



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2021 – 04:13 PM JST

PDB ID : 7DQD  
Title : Crystal structure of the AMP-PNP-bound mutant A(S23C)3B(N64C)3 complex from enterococcus hirae V-ATPase  
Authors : Maruyama, S.; Suzuki, K.; Mizutani, K.; Imai, F.L.; Ishizuka-Katsura, Y.; Shirouzu, M.; Murata, T.  
Deposited on : 2020-12-23  
Resolution : 3.38 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.25  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.25

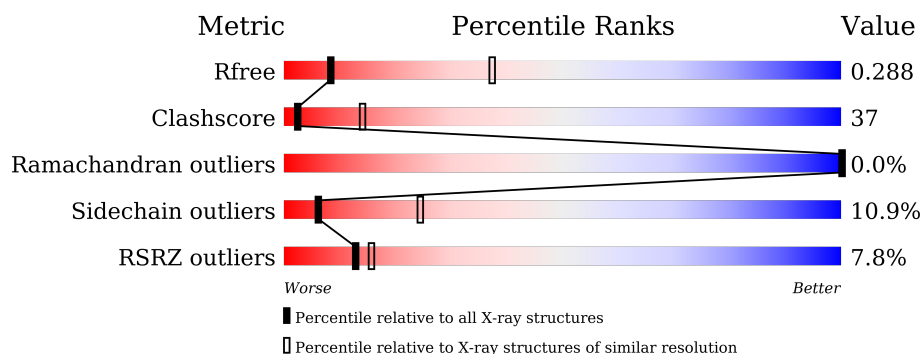
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.38 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	600	<div> <div>5%</div> <div>51% 42% 5% .</div> </div>
1	B	600	<div> <div>7%</div> <div>46% 45% 6% .</div> </div>
1	C	600	<div> <div>8%</div> <div>50% 42% 6% .</div> </div>
1	I	600	<div> <div>5%</div> <div>51% 42% . .</div> </div>
1	J	600	<div> <div>8%</div> <div>46% 47% 5% .</div> </div>
1	K	600	<div> <div>7%</div> <div>47% 46% . .</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	465	
2	E	465	
2	F	465	
2	L	465	
2	M	465	
2	N	465	

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
4	ANP	B	601	-	-	X	-
4	ANP	C	601	-	-	X	-
4	ANP	K	601	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 46492 atoms, of which 8 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 V-type sodium ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4448	2789	751	883	25			
1	B	584	Total	C	N	O	S	0	0	0
			4443	2788	752	877	26			
1	C	584	Total	C	N	O	S	0	0	0
			4274	2682	728	840	24			
1	I	583	Total	C	N	O	S	0	0	0
			4291	2687	729	853	22			
1	J	584	Total	C	N	O	S	0	0	0
			4422	2781	748	866	27			
1	K	584	Total	C	N	O	S	0	0	0
			4435	2783	749	876	27			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q08636
A	-5	SER	-	expression tag	UNP Q08636
A	-4	SER	-	expression tag	UNP Q08636
A	-3	GLY	-	expression tag	UNP Q08636
A	-2	SER	-	expression tag	UNP Q08636
A	-1	SER	-	expression tag	UNP Q08636
A	0	GLY	-	expression tag	UNP Q08636
A	23	CYS	SER	engineered mutation	UNP Q08636
B	-6	GLY	-	expression tag	UNP Q08636
B	-5	SER	-	expression tag	UNP Q08636
B	-4	SER	-	expression tag	UNP Q08636
B	-3	GLY	-	expression tag	UNP Q08636
B	-2	SER	-	expression tag	UNP Q08636
B	-1	SER	-	expression tag	UNP Q08636
B	0	GLY	-	expression tag	UNP Q08636
B	23	CYS	SER	engineered mutation	UNP Q08636
C	-6	GLY	-	expression tag	UNP Q08636

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	SER	-	expression tag	UNP Q08636
C	-4	SER	-	expression tag	UNP Q08636
C	-3	GLY	-	expression tag	UNP Q08636
C	-2	SER	-	expression tag	UNP Q08636
C	-1	SER	-	expression tag	UNP Q08636
C	0	GLY	-	expression tag	UNP Q08636
C	23	CYS	SER	engineered mutation	UNP Q08636
I	-6	GLY	-	expression tag	UNP Q08636
I	-5	SER	-	expression tag	UNP Q08636
I	-4	SER	-	expression tag	UNP Q08636
I	-3	GLY	-	expression tag	UNP Q08636
I	-2	SER	-	expression tag	UNP Q08636
I	-1	SER	-	expression tag	UNP Q08636
I	0	GLY	-	expression tag	UNP Q08636
I	23	CYS	SER	engineered mutation	UNP Q08636
J	-6	GLY	-	expression tag	UNP Q08636
J	-5	SER	-	expression tag	UNP Q08636
J	-4	SER	-	expression tag	UNP Q08636
J	-3	GLY	-	expression tag	UNP Q08636
J	-2	SER	-	expression tag	UNP Q08636
J	-1	SER	-	expression tag	UNP Q08636
J	0	GLY	-	expression tag	UNP Q08636
J	23	CYS	SER	engineered mutation	UNP Q08636
K	-6	GLY	-	expression tag	UNP Q08636
K	-5	SER	-	expression tag	UNP Q08636
K	-4	SER	-	expression tag	UNP Q08636
K	-3	GLY	-	expression tag	UNP Q08636
K	-2	SER	-	expression tag	UNP Q08636
K	-1	SER	-	expression tag	UNP Q08636
K	0	GLY	-	expression tag	UNP Q08636
K	23	CYS	SER	engineered mutation	UNP Q08636

- Molecule 2 is a protein called V-type sodium ATPase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	447	Total	C	N	O	S	0	0	0
			3383	2137	589	642	15			
2	E	453	Total	C	N	O	S	0	0	0
			3400	2152	592	643	13			
2	F	445	Total	C	N	O	S	0	0	0
			3295	2080	579	621	15			
2	L	447	Total	C	N	O	S	0	0	0
			3428	2167	591	655	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	453	Total	C	N	O	S	0	0	0
			3357	2119	586	639	13			
2	N	429	Total	C	N	O	S	0	0	0
			3162	1999	549	600	14			

There are 48 discrepancies between the modelled and reference sequences:

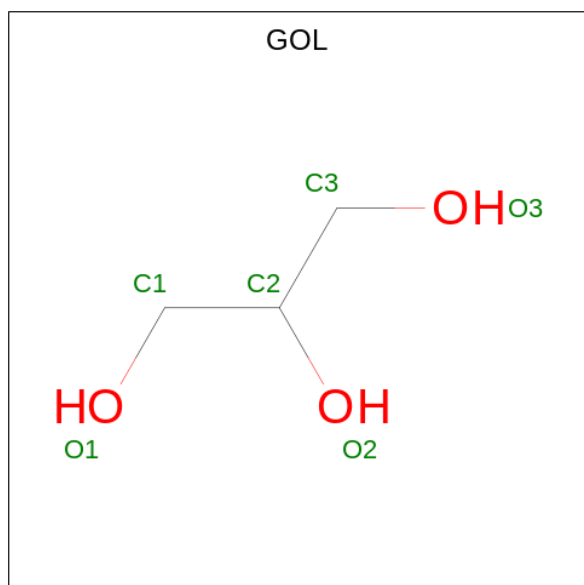
Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	GLY	-	expression tag	UNP Q08637
D	-5	SER	-	expression tag	UNP Q08637
D	-4	SER	-	expression tag	UNP Q08637
D	-3	GLY	-	expression tag	UNP Q08637
D	-2	SER	-	expression tag	UNP Q08637
D	-1	SER	-	expression tag	UNP Q08637
D	0	GLY	-	expression tag	UNP Q08637
D	64	CYS	ASN	engineered mutation	UNP Q08637
E	-6	GLY	-	expression tag	UNP Q08637
E	-5	SER	-	expression tag	UNP Q08637
E	-4	SER	-	expression tag	UNP Q08637
E	-3	GLY	-	expression tag	UNP Q08637
E	-2	SER	-	expression tag	UNP Q08637
E	-1	SER	-	expression tag	UNP Q08637
E	0	GLY	-	expression tag	UNP Q08637
E	64	CYS	ASN	engineered mutation	UNP Q08637
F	-6	GLY	-	expression tag	UNP Q08637
F	-5	SER	-	expression tag	UNP Q08637
F	-4	SER	-	expression tag	UNP Q08637
F	-3	GLY	-	expression tag	UNP Q08637
F	-2	SER	-	expression tag	UNP Q08637
F	-1	SER	-	expression tag	UNP Q08637
F	0	GLY	-	expression tag	UNP Q08637
F	64	CYS	ASN	engineered mutation	UNP Q08637
L	-6	GLY	-	expression tag	UNP Q08637
L	-5	SER	-	expression tag	UNP Q08637
L	-4	SER	-	expression tag	UNP Q08637
L	-3	GLY	-	expression tag	UNP Q08637
L	-2	SER	-	expression tag	UNP Q08637
L	-1	SER	-	expression tag	UNP Q08637
L	0	GLY	-	expression tag	UNP Q08637
L	64	CYS	ASN	engineered mutation	UNP Q08637
M	-6	GLY	-	expression tag	UNP Q08637
M	-5	SER	-	expression tag	UNP Q08637

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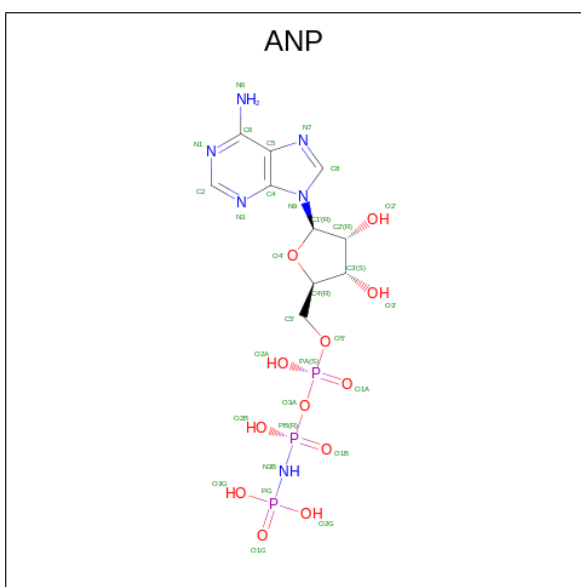
Chain	Residue	Modelled	Actual	Comment	Reference
M	-4	SER	-	expression tag	UNP Q08637
M	-3	GLY	-	expression tag	UNP Q08637
M	-2	SER	-	expression tag	UNP Q08637
M	-1	SER	-	expression tag	UNP Q08637
M	0	GLY	-	expression tag	UNP Q08637
M	64	CYS	ASN	engineered mutation	UNP Q08637
N	-6	GLY	-	expression tag	UNP Q08637
N	-5	SER	-	expression tag	UNP Q08637
N	-4	SER	-	expression tag	UNP Q08637
N	-3	GLY	-	expression tag	UNP Q08637
N	-2	SER	-	expression tag	UNP Q08637
N	-1	SER	-	expression tag	UNP Q08637
N	0	GLY	-	expression tag	UNP Q08637
N	64	CYS	ASN	engineered mutation	UNP Q08637

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula:  $C_{10}H_{17}N_6O_{12}P_3$ ).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	J	1	Total Mg 1 1	0	0
5	K	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 1 1	0	0

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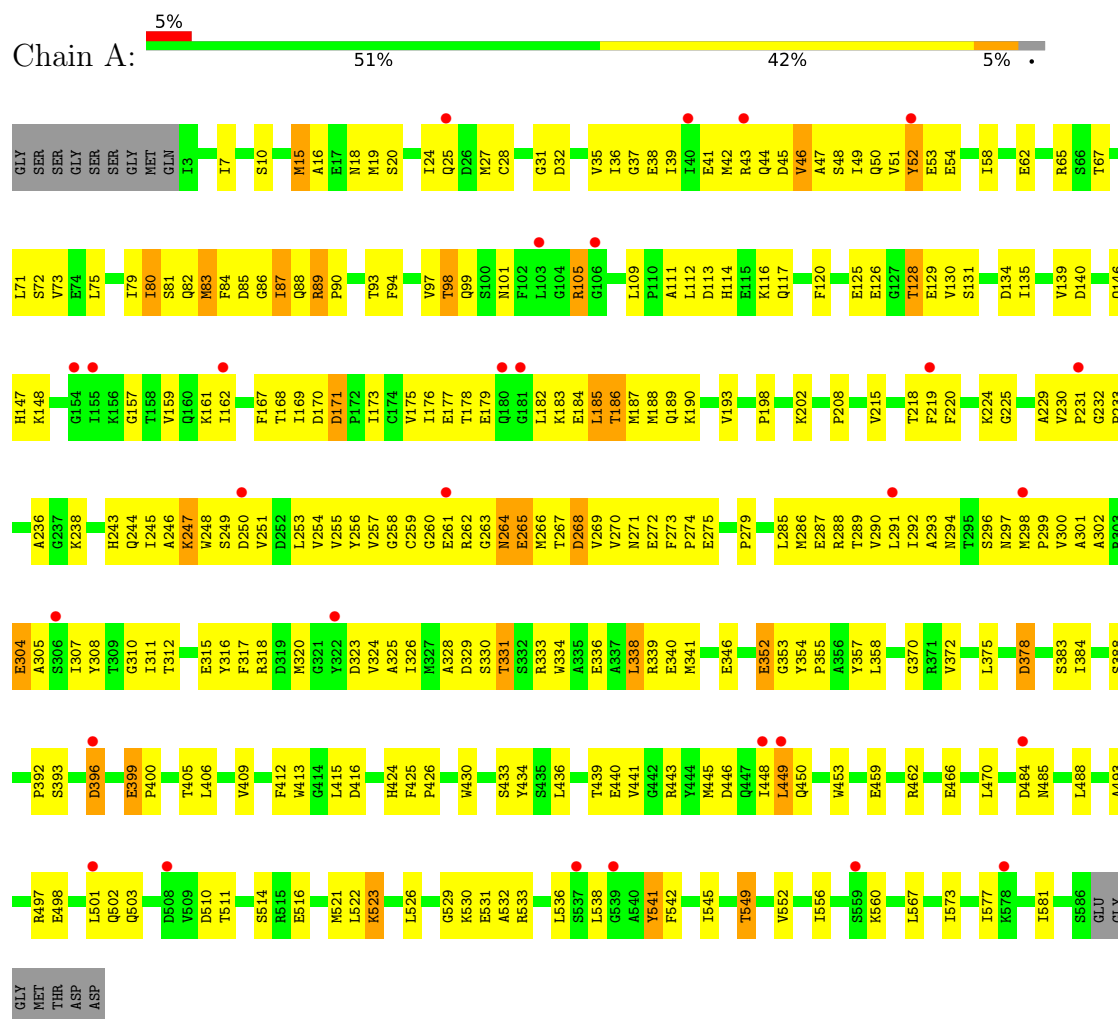
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	O 1	0	0
6	C	1	Total 1	O 1	0	0
6	E	1	Total 1	O 1	0	0
6	I	2	Total 2	O 2	0	0
6	L	1	Total 1	O 1	0	0
6	M	1	Total 1	O 1	0	0
6	N	4	Total 4	O 4	0	0

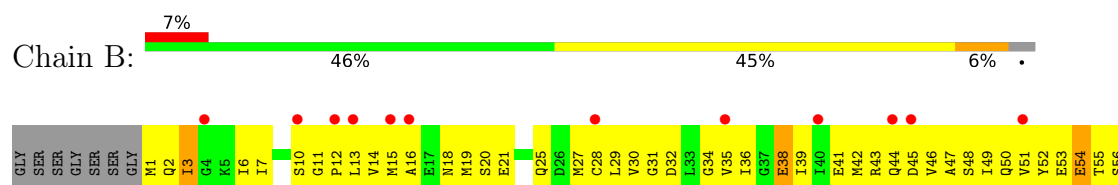
### 3 Residue-property plots [i](#)

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

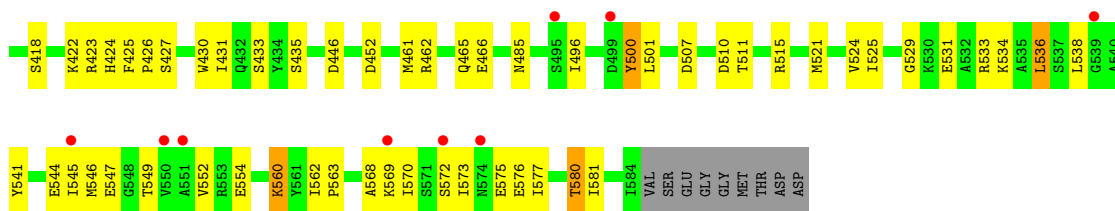
#### • Molecule 1: V-type sodium ATPase catalytic subunit A



