13	6:S:92:ASN:ND2	2.18	0.58
1:L:365:ILE:HD12	1:L:366:ASN:N	2.17	0.58
1:C:365:ILE:H	1:C:365:ILE:HD12	1.69	0.58
2:D:268:VAL:HG23	2:D:272:LEU:HD12	1.85	0.58
1:J:49:ALA:O	1:J:50:GLU:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:420:VAL:O	2:F:422:GLU:N	2.33	0.58
2:M:374:VAL:HG13	2:M:410:ILE:HG21	1.85	0.58
1:B:188:ARG:HG3	1:B:189:PHE:CD1	2.39	0.58
1:L:248:TYR:CE2	1:L:305:LEU:HD12	2.39	0.58
1:J:403:PHE:CD1	3:P:22:SER:HB2	2.38	0.58
1:K:410:LEU:N	1:K:410:LEU:HD12	2.18	0.58
2:O:227:GLY:O	2:O:230:ALA:HB3	2.04	0.58
6:W:95:LEU:O	6:W:98:THR:HG23	2.04	0.58
1:C:62:MET:H	1:C:73:VAL:CG1	2.17	0.58
2:D:170:ILE:HG13	2:D:254:PHE:CE2	2.39	0.58
2:M:41:ARG:NH1	2:M:69:LEU:HD23	2.18	0.58
1:K:113:ASN:HD22	1:K:113:ASN:H	1.52	0.58
2:N:460:VAL:HG21	2:N:466:ALA:HB2	1.86	0.58
2:M:96:ASN:ND2	2:M:98:ILE:N	2.46	0.57
1:A:7:GLU:O	1:A:8:VAL:HB	2.02	0.57
1:B:241:PRO:HA	1:B:244:TYR:HB3	1.86	0.57
2:F:72:GLY:O	2:F:73:GLN:O	2.22	0.57
4:Q:36:VAL:HG13	4:Q:65:VAL:HG13	1.86	0.57
2:E:237:LEU:HD13	2:E:253:LEU:HD22	1.86	0.57
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.39	0.57
2:D:430:LYS:HE2	2:D:465:GLU:OE1	2.03	0.57
1:K:206:ILE:HG21	1:K:274:GLN:HB2	1.86	0.57
1:C:248:TYR:CE2	1:C:305:LEU:HD12	2.39	0.57
6:S:95:LEU:O	6:S:98:THR:HG23	2.04	0.57
1:C:479:LEU:HD21	1:C:493:SER:HB3	1.85	0.57
1:J:71:VAL:HG23	2:N:71:ARG:CZ	2.34	0.57
1:L:32:LEU:CD1	1:L:42:HIS:HB2	2.34	0.57
2:F:412:ARG:HG2	2:F:458:TYR:HB2	1.86	0.57
1:C:167:ILE:HB	1:C:326:VAL:HG22	1.86	0.57
6:S:108:MSE:O	6:S:108:MSE:HE3	2.03	0.57
1:J:410:LEU:HD12	1:J:410:LEU:N	2.19	0.57
6:W:133:GLU:HB3	7:X:207:LYS:CD	2.34	0.57
1:K:101:GLU:O	1:K:104:LEU:HD12	2.04	0.57
2:M:92:GLY:HA2	2:M:206:ILE:CD1	2.34	0.57
2:M:153:GLY:HA3	2:M:329:LEU:HD13	1.84	0.57
2:O:221:GLN:HA	2:O:221:GLN:NE2	2.18	0.57
3:G:165:PHE:HB2	3:G:223:SER:OG	2.04	0.57
3:G:85:VAL:O	3:G:89:MET:HG3	2.04	0.57
2:D:31:PRO:O	2:D:34:ASN:HB2	2.03	0.57
2:N:359:ASP:HB3	2:N:362:ILE:HG13	1.86	0.57
5:R:31:LYS:HE3	5:R:35:MET:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:14:VAL:CG2	2:N:24:GLN:HB2	2.34	0.57
2:D:139:VAL:HG21	2:D:348:VAL:HB	1.86	0.57
6:S:137:VAL:HG23	7:T:207:LYS:NZ	2.19	0.57
1:A:403:PHE:CZ	3:G:25:MET:CE	2.88	0.57
1:K:66:LEU:HB2	2:O:16:VAL:CG2	2.33	0.57
1:L:199:LEU:HD12	1:L:263:HIS:O	2.05	0.57
1:B:163:GLN:O	1:B:322:THR:HG23	2.05	0.57
2:E:359:ASP:HB3	2:E:362:ILE:HG13	1.85	0.57
2:E:160:VAL:HB	2:E:335:LEU:HB3	1.85	0.57
3:G:101:LYS:N	3:G:101:LYS:HD2	2.18	0.57
1:B:460:LYS:NZ	1:B:510:ALA:HB2	2.19	0.57
2:D:413:PHE:HB2	2:D:457:PHE:HB3	1.87	0.57
1:L:180:ILE:HG12	1:L:216:LEU:HD21	1.86	0.57
2:O:282:GLN:N	2:O:282:GLN:HE21	2.02	0.57
1:C:144:GLU:O	1:C:161:ARG:HG3	2.05	0.57
4:H:116:GLN:HA	4:H:135:ILE:HD11	1.85	0.57
4:Q:116:GLN:HA	4:Q:135:ILE:HD11	1.87	0.57
8:U:85:TYR:OH	9:V:67:PRO:HD2	2.03	0.57
1:J:166:LEU:HD11	1:J:327:ILE:HG12	1.86	0.57
6:S:46:LEU:HD23	6:S:51:MSE:HE3	1.86	0.57
1:K:392:LEU:O	1:K:395:ALA:HB3	2.05	0.57
2:F:266:SER:CA	2:F:282:GLN:NE2	2.67	0.57
2:M:467:VAL:O	2:M:470:ALA:HB3	2.04	0.57
1:B:399:GLU:O	1:B:401:ALA:N	2.37	0.57
3:P:101:LYS:N	3:P:101:LYS:HD2	2.19	0.57
1:B:66:LEU:HB2	2:F:16:VAL:HB	1.86	0.57
3:G:203:ASN:OD1	5:I:11:TYR:HB2	2.04	0.57
1:C:144:GLU:HG3	1:C:311:LYS:HE2	1.87	0.57
3:G:171:TYR:O	3:G:172:LYS:CB	2.52	0.57
2:M:44:ARG:HD3	2:M:100:GLU:OE2	2.04	0.57
1:C:390:MET:HG3	1:C:390:MET:O	2.04	0.57
4:Q:103:LEU:HD23	5:R:25:ALA:O	2.04	0.57
1:A:339:PRO:O	1:A:343:ILE:HG13	2.05	0.57
4:H:78:SER:HB3	5:I:22:VAL:HG21	1.85	0.57
1:B:190:ASN:O	1:B:198:LYS:HE2	2.05	0.57
2:O:39:GLN:HG3	2:O:76:LEU:HD21	1.86	0.57
1:L:266:ILE:HD13	1:L:268:TYR:CZ	2.40	0.57
2:O:96:ASN:ND2	2:O:98:ILE:H	2.03	0.57
2:M:235:THR:HG22	2:M:236:GLY:N	2.20	0.57
1:A:403:PHE:HZ	3:G:25:MET:HE1	1.68	0.57
1:K:248:TYR:CE2	1:K:305:LEU:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ILE:HD13	1:C:121:ILE:H	1.70	0.57
8:U:69:PHE:O	8:U:73:PHE:HB2	2.04	0.57
1:C:440:GLU:OE1	1:C:473:ILE:HD11	2.05	0.57
1:A:479:LEU:HD13	1:A:496:LYS:CD	2.35	0.56
1:K:452:TYR:CD1	1:K:501:VAL:HG11	2.39	0.56
2:D:93:ARG:HH21	2:D:101:PRO:HB3	1.70	0.56
6:W:11:ILE:HG22	6:W:11:ILE:O	2.05	0.56
2:N:138:LYS:HG2	2:N:437:THR:HG23	1.85	0.56
1:L:34:ILE:HD11	1:L:79:ASP:HB2	1.87	0.56
2:E:86:VAL:O	2:E:110:THR:HG21	2.04	0.56
2:D:228:ALA:O	2:D:232:VAL:HG23	2.05	0.56
6:S:52:ALA:HA	6:S:55:LEU:HB2	1.88	0.56
2:E:415:SER:O	2:E:416:GLN:HB2	2.05	0.56
6:S:7:PRO:O	6:S:9:VAL:N	2.33	0.56
2:F:387:ILE:H	2:F:387:ILE:CD1	2.11	0.56
1:A:12:LEU:O	1:A:13:GLU:C	2.44	0.56
1:B:99:VAL:HG21	1:B:127:ARG:CG	2.36	0.56
1:A:403:PHE:N	1:A:403:PHE:CD1	2.72	0.56
2:O:266:SER:CA	2:O:282:GLN:HE22	2.18	0.56
1:A:180:ILE:HG22	1:A:181:ASP:N	2.20	0.56
3:P:204:TYR:HE2	4:Q:55:LEU:HD13	1.69	0.56
1:L:52:MET:HG3	1:L:61:GLY:O	2.04	0.56
6:W:90:ALA:HA	6:W:95:LEU:HD21	1.87	0.56
6:S:35:VAL:HG22	6:S:82:THR:HG21	1.86	0.56
6:S:61:LYS:O	6:S:65:LYS:HB2	2.05	0.56
4:Q:109:LYS:O	4:Q:112:LEU:HB3	2.05	0.56
1:J:216:LEU:HD13	1:J:220:LEU:CD1	2.35	0.56
2:M:161:GLY:HA2	12:M:600:ADP:H8	1.69	0.56
1:J:479:LEU:HD22	1:J:496:LYS:HD3	1.85	0.56
1:K:30:ARG:NH2	6:W:58:PRO:HB2	2.20	0.56
2:E:360:PRO:HB3	2:E:368:TYR:CD2	2.40	0.56
2:M:84:ILE:HD11	2:M:238:THR:CG2	2.35	0.56
7:X:165:MSE:HA	7:X:165:MSE:HE3	1.87	0.56
1:K:24:ASP:O	1:K:25:LEU:HD23	2.05	0.56
2:D:30:PRO:HG2	2:D:36:LEU:HD11	1.87	0.56
2:O:259:PHE:CE2	2:O:263:GLN:HB2	2.41	0.56
1:J:362:ARG:HA	1:J:363:PRO:C	2.24	0.56
1:B:282:SER:CB	1:B:295:PRO:HG3	2.35	0.56
2:M:104:GLU:O	2:M:105:ARG:HG3	2.05	0.56
2:O:237:LEU:HD11	2:O:296:ILE:CG1	2.24	0.56
6:S:90:ALA:HA	6:S:95:LEU:HD21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:48:GLN:HB3	2:N:68:GLY:HA2	1.86	0.56
2:O:268:VAL:HG23	2:O:272:LEU:HG	1.88	0.56
2:M:96:ASN:HB3	2:M:102:ILE:CD1	2.35	0.56
2:O:25:PHE:HB2	2:O:29:LEU:CD1	2.35	0.56
1:K:392:LEU:CD1	1:K:396:GLN:HE21	2.18	0.56
3:G:81:ILE:HD11	3:G:223:SER:O	2.04	0.56
2:N:298:THR:HG23	2:N:303:SER:HB3	1.87	0.56
1:L:90:ARG:HH21	1:L:92:GLY:HA2	1.70	0.56
1:A:56:SER:OG	1:A:86:ASP:HB3	2.05	0.56
6:W:61:LYS:O	6:W:65:LYS:HB2	2.05	0.56
2:O:25:PHE:CE1	2:O:30:PRO:CG	2.88	0.56
1:A:47:VAL:HG21	1:A:71:VAL:HG21	1.87	0.56
2:D:44:ARG:HD3	2:D:100:GLU:OE2	2.04	0.56
3:G:136:PRO:HA	3:G:140:ASP:OD2	2.06	0.56
1:C:256:TYR:HD2	1:C:257:PHE:CD1	2.24	0.56
1:A:476:HIS:C	1:A:478:ALA:N	2.59	0.56
2:N:396:LEU:HD22	2:N:396:LEU:H	1.70	0.56
2:M:91:LEU:HD21	2:M:243:PHE:HE2	1.70	0.56
1:K:464:PHE:CD2	1:K:464:PHE:C	2.78	0.56
2:D:374:VAL:HG13	2:D:410:ILE:HG21	1.88	0.56
1:A:362:ARG:HA	1:A:363:PRO:C	2.24	0.56
1:L:404:ALA:HB1	1:L:410:LEU:HD11	1.88	0.56
3:G:108:VAL:HG23	3:G:128:PHE:HB2	1.86	0.56
3:G:127:THR:HG22	3:G:128:PHE:N	2.21	0.56
2:D:467:VAL:O	2:D:470:ALA:HB3	2.05	0.56
2:F:70:VAL:HG12	2:F:71:ARG:N	2.20	0.56
2:N:170:ILE:HG21	2:N:215:VAL:CG2	2.35	0.56
4:H:48:LEU:C	4:H:50:ALA:H	2.09	0.56
1:C:32:LEU:HD11	1:C:42:HIS:HB2	1.86	0.56
1:A:133:ALA:HB2	1:A:308:ARG:HG3	1.87	0.56
3:G:203:ASN:HD21	5:I:4:TRP:HH2	1.53	0.56
7:T:198:ILE:HA	7:T:201:LEU:HD12	1.87	0.56
2:N:459:MET:O	2:N:460:VAL:HG13	2.06	0.56
1:L:78:ASN:C	1:L:78:ASN:HD22	2.09	0.56
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.87	0.56
1:J:294:TYR:HB3	1:J:298:VAL:HG11	1.87	0.56
1:A:187:LYS:HG2	1:A:188:ARG:N	2.20	0.56
2:F:364:GLY:O	2:F:366:GLU:N	2.39	0.56
6:S:116:VAL:N	6:S:117:PRO:CD	2.69	0.56
3:P:138:PHE:HA	3:P:214:TYR:HD1	1.70	0.56
2:D:33:LEU:HD22	2:D:117:HIS:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:46:GLY:C	4:H:47:ILE:HD12	2.27	0.56
2:M:93:ARG:HH21	2:M:101:PRO:HB3	1.71	0.56
2:D:440:GLY:O	2:D:444:ILE:HG13	2.06	0.56
1:C:404:ALA:HB1	1:C:410:LEU:HD11	1.87	0.56
1:B:362:ARG:HA	1:B:363:PRO:C	2.27	0.56
6:S:7:PRO:CB	6:S:108:MSE:HE1	2.36	0.55
2:O:136:GLY:HA3	2:O:431:LEU:CD2	2.34	0.55
1:J:476:HIS:HD2	1:J:496:LYS:HE2	1.70	0.55
2:E:462:PRO:HD2	2:E:465:GLU:HG3	1.88	0.55
2:O:357:ILE:O	2:O:357:ILE:HG13	2.06	0.55
2:O:348:VAL:O	2:O:350:PRO:HD3	2.05	0.55
2:M:105:ARG:O	2:M:106:GLY:O	2.24	0.55
3:P:138:PHE:HA	3:P:214:TYR:CD1	2.41	0.55
1:J:83:LYS:HD3	2:M:31:PRO:HG3	1.87	0.55
1:A:15:ARG:NH2	6:S:91:GLU:OE1	2.38	0.55
9:V:22:LYS:HZ2	9:V:30:VAL:HG13	1.71	0.55
3:G:59:THR:HG23	3:G:184:ILE:HG13	1.87	0.55
3:P:184:ILE:O	3:P:184:ILE:HD13	2.06	0.55
1:C:336:ALA:O	1:C:337:TYR:C	2.44	0.55
1:J:129:VAL:HG21	1:J:245:LEU:HD21	1.88	0.55
2:N:372:ARG:NH1	2:N:375:GLN:HE22	2.04	0.55
3:G:86:ALA:C	3:G:88:GLN:H	2.08	0.55
3:G:24:LYS:HB2	3:G:232:MET:HB3	1.87	0.55
1:A:99:VAL:CG1	1:A:256:TYR:HB2	2.35	0.55
4:H:84:VAL:HA	4:H:90:VAL:HG22	1.87	0.55
2:D:151:LYS:HA	2:D:306:SER:OG	2.06	0.55
1:L:137:ILE:CG1	1:L:138:PRO:HD3	2.25	0.55
6:S:3:LYS:O	6:S:4:LEU:HD23	2.07	0.55
1:L:336:ALA:O	1:L:337:TYR:C	2.42	0.55
3:P:31:TYR:CD1	3:P:226:SER:HB3	2.41	0.55
1:B:140:ILE:HD11	1:B:143:ARG:NH2	2.19	0.55
1:J:47:VAL:HG21	1:J:71:VAL:HG21	1.87	0.55
1:J:478:ALA:HB3	1:J:496:LYS:NZ	2.21	0.55
1:L:456:LEU:HA	1:L:509:GLU:OE2	2.06	0.55
3:P:207:TYR:CD2	4:Q:81:SER:HB3	2.42	0.55
2:O:244:ARG:CG	2:O:302:GLY:HA3	2.35	0.55
2:D:425:THR:OG1	2:D:426:GLY:N	2.39	0.55
2:E:342:LEU:HD23	2:E:342:LEU:N	2.21	0.55
2:M:475:GLU:HA	2:M:475:GLU:OE1	2.06	0.55
1:K:99:VAL:HG11	1:K:256:TYR:HB2	1.88	0.55
2:M:193:GLY:HA3	2:M:219:TYR:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:63:MET:HE1	2:N:228:ALA:HA	1.87	0.55
1:L:201:CYS:O	1:L:229:THR:HA	2.07	0.55
3:G:207:TYR:O	3:G:211:ASN:HB2	2.07	0.55
2:D:41:ARG:NH1	2:D:69:LEU:HD23	2.20	0.55
1:L:145:PRO:HB3	1:L:147:GLN:NE2	2.21	0.55
9:Z:20:ARG:C	9:Z:22:LYS:H	2.08	0.55
1:L:307:GLU:HG3	2:M:223:ASN:HB3	1.87	0.55
2:F:420:VAL:C	2:F:422:GLU:H	2.10	0.55
1:C:78:ASN:C	1:C:78:ASN:HD22	2.10	0.55
2:F:258:ILE:HG12	2:F:308:GLN:OE1	2.06	0.55
2:M:30:PRO:HG2	2:M:36:LEU:HD11	1.87	0.55
2:F:53:LEU:HD21	2:F:59:ARG:HB2	1.89	0.55
4:Q:95:GLU:O	4:Q:96:GLU:HG2	2.06	0.55
1:J:347:ASP:CB	2:N:191:ARG:HH21	2.20	0.55
1:B:180:ILE:CG1	1:B:216:LEU:HD21	2.35	0.55
1:B:392:LEU:O	1:B:395:ALA:HB3	2.07	0.55
4:Q:58:LEU:HD12	4:Q:80:GLY:H	1.71	0.55
2:N:417:PRO:O	2:N:417:PRO:HG2	2.05	0.55
3:G:59:THR:HG1	3:G:184:ILE:HD11	1.71	0.55
3:P:52:TYR:HE2	3:P:179:PHE:HD2	1.55	0.55
4:Q:46:GLY:C	4:Q:47:ILE:HD12	2.27	0.55
2:D:16:VAL:CG2	2:D:21:VAL:HG13	2.37	0.55
2:F:449:TYR:C	2:F:451:HIS:H	2.09	0.55
4:H:132:GLN:O	4:H:135:ILE:HB	2.07	0.55
1:A:144:GLU:O	1:A:161:ARG:HG3	2.06	0.55
2:O:139:VAL:HG13	2:O:414:LEU:HB3	1.89	0.55
1:B:439:GLU:O	1:B:442:VAL:HG12	2.06	0.55
1:L:206:ILE:HG12	1:L:247:PRO:HG3	1.89	0.55
1:A:23:VAL:C	1:A:25:LEU:N	2.60	0.55
1:A:190:ASN:ND2	1:A:228:TYR:CD1	2.73	0.55
1:J:476:HIS:C	1:J:478:ALA:N	2.60	0.55
1:L:358:TYR:CE2	2:O:375:GLN:NE2	2.74	0.55
1:J:213:VAL:O	1:J:217:VAL:HG13	2.06	0.55
3:P:113:ARG:C	3:P:113:ARG:HD3	2.27	0.55
1:C:45:ARG:HH11	2:D:71:ARG:HH12	1.54	0.55
7:T:164:MSE:HE1	9:V:44:LEU:HD13	1.87	0.55
7:X:198:ILE:HA	7:X:201:LEU:HD12	1.89	0.55
2:N:253:LEU:HB3	2:N:306:SER:HB2	1.86	0.55
2:N:15:ALA:HB3	2:N:22:ASP:HB2	1.88	0.55
2:D:82:ILE:HD13	2:D:98:ILE:HG22	1.87	0.55
1:J:321:LEU:HD12	1:J:322:THR:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:221:GLN:HE21	2:D:221:GLN:CA	2.18	0.55
1:C:143:ARG:O	1:C:145:PRO:HD3	2.06	0.55
2:O:89:GLU:HG3	2:O:109:LYS:O	2.06	0.55
2:M:137:ILE:HD13	2:M:418:PHE:CZ	2.41	0.55
3:P:86:ALA:C	3:P:88:GLN:H	2.09	0.55
2:N:266:SER:HB2	2:N:282:GLN:NE2	2.21	0.55
7:T:187:ALA:O	7:T:188:GLN:C	2.45	0.55
1:L:129:VAL:HG23	1:L:130:GLY:N	2.21	0.55
4:H:16:MET:HE1	4:H:90:VAL:HB	1.89	0.55
2:M:409:LYS:NZ	2:M:450:ASP:HA	2.22	0.55
6:S:7:PRO:HB2	6:S:108:MSE:CE	2.37	0.55
1:L:365:ILE:H	1:L:365:ILE:HD12	1.71	0.55
4:H:57:VAL:O	4:H:58:LEU:HD23	2.07	0.55
1:A:405:GLN:HE21	1:A:405:GLN:HA	1.72	0.55
1:C:386:VAL:HB	1:C:445:ILE:HG22	1.87	0.55
1:B:44:LEU:O	2:F:71:ARG:NH2	2.34	0.55
3:G:204:TYR:OH	4:H:83:THR:OG1	2.21	0.55
2:F:374:VAL:HG22	2:F:410:ILE:HD13	1.87	0.55
2:E:17:ILE:HD12	2:E:17:ILE:H	1.72	0.55
1:K:290:GLY:O	1:K:291:ARG:C	2.45	0.55
1:L:119:GLY:O	1:L:120:PRO:O	2.25	0.55
9:Z:41:ASP:OD1	9:Z:44:LEU:HD22	2.07	0.55
1:A:9:SER:O	1:A:10:SER:C	2.46	0.55
6:S:177:THR:HG22	9:V:15:LYS:HE3	1.89	0.55
2:F:266:SER:CA	2:F:282:GLN:HE22	2.20	0.55
3:P:59:THR:HG23	3:P:184:ILE:HG13	1.89	0.55
3:P:85:VAL:O	3:P:89:MET:HG3	2.06	0.55
2:O:351:LEU:CD1	2:O:379:GLN:HB2	2.37	0.55
1:L:78:ASN:HD22	1:L:79:ASP:N	2.05	0.55
5:I:37:THR:HG22	5:I:38:SER:N	2.22	0.55
5:R:37:THR:HG22	5:R:38:SER:N	2.22	0.55
4:Q:111:ASN:ND2	5:R:24:ASP:HB3	2.22	0.55
2:M:181:SER:O	2:M:215:VAL:HA	2.07	0.55
1:L:440:GLU:OE1	1:L:473:ILE:HD11	2.07	0.55
2:D:110:THR:OG1	2:D:112:GLN:HG2	2.07	0.55
2:O:135:THR:HB	2:O:137:ILE:HG13	1.88	0.54
6:W:114:GLY:O	6:W:115:GLU:CB	2.54	0.54
1:K:139:ARG:O	1:K:140:ILE:HB	2.07	0.54
3:G:184:ILE:HD13	3:G:184:ILE:O	2.07	0.54
2:F:89:GLU:HG3	2:F:110:THR:HA	1.88	0.54
1:A:289:PRO:HG3	2:D:275:ILE:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:228:ALA:O	2:M:232:VAL:HG23	2.06	0.54
1:C:119:GLY:O	1:C:120:PRO:O	2.25	0.54
2:O:252:LEU:HD23	2:O:305:THR:HB	1.89	0.54
2:O:377:ILE:HG21	2:O:410:ILE:HD12	1.89	0.54
6:W:22:LEU:HD23	6:W:25:ALA:HB3	1.89	0.54
1:A:156:LEU:HD13	1:A:367:VAL:CG1	2.33	0.54
1:J:156:LEU:HD13	1:J:367:VAL:CG1	2.35	0.54
3:G:113:ARG:HD3	3:G:113:ARG:C	2.28	0.54
2:O:86:VAL:HG23	2:O:87:GLY:N	2.23	0.54
1:L:468:PHE:O	1:L:468:PHE:CG	2.61	0.54
1:B:353:GLU:HB3	1:B:356:LEU:HD12	1.90	0.54
1:L:268:TYR:N	1:L:268:TYR:CD1	2.76	0.54
1:A:12:LEU:HD21	6:S:88:LEU:HD12	1.89	0.54
1:A:479:LEU:HD22	1:A:496:LYS:HD3	1.89	0.54
1:K:160:GLY:H	1:K:163:GLN:HE21	1.54	0.54
2:N:25:PHE:HB2	2:N:29:LEU:HD12	1.89	0.54
1:C:99:VAL:HG21	1:C:127:ARG:HB2	1.89	0.54
6:W:52:ALA:HA	6:W:55:LEU:HB2	1.88	0.54
7:T:181:VAL:HG21	9:V:15:LYS:NZ	2.22	0.54
2:F:282:GLN:N	2:F:282:GLN:HE21	2.05	0.54
3:G:52:TYR:HE2	3:G:179:PHE:HD2	1.55	0.54
1:J:456:LEU:HD22	1:J:505:LEU:HD11	1.87	0.54
2:N:458:TYR:CD2	2:N:459:MET:HG2	2.42	0.54
1:C:56:SER:HB2	1:C:87:ILE:H	1.72	0.54
1:B:415:GLN:HA	1:B:418:LEU:HD12	1.89	0.54
2:N:86:VAL:O	2:N:110:THR:HG21	2.08	0.54
1:B:127:ARG:HH21	1:B:131:LEU:HD22	1.69	0.54
6:S:26:ALA:O	6:S:28:LYS:N	2.40	0.54
3:G:6:ILE:HG23	3:G:246:LEU:CD2	2.38	0.54
1:A:478:ALA:HB3	1:A:496:LYS:NZ	2.22	0.54
2:E:175:LYS:HD2	2:E:431:LEU:HD23	1.88	0.54
1:C:78:ASN:HD22	1:C:79:ASP:N	2.05	0.54
6:S:135:LYS:HD2	6:S:139:LYS:NZ	2.23	0.54
4:H:95:GLU:O	4:H:96:GLU:HG2	2.07	0.54
10:O:600:ANP:O1B	10:O:600:ANP:O3G	2.25	0.54
2:N:279:VAL:O	2:N:279:VAL:HG13	2.08	0.54
2:F:221:GLN:HE21	2:F:221:GLN:CA	2.21	0.54
3:P:207:TYR:O	3:P:211:ASN:HB2	2.08	0.54
3:P:59:THR:HG1	3:P:184:ILE:HD11	1.73	0.54
2:N:23:VAL:HG12	2:N:25:PHE:CE1	2.43	0.54
1:B:160:GLY:H	1:B:163:GLN:HE21	1.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:454:GLU:O	2:E:456:ALA:N	2.40	0.54
1:C:376:SER:HA	1:C:379:GLN:HG3	1.90	0.54
2:N:39:GLN:HE21	2:N:76:LEU:HB2	1.71	0.54
2:O:163:THR:O	2:O:167:MET:HG2	2.07	0.54
2:F:450:ASP:OD1	2:F:450:ASP:N	2.41	0.54
2:M:61:ILE:CG2	2:M:227:GLY:HA2	2.38	0.54
1:C:75:VAL:HG12	1:C:77:GLY:H	1.72	0.54
2:O:258:ILE:HG12	2:O:308:GLN:OE1	2.07	0.54
2:M:282:GLN:C	2:M:284:THR:H	2.10	0.54
1:J:204:VAL:CG2	1:J:266:ILE:HD11	2.38	0.54
4:H:58:LEU:HD12	4:H:80:GLY:H	1.72	0.54
7:T:176:TRP:CZ3	9:V:22:LYS:HD3	2.43	0.54
7:T:198:ILE:CD1	9:V:11:LEU:HD21	2.37	0.54
3:G:157:GLU:HG2	3:G:158:GLY:H	1.73	0.54
1:J:188:ARG:NH1	1:J:437:ALA:HA	2.23	0.54
1:J:188:ARG:HH12	1:J:436:MET:C	2.10	0.54
2:F:153:GLY:HA3	2:F:329:LEU:HD13	1.89	0.54
2:F:264:ALA:HA	2:F:267:GLU:HG3	1.90	0.54
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.38	0.54
3:G:56:ASP:C	3:G:57:ILE:HG12	2.28	0.54
2:O:33:LEU:HD22	2:O:117:HIS:CD2	2.42	0.54
3:G:31:TYR:CB	3:G:225:GLN:HB3	2.35	0.54
3:G:31:TYR:CD1	3:G:226:SER:HB3	2.42	0.54
4:Q:57:VAL:O	4:Q:58:LEU:HD23	2.08	0.54
4:Q:106:GLY:HA3	4:Q:109:LYS:HD2	1.89	0.54
2:F:25:PHE:CD1	2:F:30:PRO:HD3	2.43	0.54
2:O:116:ILE:HG22	2:O:235:THR:HA	1.88	0.54
4:Q:104:ASP:OD2	5:R:27:LYS:HD3	2.08	0.54
2:M:170:ILE:HD11	2:M:254:PHE:CG	2.43	0.54
1:B:163:GLN:HG2	1:B:164:ARG:N	2.21	0.54
1:J:241:PRO:O	1:J:245:LEU:HB2	2.08	0.54
1:J:100:GLY:HA2	1:J:256:TYR:CE2	2.43	0.54
2:N:346:PRO:HG3	2:N:418:PHE:HZ	1.72	0.54
2:D:268:VAL:HG23	2:D:272:LEU:CD1	2.38	0.54
2:E:25:PHE:HB2	2:E:29:LEU:HD12	1.90	0.54
1:A:141:SER:O	1:A:143:ARG:HG3	2.08	0.54
2:M:168:GLU:HG3	2:M:168:GLU:O	2.08	0.54
1:K:381:ARG:O	1:K:381:ARG:HD3	2.08	0.54
1:J:405:GLN:HA	1:J:405:GLN:HE21	1.72	0.54
6:W:26:ALA:O	6:W:28:LYS:N	2.41	0.54
2:M:221:GLN:HE21	2:M:221:GLN:CA	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:26:ALA:C	6:S:28:LYS:H	2.11	0.54
1:K:140:ILE:HD11	1:K:143:ARG:NH2	2.22	0.54
1:L:66:LEU:O	2:M:16:VAL:N	2.36	0.54
1:J:180:ILE:HG22	1:J:181:ASP:N	2.21	0.54
3:P:157:GLU:HG2	3:P:158:GLY:H	1.73	0.54
1:J:28:THR:HA	1:J:88:VAL:O	2.08	0.54
4:H:75:TYR:HD2	4:H:99:THR:HG21	1.73	0.54
4:H:102:MET:HB2	5:I:26:LEU:HD22	1.89	0.54
1:J:268:TYR:CZ	1:J:305:LEU:HD11	2.43	0.54
2:F:112:GLN:N	2:F:112:GLN:HE21	1.93	0.54
1:C:186:GLN:OE1	1:C:199:LEU:HD23	2.07	0.54
4:H:21:ALA:HB2	4:H:26:VAL:HA	1.90	0.54
4:H:21:ALA:HB1	4:H:26:VAL:HA	1.90	0.54
1:A:321:LEU:HD12	1:A:322:THR:H	1.72	0.54
1:J:99:VAL:HG21	1:J:127:ARG:HB3	1.90	0.54
6:W:19:ALA:C	6:W:21:ALA:N	2.60	0.54
6:S:127:ASP:O	6:S:129:THR:N	2.41	0.54
1:K:383:MET:HG3	1:K:387:ALA:HB2	1.90	0.54
1:A:457:GLU:HG2	1:A:458:PRO:HD2	1.90	0.54
3:P:136:PRO:HA	3:P:140:ASP:OD2	2.07	0.54
2:O:471:ASP:O	2:O:474:ALA:N	2.40	0.54
1:L:56:SER:HB2	1:L:87:ILE:H	1.72	0.54
1:L:247:PRO:HB2	1:L:305:LEU:HD11	1.91	0.53
1:A:206:ILE:CD1	1:A:247:PRO:HG3	2.33	0.53
1:A:44:LEU:O	1:A:46:ASN:N	2.42	0.53
1:L:67:GLU:O	2:M:71:ARG:HD3	2.08	0.53
4:Q:33:VAL:HG11	4:Q:36:VAL:HG22	1.90	0.53
4:Q:21:ALA:HB1	4:Q:26:VAL:HA	1.88	0.53
4:H:33:VAL:HG11	4:H:36:VAL:HG22	1.90	0.53
2:O:379:GLN:O	2:O:379:GLN:HG3	2.08	0.53
1:C:272:SER:O	1:C:276:VAL:HG23	2.08	0.53
1:C:468:PHE:CG	1:C:468:PHE:O	2.61	0.53
2:D:409:LYS:NZ	2:D:450:ASP:HA	2.23	0.53
1:C:47:VAL:HG11	1:C:71:VAL:HG21	1.90	0.53
2:M:162:LYS:CB	12:M:600:ADP:O1B	2.56	0.53
4:Q:84:VAL:HA	4:Q:90:VAL:HG22	1.89	0.53
2:O:53:LEU:HD21	2:O:59:ARG:HB2	1.90	0.53
5:R:37:THR:HG22	5:R:38:SER:H	1.73	0.53
1:L:181:ASP:OD1	1:L:433:TYR:HD2	1.91	0.53
4:Q:102:MET:HB2	5:R:26:LEU:HD22	1.89	0.53
3:P:38:LEU:HD13	3:P:218:LYS:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:23:TYR:CD1	6:W:108:MSE:HE2	2.43	0.53
2:E:181:SER:O	2:E:215:VAL:HA	2.07	0.53
1:J:99:VAL:HG21	1:J:127:ARG:CB	2.38	0.53
2:O:139:VAL:CG1	2:O:414:LEU:HD22	2.38	0.53
1:J:74:VAL:HG21	1:J:281:MET:HG2	1.90	0.53
2:M:268:VAL:HG23	2:M:272:LEU:HD12	1.88	0.53
2:D:155:PHE:O	2:D:335:LEU:HB2	2.08	0.53
6:W:98:THR:HA	6:W:101:VAL:HG23	1.90	0.53
2:F:268:VAL:HG23	2:F:272:LEU:HG	1.90	0.53
6:S:7:PRO:HG2	6:S:108:MSE:HE1	1.90	0.53
1:B:392:LEU:HD11	1:B:396:GLN:HE21	1.73	0.53
1:K:83:LYS:HB2	1:K:83:LYS:HZ2	1.73	0.53
2:O:16:VAL:HG11	2:O:69:LEU:HD12	1.90	0.53
2:M:153:GLY:HA3	2:M:329:LEU:HD11	1.89	0.53
1:B:25:LEU:HD13	1:B:43:GLY:HA2	1.89	0.53
1:J:423:ARG:HG2	1:J:461:ILE:CD1	2.38	0.53
1:C:201:CYS:O	1:C:229:THR:HA	2.09	0.53
3:G:52:TYR:HD2	3:G:179:PHE:HE2	1.57	0.53
4:Q:21:ALA:HB2	4:Q:26:VAL:HA	1.89	0.53
3:G:191:SER:C	3:G:193:TYR:H	2.12	0.53
2:D:475:GLU:HA	2:D:475:GLU:OE1	2.07	0.53
1:B:464:PHE:CD2	1:B:464:PHE:C	2.81	0.53
1:B:301:LEU:HA	1:B:304:ARG:NH1	2.23	0.53
1:B:68:PRO:HD3	2:F:15:ALA:HB2	1.90	0.53
6:W:101:VAL:O	6:W:104:ALA:HB3	2.08	0.53
6:W:137:VAL:HG23	7:X:207:LYS:NZ	2.23	0.53
1:L:48:GLN:HB2	1:L:51:GLU:CB	2.37	0.53
1:L:483:ILE:O	1:L:487:GLY:HA2	2.07	0.53
4:H:106:GLY:HA3	4:H:109:LYS:HD2	1.90	0.53
1:L:186:GLN:OE1	1:L:199:LEU:HD23	2.08	0.53
2:E:63:MET:O	2:E:64:ASP:HB2	2.08	0.53
4:Q:16:MET:HE1	4:Q:90:VAL:HB	1.90	0.53
1:C:279:ARG:HG2	1:C:283:LEU:HD12	1.91	0.53
2:D:360:PRO:HD3	2:D:368:TYR:CD1	2.43	0.53
2:N:151:LYS:HG2	2:N:293:GLN:NE2	2.23	0.53
2:O:290:GLY:HA2	2:O:328:HIS:HE1	1.74	0.53
6:S:85:LEU:N	6:S:85:LEU:HD23	2.23	0.53
1:C:206:ILE:HG12	1:C:247:PRO:HG3	1.91	0.53
2:M:282:GLN:H	2:M:282:GLN:CD	2.07	0.53
1:L:71:VAL:HG12	1:L:73:VAL:HG23	1.90	0.53
1:C:352:LEU:HG	1:C:364:ALA:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:445:ILE:O	1:K:449:VAL:HG23	2.09	0.53
2:F:244:ARG:HG3	2:F:302:GLY:CA	2.38	0.53
2:N:64:ASP:OD1	2:N:65:GLY:N	2.42	0.53
2:F:421:ALA:C	2:F:423:VAL:N	2.62	0.53
4:Q:48:LEU:C	4:Q:50:ALA:H	2.10	0.53
9:Z:19:TYR:CE1	9:Z:22:LYS:HE2	2.44	0.53
3:P:265:ILE:HG22	3:P:266:ILE:N	2.24	0.53
2:N:77:ASP:OD1	2:N:79:GLY:N	2.36	0.53
1:C:206:ILE:N	1:C:206:ILE:HD12	2.22	0.53
6:S:95:LEU:C	6:S:97:ASN:H	2.12	0.53
3:G:20:THR:HG21	3:G:236:SER:N	2.24	0.53
3:P:127:THR:HG22	3:P:128:PHE:N	2.23	0.53
3:P:13:ILE:HG22	3:P:243:ILE:HD11	1.91	0.53
1:K:468:PHE:O	1:K:472:VAL:HG13	2.08	0.53
2:F:291:THR:OG1	2:F:292:MET:N	2.39	0.53
1:C:129:VAL:HG23	1:C:130:GLY:N	2.24	0.53
1:L:34:ILE:HG13	1:L:35:GLY:N	2.24	0.53
2:D:61:ILE:CG2	2:D:227:GLY:HA2	2.39	0.53
1:C:497:LEU:O	1:C:501:VAL:HG22	2.09	0.53
2:N:412:ARG:HD3	2:N:455:GLN:NE2	2.23	0.53
2:D:96:ASN:HB3	2:D:102:ILE:CD1	2.38	0.53
2:N:431:LEU:HD12	2:N:431:LEU:O	2.09	0.53
3:P:31:TYR:CB	3:P:225:GLN:HB3	2.38	0.53
2:O:266:SER:CB	2:O:282:GLN:HE22	2.22	0.53
1:L:45:ARG:NH1	2:M:71:ARG:HH12	2.07	0.53
2:M:87:GLY:O	2:M:90:THR:HG23	2.08	0.53
2:O:142:LEU:HD22	2:O:441:PHE:CD1	2.44	0.53
2:M:200:MET:SD	2:M:215:VAL:HG11	2.49	0.53
4:Q:102:MET:HB3	5:R:30:PHE:CB	2.38	0.53
1:L:399:GLU:HG3	2:M:342:LEU:HD12	1.91	0.53
1:A:255:GLU:HG3	1:A:258:ARG:CZ	2.39	0.53
2:E:151:LYS:HG2	2:E:293:GLN:NE2	2.24	0.53
2:F:382:LYS:O	2:F:385:GLN:HB2	2.08	0.53
2:F:39:GLN:HG3	2:F:76:LEU:HD21	1.89	0.53
1:K:68:PRO:HD3	2:O:15:ALA:HB2	1.90	0.53
1:L:60:LYS:O	1:L:76:PHE:HB2	2.09	0.53
1:L:144:GLU:HG3	1:L:311:LYS:CE	2.39	0.53
2:D:338:ALA:O	2:D:342:LEU:HG	2.09	0.53
1:L:279:ARG:HG2	1:L:283:LEU:HD12	1.89	0.53
1:J:188:ARG:HH12	1:J:437:ALA:N	2.07	0.53
1:J:133:ALA:HB2	1:J:308:ARG:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:MET:HG3	1:B:387:ALA:HB2	1.91	0.53
1:L:164:ARG:HD3	1:L:164:ARG:N	2.23	0.53
2:M:110:THR:OG1	2:M:112:GLN:HG2	2.09	0.53
6:S:131:LEU:HB3	6:S:134:LEU:HG	1.90	0.53
1:J:144:GLU:O	1:J:161:ARG:HG3	2.09	0.53
6:W:5:VAL:HB	6:W:24:SER:CA	2.38	0.52
6:W:85:LEU:HD23	6:W:85:LEU:N	2.24	0.52
3:G:138:PHE:HA	3:G:214:TYR:CD1	2.44	0.52
6:S:57:ASN:CG	6:S:59:TYR:CD2	2.82	0.52
2:D:221:GLN:HA	2:D:221:GLN:NE2	2.18	0.52
3:P:241:GLU:O	3:P:242:MET:C	2.47	0.52
7:T:172:HIS:O	7:T:176:TRP:HB2	2.09	0.52
3:P:54:LYS:O	3:P:55:ALA:HB2	2.09	0.52
2:N:456:ALA:HA	2:N:469:LYS:HD3	1.89	0.52
1:B:460:LYS:HZ2	1:B:510:ALA:HB2	1.75	0.52
2:O:139:VAL:HG12	2:O:414:LEU:HD22	1.90	0.52
4:H:102:MET:HB3	5:I:30:PHE:CB	2.39	0.52
1:B:176:THR:O	1:B:177:SER:C	2.48	0.52
2:O:364:GLY:O	2:O:366:GLU:N	2.40	0.52
2:F:237:LEU:HD11	2:F:296:ILE:CG1	2.29	0.52
1:L:62:MET:N	1:L:73:VAL:HG13	2.22	0.52
2:M:146:TYR:HB3	2:M:152:ILE:CD1	2.39	0.52
2:F:116:ILE:HG22	2:F:235:THR:HA	1.91	0.52
1:K:78:ASN:HD21	1:K:80:LYS:CE	2.22	0.52
2:N:441:PHE:O	2:N:445:LEU:HD12	2.09	0.52
1:A:213:VAL:O	1:A:217:VAL:HG13	2.09	0.52
1:L:376:SER:C	1:L:378:ALA:N	2.63	0.52
2:M:137:ILE:HD13	2:M:418:PHE:HZ	1.74	0.52
1:J:188:ARG:HH11	1:J:437:ALA:HA	1.75	0.52
2:M:168:GLU:N	2:M:420:VAL:HG11	2.24	0.52
3:P:191:SER:C	3:P:193:TYR:H	2.13	0.52
2:F:163:THR:O	2:F:167:MET:HG2	2.09	0.52
2:F:351:LEU:HD13	2:F:379:GLN:HB2	1.91	0.52
4:H:103:LEU:HD23	5:I:25:ALA:O	2.08	0.52
3:G:138:PHE:HA	3:G:214:TYR:HD1	1.74	0.52
1:L:302:HIS:O	1:L:306:LEU:HB2	2.10	0.52
2:M:118:ALA:H	2:M:295:ARG:HH12	1.55	0.52
4:H:113:GLU:O	4:H:115:ALA:N	2.42	0.52
3:P:129:LYS:HG2	3:P:130:GLU:H	1.74	0.52
7:X:172:HIS:O	7:X:176:TRP:HB2	2.09	0.52
6:W:137:VAL:HG22	7:X:203:LEU:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:237:LEU:HD11	2:M:295:ARG:HE	1.74	0.52
1:C:361:ILE:O	1:C:361:ILE:HG22	2.08	0.52
2:F:263:GLN:O	2:F:266:SER:HB3	2.10	0.52
2:E:456:ALA:CA	2:E:469:LYS:HD3	2.40	0.52
2:F:431:LEU:O	2:F:431:LEU:HD23	2.09	0.52
2:N:409:LYS:HD3	2:N:457:PHE:HE1	1.74	0.52
1:C:358:TYR:CE2	2:F:375:GLN:NE2	2.78	0.52
2:E:145:PRO:HD2	2:E:355:SER:HB3	1.92	0.52
1:C:42:HIS:ND1	1:C:45:ARG:NH2	2.57	0.52
4:Q:75:TYR:HD2	4:Q:99:THR:HG21	1.73	0.52
7:T:152:LYS:HE2	7:T:156:ASP:OD2	2.09	0.52
2:F:290:GLY:HA2	2:F:328:HIS:HE1	1.74	0.52
6:W:34:GLN:O	6:W:38:GLU:HG3	2.09	0.52
2:N:281:TYR:CE2	2:N:321:ALA:HB2	2.45	0.52
1:C:483:ILE:O	1:C:487:GLY:HA2	2.10	0.52
1:B:83:LYS:HB2	1:B:83:LYS:HZ2	1.74	0.52
1:L:32:LEU:HD11	1:L:42:HIS:HB2	1.91	0.52
1:A:453:LEU:HD21	1:A:464:PHE:CE2	2.45	0.52
2:F:463:ILE:O	2:F:466:ALA:HB3	2.09	0.52
7:T:151:VAL:HG11	8:U:73:PHE:CD1	2.44	0.52
2:O:161:GLY:HA2	10:O:600:ANP:PA	2.49	0.52
2:F:132:ILE:HG13	2:F:133:LEU:N	2.24	0.52
1:L:175:LYS:HB2	10:L:600:ANP:O1B	2.10	0.52
1:L:505:LEU:O	1:L:505:LEU:HD13	2.10	0.52
6:W:4:LEU:CD2	6:W:28:LYS:NZ	2.72	0.52
2:D:105:ARG:O	2:D:106:GLY:O	2.27	0.52
2:F:275:ILE:O	2:F:283:PRO:HG3	2.10	0.52
1:L:271:LEU:HD11	1:L:325:PRO:HB3	1.90	0.52
2:E:266:SER:HB2	2:E:282:GLN:HE22	1.73	0.52
1:A:7:GLU:CD	6:S:94:ARG:NH1	2.63	0.52
2:F:135:THR:HB	2:F:137:ILE:HG13	1.91	0.52
3:P:52:TYR:HD2	3:P:179:PHE:HE2	1.57	0.52
3:P:52:TYR:CE2	3:P:179:PHE:HD2	2.27	0.52
3:G:42:ARG:O	3:G:43:VAL:C	2.48	0.52
2:N:142:LEU:HG	2:N:143:LEU:HD23	1.92	0.52
1:L:419:SER:O	1:L:423:ARG:NH1	2.42	0.52
1:A:217:VAL:HB	1:A:226:MET:HE3	1.91	0.52
1:J:97:VAL:O	1:J:99:VAL:HG23	2.10	0.52
2:E:372:ARG:NH1	2:E:375:GLN:HE22	2.07	0.52
1:J:327:ILE:HD11	1:J:342:VAL:HG21	1.91	0.52
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:168:GLU:HB2	2:M:420:VAL:HG13	1.91	0.52
2:F:86:VAL:HG23	2:F:87:GLY:N	2.24	0.52
2:O:133:LEU:HB2	2:O:148:LYS:HG2	1.92	0.52
6:W:26:ALA:C	6:W:28:LYS:H	2.12	0.52
6:S:35:VAL:HG12	6:S:39:LEU:HG	1.90	0.52
6:W:137:VAL:HG23	7:X:207:LYS:HZ2	1.75	0.52
2:N:175:LYS:HD2	2:N:431:LEU:HD23	1.90	0.52
1:B:139:ARG:O	1:B:140:ILE:HB	2.10	0.52
2:O:16:VAL:CG1	2:O:21:VAL:HG13	2.39	0.52
1:L:199:LEU:HD11	1:L:265:LEU:HB2	1.92	0.52
4:H:35:GLN:HG3	4:H:47:ILE:O	2.09	0.52
2:E:237:LEU:HD13	2:E:253:LEU:CD2	2.40	0.52
2:N:404:VAL:O	2:N:408:ARG:HD3	2.09	0.52
1:C:404:ALA:HB2	1:C:410:LEU:HD21	1.92	0.52
2:D:62:ALA:O	2:D:227:GLY:HA3	2.10	0.52
2:M:294:GLU:HA	2:M:294:GLU:OE1	2.10	0.52
1:A:3:THR:HG21	6:S:14:ILE:O	2.10	0.52
8:U:33:TRP:CH2	8:U:37:LEU:HD21	2.45	0.52
6:W:35:VAL:HG12	6:W:39:LEU:HG	1.91	0.52
6:W:95:LEU:C	6:W:97:ASN:H	2.13	0.52
2:O:49:VAL:CA	2:O:60:THR:HG22	2.40	0.52
3:P:203:ASN:HB3	4:Q:57:VAL:HG21	1.91	0.52
3:G:129:LYS:HG2	3:G:130:GLU:H	1.75	0.52
2:E:142:LEU:HG	2:E:143:LEU:HD23	1.90	0.52
3:G:52:TYR:CE2	3:G:179:PHE:HD2	2.28	0.52
2:E:39:GLN:HE21	2:E:76:LEU:HB2	1.74	0.52
1:C:313:ASN:HD21	1:C:315:ALA:HB3	1.74	0.52
6:W:11:ILE:O	6:W:12:TYR:HB2	2.10	0.52
2:M:220:GLY:HA3	2:M:232:VAL:HG21	1.91	0.52
1:C:204:VAL:HG11	1:C:247:PRO:HA	1.92	0.52
3:P:44:TYR:CE2	4:Q:23:PRO:HD3	2.45	0.52
2:D:266:SER:CA	2:D:282:GLN:HE22	2.21	0.52
9:V:16:ILE:HG23	9:V:19:TYR:HB3	1.92	0.52
1:J:453:LEU:HD21	1:J:464:PHE:CE2	2.45	0.52
2:N:470:ALA:HA	2:N:473:LEU:HB2	1.92	0.52
1:C:270:ASP:OD1	1:C:272:SER:HB2	2.09	0.52
5:R:31:LYS:O	5:R:35:MET:HG3	2.10	0.52
3:P:56:ASP:C	3:P:57:ILE:HG12	2.29	0.52
2:N:167:MET:HE3	2:N:420:VAL:HG11	1.92	0.52
2:O:146:TYR:HB3	2:O:152:ILE:HD11	1.92	0.52
3:G:38:LEU:HD13	3:G:218:LYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:94:ILE:HD11	2:M:197:TYR:CD1	2.45	0.52
3:P:44:TYR:HD1	3:P:45:GLY:N	2.08	0.52
1:B:311:LYS:NZ	1:B:318:GLY:O	2.41	0.52
3:G:10:LEU:HD21	3:G:246:LEU:HB3	1.91	0.52
4:Q:35:GLN:HG3	4:Q:47:ILE:O	2.10	0.52
1:B:38:ILE:HG12	1:B:285:LEU:CD2	2.40	0.52
2:O:181:SER:O	2:O:215:VAL:HA	2.09	0.52
6:S:129:THR:HG21	6:S:135:LYS:HG3	1.91	0.52
1:J:188:ARG:NH1	1:J:437:ALA:CA	2.73	0.52
2:F:385:GLN:HE21	2:F:385:GLN:HA	1.75	0.52
2:M:307:VAL:HG12	2:M:307:VAL:O	2.10	0.52
2:M:182:VAL:HG22	2:M:216:ALA:HB3	1.92	0.52
2:D:142:LEU:HD22	2:D:441:PHE:CD1	2.45	0.52
2:D:106:GLY:O	2:D:107:PRO:O	2.27	0.51
3:G:44:TYR:HD1	3:G:45:GLY:N	2.08	0.51
2:E:278:ALA:O	2:E:279:VAL:HG12	2.10	0.51
3:P:89:MET:CG	3:P:161:ILE:HD11	2.40	0.51
2:M:145:PRO:HB2	2:M:357:ILE:HD11	1.92	0.51
4:H:84:VAL:HG12	4:H:90:VAL:CG2	2.40	0.51
1:A:255:GLU:HG3	1:A:258:ARG:NH1	2.25	0.51
2:M:155:PHE:O	2:M:335:LEU:HB2	2.10	0.51
1:C:102:GLU:OE2	1:C:123:SER:HA	2.10	0.51
2:N:422:GLU:O	2:N:423:VAL:C	2.48	0.51
2:O:277:SER:OG	2:O:278:ALA:N	2.39	0.51
2:D:163:THR:O	2:D:166:ILE:HG22	2.09	0.51
1:C:213:VAL:HG21	1:C:235:THR:HG21	1.92	0.51
1:J:107:VAL:O	1:J:115:ILE:HG12	2.09	0.51
1:L:479:LEU:HD12	1:L:500:ILE:HD11	1.92	0.51
1:C:49:ALA:N	1:C:66:LEU:HD11	2.26	0.51
1:J:457:GLU:HG2	1:J:458:PRO:HD2	1.91	0.51
1:L:52:MET:HB2	1:L:95:VAL:HG22	1.91	0.51
1:A:188:ARG:HH12	1:A:436:MET:C	2.14	0.51
1:J:187:LYS:O	1:J:189:PHE:N	2.43	0.51
1:K:353:GLU:HB3	1:K:356:LEU:HD12	1.91	0.51
1:K:202:ILE:CG2	1:K:266:ILE:HG13	2.40	0.51
1:C:133:ALA:HB2	1:C:308:ARG:HG3	1.91	0.51
3:P:24:LYS:HB2	3:P:232:MET:HB3	1.92	0.51
1:J:184:ILE:HG22	1:J:435:PRO:HG2	1.92	0.51
7:T:146:ARG:NH1	9:V:64:PHE:HA	2.20	0.51
1:A:405:GLN:CA	1:A:405:GLN:HE21	2.23	0.51
1:K:48:GLN:HB3	2:O:68:GLY:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:97:VAL:HG11	2:N:228:ALA:HB1	1.93	0.51
1:C:136:ILE:HG23	2:D:194:ASN:N	2.25	0.51
4:Q:21:ALA:HB2	4:Q:26:VAL:HG23	1.93	0.51
2:F:287:THR:O	2:F:288:ASP:C	2.48	0.51
2:N:360:PRO:HB3	2:N:368:TYR:CD2	2.45	0.51
1:B:381:ARG:HG3	1:B:487:GLY:O	2.10	0.51
1:L:404:ALA:HB2	1:L:410:LEU:HD21	1.93	0.51
2:M:36:LEU:HD22	2:M:77:ASP:HA	1.92	0.51
2:M:409:LYS:HZ3	2:M:450:ASP:HA	1.75	0.51
5:I:37:THR:HG22	5:I:38:SER:H	1.74	0.51
1:A:74:VAL:HG21	1:A:281:MET:HG2	1.92	0.51
2:F:367:HIS:HA	2:F:438:ILE:HD13	1.92	0.51
2:N:21:VAL:HB	2:N:47:LEU:HD13	1.91	0.51
1:A:472:VAL:HG23	1:A:480:LEU:HD22	1.91	0.51
6:W:4:LEU:HD22	6:W:24:SER:HG	1.75	0.51
2:F:162:LYS:N	10:F:600:ANP:O1B	2.38	0.51
1:B:392:LEU:O	1:B:392:LEU:HD12	2.10	0.51
2:D:237:LEU:HD11	2:D:295:ARG:HE	1.76	0.51
1:L:44:LEU:O	1:L:47:VAL:HG12	2.09	0.51
1:C:479:LEU:HD12	1:C:500:ILE:HD11	1.91	0.51
3:P:128:PHE:HB3	5:R:42:ILE:CG2	2.40	0.51
2:D:183:PHE:HD2	2:D:184:ALA:N	2.07	0.51
2:F:374:VAL:HG13	2:F:410:ILE:HG21	1.93	0.51
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.40	0.51
5:I:31:LYS:O	5:I:35:MET:HG3	2.10	0.51
2:M:89:GLU:CG	2:M:110:THR:HB	2.40	0.51
1:A:107:VAL:HG11	2:D:123:PHE:CE2	2.46	0.51
1:K:106:ARG:CG	1:K:106:ARG:HH11	2.15	0.51
2:O:97:VAL:O	2:O:235:THR:OG1	2.28	0.51
1:L:99:VAL:HG21	1:L:127:ARG:CB	2.39	0.51
3:G:89:MET:CG	3:G:161:ILE:HD11	2.40	0.51
2:O:142:LEU:HG	2:O:143:LEU:HD23	1.93	0.51
1:C:292:GLU:O	1:C:293:ALA:HB3	2.11	0.51
1:A:34:ILE:HG21	1:A:82:ILE:HG22	1.93	0.51
6:S:12:TYR:CE2	6:S:16:GLY:HA3	2.46	0.51
1:K:65:ASN:HA	2:O:17:ILE:HD13	1.93	0.51
1:L:110:ALA:HB2	1:L:234:ALA:HB2	1.92	0.51
1:L:363:PRO:O	1:L:365:ILE:HG13	2.11	0.51
1:L:99:VAL:HG21	1:L:127:ARG:HB2	1.93	0.51
3:P:165:PHE:HB2	3:P:223:SER:OG	2.11	0.51
2:E:409:LYS:HG2	2:E:457:PHE:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:116:VAL:N	6:S:117:PRO:HD3	2.25	0.51
1:J:189:PHE:HB3	1:J:197:LYS:O	2.11	0.51
2:M:425:THR:OG1	2:M:426:GLY:N	2.43	0.51
1:L:446:TYR:CE1	1:L:450:ARG:HG3	2.46	0.51
6:W:57:ASN:CG	6:W:59:TYR:CD2	2.84	0.51