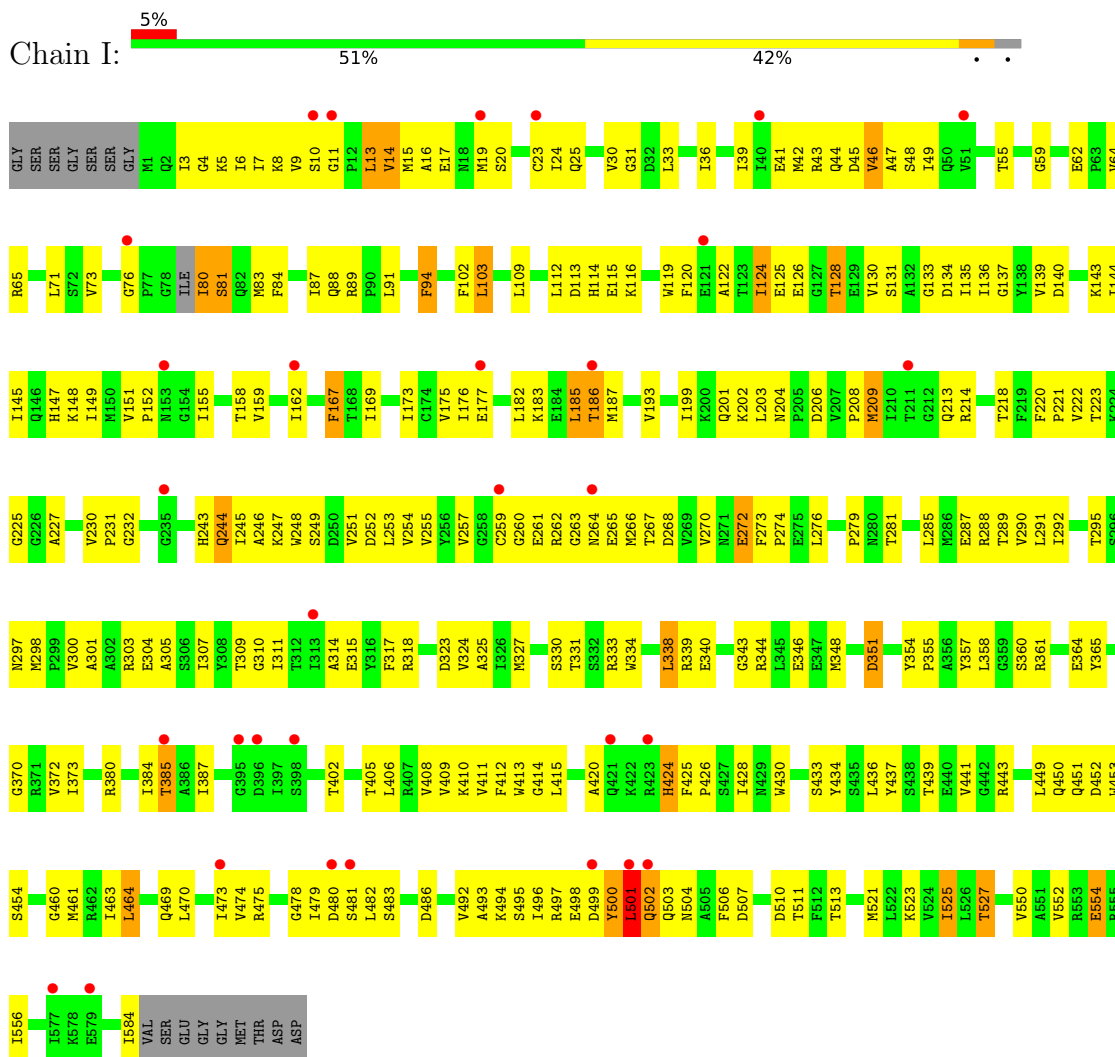
#### • Molecule 1: V-type sodium ATPase catalytic subunit A



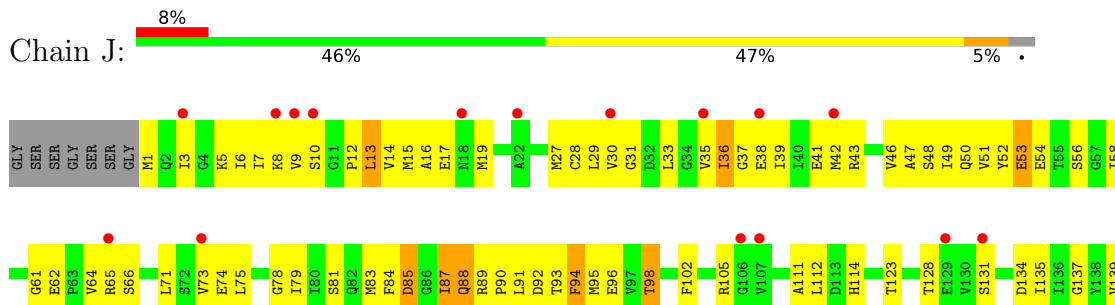


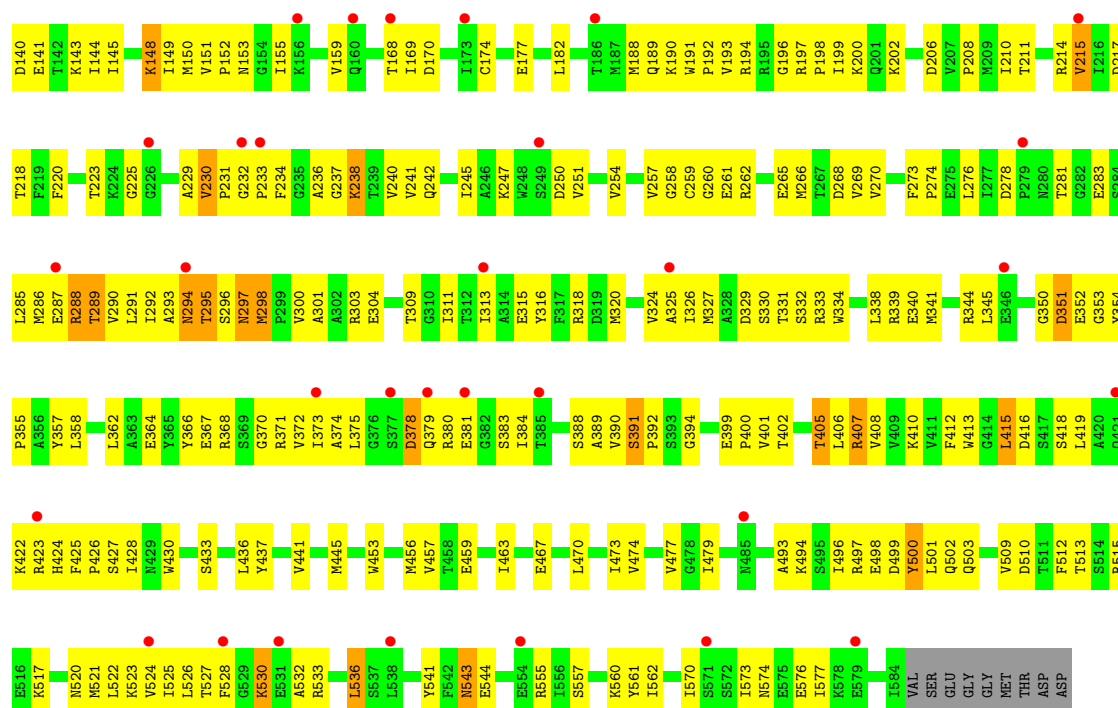


- Molecule 1: V-type sodium ATPase catalytic subunit A

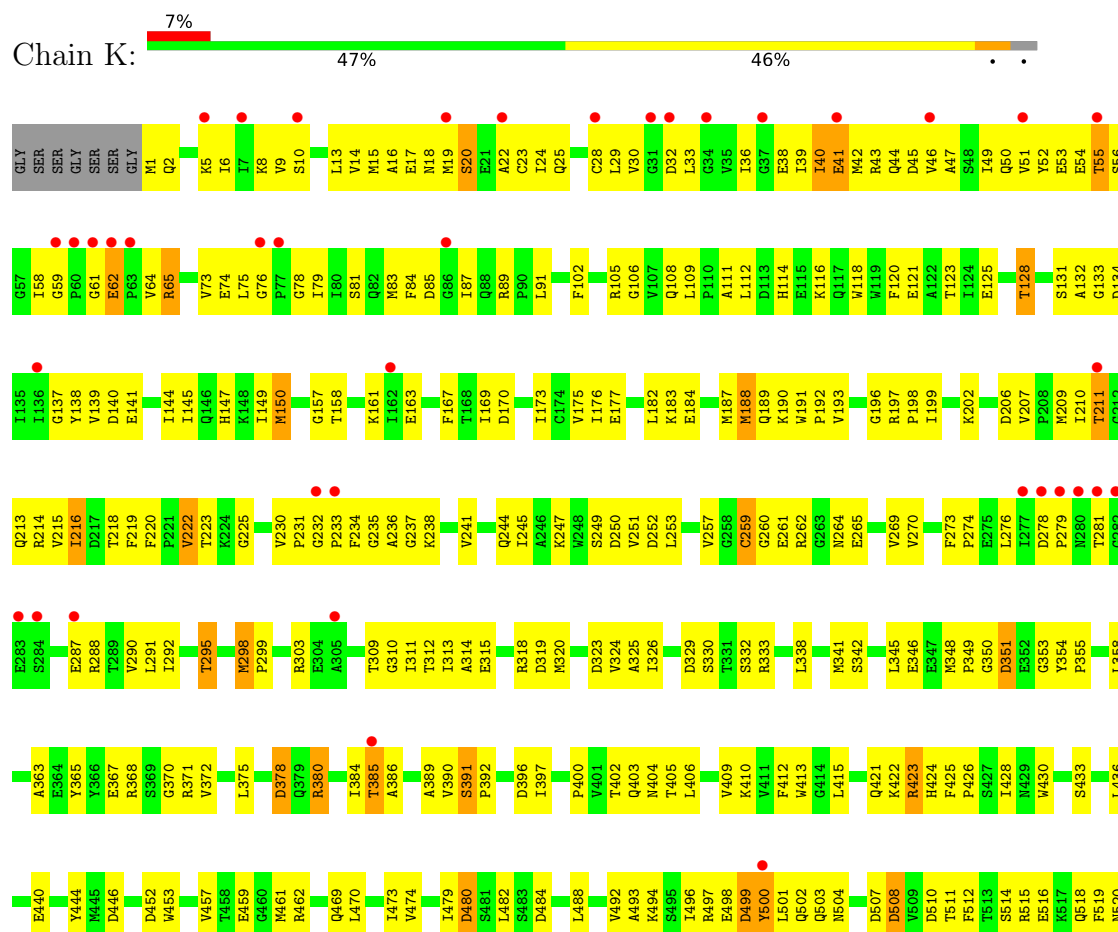


- Molecule 1: V-type sodium ATPase catalytic subunit A



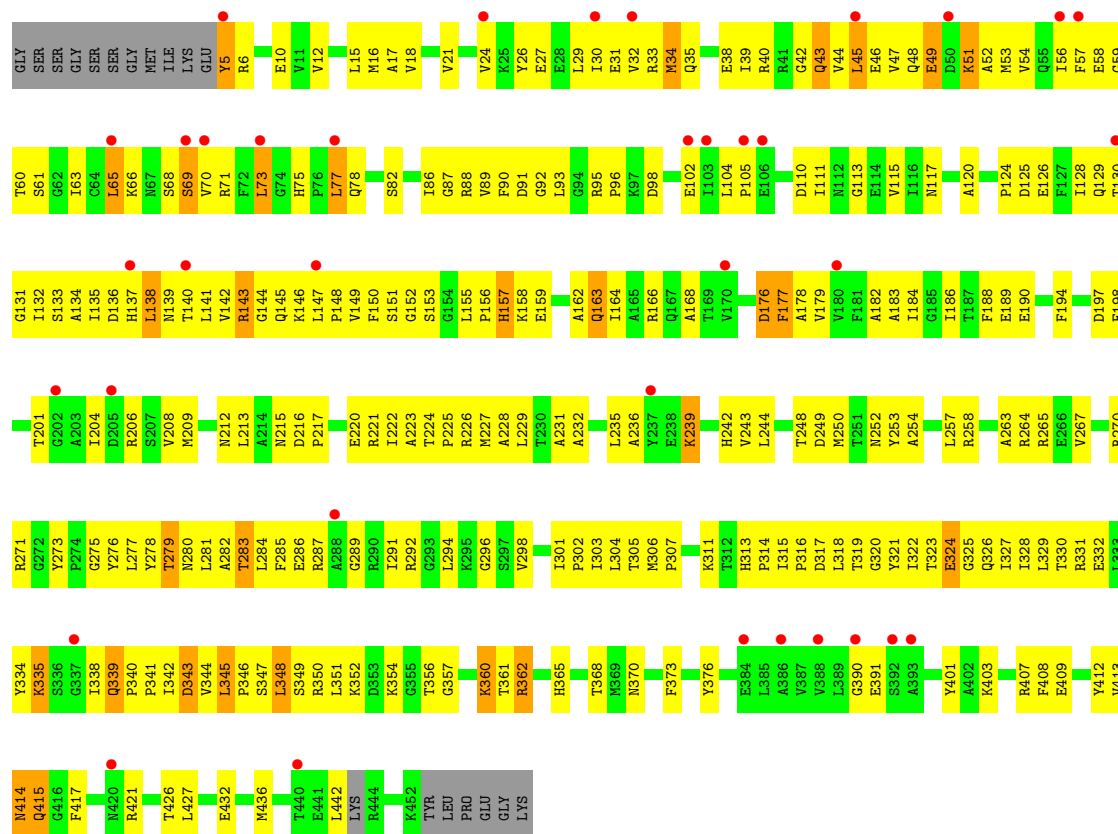


• Molecule 1: V-type sodium ATPase catalytic subunit A

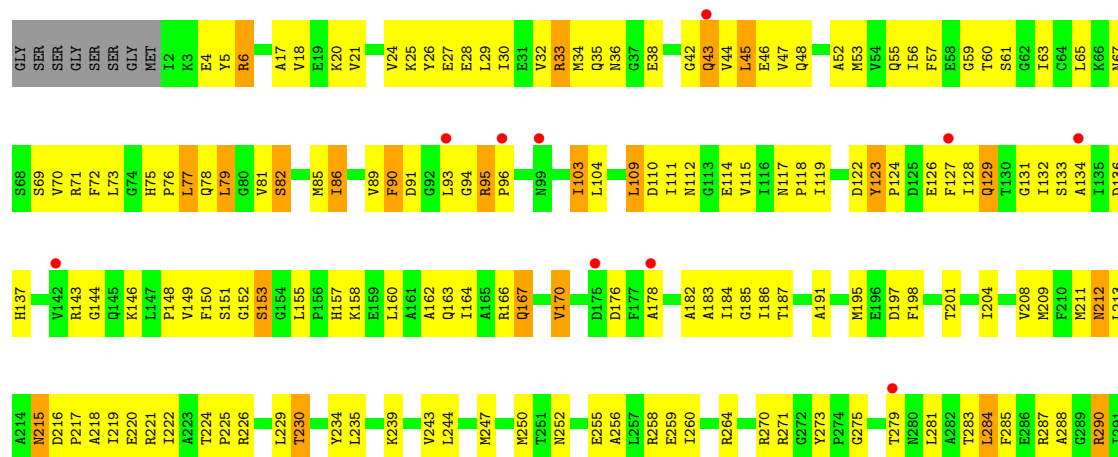
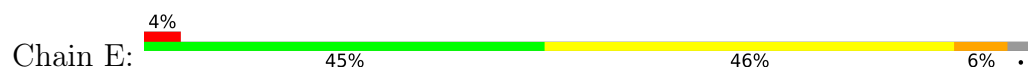


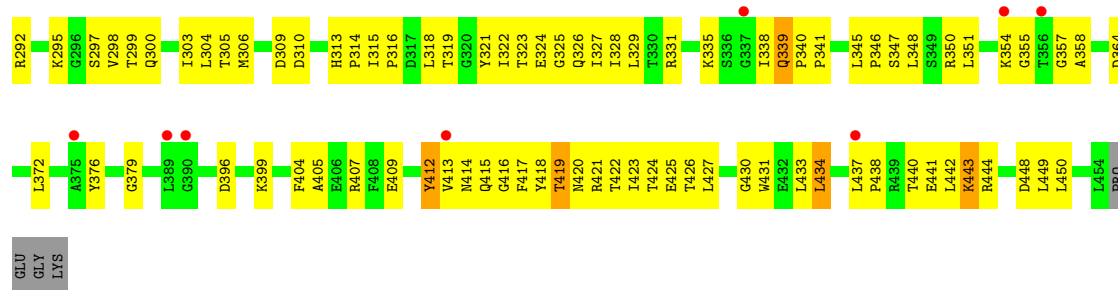


• Molecule 2: V-type sodium ATPase subunit B

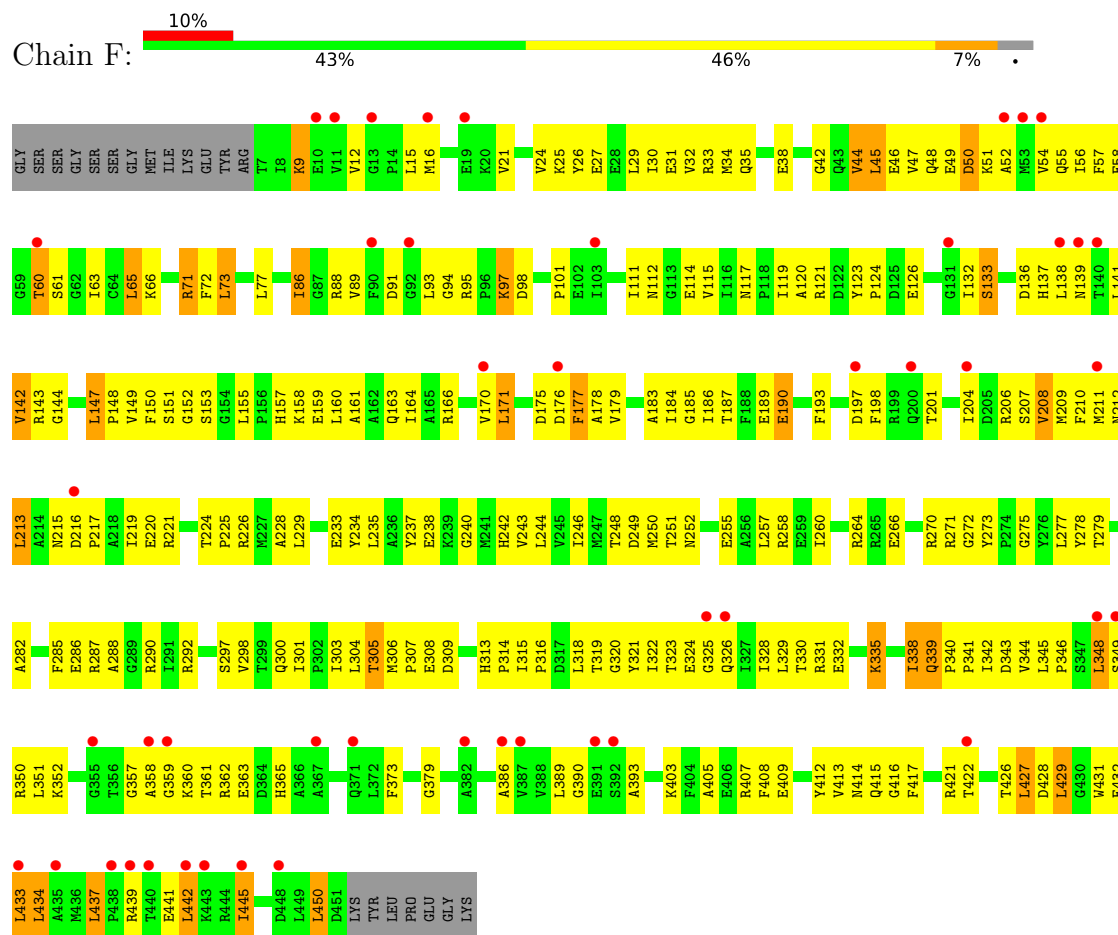


• Molecule 2: V-type sodium ATPase subunit B

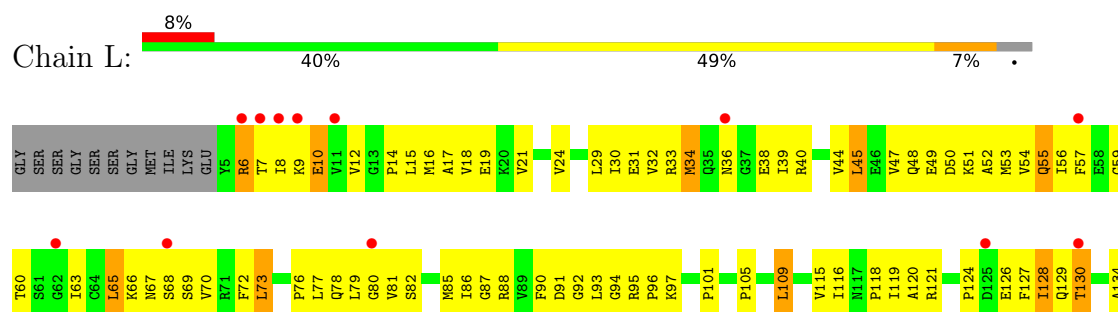


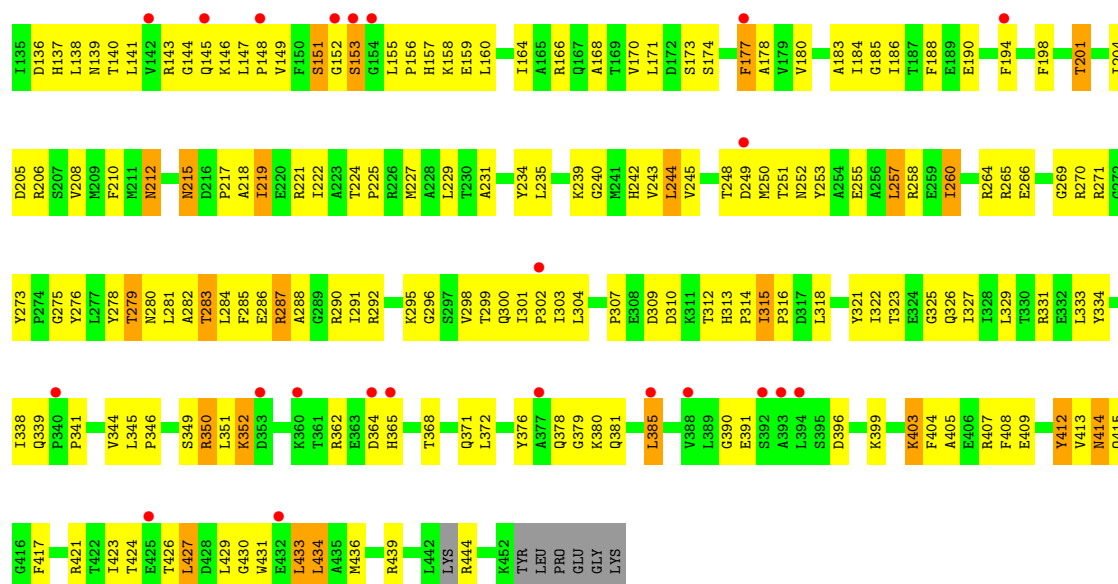


• Molecule 2: V-type sodium ATPase subunit B

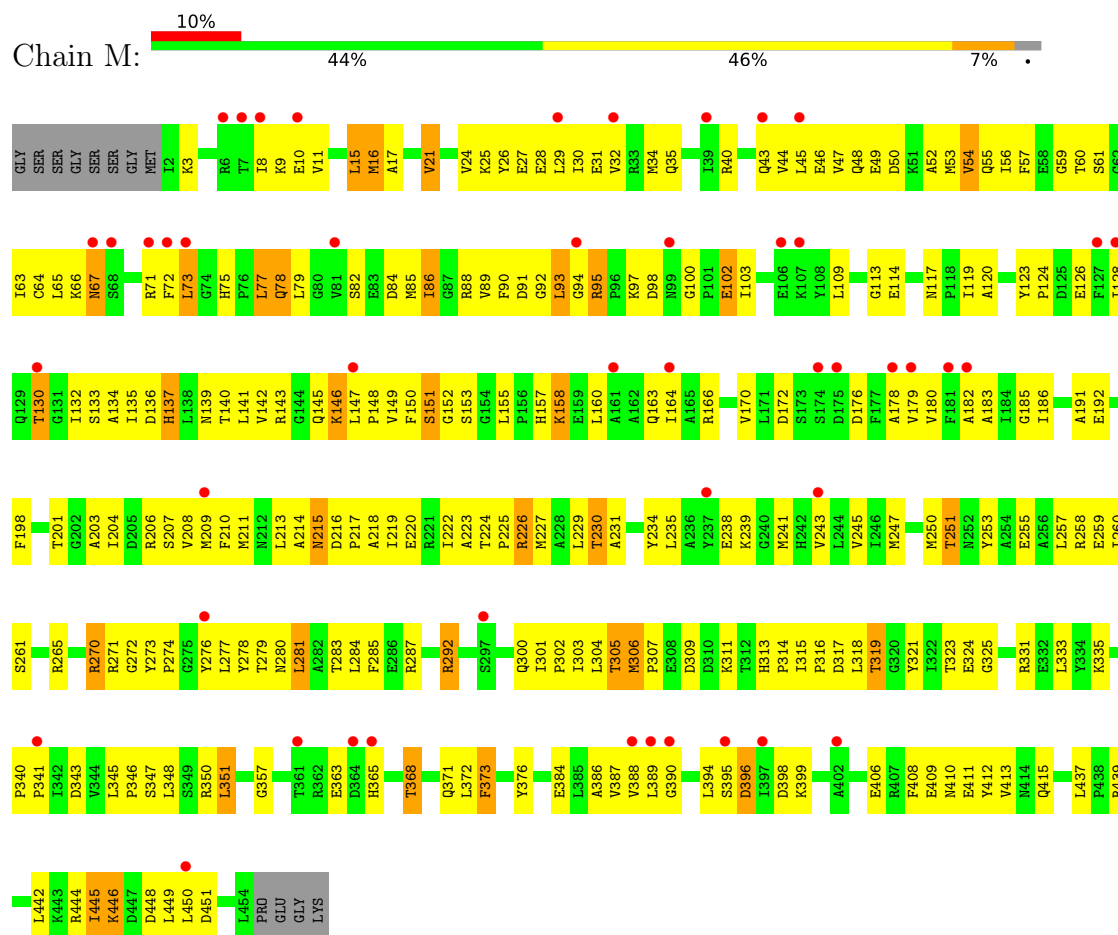


• Molecule 2: V-type sodium ATPase subunit B





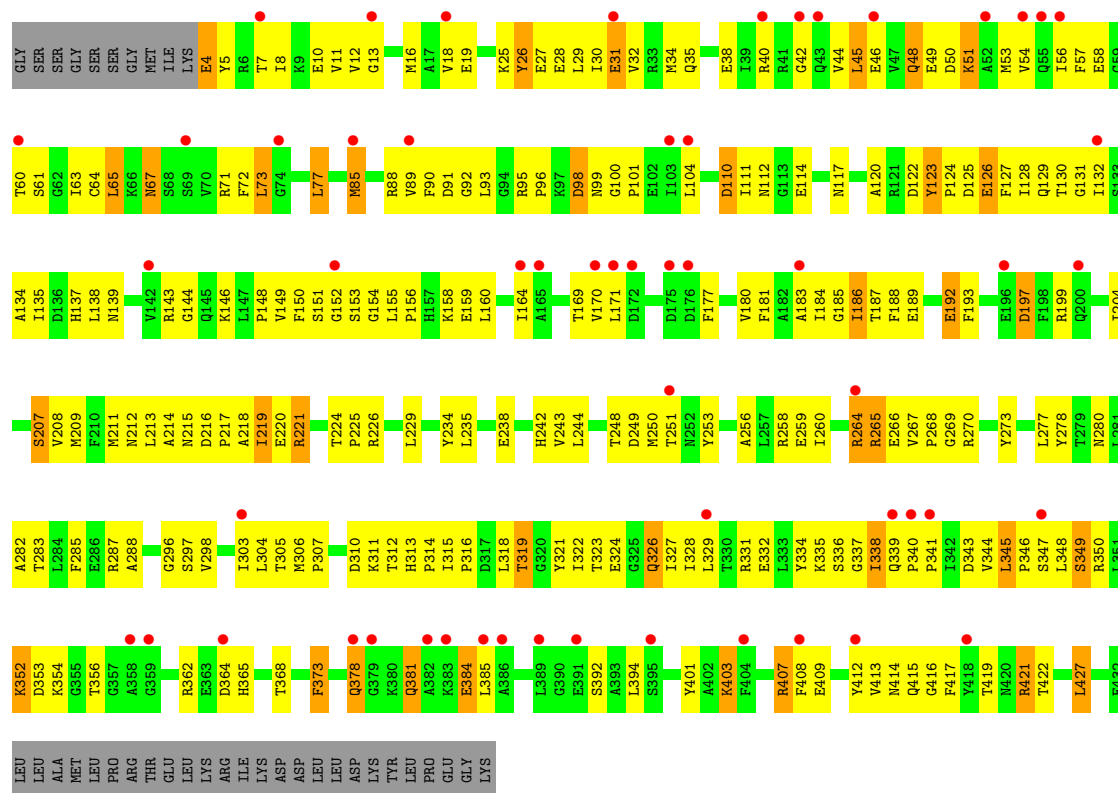
• Molecule 2: V-type sodium ATPase subunit B



• Molecule 2: V-type sodium ATPase subunit B







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.57Å 123.38Å 230.28Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	49.37 – 3.38 49.36 – 3.38	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.37-3.38) 99.3 (49.36-3.38)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.261 , 0.286 0.261 , 0.288	Depositor DCC
$R_{free}$ test set	4725 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	77.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.069 for -k,-h,-l 0.075 for k,h,-l 0.248 for h,-k,-l	Xtriage
Reported twinning fraction	0.350 for -h,-k,l	Depositor
Outliers	0 of 91940 reflections	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	46492	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, ANP

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	0.20	0/4524	0.37	0/6132
1	B	0.22	0/4519	0.39	0/6125
1	C	0.21	0/4346	0.38	0/5903
1	I	0.21	0/4361	0.40	1/5929 (0.0%)
1	J	0.25	0/4498	0.41	0/6096
1	K	0.21	0/4511	0.38	0/6115
2	D	0.24	0/3443	0.43	1/4660 (0.0%)
2	E	0.21	0/3461	0.38	0/4693
2	F	0.21	0/3351	0.39	0/4548
2	L	0.21	0/3488	0.38	0/4717
2	M	0.20	0/3413	0.38	0/4626
2	N	0.22	0/3218	0.40	0/4367
All	All	0.22	0/47133	0.39	2/63911 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	339	GLN	C-N-CD	-8.10	102.78	120.60
1	I	501	LEU	CA-CB-CG	6.77	130.86	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4448	0	4297	295	0
1	B	4443	0	4280	328	0
1	C	4274	0	3998	290	0
1	I	4291	0	4030	278	0
1	J	4422	0	4271	349	0
1	K	4435	0	4281	344	0
2	D	3383	0	3279	298	0
2	E	3400	0	3255	261	0
2	F	3295	0	3157	263	0
2	L	3428	0	3377	312	0
2	M	3357	0	3207	281	0
2	N	3162	0	2993	307	0
3	A	6	8	8	0	0
4	B	31	0	13	9	0
4	C	31	0	13	14	0
4	J	31	0	13	7	0
4	K	31	0	13	16	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	1	0	0	0	0
6	I	2	0	0	3	0
6	L	1	0	0	0	0
6	M	1	0	0	1	0
6	N	4	0	0	0	0
All	All	46484	8	44485	3401	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 37.