1:C:247:PRO:HB2	1:C:305:LEU:HD11	1.92	0.51
1:C:110:ALA:HB2	1:C:234:ALA:HB2	1.92	0.51
3:P:2:THR:HG22	3:P:4:LYS:H	1.75	0.51
7:T:176:TRP:HZ3	9:V:22:LYS:HB2	1.74	0.51
2:E:396:LEU:HD22	2:E:396:LEU:H	1.75	0.51
4:H:84:VAL:HG12	4:H:90:VAL:HG21	1.92	0.51
2:M:94:ILE:HD11	2:M:197:TYR:CE1	2.46	0.51
5:R:20:LYS:O	5:R:20:LYS:HG2	2.11	0.51
1:L:121:ILE:HD13	1:L:121:ILE:H	1.76	0.51
1:L:313:ASN:HD21	1:L:315:ALA:HB3	1.76	0.51
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.92	0.51
1:C:448:GLY:O	1:C:451:GLY:N	2.37	0.51
2:F:330:ASP:HA	2:F:356:ARG:HD3	1.93	0.51
1:L:213:VAL:HG21	1:L:235:THR:HG21	1.91	0.51
2:O:112:GLN:N	2:O:112:GLN:HE21	1.93	0.51
1:J:407:GLY:CA	1:J:410:LEU:HD21	2.39	0.51
2:O:25:PHE:CE1	2:O:30:PRO:HD3	2.46	0.51
1:J:107:VAL:HB	1:J:116:ASP:HB3	1.93	0.51
2:M:163:THR:O	2:M:166:ILE:HG22	2.11	0.51
3:P:204:TYR:CE2	4:Q:55:LEU:HD13	2.44	0.51
1:B:159:ILE:HG22	1:B:160:GLY:N	2.25	0.51
3:G:209:LEU:C	3:G:211:ASN:H	2.13	0.51
3:G:78:CYS:HA	3:G:228:ARG:HB2	1.91	0.51
1:B:148:THR:HG21	1:B:153:VAL:HG11	1.93	0.51
1:L:482:LYS:HE2	1:L:486:ASP:OD2	2.11	0.51
2:N:390:ILE:HG12	3:P:25:MET:CG	2.32	0.51
1:L:336:ALA:HB3	1:L:339:PRO:HD2	1.93	0.51
1:A:26:GLU:HB3	1:A:46:ASN:HD22	1.76	0.51
1:B:24:ASP:OD2	1:B:25:LEU:N	2.44	0.51
3:P:209:LEU:C	3:P:211:ASN:H	2.15	0.51
1:L:256:TYR:HD2	1:L:257:PHE:CD1	2.29	0.51
2:M:86:VAL:HG11	2:M:114:ALA:HB3	1.93	0.51
9:V:47:LEU:O	9:V:51:TYR:CE1	2.63	0.51
1:C:34:ILE:HG13	1:C:35:GLY:N	2.26	0.51
2:N:151:LYS:HG2	2:N:293:GLN:HE22	1.76	0.51
5:I:3:TYR:CD1	5:I:3:TYR:O	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:279:VAL:O	2:M:279:VAL:HG12	2.10	0.51
2:F:381:TYR:OH	2:F:408:ARG:NH1	2.42	0.51
2:F:146:TYR:HB3	2:F:152:ILE:HD11	1.93	0.51
1:J:157:VAL:N	1:J:158:PRO:HD3	2.26	0.51
2:O:385:GLN:HE21	2:O:385:GLN:HA	1.75	0.51
2:M:156:GLY:O	2:M:312:VAL:HG23	2.11	0.51
1:K:145:PRO:HG3	1:K:378:ALA:O	2.11	0.51
2:E:458:TYR:O	2:E:459:MET:HB2	2.11	0.51
1:L:271:LEU:CD1	1:L:325:PRO:HB3	2.41	0.51
2:D:91:LEU:HD21	2:D:243:PHE:HE2	1.75	0.51
4:Q:84:VAL:HG12	4:Q:90:VAL:CG2	2.41	0.51
1:C:376:SER:C	1:C:378:ALA:N	2.63	0.51
2:D:26:ASP:HA	6:S:6:ARG:NH1	2.26	0.51
1:L:501:VAL:HG23	1:L:502:THR:H	1.75	0.51
2:M:97:VAL:HG22	2:M:232:VAL:HG22	1.93	0.51
2:F:151:LYS:HD3	2:F:328:HIS:O	2.11	0.51
2:M:187:GLY:HA2	2:M:229:ARG:HD3	1.93	0.51
2:O:399:GLU:O	2:O:402:LEU:HB3	2.11	0.51
2:E:54:GLY:O	2:E:55:GLU:HB2	2.10	0.51
6:W:54:SER:HA	6:W:57:ASN:HB2	1.92	0.50
6:S:91:GLU:C	6:S:93:GLY:H	2.14	0.50
1:A:246:ALA:HB3	1:A:247:PRO:HD3	1.92	0.50
2:O:249:GLN:HG3	2:O:250:ASP:N	2.25	0.50
1:J:97:VAL:HG12	1:J:111:LEU:O	2.11	0.50
1:K:26:GLU:HA	1:K:45:ARG:H	1.75	0.50
2:D:89:GLU:CG	2:D:110:THR:HB	2.42	0.50
1:K:485:THR:C	1:K:487:GLY:H	2.14	0.50
2:O:382:LYS:O	2:O:385:GLN:HB2	2.11	0.50
1:K:150:ILE:O	1:K:151:LYS:C	2.50	0.50
1:A:300:TYR:CD2	1:A:304:ARG:NH1	2.78	0.50
1:L:208:GLN:O	1:L:235:THR:HB	2.10	0.50
6:S:54:SER:HA	6:S:57:ASN:HB2	1.94	0.50
1:K:99:VAL:HG21	1:K:127:ARG:CG	2.41	0.50
3:P:137:THR:O	3:P:140:ASP:HB2	2.12	0.50
2:M:338:ALA:O	2:M:342:LEU:HG	2.11	0.50
2:E:117:HIS:O	2:E:118:ALA:HB2	2.11	0.50
1:A:67:GLU:HB3	1:A:68:PRO:CD	2.41	0.50
6:W:32:LEU:HB3	6:W:109:MSE:SE	2.61	0.50
1:L:134:PRO:HG3	1:L:258:ARG:HH21	1.77	0.50
7:T:176:TRP:CD2	9:V:30:VAL:HG21	2.47	0.50
1:A:216:LEU:HD13	1:A:220:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:146:TYR:CG	2:M:152:ILE:HD13	2.47	0.50
3:P:71:VAL:HG22	3:P:108:VAL:CG1	2.41	0.50
7:X:174:ILE:O	7:X:177:VAL:HB	2.10	0.50
2:N:416:GLN:HB2	2:N:417:PRO:HD2	1.92	0.50
2:O:244:ARG:HG3	2:O:302:GLY:CA	2.41	0.50
2:E:410:ILE:HG23	2:E:441:PHE:CE2	2.46	0.50
3:P:52:TYR:HD2	3:P:179:PHE:CE2	2.29	0.50
6:S:179:ILE:HG13	6:S:184:ARG:HD2	1.93	0.50
2:N:244:ARG:HG3	2:N:303:SER:N	2.27	0.50
1:A:188:ARG:HG2	1:A:189:PHE:CD1	2.46	0.50
1:A:99:VAL:HG21	1:A:127:ARG:CB	2.41	0.50
1:A:99:VAL:HG21	1:A:127:ARG:HB3	1.93	0.50
2:F:163:THR:O	2:F:166:ILE:HG22	2.10	0.50
3:P:247:THR:CG2	3:P:247:THR:O	2.56	0.50
1:B:97:VAL:HG11	1:B:249:SER:HB3	1.92	0.50
1:L:476:HIS:C	1:L:478:ALA:N	2.64	0.50
2:F:384:LEU:O	2:F:388:ILE:HG13	2.11	0.50
2:M:390:ILE:HG22	2:M:391:LEU:CD1	2.41	0.50
6:W:62:ARG:HD3	6:W:91:GLU:O	2.11	0.50
6:S:109:MSE:HE3	6:S:109:MSE:HA	1.94	0.50
1:A:199:LEU:HD21	1:A:265:LEU:HB2	1.93	0.50
1:B:307:GLU:HG3	2:F:223:ASN:HB3	1.93	0.50
1:J:44:LEU:O	1:J:46:ASN:N	2.44	0.50
7:T:201:LEU:CD1	9:V:7:PRO:HB3	2.41	0.50
7:T:189:GLN:HA	7:T:192:GLU:OE2	2.11	0.50
3:G:81:ILE:HD13	3:G:171:TYR:CZ	2.47	0.50
6:S:125:ALA:O	6:S:126:LEU:C	2.50	0.50
4:Q:40:THR:C	4:Q:42:THR:H	2.15	0.50
1:K:415:GLN:HA	1:K:418:LEU:HD12	1.93	0.50
1:K:172:GLN:CA	10:K:600:ANP:HNB1	2.20	0.50
1:J:300:TYR:CD2	1:J:304:ARG:NH1	2.80	0.50
2:D:164:VAL:HG21	12:D:600:ADP:C8	2.46	0.50
1:C:199:LEU:HD11	1:C:265:LEU:HB2	1.92	0.50
3:G:52:TYR:HD2	3:G:179:PHE:CE2	2.30	0.50
1:L:461:ILE:O	1:L:461:ILE:CG2	2.60	0.50
6:S:114:GLY:HA2	6:S:128:GLU:HG2	1.93	0.50
1:C:476:HIS:C	1:C:478:ALA:N	2.64	0.50
1:K:267:ILE:HG12	1:K:324:LEU:HB2	1.93	0.50
6:S:7:PRO:HG2	6:S:23:TYR:CB	2.41	0.50
6:S:42:VAL:HG23	6:S:78:PHE:CZ	2.47	0.50
6:S:61:LYS:HG2	6:S:62:ARG:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:71:VAL:HG22	3:G:108:VAL:CG1	2.41	0.50
1:K:149:GLY:HA3	1:K:185:ASN:OD1	2.10	0.50
1:L:386:VAL:HB	1:L:445:ILE:HG22	1.93	0.50
2:D:183:PHE:CD2	2:D:184:ALA:N	2.80	0.50
3:G:115:ILE:O	3:G:115:ILE:CG2	2.59	0.50
3:G:209:LEU:O	3:G:212:ILE:HG22	2.11	0.50
1:A:321:LEU:HD12	1:A:322:THR:N	2.26	0.50
2:O:180:TYR:CD1	2:O:249:GLN:HG2	2.46	0.50
1:L:376:SER:HA	1:L:379:GLN:HG3	1.93	0.50
3:G:190:MET:HE2	3:G:190:MET:HA	1.94	0.50
7:T:147:VAL:HG22	9:V:62:PHE:CZ	2.47	0.50
1:C:258:ARG:HG2	1:C:259:ASP:N	2.27	0.50
1:L:47:VAL:HG11	1:L:71:VAL:HG21	1.93	0.50
3:P:6:ILE:HG23	3:P:246:LEU:CD2	2.42	0.50
9:V:6:ASP:H	9:V:7:PRO:CD	2.25	0.50
3:P:209:LEU:O	3:P:212:ILE:HG22	2.12	0.50
2:N:145:PRO:HD2	2:N:355:SER:HB3	1.94	0.50
2:O:180:TYR:CD1	2:O:243:PHE:HD2	2.29	0.50
2:M:387:ILE:HG22	2:M:388:ILE:N	2.26	0.50
2:F:252:LEU:CD2	2:F:305:THR:HB	2.42	0.50
2:D:359:ASP:O	2:D:363:VAL:HG22	2.11	0.50
1:K:144:GLU:OE2	1:K:311:LYS:NZ	2.37	0.50
7:X:193:THR:C	7:X:195:ALA:H	2.15	0.50
2:N:160:VAL:HB	2:N:335:LEU:HB3	1.92	0.50
1:C:271:LEU:HD11	1:C:325:PRO:HB3	1.94	0.50
2:N:313:PRO:HD2	2:N:322:PRO:HG3	1.93	0.50
1:B:149:GLY:HA3	1:B:185:ASN:OD1	2.11	0.50
3:G:241:GLU:O	3:G:242:MET:C	2.50	0.50
7:T:198:ILE:CD1	9:V:11:LEU:HD11	2.41	0.50
1:J:289:PRO:HG3	2:M:275:ILE:HG21	1.94	0.50
1:J:468:PHE:O	1:J:472:VAL:HG13	2.11	0.50
2:D:193:GLY:HA3	2:D:219:TYR:HE2	1.76	0.50
1:K:188:ARG:HG3	1:K:189:PHE:CE1	2.47	0.50
2:O:17:ILE:HG23	2:O:17:ILE:O	2.12	0.50
1:J:203:TYR:O	1:J:203:TYR:CD2	2.65	0.50
2:O:153:GLY:HA3	2:O:329:LEU:HD13	1.94	0.50
6:W:91:GLU:C	6:W:93:GLY:H	2.15	0.50
2:M:266:SER:CA	2:M:282:GLN:HE22	2.23	0.50
1:C:300:TYR:CZ	1:C:304:ARG:HD2	2.46	0.50
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.40	0.50
1:J:26:GLU:O	1:J:46:ASN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:GLY:HA3	2:F:431:LEU:HG	1.94	0.50
2:M:313:PRO:HG2	2:M:319:ASP:CG	2.32	0.50
1:L:140:ILE:HG22	1:L:313:ASN:HA	1.94	0.50
2:M:177:HIS:CD2	2:M:179:GLY:H	2.30	0.50
1:A:7:GLU:OE1	6:S:94:ARG:NH1	2.45	0.49
2:N:223:ASN:HD22	2:N:223:ASN:N	1.98	0.49
2:M:310:ILE:H	2:M:310:ILE:HD12	1.75	0.49
1:C:352:LEU:O	1:C:353:GLU:HB2	2.11	0.49
1:B:107:VAL:HG12	1:B:115:ILE:HD11	1.93	0.49
2:F:91:LEU:HD21	2:F:180:TYR:CD2	2.47	0.49
2:F:449:TYR:O	2:F:451:HIS:N	2.45	0.49
2:D:409:LYS:HZ3	2:D:450:ASP:HA	1.77	0.49
2:D:168:GLU:O	2:D:168:GLU:HG3	2.12	0.49
2:D:103:ASP:OD1	2:D:103:ASP:N	2.45	0.49
2:M:172:ASN:ND2	2:M:431:LEU:HD12	2.27	0.49
1:C:60:LYS:O	1:C:76:PHE:HB2	2.11	0.49
2:N:63:MET:O	2:N:64:ASP:HB2	2.11	0.49
1:A:217:VAL:HB	1:A:226:MET:HE2	1.94	0.49
4:H:67:ALA:HB3	4:H:71:THR:N	2.27	0.49
1:B:485:THR:HG22	1:B:486:ASP:N	2.26	0.49
2:E:449:TYR:HD2	2:E:452:LEU:HD12	1.77	0.49
3:G:137:THR:O	3:G:140:ASP:HB2	2.10	0.49
1:A:97:VAL:O	1:A:99:VAL:HG23	2.12	0.49
2:F:51:GLN:HB2	2:F:59:ARG:HB3	1.94	0.49
1:L:314:ASP:C	1:L:316:PHE:H	2.15	0.49
1:K:166:LEU:HB2	1:K:346:THR:HG21	1.94	0.49
1:L:204:VAL:HG11	1:L:247:PRO:HA	1.94	0.49
5:R:5:ARG:O	5:R:6:GLN:HB3	2.12	0.49
1:K:107:VAL:HG12	1:K:115:ILE:HD11	1.93	0.49
2:D:310:ILE:HD12	2:D:310:ILE:N	2.27	0.49
7:T:174:ILE:O	7:T:177:VAL:HB	2.13	0.49
1:A:479:LEU:HA	1:A:482:LYS:HB3	1.94	0.49
1:L:66:LEU:O	2:M:15:ALA:HA	2.12	0.49
2:M:428:LEU:O	2:M:429:GLY:O	2.30	0.49
3:P:42:ARG:O	3:P:43:VAL:C	2.50	0.49
4:H:129:ALA:O	4:H:133:ILE:HG13	2.12	0.49
1:C:209:LYS:HZ3	1:C:211:SER:HB2	1.77	0.49
1:L:448:GLY:O	1:L:451:GLY:N	2.37	0.49
1:A:29:GLY:HA3	1:A:42:HIS:O	2.12	0.49
6:S:7:PRO:HB2	6:S:108:MSE:HE1	1.94	0.49
6:S:39:LEU:HB3	6:S:102:ILE:CG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:203:LEU:O	7:X:207:LYS:HG3	2.12	0.49
10:K:600:ANP:H8	10:K:600:ANP:O5'	2.11	0.49
2:M:218:VAL:HG21	2:M:236:GLY:HA2	1.94	0.49
1:L:455:LYS:C	1:L:456:LEU:HD12	2.33	0.49
7:T:191:LYS:HD3	7:T:194:ILE:HD11	1.94	0.49
2:F:290:GLY:HA2	2:F:328:HIS:CE1	2.47	0.49
2:F:146:TYR:CG	2:F:152:ILE:HD13	2.47	0.49
1:L:292:GLU:O	1:L:293:ALA:HB3	2.12	0.49
2:N:117:HIS:O	2:N:118:ALA:HB2	2.13	0.49
6:W:133:GLU:CD	7:X:207:LYS:HG2	2.31	0.49
1:L:343:ILE:HG23	1:L:349:GLN:NE2	2.27	0.49
1:L:352:LEU:HG	1:L:364:ALA:O	2.13	0.49
7:T:173:MSE:HA	9:V:22:LYS:HE2	1.95	0.49
2:E:170:ILE:CG2	2:E:215:VAL:HG22	2.40	0.49
1:L:42:HIS:ND1	1:L:45:ARG:NH2	2.60	0.49
1:C:455:LYS:C	1:C:456:LEU:HD12	2.33	0.49
2:E:430:LYS:HG3	2:E:461:GLY:CA	2.42	0.49
2:E:470:ALA:HA	2:E:473:LEU:HD12	1.95	0.49
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.94	0.49
1:L:166:LEU:HD22	1:L:342:VAL:HG12	1.93	0.49
1:J:67:GLU:HB3	1:J:68:PRO:CD	2.42	0.49
2:D:187:GLY:HA2	2:D:229:ARG:HD3	1.94	0.49
1:J:167:ILE:HB	1:J:326:VAL:HG22	1.94	0.49
1:C:268:TYR:CZ	1:C:305:LEU:HD21	2.47	0.49
2:D:31:PRO:HD2	2:D:34:ASN:HD21	1.75	0.49
2:O:25:PHE:CE1	2:O:30:PRO:CD	2.96	0.49
6:S:39:LEU:CB	6:S:102:ILE:HG23	2.41	0.49
1:C:255:GLU:CG	1:C:258:ARG:HH12	2.21	0.49
2:D:452:LEU:HD22	2:D:470:ALA:CB	2.41	0.49
1:L:45:ARG:HH11	2:M:71:ARG:HH12	1.57	0.49
1:J:338:ILE:HB	1:J:339:PRO:HD3	1.95	0.49
1:C:99:VAL:HG21	1:C:127:ARG:CB	2.42	0.49
3:P:81:ILE:HD13	3:P:171:TYR:CZ	2.47	0.49
2:N:14:VAL:HG22	2:N:24:GLN:HB2	1.95	0.49
1:J:405:GLN:CA	1:J:405:GLN:HE21	2.25	0.49
1:A:107:VAL:O	1:A:115:ILE:HG12	2.11	0.49
1:B:148:THR:HA	1:B:182:THR:HG23	1.95	0.49
2:O:462:PRO:HD2	2:O:465:GLU:CD	2.33	0.49
2:M:257:ASN:O	2:M:259:PHE:N	2.45	0.49
1:C:314:ASP:C	1:C:316:PHE:H	2.15	0.49
1:J:34:ILE:HG21	1:J:82:ILE:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:O	1:B:151:LYS:C	2.51	0.49
2:D:137:ILE:HD13	2:D:418:PHE:CZ	2.47	0.49
2:F:45:LEU:HD23	2:F:69:LEU:HD21	1.94	0.49
1:B:62:MET:H	1:B:73:VAL:HG13	1.76	0.49
1:K:97:VAL:HG11	1:K:249:SER:HB3	1.95	0.49
6:S:11:ILE:HD13	6:S:104:ALA:HB1	1.93	0.49
1:B:99:VAL:HG11	1:B:256:TYR:HB2	1.93	0.49
5:R:11:TYR:O	5:R:14:TYR:HB3	2.12	0.49
2:E:381:TYR:CE2	2:E:408:ARG:HG3	2.47	0.49
1:J:26:GLU:C	1:J:27:GLU:HG2	2.33	0.49
3:G:13:ILE:HG22	3:G:243:ILE:CD1	2.42	0.49
1:L:386:VAL:HG12	1:L:449:VAL:CG1	2.40	0.49
2:E:229:ARG:O	2:E:232:VAL:HG12	2.12	0.49
1:K:24:ASP:OD2	1:K:25:LEU:N	2.45	0.49
2:M:244:ARG:HD3	2:M:304:ILE:HD11	1.94	0.49
1:J:251:CYS:O	1:J:255:GLU:HB2	2.13	0.49
1:L:212:THR:O	1:L:213:VAL:C	2.50	0.49
1:L:213:VAL:O	1:L:216:LEU:HB3	2.13	0.49
6:W:42:VAL:HG23	6:W:78:PHE:CZ	2.48	0.49
6:S:34:GLN:O	6:S:38:GLU:HG3	2.13	0.49
1:K:106:ARG:NH2	1:K:118:LYS:O	2.46	0.49
2:F:49:VAL:CA	2:F:60:THR:HG22	2.43	0.49
1:J:321:LEU:HD12	1:J:322:THR:N	2.28	0.49
1:C:357:PHE:CD2	1:C:357:PHE:C	2.86	0.49
1:B:144:GLU:OE2	1:B:311:LYS:NZ	2.40	0.49
3:P:115:ILE:CG2	3:P:115:ILE:O	2.60	0.49
3:G:54:LYS:O	3:G:55:ALA:HB2	2.12	0.49
3:G:207:TYR:CD2	4:H:81:SER:HB3	2.47	0.49
1:L:270:ASP:OD1	1:L:272:SER:HB2	2.11	0.49
2:F:443:GLN:HE22	2:F:463:ILE:HG21	1.77	0.49
2:M:313:PRO:O	2:M:314:ALA:HB3	2.12	0.49
1:A:187:LYS:O	1:A:189:PHE:N	2.46	0.49
2:O:86:VAL:HG23	2:O:242:TYR:CG	2.48	0.49
1:K:486:ASP:O	1:K:488:LYS:HB3	2.11	0.49
2:F:434:LEU:O	2:F:434:LEU:HD12	2.13	0.49
4:Q:79:SER:OG	5:R:15:SER:HA	2.13	0.49
1:C:482:LYS:HE2	1:C:486:ASP:OD2	2.12	0.49
7:T:160:SER:HA	7:T:163:ASN:HB2	1.95	0.49
4:Q:19:THR:O	4:Q:91:GLN:HA	2.13	0.49
4:H:40:THR:C	4:H:42:THR:H	2.14	0.49
1:J:407:GLY:HA3	1:J:410:LEU:CD2	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:62:MET:O	1:L:73:VAL:HA	2.12	0.49
3:P:10:LEU:HA	3:P:10:LEU:HD23	1.60	0.49
4:H:109:LYS:O	4:H:112:LEU:HB3	2.12	0.49
3:G:113:ARG:O	3:G:117:HIS:HB2	2.13	0.49
1:C:343:ILE:HG23	1:C:349:GLN:HE21	1.78	0.49
1:L:95:VAL:O	1:L:129:VAL:HG22	2.13	0.49
2:D:36:LEU:HD22	2:D:77:ASP:HA	1.94	0.49
1:B:201:CYS:O	1:B:229:THR:HA	2.13	0.49
1:A:439:GLU:HG2	1:A:440:GLU:N	2.28	0.49
2:D:244:ARG:HD3	2:D:304:ILE:HD11	1.93	0.49
1:C:446:TYR:CE1	1:C:450:ARG:HG3	2.48	0.49
2:O:223:ASN:ND2	2:O:223:ASN:N	2.58	0.49
3:G:2:THR:HG22	3:G:4:LYS:H	1.78	0.49
1:K:163:GLN:O	1:K:322:THR:HG23	2.12	0.49
2:M:27:GLU:HA	6:W:3:LYS:CD	2.41	0.49
2:E:175:LYS:HD3	2:E:431:LEU:HD23	1.95	0.49
1:K:30:ARG:NH2	6:W:58:PRO:O	2.46	0.49
2:F:377:ILE:HD11	2:F:406:ARG:HB2	1.94	0.49
1:C:164:ARG:HD3	1:C:164:ARG:N	2.28	0.49
2:O:93:ARG:NH1	2:O:108:ILE:HG12	2.27	0.49
7:T:156:ASP:HA	7:T:159:ILE:HG13	1.95	0.49
1:A:201:CYS:O	1:A:229:THR:HA	2.13	0.49
2:O:70:VAL:HG12	2:O:71:ARG:N	2.28	0.49
1:A:347:ASP:CB	2:E:191:ARG:HH21	2.25	0.49
4:Q:129:ALA:O	4:Q:133:ILE:HG13	2.13	0.49
6:W:4:LEU:HD21	6:W:28:LYS:HZ2	1.78	0.48
6:W:79:SER:N	6:W:80:PRO:CD	2.76	0.48
1:C:137:ILE:O	1:C:139:ARG:N	2.45	0.48
1:L:306:LEU:CD2	1:L:325:PRO:HG3	2.33	0.48
6:S:4:LEU:HD22	6:S:24:SER:OG	2.13	0.48
6:S:79:SER:N	6:S:80:PRO:CD	2.74	0.48
1:J:71:VAL:CG1	1:J:73:VAL:HG23	2.42	0.48
2:F:94:ILE:HG22	2:F:102:ILE:CG1	2.39	0.48
4:Q:84:VAL:HG12	4:Q:90:VAL:HG21	1.93	0.48
1:K:399:GLU:CD	1:K:399:GLU:N	2.67	0.48
1:K:30:ARG:HH22	6:W:58:PRO:HB2	1.78	0.48
1:C:45:ARG:HH11	2:D:71:ARG:NH1	2.11	0.48
7:T:151:VAL:HG11	8:U:73:PHE:CE1	2.48	0.48
4:H:54:THR:H	4:H:84:VAL:HG23	1.78	0.48
2:O:252:LEU:CD2	2:O:305:THR:HB	2.43	0.48
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:434:SER:N	1:J:435:PRO:HD3	2.28	0.48
1:K:65:ASN:ND2	2:O:17:ILE:HD13	2.26	0.48
2:D:172:ASN:ND2	2:D:431:LEU:HD12	2.28	0.48
1:J:382:ALA:HB2	1:J:487:GLY:O	2.13	0.48
4:H:19:THR:O	4:H:91:GLN:HA	2.13	0.48
2:D:428:LEU:O	2:D:429:GLY:O	2.31	0.48
2:O:189:ARG:HB2	2:O:192:GLU:HG3	1.95	0.48
6:W:61:LYS:HG2	6:W:62:ARG:H	1.78	0.48
1:A:9:SER:O	1:A:12:LEU:N	2.46	0.48
6:S:62:ARG:HD3	6:S:91:GLU:O	2.13	0.48
2:M:452:LEU:HD22	2:M:470:ALA:CB	2.41	0.48
7:T:193:THR:C	7:T:195:ALA:H	2.15	0.48
2:N:23:VAL:HG12	2:N:25:PHE:HE1	1.77	0.48
1:C:461:ILE:CG2	1:C:461:ILE:O	2.60	0.48
1:A:305:LEU:O	1:A:308:ARG:HB2	2.13	0.48
1:B:360:GLY:O	1:B:362:ARG:HG3	2.13	0.48
2:M:268:VAL:HG23	2:M:272:LEU:CD1	2.43	0.48
1:C:131:LEU:HD22	1:C:132:LYS:N	2.27	0.48
1:C:210:ARG:HB2	2:F:126:MET:CE	2.43	0.48
2:D:402:LEU:HD21	2:D:406:ARG:NH2	2.28	0.48
3:G:197:ASP:C	3:G:199:ASP:H	2.16	0.48
9:V:15:LYS:O	9:V:16:ILE:HG12	2.13	0.48
2:M:183:PHE:HD2	2:M:184:ALA:N	2.11	0.48
2:N:243:PHE:HB3	2:N:249:GLN:OE1	2.12	0.48
1:L:453:LEU:O	1:L:455:LYS:N	2.46	0.48
1:C:199:LEU:HD12	1:C:263:HIS:O	2.13	0.48
3:P:113:ARG:O	3:P:117:HIS:HB2	2.13	0.48
1:K:453:LEU:HD13	1:K:461:ILE:CD1	2.43	0.48
2:F:180:TYR:CD1	2:F:249:GLN:HG2	2.49	0.48
4:Q:67:ALA:HB3	4:Q:71:THR:N	2.26	0.48
3:P:164:ARG:HH22	3:P:166:ARG:CZ	2.26	0.48
1:A:129:VAL:HG21	1:A:245:LEU:HD21	1.96	0.48
1:C:468:PHE:O	1:C:472:VAL:HG22	2.13	0.48
2:O:290:GLY:HA2	2:O:328:HIS:CE1	2.48	0.48
1:J:439:GLU:HG2	1:J:440:GLU:N	2.28	0.48
2:D:181:SER:O	2:D:215:VAL:HA	2.13	0.48
1:B:76:PHE:CE2	1:B:245:LEU:HD22	2.49	0.48
2:F:93:ARG:NH1	2:F:108:ILE:HG12	2.28	0.48
1:J:509:GLU:O	1:J:510:ALA:CB	2.61	0.48
1:K:374:VAL:HG23	1:K:375:GLY:N	2.28	0.48
6:S:85:LEU:HD23	6:S:85:LEU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:22:LEU:HD13	6:W:85:LEU:CD1	2.20	0.48
1:C:323:ALA:O	1:C:325:PRO:HD3	2.13	0.48
2:E:279:VAL:HG11	2:E:320:PRO:HG2	1.96	0.48
1:K:256:TYR:C	1:K:256:TYR:CD2	2.86	0.48
5:I:5:ARG:O	5:I:6:GLN:HB3	2.13	0.48
2:N:449:TYR:HE2	2:N:467:VAL:HG22	1.78	0.48
3:G:58:LYS:O	3:G:184:ILE:HD11	2.13	0.48
2:O:221:GLN:CA	2:O:221:GLN:HE21	2.25	0.48
6:S:179:ILE:C	6:S:183:SER:HB2	2.33	0.48
2:N:151:LYS:HE3	2:N:296:ILE:O	2.14	0.48
1:L:140:ILE:CG2	1:L:313:ASN:HA	2.44	0.48
2:D:420:VAL:HG23	2:D:420:VAL:O	2.14	0.48
1:K:249:SER:O	1:K:253:MET:HG3	2.13	0.48
2:O:247:GLU:O	2:O:248:GLY:C	2.51	0.48
2:N:353:SER:C	2:N:354:THR:HG22	2.33	0.48
1:L:268:TYR:H	1:L:268:TYR:HD1	1.61	0.48
6:S:106:SER:O	6:S:108:MSE:N	2.46	0.48
1:A:12:LEU:CD2	6:S:88:LEU:HD12	2.44	0.48
7:T:142:GLU:O	7:T:146:ARG:HG3	2.14	0.48
2:M:204:GLY:HA2	2:M:206:ILE:O	2.13	0.48
1:L:312:MET:HB2	1:L:319:GLY:O	2.13	0.48
5:I:11:TYR:O	5:I:14:TYR:HB3	2.14	0.48
2:F:457:PHE:HD1	2:F:457:PHE:N	2.11	0.48
3:G:108:VAL:HG22	3:G:131:VAL:HG21	1.96	0.48
9:V:13:VAL:C	9:V:15:LYS:H	2.15	0.48
1:C:386:VAL:HB	1:C:445:ILE:CG2	2.43	0.48
1:L:400:VAL:O	1:L:400:VAL:HG12	2.14	0.48
1:C:458:PRO:HA	1:C:461:ILE:HG13	1.94	0.48
3:G:161:ILE:HG22	3:G:175:GLU:HA	1.95	0.48
2:D:151:LYS:HZ1	2:D:293:GLN:HB3	1.79	0.48
6:S:127:ASP:N	6:S:127:ASP:OD1	2.46	0.48
1:A:140:ILE:HD12	1:A:141:SER:H	1.78	0.48
8:U:89:VAL:O	8:U:89:VAL:HG12	2.12	0.48
2:M:251:VAL:HG23	2:M:303:SER:O	2.13	0.48
1:C:420:ARG:HG3	1:C:421:GLY:N	2.28	0.48
3:G:84:SER:HB3	3:G:173:THR:OG1	2.14	0.48
2:O:31:PRO:HD2	2:O:34:ASN:CG	2.33	0.48
1:L:136:ILE:HG23	2:M:194:ASN:CA	2.43	0.48
7:T:173:MSE:HG3	9:V:22:LYS:HG3	1.94	0.48
9:V:22:LYS:HZ2	9:V:30:VAL:CG2	2.23	0.48
3:P:161:ILE:HG22	3:P:175:GLU:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Z:22:LYS:HE3	9:Z:23:ARG:HB3	1.96	0.48
2:E:422:GLU:C	2:E:424:PHE:N	2.66	0.48
2:E:443:GLN:O	2:E:445:LEU:N	2.46	0.48
1:K:485:THR:HG22	1:K:486:ASP:N	2.28	0.48
2:O:133:LEU:HD12	2:O:133:LEU:C	2.33	0.48
1:C:314:ASP:O	1:C:316:PHE:N	2.47	0.48
1:L:131:LEU:HD22	1:L:132:LYS:N	2.28	0.48
3:P:182:ASP:HA	3:P:185:SER:HB2	1.96	0.48
1:L:107:VAL:HG12	1:L:115:ILE:HD11	1.94	0.48
1:K:27:GLU:OE2	1:K:46:ASN:ND2	2.42	0.48
2:O:356:ARG:HH11	2:O:356:ARG:CB	2.26	0.48
2:F:266:SER:CB	2:F:282:GLN:HE22	2.26	0.48
1:J:468:PHE:CE1	1:J:501:VAL:CG2	2.94	0.48
2:E:142:LEU:HD22	2:E:441:PHE:CD1	2.48	0.48
1:K:423:ARG:HD3	1:K:454:ASP:HA	1.96	0.48
1:C:419:SER:O	1:C:423:ARG:NH1	2.46	0.48
2:D:387:ILE:HG12	3:G:19:ILE:CD1	2.44	0.48
1:A:188:ARG:NH1	1:A:437:ALA:HA	2.28	0.48
2:O:86:VAL:CG2	2:O:87:GLY:N	2.77	0.48
2:D:313:PRO:O	2:D:314:ALA:HB3	2.13	0.48
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.96	0.48
6:W:4:LEU:HD23	6:W:28:LYS:HZ1	1.79	0.48
1:C:27:GLU:O	1:C:28:THR:CB	2.62	0.48
3:P:214:TYR:CZ	4:Q:23:PRO:HB3	2.49	0.48
4:Q:20:PHE:CD1	4:Q:92:LEU:HB3	2.48	0.48
1:J:25:LEU:O	1:J:26:GLU:HB2	2.12	0.48
1:K:137:ILE:C	1:K:139:ARG:H	2.17	0.48
3:P:143:VAL:HG12	3:P:143:VAL:O	2.14	0.48
1:J:214:ALA:O	1:J:217:VAL:HG22	2.14	0.48
1:C:400:VAL:HG12	1:C:400:VAL:O	2.14	0.48
6:S:184:ARG:HB3	6:S:185:ALA:H	1.57	0.48
1:B:423:ARG:HD3	1:B:454:ASP:HA	1.95	0.48
1:L:176:THR:C	1:L:178:ILE:H	2.17	0.48
7:T:155:LEU:CD2	8:U:66:VAL:HG22	2.43	0.48
1:L:102:GLU:OE2	1:L:123:SER:HA	2.14	0.48
6:S:42:VAL:HA	6:S:45:ILE:CG1	2.41	0.48
3:G:2:THR:O	3:G:6:ILE:HG12	2.13	0.48
1:K:140:ILE:HG12	1:K:141:SER:N	2.29	0.48
1:B:75:VAL:HG21	1:B:82:ILE:HD12	1.95	0.48
6:W:14:ILE:O	6:W:15:GLU:CB	2.61	0.48
2:F:137:ILE:HG23	2:F:418:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:249:GLN:HG3	2:F:250:ASP:N	2.29	0.48
2:F:377:ILE:HG12	2:F:407:ALA:HB2	1.95	0.48
1:L:218:LYS:HE2	1:L:222:ASP:CG	2.34	0.48
2:D:84:ILE:HD11	2:D:238:THR:CG2	2.43	0.48
9:Z:19:TYR:CD1	9:Z:22:LYS:HE2	2.48	0.48
6:S:135:LYS:HD2	6:S:139:LYS:HZ1	1.79	0.48
5:R:3:TYR:O	5:R:3:TYR:CD1	2.66	0.48
3:P:197:ASP:C	3:P:199:ASP:H	2.16	0.48
1:K:62:MET:H	1:K:73:VAL:HG13	1.79	0.48
3:G:182:ASP:HA	3:G:185:SER:HB2	1.95	0.48
1:K:76:PHE:CE2	1:K:245:LEU:HD22	2.49	0.48
3:P:190:MET:HE2	3:P:190:MET:HA	1.95	0.48
2:E:166:ILE:HG23	2:E:254:PHE:CE2	2.49	0.48
1:A:23:VAL:CG1	1:A:28:THR:HG23	2.36	0.48
2:M:247:GLU:HB2	2:M:249:GLN:HB2	1.93	0.48
1:K:96:ASP:HB2	1:K:127:ARG:O	2.13	0.48
1:J:115:ILE:O	2:M:124:VAL:HG13	2.13	0.48
5:R:40:SER:C	5:R:42:ILE:H	2.17	0.48
2:F:137:ILE:HG23	2:F:418:PHE:HE2	1.79	0.48
1:J:271:LEU:HA	1:J:271:LEU:HD23	1.73	0.48
2:O:384:LEU:O	2:O:388:ILE:HG13	2.14	0.48
1:J:272:SER:O	1:J:276:VAL:HG23	2.14	0.48
2:N:412:ARG:C	2:N:414:LEU:N	2.62	0.47
6:W:116:VAL:CG1	6:W:116:VAL:O	2.61	0.47
1:L:323:ALA:O	1:L:325:PRO:HD3	2.14	0.47
1:L:351:PHE:O	1:L:352:LEU:HD12	2.13	0.47
1:A:410:LEU:H	1:A:410:LEU:HD12	1.79	0.47
3:P:6:ILE:HG21	3:P:250:PHE:HB2	1.96	0.47
1:A:479:LEU:HD13	1:A:496:LYS:HZ2	1.77	0.47
1:L:218:LYS:HE2	1:L:222:ASP:OD2	2.14	0.47
6:S:18:TYR:HB2	6:S:101:VAL:HG21	1.96	0.47
1:B:442:VAL:HG11	1:B:483:ILE:HG21	1.96	0.47
2:M:61:ILE:HG21	2:M:227:GLY:HA2	1.95	0.47
2:N:54:GLY:O	2:N:55:GLU:HB2	2.14	0.47
1:K:136:ILE:HG23	2:O:194:ASN:N	2.29	0.47
2:N:16:VAL:O	2:N:16:VAL:HG12	2.14	0.47
1:J:284:LEU:C	1:J:286:ARG:H	2.18	0.47
1:K:190:ASN:O	1:K:198:LYS:HE2	2.14	0.47
2:F:277:SER:OG	2:F:278:ALA:N	2.47	0.47
2:E:103:ASP:O	2:E:105:ARG:HG3	2.14	0.47
1:L:380:THR:C	1:L:382:ALA:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:116:ILE:HA	2:E:238:THR:OG1	2.14	0.47
1:C:271:LEU:CD1	1:C:325:PRO:HB3	2.43	0.47
6:S:7:PRO:HG2	6:S:23:TYR:HB3	1.96	0.47
1:A:183:ILE:O	1:A:186:GLN:HB2	2.14	0.47
1:A:8:VAL:CG2	2:D:55:GLU:OE1	2.55	0.47
1:B:200:TYR:CD2	1:B:257:PHE:CE2	3.01	0.47
1:L:258:ARG:HG2	1:L:259:ASP:N	2.30	0.47
2:O:321:ALA:HB3	2:O:322:PRO:CD	2.41	0.47
3:G:5:ASP:N	3:G:5:ASP:OD1	2.47	0.47
1:C:365:ILE:CD1	1:C:366:ASN:N	2.76	0.47
2:O:23:VAL:HG11	2:O:75:VAL:HG21	1.95	0.47
3:P:5:ASP:N	3:P:5:ASP:OD1	2.46	0.47
1:A:227:LYS:HG3	1:A:228:TYR:HD2	1.76	0.47
1:C:453:LEU:O	1:C:455:LYS:N	2.47	0.47
1:L:453:LEU:C	1:L:455:LYS:H	2.18	0.47
3:G:51:LEU:HG	3:G:52:TYR:N	2.30	0.47
2:O:12:ARG:HB2	2:O:12:ARG:HH11	1.76	0.47
2:N:9:THR:HG21	2:N:27:GLU:HB3	1.97	0.47
1:A:62:MET:HB2	1:A:76:PHE:CE1	2.47	0.47
1:C:52:MET:HB2	1:C:95:VAL:HG22	1.95	0.47
1:C:140:ILE:CG2	1:C:313:ASN:HA	2.44	0.47
2:F:419:GLN:HA	2:F:429:GLY:HA3	1.96	0.47
2:E:110:THR:HG22	2:E:111:LYS:N	2.28	0.47
2:D:77:ASP:C	2:D:79:GLY:H	2.18	0.47
2:F:351:LEU:CD1	2:F:379:GLN:HB2	2.44	0.47
1:J:59:LEU:HA	1:J:59:LEU:HD23	1.65	0.47
1:L:97:VAL:HG23	1:L:98:PRO:O	2.14	0.47
2:N:116:ILE:HA	2:N:238:THR:OG1	2.14	0.47
6:W:5:VAL:O	6:W:7:PRO:HD3	2.15	0.47
2:O:234:LEU:HA	2:O:237:LEU:HB2	1.96	0.47
1:K:241:PRO:CG	1:K:281:MET:HE3	2.37	0.47
1:J:186:GLN:CG	1:J:199:LEU:HD23	2.44	0.47
2:E:281:TYR:CE2	2:E:321:ALA:HB2	2.49	0.47
4:Q:58:LEU:HD12	4:Q:80:GLY:N	2.29	0.47
1:K:200:TYR:CD2	1:K:257:PHE:CE2	3.01	0.47
1:J:227:LYS:HG3	1:J:228:TYR:HD2	1.79	0.47
2:F:259:PHE:CE2	2:F:263:GLN:HB2	2.49	0.47
2:O:94:ILE:HG22	2:O:102:ILE:CG1	2.40	0.47
1:J:283:LEU:O	2:M:275:ILE:HD12	2.13	0.47
1:A:44:LEU:C	1:A:46:ASN:H	2.18	0.47
4:Q:54:THR:H	4:Q:84:VAL:HG23	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:26:VAL:O	4:H:26:VAL:HG13	2.14	0.47
4:H:25:GLN:HG2	4:H:26:VAL:N	2.30	0.47
1:C:181:ASP:OD1	1:C:433:TYR:HD2	1.97	0.47
1:B:175:LYS:HB2	1:B:175:LYS:HE2	1.69	0.47
1:C:373:ARG:CZ	2:D:189:ARG:NH2	2.77	0.47
2:F:339:ILE:HG23	2:F:344:ILE:HB	1.97	0.47
1:J:65:ASN:OD1	1:J:285:LEU:HD13	2.14	0.47
1:K:125:ALA:C	1:K:126:ARG:HG2	2.34	0.47
2:N:284:THR:HB	2:N:288:ASP:OD2	2.14	0.47
1:C:176:THR:C	1:C:178:ILE:H	2.17	0.47
1:C:137:ILE:CG1	1:C:138:PRO:HD3	2.27	0.47
2:O:381:TYR:OH	2:O:408:ARG:NH1	2.47	0.47
2:O:381:TYR:CD1	2:O:404:VAL:HG22	2.49	0.47
2:D:96:ASN:ND2	2:D:98:ILE:N	2.49	0.47
2:E:266:SER:HB2	2:E:282:GLN:NE2	2.30	0.47
3:P:138:PHE:CD1	4:Q:23:PRO:HG3	2.49	0.47
2:N:461:GLY:HA3	2:N:462:PRO:HD3	1.76	0.47
3:P:58:LYS:O	3:P:184:ILE:HD11	2.15	0.47
1:L:458:PRO:HA	1:L:461:ILE:HG13	1.95	0.47
3:P:84:SER:HB3	3:P:173:THR:OG1	2.14	0.47
2:D:359:ASP:OD1	2:D:360:PRO:HD2	2.14	0.47
1:K:64:LEU:O	2:O:17:ILE:HD12	2.14	0.47
1:J:255:GLU:HG3	1:J:258:ARG:NH1	2.29	0.47
1:C:37:GLY:O	1:C:38:ILE:HD13	2.14	0.47
2:E:27:GLU:HA	2:E:27:GLU:OE2	2.14	0.47
2:D:133:LEU:HD12	2:D:133:LEU:C	2.35	0.47
1:C:107:VAL:HG12	1:C:115:ILE:HD11	1.97	0.47
1:K:41:VAL:CG1	1:K:88:VAL:HG21	2.45	0.47
2:M:136:GLY:HA2	2:M:432:VAL:O	2.14	0.47
2:M:365:SER:O	2:M:369:ASP:HB2	2.15	0.47
2:M:278:ALA:C	2:M:280:GLY:H	2.17	0.47
1:K:313:ASN:OD1	1:K:316:PHE:HD1	1.98	0.47
1:B:36:ASP:HB3	1:B:284:LEU:HD22	1.96	0.47
6:W:85:LEU:HD23	6:W:85:LEU:H	1.79	0.47
2:M:106:GLY:O	2:M:107:PRO:O	2.32	0.47
3:G:143:VAL:O	3:G:143:VAL:HG12	2.14	0.47
1:C:288:PRO:HG3	3:G:271:ALA:O	2.14	0.47
3:P:108:VAL:HG22	3:P:131:VAL:HG21	1.95	0.47
1:B:161:ARG:HA	1:B:322:THR:OG1	2.14	0.47
1:C:343:ILE:HG23	1:C:349:GLN:NE2	2.29	0.47
2:F:443:GLN:HE21	2:F:449:TYR:HE1	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:97:VAL:HG22	2:D:232:VAL:HG22	1.96	0.47
1:L:468:PHE:O	1:L:472:VAL:HG22	2.14	0.47
1:K:381:ARG:HG3	1:K:487:GLY:O	2.15	0.47
6:W:92:ASN:O	6:W:94:ARG:HG3	2.14	0.47
1:J:225:ALA:HA	1:J:228:TYR:HE2	1.72	0.47
1:L:457:GLU:H	1:L:460:LYS:NZ	2.12	0.47
7:T:150:GLU:O	7:T:154:ARG:HG2	2.14	0.47
4:H:21:ALA:HB2	4:H:26:VAL:HG23	1.96	0.47
2:F:180:TYR:CD1	2:F:243:PHE:HD2	2.33	0.47
1:K:59:LEU:HD13	1:K:75:VAL:CG1	2.44	0.47
1:K:75:VAL:HG21	1:K:82:ILE:HD12	1.96	0.47
4:H:116:GLN:O	4:H:119:LEU:HB3	2.14	0.47
1:C:295:PRO:HD2	1:C:298:VAL:HB	1.97	0.47
2:O:87:GLY:HA2	2:O:242:TYR:CE2	2.49	0.47
2:M:391:LEU:HD12	2:M:391:LEU:N	2.30	0.47
1:J:400:VAL:HG22	1:J:400:VAL:O	2.14	0.47
1:A:314:ASP:O	1:A:316:PHE:N	2.47	0.47
1:A:418:LEU:O	1:A:422:VAL:HG13	2.15	0.47
2:D:390:ILE:C	2:D:391:LEU:HD12	2.34	0.47
2:E:149:GLY:HA2	2:E:304:ILE:O	2.14	0.47
2:O:330:ASP:HA	2:O:356:ARG:HD3	1.97	0.47
6:W:22:LEU:CD2	6:W:85:LEU:HD22	2.45	0.47
1:J:403:PHE:HE1	3:P:22:SER:HB2	1.69	0.47
1:A:23:VAL:HG12	1:A:25:LEU:H	1.80	0.47
6:S:38:GLU:O	6:S:78:PHE:HE1	1.98	0.47
1:L:362:ARG:HH22	2:O:372:ARG:HB3	1.79	0.47
2:M:201:ILE:HG13	2:M:206:ILE:HB	1.96	0.47
3:G:203:ASN:O	4:H:57:VAL:HG13	2.15	0.47
9:V:22:LYS:C	9:V:24:GLN:H	2.18	0.47
2:N:462:PRO:HD2	2:N:465:GLU:HG3	1.95	0.47
1:A:71:VAL:HG23	2:E:71:ARG:CZ	2.44	0.47
4:Q:26:VAL:HG13	4:Q:26:VAL:O	2.13	0.47
1:B:48:GLN:HG3	1:B:51:GLU:HB2	1.96	0.47
2:F:181:SER:O	2:F:215:VAL:HA	2.14	0.47
2:F:463:ILE:O	2:F:467:VAL:HG23	2.15	0.47
1:B:485:THR:C	1:B:487:GLY:H	2.17	0.47
9:Z:17:ARG:HA	9:Z:20:ARG:HB2	1.96	0.47
2:N:168:GLU:HG2	2:N:418:PHE:CD2	2.50	0.47
1:C:140:ILE:HG22	1:C:313:ASN:HA	1.95	0.47
2:E:449:TYR:HE2	2:E:467:VAL:HG23	1.79	0.47
2:E:244:ARG:HG3	2:E:303:SER:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:158:ALA:HB2	2:M:311:TYR:HE1	1.80	0.47
2:M:35:ALA:C	2:M:36:LEU:HD23	2.35	0.47
2:F:408:ARG:HB3	2:F:454:GLU:OE1	2.15	0.47
1:L:176:THR:C	1:L:178:ILE:N	2.68	0.47
1:C:176:THR:C	1:C:178:ILE:N	2.68	0.47
2:D:390:ILE:HG22	2:D:391:LEU:CD1	2.44	0.47
1:K:157:VAL:N	1:K:158:PRO:CD	2.77	0.47
2:D:294:GLU:HA	2:D:294:GLU:OE1	2.14	0.47
2:D:307:VAL:HG12	2:D:307:VAL:O	2.14	0.47
2:E:317:LEU:HA	2:E:317:LEU:HD23	1.77	0.47
1:A:101:GLU:H	1:A:101:GLU:HG2	1.50	0.47
6:S:171:VAL:O	6:S:172:ASP:CB	2.62	0.47
1:A:286:ARG:NH2	3:G:272:LEU:HD13	2.29	0.47
1:A:294:TYR:HB3	1:A:298:VAL:HG11	1.96	0.47
1:L:420:ARG:HG3	1:L:421:GLY:N	2.30	0.47
2:D:94:ILE:HD11	2:D:197:TYR:CD1	2.49	0.47
2:M:408:ARG:NE	2:M:454:GLU:OE1	2.47	0.47
1:C:179:ALA:HB1	1:C:267:ILE:CD1	2.16	0.47
6:W:4:LEU:CD2	6:W:28:LYS:HZ1	2.27	0.47
1:L:247:PRO:CB	1:L:268:TYR:HD2	2.26	0.47
1:B:106:ARG:HH11	1:B:106:ARG:CG	2.14	0.47
2:M:154:LEU:CD1	2:M:165:LEU:HD23	2.40	0.47
1:C:386:VAL:HG12	1:C:449:VAL:CG1	2.41	0.47
2:O:116:ILE:HA	2:O:238:THR:OG1	2.15	0.47
2:D:13:ILE:HD13	2:D:69:LEU:HD13	1.95	0.47
1:L:78:ASN:ND2	1:L:78:ASN:C	2.67	0.47
2:D:61:ILE:HG21	2:D:227:GLY:HA2	1.95	0.47
2:M:390:ILE:C	2:M:391:LEU:HD12	2.34	0.47
5:R:33:ASN:N	5:R:33:ASN:HD22	2.13	0.47
5:I:40:SER:C	5:I:42:ILE:H	2.18	0.47
1:B:172:GLN:HA	10:B:600:ANP:HNB1	1.80	0.47
1:C:268:TYR:CD1	1:C:268:TYR:N	2.83	0.47
1:L:357:PHE:CD2	1:L:357:PHE:C	2.88	0.47
2:D:118:ALA:H	2:D:295:ARG:HH12	1.56	0.47
1:L:365:ILE:CD1	1:L:366:ASN:N	2.77	0.47
1:K:137:ILE:CB	1:K:138:PRO:HD3	2.45	0.47
1:L:276:VAL:O	1:L:279:ARG:HB3	2.14	0.47
2:E:454:GLU:C	2:E:456:ALA:H	2.18	0.47
1:K:34:ILE:CG2	2:N:52:HIS:HB2	2.45	0.47
2:O:249:GLN:HG3	2:O:250:ASP:H	1.79	0.47
1:K:360:GLY:O	1:K:362:ARG:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:HH12	1:A:437:ALA:N	2.12	0.47
2:M:160:VAL:HG23	2:M:335:LEU:HD23	1.97	0.47
1:L:475:GLN:OE1	1:L:476:HIS:CE1	2.68	0.47
7:T:155:LEU:HD23	8:U:66:VAL:HG22	1.96	0.47
2:N:103:ASP:O	2:N:105:ARG:HG3	2.15	0.47
4:Q:56:GLN:O	4:Q:82:VAL:HG12	2.15	0.47
1:A:186:GLN:CG	1:A:199:LEU:HD23	2.45	0.47
2:N:431:LEU:O	2:N:433:PRO:HD3	2.15	0.47
2:D:282:GLN:C	2:D:284:THR:H	2.18	0.47
1:L:44:LEU:HD11	1:L:53:VAL:HG11	1.97	0.47
4:H:58:LEU:HD12	4:H:80:GLY:N	2.29	0.47
3:P:2:THR:HG22	3:P:4:LYS:N	2.31	0.47
6:S:182:LEU:HD21	7:T:202:LYS:HZ1	1.78	0.47
2:O:287:THR:O	2:O:288:ASP:C	2.53	0.47
2:D:193:GLY:HA3	2:D:219:TYR:CE2	2.51	0.47
2:E:465:GLU:O	2:E:469:LYS:HB2	2.15	0.47
1:K:188:ARG:HG3	1:K:189:PHE:HD1	1.80	0.47
2:F:449:TYR:C	2:F:451:HIS:N	2.68	0.47
1:J:106:ARG:NH2	1:J:118:LYS:HB2	2.29	0.47
1:A:251:CYS:O	1:A:255:GLU:HB2	2.15	0.47
2:F:133:LEU:HB2	2:F:148:LYS:HG2	1.96	0.47
2:F:246:GLN:O	2:F:247:GLU:HB2	2.15	0.47
2:M:402:LEU:HD21	2:M:406:ARG:NH2	2.30	0.47
1:L:180:ILE:CD1	1:L:216:LEU:HD21	2.44	0.46
1:J:367:VAL:CG1	1:J:367:VAL:O	2.63	0.46
9:V:16:ILE:HG22	9:V:16:ILE:O	2.15	0.46
1:J:472:VAL:CG2	1:J:480:LEU:HD13	2.46	0.46
1:B:48:GLN:HE21	2:F:68:GLY:HA2	1.77	0.46
2:D:145:PRO:HB2	2:D:357:ILE:HD11	1.97	0.46
1:A:338:ILE:HB	1:A:339:PRO:HD3	1.96	0.46
2:D:377:ILE:HG21	2:D:410:ILE:HD12	1.96	0.46
1:C:78:ASN:C	1:C:78:ASN:ND2	2.68	0.46
1:K:142:VAL:CG2	1:K:374:VAL:HB	2.45	0.46
8:U:86:THR:O	8:U:86:THR:HG22	2.16	0.46
1:B:505:LEU:O	1:B:505:LEU:HD23	2.15	0.46
2:M:192:GLU:HA	2:M:195:ASP:HB2	1.98	0.46
2:D:87:GLY:O	2:D:90:THR:HG23	2.14	0.46
2:E:434:LEU:O	2:E:438:ILE:HG13	2.15	0.46
1:A:9:SER:CB	2:D:55:GLU:OE1	2.56	0.46
4:H:20:PHE:CD1	4:H:92:LEU:HB3	2.49	0.46
1:A:407:GLY:CA	1:A:410:LEU:HD21	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:64:ASP:OD1	2:E:65:GLY:N	2.48	0.46
3:P:51:LEU:HD22	3:P:204:TYR:CE2	2.51	0.46
1:C:99:VAL:CG1	1:C:100:GLY:N	2.78	0.46
1:K:148:THR:HA	1:K:182:THR:HG23	1.97	0.46
2:N:336:SER:HB3	2:N:339:ILE:HG12	1.97	0.46
6:S:116:VAL:H	6:S:117:PRO:HD3	1.80	0.46
2:M:77:ASP:O	2:M:79:GLY:N	2.48	0.46
2:O:162:LYS:HE3	2:O:257:ASN:HD21	1.79	0.46
1:C:373:ARG:NH2	2:D:189:ARG:NH2	2.63	0.46
1:L:401:ALA:HA	1:L:418:LEU:HD11	1.97	0.46
2:M:316:ASP:C	2:M:318:THR:H	2.18	0.46
1:K:111:LEU:HD23	1:K:111:LEU:HA	1.73	0.46
6:S:186:MSE:HB2	6:S:187:ARG:H	1.44	0.46
6:W:106:SER:C	6:W:108:MSE:N	2.69	0.46
1:B:104:LEU:HD21	1:B:200:TYR:HD2	1.79	0.46
3:P:31:TYR:CD2	3:P:31:TYR:C	2.89	0.46
1:B:389:THR:HG23	1:B:449:VAL:HG11	1.98	0.46
2:E:400:ASP:C	2:E:402:LEU:N	2.68	0.46
1:C:445:ILE:O	1:C:449:VAL:HG12	2.15	0.46
1:L:99:VAL:CG1	1:L:100:GLY:N	2.77	0.46