All (3401) 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:I:20:SER:HB3	1:I:45:ASP:HB2	1.25	1.16
1:K:497:ARG:HA	1:K:501:LEU:HG	1.28	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:9:VAL:HG21	1:J:58:ILE:HB	1.27	1.16
1:J:215:VAL:HB	1:J:501:LEU:HA	1.23	1.15
1:B:497:ARG:HA	1:B:501:LEU:HB2	1.29	1.14
1:C:10:SER:HB2	2:F:46:GLU:HG3	1.30	1.13
2:L:18:VAL:HB	2:L:52:ALA:HB3	1.25	1.12
1:K:24:ILE:HD12	1:K:41:GLU:HA	1.32	1.11
2:M:82:SER:HB3	2:M:103:ILE:HD11	1.13	1.11
1:C:577:ILE:HG22	1:C:581:ILE:HD11	1.30	1.10
1:K:232:GLY:HA3	1:K:415:LEU:HD12	1.25	1.10
4:K:601:ANP:H5'2	2:N:350:ARG:HD3	1.32	1.10
2:M:128:ILE:HG13	2:M:143:ARG:HG2	1.32	1.10
2:F:198:PHE:HB3	2:F:204:ILE:HB	1.25	1.09
2:N:128:ILE:HA	2:N:170:VAL:HA	1.36	1.08
1:A:264:ASN:HD21	2:D:324:GLU:HG2	1.10	1.06
2:N:338:ILE:HB	2:N:414:ASN:HD22	1.15	1.06
2:N:326:GLN:HG3	2:N:348:LEU:HB3	1.38	1.06
1:K:55:THR:HG22	1:K:58:ILE:HD12	1.39	1.05
2:E:132:ILE:HG12	2:E:340:PRO:HG3	1.39	1.04
1:B:27:MET:HE1	1:B:38:GLU:HG2	1.40	1.03
1:I:264:ASN:HB3	2:L:351:LEU:HD11	1.38	1.03
1:K:41:GLU:HG2	2:L:12:VAL:HG13	1.36	1.03
2:F:44:VAL:HG22	2:F:54:VAL:HG12	1.36	1.03
2:L:149:VAL:HA	2:L:327:ILE:HB	1.41	1.02
1:K:43:ARG:HA	2:L:10:GLU:HB3	1.38	1.02
2:E:270:ARG:HG2	2:E:271:ARG:HG2	1.38	1.01
1:K:8:LYS:HB2	2:N:48:GLN:HB3	1.39	1.01
1:J:17:GLU:HA	1:J:46:VAL:HG22	1.37	1.00
1:B:202:LYS:HG2	1:B:372:VAL:HG12	1.44	1.00
2:L:6:ARG:HB3	2:L:6:ARG:HH21	1.27	1.00
1:J:392:PRO:HB3	1:J:399:GLU:HB2	1.42	1.00
1:A:39:ILE:HG12	1:A:49:ILE:HG23	1.40	0.99
1:B:11:GLY:HA2	1:B:55:THR:HG21	1.42	0.99
2:F:338:ILE:HB	2:F:414:ASN:HD22	1.29	0.98
2:F:93:LEU:HD12	2:F:95:ARG:HH22	1.28	0.98
2:E:21:VAL:HG11	2:E:52:ALA:HB2	1.43	0.97
1:J:73:VAL:HG12	1:J:88:GLN:HG3	1.46	0.97
1:J:262:ARG:NH2	2:M:321:TYR:O	1.96	0.97
1:B:13:LEU:HD22	1:B:345:LEU:HD22	1.43	0.97
1:C:83:MET:HG3	2:F:119:ILE:HD11	1.46	0.97
2:F:325:GLY:HA3	2:F:326:GLN:HG2	1.47	0.96
2:L:32:VAL:HG22	2:L:70:VAL:HG22	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ASN:ND2	2:D:351:LEU:HD11	1.81	0.95
2:E:166:ARG:HD2	2:E:201:THR:HG21	1.48	0.95
2:D:140:THR:CB	2:D:352:LYS:HB2	1.97	0.95
1:C:135:ILE:HD11	1:C:150:MET:HA	1.48	0.95
2:D:304:LEU:HD22	2:D:315:ILE:HG22	1.51	0.93
1:B:285:LEU:CD1	1:B:288:ARG:HD2	1.98	0.93
2:E:372:LEU:HD21	2:E:412:TYR:HE1	1.33	0.92
1:B:230:VAL:HG22	1:B:413:TRP:HB2	1.50	0.91
1:B:249:SER:O	1:B:288:ARG:NH1	2.02	0.91
1:C:139:VAL:HG23	1:C:149:ILE:HD11	1.52	0.91
1:J:35:VAL:HB	1:J:53:GLU:HB2	1.52	0.91
1:C:572:SER:O	1:C:576:GLU:N	2.03	0.91
1:A:264:ASN:HD21	2:D:324:GLU:CG	1.82	0.91
1:A:297:ASN:HB2	2:D:286:GLU:HG3	1.53	0.90
2:M:345:LEU:HA	2:M:373:PHE:HZ	1.37	0.90
2:D:140:THR:HB	2:D:352:LYS:HB2	1.53	0.90
2:L:6:ARG:CZ	2:L:69:SER:HA	2.01	0.90
2:L:16:MET:HB2	2:L:54:VAL:HG22	1.52	0.89
2:L:148:PRO:HG2	2:L:326:GLN:HA	1.51	0.89
1:A:73:VAL:HG13	1:A:193:VAL:HG12	1.54	0.89
2:L:352:LYS:H	2:L:352:LYS:HZ3	0.93	0.89
1:J:362:LEU:HD13	1:J:405:THR:HG23	1.52	0.89
2:F:338:ILE:HB	2:F:414:ASN:ND2	1.87	0.89
2:M:145:GLN:HB2	2:M:351:LEU:HD12	1.53	0.89
1:C:202:LYS:HG3	1:C:372:VAL:HG12	1.52	0.89
2:N:91:ASP:N	2:N:95:ARG:O	2.06	0.89
2:N:44:VAL:CG2	2:N:54:VAL:HG12	2.03	0.88
1:A:24:ILE:HG22	1:A:25:GLN:HG2	1.53	0.88
2:D:29:LEU:HB2	2:D:73:LEU:HD11	1.53	0.88
1:B:208:PRO:HA	1:B:223:THR:HA	1.55	0.88
1:A:126:GLU:HG2	1:A:162:ILE:HG22	1.56	0.88
4:C:601:ANP:O3'	2:F:350:ARG:HA	1.73	0.87
1:I:318:ARG:HG3	1:I:384:ILE:HG13	1.55	0.87
1:A:215:VAL:HG23	1:A:219:PHE:HD2	1.39	0.87
2:N:152:GLY:H	2:N:155:LEU:HD12	1.36	0.87
1:J:358:LEU:HD21	1:J:401:VAL:HG22	1.56	0.87
2:N:150:PHE:HB2	2:N:328:ILE:HD13	1.56	0.87
1:C:355:PRO:HG2	1:C:358:LEU:HB2	1.57	0.86
1:J:150:MET:O	1:J:152:PRO:HD3	1.75	0.86
2:F:16:MET:HB2	2:F:54:VAL:HG23	1.57	0.86
2:N:8:ILE:HA	2:N:18:VAL:HA	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:VAL:HG12	1:C:88:GLN:HG3	1.56	0.86
2:D:362:ARG:HG3	2:D:427:LEU:HD13	1.56	0.86
2:M:179:VAL:HB	2:M:207:SER:HB3	1.58	0.86
2:N:138:LEU:HD13	2:N:344:VAL:HG11	1.55	0.86
2:D:145:GLN:HG3	2:D:351:LEU:HD12	1.55	0.86
1:K:211:THR:HB	1:K:216:ILE:HD13	1.57	0.86
1:I:81:SER:HB3	1:I:287:GLU:HA	1.58	0.85
2:D:128:ILE:HD11	2:D:143:ARG:HA	1.57	0.85
1:K:213:GLN:CB	1:K:216:ILE:HD11	2.05	0.85
1:K:231:PRO:HB3	1:K:390:VAL:HB	1.58	0.85
1:J:84:PHE:HB2	1:J:292:ILE:HG13	1.57	0.85
2:M:15:LEU:HD22	2:M:55:GLN:HB2	1.56	0.85
1:B:496:ILE:HG12	1:B:525:ILE:HG21	1.57	0.85
1:B:497:ARG:O	1:B:502:GLN:N	2.09	0.85
1:C:251:VAL:HG21	1:C:325:ALA:HB2	1.57	0.85
2:E:132:ILE:HG12	2:E:340:PRO:CG	2.08	0.84
2:F:152:GLY:H	2:F:155:LEU:HD12	1.41	0.84
1:K:85:ASP:OD1	1:K:89:ARG:N	2.11	0.84
1:A:231:PRO:HG2	1:A:415:LEU:H	1.40	0.84
1:B:31:GLY:HA2	1:B:62:GLU:HB3	1.58	0.84
1:A:264:ASN:ND2	2:D:324:GLU:HG2	1.91	0.84
1:C:577:ILE:HG22	1:C:581:ILE:CD1	2.07	0.84
1:C:10:SER:HB2	2:F:46:GLU:CG	2.07	0.84
2:L:278:TYR:HE1	2:L:322:ILE:HG12	1.40	0.84
1:J:6:ILE:HG23	1:J:16:ALA:HB2	1.57	0.84
1:K:231:PRO:HA	1:K:390:VAL:O	1.77	0.84
2:L:148:PRO:HA	2:L:302:PRO:HG2	1.59	0.84
2:N:282:ALA:HA	2:N:322:ILE:HG21	1.58	0.84
2:E:151:SER:O	2:E:306:MET:N	2.11	0.83
1:I:8:LYS:HB3	1:I:15:MET:HB2	1.60	0.83
2:D:179:VAL:HG22	2:D:244:LEU:HB3	1.59	0.83
2:E:29:LEU:HB3	2:E:73:LEU:HD21	1.60	0.83
2:E:35:GLN:HB3	2:E:67:ASN:HB3	1.60	0.83
1:A:497:ARG:HG2	1:A:501:LEU:HD12	1.60	0.83
4:C:601:ANP:H4'	2:F:348:LEU:HD21	1.60	0.83
1:J:16:ALA:HB3	1:J:19:MET:HE2	1.61	0.83
1:K:9:VAL:HG22	1:K:14:VAL:HG13	1.61	0.83
2:M:371:GLN:HG2	2:M:445:ILE:HD11	1.61	0.83
2:F:358:ALA:N	2:F:359:GLY:HA3	1.93	0.83
2:N:126:GLU:HB3	2:N:143:ARG:HG3	1.61	0.83
1:I:340:GLU:HG3	2:L:276:TYR:HA	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:415:LEU:HD22	1:J:428:ILE:HG13	1.58	0.82
2:M:82:SER:HB3	2:M:103:ILE:CD1	2.05	0.82
2:E:132:ILE:CG1	2:E:340:PRO:HG3	2.09	0.82
1:K:8:LYS:CB	2:N:48:GLN:HB3	2.10	0.82
1:A:297:ASN:CB	2:D:286:GLU:HG3	2.08	0.82
1:J:392:PRO:HB3	1:J:399:GLU:CB	2.09	0.82
2:M:130:THR:HG21	2:M:135:ILE:HG21	1.61	0.82
1:B:50:GLN:NE2	1:B:341:MET:SD	2.53	0.82
2:F:409:GLU:HA	2:F:413:VAL:HB	1.62	0.82
2:L:80:GLY:HA3	2:L:105:PRO:HG3	1.61	0.82
1:J:9:VAL:HG21	1:J:58:ILE:CB	2.09	0.81
1:C:39:ILE:HG12	1:C:49:ILE:HG12	1.62	0.81
2:E:124:PRO:HB3	2:E:143:ARG:O	1.79	0.81
1:I:257:VAL:HG21	1:I:310:GLY:HA3	1.62	0.81
2:M:439:ARG:NH2	2:M:451:ASP:OD2	2.13	0.81
2:N:217:PRO:HB2	2:N:220:GLU:HG3	1.61	0.81
1:I:424:HIS:CE1	1:I:501:LEU:HD22	2.15	0.81
2:N:127:PHE:O	2:N:171:LEU:N	2.13	0.81
1:A:202:LYS:HG3	1:A:372:VAL:HG12	1.62	0.81
2:L:6:ARG:HD3	2:L:70:VAL:H	1.46	0.81
2:N:338:ILE:HB	2:N:414:ASN:ND2	1.95	0.81
1:J:497:ARG:O	1:J:502:GLN:HG3	1.81	0.81
2:N:349:SER:HB3	2:N:352:LYS:HD3	1.62	0.81
2:D:329:LEU:HA	2:D:342:ILE:HA	1.62	0.81
2:E:24:VAL:HG22	2:E:72:PHE:HE1	1.45	0.81
1:B:214:ARG:HB3	1:B:500:TYR:CE2	2.16	0.81
1:J:218:THR:CG2	1:J:457:VAL:HG22	2.11	0.80
2:M:85:MET:HG2	2:M:103:ILE:CD1	2.10	0.80
1:J:202:LYS:HG2	1:J:372:VAL:HG12	1.64	0.80
2:N:138:LEU:HD11	2:N:408:PHE:HZ	1.44	0.80
1:K:220:PHE:HZ	1:K:430:TRP:HA	1.46	0.80
2:N:381:GLN:HE21	2:N:381:GLN:H	1.27	0.80
1:J:144:ILE:HG13	1:J:145:ILE:HG12	1.64	0.80
2:L:155:LEU:HD13	2:L:329:LEU:HB3	1.63	0.80
2:N:346:PRO:HB2	2:N:347:SER:C	2.02	0.80
1:A:497:ARG:HA	1:A:501:LEU:HB2	1.63	0.80
1:B:41:GLU:HB2	1:B:48:SER:HB3	1.64	0.80
2:E:409:GLU:HA	2:E:413:VAL:HG23	1.62	0.79
2:M:340:PRO:HD3	2:M:415:GLN:CB	2.12	0.79
2:D:44:VAL:HG22	2:D:54:VAL:HG12	1.63	0.79
1:K:74:GLU:HB2	1:K:111:ALA:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:250:MET:HB2	2:L:304:LEU:HB3	1.65	0.79
2:N:8:ILE:HD11	2:N:65:LEU:HA	1.64	0.79
1:C:40:ILE:HD12	1:C:345:LEU:HD11	1.64	0.79
1:J:295:THR:OG1	1:J:298:MET:SD	2.41	0.79
1:A:176:ILE:HD12	1:A:185:LEU:HD21	1.62	0.79
2:F:139:ASN:HB3	2:F:349:SER:HB2	1.64	0.79
1:B:298:MET:HB3	1:B:299:PRO:HD2	1.64	0.79
1:I:202:LYS:HG3	1:I:372:VAL:HG12	1.65	0.79
1:K:5:LYS:O	1:K:17:GLU:N	2.10	0.79
2:N:26:TYR:CD1	2:N:27:GLU:HG2	2.17	0.79
2:M:34:MET:SD	2:M:40:ARG:NH2	2.56	0.79
2:F:325:GLY:H	2:F:350:ARG:HE	1.29	0.79
2:D:407:ARG:HD3	2:D:436:MET:HE1	1.64	0.78
1:I:144:ILE:HG12	1:I:281:THR:HG21	1.65	0.78
1:K:497:ARG:HA	1:K:501:LEU:CG	2.12	0.78
1:I:125:GLU:O	1:I:128:THR:OG1	2.01	0.78
1:I:204:ASN:HD21	2:M:192:GLU:HG3	1.47	0.78
1:K:19:MET:HG2	1:K:47:ALA:HB3	1.64	0.78
2:D:281:LEU:HD22	2:D:285:PHE:HE2	1.49	0.78
1:I:43:ARG:HB3	1:I:44:GLN:C	2.03	0.78
2:L:93:LEU:HD12	2:L:95:ARG:CZ	2.14	0.78
2:M:250:MET:HB2	2:M:304:LEU:HB3	1.66	0.78
2:N:264:ARG:HG2	2:N:266:GLU:HG3	1.66	0.78
2:E:127:PHE:CZ	2:E:129:GLN:HA	2.18	0.78
1:A:220:PHE:CZ	1:A:433:SER:HB2	2.19	0.78
2:M:34:MET:HB2	2:M:40:ARG:HH21	1.49	0.78
2:D:166:ARG:HD2	2:D:201:THR:HG21	1.66	0.77
2:N:123:TYR:CD1	2:N:124:PRO:HD2	2.19	0.77
1:C:238:LYS:HG2	1:C:415:LEU:HD12	1.64	0.77
2:D:338:ILE:HG23	2:D:414:ASN:HB3	1.66	0.77
2:F:123:TYR:O	2:F:290:ARG:NH1	2.17	0.77
2:N:336:SER:HB2	2:N:337:GLY:HA2	1.66	0.77
1:A:130:VAL:HG22	1:A:157:GLY:O	1.85	0.77
1:C:300:VAL:HG12	1:C:337:ALA:HB2	1.65	0.77
2:F:77:LEU:HD23	2:F:111:ILE:HD13	1.66	0.77
2:F:93:LEU:HD12	2:F:95:ARG:NH2	1.99	0.77
1:K:262:ARG:NH2	2:N:321:TYR:O	2.16	0.77
1:B:12:PRO:HB3	1:B:344:ARG:HD2	1.65	0.77
1:K:237:GLY:CA	4:K:601:ANP:H8	2.14	0.77
2:N:129:GLN:HE22	2:N:422:THR:HA	1.48	0.77
1:B:246:ALA:HB1	1:B:254:VAL:HG11	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:232:GLY:CA	1:K:415:LEU:HD12	2.09	0.77
1:I:84:PHE:HB2	1:I:292:ILE:CD1	2.15	0.77
1:J:43:ARG:HA	2:N:10:GLU:HB2	1.65	0.77
1:J:555:ARG:HH21	1:J:573:ILE:HG12	1.50	0.77
2:N:123:TYR:HD1	2:N:124:PRO:HD2	1.50	0.77
1:A:424:HIS:CE1	1:A:502:GLN:HG2	2.19	0.77
1:K:220:PHE:CZ	1:K:430:TRP:HA	2.20	0.77
1:J:232:GLY:HA3	1:J:238:LYS:HG2	1.67	0.77
1:I:83:MET:HE3	2:L:119:ILE:HG21	1.64	0.76
1:J:332:SER:OG	1:J:391:SER:N	2.18	0.76
1:K:233:PRO:HD2	1:K:236:ALA:HB2	1.67	0.76
2:M:65:LEU:H	2:M:65:LEU:HD12	1.49	0.76
1:C:577:ILE:CG2	1:C:581:ILE:HD11	2.12	0.76
1:I:497:ARG:CA	1:I:501:LEU:HB3	2.14	0.76
1:I:220:PHE:HZ	1:I:430:TRP:HA	1.48	0.76
1:I:285:LEU:HD21	1:I:288:ARG:HH21	1.50	0.76
1:I:20:SER:HB3	1:I:45:ASP:CB	2.10	0.76
1:K:5:LYS:HG3	1:K:61:GLY:HA2	1.66	0.76
2:L:6:ARG:CD	2:L:70:VAL:HB	2.16	0.76
1:K:202:LYS:HG3	1:K:372:VAL:HG12	1.68	0.76
2:N:340:PRO:HD3	2:N:416:GLY:H	1.51	0.76
1:I:80:ILE:HA	1:I:290:VAL:HG22	1.68	0.76
1:I:119:TRP:O	1:I:139:VAL:HG13	1.85	0.76
1:J:220:PHE:HB3	1:J:413:TRP:NE1	2.00	0.76
4:K:601:ANP:H5'2	2:N:350:ARG:CD	2.14	0.76
2:L:152:GLY:H	2:L:155:LEU:HD12	1.51	0.76
1:B:28:CYS:CB	1:B:66:SER:HA	2.17	0.75
2:E:29:LEU:HD11	2:E:77:LEU:HG	1.66	0.75
2:L:14:PRO:HB2	2:L:55:GLN:HG2	1.68	0.75
2:E:55:GLN:HE22	2:E:260:ILE:HG23	1.51	0.75
2:E:153:SER:O	2:E:331:ARG:NH2	2.18	0.75
2:N:129:GLN:HB3	2:N:169:THR:H	1.50	0.75
1:B:27:MET:CE	1:B:38:GLU:HG2	2.14	0.75
1:C:214:ARG:HD2	1:C:501:LEU:H	1.49	0.75
1:J:17:GLU:CA	1:J:46:VAL:HG22	2.13	0.75
2:L:149:VAL:HB	2:L:303:ILE:HG12	1.67	0.75
2:N:138:LEU:HD11	2:N:408:PHE:CZ	2.20	0.75
2:D:158:LYS:HD3	2:D:190:GLU:HG3	1.68	0.75
1:J:220:PHE:HZ	1:J:430:TRP:HA	1.49	0.75
1:K:516:GLU:O	1:K:520:ASN:ND2	2.19	0.75
1:B:497:ARG:CA	1:B:501:LEU:HB2	2.14	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:O	1:A:50:GLN:N	2.19	0.75
1:C:149:ILE:H	1:C:149:ILE:HD12	1.52	0.75
2:E:65:LEU:H	2:E:65:LEU:HD12	1.52	0.75
1:K:410:LYS:HD3	1:K:436:LEU:HD12	1.68	0.75
2:N:148:PRO:HG3	2:N:323:THR:HG21	1.68	0.75
2:L:80:GLY:CA	2:L:105:PRO:HG3	2.16	0.75
2:N:326:GLN:CG	2:N:348:LEU:HB3	2.16	0.75
1:B:536:LEU:HD21	1:B:542:PHE:HB2	1.67	0.75
2:N:77:LEU:HD11	2:N:111:ILE:HD13	1.69	0.75
2:D:140:THR:HG21	2:D:356:THR:HG23	1.69	0.74
1:I:259:CYS:SG	1:I:334:TRP:HB2	2.26	0.74
2:M:446:LYS:HE2	2:M:446:LYS:HA	1.66	0.74
1:A:264:ASN:HB2	2:D:351:LEU:CD1	2.17	0.74
1:A:536:LEU:HD21	1:A:542:PHE:HA	1.69	0.74
1:K:210:ILE:N	1:K:250:ASP:OD1	2.20	0.74
2:F:185:GLY:O	2:F:252:ASN:ND2	2.20	0.74
1:K:6:ILE:HA	1:K:16:ALA:HA	1.68	0.74
2:L:91:ASP:OD1	2:L:95:ARG:N	2.21	0.74
2:M:35:GLN:HB3	2:M:67:ASN:HB3	1.68	0.74
1:A:159:VAL:HG22	1:A:176:ILE:HG12	1.69	0.74
1:B:12:PRO:CB	1:B:344:ARG:HD2	2.18	0.74
1:I:4:GLY:HA3	1:I:19:MET:HE1	1.69	0.74
1:K:232:GLY:HA2	1:K:415:LEU:HB2	1.69	0.74
2:E:86:ILE:HA	2:E:208:VAL:HG22	1.68	0.74
1:I:339:ARG:HB2	1:I:354:TYR:HD1	1.52	0.74
2:L:6:ARG:HB3	2:L:6:ARG:NH2	2.00	0.74
1:C:220:PHE:HZ	1:C:430:TRP:HA	1.53	0.74
2:L:6:ARG:HG2	2:L:7:THR:N	2.02	0.74
1:A:259:CYS:CB	1:A:294:ASN:HB2	2.17	0.74
1:C:573:ILE:HG22	1:C:577:ILE:HD11	1.70	0.74
1:J:12:PRO:CD	1:J:344:ARG:HD3	2.18	0.74
1:I:83:MET:CE	2:L:119:ILE:HG21	2.18	0.74
1:B:324:VAL:HB	1:B:384:ILE:HG12	1.69	0.73
1:I:91:LEU:H	1:I:91:LEU:HD12	1.52	0.73
1:J:12:PRO:HG3	1:J:344:ARG:HD3	1.69	0.73
1:J:259:CYS:HA	1:J:294:ASN:HB3	1.68	0.73
1:K:18:ASN:ND2	1:K:20:SER:HB2	2.02	0.73
1:K:260:GLY:HA3	1:K:333:ARG:HG3	1.70	0.73
1:B:513:THR:HG23	1:B:517:LYS:HE2	1.70	0.73
1:K:43:ARG:HA	2:L:10:GLU:CB	2.18	0.73
1:A:264:ASN:HD22	2:D:351:LEU:HD11	1.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:VAL:HG21	1:B:314:ALA:HB2	1.70	0.73
1:K:188:MET:HE3	1:K:190:LYS:HG3	1.68	0.73
2:L:44:VAL:HG22	2:L:54:VAL:HG12	1.70	0.73
2:D:141:LEU:HD22	2:D:147:LEU:HD22	1.69	0.73
1:J:215:VAL:HG23	1:J:501:LEU:HD23	1.70	0.73
1:K:213:GLN:HB2	1:K:216:ILE:HD11	1.68	0.73
1:A:264:ASN:HB2	2:D:351:LEU:HD11	1.70	0.73
1:K:261:GLU:HG3	1:K:265:GLU:OE2	1.89	0.73
2:M:78:GLN:NE2	2:M:109:LEU:O	2.21	0.73
2:N:4:GLU:HB3	2:N:71:ARG:HB3	1.68	0.73
1:C:570:ILE:CB	1:C:573:ILE:HG13	2.19	0.73
2:F:45:LEU:HD22	2:F:264:ARG:NH2	2.04	0.73
1:A:38:GLU:N	1:A:50:GLN:O	2.17	0.73
1:A:43:ARG:CB	1:A:46:VAL:HG13	2.19	0.73
2:E:122:ASP:HB2	2:E:292:ARG:HG2	1.71	0.73
2:E:326:GLN:HB2	2:E:348:LEU:H	1.54	0.73
2:E:409:GLU:HA	2:E:413:VAL:CG2	2.17	0.73
2:L:253:TYR:CZ	2:L:284:LEU:HD11	2.23	0.73
1:K:209:MET:SD	1:K:385:THR:HG21	2.28	0.73
2:L:352:LYS:HZ3	2:L:352:LYS:N	1.78	0.73
1:J:144:ILE:HG23	1:J:283:GLU:HG3	1.71	0.72
2:F:124:PRO:HB2	2:F:142:VAL:CG1	2.20	0.72
1:J:42:MET:SD	1:J:47:ALA:HB2	2.29	0.72
2:F:47:VAL:HG23	2:F:52:ALA:HA	1.71	0.72
2:F:139:ASN:HB3	2:F:349:SER:CB	2.18	0.72
1:C:41:GLU:OE1	1:C:43:ARG:NH1	2.21	0.72
2:F:26:TYR:CE1	2:F:27:GLU:HG2	2.24	0.72
1:I:346:GLU:O	2:M:265:ARG:NH2	2.22	0.72
1:J:233:PRO:HD2	1:J:236:ALA:CB	2.19	0.72
2:D:140:THR:HB	2:D:352:LYS:CB	2.19	0.72
1:J:350:GLY:N	1:J:354:TYR:O	2.22	0.72
1:K:55:THR:HG22	1:K:58:ILE:CD1	2.18	0.72
2:D:338:ILE:HG23	2:D:414:ASN:CB	2.20	0.72
1:K:350:GLY:N	1:K:354:TYR:O	2.22	0.72
1:B:10:SER:HA	2:E:46:GLU:CB	2.20	0.72
1:K:211:THR:HB	1:K:216:ILE:CD1	2.19	0.72
1:A:338:LEU:HD22	1:A:355:PRO:HG3	1.70	0.72
2:E:131:GLY:H	2:E:167:GLN:HB3	1.53	0.72
1:J:134:ASP:O	1:J:151:VAL:HG23	1.90	0.72
1:A:262:ARG:NH2	2:D:320:GLY:O	2.22	0.72
1:A:264:ASN:CG	2:D:351:LEU:HD11	2.09	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:12:PRO:HD3	1:J:344:ARG:HD3	1.71	0.71
1:J:215:VAL:CG1	1:J:426:PRO:HG2	2.19	0.71
1:B:35:VAL:HB	1:B:53:GLU:HB2	1.72	0.71
1:B:503:GLN:NE2	1:B:510:ASP:O	2.24	0.71
1:C:352:GLU:HB2	1:C:400:PRO:HG2	1.72	0.71
1:B:97:VAL:HG21	1:B:109:LEU:HD21	1.70	0.71
2:D:250:MET:HB2	2:D:304:LEU:HB3	1.71	0.71
1:I:177:GLU:HA	1:I:182:LEU:HA	1.71	0.71
2:L:6:ARG:HD3	2:L:70:VAL:HB	1.71	0.71
2:L:282:ALA:O	2:L:286:GLU:N	2.23	0.71
2:L:352:LYS:H	2:L:352:LYS:NZ	1.81	0.71
2:M:57:PHE:HA	2:M:219:ILE:HD13	1.70	0.71
2:N:130:THR:HG21	2:N:135:ILE:O	1.90	0.71
1:C:260:GLY:HA2	1:C:296:SER:HA	1.72	0.71
2:E:407:ARG:HG2	2:E:433:LEU:HD21	1.71	0.71
1:J:6:ILE:HD11	1:J:62:GLU:HB2	1.71	0.71
2:M:86:ILE:HA	2:M:208:VAL:HG22	1.71	0.71
1:C:295:THR:HB	1:C:297:ASN:OD1	1.90	0.71
2:E:218:ALA:HB3	2:E:260:ILE:HD11	1.72	0.71
1:J:232:GLY:CA	1:J:238:LYS:HD3	2.19	0.71
2:L:338:ILE:HG23	2:L:414:ASN:ND2	2.05	0.71
2:N:26:TYR:HD1	2:N:27:GLU:N	1.88	0.71
1:B:297:ASN:OD1	1:B:297:ASN:N	2.23	0.71
1:J:12:PRO:HD3	1:J:344:ARG:HH11	1.54	0.71
1:K:213:GLN:HB2	1:K:216:ILE:CG1	2.20	0.71
2:N:250:MET:HB2	2:N:304:LEU:HB3	1.73	0.71
1:C:36:ILE:HG23	1:C:52:TYR:HB2	1.71	0.71
1:I:295:THR:H	1:I:298:MET:HG3	1.53	0.71
1:J:6:ILE:CG2	1:J:16:ALA:HB2	2.21	0.71
1:K:188:MET:CE	1:K:190:LYS:HG3	2.19	0.71
2:L:240:GLY:O	2:L:295:LYS:NZ	2.24	0.71
1:A:43:ARG:HB2	1:A:46:VAL:HG13	1.72	0.71
2:E:91:ASP:OD1	2:E:95:ARG:N	2.23	0.71
1:J:54:GLU:OE1	1:J:56:SER:N	2.22	0.71
2:L:15:LEU:HD23	2:L:55:GLN:HG3	1.72	0.71
1:A:488:LEU:HD23	1:A:533:ARG:HG3	1.73	0.71
1:B:143:LYS:H	1:B:143:LYS:HD2	1.54	0.71
2:D:111:ILE:O	2:D:287:ARG:NH2	2.24	0.71
2:F:58:GLU:OE1	2:F:58:GLU:N	2.24	0.71
1:I:39:ILE:HG12	1:I:49:ILE:HG12	1.73	0.71
1:I:507:ASP:HB3	1:I:510:ASP:HB3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:500:TYR:HE2	1:K:522:LEU:HB2	1.53	0.71
2:D:146:LYS:HD3	2:D:285:PHE:O	1.91	0.70
2:D:148:PRO:HG3	2:D:323:THR:HB	1.73	0.70
2:D:198:PHE:HB3	2:D:204:ILE:HB	1.72	0.70
2:F:177:PHE:HE1	2:F:243:VAL:CA	2.04	0.70
1:I:264:ASN:CB	2:L:351:LEU:HD11	2.18	0.70
2:L:178:ALA:O	2:L:243:VAL:HA	1.90	0.70
1:C:234:PHE:HB3	2:F:321:TYR:CD2	2.26	0.70
1:I:173:ILE:HD13	1:I:187:MET:HG2	1.71	0.70
1:A:267:THR:O	1:A:271:ASN:ND2	2.23	0.70
1:B:443:ARG:NH1	1:B:443:ARG:HB2	2.06	0.70
2:D:6:ARG:HA	2:D:69:SER:HA	1.72	0.70
2:E:437:LEU:HB2	2:E:442:LEU:HD21	1.73	0.70
1:I:339:ARG:HB2	1:I:354:TYR:CD1	2.26	0.70
2:M:29:LEU:HB3	2:M:73:LEU:HD23	1.72	0.70
2:N:146:LYS:NZ	2:N:324:GLU:OE1	2.21	0.70
1:B:114:HIS:HD2	1:B:169:ILE:HD11	1.56	0.70
1:J:498:GLU:HA	1:J:502:GLN:CD	2.11	0.70
2:L:18:VAL:O	2:L:52:ALA:N	2.24	0.70
1:I:214:ARG:HB3	1:I:500:TYR:CZ	2.27	0.70
1:J:418:SER:O	1:J:422:LYS:HG3	1.92	0.70
1:K:298:MET:HB3	1:K:299:PRO:HD2	1.73	0.70
2:D:91:ASP:OD1	2:D:95:ARG:N	2.24	0.70
2:E:144:GLY:HA2	2:E:298:VAL:O	1.92	0.70
2:M:218:ALA:HB3	2:M:260:ILE:HD11	1.74	0.70
2:N:26:TYR:CE1	2:N:27:GLU:HG2	2.27	0.70
1:A:253:LEU:HB3	1:A:324:VAL:HG13	1.73	0.70
2:E:132:ILE:HD12	2:E:132:ILE:H	1.55	0.70
1:K:213:GLN:H	1:K:216:ILE:HD11	1.57	0.70
2:L:32:VAL:HG22	2:L:70:VAL:CG2	2.22	0.70
2:N:229:LEU:HD13	2:N:287:ARG:HG3	1.74	0.70
1:I:44:GLN:CB	1:I:45:ASP:HA	2.20	0.70
2:L:6:ARG:NH1	2:L:68:SER:O	2.25	0.70
2:N:129:GLN:HB3	2:N:169:THR:N	2.06	0.70
2:D:133:SER:HB3	2:D:426:THR:HG23	1.73	0.70
2:E:151:SER:OG	2:E:157:HIS:HB3	1.92	0.70
1:I:4:GLY:HA3	1:I:19:MET:CE	2.22	0.70
1:J:208:PRO:HA	1:J:223:THR:HA	1.74	0.70
2:N:352:LYS:O	2:N:356:THR:N	2.24	0.70
1:I:297:ASN:HB2	2:L:286:GLU:HG3	1.72	0.70
1:J:296:SER:HA	1:J:303:ARG:HH21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:326:GLN:HE22	2:N:346:PRO:HB3	1.57	0.70
1:B:202:LYS:NZ	1:B:367:GLU:O	2.25	0.69
1:I:177:GLU:HG3	1:I:182:LEU:HA	1.72	0.69
1:J:437:TYR:OH	2:N:189:GLU:OE2	2.09	0.69
1:B:214:ARG:NH1	1:B:513:THR:OG1	2.24	0.69
2:E:45:LEU:H	2:E:45:LEU:HD22	1.56	0.69
2:F:177:PHE:CZ	2:F:244:LEU:HB2	2.27	0.69
2:N:213:LEU:H	2:N:213:LEU:HD12	1.57	0.69
2:F:86:ILE:HG22	2:F:208:VAL:HG22	1.74	0.69
1:A:41:GLU:HB2	1:A:48:SER:HB2	1.72	0.69
1:B:233:PRO:HG3	1:B:417:SER:HB2	1.74	0.69
1:C:568:ALA:C	1:C:570:ILE:HA	2.12	0.69
1:I:254:VAL:H	1:I:289:THR:HG22	1.57	0.69
1:I:494:LYS:HG2	1:I:498:GLU:OE1	1.92	0.69
2:L:33:ARG:NH2	2:L:67:ASN:O	2.25	0.69
2:M:153:SER:O	2:M:331:ARG:NH2	2.25	0.69
2:M:277:LEU:HD23	2:M:318:LEU:HD12	1.75	0.69
2:M:345:LEU:HA	2:M:373:PHE:CZ	2.26	0.69
2:N:126:GLU:OE1	2:N:143:ARG:HD2	1.92	0.69
1:C:14:VAL:N	1:C:49:ILE:O	2.22	0.69
1:J:406:LEU:HD21	1:J:412:PHE:CD1	2.27	0.69
2:N:138:LEU:HD13	2:N:344:VAL:CG1	2.22	0.69
1:A:36:ILE:H	1:A:36:ILE:HD12	1.56	0.69
2:N:149:VAL:HA	2:N:327:ILE:HB	1.73	0.69
2:N:378:GLN:HB3	2:N:401:TYR:CE1	2.27	0.69
2:D:325:GLY:HA2	2:D:349:SER:HA	1.75	0.69
2:F:60:THR:HA	2:F:63:ILE:HD12	1.75	0.69
1:J:415:LEU:HA	1:J:428:ILE:HA	1.73	0.69
2:N:44:VAL:HG22	2:N:54:VAL:HA	1.72	0.69
1:A:488:LEU:CD2	1:A:533:ARG:HG3	2.23	0.69
1:K:8:LYS:HG3	2:N:48:GLN:CG	2.23	0.69
1:K:14:VAL:O	1:K:49:ILE:N	2.22	0.69
2:L:45:LEU:HD13	2:L:260:ILE:HG22	1.74	0.69
2:D:338:ILE:HG23	2:D:414:ASN:CG	2.13	0.69
1:K:8:LYS:HG3	2:N:48:GLN:HG2	1.74	0.69
2:L:91:ASP:OD1	2:L:94:GLY:N	2.26	0.69
1:C:43:ARG:CZ	2:D:12:VAL:HG21	2.23	0.69
1:K:213:GLN:N	1:K:216:ILE:HD11	2.08	0.69
2:L:16:MET:HB2	2:L:54:VAL:CG2	2.23	0.69
1:I:20:SER:HA	1:I:42:MET:HE1	1.74	0.68