2:O:441:PHE:O	2:O:442:GLN:C	2.53	0.46
2:M:366:GLU:O	2:M:370:VAL:HG23	2.14	0.46
6:S:129:THR:HG21	6:S:135:LYS:CD	2.45	0.46
2:M:316:ASP:O	2:M:318:THR:N	2.48	0.46
6:S:71:ASP:C	6:S:73:THR:H	2.19	0.46
2:O:154:LEU:HD13	2:O:165:LEU:HD23	1.97	0.46
1:L:299:PHE:CE1	1:L:345:ILE:HD11	2.50	0.46
2:D:235:THR:HG22	2:D:236:GLY:N	2.31	0.46
6:W:45:ILE:O	6:W:51:MSE:HG3	2.15	0.46
6:W:38:GLU:O	6:W:78:PHE:HE1	1.99	0.46
2:F:164:VAL:HG11	10:F:600:ANP:N6	2.30	0.46
1:L:300:TYR:O	1:L:304:ARG:HG2	2.15	0.46
1:A:6:ALA:O	1:A:11:ILE:HB	2.14	0.46
6:S:137:VAL:HG12	6:S:141:PHE:CE2	2.50	0.46
3:G:31:TYR:CD2	3:G:31:TYR:C	2.85	0.46
1:L:44:LEU:CD1	1:L:53:VAL:HG11	2.45	0.46
1:L:343:ILE:HG23	1:L:349:GLN:HE21	1.80	0.46
1:C:351:PHE:O	1:C:352:LEU:HD12	2.15	0.46
2:E:396:LEU:HB3	2:E:400:ASP:CB	2.44	0.46
1:J:479:LEU:HA	1:J:482:LYS:HB3	1.97	0.46
1:L:200:TYR:HE1	1:L:262:LYS:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:5:LEU:HD23	9:V:9:GLN:NE2	2.30	0.46
1:L:221:THR:HG22	1:L:222:ASP:N	2.31	0.46
1:B:142:VAL:CG2	1:B:374:VAL:HB	2.45	0.46
2:M:393:MET:O	2:M:396:LEU:HG	2.16	0.46
2:F:86:VAL:HG23	2:F:242:TYR:CG	2.49	0.46
1:B:220:LEU:HA	1:B:220:LEU:HD23	1.65	0.46
2:F:317:LEU:HD23	2:F:317:LEU:HA	1.65	0.46
6:W:71:ASP:O	6:W:75:LYS:HB2	2.15	0.46
1:B:272:SER:O	1:B:276:VAL:HG23	2.15	0.46
1:B:41:VAL:CG1	1:B:88:VAL:HG21	2.45	0.46
2:F:234:LEU:HA	2:F:237:LEU:HB2	1.97	0.46
1:L:286:ARG:O	1:L:288:PRO:HD3	2.16	0.46
2:F:413:PHE:HB2	2:F:457:PHE:HB3	1.97	0.46
3:G:127:THR:HG22	3:G:128:PHE:H	1.81	0.46
1:B:43:GLY:O	1:B:44:LEU:C	2.53	0.46
2:M:243:PHE:H	2:M:243:PHE:HD1	1.63	0.46
4:Q:113:GLU:O	4:Q:115:ALA:N	2.46	0.46
2:M:87:GLY:HA2	2:M:242:TYR:CE2	2.50	0.46
1:J:164:ARG:HH12	1:J:307:GLU:HA	1.80	0.46
2:O:146:TYR:CG	2:O:152:ILE:HD13	2.50	0.46
2:O:462:PRO:HD2	2:O:465:GLU:OE2	2.16	0.46
1:B:136:ILE:HG23	2:F:194:ASN:N	2.29	0.46
4:Q:62:LEU:HD23	4:Q:76:PHE:HB2	1.96	0.46
1:L:209:LYS:HZ3	1:L:211:SER:HB2	1.80	0.46
6:W:23:TYR:CG	6:W:108:MSE:HE2	2.51	0.46
6:S:137:VAL:HG22	7:T:203:LEU:HB3	1.98	0.46
3:G:31:TYR:CD2	3:G:32:ALA:N	2.83	0.46
1:A:411:ASP:N	1:A:411:ASP:OD1	2.49	0.46
1:L:460:LYS:O	1:L:462:THR:N	2.49	0.46
1:K:392:LEU:HD12	1:K:392:LEU:O	2.16	0.46
2:M:243:PHE:N	2:M:243:PHE:CD1	2.84	0.46
6:S:179:ILE:HG22	6:S:180:GLN:OE1	2.16	0.46
1:J:99:VAL:HG13	1:J:256:TYR:HB2	1.97	0.46
1:J:187:LYS:HG2	1:J:188:ARG:N	2.31	0.46
1:A:3:THR:OG1	1:A:4:GLY:N	2.49	0.46
2:D:391:LEU:N	2:D:391:LEU:HD12	2.30	0.46
1:A:59:LEU:HA	1:A:59:LEU:HD23	1.60	0.46
5:I:20:LYS:HG2	5:I:20:LYS:O	2.15	0.46
5:I:33:ASN:HD22	5:I:33:ASN:N	2.14	0.46
1:A:312:MET:HA	1:A:312:MET:HE3	1.97	0.46
1:K:176:THR:O	1:K:177:SER:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:86:VAL:HG11	2:D:114:ALA:HB3	1.97	0.46
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.51	0.46
6:W:7:PRO:HG3	6:W:23:TYR:HB2	1.98	0.46
1:L:137:ILE:C	1:L:139:ARG:H	2.19	0.46
2:D:247:GLU:HB2	2:D:249:GLN:HB2	1.96	0.46
1:B:104:LEU:HD22	1:B:228:TYR:HA	1.98	0.46
2:M:92:GLY:CA	2:M:206:ILE:HG23	2.46	0.46
1:L:136:ILE:CG2	2:M:194:ASN:HA	2.46	0.46
2:M:360:PRO:HD3	2:M:368:TYR:CD1	2.51	0.46
2:F:137:ILE:HA	2:F:416:GLN:NE2	2.25	0.46
4:H:113:GLU:C	4:H:115:ALA:N	2.66	0.46
2:E:32:ILE:HG22	2:E:33:LEU:HG	1.98	0.46
2:E:336:SER:CB	2:E:339:ILE:HG12	2.46	0.46
2:D:77:ASP:O	2:D:79:GLY:N	2.48	0.46
6:S:129:THR:HG21	6:S:135:LYS:HD2	1.98	0.46
7:X:168:LYS:O	7:X:171:GLU:HB2	2.16	0.46
2:F:281:TYR:HD1	2:F:320:PRO:HG2	1.81	0.46
2:E:77:ASP:OD1	2:E:79:GLY:N	2.40	0.46
2:D:54:GLY:O	2:D:55:GLU:C	2.53	0.46
3:P:31:TYR:CD2	3:P:32:ALA:N	2.84	0.46
1:K:389:THR:HG23	1:K:449:VAL:HG11	1.97	0.46
1:A:478:ALA:HB1	1:A:479:LEU:HD12	1.98	0.46
2:O:94:ILE:HG22	2:O:102:ILE:CD1	2.45	0.46
4:Q:35:GLN:HB3	4:Q:35:GLN:HE21	1.58	0.46
2:N:29:LEU:HA	2:N:30:PRO:HD3	1.77	0.46
2:N:170:ILE:CG2	2:N:215:VAL:HG22	2.44	0.46
4:H:35:GLN:HB3	4:H:35:GLN:HE21	1.57	0.46
3:G:105:ILE:HD12	3:G:124:PHE:CD1	2.51	0.46
1:L:423:ARG:HB3	1:L:461:ILE:CD1	2.46	0.46
4:Q:113:GLU:C	4:Q:115:ALA:N	2.68	0.46
2:M:77:ASP:C	2:M:79:GLY:H	2.19	0.46
2:O:410:ILE:HG12	2:O:444:ILE:HG21	1.98	0.46
1:C:418:LEU:C	1:C:420:ARG:H	2.19	0.46
2:N:424:PHE:CD1	2:N:424:PHE:O	2.69	0.46
1:A:96:ASP:OD2	1:A:126:ARG:HD3	2.15	0.46
2:D:177:HIS:CD2	2:D:179:GLY:H	2.34	0.46
1:J:303:SER:HA	1:J:345:ILE:HD13	1.98	0.46
1:L:137:ILE:N	1:L:138:PRO:CD	2.78	0.46
6:S:9:VAL:O	6:S:11:ILE:N	2.42	0.46
1:J:410:LEU:O	1:J:411:ASP:C	2.54	0.46
6:S:91:GLU:O	6:S:93:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:278:ALA:O	2:N:279:VAL:HG12	2.16	0.46
7:T:203:LEU:O	7:T:207:LYS:HG3	2.15	0.46
1:J:107:VAL:HG12	1:J:115:ILE:CG1	2.46	0.46
1:L:258:ARG:HE	1:L:312:MET:HE2	1.81	0.46
1:L:479:LEU:CD2	1:L:493:SER:HB3	2.46	0.46
5:R:42:ILE:HG22	5:R:43:LYS:N	2.30	0.46
2:O:180:TYR:HD1	2:O:249:GLN:HG2	1.81	0.46
3:P:105:ILE:HD12	3:P:124:PHE:CD1	2.51	0.46
2:E:457:PHE:HE2	2:E:463:ILE:HD11	1.80	0.46
4:Q:116:GLN:O	4:Q:119:LEU:HB3	2.16	0.46
2:M:311:TYR:CE2	2:M:313:PRO:HA	2.51	0.46
2:E:25:PHE:O	2:E:56:SER:HB3	2.16	0.46
1:K:190:ASN:HA	1:K:198:LYS:HG2	1.98	0.46
2:D:175:LYS:C	2:D:177:HIS:H	2.19	0.46
2:E:152:ILE:HD12	2:E:152:ILE:N	2.31	0.46
1:C:212:THR:O	1:C:213:VAL:C	2.54	0.46
6:W:23:TYR:CE1	6:W:105:PHE:HA	2.51	0.46
2:O:234:LEU:O	2:O:237:LEU:HB3	2.16	0.46
3:P:44:TYR:CD1	3:P:44:TYR:C	2.90	0.46
1:C:62:MET:HB2	1:C:76:PHE:HE1	1.80	0.46
2:D:32:ILE:HG12	2:D:32:ILE:H	1.30	0.46
6:S:182:LEU:HD21	7:T:202:LYS:HZ3	1.77	0.46
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.96	0.46
3:P:204:TYR:O	3:P:208:SER:HB3	2.17	0.46
3:P:51:LEU:O	3:P:52:TYR:C	2.54	0.46
4:Q:25:GLN:HG2	4:Q:26:VAL:N	2.31	0.46
1:B:113:ASN:ND2	1:B:113:ASN:H	2.12	0.46
3:G:193:TYR:CD2	4:H:53:PRO:HB3	2.51	0.46
1:J:103:LEU:O	1:J:106:ARG:HG2	2.16	0.46
4:Q:108:ALA:HB2	5:R:25:ALA:HA	1.98	0.46
1:K:25:LEU:O	1:K:45:ARG:HG2	2.16	0.46
1:A:268:TYR:CZ	1:A:305:LEU:HD11	2.51	0.46
4:H:95:GLU:O	4:H:95:GLU:HG3	2.16	0.46
2:M:62:ALA:O	2:M:227:GLY:HA3	2.15	0.46
3:G:217:LEU:HA	3:G:217:LEU:HD12	1.54	0.46
9:V:50:MSE:HG2	9:V:50:MSE:O	2.16	0.46
2:F:357:ILE:HG13	2:F:357:ILE:O	2.15	0.46
2:D:234:LEU:HD23	2:D:234:LEU:N	2.31	0.46
1:K:352:LEU:HA	1:K:364:ALA:O	2.16	0.46
2:D:11:GLY:N	2:D:75:VAL:O	2.41	0.46
6:W:42:VAL:HA	6:W:45:ILE:CG1	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ILE:C	1:C:139:ARG:H	2.18	0.45
2:F:237:LEU:HA	2:F:237:LEU:HD12	1.57	0.45
1:J:411:ASP:N	1:J:411:ASP:OD1	2.48	0.45
6:S:133:GLU:HA	6:S:136:THR:HG21	1.95	0.45
2:N:136:GLY:HA3	2:N:431:LEU:CD1	2.37	0.45
2:M:218:VAL:O	2:M:219:TYR:CD1	2.70	0.45
2:D:12:ARG:HH21	6:S:10:GLN:HE21	1.64	0.45
1:C:453:LEU:C	1:C:455:LYS:H	2.19	0.45
6:W:120:VAL:HG12	6:W:121:THR:CG2	2.45	0.45
3:P:51:LEU:HG	3:P:52:TYR:N	2.31	0.45
2:D:155:PHE:HB2	2:D:334:VAL:HG22	1.98	0.45
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.97	0.45
2:O:17:ILE:O	2:O:17:ILE:CG2	2.63	0.45
5:I:42:ILE:HG22	5:I:43:LYS:N	2.30	0.45
2:O:422:GLU:OE2	2:O:428:LEU:HD23	2.14	0.45
1:J:96:ASP:OD2	1:J:126:ARG:HD3	2.16	0.45
2:F:356:ARG:HH11	2:F:356:ARG:CB	2.30	0.45
6:W:98:THR:O	6:W:102:ILE:HG13	2.16	0.45
6:S:7:PRO:CG	6:S:108:MSE:HE1	2.46	0.45
2:M:154:LEU:HD13	2:M:165:LEU:CD2	2.40	0.45
5:I:12:ILE:H	5:I:12:ILE:HG12	1.57	0.45
1:C:168:ILE:HG23	1:C:351:PHE:CD1	2.51	0.45
3:G:59:THR:CG2	3:G:184:ILE:HG13	2.47	0.45
3:G:164:ARG:HH22	3:G:166:ARG:CZ	2.29	0.45
2:N:404:VAL:O	2:N:408:ARG:CD	2.65	0.45
1:A:78:ASN:OD1	1:A:79:ASP:N	2.50	0.45
1:K:62:MET:HG3	1:K:95:VAL:HG21	1.98	0.45
2:M:133:LEU:HD12	2:M:134:VAL:O	2.16	0.45
4:Q:72:THR:HG22	4:Q:72:THR:O	2.17	0.45
2:N:53:LEU:HD23	2:N:53:LEU:HA	1.69	0.45
1:L:249:SER:O	1:L:253:MET:HG3	2.16	0.45
2:N:139:VAL:HA	2:N:414:LEU:CD2	2.46	0.45
2:O:404:VAL:HG12	2:O:405:SER:N	2.30	0.45
2:E:434:LEU:HD12	2:E:434:LEU:O	2.16	0.45
6:S:45:ILE:O	6:S:51:MSE:HG3	2.16	0.45
6:S:88:LEU:HD22	6:S:88:LEU:HA	1.70	0.45
2:M:183:PHE:CD2	2:M:184:ALA:N	2.85	0.45
2:F:431:LEU:HD23	2:F:431:LEU:C	2.37	0.45
6:S:129:THR:HG21	6:S:135:LYS:CG	2.46	0.45
2:E:151:LYS:HE3	2:E:296:ILE:O	2.16	0.45
2:E:146:TYR:CD1	2:E:152:ILE:HG12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:473:LEU:HD23	2:O:473:LEU:HA	1.73	0.45
1:L:489:ILE:O	1:L:489:ILE:HG22	2.15	0.45
1:J:282:SER:CB	1:J:295:PRO:HG3	2.45	0.45
1:J:29:GLY:CA	1:J:42:HIS:O	2.64	0.45
2:D:257:ASN:O	2:D:259:PHE:N	2.49	0.45
2:E:434:LEU:HD12	2:E:434:LEU:C	2.35	0.45
2:E:139:VAL:HG22	2:E:414:LEU:O	2.16	0.45
6:S:54:SER:HB2	6:S:65:LYS:HE3	1.99	0.45
6:S:78:PHE:CA	6:S:80:PRO:HD3	2.46	0.45
2:E:180:TYR:H	2:E:249:GLN:HE22	1.61	0.45
2:O:359:ASP:OD1	2:O:360:PRO:HD2	2.16	0.45
2:F:29:LEU:HD23	2:F:52:HIS:ND1	2.32	0.45
3:P:54:LYS:HD2	4:Q:85:ASN:ND2	2.32	0.45
2:N:181:SER:O	2:N:215:VAL:HA	2.16	0.45
1:J:87:ILE:HG13	6:W:1:PHE:HE1	1.80	0.45
2:M:377:ILE:HG21	2:M:410:ILE:HD12	1.98	0.45
1:C:270:ASP:HB2	1:C:326:VAL:O	2.17	0.45
2:N:419:GLN:HA	2:N:422:GLU:HG3	1.97	0.45
1:A:300:TYR:CE2	1:A:304:ARG:NH1	2.84	0.45
2:N:126:MET:HB3	2:N:126:MET:HE2	1.52	0.45
2:D:365:SER:O	2:D:369:ASP:HB2	2.16	0.45
2:D:73:GLN:HB2	2:D:73:GLN:HE21	1.59	0.45
2:D:408:ARG:NE	2:D:454:GLU:OE1	2.48	0.45
2:O:339:ILE:HG23	2:O:344:ILE:HB	1.98	0.45
1:B:385:GLN:NE2	1:B:489:ILE:N	2.50	0.45
1:C:307:GLU:CG	2:D:223:ASN:HB3	2.45	0.45
3:P:171:TYR:O	3:P:172:LYS:HB3	2.16	0.45
2:M:346:PRO:O	2:M:348:VAL:N	2.44	0.45
2:N:408:ARG:NE	2:N:454:GLU:OE1	2.49	0.45
2:M:374:VAL:HG13	2:M:410:ILE:CG2	2.47	0.45
1:B:190:ASN:HA	1:B:198:LYS:HG2	1.98	0.45
1:L:468:PHE:CD2	1:L:468:PHE:O	2.70	0.45
2:O:162:LYS:NZ	10:O:600:ANP:O1B	2.40	0.45
4:H:28:PHE:HE2	4:H:75:TYR:HH	1.62	0.45
2:F:133:LEU:HD12	2:F:133:LEU:C	2.36	0.45
2:M:157:GLY:O	2:M:160:VAL:HG22	2.16	0.45
3:P:77:LEU:HD13	3:P:232:MET:HE2	1.98	0.45
2:M:256:ASP:HA	2:M:257:ASN:HA	1.80	0.45
1:A:490:SER:O	1:A:491:GLU:C	2.55	0.45
1:B:417:LEU:HD23	1:B:417:LEU:HA	1.66	0.45
1:L:133:ALA:HB2	1:L:308:ARG:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:275:ALA:HB2	1:L:302:HIS:HE1	1.82	0.45
1:J:403:PHE:HB3	1:J:410:LEU:CD2	2.47	0.45
2:M:282:GLN:C	2:M:284:THR:N	2.69	0.45
6:S:98:THR:O	6:S:102:ILE:HG13	2.17	0.45
2:D:92:GLY:CA	2:D:206:ILE:HG23	2.44	0.45
3:G:2:THR:HG22	3:G:4:LYS:N	2.31	0.45
1:B:137:ILE:CB	1:B:138:PRO:HD3	2.43	0.45
2:M:359:ASP:O	2:M:363:VAL:HG22	2.16	0.45
2:E:97:VAL:HG11	2:E:228:ALA:HB1	1.99	0.45
7:T:192:GLU:O	7:T:195:ALA:HB3	2.17	0.45
2:M:51:GLN:HG3	2:M:59:ARG:HB3	1.98	0.45
1:L:501:VAL:CG2	1:L:502:THR:N	2.79	0.45
2:F:409:LYS:NZ	2:F:450:ASP:HA	2.31	0.45
7:T:157:TYR:HE1	9:V:48:LYS:HA	1.81	0.45
1:J:341:ASN:O	1:J:345:ILE:HG13	2.17	0.45
1:C:284:LEU:HA	1:C:284:LEU:HD23	1.74	0.45
1:C:380:THR:C	1:C:382:ALA:H	2.20	0.45
1:A:110:ALA:HB2	1:A:234:ALA:HB2	1.98	0.45
1:B:46:ASN:HB2	1:B:90:ARG:HH11	1.82	0.45
1:K:292:GLU:O	1:K:293:ALA:HB3	2.16	0.45
1:L:236:ALA:HB3	2:O:294:GLU:HG3	1.98	0.45
1:B:256:TYR:CD2	1:B:256:TYR:C	2.90	0.45
1:C:258:ARG:HE	1:C:312:MET:HE2	1.82	0.45
1:L:49:ALA:N	1:L:66:LEU:HD11	2.31	0.45
6:W:15:GLU:HB3	6:W:16:GLY:H	1.58	0.45
3:P:179:PHE:HB3	3:P:184:ILE:HG23	1.99	0.45
1:A:87:ILE:HD12	1:A:87:ILE:N	2.29	0.45
1:C:336:ALA:HB3	1:C:339:PRO:HD2	1.98	0.45
2:E:336:SER:HB3	2:E:339:ILE:HG12	1.98	0.45
4:Q:126:ALA:C	4:Q:128:ARG:H	2.20	0.45
6:W:12:TYR:HB3	6:W:13:GLY:H	1.30	0.45
1:A:140:ILE:HA	1:A:140:ILE:HD12	1.76	0.45
1:J:133:ALA:HB2	1:J:308:ARG:CG	2.46	0.45
1:J:34:ILE:HD11	1:J:79:ASP:HB2	1.99	0.45
1:J:55:PHE:CE2	1:J:82:ILE:HD13	2.51	0.45
1:L:418:LEU:C	1:L:420:ARG:H	2.17	0.45
2:N:317:LEU:HA	2:N:317:LEU:HD23	1.75	0.45
2:M:29:LEU:HD12	2:M:29:LEU:HA	1.79	0.45
2:M:285:LEU:C	2:M:285:LEU:HD23	2.37	0.45
1:J:231:VAL:O	1:J:231:VAL:HG12	2.16	0.45
1:K:427:LEU:HD11	1:K:448:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:149:GLY:HA2	2:N:304:ILE:O	2.16	0.45
1:B:352:LEU:HA	1:B:364:ALA:O	2.17	0.45
6:S:111:VAL:HG12	6:S:111:VAL:O	2.15	0.45
1:B:106:ARG:NH2	1:B:118:LYS:O	2.50	0.45
2:D:285:LEU:HD23	2:D:285:LEU:C	2.37	0.45
1:C:71:VAL:HG12	1:C:73:VAL:HG23	1.98	0.45
1:B:313:ASN:OD1	1:B:315:ALA:HB3	2.16	0.45
3:P:5:ASP:O	3:P:6:ILE:C	2.55	0.45
2:E:12:ARG:O	2:E:14:VAL:HG13	2.17	0.45
5:R:9:LEU:HD11	5:R:13:ARG:HG2	1.98	0.45
1:C:144:GLU:HG3	1:C:311:LYS:CE	2.47	0.45
4:Q:35:GLN:HG2	4:Q:36:VAL:H	1.82	0.45
2:D:223:ASN:OD1	2:D:224:GLU:HG2	2.17	0.45
1:A:166:LEU:HD22	1:A:342:VAL:HG12	1.99	0.45
3:G:78:CYS:HB3	3:G:228:ARG:HB2	1.99	0.45
6:S:116:VAL:O	6:S:116:VAL:HG12	2.17	0.45
6:S:131:LEU:HD12	6:S:134:LEU:HD11	1.98	0.45
2:D:420:VAL:O	2:D:420:VAL:CG2	2.65	0.45
3:G:84:SER:O	3:G:173:THR:HG21	2.17	0.45
1:L:150:ILE:O	1:L:151:LYS:C	2.56	0.45
1:J:314:ASP:O	1:J:316:PHE:N	2.49	0.45
1:K:301:LEU:HA	1:K:304:ARG:NH1	2.31	0.45
2:E:256:ASP:HA	2:E:257:ASN:HA	1.58	0.45
6:W:59:TYR:N	6:W:59:TYR:CD2	2.85	0.45
1:C:202:ILE:HB	1:C:266:ILE:HG13	1.99	0.45
1:L:268:TYR:CE2	1:L:305:LEU:HD11	2.52	0.45
2:N:172:ASN:CG	2:N:431:LEU:HD22	2.38	0.45
2:M:275:ILE:HG23	3:P:269:ALA:CB	2.45	0.45
1:C:49:ALA:HB2	1:C:66:LEU:CD1	2.47	0.45
1:L:279:ARG:CG	1:L:283:LEU:HD12	2.47	0.45
1:L:419:SER:C	1:L:423:ARG:NH1	2.71	0.45
1:C:397:TYR:HA	1:C:417:LEU:HD23	1.99	0.45
1:L:218:LYS:HG2	2:O:128:VAL:HG21	1.99	0.45
1:A:303:SER:HA	1:A:345:ILE:HD13	1.98	0.45
2:O:188:GLU:HG3	2:O:256:ASP:OD2	2.17	0.45
1:J:188:ARG:HG2	1:J:189:PHE:CD1	2.52	0.45
3:P:232:MET:O	3:P:233:ASP:C	2.55	0.45
2:O:246:GLN:O	2:O:247:GLU:HB2	2.16	0.45
8:U:66:VAL:O	8:U:66:VAL:HG12	2.17	0.45
2:D:94:ILE:HD11	2:D:197:TYR:CE1	2.51	0.45
4:Q:127:THR:HG22	4:Q:127:THR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:201:CYS:O	1:K:229:THR:HA	2.16	0.45
1:C:180:ILE:CG1	1:C:216:LEU:HD21	2.46	0.45
2:F:161:GLY:HA2	10:F:600:ANP:PA	2.57	0.45
2:M:31:PRO:HD2	2:M:34:ASN:HD21	1.77	0.45
1:K:240:ALA:HB3	1:K:241:PRO:HD3	1.98	0.45
1:A:15:ARG:HH11	1:A:15:ARG:HG3	1.82	0.45
1:K:66:LEU:HD12	2:O:16:VAL:CG2	2.47	0.45
2:F:97:VAL:O	2:F:235:THR:OG1	2.34	0.45
3:G:51:LEU:HD22	3:G:204:TYR:CE2	2.52	0.45
2:M:90:THR:O	2:M:93:ARG:HB2	2.18	0.45
2:F:377:ILE:CG2	2:F:410:ILE:HD12	2.47	0.45
1:J:62:MET:HB2	1:J:76:PHE:CE1	2.50	0.45
1:B:188:ARG:HG3	1:B:189:PHE:CE1	2.51	0.45
2:D:168:GLU:HB2	2:D:420:VAL:HG13	1.99	0.45
4:H:127:THR:HG22	4:H:127:THR:O	2.16	0.45
1:C:113:ASN:OD1	1:C:113:ASN:N	2.50	0.45
2:E:275:ILE:HA	2:E:276:PRO:HD3	1.81	0.45
2:E:275:ILE:O	2:E:283:PRO:HG3	2.17	0.45
6:W:78:PHE:CA	6:W:80:PRO:HD3	2.47	0.44
1:C:501:VAL:O	1:C:503:ASN:N	2.50	0.44
1:L:137:ILE:HG12	1:L:138:PRO:CD	2.25	0.44
1:B:267:ILE:HG12	1:B:324:LEU:HB2	1.99	0.44
1:C:247:PRO:CB	1:C:268:TYR:HD2	2.27	0.44
1:C:306:LEU:CD2	1:C:325:PRO:HG3	2.31	0.44
2:O:11:GLY:HA3	2:O:25:PHE:HE2	1.75	0.44
1:K:128:ARG:HB2	1:K:131:LEU:HD12	1.99	0.44
6:W:138:LEU:HA	6:W:141:PHE:HD2	1.82	0.44
1:L:460:LYS:C	1:L:462:THR:H	2.21	0.44
1:L:386:VAL:HB	1:L:445:ILE:CG2	2.46	0.44
1:J:472:VAL:HG21	1:J:480:LEU:HD13	1.99	0.44
2:N:396:LEU:HB3	2:N:400:ASP:CB	2.46	0.44
1:K:473:ILE:O	1:K:477:GLN:HG2	2.17	0.44
1:K:159:ILE:HG22	1:K:160:GLY:N	2.31	0.44
1:L:241:PRO:HA	1:L:281:MET:SD	2.58	0.44
2:M:151:LYS:HZ1	2:M:293:GLN:HB3	1.82	0.44
4:H:48:LEU:C	4:H:50:ALA:N	2.70	0.44
1:K:442:VAL:HG11	1:K:483:ILE:HG21	1.98	0.44
2:F:443:GLN:NE2	2:F:463:ILE:HG21	2.32	0.44
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.33	0.44
1:B:460:LYS:NZ	1:B:510:ALA:CB	2.80	0.44
1:J:436:MET:HE2	1:J:441:GLN:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:175:LYS:C	2:M:177:HIS:H	2.20	0.44
1:A:138:PRO:O	1:A:312:MET:HE3	2.17	0.44
2:M:248:GLY:HA2	2:M:301:LYS:O	2.17	0.44
1:A:498:LYS:O	1:A:502:THR:HG23	2.17	0.44
1:J:428:LEU:HD23	1:J:428:LEU:HA	1.73	0.44
1:K:288:PRO:HA	1:K:289:PRO:HD3	1.76	0.44
1:A:214:ALA:O	1:A:215:GLN:C	2.56	0.44
1:J:137:ILE:C	1:J:139:ARG:H	2.21	0.44
6:S:9:VAL:CB	6:S:108:MSE:HG2	2.35	0.44
2:D:204:GLY:HA2	2:D:206:ILE:O	2.16	0.44
3:G:10:LEU:HD23	3:G:10:LEU:HA	1.58	0.44
2:O:23:VAL:HG23	2:O:58:VAL:CG2	2.43	0.44
1:K:161:ARG:HA	1:K:322:THR:OG1	2.17	0.44
3:G:212:ILE:HG23	3:G:213:ILE:H	1.77	0.44
3:G:42:ARG:NH2	3:G:219:GLU:OE2	2.50	0.44
2:N:409:LYS:NZ	2:N:450:ASP:O	2.51	0.44
3:G:191:SER:C	3:G:193:TYR:N	2.71	0.44
2:E:445:LEU:C	2:E:447:GLY:H	2.21	0.44
1:B:202:ILE:HG22	1:B:266:ILE:HG13	1.99	0.44
1:K:278:TYR:CG	1:K:301:LEU:HD13	2.52	0.44
1:B:290:GLY:O	1:B:291:ARG:C	2.54	0.44
2:E:155:PHE:N	2:E:155:PHE:CD1	2.84	0.44
2:F:333:THR:HA	2:F:353:SER:OG	2.17	0.44
2:M:12:ARG:NH2	6:W:10:GLN:NE2	2.65	0.44
4:H:62:LEU:HD23	4:H:76:PHE:HB2	1.99	0.44
1:L:381:ARG:NH1	1:L:385:GLN:HE21	2.15	0.44
6:W:23:TYR:CD2	6:W:108:MSE:SE	3.20	0.44
3:G:44:TYR:CD1	3:G:44:TYR:C	2.91	0.44
1:B:256:TYR:HD2	1:B:257:PHE:CD1	2.35	0.44
4:Q:58:LEU:HD13	4:Q:77:VAL:HG11	1.99	0.44
2:D:100:GLU:HA	2:D:101:PRO:HD3	1.71	0.44
2:E:377:ILE:CG2	2:E:378:LEU:N	2.80	0.44
3:P:164:ARG:O	3:P:171:TYR:HB2	2.16	0.44
2:E:101:PRO:HG2	2:E:107:PRO:HA	2.00	0.44
1:A:241:PRO:O	1:A:245:LEU:HB2	2.18	0.44
1:A:188:ARG:NH1	1:A:437:ALA:CA	2.81	0.44
4:Q:95:GLU:O	4:Q:95:GLU:HG3	2.17	0.44
1:J:305:LEU:O	1:J:308:ARG:HB2	2.17	0.44
1:A:472:VAL:HG21	1:A:480:LEU:HD13	1.98	0.44
1:C:489:ILE:O	1:C:489:ILE:HG22	2.15	0.44
3:P:3:LEU:HD23	3:P:3:LEU:HA	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:113:ASN:OD1	1:L:113:ASN:N	2.51	0.44
1:L:189:PHE:HB3	1:L:197:LYS:O	2.17	0.44
1:C:166:LEU:HD22	1:C:342:VAL:HG12	1.99	0.44
3:P:214:TYR:C	3:P:214:TYR:CD2	2.90	0.44
6:S:61:LYS:HB2	6:S:61:LYS:HE3	1.81	0.44
1:A:403:PHE:HB3	1:A:410:LEU:CD2	2.48	0.44
1:L:49:ALA:HB2	1:L:66:LEU:CD1	2.48	0.44
2:D:93:ARG:NH2	2:D:101:PRO:HB3	2.31	0.44
2:F:12:ARG:HB3	2:F:72:GLY:O	2.18	0.44
3:P:59:THR:CG2	3:P:184:ILE:HG13	2.47	0.44
3:G:166:ARG:H	3:G:171:TYR:HA	1.81	0.44
2:M:86:VAL:HG23	2:M:242:TYR:CG	2.52	0.44
1:J:100:GLY:O	1:J:103:LEU:HD12	2.16	0.44
2:N:14:VAL:HG21	2:N:24:GLN:HB2	2.00	0.44
1:C:200:TYR:CD1	1:C:257:PHE:HD2	2.35	0.44
2:D:314:ALA:O	2:D:315:ASP:HB2	2.18	0.44
2:M:226:PRO:HB2	2:M:268:VAL:CG1	2.48	0.44
1:A:34:ILE:HD11	1:A:79:ASP:HB2	1.98	0.44
1:J:314:ASP:C	1:J:316:PHE:H	2.21	0.44
3:P:217:LEU:HD12	3:P:217:LEU:HA	1.55	0.44
1:K:424:LEU:HA	1:K:424:LEU:HD23	1.64	0.44
1:L:104:LEU:HD13	1:L:228:TYR:HA	2.00	0.44
1:L:210:ARG:HB2	2:O:126:MET:CE	2.48	0.44
1:L:180:ILE:CG1	1:L:216:LEU:HD21	2.48	0.44
6:W:39:LEU:HB3	6:W:102:ILE:HG23	1.99	0.44
2:N:390:ILE:CG1	3:P:25:MET:HG2	2.36	0.44
1:L:62:MET:O	1:L:73:VAL:HG13	2.18	0.44
1:L:168:ILE:HD11	1:L:339:PRO:HB3	1.99	0.44
1:C:460:LYS:O	1:C:462:THR:N	2.50	0.44
1:J:114:ALA:HB2	1:J:121:ILE:CD1	2.45	0.44
1:C:338:ILE:HG22	1:C:339:PRO:N	2.31	0.44
6:W:139:LYS:HG2	6:W:142:LEU:CD1	2.46	0.44
6:S:184:ARG:N	6:S:184:ARG:HE	2.16	0.44
1:B:486:ASP:O	1:B:488:LYS:HB3	2.17	0.44
1:C:475:GLN:OE1	1:C:476:HIS:CE1	2.71	0.44
6:W:71:ASP:C	6:W:73:THR:H	2.20	0.44
1:L:37:GLY:O	1:L:38:ILE:HD13	2.17	0.44
6:W:131:LEU:HB3	6:W:132:THR:H	1.64	0.44
2:O:452:LEU:HB3	2:O:453:PRO:CD	2.48	0.44
1:J:403:PHE:N	1:J:403:PHE:HD1	2.13	0.44
2:E:243:PHE:HB3	2:E:249:GLN:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:176:TRP:CE3	9:V:22:LYS:HB2	2.52	0.44
1:A:476:HIS:HD2	1:A:496:LYS:CE	2.30	0.44
2:M:153:GLY:CA	2:M:329:LEU:HD13	2.47	0.44
2:M:93:ARG:NH2	2:M:101:PRO:HB3	2.33	0.44
1:K:59:LEU:HD23	1:K:59:LEU:HA	1.80	0.44
9:Z:22:LYS:CE	9:Z:23:ARG:HB3	2.48	0.44
2:E:443:GLN:O	2:E:444:ILE:C	2.56	0.44
6:S:186:MSE:O	6:S:188:GLU:N	2.51	0.44
2:F:256:ASP:HA	2:F:257:ASN:HA	1.80	0.44
2:F:189:ARG:HB2	2:F:192:GLU:HG3	1.99	0.44
9:V:18:GLU:C	9:V:20:ARG:N	2.71	0.44
6:W:28:LYS:O	6:W:29:GLN:CB	2.57	0.44
1:C:501:VAL:O	1:C:502:THR:C	2.55	0.44
6:S:5:VAL:HG23	6:S:24:SER:OG	2.17	0.44
1:A:24:ASP:O	1:A:25:LEU:HB2	2.17	0.44
2:E:139:VAL:CA	2:E:414:LEU:HD23	2.37	0.44
1:B:106:ARG:NH1	1:B:121:ILE:HG12	2.33	0.44
1:J:202:ILE:HB	1:J:266:ILE:HD12	1.98	0.44
6:S:137:VAL:HG22	7:T:203:LEU:CD1	2.43	0.44
2:O:431:LEU:HD23	2:O:431:LEU:HA	1.56	0.44
1:L:338:ILE:HG22	1:L:339:PRO:N	2.32	0.44
1:L:352:LEU:O	1:L:353:GLU:HB2	2.17	0.44
2:M:218:VAL:O	2:M:219:TYR:HD1	2.01	0.44
1:B:137:ILE:C	1:B:139:ARG:H	2.20	0.44
1:K:392:LEU:HD11	1:K:396:GLN:HE21	1.82	0.44
2:N:410:ILE:HG22	2:N:411:GLN:N	2.32	0.44
1:K:189:PHE:CD1	1:K:189:PHE:N	2.86	0.44
4:H:126:ALA:C	4:H:128:ARG:H	2.21	0.44
2:N:336:SER:CB	2:N:339:ILE:HG12	2.47	0.44
3:G:232:MET:O	3:G:233:ASP:C	2.54	0.44
1:A:100:GLY:O	1:A:103:LEU:HD12	2.17	0.44
1:J:188:ARG:NH1	1:J:437:ALA:N	2.65	0.44
2:E:151:LYS:HG2	2:E:293:GLN:HE22	1.82	0.44
2:F:45:LEU:CD2	2:F:69:LEU:HD21	2.48	0.44
2:F:188:GLU:O	2:F:222:MET:HG2	2.18	0.44
1:A:203:TYR:CD2	1:A:203:TYR:O	2.71	0.44
5:R:23:ARG:HG2	5:R:34:ALA:HB1	2.00	0.44
7:T:168:LYS:O	7:T:171:GLU:HB2	2.18	0.44
2:M:96:ASN:HD22	2:M:98:ILE:H	1.59	0.44
6:S:5:VAL:HB	6:S:24:SER:HA	2.00	0.44
1:J:183:ILE:HG23	1:J:201:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:25:MET:HE2	3:G:25:MET:HB2	1.86	0.44
1:K:394:LEU:O	1:K:398:ARG:HG3	2.17	0.44
3:P:71:VAL:HG22	3:P:108:VAL:HG12	2.00	0.44
6:S:176:LYS:O	6:S:179:ILE:HG22	2.18	0.44
1:C:438:ILE:O	1:C:442:VAL:HG23	2.18	0.44
6:S:18:TYR:HB2	6:S:101:VAL:CG2	2.47	0.44
6:S:18:TYR:N	6:S:18:TYR:CD2	2.86	0.44
1:L:427:LEU:HD23	1:L:427:LEU:HA	1.86	0.44
1:C:101:GLU:C	1:C:103:LEU:H	2.20	0.44
2:M:25:PHE:CZ	2:M:36:LEU:HD13	2.52	0.44
2:N:85:PRO:O	2:N:86:VAL:HG12	2.18	0.44
1:J:255:GLU:HG3	1:J:258:ARG:CZ	2.47	0.44
1:C:401:ALA:HA	1:C:418:LEU:HD11	1.99	0.44
1:A:397:TYR:CG	1:A:421:GLY:HA3	2.53	0.44
1:J:43:GLY:C	1:J:45:ARG:N	2.71	0.44
1:A:505:LEU:O	1:A:506:ALA:C	2.55	0.44
1:L:284:LEU:HA	1:L:284:LEU:HD23	1.81	0.44
1:J:349:GLN:HB2	1:J:351:PHE:CE1	2.52	0.44
6:W:22:LEU:HB2	6:W:105:PHE:CE2	2.53	0.44
1:C:497:LEU:O	1:C:499:GLU:N	2.51	0.44
5:R:5:ARG:HB3	5:R:6:GLN:H	1.55	0.44
1:C:44:LEU:HD11	1:C:53:VAL:HG11	2.00	0.44
7:T:127:VAL:HG13	8:U:34:ASN:ND2	2.30	0.44
3:P:42:ARG:NH2	3:P:219:GLU:OE2	2.51	0.44
1:L:501:VAL:CG2	1:L:502:THR:H	2.30	0.44
1:K:305:LEU:O	1:K:305:LEU:HG	2.17	0.44
1:L:78:ASN:ND2	1:L:80:LYS:H	2.15	0.44
1:A:188:ARG:HH11	1:A:437:ALA:HA	1.82	0.44
4:Q:75:TYR:HD2	4:Q:99:THR:CG2	2.31	0.44
1:A:440:GLU:O	1:A:444:VAL:HG12	2.17	0.44
1:C:210:ARG:HB2	2:F:126:MET:HE3	1.99	0.44
1:K:136:ILE:HG23	2:O:194:ASN:CA	2.48	0.44
1:A:314:ASP:C	1:A:316:PHE:H	2.20	0.44
3:P:176:LYS:HA	3:P:177:PRO:HD3	1.78	0.44
3:G:250:PHE:CD1	3:G:250:PHE:C	2.91	0.44
1:J:424:LEU:HD23	1:J:424:LEU:HA	1.72	0.44
1:K:187:LYS:NZ	1:K:224:ASP:HB3	2.32	0.44
4:H:56:GLN:O	4:H:82:VAL:HG12	2.18	0.44
1:C:135:GLY:O	1:C:139:ARG:HD2	2.18	0.43
1:K:180:ILE:HA	1:K:180:ILE:HD13	1.69	0.43
1:A:476:HIS:C	1:A:478:ALA:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:48:GLN:HG3	1:K:51:GLU:HB2	2.00	0.43
7:T:132:ILE:HG13	8:U:88:GLN:NE2	2.25	0.43
1:C:457:GLU:H	1:C:460:LYS:NZ	2.16	0.43
1:J:501:VAL:HG12	1:J:502:THR:N	2.32	0.43
2:F:29:LEU:HA	2:F:30:PRO:HD3	1.81	0.43
4:Q:48:LEU:C	4:Q:50:ALA:N	2.71	0.43
2:N:9:THR:HB	2:N:27:GLU:CG	2.48	0.43
6:W:139:LYS:CG	6:W:142:LEU:HD12	2.46	0.43
1:B:386:VAL:CG2	1:B:387:ALA:N	2.78	0.43
2:F:86:VAL:CG2	2:F:87:GLY:N	2.79	0.43
2:M:155:PHE:HB2	2:M:334:VAL:HG22	1.99	0.43
2:O:189:ARG:HB2	2:O:192:GLU:CG	2.48	0.43
1:K:41:VAL:HG23	1:K:71:VAL:HB	2.00	0.43
10:J:600:ANP:O2B	10:J:600:ANP:O2G	2.36	0.43
3:G:248:LEU:HD23	3:G:248:LEU:HA	1.53	0.43
2:O:317:LEU:HA	2:O:317:LEU:HD23	1.60	0.43
1:K:43:GLY:O	1:K:44:LEU:C	2.57	0.43
2:F:415:SER:HB2	2:F:459:MET:CE	2.48	0.43
2:D:138:LYS:HG2	2:D:437:THR:HG23	1.98	0.43
1:K:309:ALA:HA	1:K:321:LEU:HB3	2.00	0.43
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.48	0.43
2:O:405:SER:O	2:O:409:LYS:HG3	2.17	0.43
1:L:248:TYR:O	1:L:251:CYS:HB3	2.18	0.43
6:S:59:TYR:CD2	6:S:59:TYR:N	2.86	0.43
2:D:284:THR:O	2:D:285:LEU:C	2.55	0.43
1:L:168:ILE:HG23	1:L:351:PHE:CD1	2.53	0.43
1:J:66:LEU:HB3	2:N:71:ARG:HD3	1.99	0.43
1:C:383:MET:O	1:C:386:VAL:HG23	2.18	0.43
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.18	0.43
1:J:472:VAL:HG23	1:J:480:LEU:HD22	2.00	0.43
2:M:243:PHE:N	2:M:243:PHE:HD1	2.15	0.43
1:L:100:GLY:HA2	1:L:256:TYR:CE2	2.53	0.43
1:C:45:ARG:NH1	2:D:71:ARG:HH12	2.17	0.43
1:B:151:LYS:HB2	1:B:151:LYS:HE3	1.81	0.43
1:J:509:GLU:O	1:J:510:ALA:HB3	2.18	0.43
1:K:47:VAL:HG23	1:K:90:ARG:HG2	2.00	0.43
3:G:200:VAL:HG22	4:H:56:GLN:HA	2.00	0.43
1:K:335:SER:HA	1:K:340:THR:HG23	1.99	0.43
4:H:72:THR:O	4:H:72:THR:HG22	2.17	0.43
2:E:129:GLU:HA	2:E:129:GLU:OE1	2.17	0.43
1:K:220:LEU:HD23	1:K:220:LEU:HA	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:335:LEU:HA	2:F:347:ALA:O	2.18	0.43
1:A:43:GLY:C	1:A:45:ARG:N	2.71	0.43
1:B:468:PHE:O	1:B:472:VAL:HG13	2.18	0.43
2:E:313:PRO:HD2	2:E:322:PRO:HG3	2.00	0.43
2:E:319:ASP:HA	3:G:255:GLN:NE2	2.33	0.43
2:D:201:ILE:HG13	2:D:206:ILE:HB	2.00	0.43
3:G:242:MET:O	3:G:246:LEU:HB2	2.19	0.43
2:F:312:VAL:HG13	2:F:322:PRO:HG2	2.00	0.43
2:F:241:GLU:HG2	2:F:244:ARG:HH21	1.81	0.43
2:N:396:LEU:HD22	2:N:396:LEU:N	2.33	0.43
3:P:20:THR:HG21	3:P:236:SER:N	2.32	0.43
2:F:73:GLN:HB2	2:F:73:GLN:HE21	1.64	0.43
3:G:157:GLU:HG2	3:G:158:GLY:N	2.33	0.43
2:E:39:GLN:HE21	2:E:76:LEU:HB3	1.81	0.43
1:L:295:PRO:HD2	1:L:298:VAL:HB	2.00	0.43
2:M:223:ASN:OD1	2:M:224:GLU:HG2	2.19	0.43
1:C:279:ARG:CG	1:C:283:LEU:HD12	2.48	0.43
1:K:485:THR:C	1:K:487:GLY:N	2.72	0.43
1:J:78:ASN:OD1	1:J:79:ASP:N	2.50	0.43
2:D:137:ILE:HD13	2:D:418:PHE:HZ	1.82	0.43
2:F:247:GLU:O	2:F:248:GLY:C	2.55	0.43
6:S:71:ASP:O	6:S:75:LYS:HB2	2.19	0.43
2:E:16:VAL:HG22	2:E:21:VAL:HG22	2.00	0.43
2:N:152:ILE:HD12	2:N:152:ILE:N	2.33	0.43
6:W:76:GLU:HB3	6:W:77:LYS:H	1.61	0.43
4:H:29:ASN:O	4:H:30:SER:C	2.57	0.43
3:P:150:ASN:O	3:P:152:GLY:N	2.52	0.43
1:C:180:ILE:HD11	1:C:216:LEU:HD11	2.00	0.43
1:K:165:GLU:O	1:K:325:PRO:HD2	2.19	0.43
2:O:29:LEU:HA	2:O:30:PRO:HD3	1.78	0.43
2:E:31:PRO:HD2	2:E:34:ASN:CG	2.39	0.43
2:N:312:VAL:HG12	2:N:316:ASP:H	1.84	0.43
2:O:432:VAL:HA	2:O:433:PRO:HD3	1.75	0.43
4:H:58:LEU:HB2	4:H:80:GLY:H	1.84	0.43
7:T:183:GLN:O	7:T:187:ALA:HB3	2.19	0.43
2:F:142:LEU:HG	2:F:143:LEU:HD23	2.00	0.43
3:G:51:LEU:O	3:G:52:TYR:C	2.56	0.43
2:F:180:TYR:HD1	2:F:249:GLN:HG2	1.83	0.43
9:V:32:ALA:HB1	9:V:36:TYR:CB	2.49	0.43
1:C:200:TYR:HE1	1:C:262:LYS:HD2	1.82	0.43
1:A:189:PHE:HB3	1:A:197:LYS:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:188:ARG:HE	1:J:188:ARG:HB3	1.44	0.43
4:Q:28:PHE:HE2	4:Q:75:TYR:HH	1.63	0.43
1:K:46:ASN:HB2	1:K:90:ARG:HH11	1.84	0.43
1:K:460:LYS:NZ	1:K:510:ALA:HB2	2.33	0.43
6:S:64:VAL:O	6:S:64:VAL:HG12	2.18	0.43
1:K:417:LEU:HA	1:K:417:LEU:HD23	1.57	0.43
1:C:381:ARG:NH1	1:C:385:GLN:HE21	2.17	0.43
1:K:28:THR:CG2	1:K:29:GLY:N	2.81	0.43
1:J:484:ARG:HG2	1:J:485:THR:N	2.34	0.43
1:J:179:ALA:O	1:J:182:THR:HB	2.18	0.43
1:C:214:ALA:HA	2:F:123:PHE:CZ	2.54	0.43
6:W:8:PRO:HD2	6:W:108:MSE:CE	2.48	0.43
6:S:98:THR:N	6:S:99:PRO:CD	2.82	0.43
2:N:20:VAL:O	2:N:20:VAL:HG12	2.16	0.43
1:J:266:ILE:HG13	1:J:267:ILE:N	2.32	0.43
1:B:441:GLN:O	1:B:445:ILE:HG13	2.19	0.43
1:A:172:GLN:CA	10:A:600:ANP:HNB1	2.28	0.43
2:D:464:GLU:HA	2:D:467:VAL:HG23	1.99	0.43
3:G:130:GLU:HB3	5:I:41:THR:O	2.19	0.43
2:N:101:PRO:HG2	2:N:107:PRO:HA	2.01	0.43
1:L:74:VAL:O	1:L:74:VAL:HG23	2.18	0.43
1:K:399:GLU:OE2	1:K:399:GLU:N	2.50	0.43
3:G:171:TYR:CD2	3:G:171:TYR:N	2.86	0.43
2:O:91:LEU:HD21	2:O:180:TYR:CD2	2.54	0.43
1:J:433:TYR:C	1:J:435:PRO:HD3	2.38	0.43
2:F:434:LEU:HD12	2:F:438:ILE:HG13	2.01	0.43
1:C:447:ALA:O	1:C:452:TYR:HB2	2.18	0.43
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.71	0.43
2:D:278:ALA:C	2:D:280:GLY:H	2.22	0.43
1:B:300:TYR:HA	1:B:303:SER:OG	2.19	0.43
1:B:187:LYS:NZ	1:B:224:ASP:HB3	2.34	0.43
1:A:210:ARG:C	1:A:212:THR:N	2.71	0.43
2:N:195:ASP:O	2:N:199:GLU:HG3	2.18	0.43
3:G:44:TYR:CD1	3:G:45:GLY:N	2.86	0.43
1:C:302:HIS:O	1:C:306:LEU:HB2	2.18	0.43
1:A:8:VAL:HG23	6:S:17:ARG:CB	2.43	0.43
2:N:279:VAL:HG12	2:N:281:TYR:HD1	1.84	0.43
1:J:300:TYR:CE2	1:J:304:ARG:NH1	2.86	0.43
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.54	0.43
2:E:281:TYR:CZ	2:E:321:ALA:HB2	2.53	0.43
1:C:62:MET:O	1:C:73:VAL:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:PHE:O	1:C:365:ILE:O	2.36	0.43
2:F:35:ALA:CB	2:F:82:ILE:HG13	2.46	0.43
1:A:225:ALA:HA	1:A:228:TYR:HE2	1.81	0.43
1:J:458:PRO:HA	1:J:461:ILE:HG13	1.99	0.43
1:B:48:GLN:HB3	2:F:68:GLY:O	2.19	0.43
1:C:42:HIS:CE1	1:C:45:ARG:HH21	2.36	0.43
2:O:39:GLN:HG3	2:O:76:LEU:CD2	2.47	0.43
1:A:100:GLY:HA2	1:A:256:TYR:CE2	2.53	0.43
1:L:476:HIS:C	1:L:478:ALA:H	2.21	0.43
1:C:176:THR:O	1:C:178:ILE:N	2.52	0.43
2:D:37:GLU:O	2:D:75:VAL:HA	2.18	0.43
1:K:246:ALA:O	1:K:247:PRO:C	2.55	0.43
2:D:471:ASP:N	2:D:471:ASP:OD2	2.52	0.43
3:P:248:LEU:HA	3:P:248:LEU:HD23	1.50	0.43
1:J:371:VAL:HG22	1:J:372:SER:N	2.33	0.43
2:N:367:HIS:HA	2:N:438:ILE:HD13	2.00	0.43
2:D:251:VAL:HG23	2:D:303:SER:O	2.18	0.43
6:S:22:LEU:HB2	6:S:105:PHE:CE2	2.54	0.43
1:C:266:ILE:HD13	1:C:268:TYR:CZ	2.53	0.43
2:O:25:PHE:CD1	2:O:30:PRO:CD	2.97	0.43
1:A:5:THR:O	1:A:6:ALA:HB3	2.19	0.43
6:S:51:MSE:HE1	6:S:69:LEU:CD2	2.45	0.43
1:L:134:PRO:CG	1:L:258:ARG:HH21	2.31	0.43
2:M:49:VAL:HA	2:M:60:THR:HG22	2.01	0.43
1:L:351:PHE:O	1:L:365:ILE:O	2.37	0.43
1:B:140:ILE:HD13	1:B:143:ARG:HE	1.82	0.43
2:F:94:ILE:HG22	2:F:102:ILE:CD1	2.48	0.43
6:S:177:THR:O	6:S:181:LYS:HG3	2.18	0.43
5:R:40:SER:O	5:R:42:ILE:N	2.52	0.43
1:C:264:ALA:HB3	1:C:321:LEU:HD13	2.00	0.43
1:A:46:ASN:HB3	1:A:90:ARG:HH11	1.83	0.43
3:P:51:LEU:O	3:P:53:GLU:N	2.52	0.43
1:C:74:VAL:O	1:C:74:VAL:HG23	2.19	0.43
2:M:234:LEU:HA	2:M:234:LEU:HD22	1.41	0.43
3:P:157:GLU:HG2	3:P:158:GLY:N	2.34	0.43
2:E:145:PRO:HD2	2:E:355:SER:CB	2.49	0.43
2:N:454:GLU:O	2:N:456:ALA:N	2.47	0.43
1:C:200:TYR:CD1	1:C:257:PHE:CD2	3.06	0.43
4:H:75:TYR:HD2	4:H:99:THR:CG2	2.31	0.43
1:C:209:LYS:NZ	1:C:211:SER:HB2	2.34	0.43
1:K:41:VAL:HG23	1:K:71:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:422:GLU:O	2:O:423:VAL:C	2.56	0.43
2:N:155:PHE:CD1	2:N:155:PHE:N	2.87	0.43
1:A:381:ARG:HB2	1:A:381:ARG:HE	1.57	0.43
4:H:108:ALA:C	4:H:110:ALA:N	2.72	0.43
1:A:167:ILE:HB	1:A:326:VAL:HG22	2.00	0.43
3:G:150:ASN:O	3:G:152:GLY:N	2.52	0.43
4:H:138:ASN:O	4:H:141:LEU:HB2	2.19	0.43
1:A:371:VAL:HG22	1:A:372:SER:N	2.33	0.43
6:W:91:GLU:O	6:W:93:GLY:N	2.51	0.43
6:S:7:PRO:HA	6:S:8:PRO:HD3	1.88	0.43
3:P:25:MET:HE2	3:P:25:MET:HB2	1.86	0.43
1:K:106:ARG:NH1	1:K:121:ILE:HG12	2.34	0.43
1:C:44:LEU:CD1	1:C:53:VAL:HG11	2.47	0.43
9:V:16:ILE:HA	9:V:19:TYR:CB	2.48	0.43
1:K:34:ILE:HD13	1:K:39:ALA:HB2	2.00	0.43
2:D:393:MET:O	2:D:396:LEU:HG	2.18	0.43
2:O:89:GLU:O	2:O:108:ILE:HG23	2.19	0.43
1:C:269:ASP:HA	1:C:270:ASP:HA	1.71	0.43
7:T:139:THR:OG1	9:V:67:PRO:HB3	2.18	0.43
2:M:420:VAL:O	2:M:420:VAL:HG23	2.19	0.43
1:C:102:GLU:OE2	1:C:122:GLY:O	2.36	0.43
1:K:353:GLU:CB	1:K:356:LEU:HD12	2.49	0.43
1:J:390:MET:HE3	1:J:424:LEU:HD22	2.00	0.43
1:J:172:GLN:HA	10:J:600:ANP:HNB1	1.83	0.43
1:C:203:TYR:CD2	1:C:203:TYR:O	2.72	0.43
1:A:428:LEU:HA	1:A:428:LEU:HD23	1.75	0.43
4:Q:138:ASN:O	4:Q:141:LEU:HB2	2.18	0.43
2:M:103:ASP:N	2:M:103:ASP:OD1	2.47	0.43
6:S:26:ALA:C	6:S:28:LYS:N	2.72	0.43
1:B:184:ILE:HG22	1:B:435:PRO:CG	2.42	0.43
1:L:383:MET:O	1:L:384:LYS:C	2.58	0.43
2:O:390:ILE:HD11	3:P:239:ALA:HA	2.01	0.43
3:G:179:PHE:HB3	3:G:184:ILE:HG23	1.99	0.43
1:L:270:ASP:HB2	1:L:326:VAL:O	2.19	0.43