1:I:297:ASN:CB	2:L:286:GLU:HG3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:233:PRO:HD3	1:K:415:LEU:HB2	1.75	0.68
1:A:126:GLU:CG	1:A:162:ILE:HG22	2.23	0.68
2:F:44:VAL:HG22	2:F:54:VAL:CG1	2.17	0.68
1:I:497:ARG:HB3	1:I:501:LEU:HG	1.74	0.68
1:J:200:LYS:NZ	1:J:379:GLN:OE1	2.25	0.68
2:E:134:ALA:HB2	2:E:412:TYR:CD2	2.28	0.68
1:I:6:ILE:HG13	1:I:64:VAL:HG22	1.75	0.68
1:I:497:ARG:HA	1:I:501:LEU:HB3	1.74	0.68
2:L:313:HIS:CG	2:L:314:PRO:HD2	2.28	0.68
1:B:56:SER:HA	2:E:26:TYR:HB3	1.75	0.68
2:E:167:GLN:HG3	2:E:420:ASN:HB2	1.76	0.68
1:K:232:GLY:CA	1:K:238:LYS:HD3	2.23	0.68
1:K:241:VAL:O	1:K:245:ILE:HG12	1.92	0.68
1:B:14:VAL:N	1:B:49:ILE:O	2.25	0.68
2:E:146:LYS:HB2	2:E:324:GLU:HG2	1.74	0.68
2:F:121:ARG:NH1	2:F:288:ALA:O	2.26	0.68
2:F:408:PHE:CD1	2:F:413:VAL:HG23	2.29	0.68
1:I:291:LEU:HD23	1:I:292:ILE:N	2.09	0.68
2:L:18:VAL:CG1	2:L:21:VAL:HG11	2.22	0.68
1:K:252:ASP:H	1:K:323:ASP:HB2	1.59	0.68
1:C:27:MET:HE1	1:C:38:GLU:HB2	1.75	0.68
1:I:497:ARG:O	1:I:501:LEU:HB3	1.92	0.68
1:A:39:ILE:CD1	1:A:49:ILE:HG12	2.24	0.68
1:B:494:LYS:HA	1:B:497:ARG:HH11	1.59	0.68
1:C:300:VAL:HG13	1:C:303:ARG:HD2	1.74	0.68
1:J:38:GLU:O	1:J:50:GLN:N	2.26	0.68
1:J:73:VAL:CG1	1:J:88:GLN:HG3	2.21	0.68
2:M:146:LYS:HB2	2:M:323:THR:O	1.94	0.68
1:A:257:VAL:HG21	1:A:310:GLY:HA3	1.76	0.68
1:B:198:PRO:HB2	1:B:375:LEU:HD11	1.75	0.68
2:F:234:TYR:CD1	2:F:238:GLU:HG3	2.28	0.68
2:M:198:PHE:HB3	2:M:204:ILE:HB	1.76	0.68
1:I:5:LYS:NZ	1:I:17:GLU:OE2	2.27	0.68
1:J:278:ASP:O	1:J:281:THR:HG22	1.94	0.68
2:N:315:ILE:O	2:N:319:THR:OG1	2.11	0.68
1:A:264:ASN:CB	2:D:351:LEU:HD11	2.23	0.67
1:A:44:GLN:CB	1:A:45:ASP:HA	2.23	0.67
2:D:5:TYR:N	2:D:70:VAL:HB	2.08	0.67
2:D:148:PRO:O	2:D:327:ILE:HB	1.94	0.67
1:J:79:ILE:HB	1:J:112:LEU:HD21	1.76	0.67
1:K:9:VAL:HG13	1:K:14:VAL:HG22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:PRO:HA	1:C:223:THR:HA	1.75	0.67
1:J:557:SER:O	1:J:560:LYS:NZ	2.26	0.67
1:K:237:GLY:HA2	4:K:601:ANP:H8	1.75	0.67
1:A:257:VAL:HG12	1:A:258:GLY:H	1.59	0.67
1:A:296:SER:OG	2:D:286:GLU:OE2	2.10	0.67
1:C:211:THR:HG21	1:C:216:ILE:CG2	2.24	0.67
1:C:350:GLY:N	1:C:354:TYR:O	2.25	0.67
1:J:73:VAL:HG13	1:J:193:VAL:CG1	2.24	0.67
1:K:262:ARG:NH1	4:K:601:ANP:O2G	2.27	0.67
2:L:6:ARG:HE	2:L:8:ILE:HG13	1.58	0.67
1:A:440:GLU:HA	1:A:443:ARG:HH12	1.59	0.67
1:K:233:PRO:HD2	1:K:236:ALA:CB	2.24	0.67
2:N:92:GLY:O	2:N:93:LEU:HD23	1.95	0.67
2:N:409:GLU:HA	2:N:413:VAL:HB	1.77	0.67
2:D:282:ALA:C	2:D:286:GLU:HG2	2.15	0.67
1:I:20:SER:HB2	2:M:66:LYS:HZ2	1.60	0.67
1:I:135:ILE:CD1	1:I:148:LYS:HD3	2.24	0.67
1:I:338:LEU:HD22	1:I:355:PRO:HG3	1.77	0.67
1:J:232:GLY:HA3	1:J:238:LYS:CG	2.25	0.67
1:B:38:GLU:O	1:B:50:GLN:N	2.27	0.67
1:B:499:ASP:OD1	1:B:556:ILE:HG22	1.94	0.67
2:F:137:HIS:ND1	2:F:412:TYR:OH	2.28	0.67
2:F:153:SER:O	2:F:331:ARG:NH2	2.23	0.67
1:J:10:SER:CB	2:M:46:GLU:HA	2.24	0.67
1:J:218:THR:HG23	1:J:457:VAL:HG22	1.77	0.67
2:L:307:PRO:HG2	2:L:313:HIS:CE1	2.30	0.67
2:M:273:TYR:HD2	2:M:314:PRO:HG2	1.59	0.67
1:I:177:GLU:HG3	1:I:182:LEU:CA	2.24	0.67
1:A:86:GLY:H	1:A:294:ASN:HD21	1.42	0.67
2:D:125:ASP:OD1	2:D:126:GLU:HG2	1.95	0.67
1:I:84:PHE:HB2	1:I:292:ILE:HD13	1.76	0.67
1:J:13:LEU:HD21	1:J:48:SER:HB2	1.76	0.67
2:D:29:LEU:HD21	2:D:77:LEU:HG	1.76	0.67
2:M:152:GLY:H	2:M:155:LEU:HD12	1.60	0.67
2:N:150:PHE:HB3	2:N:306:MET:SD	2.35	0.67
2:N:185:GLY:HA2	2:N:214:ALA:HA	1.76	0.67
2:F:224:THR:HB	2:F:225:PRO:HD3	1.77	0.66
1:J:41:GLU:OE2	1:J:43:ARG:NH1	2.28	0.66
1:J:555:ARG:NH2	1:J:573:ILE:HG12	2.09	0.66
2:N:307:PRO:HG2	2:N:313:HIS:CE1	2.30	0.66
1:B:29:LEU:N	1:B:65:ARG:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASP:N	1:B:62:GLU:OE1	2.23	0.66
1:B:119:TRP:O	1:B:139:VAL:HG22	1.95	0.66
1:B:262:ARG:NH1	1:B:265:GLU:OE2	2.28	0.66
1:B:412:PHE:CD2	1:B:433:SER:HA	2.29	0.66
2:F:229:LEU:HB2	2:F:287:ARG:NH2	2.09	0.66
1:J:36:ILE:HB	1:J:52:TYR:HB2	1.78	0.66
1:J:215:VAL:CG2	1:J:501:LEU:HD23	2.23	0.66
2:N:128:ILE:HD11	2:N:143:ARG:HG2	1.77	0.66
1:A:271:ASN:OD1	2:D:292:ARG:NH2	2.27	0.66
2:E:219:ILE:H	2:E:219:ILE:HD12	1.59	0.66
1:B:253:LEU:HB3	1:B:324:VAL:HG13	1.75	0.66
2:D:282:ALA:O	2:D:286:GLU:N	2.29	0.66
2:E:93:LEU:HD12	2:E:95:ARG:NH2	2.11	0.66
2:F:313:HIS:CE1	2:F:315:ILE:HG12	2.31	0.66
1:I:39:ILE:HG21	1:I:47:ALA:HB1	1.77	0.66
1:J:58:ILE:O	2:M:25:LYS:HA	1.96	0.66
2:M:79:LEU:HB2	2:M:227:MET:CE	2.26	0.66
1:C:300:VAL:CG2	2:F:279:THR:HG21	2.26	0.66
1:J:12:PRO:CG	1:J:344:ARG:HD3	2.26	0.66
1:K:114:HIS:ND1	1:K:170:ASP:OD1	2.29	0.66
2:M:44:VAL:HG22	2:M:54:VAL:CG1	2.26	0.66
1:A:31:GLY:HA2	1:A:62:GLU:HB3	1.77	0.66
1:B:210:ILE:HG23	1:B:515:ARG:HH21	1.60	0.66
2:D:45:LEU:HD22	2:D:264:ARG:HG3	1.77	0.66
1:J:7:ILE:HD12	1:J:8:LYS:H	1.60	0.66
1:J:497:ARG:HA	1:J:501:LEU:HD12	1.76	0.66
1:A:215:VAL:HG23	1:A:219:PHE:CD2	2.26	0.66
2:N:8:ILE:HG22	2:N:18:VAL:HG22	1.77	0.66
1:B:80:ILE:HB	1:B:141:GLU:OE1	1.96	0.66
1:B:216:ILE:HD12	1:B:245:ILE:HD11	1.77	0.66
2:E:364:ASP:CB	2:E:449:LEU:HD13	2.26	0.66
1:K:423:ARG:NH2	2:N:352:LYS:HE3	2.09	0.66
1:C:73:VAL:HB	1:C:88:GLN:NE2	2.11	0.66
1:C:348:MET:HG3	2:D:265:ARG:HA	1.76	0.66
2:D:362:ARG:CG	2:D:427:LEU:HD13	2.25	0.66
1:J:36:ILE:O	1:J:52:TYR:N	2.29	0.66
1:J:56:SER:O	1:J:105:ARG:NH2	2.29	0.66
1:J:498:GLU:HA	1:J:502:GLN:NE2	2.11	0.66
2:N:381:GLN:H	2:N:381:GLN:NE2	1.93	0.66
1:A:339:ARG:NH2	1:A:352:GLU:O	2.25	0.66
2:D:140:THR:OG1	2:D:352:LYS:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:214:ARG:HD3	1:I:513:THR:OG1	1.95	0.66
1:J:79:ILE:HG13	1:J:84:PHE:CZ	2.31	0.66
1:K:230:VAL:HG13	1:K:413:TRP:HE3	1.61	0.66
2:L:6:ARG:NH2	2:L:69:SER:HA	2.10	0.66
1:A:169:ILE:O	1:A:186:THR:OG1	2.12	0.65
2:D:125:ASP:O	2:D:360:LYS:NZ	2.22	0.65
2:D:138:LEU:HG	2:D:344:VAL:HB	1.77	0.65
1:K:237:GLY:HA3	4:K:601:ANP:H8	1.78	0.65
2:M:395:SER:OG	2:M:398:ASP:OD2	2.14	0.65
2:N:313:HIS:CE1	2:N:315:ILE:HG12	2.31	0.65
1:C:135:ILE:HG13	1:C:149:ILE:O	1.97	0.65
2:F:177:PHE:HE1	2:F:243:VAL:HA	1.61	0.65
1:K:133:GLY:O	1:K:380:ARG:NH2	2.28	0.65
2:L:6:ARG:HD3	2:L:70:VAL:N	2.11	0.65
1:A:157:GLY:HA3	1:A:177:GLU:O	1.95	0.65
1:B:12:PRO:HB3	1:B:344:ARG:CD	2.25	0.65
1:C:87:ILE:HG21	1:C:89:ARG:HE	1.62	0.65
2:D:149:VAL:HB	2:D:303:ILE:HG12	1.79	0.65
1:I:297:ASN:HB2	2:L:286:GLU:OE1	1.96	0.65
2:L:325:GLY:HA3	2:L:349:SER:HA	1.79	0.65
2:E:133:SER:CB	2:E:426:THR:HG23	2.26	0.65
1:J:366:TYR:HH	1:J:388:SER:HG	1.42	0.65
1:J:453:TRP:O	1:J:457:VAL:HG23	1.96	0.65
1:K:214:ARG:O	1:K:218:THR:HG22	1.95	0.65
1:A:101:ASN:O	2:D:117:ASN:HB2	1.96	0.65
1:C:251:VAL:O	1:C:288:ARG:NH1	2.30	0.65
2:D:130:THR:OG1	2:D:136:ASP:OD1	2.14	0.65
2:F:138:LEU:HD21	2:F:408:PHE:HZ	1.60	0.65
2:F:339:GLN:HA	2:F:341:PRO:HD3	1.78	0.65
1:J:202:LYS:HG2	1:J:372:VAL:CG1	2.26	0.65
2:M:47:VAL:HA	2:M:52:ALA:HA	1.77	0.65
1:A:249:SER:HB3	1:A:251:VAL:HG22	1.79	0.65
1:B:304:GLU:HG3	1:B:334:TRP:HE1	1.61	0.65
2:D:338:ILE:CG2	2:D:414:ASN:HB3	2.26	0.65
1:I:251:VAL:HG21	1:I:325:ALA:HB2	1.79	0.65
1:J:366:TYR:OH	1:J:388:SER:OG	2.15	0.65
2:L:409:GLU:HA	2:L:413:VAL:HB	1.79	0.65
1:A:353:GLY:HA3	2:D:270:ARG:HD3	1.77	0.65
2:E:313:HIS:HB3	2:E:316:PRO:CG	2.27	0.65
1:J:318:ARG:HD3	1:J:384:ILE:HD11	1.78	0.65
2:F:151:SER:O	2:F:306:MET:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:344:ARG:HG2	2:L:276:TYR:HB3	1.78	0.65
2:L:19:GLU:HG2	2:L:50:ASP:O	1.97	0.65
2:N:364:ASP:O	2:N:368:THR:N	2.20	0.65
1:B:246:ALA:HB2	1:B:327:MET:HG3	1.79	0.64
2:E:338:ILE:HG23	2:E:414:ASN:CG	2.17	0.64
1:K:41:GLU:CB	2:L:12:VAL:HA	2.26	0.64
1:K:225:GLY:CA	1:K:370:GLY:HA2	2.27	0.64
2:N:138:LEU:CD1	2:N:344:VAL:HG11	2.27	0.64
1:A:105:ARG:NH1	2:D:113:GLY:O	2.28	0.64
1:B:544:GLU:OE1	1:B:544:GLU:N	2.29	0.64
2:D:130:THR:CG2	2:D:141:LEU:HD23	2.27	0.64
1:K:10:SER:HA	2:N:46:GLU:CB	2.27	0.64
1:K:235:GLY:HA2	4:K:601:ANP:H5'1	1.79	0.64
2:L:93:LEU:HD12	2:L:95:ARG:NH2	2.13	0.64
1:A:220:PHE:HZ	1:A:430:TRP:HA	1.61	0.64
1:C:87:ILE:HB	1:C:89:ARG:HG2	1.78	0.64
2:E:18:VAL:HB	2:E:52:ALA:HB3	1.79	0.64
2:E:91:ASP:OD2	2:E:93:LEU:HB2	1.97	0.64
1:I:177:GLU:HB2	1:I:182:LEU:HD23	1.79	0.64
1:K:213:GLN:HB2	1:K:216:ILE:CD1	2.28	0.64
2:L:139:ASN:HB3	2:L:349:SER:HB2	1.80	0.64
1:B:362:LEU:HD13	1:B:405:THR:HG23	1.79	0.64
1:C:73:VAL:CG1	1:C:88:GLN:HG3	2.26	0.64
1:I:415:LEU:HD23	1:I:428:ILE:HG12	1.78	0.64
1:J:232:GLY:N	1:J:238:LYS:HD3	2.12	0.64
1:K:144:ILE:HD11	1:K:288:ARG:HB3	1.77	0.64
2:M:29:LEU:HB3	2:M:73:LEU:CD2	2.27	0.64
1:B:152:PRO:HD2	1:B:185:LEU:HD22	1.79	0.64
1:I:159:VAL:CB	1:I:176:ILE:HG12	2.27	0.64
1:J:29:LEU:N	1:J:65:ARG:O	2.30	0.64
2:M:270:ARG:HD3	2:M:271:ARG:HG2	1.80	0.64
2:N:315:ILE:HB	2:N:316:PRO:HD3	1.78	0.64
2:N:338:ILE:CB	2:N:414:ASN:HD22	2.01	0.64
1:C:577:ILE:O	1:C:581:ILE:HG13	1.98	0.64
1:J:143:LYS:N	1:J:283:GLU:OE1	2.23	0.64
2:M:132:ILE:HD12	2:M:132:ILE:H	1.62	0.64
2:D:277:LEU:HD23	2:D:318:LEU:HD12	1.80	0.64
2:F:408:PHE:CD1	2:F:412:TYR:HB3	2.33	0.64
1:J:27:MET:SD	1:J:28:CYS:N	2.71	0.64
1:B:218:THR:HB	1:B:219:PHE:HD2	1.62	0.64
2:E:198:PHE:HB3	2:E:204:ILE:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:497:ARG:C	1:I:501:LEU:HB3	2.17	0.64
1:J:189:GLN:OE1	1:J:197:ARG:NH2	2.30	0.64
2:L:18:VAL:HG12	2:L:21:VAL:HG11	1.80	0.64
2:M:406:GLU:O	2:M:410:ASN:ND2	2.25	0.64
2:E:44:VAL:HG23	2:E:53:MET:O	1.98	0.64
2:E:89:VAL:HG22	2:E:209:MET:HB2	1.79	0.64
1:J:83:MET:SD	1:J:91:LEU:HD12	2.38	0.64
1:K:42:MET:CE	2:L:65:LEU:HD11	2.27	0.64
2:N:88:ARG:NH1	2:N:101:PRO:O	2.30	0.64
1:B:13:LEU:HD21	1:B:48:SER:OG	1.97	0.64
2:F:132:ILE:HA	2:F:415:GLN:NE2	2.13	0.64
2:F:324:GLU:HA	2:F:350:ARG:HE	1.63	0.64
1:I:262:ARG:NH1	1:I:265:GLU:OE1	2.28	0.64
2:N:408:PHE:O	2:N:413:VAL:N	2.21	0.64
1:C:14:VAL:O	1:C:49:ILE:N	2.32	0.63
2:F:26:TYR:CD1	2:F:27:GLU:HG2	2.32	0.63
2:L:57:PHE:CE2	2:L:219:ILE:HD12	2.32	0.63
1:C:423:ARG:HH12	2:F:348:LEU:HB2	1.63	0.63
1:C:431:ILE:O	2:D:335:LYS:NZ	2.31	0.63
2:D:273:TYR:OH	2:D:315:ILE:HD11	1.99	0.63
2:F:258:ARG:HH21	2:F:272:GLY:HA3	1.63	0.63
1:J:8:LYS:HB2	2:M:48:GLN:CB	2.28	0.63
2:M:93:LEU:HG	2:M:95:ARG:NH2	2.13	0.63