2:E:453:PRO:HB2	2:E:454:GLU:H	1.45	0.43
2:F:249:GLN:HG3	2:F:250:ASP:H	1.82	0.43
1:A:256:TYR:CD2	1:A:257:PHE:N	2.87	0.43
2:O:163:THR:OG1	10:O:600:ANP:O2B	2.35	0.43
2:O:151:LYS:HD3	2:O:328:HIS:O	2.18	0.43
2:F:140:VAL:HG11	2:F:146:TYR:CZ	2.54	0.43
1:B:97:VAL:HG11	1:B:249:SER:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:373:ARG:HB2	1:K:374:VAL:H	1.58	0.43
1:A:109:ASP:C	1:A:109:ASP:OD2	2.57	0.43
9:V:39:ASP:C	9:V:41:ASP:H	2.21	0.43
1:J:165:GLU:OE1	1:J:348:GLY:HA3	2.18	0.43
6:S:36:GLU:HG3	6:S:109:MSE:HG3	2.00	0.43
2:M:9:THR:O	2:M:76:LEU:HD23	2.19	0.43
1:A:8:VAL:CG2	6:S:17:ARG:HD3	2.48	0.43
6:S:80:PRO:HB2	6:S:81:LEU:H	1.64	0.43
2:N:259:PHE:CE1	2:N:313:PRO:HG3	2.54	0.43
1:K:104:LEU:HD21	1:K:200:TYR:HD2	1.84	0.43
2:M:32:ILE:HA	2:M:49:VAL:HG12	2.00	0.43
1:A:410:LEU:O	1:A:411:ASP:C	2.56	0.43
2:O:45:LEU:HD23	2:O:69:LEU:HD21	2.01	0.43
1:A:479:LEU:HD13	1:A:496:LYS:CE	2.49	0.43
1:C:383:MET:O	1:C:384:LYS:C	2.58	0.43
2:D:170:ILE:CD1	2:D:183:PHE:HD1	2.32	0.43
3:P:125:LEU:O	3:P:126:VAL:HG13	2.19	0.43
2:O:390:ILE:HG22	2:O:391:LEU:HG	1.99	0.43
1:J:87:ILE:N	1:J:87:ILE:HD12	2.32	0.43
2:M:430:LYS:HA	2:M:430:LYS:HD3	1.84	0.43
1:C:218:LYS:HG2	2:F:128:VAL:HG21	2.00	0.43
2:F:452:LEU:HD22	2:F:470:ALA:HB1	2.00	0.43
6:W:11:ILE:CG2	6:W:11:ILE:O	2.67	0.43
1:A:29:GLY:CA	1:A:42:HIS:O	2.67	0.43
7:X:168:LYS:HD3	7:X:171:GLU:OE2	2.18	0.43
6:S:76:GLU:HB3	6:S:77:LYS:H	1.61	0.43
1:B:476:HIS:C	1:B:478:ALA:N	2.70	0.43
1:B:292:GLU:O	1:B:293:ALA:HB3	2.19	0.43
1:L:231:VAL:O	1:L:231:VAL:HG12	2.19	0.43
1:K:36:ASP:HB3	1:K:284:LEU:HD22	2.00	0.43
1:B:424:LEU:HA	1:B:424:LEU:HD23	1.74	0.43
1:C:148:THR:HG21	1:C:153:VAL:HG11	2.01	0.43
3:P:141:ALA:CB	3:P:214:TYR:HB2	2.49	0.42
2:E:312:VAL:HA	2:E:313:PRO:HD2	1.89	0.42
1:L:136:ILE:O	2:M:194:ASN:HB2	2.19	0.42
2:F:70:VAL:CG1	2:F:71:ARG:N	2.82	0.42
3:G:51:LEU:O	3:G:53:GLU:N	2.52	0.42
1:A:202:ILE:O	1:A:266:ILE:HA	2.19	0.42
1:A:204:VAL:CG2	1:A:266:ILE:HD11	2.49	0.42
2:D:26:ASP:CA	6:S:6:ARG:HH12	2.30	0.42
3:P:172:LYS:HG3	3:P:173:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:35:ALA:C	2:D:36:LEU:HD23	2.40	0.42
1:J:276:VAL:O	1:J:279:ARG:HB3	2.19	0.42
5:I:40:SER:O	5:I:42:ILE:N	2.52	0.42
1:B:206:ILE:HG21	1:B:274:GLN:HB2	2.00	0.42
4:Q:29:ASN:O	4:Q:30:SER:C	2.58	0.42
2:O:77:ASP:OD1	2:O:78:SER:N	2.52	0.42
1:A:184:ILE:HG22	1:A:435:PRO:HG2	1.99	0.42
1:A:165:GLU:OE1	1:A:348:GLY:HA3	2.18	0.42
6:S:11:ILE:HD11	6:S:108:MSE:HB2	2.01	0.42
1:J:186:GLN:HG2	1:J:199:LEU:HD23	2.01	0.42
1:L:47:VAL:O	2:M:70:VAL:HG13	2.19	0.42
4:H:57:VAL:CG1	5:I:11:TYR:CE1	2.98	0.42
1:L:182:THR:HG22	1:L:183:ILE:N	2.34	0.42
1:A:202:ILE:HB	1:A:266:ILE:HD12	2.00	0.42
3:G:192:ILE:O	4:H:53:PRO:HB2	2.19	0.42
2:D:51:GLN:HG3	2:D:59:ARG:HB3	2.00	0.42
2:O:379:GLN:CG	2:O:379:GLN:O	2.67	0.42
2:D:370:VAL:O	2:D:374:VAL:HG23	2.19	0.42
1:B:353:GLU:CB	1:B:356:LEU:HD12	2.48	0.42
7:T:152:LYS:HG2	7:T:152:LYS:O	2.19	0.42
2:O:132:ILE:HG13	2:O:133:LEU:N	2.33	0.42
2:D:168:GLU:N	2:D:420:VAL:HG11	2.34	0.42
1:L:314:ASP:O	1:L:316:PHE:N	2.52	0.42
2:N:146:TYR:CD1	2:N:152:ILE:HG12	2.55	0.42
1:K:175:LYS:HB2	1:K:175:LYS:HE2	1.68	0.42
4:H:120:LEU:O	4:H:122:ALA:N	2.51	0.42
1:K:186:GLN:CD	1:K:199:LEU:HD23	2.39	0.42
2:D:182:VAL:HG22	2:D:216:ALA:HB3	2.01	0.42
2:E:195:ASP:O	2:E:199:GLU:HG3	2.19	0.42
2:D:336:SER:OG	2:D:339:ILE:HG13	2.19	0.42
6:W:22:LEU:HD21	6:W:85:LEU:HD22	2.00	0.42
6:W:88:LEU:HD22	6:W:88:LEU:HA	1.66	0.42
1:L:137:ILE:O	1:L:139:ARG:N	2.52	0.42
1:L:271:LEU:HD13	1:L:302:HIS:CD2	2.54	0.42
1:J:410:LEU:H	1:J:410:LEU:HD12	1.83	0.42
2:D:247:GLU:HB3	2:D:249:GLN:CB	2.39	0.42
1:B:313:ASN:OD1	1:B:316:PHE:HD1	2.02	0.42
2:E:170:ILE:HD13	2:E:215:VAL:HG21	2.00	0.42
3:G:125:LEU:O	3:G:126:VAL:HG13	2.19	0.42
2:O:35:ALA:CB	2:O:82:ILE:HG13	2.47	0.42
2:M:162:LYS:HB3	2:M:162:LYS:HE2	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:264:ALA:HB3	1:L:321:LEU:HD13	2.01	0.42
4:H:35:GLN:HG2	4:H:36:VAL:H	1.83	0.42
2:M:100:GLU:HA	2:M:101:PRO:HD3	1.74	0.42
3:P:129:LYS:HG2	3:P:130:GLU:N	2.33	0.42
1:C:276:VAL:O	1:C:279:ARG:HB3	2.20	0.42
1:A:283:LEU:O	2:D:275:ILE:HD12	2.19	0.42
2:N:110:THR:HG22	2:N:111:LYS:N	2.33	0.42
1:C:476:HIS:C	1:C:478:ALA:H	2.20	0.42
1:K:136:ILE:HG23	2:O:194:ASN:HA	2.02	0.42
1:J:366:ASN:OD1	1:J:366:ASN:C	2.58	0.42
3:P:72:SER:OG	3:P:73:SER:N	2.51	0.42
1:J:333:ASP:OD1	1:J:336:ALA:N	2.52	0.42
2:F:234:LEU:O	2:F:237:LEU:HB3	2.18	0.42
2:F:96:ASN:ND2	2:F:98:ILE:N	2.68	0.42
2:E:279:VAL:CG1	2:E:320:PRO:HG2	2.49	0.42
1:K:104:LEU:HD22	1:K:228:TYR:HA	2.01	0.42
2:M:32:ILE:H	2:M:32:ILE:HG12	1.33	0.42
1:C:479:LEU:CD2	1:C:493:SER:HB3	2.49	0.42
1:C:460:LYS:C	1:C:462:THR:H	2.22	0.42
4:Q:37:ASP:OD2	4:Q:64:VAL:HG12	2.20	0.42
4:H:37:ASP:OD2	4:H:64:VAL:HG12	2.19	0.42
2:F:172:ASN:CG	2:F:431:LEU:HD12	2.39	0.42
2:N:409:LYS:HB3	2:N:457:PHE:CD1	2.54	0.42
1:J:164:ARG:H	1:J:164:ARG:HD3	1.84	0.42
6:S:19:ALA:C	6:S:21:ALA:H	2.22	0.42
2:D:313:PRO:HG2	2:D:319:ASP:CG	2.39	0.42
3:P:191:SER:C	3:P:193:TYR:N	2.73	0.42
1:L:174:GLY:HA2	10:L:600:ANP:PA	2.59	0.42
1:A:284:LEU:C	1:A:286:ARG:H	2.23	0.42
1:A:490:SER:C	1:A:492:GLU:N	2.72	0.42
1:J:137:ILE:N	1:J:138:PRO:HD2	2.35	0.42
2:N:129:GLU:OE1	2:N:129:GLU:HA	2.19	0.42
2:O:430:LYS:HA	2:O:430:LYS:HD3	1.76	0.42
2:E:196:LEU:O	2:E:200:MET:HG3	2.20	0.42
2:E:197:TYR:O	2:E:201:ILE:HG13	2.18	0.42
6:W:145:GLY:O	6:W:146:GLN:C	2.57	0.42
1:C:502:THR:C	1:C:504:PHE:H	2.22	0.42
2:M:96:ASN:CB	2:M:102:ILE:HD11	2.46	0.42
1:C:80:LYS:HG2	1:C:81:LEU:HD23	2.02	0.42
2:D:162:LYS:HE2	2:D:162:LYS:HB3	1.71	0.42
1:L:479:LEU:CD1	1:L:496:LYS:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:1:VAL:HG11	5:I:6:GLN:OE1	2.20	0.42
3:P:250:PHE:CD1	3:P:250:PHE:C	2.93	0.42
1:K:137:ILE:HA	1:K:137:ILE:HD13	1.93	0.42
2:O:16:VAL:HG12	2:O:21:VAL:HG13	2.02	0.42
1:L:182:THR:O	1:L:185:ASN:HB3	2.18	0.42
5:I:9:LEU:HD11	5:I:13:ARG:HG2	2.00	0.42
2:E:377:ILE:HG23	2:E:378:LEU:N	2.33	0.42
1:L:75:VAL:HG12	1:L:77:GLY:N	2.31	0.42
4:Q:27:PHE:HE2	4:Q:97:ALA:CB	2.30	0.42
2:O:73:GLN:HB2	2:O:73:GLN:HE21	1.64	0.42
1:L:80:LYS:HG2	1:L:81:LEU:HD23	2.00	0.42
1:A:383:MET:CE	1:A:441:GLN:HE21	2.32	0.42
2:M:25:PHE:HZ	2:M:36:LEU:HD13	1.84	0.42
2:M:137:ILE:HA	2:M:416:GLN:HE22	1.84	0.42
1:B:278:TYR:CG	1:B:301:LEU:HD13	2.54	0.42
1:L:280:GLN:HG2	1:L:284:LEU:CD1	2.50	0.42
2:D:17:ILE:O	2:D:19:ALA:N	2.52	0.42
2:D:296:ILE:HG22	2:D:296:ILE:O	2.18	0.42
2:N:211:ALA:C	2:N:213:SER:H	2.22	0.42
1:L:148:THR:HG21	1:L:153:VAL:HG11	2.02	0.42
3:G:176:LYS:HA	3:G:177:PRO:HD3	1.80	0.42
1:C:249:SER:O	1:C:253:MET:HG3	2.19	0.42
6:W:4:LEU:HB3	6:W:5:VAL:H	1.65	0.42
1:J:204:VAL:HG21	1:J:266:ILE:HD11	2.01	0.42
1:C:312:MET:HB2	1:C:319:GLY:O	2.20	0.42
1:C:303:SER:OG	1:C:304:ARG:N	2.53	0.42
4:H:20:PHE:HD1	4:H:92:LEU:HB3	1.85	0.42
1:J:44:LEU:C	1:J:46:ASN:H	2.20	0.42
3:G:129:LYS:HG2	3:G:130:GLU:N	2.34	0.42
1:J:478:ALA:HB1	1:J:479:LEU:HD12	2.00	0.42
1:L:508:PHE:HB3	1:L:509:GLU:H	1.69	0.42
7:T:188:GLN:OE1	7:T:191:LYS:HG3	2.20	0.42
2:N:343:GLY:O	2:N:458:TYR:OH	2.23	0.42
1:B:418:LEU:O	1:B:421:GLY:N	2.53	0.42
2:O:188:GLU:O	2:O:222:MET:HG2	2.19	0.42
2:O:258:ILE:O	2:O:261:PHE:HB3	2.19	0.42
6:S:131:LEU:HD12	6:S:134:LEU:CD1	2.50	0.42
1:A:468:PHE:CD2	1:A:468:PHE:C	2.92	0.42
1:A:282:SER:CB	1:A:295:PRO:HG3	2.49	0.42
1:B:505:LEU:CG	1:B:505:LEU:O	2.67	0.42
1:J:139:ARG:CZ	1:J:310:ALA:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:VAL:HG11	1:C:465:GLU:HG3	2.02	0.42
2:O:472:LYS:HE3	2:O:472:LYS:HB3	1.82	0.42
1:J:274:GLN:HB3	1:J:274:GLN:HE21	1.45	0.42
2:F:17:ILE:HG23	2:F:17:ILE:O	2.19	0.42
4:Q:68:GLU:HG3	4:Q:68:GLU:O	2.18	0.42
1:B:125:ALA:C	1:B:126:ARG:HG2	2.39	0.42
2:N:10:THR:CG2	2:N:11:GLY:N	2.82	0.42
2:D:185:GLY:HA2	2:D:256:ASP:O	2.19	0.42
2:O:237:LEU:HD12	2:O:237:LEU:HA	1.68	0.42
6:S:92:ASN:O	6:S:94:ARG:HG3	2.20	0.42
1:C:134:PRO:HG3	1:C:258:ARG:HH21	1.85	0.42
2:N:417:PRO:O	2:N:417:PRO:CG	2.67	0.42
1:J:479:LEU:HD13	1:J:496:LYS:CE	2.49	0.42
2:E:410:ILE:HG23	2:E:441:PHE:CD2	2.55	0.42
2:N:32:ILE:HG22	2:N:33:LEU:HG	2.00	0.42
1:J:442:VAL:CG1	1:J:489:ILE:HD11	2.48	0.42
2:F:136:GLY:HA2	2:F:432:VAL:O	2.20	0.42
2:M:93:ARG:HG3	2:M:108:ILE:CD1	2.49	0.42
2:M:348:VAL:O	2:M:350:PRO:HD3	2.20	0.42
9:V:51:TYR:N	9:V:51:TYR:CD1	2.88	0.42
4:Q:135:ILE:HG22	4:Q:136:GLU:N	2.35	0.42
2:M:314:ALA:O	2:M:315:ASP:HB2	2.19	0.42
2:D:220:GLY:HA3	2:D:232:VAL:HG21	2.01	0.42
2:N:85:PRO:C	2:N:86:VAL:CG1	2.87	0.42
2:D:311:TYR:CE2	2:D:313:PRO:HA	2.54	0.42
7:T:138:VAL:HG21	8:U:37:LEU:HD22	2.02	0.42
3:G:37:GLU:HB3	3:G:218:LYS:HE3	2.02	0.42
1:K:313:ASN:OD1	1:K:315:ALA:HB3	2.20	0.42
6:S:73:THR:HB	6:S:83:SER:HB2	2.01	0.42
1:J:341:ASN:O	1:J:344:SER:HB3	2.19	0.42
1:B:292:GLU:HB2	1:B:294:TYR:CD1	2.55	0.42
2:D:200:MET:HE2	2:D:200:MET:HB2	1.88	0.42
1:B:492:GLU:O	1:B:493:SER:C	2.58	0.42
1:J:102:GLU:HG3	1:J:123:SER:HA	2.01	0.42
1:L:55:PHE:CE2	1:L:82:ILE:HD13	2.54	0.42
1:J:202:ILE:O	1:J:266:ILE:HA	2.20	0.42
3:G:203:ASN:HB3	4:H:57:VAL:HG21	2.02	0.42
1:B:145:PRO:HG3	1:B:378:ALA:O	2.20	0.42
1:L:67:GLU:HB3	1:L:68:PRO:CD	2.47	0.42
2:D:93:ARG:HG3	2:D:108:ILE:CD1	2.50	0.42
4:H:27:PHE:HE2	4:H:97:ALA:CB	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:39:GLN:HE21	2:N:76:LEU:HB3	1.82	0.42
9:V:29:PRO:HG2	9:V:36:TYR:CZ	2.55	0.42
9:Z:17:ARG:N	9:Z:20:ARG:HD2	2.35	0.42
2:D:413:PHE:CD2	2:D:444:ILE:HD11	2.55	0.42
2:F:258:ILE:O	2:F:261:PHE:HB3	2.20	0.42
2:N:237:LEU:HD13	2:N:253:LEU:HD22	2.02	0.42
2:O:87:GLY:HA2	2:O:242:TYR:CZ	2.55	0.42
1:J:133:ALA:CB	1:J:308:ARG:HA	2.50	0.42
1:L:175:LYS:HB2	1:L:175:LYS:HE2	1.83	0.42
6:S:186:MSE:C	6:S:188:GLU:H	2.22	0.42
6:W:9:VAL:O	6:W:10:GLN:HB2	2.19	0.42
4:Q:134:ARG:HG2	4:Q:138:ASN:HD22	1.85	0.42
1:K:168:ILE:O	1:K:168:ILE:HG23	2.19	0.42
2:N:398:GLU:OE2	2:N:401:LYS:HD2	2.20	0.42
1:K:49:ALA:C	1:K:50:GLU:HG3	2.40	0.42
2:N:257:ASN:HB2	2:N:309:ALA:HB3	2.01	0.42
1:L:101:GLU:C	1:L:103:LEU:H	2.23	0.42
1:A:191:ASP:N	1:A:192:GLY:N	2.68	0.42
2:N:279:VAL:HG11	2:N:320:PRO:HG2	2.02	0.42
1:B:395:ALA:HA	1:B:398:ARG:HH12	1.78	0.42
2:D:162:LYS:CB	12:D:600:ADP:O1B	2.60	0.42
1:L:136:ILE:HD11	2:M:219:TYR:CE2	2.53	0.42
1:K:185:ASN:HB2	1:K:435:PRO:HB3	2.01	0.42
1:K:285:LEU:O	1:K:286:ARG:HB2	2.19	0.42
1:L:200:TYR:CD1	1:L:257:PHE:HD2	2.37	0.42
2:M:429:GLY:O	2:M:430:LYS:HG2	2.20	0.42
1:L:397:TYR:HA	1:L:417:LEU:HD23	2.01	0.42
6:S:180:GLN:C	6:S:183:SER:OG	2.58	0.42
5:I:32:ALA:HA	5:I:35:MET:CE	2.50	0.42
2:D:139:VAL:HG21	2:D:348:VAL:CB	2.50	0.42
2:O:252:LEU:HA	2:O:252:LEU:HD23	1.80	0.42
2:D:319:ASP:O	2:D:321:ALA:N	2.53	0.42
1:L:380:THR:OG1	1:L:382:ALA:HB3	2.19	0.42
6:W:73:THR:HB	6:W:83:SER:HB2	2.02	0.42
1:C:380:THR:OG1	1:C:382:ALA:HB3	2.20	0.42
1:B:90:ARG:HH21	1:B:92:GLY:HA2	1.85	0.42
1:K:28:THR:HG22	1:K:29:GLY:N	2.35	0.42
2:D:337:ARG:HB2	2:D:337:ARG:HE	1.60	0.42
2:O:83:ARG:HA	2:O:114:ALA:O	2.20	0.42
2:E:211:ALA:C	2:E:213:SER:H	2.24	0.42
2:O:41:ARG:C	2:O:43:THR:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:180:ILE:HD11	1:L:216:LEU:HD11	2.02	0.42
6:S:22:LEU:CD2	6:S:85:LEU:HD22	2.50	0.42
6:W:26:ALA:C	6:W:28:LYS:N	2.73	0.42
6:S:9:VAL:HG11	6:S:107:THR:O	2.19	0.42
2:O:33:LEU:HA	2:O:33:LEU:HD23	1.88	0.42
1:A:15:ARG:NH1	1:A:15:ARG:HG3	2.35	0.42
6:S:97:ASN:C	6:S:99:PRO:HD2	2.40	0.42
4:Q:58:LEU:HB2	4:Q:80:GLY:H	1.84	0.42
4:Q:80:GLY:HA3	4:Q:93:LEU:O	2.20	0.42
5:R:1:VAL:HG11	5:R:6:GLN:OE1	2.20	0.42
2:M:367:HIS:O	2:M:368:TYR:C	2.58	0.42
4:Q:47:ILE:HD12	4:Q:47:ILE:N	2.35	0.42
1:L:419:SER:HA	1:L:423:ARG:HH12	1.85	0.42
9:V:5:LEU:HD23	9:V:5:LEU:O	2.20	0.42
2:M:234:LEU:N	2:M:234:LEU:HD23	2.31	0.42
2:E:449:TYR:CD2	2:E:452:LEU:HD12	2.54	0.42
2:M:319:ASP:O	2:M:321:ALA:N	2.52	0.42
1:L:78:ASN:ND2	1:L:80:LYS:HB3	2.34	0.42
1:C:55:PHE:O	1:C:56:SER:C	2.57	0.42
2:O:162:LYS:HB2	2:O:162:LYS:HE2	1.76	0.42
2:O:256:ASP:HA	2:O:257:ASN:HA	1.85	0.42
2:D:313:PRO:HG2	2:D:319:ASP:OD1	2.20	0.42
1:K:144:GLU:HA	1:K:145:PRO:HD3	1.85	0.42
1:K:97:VAL:HG11	1:K:249:SER:CB	2.49	0.42
7:T:168:LYS:HD3	7:T:171:GLU:OE2	2.20	0.42
1:A:400:VAL:HG22	1:A:400:VAL:O	2.20	0.42
6:W:64:VAL:O	6:W:64:VAL:HG12	2.20	0.42
1:L:203:TYR:O	1:L:203:TYR:CD2	2.73	0.42
1:L:490:SER:C	1:L:492:GLU:N	2.74	0.42
2:D:249:GLN:OE1	2:D:249:GLN:HA	2.20	0.41
2:E:223:ASN:N	2:E:223:ASN:ND2	2.66	0.41
1:K:256:TYR:HD2	1:K:257:PHE:CD1	2.36	0.41
1:L:62:MET:HB2	1:L:76:PHE:HE1	1.84	0.41
1:A:407:GLY:HA3	1:A:410:LEU:CD2	2.44	0.41
1:B:140:ILE:HG12	1:B:141:SER:N	2.34	0.41
3:G:71:VAL:HG22	3:G:108:VAL:HG12	2.02	0.41
1:B:473:ILE:O	1:B:477:GLN:HG2	2.19	0.41
3:P:108:VAL:CG2	3:P:131:VAL:HG21	2.50	0.41
1:J:479:LEU:HD13	1:J:496:LYS:HD3	2.02	0.41
6:W:15:GLU:C	6:W:17:ARG:H	2.22	0.41
1:J:56:SER:HA	1:J:89:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:93:ARG:HA	2:O:103:ASP:OD2	2.20	0.41
3:P:134:ARG:HB2	5:R:41:THR:HG21	2.02	0.41
2:D:77:ASP:C	2:D:79:GLY:N	2.73	0.41
2:O:161:GLY:HA2	10:O:600:ANP:O2A	2.20	0.41
2:F:39:GLN:HG3	2:F:76:LEU:CD2	2.50	0.41
1:K:418:LEU:O	1:K:421:GLY:N	2.53	0.41
1:A:185:ASN:HB2	1:A:435:PRO:HB3	2.01	0.41
1:B:59:LEU:HA	1:B:59:LEU:HD23	1.81	0.41
2:O:333:THR:HA	2:O:353:SER:OG	2.20	0.41
1:L:497:LEU:O	1:L:499:GLU:N	2.53	0.41
1:A:292:GLU:O	1:A:293:ALA:HB3	2.20	0.41
6:W:54:SER:HB2	6:W:65:LYS:HE3	2.02	0.41
6:W:94:ARG:O	6:W:97:ASN:HB2	2.20	0.41
2:O:25:PHE:CB	2:O:29:LEU:HD12	2.42	0.41
1:B:394:LEU:O	1:B:398:ARG:HG3	2.20	0.41
2:E:279:VAL:HG12	2:E:281:TYR:HD1	1.84	0.41
7:T:143:ARG:HG2	7:T:146:ARG:NE	2.35	0.41
3:G:108:VAL:CG2	3:G:131:VAL:HG21	2.50	0.41
1:L:445:ILE:O	1:L:449:VAL:HG12	2.20	0.41
2:N:416:GLN:CB	2:N:417:PRO:HD2	2.50	0.41
2:M:200:MET:HE2	2:M:200:MET:HB2	1.92	0.41
1:L:440:GLU:O	1:L:443:ALA:HB3	2.20	0.41
1:B:62:MET:HG3	1:B:95:VAL:HG21	2.01	0.41
1:K:62:MET:HG3	1:K:95:VAL:CG2	2.49	0.41
1:A:210:ARG:C	1:A:212:THR:H	2.23	0.41
1:B:424:LEU:O	1:B:428:LEU:HD12	2.20	0.41
1:L:504:PHE:O	1:L:504:PHE:CD1	2.74	0.41
2:M:412:ARG:HH11	2:M:412:ARG:HG3	1.84	0.41
1:J:242:LEU:HA	1:J:242:LEU:HD23	1.79	0.41
1:B:466:ASN:HA	1:B:466:ASN:HD22	1.64	0.41
2:D:443:GLN:O	2:D:446:ALA:N	2.53	0.41
1:K:476:HIS:C	1:K:478:ALA:N	2.74	0.41
1:C:85:GLY:O	1:C:86:ASP:O	2.38	0.41
1:C:236:ALA:HB3	2:F:294:GLU:HG3	2.02	0.41
2:E:164:VAL:HA	2:E:167:MET:HE2	2.01	0.41
3:G:138:PHE:O	3:G:141:ALA:N	2.53	0.41
3:P:44:TYR:CD1	3:P:45:GLY:N	2.87	0.41
2:N:31:PRO:HD2	2:N:34:ASN:CG	2.40	0.41
1:J:201:CYS:HB2	1:J:229:THR:OG1	2.20	0.41
1:B:139:ARG:O	1:B:313:ASN:HB3	2.21	0.41
1:C:288:PRO:HA	1:C:289:PRO:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:127:THR:HG22	3:P:128:PHE:H	1.83	0.41
2:M:434:LEU:HD12	2:M:438:ILE:HG13	2.02	0.41
1:J:468:PHE:HE1	1:J:501:VAL:HG23	1.78	0.41
3:G:204:TYR:O	3:G:208:SER:HB3	2.20	0.41
4:H:38:VAL:HA	4:H:39:PRO:HD3	1.92	0.41
4:H:47:ILE:N	4:H:47:ILE:HD12	2.34	0.41
1:K:423:ARG:HG2	1:K:461:ILE:HD11	2.01	0.41
2:N:409:LYS:HB3	2:N:457:PHE:CE1	2.56	0.41
2:M:321:ALA:HB3	2:M:322:PRO:HD3	2.01	0.41
2:D:275:ILE:HG23	3:G:269:ALA:CB	2.50	0.41
1:C:409:ASP:C	1:C:410:LEU:HG	2.40	0.41
3:P:247:THR:O	3:P:247:THR:HG23	2.20	0.41
1:B:427:LEU:HD22	1:B:444:VAL:HG23	2.02	0.41
1:B:505:LEU:O	1:B:505:LEU:HG	2.21	0.41
6:W:143:SER:C	6:W:145:GLY:N	2.73	0.41
2:E:169:LEU:HD23	2:E:169:LEU:HA	1.90	0.41
3:G:160:ILE:CG2	3:G:160:ILE:O	2.68	0.41
2:M:138:LYS:HG2	2:M:437:THR:HG23	2.01	0.41
1:B:168:ILE:HG21	1:B:168:ILE:HD13	1.78	0.41
1:C:105:GLY:HA2	1:C:226:MET:O	2.20	0.41
1:A:106:ARG:NH2	1:A:118:LYS:HB2	2.35	0.41
6:W:20:THR:HA	6:W:23:TYR:CE2	2.55	0.41
2:F:161:GLY:HA2	10:F:600:ANP:O2A	2.20	0.41
1:L:428:LEU:HD12	1:L:428:LEU:H	1.83	0.41
3:G:214:TYR:CD2	3:G:214:TYR:C	2.92	0.41
1:K:257:PHE:N	1:K:257:PHE:CD1	2.89	0.41
1:C:48:GLN:HB2	1:C:51:GLU:CB	2.43	0.41
1:L:361:ILE:O	1:L:364:ALA:HA	2.20	0.41
5:I:11:TYR:O	5:I:12:ILE:C	2.59	0.41
1:C:49:ALA:HA	1:C:66:LEU:HD21	2.02	0.41
2:D:243:PHE:N	2:D:243:PHE:CD1	2.88	0.41
3:G:164:ARG:O	3:G:171:TYR:HB2	2.21	0.41
1:A:327:ILE:HD11	1:A:342:VAL:HG21	2.03	0.41
1:J:142:VAL:HG13	1:J:161:ARG:O	2.19	0.41
1:J:440:GLU:O	1:J:443:ALA:HB3	2.20	0.41
1:L:418:LEU:C	1:L:420:ARG:N	2.73	0.41
4:H:68:GLU:HG3	4:H:68:GLU:O	2.20	0.41
1:B:204:VAL:HG13	1:B:232:VAL:HB	2.02	0.41
1:J:210:ARG:C	1:J:212:THR:N	2.73	0.41
1:A:102:GLU:HG3	1:A:123:SER:HA	2.01	0.41
1:C:213:VAL:O	1:C:216:LEU:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ILE:CA	1:C:163:GLN:NE2	2.80	0.41
1:C:80:LYS:HD2	2:F:33:LEU:HD12	2.02	0.41
2:N:134:VAL:HG12	2:N:136:GLY:H	1.86	0.41
4:Q:20:PHE:HD1	4:Q:92:LEU:HB3	1.84	0.41
2:M:140:VAL:HG11	2:M:146:TYR:CZ	2.55	0.41
1:L:45:ARG:NH1	2:M:71:ARG:NH1	2.62	0.41
4:Q:54:THR:HG22	4:Q:55:LEU:N	2.35	0.41
1:K:59:LEU:HD21	1:K:77:GLY:HA3	2.03	0.41
1:C:164:ARG:NH1	1:C:307:GLU:HA	2.36	0.41
6:S:180:GLN:N	6:S:180:GLN:OE1	2.53	0.41
1:A:303:SER:CA	1:A:345:ILE:HD13	2.51	0.41
2:M:84:ILE:HD11	2:M:238:THR:HG22	2.02	0.41
2:O:89:GLU:HG3	2:O:110:THR:CA	2.49	0.41
4:H:78:SER:O	4:H:79:SER:HB3	2.21	0.41
1:C:440:GLU:O	1:C:443:ALA:HB3	2.20	0.41
1:J:347:ASP:HB3	2:N:191:ARG:HH21	1.86	0.41
1:C:468:PHE:CD2	1:C:468:PHE:O	2.73	0.41
1:J:293:ALA:HB2	3:P:265:ILE:HD13	2.02	0.41
2:O:464:GLU:O	2:O:467:VAL:N	2.52	0.41
1:A:231:VAL:O	1:A:231:VAL:HG12	2.19	0.41
2:N:432:VAL:HG12	2:N:436:GLU:HB2	2.02	0.41
2:N:176:ALA:O	2:N:177:HIS:ND1	2.53	0.41
2:D:432:VAL:HA	2:D:433:PRO:HD3	1.85	0.41
6:W:42:VAL:CG2	6:W:45:ILE:HD12	2.50	0.41
1:C:247:PRO:HB3	1:C:268:TYR:CD2	2.45	0.41
2:O:49:VAL:HA	2:O:60:THR:CG2	2.50	0.41
2:O:136:GLY:HA2	2:O:432:VAL:O	2.21	0.41
1:B:436:MET:HE2	1:B:441:GLN:HG3	2.03	0.41
1:L:69:ASP:OD1	1:L:69:ASP:C	2.58	0.41
2:D:243:PHE:N	2:D:243:PHE:HD1	2.19	0.41
1:K:163:GLN:CG	1:K:164:ARG:N	2.82	0.41
1:B:163:GLN:CG	1:B:164:ARG:N	2.84	0.41
4:H:37:ASP:O	4:H:63:VAL:HG13	2.20	0.41
2:E:469:LYS:O	2:E:473:LEU:HG	2.20	0.41
1:L:419:SER:O	1:L:423:ARG:CZ	2.69	0.41
1:C:218:LYS:HE2	1:C:222:ASP:CG	2.41	0.41
2:M:313:PRO:HG2	2:M:319:ASP:OD1	2.20	0.41
2:F:420:VAL:C	2:F:422:GLU:N	2.74	0.41
2:N:458:TYR:CE2	2:N:459:MET:HG2	2.54	0.41
1:L:46:ASN:O	1:L:90:ARG:NH1	2.53	0.41
1:C:101:GLU:OE1	1:C:262:LYS:HE3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ARG:NH1	1:A:437:ALA:N	2.68	0.41
10:O:600:ANP:O1A	10:O:600:ANP:N3B	2.54	0.41
3:P:190:MET:HA	3:P:190:MET:CE	2.50	0.41
1:B:41:VAL:HG23	1:B:71:VAL:O	2.21	0.41
1:J:333:ASP:OD1	1:J:333:ASP:C	2.59	0.41
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.76	0.41
1:K:446:TYR:CZ	1:K:497:LEU:HD23	2.56	0.41
1:J:397:TYR:CG	1:J:421:GLY:HA3	2.54	0.41
1:A:16:ILE:HG12	6:S:85:LEU:HD23	2.01	0.41
2:D:96:ASN:HD22	2:D:98:ILE:H	1.58	0.41
6:S:9:VAL:HG22	6:S:111:VAL:CG1	2.51	0.41
5:R:14:TYR:C	5:R:14:TYR:CD1	2.94	0.41
2:D:32:ILE:HA	2:D:49:VAL:HG12	2.01	0.41
2:M:193:GLY:HA2	2:M:219:TYR:OH	2.20	0.41
1:B:83:LYS:CB	1:B:83:LYS:NZ	2.78	0.41
1:B:137:ILE:O	1:B:139:ARG:N	2.53	0.41
1:J:46:ASN:HB3	1:J:90:ARG:HH11	1.85	0.41
3:P:2:THR:O	3:P:6:ILE:HG12	2.20	0.41
7:T:198:ILE:HD12	9:V:11:LEU:HD11	2.01	0.41
4:Q:54:THR:HG22	4:Q:55:LEU:H	1.85	0.41
3:G:46:VAL:O	3:G:49:LEU:HB2	2.21	0.41
1:J:442:VAL:HG12	1:J:489:ILE:HD11	2.03	0.41
2:E:471:ASP:C	2:E:473:LEU:H	2.24	0.41
3:G:171:TYR:O	3:G:172:LYS:HB3	2.19	0.41
3:P:163:ASN:HB3	3:P:171:TYR:HD1	1.85	0.41
2:N:408:ARG:NH2	2:N:454:GLU:OE1	2.53	0.41
2:M:35:ALA:O	2:M:36:LEU:HD23	2.21	0.41
2:E:216:ALA:C	2:E:217:LEU:HD23	2.41	0.41
7:X:193:THR:HG23	7:X:194:ILE:N	2.36	0.41
3:P:188:GLU:O	3:P:190:MET:N	2.54	0.41
2:D:234:LEU:HD22	2:D:234:LEU:HA	1.45	0.41
4:Q:138:ASN:OD1	5:R:21:ALA:HB1	2.21	0.41
2:M:37:GLU:O	2:M:75:VAL:HA	2.20	0.41
1:J:109:ASP:C	1:J:109:ASP:OD2	2.59	0.41
2:O:419:GLN:HG3	2:O:419:GLN:O	2.16	0.41
1:A:274:GLN:HB3	1:A:274:GLN:HE21	1.57	0.41
1:B:271:LEU:HD23	1:B:271:LEU:HA	1.81	0.41
6:S:22:LEU:HA	6:S:25:ALA:HB3	2.03	0.41
1:K:166:LEU:HD12	1:K:325:PRO:O	2.21	0.41
6:S:94:ARG:O	6:S:97:ASN:HB2	2.20	0.41
2:N:312:VAL:HA	2:N:313:PRO:HD2	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:288:PRO:HA	1:J:289:PRO:HD3	1.87	0.41
1:J:180:ILE:HA	1:J:180:ILE:HD13	1.80	0.41
4:H:104:ASP:OD2	5:I:27:LYS:HD3	2.21	0.41
3:G:212:ILE:HD12	3:G:212:ILE:HA	1.85	0.41
4:H:54:THR:HG22	4:H:55:LEU:N	2.36	0.41
1:A:472:VAL:CG2	1:A:480:LEU:HD13	2.51	0.41
4:H:133:ILE:HG13	4:H:133:ILE:H	1.66	0.41
1:K:245:LEU:HD12	1:K:245:LEU:O	2.20	0.41
2:D:86:VAL:HG23	2:D:242:TYR:CG	2.55	0.41
1:J:312:MET:HB3	1:J:312:MET:HE2	1.84	0.41
1:C:166:LEU:HB2	1:C:346:THR:HG21	2.03	0.41
1:B:292:GLU:HB2	1:B:294:TYR:HD1	1.86	0.41
1:A:434:SER:N	1:A:435:PRO:HD3	2.36	0.41
2:E:53:LEU:HD23	2:E:53:LEU:HA	1.76	0.41
3:P:160:ILE:CG2	3:P:160:ILE:O	2.68	0.41
1:A:272:SER:O	1:A:276:VAL:HG23	2.20	0.41
6:W:97:ASN:C	6:W:99:PRO:HD2	2.41	0.41
2:F:301:LYS:HZ3	9:V:46:LYS:HZ1	1.69	0.41
1:J:411:ASP:C	1:J:413:ALA:N	2.74	0.41
2:O:32:ILE:HG13	2:O:52:HIS:CD2	2.56	0.41
6:S:38:GLU:O	6:S:78:PHE:CE1	2.74	0.41
6:S:42:VAL:CG2	6:S:45:ILE:HD12	2.50	0.41
1:J:201:CYS:O	1:J:229:THR:HA	2.21	0.41
5:R:11:TYR:O	5:R:12:ILE:C	2.59	0.41
2:D:140:VAL:HG11	2:D:146:TYR:CZ	2.56	0.41
2:F:455:GLN:O	2:F:457:PHE:N	2.53	0.41
1:C:361:ILE:O	1:C:364:ALA:HA	2.21	0.41
3:P:242:MET:O	3:P:246:LEU:HB2	2.21	0.41
1:K:396:GLN:HG3	1:K:396:GLN:H	1.75	0.41
2:M:153:GLY:N	2:M:329:LEU:HD13	2.36	0.41
6:W:15:GLU:C	6:W:17:ARG:N	2.74	0.41
2:D:93:ARG:HH21	2:D:101:PRO:CB	2.33	0.41
4:Q:37:ASP:O	4:Q:63:VAL:HG13	2.21	0.41
1:C:423:ARG:HB3	1:C:461:ILE:CD1	2.50	0.41
6:W:119:THR:HG23	6:W:125:ALA:CB	2.49	0.41
3:P:105:ILE:HG13	3:P:123:GLN:HB2	2.03	0.41
3:P:166:ARG:H	3:P:171:TYR:HA	1.86	0.41
3:P:171:TYR:CD2	3:P:171:TYR:N	2.88	0.41
2:M:139:VAL:HG21	2:M:348:VAL:CB	2.50	0.41
2:O:142:LEU:HB2	2:O:437:THR:CG2	2.51	0.41
2:D:357:ILE:HB	2:D:362:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:252:LEU:HD23	2:F:252:LEU:HA	1.80	0.41
2:F:419:GLN:O	2:F:422:GLU:HG3	2.21	0.41
1:J:166:LEU:HD22	1:J:342:VAL:HG12	2.03	0.41
2:N:297:THR:OG1	2:N:298:THR:N	2.54	0.41
1:A:436:MET:HE2	1:A:441:GLN:CG	2.51	0.41
1:J:436:MET:HB3	1:J:436:MET:HE3	1.91	0.41
2:N:151:LYS:HE2	2:N:296:ILE:HB	2.03	0.41
1:C:131:LEU:O	1:C:308:ARG:HD2	2.21	0.41
1:C:251:CYS:HB3	1:C:308:ARG:NH2	2.35	0.41
1:A:107:VAL:HG12	1:A:115:ILE:CG1	2.50	0.41
3:G:190:MET:CE	3:G:190:MET:HA	2.50	0.41
2:N:335:LEU:HA	2:N:347:ALA:O	2.21	0.41
2:O:154:LEU:HB2	2:O:309:ALA:HA	2.02	0.41
1:J:138:PRO:O	1:J:312:MET:HE3	2.21	0.41
4:H:120:LEU:C	4:H:122:ALA:H	2.25	0.41
2:F:231:ARG:HD3	2:F:231:ARG:HA	1.81	0.41
2:N:209:LYS:HD3	2:N:209:LYS:HA	1.80	0.41
7:T:161:VAL:HG12	7:T:161:VAL:O	2.21	0.41
1:K:272:SER:O	1:K:276:VAL:HG23	2.21	0.41
1:K:32:LEU:HD21	1:K:42:HIS:HB2	2.02	0.41
2:D:23:VAL:O	2:D:57:THR:HA	2.21	0.41
1:L:108:VAL:O	1:L:232:VAL:HA	2.21	0.41
1:B:91:THR:C	1:B:93:ALA:H	2.25	0.41
1:A:349:GLN:HB2	1:A:351:PHE:CE1	2.56	0.41
4:H:105:LEU:C	4:H:107:ALA:H	2.24	0.41
2:F:154:LEU:HB2	2:F:309:ALA:HA	2.03	0.41
2:M:252:LEU:HD23	2:M:305:THR:HB	2.03	0.41
1:B:242:LEU:HD23	1:B:242:LEU:HA	1.69	0.41
2:O:231:ARG:HD3	2:O:231:ARG:HA	1.83	0.41
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.71	0.41
2:D:412:ARG:HG3	2:D:412:ARG:HH11	1.85	0.41
2:F:162:LYS:HB2	2:F:162:LYS:HE2	1.83	0.41
1:C:479:LEU:CD1	1:C:496:LYS:HB3	2.51	0.41
5:I:14:TYR:C	5:I:14:TYR:CD1	2.94	0.41
3:G:2:THR:O	3:G:3:LEU:C	2.57	0.41
2:O:434:LEU:HD23	2:O:434:LEU:C	2.40	0.41
2:E:134:VAL:HG12	2:E:136:GLY:H	1.86	0.41
1:C:419:SER:C	1:C:423:ARG:NH1	2.74	0.41
6:W:124:SER:O	6:W:125:ALA:HB2	2.21	0.41
1:K:386:VAL:HG11	1:K:442:VAL:HG22	2.01	0.41
2:M:370:VAL:O	2:M:374:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PHE:N	1:B:189:PHE:CD1	2.89	0.41
5:R:32:ALA:HA	5:R:35:MET:CE	2.51	0.41
1:J:405:GLN:HB2	1:J:406:PHE:H	1.72	0.41
1:J:440:GLU:O	1:J:444:VAL:HG12	2.21	0.41
1:K:90:ARG:HH21	1:K:92:GLY:HA2	1.86	0.41
1:J:29:GLY:HA3	1:J:42:HIS:O	2.21	0.41
1:B:96:ASP:CG	1:B:126:ARG:HH21	2.25	0.41
2:N:398:GLU:HA	2:N:401:LYS:HB2	2.02	0.41
2:E:44:ARG:HB3	2:E:44:ARG:HE	1.71	0.41
2:D:122:GLU:H	2:D:122:GLU:HG2	1.66	0.41
1:B:446:TYR:CZ	1:B:497:LEU:HD23	2.56	0.41
2:N:235:THR:O	2:N:239:VAL:HG23	2.20	0.41
1:B:157:VAL:N	1:B:158:PRO:CD	2.84	0.41
2:M:299:THR:O	2:M:302:GLY:O	2.39	0.41
2:N:40:GLY:O	2:N:41:ARG:HG3	2.21	0.41
6:W:38:GLU:O	6:W:78:PHE:CE1	2.75	0.40
6:W:98:THR:N	6:W:99:PRO:CD	2.84	0.40
2:M:103:ASP:OD2	2:M:105:ARG:HD3	2.21	0.40
1:L:136:ILE:CG2	2:M:194:ASN:CA	3.00	0.40
3:G:5:ASP:O	3:G:6:ILE:C	2.59	0.40
1:C:363:PRO:O	1:C:365:ILE:HG13	2.21	0.40
1:K:441:GLN:O	1:K:445:ILE:HG13	2.20	0.40
2:M:464:GLU:HA	2:M:467:VAL:HG23	2.03	0.40
2:M:91:LEU:HD21	2:M:243:PHE:CE2	2.54	0.40
7:T:193:THR:HG23	7:T:194:ILE:N	2.35	0.40
4:H:48:LEU:O	4:H:50:ALA:N	2.53	0.40
1:B:423:ARG:HG2	1:B:461:ILE:HD11	2.03	0.40
9:Z:17:ARG:HG3	9:Z:20:ARG:NH1	2.36	0.40
1:C:140:ILE:HD11	1:C:143:ARG:NH2	2.36	0.40
2:E:89:GLU:OE2	2:E:110:THR:HG23	2.21	0.40
1:L:409:ASP:C	1:L:410:LEU:HG	2.41	0.40
2:F:87:GLY:HA2	2:F:242:TYR:CZ	2.55	0.40
7:T:155:LEU:C	7:T:157:TYR:N	2.75	0.40
1:K:41:VAL:CG2	1:K:71:VAL:O	2.69	0.40
1:A:137:ILE:C	1:A:139:ARG:H	2.25	0.40
1:C:444:VAL:O	1:C:447:ALA:HB3	2.21	0.40
2:N:256:ASP:HA	2:N:257:ASN:HA	1.66	0.40
2:D:279:VAL:HG12	2:D:279:VAL:O	2.21	0.40
1:L:157:VAL:HG12	1:L:372:SER:N	2.36	0.40
1:J:163:GLN:OE1	1:J:374:VAL:HG21	2.21	0.40
2:N:83:ARG:HA	2:N:114:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:ALA:HB2	1:J:234:ALA:HB2	2.01	0.40
4:Q:105:LEU:C	4:Q:107:ALA:H	2.24	0.40
5:R:45:VAL:HG13	5:R:47:VAL:HG23	2.03	0.40
2:F:461:GLY:HA3	2:F:462:PRO:HD3	1.89	0.40
1:J:414:THR:HA	1:J:417:LEU:HG	2.04	0.40
1:B:269:ASP:HA	1:B:270:ASP:HA	1.73	0.40
1:C:214:ALA:C	1:C:216:LEU:N	2.75	0.40
2:E:412:ARG:O	2:E:415:SER:HB3	2.20	0.40
1:C:268:TYR:CE2	1:C:305:LEU:HD11	2.56	0.40
6:S:106:SER:C	6:S:108:MSE:N	2.73	0.40
1:A:5:THR:C	1:A:7:GLU:H	2.23	0.40
1:A:403:PHE:N	1:A:403:PHE:HD1	2.16	0.40
1:J:228:TYR:CD2	1:J:228:TYR:N	2.89	0.40
6:W:141:PHE:HE1	6:W:144:LYS:HZ2	1.64	0.40
1:J:476:HIS:C	1:J:478:ALA:H	2.24	0.40
6:W:14:ILE:N	6:W:14:ILE:CD1	2.76	0.40
1:C:68:PRO:HD3	2:D:15:ALA:HB2	2.02	0.40
2:E:431:LEU:HD12	2:E:432:VAL:N	2.36	0.40
2:E:151:LYS:CD	2:E:151:LYS:N	2.84	0.40
2:F:188:GLU:HG3	2:F:256:ASP:OD2	2.21	0.40
2:N:434:LEU:O	2:N:438:ILE:HG13	2.21	0.40
1:A:84:GLU:HB3	2:D:29:LEU:CD2	2.51	0.40
1:K:91:THR:C	1:K:93:ALA:H	2.25	0.40
3:G:138:PHE:O	3:G:139:GLY:C	2.59	0.40
2:O:49:VAL:N	2:O:60:THR:HG22	2.36	0.40
1:B:128:ARG:HB2	1:B:131:LEU:HD12	2.03	0.40
1:B:307:GLU:OE1	2:F:190:THR:HB	2.21	0.40
1:B:185:ASN:HB2	1:B:435:PRO:HB3	2.03	0.40
2:F:444:ILE:HD11	2:F:457:PHE:HD2	1.87	0.40
1:K:438:ILE:O	1:K:441:GLN:HB2	2.22	0.40
9:V:22:LYS:HZ2	9:V:30:VAL:CG1	2.34	0.40
2:E:396:LEU:HD22	2:E:396:LEU:N	2.36	0.40
1:L:383:MET:O	1:L:386:VAL:HG23	2.20	0.40
1:K:38:ILE:H	1:K:38:ILE:HD12	1.85	0.40
3:P:52:TYR:CE2	3:P:179:PHE:CD2	3.09	0.40
4:H:39:PRO:HD3	4:H:63:VAL:HG22	2.03	0.40
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.89	0.40
1:L:200:TYR:CD1	1:L:257:PHE:CD2	3.09	0.40
2:F:128:VAL:O	2:F:128:VAL:CG2	2.69	0.40
2:M:234:LEU:HD21	2:M:292:MET:HG2	2.03	0.40
2:E:447:GLY:C	2:E:449:TYR:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:163:THR:O	2:O:166:ILE:HG22	2.22	0.40
1:A:468:PHE:O	1:A:472:VAL:HG13	2.21	0.40
2:F:278:ALA:C	2:F:279:VAL:HG23	2.41	0.40
2:D:390:ILE:HG23	2:F:391:LEU:HD11	2.03	0.40
1:A:294:TYR:HA	1:A:295:PRO:HD3	1.85	0.40
6:S:188:GLU:O	6:S:189:ILE:O	2.40	0.40
1:A:137:ILE:N	1:A:138:PRO:HD2	2.37	0.40
2:F:189:ARG:HB2	2:F:192:GLU:CG	2.51	0.40
2:E:199:GLU:O	2:E:203:SER:HB3	2.21	0.40
2:D:399:GLU:OE1	2:D:399:GLU:HA	2.21	0.40
1:A:14:GLU:H	1:A:14:GLU:HG2	1.46	0.40
1:B:165:GLU:O	1:B:325:PRO:HD2	2.21	0.40
3:G:33:ARG:C	3:G:35:GLU:N	2.74	0.40
2:D:147:ALA:O	2:D:148:LYS:C	2.59	0.40
1:L:214:ALA:C	1:L:216:LEU:H	2.25	0.40
1:K:165:GLU:HB3	1:K:324:LEU:CD2	2.51	0.40
3:P:138:PHE:O	3:P:141:ALA:N	2.54	0.40
1:J:83:LYS:HG2	2:M:52:HIS:HE1	1.87	0.40
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.46	0.40
2:D:32:ILE:O	2:D:33:LEU:CB	2.58	0.40
2:O:266:SER:N	2:O:282:GLN:NE2	2.69	0.40
1:B:469:LEU:HD11	1:B:473:ILE:HD11	2.03	0.40
1:A:476:HIS:CD2	1:A:496:LYS:HE2	2.50	0.40
2:N:25:PHE:HB2	2:N:29:LEU:CD1	2.50	0.40
2:O:180:TYR:CD1	2:O:243:PHE:CD2	3.09	0.40
2:D:387:ILE:HG22	2:D:388:ILE:N	2.36	0.40
2:O:400:ASP:O	2:O:401:LYS:C	2.56	0.40
1:L:425:THR:C	1:L:427:LEU:N	2.74	0.40
1:K:108:VAL:HB	1:K:113:ASN:O	2.22	0.40
1:C:200:TYR:HD1	1:C:257:PHE:HD2	1.69	0.40
1:A:99:VAL:HG13	1:A:256:TYR:HB2	2.03	0.40
2:M:420:VAL:CG2	2:M:420:VAL:O	2.69	0.40
3:P:37:GLU:HB3	3:P:218:LYS:HE3	2.01	0.40
2:D:445:LEU:HA	2:D:445:LEU:HD23	1.95	0.40
1:J:381:ARG:HE	1:J:381:ARG:HB2	1.60	0.40
1:A:366:ASN:C	1:A:366:ASN:OD1	2.59	0.40
2:M:471:ASP:N	2:M:471:ASP:OD2	2.53	0.40
1:J:387:ALA:O	1:J:388:GLY:C	2.59	0.40
2:N:275:ILE:O	2:N:283:PRO:HG3	2.21	0.40
6:W:85:LEU:CD2	6:W:85:LEU:H	2.34	0.40
6:W:98:THR:HA	6:W:101:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:20:VAL:HA	2:N:60:THR:O	2.22	0.40
1:A:156:LEU:HA	1:A:156:LEU:HD23	1.73	0.40
6:S:133:GLU:OE1	7:T:207:LYS:HG2	2.22	0.40
1:B:144:GLU:HA	1:B:145:PRO:HD3	1.88	0.40
1:A:405:GLN:C	1:A:407:GLY:H	2.23	0.40
1:A:411:ASP:C	1:A:413:ALA:N	2.75	0.40
2:F:116:ILE:HA	2:F:238:THR:OG1	2.21	0.40
2:M:163:THR:CB	12:M:600:ADP:O2B	2.69	0.40
1:A:71:VAL:CG1	1:A:73:VAL:HG23	2.48	0.40
1:A:133:ALA:CB	1:A:308:ARG:HA	2.52	0.40
1:A:133:ALA:HB2	1:A:308:ARG:CG	2.50	0.40
2:M:450:ASP:N	2:M:450:ASP:OD1	2.54	0.40
2:F:367:HIS:CG	2:F:438:ILE:HD11	2.56	0.40
3:G:188:GLU:O	3:G:190:MET:N	2.54	0.40
1:K:374:VAL:HG23	1:K:375:GLY:H	1.86	0.40
4:H:134:ARG:HG2	4:H:138:ASN:HD22	1.87	0.40
2:F:390:ILE:HA	2:F:390:ILE:HD13	1.85	0.40
1:C:189:PHE:HB3	1:C:197:LYS:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	508/510 (100%)	423 (83%)	61 (12%)	24 (5%)	3	22
1	B	476/510 (93%)	410 (86%)	60 (13%)	6 (1%)	15	59
1	C	482/510 (94%)	365 (76%)	88 (18%)	29 (6%)	2	16
1	J	485/510 (95%)	404 (83%)	61 (13%)	20 (4%)	3	27
1	K	476/510 (93%)	414 (87%)	54 (11%)	8 (2%)	11	52
1	L	479/510 (94%)	354 (74%)	100 (21%)	25 (5%)	2	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	465/482 (96%)	360 (77%)	84 (18%)	21 (4%)	3	24
2	E	464/482 (96%)	392 (84%)	61 (13%)	11 (2%)	7	43
2	F	465/482 (96%)	368 (79%)	78 (17%)	19 (4%)	3	27
2	M	465/482 (96%)	356 (77%)	79 (17%)	30 (6%)	1	13
2	N	464/482 (96%)	392 (84%)	60 (13%)	12 (3%)	7	40
2	O	464/482 (96%)	375 (81%)	70 (15%)	19 (4%)	3	27
3	G	254/272 (93%)	172 (68%)	65 (26%)	17 (7%)	1	12
3	P	254/272 (93%)	175 (69%)	62 (24%)	17 (7%)	1	12
4	H	129/146 (88%)	95 (74%)	22 (17%)	12 (9%)	1	5
4	Q	129/146 (88%)	95 (74%)	22 (17%)	12 (9%)	1	5
5	I	45/50 (90%)	28 (62%)	13 (29%)	4 (9%)	1	5
5	R	45/50 (90%)	28 (62%)	13 (29%)	4 (9%)	1	5
6	S	163/190 (86%)	97 (60%)	44 (27%)	22 (14%)	0	1
6	W	144/190 (76%)	81 (56%)	37 (26%)	26 (18%)	0	0
7	T	84/116 (72%)	68 (81%)	12 (14%)	4 (5%)	3	22
7	X	37/116 (32%)	25 (68%)	10 (27%)	2 (5%)	2	19
8	U	22/118 (19%)	20 (91%)	2 (9%)	0	100	100
9	V	64/76 (84%)	43 (67%)	19 (30%)	2 (3%)	5	34
9	Z	13/76 (17%)	5 (38%)	8 (62%)	0	100	100
All	All	7076/7770 (91%)	5545 (78%)	1185 (17%)	346 (5%)	3	22

All (346) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	22	SER
1	A	24	ASP
1	A	361	ILE
1	A	409	ASP
1	A	452	TYR
1	A	475	GLN
1	A	478	ALA
1	C	28	THR
1	C	86	ASP
1	C	120	PRO

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Mol	Chain	Res	Type
2	D	107	PRO
2	D	210	ASP
2	D	474	ALA
2	E	453	PRO
2	E	455	GLN
2	F	33	LEU
2	F	73	GLN
2	F	247	GLU
3	G	41	ALA
3	G	51	LEU
3	G	55	ALA
3	G	172	LYS
4	H	105	LEU
1	J	26	GLU
1	J	315	ALA
1	J	361	ILE
1	J	409	ASP
1	J	452	TYR
1	J	475	GLN
1	J	478	ALA
1	L	86	ASP
1	L	120	PRO
1	L	315	ALA
2	M	106	GLY
2	M	107	PRO
2	M	210	ASP
2	M	474	ALA
2	N	27	GLU
2	N	423	VAL
2	O	33	LEU
2	O	73	GLN
2	O	247	GLU
3	P	41	ALA
3	P	51	LEU
3	P	55	ALA
3	P	172	LYS
4	Q	87	ASP
4	Q	105	LEU
6	S	29	GLN
6	S	76	GLU
6	S	128	GLU
6	S	171	VAL