1:B:3:ILE:HG23	1:B:64:VAL:O	1.98	0.63
1:B:300:VAL:HG22	2:E:279:THR:HG21	1.80	0.63
1:C:259:CYS:N	1:C:329:ASP:O	2.24	0.63
2:E:415:GLN:O	2:E:419:THR:OG1	2.11	0.63
2:F:340:PRO:HD3	2:F:416:GLY:H	1.63	0.63
1:I:135:ILE:HD13	1:I:148:LYS:HD3	1.81	0.63
1:I:412:PHE:HD2	1:I:433:SER:HA	1.62	0.63
1:K:177:GLU:HA	1:K:182:LEU:HA	1.80	0.63
2:M:85:MET:HG2	2:M:103:ILE:HD12	1.80	0.63
1:B:83:MET:SD	1:B:91:LEU:HD12	2.39	0.63
1:C:531:GLU:HB3	1:C:581:ILE:HD13	1.79	0.63
2:D:222:ILE:HG23	2:D:253:TYR:CE1	2.34	0.63
2:F:251:THR:HG23	2:F:304:LEU:HB2	1.79	0.63
1:K:76:GLY:H	1:K:112:LEU:HD13	1.63	0.63
1:K:500:TYR:CE2	1:K:522:LEU:HB2	2.32	0.63
2:M:152:GLY:N	2:M:155:LEU:HD12	2.12	0.63
1:C:87:ILE:HB	1:C:89:ARG:CG	2.28	0.63
1:C:569:LYS:N	1:C:570:ILE:HA	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:124:PRO:HA	2:E:290:ARG:HD3	1.81	0.63
2:F:48:GLN:N	2:F:51:LYS:O	2.31	0.63
2:F:282:ALA:O	2:F:286:GLU:N	2.30	0.63
1:I:44:GLN:N	2:M:9:LYS:O	2.25	0.63
2:L:302:PRO:HG3	2:L:323:THR:HG21	1.79	0.63
2:M:445:ILE:HB	2:M:450:LEU:HD21	1.81	0.63
2:N:159:GLU:N	2:N:159:GLU:OE2	2.30	0.63
2:N:364:ASP:CG	2:N:427:LEU:HD11	2.18	0.63
1:B:241:VAL:O	1:B:245:ILE:HG12	1.98	0.63
1:B:285:LEU:HD13	1:B:288:ARG:HD2	1.81	0.63
1:C:238:LYS:HG2	1:C:415:LEU:CD1	2.27	0.63
2:D:408:PHE:HD1	2:D:412:TYR:HB3	1.62	0.63
2:F:339:GLN:CB	2:F:341:PRO:HD3	2.28	0.63
2:L:273:TYR:HE1	2:L:315:ILE:HG12	1.62	0.63
2:M:15:LEU:HA	2:M:55:GLN:HA	1.79	0.63
2:N:128:ILE:HD11	2:N:143:ARG:HA	1.80	0.63
2:N:151:SER:O	2:N:306:MET:N	2.31	0.63
2:N:152:GLY:H	2:N:155:LEU:CD1	2.11	0.63
2:F:86:ILE:HA	2:F:208:VAL:HG22	1.80	0.63
2:F:124:PRO:HB3	2:F:143:ARG:O	1.98	0.63
1:K:235:GLY:H	4:K:601:ANP:HNB1	1.46	0.63
2:L:403:LYS:HA	2:L:403:LYS:HE3	1.79	0.63
2:M:182:ALA:HB3	2:M:247:MET:HG2	1.81	0.63
1:A:556:ILE:HG12	1:A:573:ILE:HG21	1.80	0.63
1:B:202:LYS:HG2	1:B:372:VAL:CG1	2.25	0.63
1:J:35:VAL:HB	1:J:53:GLU:CB	2.28	0.63
2:L:90:PHE:HE1	2:L:96:PRO:HB3	1.63	0.63
2:N:30:ILE:HG12	2:N:54:VAL:HB	1.80	0.63
1:C:373:ILE:HG12	1:C:381:GLU:HG2	1.80	0.63
2:D:313:HIS:ND1	2:D:314:PRO:HD2	2.13	0.63
2:E:24:VAL:HB	2:E:47:VAL:CB	2.29	0.63
2:E:91:ASP:OD2	2:E:95:ARG:NE	2.31	0.63
2:F:88:ARG:NH1	2:F:101:PRO:O	2.32	0.63
2:F:278:TYR:HB2	2:F:318:LEU:HD22	1.81	0.63
1:K:498:GLU:O	1:K:502:GLN:HB2	1.99	0.63
2:L:170:VAL:CG1	2:L:173:SER:HB3	2.28	0.63
2:M:92:GLY:O	2:M:227:MET:HG3	1.98	0.63
2:N:124:PRO:HB2	2:N:143:ARG:O	1.99	0.63
1:C:218:THR:HG21	1:C:500:TYR:CE2	2.34	0.62
2:E:150:PHE:HD2	2:E:306:MET:SD	2.21	0.62
2:F:340:PRO:HD3	2:F:416:GLY:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:ILE:HG13	1:I:64:VAL:CG2	2.28	0.62
1:J:297:ASN:OD1	1:J:297:ASN:N	2.26	0.62
2:L:159:GLU:OE1	2:L:159:GLU:N	2.31	0.62
2:N:134:ALA:O	2:N:138:LEU:HB2	1.98	0.62
2:N:346:PRO:O	2:N:348:LEU:HD12	1.99	0.62
1:B:58:ILE:O	2:E:25:LYS:HA	1.99	0.62
2:F:184:ILE:HD13	2:F:225:PRO:HG3	1.80	0.62
1:K:213:GLN:NE2	1:K:244:GLN:HB3	2.14	0.62
1:A:262:ARG:HB2	1:A:265:GLU:HB2	1.81	0.62
1:B:13:LEU:HD22	1:B:345:LEU:CD2	2.25	0.62
2:F:304:LEU:HD22	2:F:315:ILE:HG22	1.81	0.62
1:J:233:PRO:HD2	1:J:236:ALA:HB2	1.81	0.62
1:J:354:TYR:HB3	1:J:355:PRO:HD2	1.81	0.62
2:L:155:LEU:HD21	2:L:331:ARG:HA	1.81	0.62
2:N:326:GLN:NE2	2:N:346:PRO:HB3	2.15	0.62
2:N:313:HIS:ND1	2:N:315:ILE:HG12	2.14	0.62
1:A:231:PRO:CG	1:A:415:LEU:H	2.11	0.62
1:B:79:ILE:HA	1:B:112:LEU:HD22	1.82	0.62
1:B:285:LEU:HD12	1:B:285:LEU:O	1.98	0.62
1:B:352:GLU:HB3	1:B:400:PRO:HG3	1.82	0.62
1:C:235:GLY:H	4:C:601:ANP:HNB1	1.48	0.62
1:C:300:VAL:HG12	1:C:337:ALA:CB	2.28	0.62
1:J:7:ILE:HD12	1:J:8:LYS:N	2.14	0.62
2:L:152:GLY:N	2:L:155:LEU:HD12	2.13	0.62
2:L:183:ALA:HB1	2:L:186:ILE:HD13	1.82	0.62
1:B:327:MET:N	1:B:327:MET:SD	2.72	0.62
1:B:443:ARG:H	1:B:443:ARG:CZ	2.12	0.62
1:C:531:GLU:HB3	1:C:581:ILE:CD1	2.29	0.62
2:E:328:ILE:H	2:E:347:SER:HB3	1.64	0.62
1:J:12:PRO:HD3	1:J:344:ARG:NH1	2.14	0.62
2:L:8:ILE:HG23	2:L:17:ALA:O	1.98	0.62
2:L:253:TYR:OH	2:L:280:ASN:OD1	2.14	0.62
2:N:131:GLY:O	2:N:415:GLN:NE2	2.33	0.62
1:C:295:THR:N	1:C:298:MET:SD	2.72	0.62
1:C:562:ILE:HG23	1:C:563:PRO:HD2	1.81	0.62
1:C:573:ILE:O	1:C:577:ILE:HG13	1.99	0.62
2:D:326:GLN:O	2:D:347:SER:HB2	2.00	0.62
1:I:523:LYS:O	1:I:527:THR:OG1	2.17	0.62
1:J:9:VAL:HG11	1:J:58:ILE:O	1.99	0.62
2:N:315:ILE:HB	2:N:316:PRO:CD	2.29	0.62
1:A:39:ILE:HG12	1:A:49:ILE:CG2	2.22	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PHE:O	1:A:98:THR:OG1	2.16	0.62
2:E:132:ILE:HA	2:E:415:GLN:NE2	2.15	0.62
2:M:78:GLN:NE2	2:M:79:LEU:H	1.97	0.62
2:M:368:THR:O	2:M:372:LEU:HB2	1.99	0.62
1:A:244:GLN:OE1	1:A:511:THR:OG1	2.18	0.62
1:B:498:GLU:HA	1:B:502:GLN:HB2	1.80	0.62
1:C:75:LEU:HB2	1:C:189:GLN:HB3	1.80	0.62
2:D:222:ILE:HD11	2:D:257:LEU:HA	1.81	0.62
2:F:30:ILE:HG21	2:F:54:VAL:HG11	1.82	0.62
1:I:43:ARG:HB3	1:I:44:GLN:CA	2.30	0.62
1:J:39:ILE:HG12	1:J:49:ILE:HG12	1.80	0.62
1:K:397:ILE:O	1:K:403:GLN:NE2	2.32	0.62
1:C:332:SER:HB2	1:C:391:SER:H	1.64	0.62
2:E:288:ALA:HB2	2:E:300:GLN:HG3	1.80	0.62
2:F:57:PHE:O	2:F:217:PRO:HB3	1.99	0.62
2:F:183:ALA:HB1	2:F:186:ILE:HD11	1.82	0.62
1:I:218:THR:HA	1:I:453:TRP:HZ2	1.64	0.62
1:I:230:VAL:HG22	1:I:413:TRP:HB2	1.81	0.62
1:J:208:PRO:HG3	1:J:441:VAL:HG13	1.81	0.62
1:K:318:ARG:HD3	1:K:384:ILE:HG13	1.81	0.62
2:L:138:LEU:HD23	2:L:344:VAL:HB	1.80	0.62
2:M:15:LEU:CD2	2:M:55:GLN:HG3	2.29	0.62
1:B:412:PHE:CE2	1:B:433:SER:HA	2.35	0.61
2:D:144:GLY:HA2	2:D:298:VAL:O	1.99	0.61
1:J:19:MET:HE3	1:J:64:VAL:HG11	1.82	0.61
1:J:555:ARG:NH1	1:J:576:GLU:OE2	2.33	0.61
1:C:290:VAL:HG11	1:C:313:ILE:HG21	1.81	0.61
1:J:131:SER:N	1:J:134:ASP:OD2	2.32	0.61
1:K:497:ARG:HG2	1:K:501:LEU:HD12	1.81	0.61
1:K:567:LEU:N	1:K:568:ALA:HA	2.15	0.61
2:L:8:ILE:HD13	2:L:16:MET:CE	2.30	0.61
2:L:90:PHE:CE1	2:L:96:PRO:HB3	2.35	0.61
2:M:176:ASP:O	2:M:241:MET:HB2	2.01	0.61
1:A:340:GLU:OE2	2:D:279:THR:OG1	2.17	0.61
1:B:28:CYS:HB2	1:B:66:SER:HA	1.83	0.61
1:C:367:GLU:HG2	2:D:215:ASN:HD22	1.65	0.61
2:D:151:SER:O	2:D:305:THR:HA	2.00	0.61
2:E:338:ILE:CG2	2:E:414:ASN:HB3	2.30	0.61
1:J:81:SER:OG	1:J:287:GLU:HA	2.00	0.61
1:K:232:GLY:O	1:K:238:LYS:HD3	2.00	0.61
2:M:143:ARG:NH2	2:M:172:ASP:OD2	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:225:PRO:O	2:F:229:LEU:HG	2.01	0.61
1:J:258:GLY:HA3	1:J:266:MET:SD	2.41	0.61
1:K:8:LYS:HD3	1:K:10:SER:OG	1.99	0.61
1:K:213:GLN:CA	1:K:216:ILE:HD11	2.30	0.61
1:K:494:LYS:O	1:K:498:GLU:HG2	2.00	0.61
1:A:262:ARG:HH12	2:D:350:ARG:CZ	2.13	0.61
2:E:128:ILE:O	2:E:129:GLN:HG3	1.99	0.61
1:I:262:ARG:H	1:I:262:ARG:HD2	1.66	0.61
1:I:439:THR:O	1:I:443:ARG:NH1	2.33	0.61
1:K:214:ARG:NH1	1:K:521:MET:HE1	2.15	0.61
2:E:126:GLU:O	2:E:143:ARG:N	2.31	0.61
2:F:139:ASN:OD1	2:F:348:LEU:HA	2.01	0.61
2:F:151:SER:HA	2:F:329:LEU:HD12	1.83	0.61
2:F:318:LEU:O	2:F:322:ILE:HG13	2.01	0.61
2:F:325:GLY:H	2:F:350:ARG:NE	1.99	0.61
1:I:232:GLY:HA2	1:I:415:LEU:HB2	1.82	0.61
1:J:150:MET:HE2	1:J:320:MET:HA	1.81	0.61
1:J:273:PHE:HB3	1:J:286:MET:HB2	1.81	0.61
2:M:78:GLN:HA	2:M:78:GLN:HE21	1.66	0.61
1:A:85:ASP:OD2	1:A:89:ARG:N	2.32	0.61
4:B:601:ANP:HNB1	2:E:350:ARG:NH2	1.99	0.61
1:C:297:ASN:OD1	1:C:297:ASN:N	2.24	0.61
2:F:26:TYR:CE1	2:F:45:LEU:HA	2.36	0.61
1:K:348:MET:HG3	2:L:265:ARG:HA	1.82	0.61
2:L:231:ALA:O	2:L:235:LEU:HG	2.00	0.61
2:M:21:VAL:HG12	2:M:50:ASP:O	2.01	0.61
2:N:126:GLU:CB	2:N:143:ARG:HG3	2.29	0.61
1:A:86:GLY:HA3	1:A:302:ALA:O	2.00	0.61
1:B:273:PHE:HB2	1:B:274:PRO:HD3	1.83	0.61
2:E:28:GLU:O	2:E:44:VAL:HG12	2.01	0.61
2:F:86:ILE:HG22	2:F:208:VAL:CG2	2.31	0.61
1:J:9:VAL:HA	1:J:14:VAL:HG13	1.83	0.61
1:J:257:VAL:HG22	1:J:292:ILE:HB	1.82	0.61
1:A:262:ARG:O	1:A:266:MET:N	2.29	0.61
1:B:355:PRO:HG2	1:B:358:LEU:HB2	1.83	0.61
1:C:51:VAL:HG21	1:C:55:THR:HG23	1.83	0.61
2:D:21:VAL:HG21	2:D:52:ALA:HB2	1.83	0.61
2:E:34:MET:SD	2:E:63:ILE:HG12	2.41	0.61
1:J:36:ILE:N	1:J:53:GLU:OE1	2.27	0.61
2:L:29:LEU:HD11	2:L:77:LEU:HD23	1.83	0.61
2:D:92:GLY:HA3	2:D:224:THR:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:ASN:HB3	2:D:349:SER:HB2	1.82	0.61
1:I:483:SER:OG	1:I:486:ASP:OD1	2.19	0.61
1:I:501:LEU:HD12	1:I:502:GLN:HG2	1.83	0.61
1:J:496:ILE:HA	1:J:525:ILE:HD13	1.81	0.61
1:K:55:THR:CG2	1:K:58:ILE:HD12	2.25	0.61
1:K:238:LYS:HG2	1:K:415:LEU:HD12	1.82	0.61
2:L:396:ASP:O	2:L:399:LYS:HE2	2.01	0.61
2:M:357:GLY:HA2	2:M:363:GLU:HA	1.83	0.61
2:N:415:GLN:CD	2:N:421:ARG:HD2	2.22	0.61
1:A:80:ILE:H	1:A:80:ILE:HD12	1.65	0.60
1:A:304:GLU:O	1:A:334:TRP:NE1	2.32	0.60
1:J:73:VAL:HG13	1:J:193:VAL:HG11	1.82	0.60
1:J:234:PHE:HZ	2:M:311:LYS:HD3	1.66	0.60
1:K:53:GLU:HG2	1:K:106:GLY:H	1.65	0.60
2:N:188:PHE:O	2:N:192:GLU:N	2.34	0.60
1:A:218:THR:HG23	1:A:453:TRP:CZ2	2.36	0.60
1:A:231:PRO:HG2	1:A:415:LEU:N	2.14	0.60
1:B:262:ARG:NH2	2:E:321:TYR:O	2.35	0.60
1:C:114:HIS:O	1:C:168:THR:OG1	2.18	0.60
2:D:18:VAL:O	2:D:52:ALA:N	2.32	0.60
2:D:125:ASP:OD1	2:D:126:GLU:N	2.33	0.60
1:K:257:VAL:HG21	1:K:310:GLY:HA3	1.82	0.60
2:L:79:LEU:HD13	2:L:227:MET:HE3	1.83	0.60
2:M:149:VAL:HB	2:M:303:ILE:HG12	1.82	0.60
1:C:101:ASN:O	2:F:117:ASN:HB2	2.01	0.60
2:D:148:PRO:HG3	2:D:323:THR:CB	2.30	0.60
2:D:356:THR:HA	2:D:361:THR:OG1	2.01	0.60
1:J:562:ILE:HD12	1:J:570:ILE:HG12	1.83	0.60
1:K:42:MET:HG2	1:K:47:ALA:HB2	1.83	0.60
2:L:18:VAL:HG12	2:L:21:VAL:CG1	2.31	0.60
2:N:226:ARG:NH2	2:N:253:TYR:OH	2.34	0.60
1:B:27:MET:HE1	1:B:38:GLU:CG	2.26	0.60
1:C:255:VAL:N	1:C:325:ALA:O	2.27	0.60
1:C:529:GLY:O	1:C:533:ARG:HB2	2.02	0.60
2:E:73:LEU:HD13	2:E:75:HIS:CE1	2.37	0.60
2:E:376:TYR:OH	2:E:409:GLU:OE2	2.18	0.60
1:I:244:GLN:OE1	1:I:511:THR:OG1	2.19	0.60
1:J:215:VAL:HG11	1:J:426:PRO:HG2	1.83	0.60
2:L:6:ARG:HD2	2:L:70:VAL:HB	1.83	0.60
2:M:343:ASP:O	2:M:347:SER:OG	2.19	0.60
1:C:41:GLU:HB2	2:D:12:VAL:HA	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:LYS:HB3	2:D:188:PHE:CZ	2.36	0.60
1:C:269:VAL:O	1:C:273:PHE:HB2	2.01	0.60
2:L:9:LYS:HG3	2:L:19:GLU:HG3	1.83	0.60
2:N:177:PHE:HA	2:N:242:HIS:HB2	1.82	0.60
1:C:135:ILE:HD11	1:C:150:MET:CA	2.26	0.60
2:E:89:VAL:CG1	2:E:211:MET:HG2	2.31	0.60