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Mol	Chain	Res	Type
6	S	172	ASP
6	S	181	LYS
6	S	186	MSE
7	T	197	CYS
6	W	11	ILE
6	W	12	TYR
6	W	14	ILE
6	W	15	GLU
6	W	29	GLN
6	W	76	GLU
6	W	106	SER
6	W	114	GLY
6	W	115	GLU
6	W	116	VAL
6	W	121	THR
7	X	197	CYS
1	A	23	VAL
1	A	110	ALA
1	A	188	ARG
1	A	300	TYR
1	A	315	ALA
1	C	135	GLY
1	C	188	ARG
1	C	236	ALA
1	C	315	ALA
1	C	333	ASP
1	C	368	GLY
1	C	377	ALA
1	C	411	ASP
1	C	501	VAL
1	C	502	THR
1	C	503	ASN
1	C	508	PHE
2	D	18	GLY
2	D	78	SER
2	D	81	PRO
2	D	92	GLY
2	D	97	VAL
2	D	106	GLY
2	D	279	VAL
2	D	292	MET
2	D	429	GLY

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Mol	Chain	Res	Type
2	E	279	VAL
2	E	391	LEU
2	E	444	ILE
2	E	448	GLU
2	F	290	GLY
2	F	301	LYS
2	F	365	SER
2	F	421	ALA
3	G	52	TYR
3	G	72	SER
4	H	57	VAL
4	H	79	SER
4	H	87	ASP
4	H	114	LYS
4	H	137	ALA
5	I	5	ARG
5	I	31	LYS
5	I	41	THR
1	J	188	ARG
1	K	500	ILE
1	L	188	ARG
1	L	236	ALA
1	L	333	ASP
1	L	368	GLY
1	L	377	ALA
1	L	411	ASP
1	L	454	ASP
1	L	478	ALA
2	M	78	SER
2	M	81	PRO
2	M	92	GLY
2	M	97	VAL
2	M	279	VAL
2	M	292	MET
2	M	317	LEU
2	M	347	ALA
2	M	425	THR
2	M	429	GLY
2	N	279	VAL
2	N	391	LEU
2	N	461	GLY
2	O	290	GLY

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Mol	Chain	Res	Type
2	O	301	LYS
2	O	365	SER
3	P	52	TYR
3	P	72	SER
4	Q	57	VAL
4	Q	79	SER
4	Q	114	LYS
4	Q	137	ALA
5	R	5	ARG
5	R	31	LYS
5	R	41	THR
6	S	11	ILE
6	S	12	TYR
6	S	27	SER
6	S	72	MSE
6	S	75	LYS
6	S	80	PRO
6	S	92	ASN
6	S	121	THR
6	S	184	ARG
7	T	188	GLN
7	T	204	LEU
6	W	27	SER
6	W	72	MSE
6	W	75	LYS
6	W	80	PRO
6	W	92	ASN
6	W	107	THR
6	W	124	SER
6	W	125	ALA
6	W	128	GLU
7	X	204	LEU
1	A	13	GLU
1	A	44	LEU
1	A	45	ARG
1	A	120	PRO
1	A	211	SER
1	A	405	GLN
1	B	361	ILE
1	B	385	GLN
1	C	138	PRO
1	C	454	ASP

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Mol	Chain	Res	Type
1	C	478	ALA
2	D	121	PRO
2	D	317	LEU
2	D	347	ALA
2	D	425	THR
2	E	459	MET
2	F	121	PRO
2	F	371	ALA
2	F	450	ASP
2	F	456	ALA
3	G	40	PRO
3	G	44	TYR
3	G	88	GLN
3	G	204	TYR
4	H	49	ALA
1	J	120	PRO
1	J	477	GLN
1	K	385	GLN
1	L	44	LEU
1	L	119	GLY
2	M	69	LEU
2	M	121	PRO
2	N	454	GLU
2	O	121	PRO
2	O	371	ALA
3	P	40	PRO
3	P	44	TYR
3	P	88	GLN
3	P	204	TYR
4	Q	49	ALA
6	S	8	PRO
6	S	126	LEU
6	S	187	ARG
7	T	187	ALA
1	A	10	SER
1	A	406	PHE
1	A	476	HIS
1	C	44	LEU
1	C	119	GLY
1	C	492	GLU
2	D	33	LEU
2	E	160	VAL

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Mol	Chain	Res	Type
2	E	472	LYS
2	F	55	GLU
2	F	225	PRO
3	G	151	SER
4	H	126	ALA
1	J	45	ARG
1	J	110	ALA
1	J	184	ILE
1	J	405	GLN
1	L	138	PRO
1	L	215	GLN
1	L	373	ARG
2	M	77	ASP
2	M	168	GLU
2	M	236	GLY
2	M	367	HIS
2	O	69	LEU
2	O	279	VAL
2	O	453	PRO
3	P	151	SER
4	Q	126	ALA
6	S	54	SER
6	W	54	SER
6	W	61	LYS
6	W	122	THR
1	A	8	VAL
1	A	9	SER
1	C	187	LYS
1	C	215	GLN
1	C	337	TYR
1	C	435	PRO
1	C	498	LYS
2	D	397	SER
2	F	232	VAL
3	G	152	GLY
3	G	177	PRO
3	G	187	ALA
3	G	196	ILE
4	H	101	ASP
1	J	44	LEU
1	J	214	ALA
1	K	361	ILE

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Mol	Chain	Res	Type
1	K	400	VAL
1	L	177	SER
1	L	187	LYS
1	L	367	VAL
1	L	461	ILE
1	L	492	GLU
2	M	33	LEU
2	M	397	SER
2	M	431	LEU
2	N	160	VAL
2	N	210	ASP
2	N	413	PHE
2	O	28	GLY
2	O	225	PRO
3	P	152	GLY
3	P	177	PRO
3	P	187	ALA
3	P	196	ILE
4	Q	101	ASP
6	S	61	LYS
6	S	107	THR
6	W	20	THR
1	B	138	PRO
1	B	140	ILE
1	B	400	VAL
1	C	373	ARG
1	C	461	ILE
2	D	168	GLU
2	F	81	PRO
3	G	123	GLN
4	H	50	ALA
1	J	300	TYR
1	J	406	PHE
1	K	120	PRO
1	K	138	PRO
1	L	135	GLY
1	L	337	TYR
2	M	55	GLU
2	M	172	ASN
2	O	81	PRO
2	O	288	ASP
3	P	43	VAL

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Mol	Chain	Res	Type
3	P	271	ALA
4	Q	50	ALA
5	R	12	ILE
6	W	30	ASN
2	E	363	VAL
2	F	279	VAL
2	F	321	ALA
5	I	12	ILE
1	K	68	PRO
2	M	18	GLY
2	O	40	GLY
4	Q	121	GLY
9	V	6	ASP
1	B	120	PRO
1	C	367	VAL
2	E	423	VAL
2	F	40	GLY
4	H	121	GLY
1	J	138	PRO
2	M	362	ILE
2	M	392	GLY
2	N	363	VAL
9	V	7	PRO
6	W	8	PRO
2	D	320	PRO
2	D	392	GLY
4	H	106	GLY
1	L	213	VAL
1	L	435	PRO
2	O	232	VAL
2	F	404	VAL
1	J	180	ILE
1	K	140	ILE
2	M	85	PRO
2	M	201	ILE
2	N	107	PRO
2	N	268	VAL
2	O	187	GLY
2	O	460	VAL
4	Q	106	GLY
3	G	43	VAL

### 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	412/412 (100%)	358 (87%)	54 (13%)	5	24
1	B	389/412 (94%)	335 (86%)	54 (14%)	4	20
1	C	388/412 (94%)	333 (86%)	55 (14%)	4	19
1	J	393/412 (95%)	339 (86%)	54 (14%)	4	21
1	K	389/412 (94%)	333 (86%)	56 (14%)	4	19
1	L	388/412 (94%)	331 (85%)	57 (15%)	4	18
2	D	377/386 (98%)	321 (85%)	56 (15%)	4	17
2	E	376/386 (97%)	326 (87%)	50 (13%)	5	23
2	F	377/386 (98%)	332 (88%)	45 (12%)	6	28
2	M	377/386 (98%)	317 (84%)	60 (16%)	3	14
2	N	376/386 (97%)	330 (88%)	46 (12%)	6	27
2	O	376/386 (97%)	329 (88%)	47 (12%)	6	26
3	G	222/230 (96%)	184 (83%)	38 (17%)	2	12
3	P	222/230 (96%)	183 (82%)	39 (18%)	2	11
4	H	104/109 (95%)	95 (91%)	9 (9%)	13	45
4	Q	104/109 (95%)	95 (91%)	9 (9%)	13	45
5	I	38/41 (93%)	35 (92%)	3 (8%)	15	53
5	R	38/41 (93%)	34 (90%)	4 (10%)	8	35
6	S	146/158 (92%)	120 (82%)	26 (18%)	2	11
6	W	127/158 (80%)	107 (84%)	20 (16%)	3	15
7	T	81/100 (81%)	76 (94%)	5 (6%)	23	64
7	X	39/100 (39%)	37 (95%)	2 (5%)	29	70
8	U	26/100 (26%)	23 (88%)	3 (12%)	7	30
9	V	60/68 (88%)	55 (92%)	5 (8%)	14	49
9	Z	17/68 (25%)	14 (82%)	3 (18%)	2	11
All	All	5842/6300 (93%)	5042 (86%)	800 (14%)	4	21



All (800) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	9	SER
1	A	14	GLU
1	A	17	LEU
1	A	24	ASP
1	A	28	THR
1	A	34	ILE
1	A	47	VAL
1	A	70	ASN
1	A	79	ASP
1	A	89	LYS
1	A	94	ILE
1	A	101	GLU
1	A	102	GLU
1	A	103	LEU
1	A	121	ILE
1	A	126	ARG
1	A	128	ARG
1	A	140	ILE
1	A	147	GLN
1	A	164	ARG
1	A	186	GLN
1	A	187	LYS
1	A	188	ARG
1	A	208	GLN
1	A	211	SER
1	A	216	LEU
1	A	220	LEU
1	A	229	THR
1	A	235	THR
1	A	245	LEU
1	A	252	SER
1	A	266	ILE
1	A	274	GLN
1	A	282	SER
1	A	292	GLU
1	A	347	ASP
1	A	354	THR
1	A	355	GLU
1	A	376	SER
1	A	380	THR
1	A	381	ARG

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Mol	Chain	Res	Type
1	A	405	GLN
1	A	408	SER
1	A	410	LEU
1	A	444	VAL
1	A	450	ARG
1	A	459	SER
1	A	462	THR
1	A	465	GLU
1	A	472	VAL
1	A	475	GLN
1	A	490	SER
1	A	493	SER
1	B	25	LEU
1	B	28	THR
1	B	30	ARG
1	B	38	ILE
1	B	40	ARG
1	B	41	VAL
1	B	47	VAL
1	B	48	GLN
1	B	65	ASN
1	B	80	LYS
1	B	83	LYS
1	B	99	VAL
1	B	128	ARG
1	B	131	LEU
1	B	140	ILE
1	B	141	SER
1	B	144	GLU
1	B	164	ARG
1	B	177	SER
1	B	185	ASN
1	B	189	PHE
1	B	208	GLN
1	B	211	SER
1	B	216	LEU
1	B	221	THR
1	B	233	SER
1	B	235	THR
1	B	256	TYR
1	B	286	ARG
1	B	287	ARG

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Mol	Chain	Res	Type
1	B	291	ARG
1	B	301	LEU
1	B	344	SER
1	B	347	ASP
1	B	349	GLN
1	B	354	THR
1	B	380	THR
1	B	386	VAL
1	B	399	GLU
1	B	410	LEU
1	B	411	ASP
1	B	419	SER
1	B	423	ARG
1	B	434	SER
1	B	444	VAL
1	B	449	VAL
1	B	462	THR
1	B	479	LEU
1	B	484	ARG
1	B	490	SER
1	B	494	ASP
1	B	502	THR
1	B	508	PHE
1	B	509	GLU
1	C	34	ILE
1	C	64	LEU
1	C	78	ASN
1	C	87	ILE
1	C	89	LYS
1	C	97	VAL
1	C	101	GLU
1	C	102	GLU
1	C	113	ASN
1	C	121	ILE
1	C	131	LEU
1	C	136	ILE
1	C	137	ILE
1	C	157	VAL
1	C	173	THR
1	C	176	THR
1	C	182	THR
1	C	193	THR

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Mol	Chain	Res	Type
1	C	206	ILE
1	C	226	MET
1	C	237	SER
1	C	242	LEU
1	C	245	LEU
1	C	258	ARG
1	C	268	TYR
1	C	283	LEU
1	C	304	ARG
1	C	313	ASN
1	C	335	SER
1	C	337	TYR
1	C	340	THR
1	C	349	GLN
1	C	350	ILE
1	C	354	THR
1	C	365	ILE
1	C	369	LEU
1	C	371	VAL
1	C	381	ARG
1	C	386	VAL
1	C	390	MET
1	C	396	GLN
1	C	397	TYR
1	C	410	LEU
1	C	418	LEU
1	C	424	LEU
1	C	425	THR
1	C	444	VAL
1	C	455	LYS
1	C	462	THR
1	C	479	LEU
1	C	483	ILE
1	C	491	GLU
1	C	500	ILE
1	C	502	THR
1	C	504	PHE
2	D	10	THR
2	D	12	ARG
2	D	14	VAL
2	D	17	ILE
2	D	22	ASP

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Mol	Chain	Res	Type
2	D	26	ASP
2	D	32	ILE
2	D	43	THR
2	D	45	LEU
2	D	51	GLN
2	D	53	LEU
2	D	67	GLU
2	D	74	LYS
2	D	78	SER
2	D	86	VAL
2	D	89	GLU
2	D	96	ASN
2	D	98	ILE
2	D	102	ILE
2	D	112	GLN
2	D	128	VAL
2	D	132	ILE
2	D	133	LEU
2	D	162	LYS
2	D	183	PHE
2	D	190	THR
2	D	194	ASN
2	D	196	LEU
2	D	200	MET
2	D	201	ILE
2	D	205	VAL
2	D	221	GLN
2	D	234	LEU
2	D	237	LEU
2	D	249	GLN
2	D	251	VAL
2	D	262	THR
2	D	271	LEU
2	D	274	ARG
2	D	282	GLN
2	D	289	MET
2	D	292	MET
2	D	335	LEU
2	D	336	SER
2	D	337	ARG
2	D	342	LEU
2	D	344	ILE

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Mol	Chain	Res	Type
2	D	354	THR
2	D	405	SER
2	D	414	LEU
2	D	420	VAL
2	D	423	VAL
2	D	435	LYS
2	D	471	ASP
2	D	473	LEU
2	D	475	GLU
2	E	17	ILE
2	E	43	THR
2	E	71	ARG
2	E	74	LYS
2	E	109	LYS
2	E	111	LYS
2	E	124	VAL
2	E	127	SER
2	E	128	VAL
2	E	131	GLU
2	E	132	ILE
2	E	151	LYS
2	E	160	VAL
2	E	175	LYS
2	E	203	SER
2	E	213	SER
2	E	223	ASN
2	E	237	LEU
2	E	257	ASN
2	E	258	ILE
2	E	275	ILE
2	E	279	VAL
2	E	282	GLN
2	E	284	THR
2	E	298	THR
2	E	306	SER
2	E	310	ILE
2	E	336	SER
2	E	341	GLU
2	E	342	LEU
2	E	352	ASP
2	E	354	THR
2	E	381	TYR

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Mol	Chain	Res	Type
2	E	385	GLN
2	E	390	ILE
2	E	391	LEU
2	E	396	LEU
2	E	405	SER
2	E	412	ARG
2	E	414	LEU
2	E	419	GLN
2	E	420	VAL
2	E	423	VAL
2	E	428	LEU
2	E	431	LEU
2	E	437	THR
2	E	439	LYS
2	E	460	VAL
2	E	464	GLU
2	E	467	VAL
2	F	10	THR
2	F	21	VAL
2	F	26	ASP
2	F	41	ARG
2	F	42	GLU
2	F	43	THR
2	F	58	VAL
2	F	64	ASP
2	F	73	GLN
2	F	78	SER
2	F	83	ARG
2	F	86	VAL
2	F	91	LEU
2	F	96	ASN
2	F	112	GLN
2	F	124	VAL
2	F	127	SER
2	F	128	VAL
2	F	132	ILE
2	F	133	LEU
2	F	139	VAL
2	F	190	THR
2	F	191	ARG
2	F	221	GLN
2	F	223	ASN

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Mol	Chain	Res	Type
2	F	224	GLU
2	F	241	GLU
2	F	246	GLN
2	F	247	GLU
2	F	258	ILE
2	F	271	LEU
2	F	274	ARG
2	F	282	GLN
2	F	356	ARG
2	F	357	ILE
2	F	385	GLN
2	F	386	ASP
2	F	390	ILE
2	F	401	LYS
2	F	402	LEU
2	F	412	ARG
2	F	434	LEU
2	F	450	ASP
2	F	457	PHE
2	F	467	VAL
3	G	4	LYS
3	G	5	ASP
3	G	7	THR
3	G	8	ARG
3	G	22	SER
3	G	31	TYR
3	G	48	SER
3	G	56	ASP
3	G	77	LEU
3	G	88	GLN
3	G	91	SER
3	G	95	ASN
3	G	125	LEU
3	G	130	GLU
3	G	138	PHE
3	G	146	LEU
3	G	155	PHE
3	G	166	ARG
3	G	168	VAL
3	G	169	ILE
3	G	174	GLU
3	G	175	GLU

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Mol	Chain	Res	Type
3	G	184	ILE
3	G	197	ASP
3	G	200	VAL
3	G	205	GLN
3	G	208	SER
3	G	211	ASN
3	G	217	LEU
3	G	220	SER
3	G	225	GLN
3	G	230	THR
3	G	232	MET
3	G	240	SER
3	G	242	MET
3	G	246	LEU
3	G	247	THR
3	G	249	THR
4	H	35	GLN
4	H	40	THR
4	H	57	VAL
4	H	64	VAL
4	H	95	GLU
4	H	99	THR
4	H	118	GLU
4	H	124	ASP
4	H	141	LEU
5	I	14	TYR
5	I	17	ILE
5	I	35	MET
1	J	25	LEU
1	J	34	ILE
1	J	46	ASN
1	J	47	VAL
1	J	70	ASN
1	J	79	ASP
1	J	89	LYS
1	J	94	ILE
1	J	101	GLU
1	J	102	GLU
1	J	103	LEU
1	J	121	ILE
1	J	126	ARG
1	J	140	ILE

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Mol	Chain	Res	Type
1	J	147	GLN
1	J	150	ILE
1	J	161	ARG
1	J	164	ARG
1	J	186	GLN
1	J	187	LYS
1	J	188	ARG
1	J	208	GLN
1	J	211	SER
1	J	216	LEU
1	J	220	LEU
1	J	229	THR
1	J	235	THR
1	J	245	LEU
1	J	252	SER
1	J	266	ILE
1	J	274	GLN
1	J	282	SER
1	J	292	GLU
1	J	347	ASP
1	J	354	THR
1	J	355	GLU
1	J	376	SER
1	J	380	THR
1	J	381	ARG
1	J	392	LEU
1	J	403	PHE
1	J	405	GLN
1	J	408	SER
1	J	410	LEU
1	J	444	VAL
1	J	449	VAL
1	J	450	ARG
1	J	459	SER
1	J	462	THR
1	J	465	GLU
1	J	475	GLN
1	J	490	SER
1	J	493	SER
1	J	501	VAL
1	K	23	VAL
1	K	26	GLU

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Mol	Chain	Res	Type
1	K	30	ARG
1	K	38	ILE
1	K	40	ARG
1	K	41	VAL
1	K	47	VAL
1	K	48	GLN
1	K	65	ASN
1	K	80	LYS
1	K	83	LYS
1	K	99	VAL
1	K	115	ILE
1	K	128	ARG
1	K	131	LEU
1	K	140	ILE
1	K	141	SER
1	K	144	GLU
1	K	164	ARG
1	K	171	ARG
1	K	177	SER
1	K	185	ASN
1	K	189	PHE
1	K	208	GLN
1	K	211	SER
1	K	216	LEU
1	K	221	THR
1	K	233	SER
1	K	235	THR
1	K	256	TYR
1	K	286	ARG
1	K	287	ARG
1	K	291	ARG
1	K	301	LEU
1	K	344	SER
1	K	347	ASP
1	K	349	GLN
1	K	354	THR
1	K	380	THR
1	K	386	VAL
1	K	399	GLU
1	K	410	LEU
1	K	411	ASP
1	K	419	SER

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Mol	Chain	Res	Type
1	K	423	ARG
1	K	434	SER
1	K	444	VAL
1	K	449	VAL
1	K	462	THR
1	K	472	VAL
1	K	479	LEU
1	K	484	ARG
1	K	490	SER
1	K	494	ASP
1	K	496	LYS
1	K	501	VAL
1	L	34	ILE
1	L	64	LEU
1	L	78	ASN
1	L	83	LYS
1	L	87	ILE
1	L	89	LYS
1	L	97	VAL
1	L	101	GLU
1	L	102	GLU
1	L	113	ASN
1	L	121	ILE
1	L	131	LEU
1	L	136	ILE
1	L	137	ILE
1	L	157	VAL
1	L	176	THR
1	L	182	THR
1	L	193	THR
1	L	206	ILE
1	L	226	MET
1	L	233	SER
1	L	237	SER
1	L	242	LEU
1	L	245	LEU
1	L	258	ARG
1	L	268	TYR
1	L	283	LEU
1	L	304	ARG
1	L	313	ASN
1	L	335	SER

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Mol	Chain	Res	Type
1	L	337	TYR
1	L	340	THR
1	L	349	GLN
1	L	350	ILE
1	L	354	THR
1	L	365	ILE
1	L	369	LEU
1	L	371	VAL
1	L	381	ARG
1	L	386	VAL
1	L	390	MET
1	L	396	GLN
1	L	397	TYR
1	L	410	LEU
1	L	418	LEU
1	L	424	LEU
1	L	425	THR
1	L	444	VAL
1	L	455	LYS
1	L	462	THR
1	L	468	PHE
1	L	479	LEU
1	L	483	ILE
1	L	491	GLU
1	L	504	PHE
1	L	505	LEU
1	L	508	PHE
2	M	9	THR
2	M	10	THR
2	M	12	ARG
2	M	14	VAL
2	M	17	ILE
2	M	20	VAL
2	M	32	ILE
2	M	43	THR
2	M	45	LEU
2	M	51	GLN
2	M	53	LEU
2	M	67	GLU
2	M	73	GLN
2	M	74	LYS
2	M	78	SER

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Mol	Chain	Res	Type
2	M	86	VAL
2	M	89	GLU
2	M	96	ASN
2	M	98	ILE
2	M	102	ILE
2	M	112	GLN
2	M	128	VAL
2	M	132	ILE
2	M	133	LEU
2	M	162	LYS
2	M	183	PHE
2	M	190	THR
2	M	194	ASN
2	M	196	LEU
2	M	200	MET
2	M	201	ILE
2	M	205	VAL
2	M	221	GLN
2	M	234	LEU
2	M	237	LEU
2	M	249	GLN
2	M	251	VAL
2	M	262	THR
2	M	271	LEU
2	M	274	ARG
2	M	282	GLN
2	M	289	MET
2	M	292	MET
2	M	310	ILE
2	M	315	ASP
2	M	335	LEU
2	M	336	SER
2	M	337	ARG
2	M	342	LEU
2	M	344	ILE
2	M	354	THR
2	M	390	ILE
2	M	405	SER
2	M	414	LEU
2	M	420	VAL
2	M	423	VAL
2	M	435	LYS

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Mol	Chain	Res	Type
2	M	471	ASP
2	M	473	LEU
2	M	475	GLU
2	N	14	VAL
2	N	17	ILE
2	N	29	LEU
2	N	43	THR
2	N	71	ARG
2	N	74	LYS
2	N	109	LYS
2	N	111	LYS
2	N	124	VAL
2	N	127	SER
2	N	131	GLU
2	N	132	ILE
2	N	151	LYS
2	N	160	VAL
2	N	175	LYS
2	N	203	SER
2	N	213	SER
2	N	223	ASN
2	N	237	LEU
2	N	257	ASN
2	N	258	ILE
2	N	275	ILE
2	N	279	VAL
2	N	282	GLN
2	N	284	THR
2	N	298	THR
2	N	306	SER
2	N	310	ILE
2	N	336	SER
2	N	341	GLU
2	N	342	LEU
2	N	352	ASP
2	N	354	THR
2	N	381	TYR
2	N	385	GLN
2	N	390	ILE
2	N	391	LEU
2	N	396	LEU
2	N	404	VAL

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Mol	Chain	Res	Type
2	N	410	ILE
2	N	412	ARG
2	N	428	LEU
2	N	431	LEU
2	N	434	LEU
2	N	448	GLU
2	N	460	VAL
2	O	12	ARG
2	O	14	VAL
2	O	16	VAL
2	O	20	VAL
2	O	23	VAL
2	O	41	ARG
2	O	43	THR
2	O	58	VAL
2	O	64	ASP
2	O	73	GLN
2	O	78	SER
2	O	83	ARG
2	O	86	VAL
2	O	91	LEU
2	O	96	ASN
2	O	112	GLN
2	O	124	VAL
2	O	127	SER
2	O	128	VAL
2	O	133	LEU
2	O	139	VAL
2	O	190	THR
2	O	191	ARG
2	O	194	ASN
2	O	221	GLN
2	O	223	ASN
2	O	224	GLU
2	O	241	GLU
2	O	246	GLN
2	O	247	GLU
2	O	258	ILE
2	O	271	LEU
2	O	274	ARG
2	O	282	GLN
2	O	297	THR

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Mol	Chain	Res	Type
2	O	356	ARG
2	O	357	ILE
2	O	385	GLN
2	O	386	ASP
2	O	390	ILE
2	O	401	LYS
2	O	419	GLN
2	O	420	VAL
2	O	423	VAL
2	O	428	LEU
2	O	431	LEU
2	O	460	VAL
3	P	4	LYS
3	P	5	ASP
3	P	7	THR
3	P	8	ARG
3	P	22	SER
3	P	31	TYR
3	P	48	SER
3	P	56	ASP
3	P	77	LEU
3	P	88	GLN
3	P	91	SER
3	P	95	ASN
3	P	125	LEU
3	P	130	GLU
3	P	138	PHE
3	P	146	LEU
3	P	155	PHE
3	P	166	ARG
3	P	168	VAL
3	P	169	ILE
3	P	174	GLU
3	P	175	GLU
3	P	184	ILE
3	P	190	MET
3	P	197	ASP
3	P	200	VAL
3	P	205	GLN
3	P	208	SER
3	P	217	LEU
3	P	220	SER

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Mol	Chain	Res	Type
3	P	225	GLN
3	P	230	THR
3	P	232	MET
3	P	240	SER
3	P	242	MET
3	P	246	LEU
3	P	247	THR
3	P	248	LEU
3	P	249	THR
4	Q	35	GLN
4	Q	40	THR
4	Q	57	VAL
4	Q	64	VAL
4	Q	95	GLU
4	Q	99	THR
4	Q	118	GLU
4	Q	124	ASP
4	Q	141	LEU
5	R	14	TYR
5	R	17	ILE
5	R	35	MET
5	R	46	LYS
6	S	1	PHE
6	S	4	LEU
6	S	15	GLU
6	S	42	VAL
6	S	55	LEU
6	S	65	LYS
6	S	68	SER
6	S	72	MSE
6	S	79	SER
6	S	82	THR
6	S	85	LEU
6	S	88	LEU
6	S	98	THR
6	S	101	VAL
6	S	107	THR
6	S	108	MSE
6	S	109	MSE
6	S	122	THR
6	S	127	ASP
6	S	177	THR

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Mol	Chain	Res	Type
6	S	178	LYS
6	S	179	ILE
6	S	182	LEU
6	S	183	SER
6	S	184	ARG
6	S	186	MSE
7	T	122	HIS
7	T	153	ASN
7	T	154	ARG
7	T	164	MSE
7	T	198	ILE
8	U	31	LYS
8	U	40	ARG
8	U	67	ASP
9	V	5	LEU
9	V	12	PHE
9	V	20	ARG
9	V	21	THR
9	V	23	ARG
6	W	1	PHE
6	W	9	VAL
6	W	14	ILE
6	W	15	GLU
6	W	42	VAL
6	W	55	LEU
6	W	65	LYS
6	W	68	SER
6	W	72	MSE
6	W	79	SER
6	W	82	THR
6	W	85	LEU
6	W	88	LEU
6	W	98	THR
6	W	105	PHE
6	W	108	MSE
6	W	109	MSE
6	W	111	VAL
6	W	121	THR
6	W	129	THR
7	X	164	MSE
7	X	198	ILE
9	Z	22	LYS

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Mol	Chain	Res	Type
9	Z	41	ASP
9	Z	46	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (167) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	208	GLN
1	A	263	HIS
1	A	274	GLN
1	A	349	GLN
1	A	396	GLN
1	A	405	GLN
1	A	430	GLN
1	A	432	GLN
1	A	441	GLN
1	A	475	GLN
1	B	42	HIS
1	B	48	GLN
1	B	65	ASN
1	B	78	ASN
1	B	113	ASN
1	B	163	GLN
1	B	172	GLN
1	B	302	HIS
1	B	385	GLN
1	B	396	GLN
1	B	415	GLN
1	B	432	GLN
1	B	466	ASN
1	C	78	ASN
1	C	163	GLN
1	C	215	GLN
1	C	302	HIS
1	C	313	ASN
1	C	341	ASN
1	C	385	GLN
1	C	405	GLN
1	C	416	GLN
1	C	471	HIS
1	C	476	HIS
2	D	39	GLN

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Mol	Chain	Res	Type
2	D	73	GLN
2	D	96	ASN
2	D	130	GLN
2	D	194	ASN
2	D	198	HIS
2	D	221	GLN
2	D	282	GLN
2	D	419	GLN
2	E	39	GLN
2	E	223	ASN
2	E	249	GLN
2	E	282	GLN
2	E	293	GLN
2	E	367	HIS
2	E	375	GLN
2	E	379	GLN
2	E	385	GLN
2	E	442	GLN
2	E	455	GLN
2	F	34	ASN
2	F	39	GLN
2	F	51	GLN
2	F	73	GLN
2	F	96	ASN
2	F	112	GLN
2	F	130	GLN
2	F	194	ASN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	385	GLN
2	F	419	GLN
2	F	443	GLN
2	F	455	GLN
3	G	82	HIS
3	G	88	GLN
3	G	163	ASN
3	G	205	GLN
3	G	234	ASN
4	H	35	GLN
4	H	66	HIS
4	H	138	ASN

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Mol	Chain	Res	Type
5	I	33	ASN
1	J	46	ASN
1	J	208	GLN
1	J	274	GLN
1	J	396	GLN
1	J	405	GLN
1	J	430	GLN
1	J	432	GLN
1	J	441	GLN
1	J	475	GLN
1	K	48	GLN
1	K	65	ASN
1	K	78	ASN
1	K	113	ASN
1	K	163	GLN
1	K	172	GLN
1	K	280	GLN
1	K	302	HIS
1	K	385	GLN
1	K	415	GLN
1	K	432	GLN
1	K	466	ASN
1	K	503	ASN
1	L	78	ASN
1	L	163	GLN
1	L	215	GLN
1	L	302	HIS
1	L	313	ASN
1	L	341	ASN
1	L	385	GLN
1	L	405	GLN
1	L	416	GLN
1	L	471	HIS
1	L	476	HIS
2	M	39	GLN
2	M	73	GLN
2	M	96	ASN
2	M	130	GLN
2	M	194	ASN
2	M	198	HIS
2	M	221	GLN
2	M	282	GLN

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Mol	Chain	Res	Type
2	M	419	GLN
2	N	39	GLN
2	N	223	ASN
2	N	249	GLN
2	N	282	GLN
2	N	293	GLN
2	N	367	HIS
2	N	375	GLN
2	N	379	GLN
2	N	385	GLN
2	N	411	GLN
2	N	442	GLN
2	N	455	GLN
2	O	39	GLN
2	O	51	GLN
2	O	73	GLN
2	O	96	ASN
2	O	112	GLN
2	O	130	GLN
2	O	194	ASN
2	O	221	GLN
2	O	223	ASN
2	O	282	GLN
2	O	385	GLN
2	O	416	GLN
2	O	443	GLN
2	O	451	HIS
3	P	82	HIS
3	P	88	GLN
3	P	163	ASN
3	P	205	GLN
3	P	225	GLN
3	P	234	ASN
4	Q	35	GLN
4	Q	66	HIS
4	Q	85	ASN
4	Q	111	ASN
5	R	33	ASN
6	S	10	GLN
7	T	153	ASN
7	T	162	GLN
8	U	34	ASN

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Mol	Chain	Res	Type
8	U	88	GLN
9	V	9	GLN
9	V	49	GLN
6	W	10	GLN
7	X	162	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\# Z  > 2$
10	ANP	A	600	11	27,33,33	4.07	12 (44%)	30,52,52	2.40	6 (20%)
10	ANP	B	600	11	27,33,33	4.11	12 (44%)	30,52,52	2.79	9 (30%)
10	ANP	C	600	11	27,33,33	3.98	12 (44%)	30,52,52	2.85	8 (26%)
12	ADP	D	600	11	22,29,29	1.95	6 (27%)	27,45,45	2.70	8 (29%)
10	ANP	F	600	11	27,33,33	3.72	12 (44%)	30,52,52	2.44	8 (26%)
10	ANP	J	600	11	27,33,33	3.98	12 (44%)	30,52,52	2.65	8 (26%)
10	ANP	K	600	11	27,33,33	3.95	12 (44%)	30,52,52	2.51	6 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	ANP	L	600	11	27,33,33	4.14	12 (44%)	30,52,52	3.01	10 (33%)
12	ADP	M	600	11	22,29,29	2.18	7 (31%)	27,45,45	2.76	7 (25%)
10	ANP	O	600	11	27,33,33	3.68	12 (44%)	30,52,52	2.66	8 (26%)

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
10	ANP	A	600	11	-	1/12/38/38	0/3/3/3
10	ANP	B	600	11	2/2/7/8	1/12/38/38	0/3/3/3
10	ANP	C	600	11	-	0/12/38/38	0/3/3/3
12	ADP	D	600	11	-	0/12/32/32	0/3/3/3
10	ANP	F	600	11	-	0/12/38/38	0/3/3/3
10	ANP	J	600	11	-	1/12/38/38	0/3/3/3
10	ANP	K	600	11	-	0/12/38/38	0/3/3/3
10	ANP	L	600	11	-	0/12/38/38	0/3/3/3
12	ADP	M	600	11	-	0/12/32/32	0/3/3/3
10	ANP	O	600	11	-	0/12/38/38	0/3/3/3

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	600	ANP	PB-O2B	-3.73	1.46	1.56
10	A	600	ANP	PB-O2B	-3.60	1.46	1.56
10	K	600	ANP	PB-O2B	-3.47	1.47	1.56
10	L	600	ANP	PB-O2B	-3.46	1.47	1.56
10	C	600	ANP	PB-O2B	-3.43	1.47	1.56
10	O	600	ANP	PB-O2B	-3.42	1.47	1.56
10	F	600	ANP	PB-O2B	-3.29	1.47	1.56
10	J	600	ANP	PB-O2B	-3.15	1.47	1.56
10	F	600	ANP	PA-O2A	2.15	1.64	1.54
12	M	600	ADP	PA-O2A	2.21	1.64	1.54
12	M	600	ADP	C2-N3	2.25	1.36	1.32
12	D	600	ADP	PA-O2A	2.27	1.64	1.54
10	O	600	ANP	PA-O2A	2.29	1.64	1.54
10	K	600	ANP	PB-N3B	2.49	1.69	1.63
10	A	600	ANP	PA-O2A	2.49	1.65	1.54
10	O	600	ANP	PB-N3B	2.52	1.70	1.63
10	L	600	ANP	PA-O2A	2.62	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	600	ANP	PA-O2A	2.64	1.66	1.54
10	B	600	ANP	PA-O2A	2.66	1.66	1.54
10	K	600	ANP	PA-O2A	2.70	1.66	1.54
10	F	600	ANP	PB-N3B	2.71	1.70	1.63
10	O	600	ANP	PG-N3B	2.74	1.70	1.63
10	A	600	ANP	PB-N3B	2.77	1.70	1.63
10	C	600	ANP	PG-N3B	2.78	1.70	1.63
10	J	600	ANP	PA-O2A	2.82	1.67	1.54
10	C	600	ANP	PB-N3B	2.84	1.70	1.63
12	D	600	ADP	C2-N1	2.95	1.39	1.33
10	A	600	ANP	PG-N3B	2.98	1.71	1.63
10	B	600	ANP	PB-N3B	3.00	1.71	1.63
10	L	600	ANP	PG-N3B	3.04	1.71	1.63
10	J	600	ANP	PG-N3B	3.07	1.71	1.63
12	D	600	ADP	PB-O2B	3.09	1.65	1.54
12	D	600	ADP	PB-O3B	3.11	1.65	1.54
10	F	600	ANP	PG-N3B	3.11	1.71	1.63
10	O	600	ANP	PG-O3G	3.11	1.65	1.56
10	J	600	ANP	PB-N3B	3.14	1.71	1.63
12	M	600	ADP	PB-O2B	3.17	1.66	1.54
10	B	600	ANP	PG-N3B	3.22	1.71	1.63
12	D	600	ADP	C6-N6	3.23	1.44	1.34
10	L	600	ANP	PB-N3B	3.26	1.72	1.63
10	O	600	ANP	C6-N6	3.30	1.45	1.34
10	K	600	ANP	PG-N3B	3.33	1.72	1.63
10	F	600	ANP	PG-O2G	3.41	1.66	1.56
10	F	600	ANP	C6-N6	3.42	1.45	1.34
10	J	600	ANP	PG-O3G	3.44	1.66	1.56
12	M	600	ADP	C6-N6	3.45	1.45	1.34
10	J	600	ANP	PG-O2G	3.46	1.66	1.56
10	C	600	ANP	PG-O2G	3.49	1.66	1.56
10	A	600	ANP	PG-O2G	3.54	1.66	1.56
10	L	600	ANP	PG-O2G	3.55	1.66	1.56
10	O	600	ANP	PB-O3A	3.58	1.63	1.59
10	K	600	ANP	PG-O2G	3.63	1.66	1.56
10	C	600	ANP	PG-O3G	3.65	1.66	1.56
10	O	600	ANP	PG-O2G	3.72	1.67	1.56
10	C	600	ANP	PB-O3A	3.72	1.63	1.59
12	M	600	ADP	PB-O3B	3.73	1.68	1.54
10	C	600	ANP	C6-N6	3.73	1.46	1.34
10	B	600	ANP	PG-O2G	3.74	1.67	1.56
10	K	600	ANP	C6-N6	3.84	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	600	ANP	C6-N6	3.90	1.47	1.34
10	F	600	ANP	PG-O3G	3.97	1.67	1.56
10	B	600	ANP	PG-O3G	3.98	1.67	1.56
10	J	600	ANP	C6-N6	4.02	1.47	1.34
10	A	600	ANP	PG-O3G	4.05	1.67	1.56
12	M	600	ADP	C2-N1	4.07	1.41	1.33
10	O	600	ANP	C2-N1	4.12	1.41	1.33
10	K	600	ANP	PG-O3G	4.14	1.68	1.56
10	F	600	ANP	C2-N3	4.15	1.39	1.32
10	L	600	ANP	PG-O3G	4.15	1.68	1.56
10	F	600	ANP	C2-N1	4.18	1.41	1.33
10	J	600	ANP	C2-N1	4.18	1.41	1.33
10	B	600	ANP	C6-N6	4.19	1.47	1.34
10	A	600	ANP	C6-N6	4.19	1.47	1.34
10	C	600	ANP	C2-N3	4.21	1.39	1.32
10	A	600	ANP	PB-O3A	4.24	1.64	1.59
10	L	600	ANP	C2-N3	4.26	1.39	1.32
10	O	600	ANP	C2-N3	4.26	1.39	1.32
10	K	600	ANP	PB-O3A	4.27	1.64	1.59
10	J	600	ANP	PB-O3A	4.28	1.64	1.59
10	C	600	ANP	C2-N1	4.39	1.42	1.33
10	A	600	ANP	C2-N3	4.46	1.40	1.32
10	J	600	ANP	C2-N3	4.47	1.40	1.32
10	K	600	ANP	C2-N3	4.49	1.40	1.32
10	B	600	ANP	C2-N3	4.50	1.40	1.32
12	D	600	ADP	C4-N3	4.53	1.42	1.35
10	K	600	ANP	C2-N1	4.56	1.42	1.33
10	A	600	ANP	C2-N1	4.59	1.42	1.33
10	L	600	ANP	C2-N1	4.64	1.42	1.33
10	B	600	ANP	C2-N1	4.85	1.43	1.33
10	O	600	ANP	C4-N3	4.97	1.43	1.35
10	F	600	ANP	C4-N3	5.00	1.43	1.35
10	F	600	ANP	PB-O3A	5.09	1.65	1.59
10	J	600	ANP	C4-N3	5.36	1.43	1.35
10	B	600	ANP	PB-O3A	5.50	1.66	1.59
12	M	600	ADP	C4-N3	5.69	1.44	1.35
10	C	600	ANP	C4-N3	5.88	1.44	1.35
10	A	600	ANP	C4-N3	5.93	1.44	1.35
10	L	600	ANP	C4-N3	5.98	1.44	1.35
10	L	600	ANP	PB-O3A	6.05	1.66	1.59
10	B	600	ANP	C4-N3	6.23	1.44	1.35
10	K	600	ANP	C4-N3	6.47	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	600	ANP	PB-O1B	14.19	1.62	1.46
10	O	600	ANP	PB-O1B	14.57	1.62	1.46
10	K	600	ANP	PB-O1B	14.82	1.63	1.46
10	B	600	ANP	PB-O1B	15.36	1.63	1.46
10	J	600	ANP	PB-O1B	15.81	1.64	1.46
10	C	600	ANP	PB-O1B	15.96	1.64	1.46
10	L	600	ANP	PB-O1B	15.98	1.64	1.46
10	A	600	ANP	PB-O1B	16.01	1.64	1.46

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	600	ANP	N3-C2-N1	-12.23	119.53	128.89
10	C	600	ANP	N3-C2-N1	-12.22	119.54	128.89
10	B	600	ANP	N3-C2-N1	-11.63	119.99	128.89
12	D	600	ADP	N3-C2-N1	-11.26	120.28	128.89
12	M	600	ADP	N3-C2-N1	-10.97	120.50	128.89
10	K	600	ANP	N3-C2-N1	-10.96	120.50	128.89
10	J	600	ANP	N3-C2-N1	-10.90	120.55	128.89
10	A	600	ANP	N3-C2-N1	-10.07	121.18	128.89
10	O	600	ANP	N3-C2-N1	-9.93	121.29	128.89
10	F	600	ANP	N3-C2-N1	-9.81	121.39	128.89
10	O	600	ANP	PA-O3A-PB	-6.65	110.36	132.67
10	C	600	ANP	PA-O3A-PB	-5.35	114.74	132.67
10	L	600	ANP	PA-O3A-PB	-4.71	116.89	132.67
10	J	600	ANP	PA-O3A-PB	-4.66	117.03	132.67
10	O	600	ANP	O1G-PG-N3B	-4.63	104.80	111.90
10	A	600	ANP	PA-O3A-PB	-4.10	118.94	132.67
12	M	600	ADP	PA-O3A-PB	-4.05	119.10	132.67
10	F	600	ANP	PA-O3A-PB	-4.01	119.22	132.67
12	D	600	ADP	PA-O3A-PB	-3.94	119.44	132.67
10	L	600	ANP	O1G-PG-N3B	-3.60	106.38	111.90
10	K	600	ANP	PA-O3A-PB	-3.49	120.97	132.67
10	B	600	ANP	PA-O3A-PB	-3.40	121.27	132.67
10	L	600	ANP	C1'-N9-C4	-2.96	122.48	126.94
10	A	600	ANP	C2'-C1'-N9	-2.79	110.03	114.29
10	B	600	ANP	C4'-O4'-C1'	-2.65	106.81	109.72
10	J	600	ANP	C2'-C3'-C4'	-2.57	97.32	102.61
10	B	600	ANP	O4'-C4'-C3'	-2.47	100.16	105.15
10	K	600	ANP	O1G-PG-N3B	-2.47	108.11	111.90
10	O	600	ANP	C4-C5-N7	-2.44	107.24	109.48
12	D	600	ADP	C2'-C1'-N9	-2.39	110.64	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	600	ANP	O1G-PG-N3B	-2.38	108.25	111.90
10	L	600	ANP	O4'-C1'-N9	-2.32	103.25	108.10
10	L	600	ANP	O3G-PG-O1G	-2.18	107.69	113.49
10	C	600	ANP	O1G-PG-N3B	-2.17	108.58	111.90
10	C	600	ANP	O2G-PG-O1G	-2.13	107.82	113.49
10	F	600	ANP	O2B-PB-O1B	-2.09	105.65	110.00
10	A	600	ANP	O2G-PG-O1G	-2.00	108.16	113.49
10	O	600	ANP	O3'-C3'-C2'	2.00	118.33	111.83
10	C	600	ANP	O2'-C2'-C3'	2.01	118.37	111.83
10	J	600	ANP	O4'-C1'-N9	2.06	112.41	108.10
12	D	600	ADP	O3B-PB-O3A	2.11	114.68	105.09
12	D	600	ADP	O3'-C3'-C2'	2.12	118.71	111.83
10	J	600	ANP	O3A-PA-O5'	2.13	108.59	102.94
10	B	600	ANP	O3'-C3'-C2'	2.14	118.78	111.83
12	D	600	ADP	O2B-PB-O3A	2.17	114.94	105.09
10	B	600	ANP	O3A-PA-O5'	2.22	108.83	102.94
10	F	600	ANP	O3'-C3'-C4'	2.23	117.73	111.05
10	K	600	ANP	O2'-C2'-C3'	2.24	119.13	111.83
10	A	600	ANP	O4'-C4'-C5'	2.28	117.47	109.32
10	O	600	ANP	O1B-PB-N3B	2.30	115.42	111.90
10	F	600	ANP	O4'-C4'-C5'	2.32	117.62	109.32
10	O	600	ANP	O2B-PB-O3A	2.33	115.65	105.09
10	L	600	ANP	O3'-C3'-C4'	2.40	118.26	111.05
12	M	600	ADP	O3'-C3'-C4'	2.45	118.39	111.05
10	B	600	ANP	O5'-C5'-C4'	2.48	118.26	109.12
10	C	600	ANP	C2'-C3'-C4'	2.48	107.72	102.61
12	D	600	ADP	O4'-C4'-C5'	2.54	118.41	109.32
10	B	600	ANP	C5'-C4'-C3'	2.58	125.47	115.21
10	C	600	ANP	O3'-C3'-C2'	2.70	120.59	111.83
10	L	600	ANP	C2'-C1'-N9	2.76	118.50	114.29
12	M	600	ADP	O3'-C3'-C2'	2.77	120.85	111.83
10	A	600	ANP	O3'-C3'-C4'	2.90	119.75	111.05
10	J	600	ANP	O3'-C3'-C4'	2.95	119.91	111.05
10	F	600	ANP	O3'-C3'-C2'	3.03	121.67	111.83
10	L	600	ANP	O3'-C3'-C2'	3.03	121.68	111.83
10	F	600	ANP	O3A-PA-O5'	3.06	111.06	102.94
10	K	600	ANP	O3'-C3'-C2'	3.14	122.03	111.83
10	K	600	ANP	O3'-C3'-C4'	3.21	120.69	111.05
10	O	600	ANP	O3A-PA-O5'	3.22	111.47	102.94
10	J	600	ANP	O3'-C3'-C2'	3.23	122.34	111.83
12	M	600	ADP	C2'-C1'-N9	3.30	119.33	114.29
10	J	600	ANP	O2'-C2'-C3'	3.45	123.03	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	600	ADP	C4'-O4'-C1'	3.47	113.53	109.72
12	D	600	ADP	O3A-PA-O5'	3.63	112.58	102.94
12	M	600	ADP	O3A-PA-O5'	3.95	113.41	102.94
10	C	600	ANP	O3'-C3'-C4'	4.02	123.11	111.05
10	L	600	ANP	O3A-PA-O5'	4.23	114.15	102.94
10	B	600	ANP	O3'-C3'-C4'	5.06	126.22	111.05

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	600	ANP	C4'
10	B	600	ANP	C3'

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	J	600	ANP	O1B-PB-N3B-PG
10	B	600	ANP	O1B-PB-N3B-PG
10	A	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

9 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	600	ANP	2	0
10	B	600	ANP	1	0
12	D	600	ADP	3	0
10	F	600	ANP	9	0
10	J	600	ANP	2	0
10	K	600	ANP	4	0
10	L	600	ANP	2	0
12	M	600	ADP	4	0
10	O	600	ANP	6	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	510/510 (100%)	-0.40	1 (0%) 95 94	32, 60, 113, 179	0
1	B	480/510 (94%)	-0.54	0 100 100	34, 59, 91, 147	0
1	C	484/510 (94%)	-0.14	15 (3%) 52 38	50, 86, 171, 227	0
1	J	487/510 (95%)	-0.43	5 (1%) 84 75	32, 62, 98, 132	0
1	K	480/510 (94%)	-0.49	1 (0%) 95 94	33, 59, 95, 144	0
1	L	481/510 (94%)	-0.03	24 (4%) 32 19	51, 87, 170, 227	0
2	D	467/482 (96%)	-0.33	0 100 100	46, 79, 126, 169	0
2	E	466/482 (96%)	-0.45	4 (0%) 85 78	30, 64, 113, 174	0
2	F	466/482 (96%)	-0.27	0 100 100	39, 71, 105, 130	0
2	M	467/482 (96%)	-0.22	12 (2%) 59 45	46, 82, 127, 168	0
2	N	466/482 (96%)	-0.40	1 (0%) 95 94	31, 65, 119, 173	0
2	O	466/482 (96%)	-0.40	0 100 100	40, 71, 106, 139	0
3	G	260/272 (95%)	0.19	16 (6%) 24 13	33, 119, 237, 251	0
3	P	260/272 (95%)	0.32	21 (8%) 15 8	34, 118, 236, 252	0
4	H	131/146 (89%)	1.23	28 (21%) 1 1	117, 199, 238, 252	0
4	Q	131/146 (89%)	1.57	40 (30%) 1 0	123, 201, 239, 254	0
5	I	47/50 (94%)	0.62	5 (10%) 8 4	125, 193, 238, 252	0
5	R	47/50 (94%)	1.27	10 (21%) 1 1	124, 195, 239, 251	0
6	S	161/190 (84%)	0.66	20 (12%) 5 3	113, 159, 188, 206	0
6	W	142/190 (74%)	1.05	28 (19%) 1 1	115, 157, 191, 203	0
7	T	82/116 (70%)	2.44	49 (59%) 0 0	165, 233, 275, 288	0
7	X	38/116 (32%)	1.94	19 (50%) 0 0	164, 217, 238, 239	0
8	U	28/118 (23%)	2.58	21 (75%) 0 0	195, 232, 254, 261	0
9	V	64/76 (84%)	3.10	34 (53%) 0 0	157, 221, 291, 302	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
9	Z	17/76 (22%)	1.70	8 (47%) 0 0	175, 211, 230, 238	0
All	All	7128/7770 (91%)	-0.08	362 (5%) 32 18	30, 76, 216, 302	0

All (362) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	V	70	GLU	12.3
5	R	9	LEU	10.0
9	V	67	PRO	9.3
3	G	180	SER	9.2
9	V	8	VAL	9.1
9	V	7	PRO	8.8
9	V	69	PHE	8.7
9	V	66	ASP	8.6
7	X	161	VAL	8.5
4	Q	80	GLY	8.1
5	R	8	GLY	8.0
9	V	13	VAL	7.9
9	V	68	LYS	7.7
4	Q	145	LEU	7.6
1	L	409	ASP	7.4
1	C	412	ALA	7.3
7	T	124	LEU	7.0
4	Q	127	THR	7.0
4	Q	54	THR	6.8
3	P	104	LYS	6.7
1	C	413	ALA	6.6
1	L	410	LEU	6.5
7	T	157	TYR	6.1
7	T	203	LEU	6.1
1	C	414	THR	6.1
1	L	411	ASP	6.0
7	T	147	VAL	6.0
6	S	184	ARG	6.0
9	V	5	LEU	5.8
7	T	155	LEU	5.8
4	Q	56	GLN	5.8
5	R	1	VAL	5.7
7	X	186	SER	5.7
4	Q	114	LYS	5.6
9	V	6	ASP	5.6
1	C	510	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
9	V	61	ASN	5.6
4	H	56	GLN	5.5
3	P	102	GLU	5.4
4	Q	98	VAL	5.4
7	T	149	ARG	5.3
1	L	414	THR	5.3
9	V	59	PHE	5.1
9	V	15	LYS	5.1
5	R	2	ALA	5.0
4	H	55	LEU	5.0
4	Q	104	ASP	4.9
4	H	124	ASP	4.9
4	Q	58	LEU	4.9
1	L	510	ALA	4.8
6	W	123	ALA	4.8
7	T	185	ILE	4.7
4	Q	31	ALA	4.7
2	M	108	ILE	4.6
7	T	170	GLN	4.5
7	T	138	VAL	4.5
6	W	10	GLN	4.5
7	T	161	VAL	4.5
3	P	121	SER	4.5
9	V	36	TYR	4.5
7	T	144	LEU	4.5
4	Q	33	VAL	4.4
7	X	172	HIS	4.4
7	T	166	ARG	4.4
3	P	90	LYS	4.4
6	W	49	PRO	4.4
1	L	452	TYR	4.4
9	V	65	GLU	4.4
4	Q	82	VAL	4.4
4	H	123	ALA	4.3
2	M	215	VAL	4.3
4	Q	55	LEU	4.3
8	U	90	ASP	4.2
3	P	193	TYR	4.2
8	U	33	TRP	4.2
9	V	57	ASN	4.2
4	H	104	ASP	4.2
7	T	199	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
4	Q	124	ASP	4.2
1	J	406	PHE	4.2
4	Q	32	ASN	4.2
3	P	103	VAL	4.2
3	G	126	VAL	4.2
4	H	65	VAL	4.2
9	V	60	PRO	4.1
4	Q	118	GLU	4.1
8	U	88	GLN	4.1
4	Q	76	PHE	4.0
5	R	47	VAL	4.0
7	T	189	GLN	4.0
6	W	112	HIS	4.0
3	P	59	THR	4.0
1	L	389	THR	3.9
5	R	28	THR	3.9
5	I	47	VAL	3.9
3	G	102	GLU	3.9
7	T	158	HIS	3.9
4	Q	57	VAL	3.9
1	J	91	THR	3.9
4	Q	81	SER	3.9
7	T	198	ILE	3.9
1	C	411	ASP	3.9
9	V	63	THR	3.8
4	Q	84	VAL	3.8
7	T	190	GLU	3.8
3	P	122	ASP	3.8
7	T	125	PHE	3.8
7	X	199	ALA	3.8
7	T	188	GLN	3.8
6	W	9	VAL	3.8
7	T	154	ARG	3.7
1	L	412	ALA	3.7
4	H	127	THR	3.7
1	C	509	GLU	3.7
7	T	136	LEU	3.7
5	R	7	ALA	3.7
3	P	117	HIS	3.6
1	L	413	ALA	3.6
9	Z	47	LEU	3.6
7	T	151	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
7	X	175	ASN	3.6
4	H	71	THR	3.6
8	U	74	ASN	3.6
3	P	196	ILE	3.5
5	R	6	GLN	3.5
8	U	65	LEU	3.5
9	V	46	LYS	3.5
7	T	202	LYS	3.5
9	V	51	TYR	3.5
9	V	62	PHE	3.4
1	L	509	GLU	3.4
9	V	47	LEU	3.4
4	Q	59	ARG	3.4
4	H	66	HIS	3.4
7	X	163	ASN	3.4
3	G	90	LYS	3.4
7	T	139	THR	3.4
8	U	91	ALA	3.4
7	T	135	ALA	3.4
3	P	105	ILE	3.3
9	Z	17	ARG	3.3
8	U	73	PHE	3.3
4	H	138	ASN	3.3
5	I	9	LEU	3.3
7	X	169	GLU	3.3
1	L	501	VAL	3.3
6	S	132	THR	3.3
1	L	472	VAL	3.2
6	W	85	LEU	3.2
9	Z	43	GLU	3.2
4	H	99	THR	3.2
6	S	23	TYR	3.2
8	U	67	ASP	3.2
3	P	70	GLY	3.2
7	T	187	ALA	3.2
9	V	58	THR	3.2
7	T	145	HIS	3.2
4	H	78	SER	3.2
8	U	69	PHE	3.1
6	S	136	THR	3.1
2	M	213	SER	3.1
9	V	32	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
6	W	128	GLU	3.1
8	U	86	THR	3.1
9	V	14	ASP	3.1
6	W	135	LYS	3.0
4	H	81	SER	3.0
6	W	146	GLN	3.0
6	W	12	TYR	3.0
6	S	49	PRO	3.0
8	U	66	VAL	3.0
4	H	80	GLY	3.0
6	S	62	ARG	3.0
4	Q	74	LYS	3.0
4	H	72	THR	3.0
9	V	22	LYS	2.9
1	L	505	LEU	2.9
4	Q	94	ALA	2.9
8	U	37	LEU	2.9
6	W	11	ILE	2.9
4	Q	121	GLY	2.9
7	T	128	GLN	2.9
4	Q	85	ASN	2.9
6	S	59	TYR	2.9
2	M	14	VAL	2.9
6	W	138	LEU	2.9
4	Q	60	PRO	2.9
2	M	109	LYS	2.9
3	G	154	GLU	2.9
1	L	319	GLY	2.8
4	H	101	ASP	2.8
4	Q	97	ALA	2.8
1	L	262	LYS	2.8
6	W	139	LYS	2.8
6	W	39	LEU	2.8
1	J	94	ILE	2.8
6	S	185	ALA	2.8
7	X	166	ARG	2.8
9	Z	45	PHE	2.8
8	U	68	ASP	2.8
6	W	120	VAL	2.8
3	P	180	SER	2.8
4	Q	107	ALA	2.7
4	Q	102	MET	2.7

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Mol	Chain	Res	Type	RSRZ
7	T	174	ILE	2.7
6	S	188	GLU	2.7
9	V	53	LYS	2.7
5	R	23	ARG	2.7
3	P	93	ALA	2.7
9	Z	46	LYS	2.7
4	H	34	ARG	2.7
7	T	143	ARG	2.7
7	X	162	GLN	2.7
8	U	71	LYS	2.7
3	G	183	THR	2.7
9	V	43	GLU	2.7
7	T	184	SER	2.7
7	X	183	GLN	2.7
6	W	113	ARG	2.7
3	P	179	PHE	2.7
4	Q	115	ALA	2.7
7	T	197	CYS	2.7
8	U	85	TYR	2.7
1	C	193	THR	2.7
6	W	134	LEU	2.6
6	W	116	VAL	2.6
3	G	179	PHE	2.6
6	W	8	PRO	2.6
8	U	40	ARG	2.6
3	G	188	GLU	2.6
3	G	208	SER	2.6
6	S	39	LEU	2.6
3	G	125	LEU	2.6
1	L	92	GLY	2.6
4	H	122	ALA	2.6
1	L	41	VAL	2.6
8	U	36	THR	2.6
1	A	406	PHE	2.6
1	C	446	TYR	2.5
7	X	182	VAL	2.5
2	M	180	TYR	2.5
2	M	214	LYS	2.5
7	X	185	ILE	2.5
1	L	60	LYS	2.5
7	X	180	ARG	2.5
4	H	54	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	451	HIS	2.5
4	Q	78	SER	2.5
6	S	133	GLU	2.5
9	V	54	ALA	2.5
3	P	106	ILE	2.5
3	P	199	ASP	2.5
6	S	112	HIS	2.5
6	S	14	ILE	2.5
6	W	79	SER	2.5
4	H	145	LEU	2.5
3	G	182	ASP	2.5
5	R	36	LYS	2.5
6	S	134	LEU	2.5
4	Q	79	SER	2.4
3	G	107	GLY	2.4
8	U	87	ALA	2.4
7	T	146	ARG	2.4
3	G	93	ALA	2.4
7	T	153	ASN	2.4
1	C	489	ILE	2.4
3	G	48	SER	2.4
7	T	142	GLU	2.4
7	X	200	ASP	2.4
6	W	18	TYR	2.4
5	I	1	VAL	2.4
6	W	50	LYS	2.4
7	X	176	TRP	2.4
8	U	34	ASN	2.4
1	C	452	TYR	2.4
1	L	502	THR	2.4
7	T	122	HIS	2.4
5	I	46	LYS	2.3
3	P	91	SER	2.3
9	V	12	PHE	2.3
2	E	458	TYR	2.3
4	H	74	LYS	2.3
3	P	147	GLU	2.3
9	V	28	GLY	2.3
1	L	468	PHE	2.3
6	S	87	ASN	2.3
6	W	56	LEU	2.3
5	I	3	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
6	W	42	VAL	2.3
6	S	13	GLY	2.3
6	S	127	ASP	2.3
9	Z	20	ARG	2.3
4	H	100	LEU	2.3
4	H	105	LEU	2.3
2	M	107	PRO	2.3
4	Q	83	THR	2.3
9	V	55	ASP	2.3
7	T	140	TYR	2.3
7	T	192	GLU	2.3
1	L	508	PHE	2.3
6	S	143	SER	2.3
3	G	204	TYR	2.3
1	K	25	LEU	2.2
7	T	123	TYR	2.2
7	T	131	ASN	2.2
7	T	148	TYR	2.2
1	J	124	LYS	2.2
4	H	16	MET	2.2
2	M	174	ALA	2.2
7	T	204	LEU	2.2
7	T	168	LYS	2.2
2	M	205	VAL	2.2
6	W	59	TYR	2.2
2	E	393	MET	2.2
6	W	91	GLU	2.2
3	G	150	ASN	2.2
2	M	12	ARG	2.2
3	P	197	ASP	2.2
4	Q	93	LEU	2.2
7	X	201	LEU	2.2
4	Q	17	SER	2.2
1	L	392	LEU	2.2
7	T	201	LEU	2.2
8	U	31	LYS	2.2
9	Z	42	ARG	2.2
4	H	132	GLN	2.1
6	W	44	GLN	2.1
4	Q	38	VAL	2.1
7	T	133	ALA	2.1
1	J	403	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
7	T	169	GLU	2.1
1	C	450	ARG	2.1
6	W	126	LEU	2.1
7	X	178	GLU	2.1
1	C	497	LEU	2.1
6	S	66	VAL	2.1
7	T	162	GLN	2.1
8	U	35	GLU	2.1
4	H	79	SER	2.1
1	L	318	GLY	2.1
1	C	407	GLY	2.1
4	Q	138	ASN	2.1
4	H	86	ALA	2.1
4	Q	36	VAL	2.1
7	T	127	VAL	2.1
2	E	344	ILE	2.1
2	M	206	ILE	2.1
2	N	36	LEU	2.1
9	V	27	GLY	2.1
1	C	195	GLU	2.1
3	P	58	LYS	2.1
7	X	203	LEU	2.0
7	T	186	SER	2.0
1	L	196	LYS	2.0
4	Q	134	ARG	2.0
4	Q	18	PHE	2.0
6	S	65	LYS	2.0
1	C	469	LEU	2.0
7	X	197	CYS	2.0
9	V	11	LEU	2.0
4	H	69	ASP	2.0
9	Z	41	ASP	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	MG	O	601	1/1	0.98	0.39	6.80	51,51,51,51	0
11	MG	D	601	1/1	0.98	0.50	5.21	66,66,66,66	0
11	MG	F	601	1/1	0.98	0.40	3.42	52,52,52,52	0
11	MG	M	601	1/1	0.97	0.42	3.03	64,64,64,64	0
12	ADP	M	600	27/27	0.92	0.28	1.55	46,66,79,86	0
12	ADP	D	600	27/27	0.95	0.27	1.05	53,70,80,84	0
10	ANP	A	600	31/31	0.96	0.22	0.91	51,64,82,93	0
10	ANP	J	600	31/31	0.96	0.21	0.72	50,70,85,95	0
10	ANP	K	600	31/31	0.95	0.19	0.68	40,95,115,117	0
10	ANP	B	600	31/31	0.94	0.19	0.68	44,92,104,109	0
10	ANP	O	600	31/31	0.97	0.19	0.21	44,55,67,81	0
10	ANP	L	600	31/31	0.94	0.20	-0.12	54,91,101,115	0
10	ANP	C	600	31/31	0.96	0.17	-0.16	78,98,114,115	0
10	ANP	F	600	31/31	0.96	0.20	-0.42	41,52,63,78	0
11	MG	J	601	1/1	0.98	0.37	-	81,81,81,81	0
11	MG	B	601	1/1	0.95	0.28	-	84,84,84,84	0
11	MG	A	601	1/1	0.96	0.31	-	49,49,49,49	0
11	MG	L	601	1/1	0.93	0.64	-	81,81,81,81	0
11	MG	C	601	1/1	0.96	0.36	-	76,76,76,76	0
11	MG	K	601	1/1	0.95	0.35	-	65,65,65,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.