1:J:85:ASP:OD1	1:J:89:ARG:N	2.30	0.60
1:J:425:PHE:HA	1:J:426:PRO:C	2.22	0.60
4:J:601:ANP:O2G	2:M:321:TYR:O	2.20	0.60
1:K:29:LEU:HD13	1:K:65:ARG:HH21	1.66	0.60
2:L:32:VAL:CG2	2:L:70:VAL:HG22	2.27	0.60
2:L:45:LEU:HD21	2:L:55:GLN:HB2	1.84	0.60
1:A:20:SER:HA	1:A:42:MET:HE1	1.83	0.60
1:A:245:ILE:O	1:A:249:SER:OG	2.19	0.60
1:B:371:ARG:NH1	1:B:381:GLU:OE2	2.35	0.60
2:D:159:GLU:OE1	2:D:159:GLU:N	2.33	0.60
2:F:21:VAL:HG21	2:F:52:ALA:HB2	1.83	0.60
2:F:408:PHE:HD1	2:F:412:TYR:HB3	1.66	0.60
1:J:240:VAL:HG23	4:J:601:ANP:O2A	2.02	0.60
1:C:39:ILE:HG12	1:C:49:ILE:CG1	2.32	0.60
1:C:235:GLY:HA2	4:C:601:ANP:H5'1	1.82	0.60
2:F:177:PHE:HD1	2:F:178:ALA:N	2.00	0.60
1:J:36:ILE:HG22	1:J:52:TYR:CD1	2.37	0.60
1:C:241:VAL:O	1:C:245:ILE:HG12	2.02	0.60
2:E:134:ALA:HA	2:E:412:TYR:CE2	2.37	0.60
2:E:250:MET:HB2	2:E:304:LEU:HB3	1.84	0.60
2:F:217:PRO:HB2	2:F:220:GLU:HB2	1.82	0.60
2:F:328:ILE:O	2:F:342:ILE:HG23	2.01	0.60
1:J:39:ILE:HG12	1:J:49:ILE:HG23	1.84	0.60
1:K:262:ARG:NH2	2:N:350:ARG:HH12	1.99	0.60
2:M:89:VAL:HG22	2:M:209:MET:HB2	1.83	0.60
1:A:25:GLN:HG3	2:E:61:SER:HA	1.84	0.60
1:B:500:TYR:OH	1:B:518:GLN:HA	2.01	0.60
1:C:120:PHE:CD1	1:C:173:ILE:HD11	2.37	0.60
1:C:251:VAL:HG12	1:C:323:ASP:HB3	1.83	0.60
1:I:301:ALA:O	1:I:305:ALA:N	2.35	0.60
1:J:31:GLY:HA2	1:J:62:GLU:HB3	1.84	0.60
1:J:237:GLY:HA3	4:J:601:ANP:H8	1.84	0.60
1:J:424:HIS:NE2	1:J:502:GLN:HG2	2.17	0.60
2:N:8:ILE:HD11	2:N:65:LEU:CA	2.31	0.60
2:D:65:LEU:HD12	2:D:66:LYS:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:57:PHE:HE2	2:L:219:ILE:HD12	1.66	0.59
2:M:224:THR:HB	2:M:225:PRO:HD3	1.84	0.59
2:D:89:VAL:HG22	2:D:209:MET:HB2	1.83	0.59
2:E:90:PHE:HA	2:E:96:PRO:HA	1.84	0.59
1:I:6:ILE:HA	1:I:16:ALA:HA	1.84	0.59
1:K:18:ASN:HD21	1:K:20:SER:HB2	1.67	0.59
1:K:238:LYS:HG2	1:K:415:LEU:CD1	2.32	0.59
1:A:39:ILE:CG1	1:A:49:ILE:HG23	2.25	0.59
1:B:521:MET:CE	1:B:560:LYS:HB3	2.31	0.59
1:C:84:PHE:HB2	1:C:292:ILE:HG13	1.85	0.59
2:D:88:ARG:NE	2:D:98:ASP:OD2	2.32	0.59
2:E:29:LEU:HB2	2:E:73:LEU:HD11	1.83	0.59
1:I:351:ASP:OD1	2:M:258:ARG:NH1	2.30	0.59
1:B:550:VAL:HG12	1:B:553:ARG:NH2	2.18	0.59
1:C:132:ALA:O	1:C:375:LEU:HB3	2.02	0.59
2:D:137:HIS:HA	2:D:365:HIS:NE2	2.17	0.59
2:E:345:LEU:HB2	2:E:346:PRO:HD3	1.83	0.59
1:K:459:GLU:OE2	1:K:462:ARG:NH1	2.36	0.59
2:M:40:ARG:HG2	2:M:56:ILE:HG21	1.84	0.59
2:M:270:ARG:HD3	2:M:271:ARG:CG	2.32	0.59
1:C:83:MET:HE3	1:C:91:LEU:HD12	1.83	0.59
2:D:176:ASP:HB3	2:D:206:ARG:HD2	1.85	0.59
1:I:20:SER:CB	1:I:45:ASP:HB2	2.18	0.59
1:J:532:ALA:O	1:J:536:LEU:N	2.35	0.59
2:M:226:ARG:HA	2:M:229:LEU:HD12	1.83	0.59
2:N:10:GLU:HA	2:N:65:LEU:HD13	1.84	0.59
1:B:497:ARG:HA	1:B:501:LEU:CB	2.19	0.59
2:F:29:LEU:HD23	2:F:73:LEU:HD23	1.84	0.59
2:M:223:ALA:O	2:M:227:MET:HG2	2.02	0.59
1:B:12:PRO:HB2	1:B:344:ARG:CB	2.33	0.59
1:B:240:VAL:HG23	4:B:601:ANP:O2A	2.02	0.59
1:B:565:GLU:OE1	1:B:565:GLU:N	2.27	0.59
4:B:601:ANP:H5'2	2:E:350:ARG:HD3	1.84	0.59
2:D:282:ALA:O	2:D:286:GLU:HG2	2.02	0.59
2:D:315:ILE:HB	2:D:316:PRO:HD3	1.85	0.59
2:E:339:GLN:O	2:E:414:ASN:HB2	2.02	0.59
2:F:89:VAL:HG22	2:F:209:MET:HB2	1.84	0.59
2:F:339:GLN:HA	2:F:341:PRO:CD	2.33	0.59
1:I:87:ILE:N	1:I:88:GLN:HA	2.17	0.59
1:I:255:VAL:N	1:I:325:ALA:O	2.31	0.59
1:I:424:HIS:O	1:I:425:PHE:HD1	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:497:ARG:O	1:I:501:LEU:N	2.36	0.59
1:J:318:ARG:HB2	1:J:384:ILE:HD11	1.84	0.59
1:K:75:LEU:O	1:K:188:MET:HA	2.02	0.59
1:K:244:GLN:NE2	1:K:511:THR:OG1	2.31	0.59
2:N:57:PHE:HD1	2:N:219:ILE:HB	1.67	0.59
2:N:98:ASP:OD1	2:N:100:GLY:N	2.35	0.59
2:N:341:PRO:HD2	2:N:417:PHE:CZ	2.37	0.59
1:J:8:LYS:HD3	2:M:48:GLN:CB	2.33	0.59
1:K:24:ILE:CD1	1:K:41:GLU:HA	2.19	0.59
1:K:230:VAL:HG23	1:K:389:ALA:HA	1.84	0.59
1:K:230:VAL:CG1	1:K:413:TRP:HE3	2.15	0.59
1:K:424:HIS:CD2	1:K:502:GLN:HG2	2.38	0.59
2:N:89:VAL:HG22	2:N:209:MET:HB2	1.84	0.59
1:A:39:ILE:HD13	1:A:49:ILE:HG12	1.85	0.59
1:A:117:GLN:HG2	1:A:168:THR:HG22	1.85	0.59
1:B:354:TYR:HB3	1:B:355:PRO:HD2	1.85	0.59
1:C:83:MET:HG3	2:F:119:ILE:CD1	2.27	0.59
1:C:393:SER:H	1:C:399:GLU:HG3	1.67	0.59
2:E:29:LEU:CB	2:E:73:LEU:HD11	2.33	0.59
2:E:357:GLY:N	2:E:358:ALA:HA	2.17	0.59
1:I:7:ILE:HB	2:L:49:GLU:CG	2.31	0.59
1:I:175:VAL:HG12	1:I:182:LEU:HD22	1.85	0.59
1:A:231:PRO:HD3	1:A:413:TRP:O	2.03	0.59
1:B:562:ILE:HD12	1:B:570:ILE:HG12	1.85	0.59
2:F:325:GLY:O	2:F:349:SER:HA	2.02	0.59
1:J:8:LYS:HG2	1:J:10:SER:H	1.67	0.59
2:L:87:GLY:HA2	2:L:204:ILE:O	2.03	0.59
2:L:350:ARG:N	2:L:352:LYS:HZ1	2.00	0.59
2:L:423:ILE:O	2:L:427:LEU:HG	2.03	0.59
2:N:183:ALA:HB3	2:N:211:MET:HA	1.85	0.59
1:C:1:MET:HG2	1:C:2:GLN:H	1.66	0.58
2:F:213:LEU:N	2:F:216:ASP:OD2	2.36	0.58
2:L:90:PHE:O	2:L:210:PHE:HA	2.03	0.58
2:L:244:LEU:HD12	2:L:299:THR:HB	1.84	0.58
1:A:357:TYR:HB3	2:E:259:GLU:HG3	1.85	0.58
1:B:285:LEU:HD11	1:B:288:ARG:HD2	1.84	0.58
1:C:124:ILE:CG2	1:C:136:ILE:HB	2.33	0.58
2:D:48:GLN:HB2	2:D:51:LYS:HG2	1.85	0.58
2:D:315:ILE:HB	2:D:316:PRO:CD	2.32	0.58
2:F:97:LYS:HE2	2:F:211:MET:HB2	1.85	0.58
2:F:285:PHE:CE2	2:F:319:THR:HG23	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:340:PRO:HA	2:F:417:PHE:CE1	2.37	0.58
1:J:27:MET:CE	1:J:36:ILE:HG23	2.33	0.58
1:J:238:LYS:HE3	4:J:601:ANP:O2B	2.03	0.58
1:K:42:MET:HE2	2:L:65:LEU:HD11	1.83	0.58
1:A:42:MET:SD	1:A:47:ALA:HB2	2.42	0.58
2:L:325:GLY:CA	2:L:349:SER:HA	2.33	0.58
2:M:183:ALA:HB3	2:M:211:MET:HA	1.85	0.58
2:N:153:SER:O	2:N:331:ARG:NH2	2.35	0.58
1:A:440:GLU:HA	1:A:443:ARG:NH1	2.19	0.58
1:B:15:MET:HA	1:B:47:ALA:O	2.04	0.58
1:B:495:SER:O	1:B:499:ASP:HB2	2.04	0.58
1:B:497:ARG:HA	1:B:501:LEU:HD13	1.85	0.58
1:I:9:VAL:HB	2:L:47:VAL:HG22	1.86	0.58
1:J:27:MET:HE1	1:J:36:ILE:HG23	1.85	0.58
1:K:41:GLU:CG	2:L:12:VAL:HG13	2.22	0.58
2:N:137:HIS:HA	2:N:365:HIS:CD2	2.38	0.58
1:C:251:VAL:HG21	1:C:325:ALA:CB	2.32	0.58
2:E:82:SER:O	2:E:85:MET:HB2	2.04	0.58
1:I:20:SER:HA	1:I:42:MET:CE	2.34	0.58
1:J:9:VAL:HG11	1:J:58:ILE:C	2.24	0.58
2:L:8:ILE:HD13	2:L:16:MET:HE1	1.85	0.58
2:L:124:PRO:HB3	2:L:143:ARG:O	2.03	0.58
1:B:169:ILE:O	1:B:186:THR:HB	2.03	0.58
1:B:441:VAL:N	1:B:443:ARG:HH22	2.01	0.58
2:F:34:MET:SD	2:F:63:ILE:HG12	2.43	0.58
2:F:124:PRO:HB2	2:F:142:VAL:HG12	1.83	0.58
1:K:264:ASN:ND2	2:N:324:GLU:OE1	2.36	0.58
1:K:278:ASP:HB3	1:K:281:THR:HG21	1.84	0.58
2:M:166:ARG:HD2	2:M:201:THR:HG21	1.86	0.58
2:N:44:VAL:HG13	2:N:53:MET:O	2.04	0.58
1:A:545:ILE:O	1:A:549:THR:OG1	2.18	0.58
2:D:60:THR:HA	2:D:63:ILE:HD13	1.85	0.58
2:D:86:ILE:HD13	2:D:208:VAL:HG23	1.85	0.58
2:D:111:ILE:HG21	2:D:227:MET:HG2	1.84	0.58
2:D:140:THR:HB	2:D:352:LYS:CA	2.33	0.58
1:I:84:PHE:HB3	1:I:88:GLN:CB	2.33	0.58
1:J:261:GLU:HB3	1:J:265:GLU:OE1	2.03	0.58
1:K:214:ARG:NH2	1:K:510:ASP:OD1	2.36	0.58
1:K:222:VAL:HG22	1:K:413:TRP:CZ2	2.39	0.58
2:L:126:GLU:HB2	2:L:143:ARG:HD2	1.84	0.58
2:L:345:LEU:HB2	2:L:346:PRO:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:45:LEU:HD13	2:N:45:LEU:H	1.67	0.58
1:A:297:ASN:HB2	2:D:286:GLU:CG	2.32	0.58
1:C:576:GLU:O	1:C:580:THR:OG1	2.20	0.58
2:F:160:LEU:HD22	2:F:342:ILE:HD11	1.85	0.58
1:J:6:ILE:CD1	1:J:62:GLU:HB2	2.34	0.58
1:K:49:ILE:HD11	1:K:64:VAL:HG11	1.86	0.58
1:K:499:ASP:OD2	1:K:557:SER:HA	2.02	0.58
2:M:324:GLU:CB	2:M:350:ARG:HD2	2.34	0.58
2:N:313:HIS:CG	2:N:314:PRO:HD2	2.39	0.58
1:A:311:ILE:O	1:A:315:GLU:HG3	2.04	0.58
1:A:393:SER:HB2	2:D:321:TYR:HE1	1.69	0.58
1:C:546:MET:O	1:C:549:THR:OG1	2.22	0.58
2:D:153:SER:O	2:D:331:ARG:NH2	2.30	0.58
2:D:156:PRO:HG3	2:D:334:TYR:CE1	2.39	0.58
2:E:93:LEU:HD12	2:E:95:ARG:HH22	1.67	0.58
2:F:15:LEU:HD12	2:F:55:GLN:HG3	1.84	0.58
1:I:225:GLY:HA2	1:I:384:ILE:O	2.03	0.58
1:K:145:ILE:HD11	1:K:252:ASP:O	2.04	0.58
2:L:146:LYS:HD3	2:L:285:PHE:O	2.04	0.58
2:N:264:ARG:HG2	2:N:266:GLU:CG	2.34	0.58
2:E:409:GLU:O	2:E:413:VAL:HB	2.04	0.58
1:J:128:THR:H	1:J:159:VAL:CB	2.17	0.58
1:K:49:ILE:CD1	1:K:64:VAL:HG11	2.34	0.58
2:L:198:PHE:HB3	2:L:204:ILE:HB	1.85	0.58
2:L:278:TYR:CE1	2:L:322:ILE:HG12	2.29	0.58
2:N:183:ALA:HB3	2:N:212:ASN:H	1.69	0.58
1:B:209:MET:HB2	1:B:224:LYS:HD3	1.86	0.57
2:D:254:ALA:HB1	2:D:273:TYR:CE1	2.38	0.57
1:I:43:ARG:HB2	1:I:46:VAL:O	2.04	0.57
1:J:415:LEU:HD23	1:J:415:LEU:N	2.18	0.57
1:K:76:GLY:N	1:K:112:LEU:HD13	2.18	0.57
2:L:8:ILE:HD11	2:L:70:VAL:HG23	1.86	0.57
2:M:8:ILE:CB	2:M:65:LEU:HB3	2.34	0.57
2:M:255:GLU:O	2:M:258:ARG:HG2	2.03	0.57
1:C:29:LEU:N	1:C:65:ARG:O	2.37	0.57
2:D:78:GLN:HG2	2:D:110:ASP:HA	1.85	0.57
2:F:408:PHE:O	2:F:413:VAL:N	2.19	0.57
1:I:330:SER:HB3	1:I:333:ARG:HG2	1.84	0.57
1:J:38:GLU:OE1	1:J:194:ARG:NH2	2.31	0.57
2:L:91:ASP:OD2	2:L:93:LEU:HB2	2.03	0.57
1:B:374:ALA:HB3	1:B:380:ARG:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:422:THR:O	2:F:426:THR:OG1	2.20	0.57
1:J:197:ARG:HG3	1:J:315:GLU:HB3	1.85	0.57
1:J:220:PHE:HB3	1:J:413:TRP:HE1	1.67	0.57
1:K:14:VAL:HB	1:K:49:ILE:HB	1.85	0.57
1:K:157:GLY:HA3	1:K:177:GLU:O	2.04	0.57
2:M:386:ALA:O	2:M:390:GLY:N	2.37	0.57
1:B:2:GLN:NE2	1:B:18:ASN:O	2.37	0.57
2:D:31:GLU:O	2:D:71:ARG:N	2.37	0.57
2:E:24:VAL:HG22	2:E:72:PHE:CE1	2.33	0.57
1:I:248:TRP:CZ3	1:I:279:PRO:HG2	2.39	0.57
1:I:420:ALA:HA	1:I:425:PHE:HE1	1.70	0.57
1:J:340:GLU:OE2	1:J:344:ARG:NE	2.35	0.57
2:L:148:PRO:CA	2:L:302:PRO:HG2	2.32	0.57
1:B:218:THR:HB	1:B:219:PHE:CD2	2.39	0.57
2:E:137:HIS:ND1	2:E:412:TYR:OH	2.37	0.57
1:K:42:MET:CG	1:K:47:ALA:HB2	2.34	0.57
1:K:139:VAL:O	1:K:147:HIS:HB3	2.05	0.57
2:L:229:LEU:HD13	2:L:287:ARG:HD3	1.86	0.57
2:M:29:LEU:HB2	2:M:75:HIS:O	2.04	0.57
2:N:148:PRO:HB2	2:N:150:PHE:HE1	1.68	0.57
2:N:242:HIS:ND1	2:N:296:GLY:HA2	2.20	0.57
1:B:42:MET:HG2	2:F:65:LEU:HD21	1.85	0.57
1:C:378:ASP:HB2	1:C:380:ARG:HH21	1.70	0.57
1:J:301:ALA:HB2	1:J:341:MET:CE	2.35	0.57
2:L:6:ARG:HD3	2:L:70:VAL:CB	2.34	0.57
2:L:143:ARG:HD3	2:L:290:ARG:HH11	1.69	0.57
1:A:256:TYR:CE2	1:A:269:VAL:HG11	2.39	0.57
1:B:258:GLY:N	1:B:292:ILE:O	2.33	0.57
1:B:563:PRO:HB2	1:B:566:GLU:HG3	1.86	0.57
1:C:485:ASN:O	1:C:533:ARG:NH1	2.31	0.57
2:E:166:ARG:HH22	2:E:418:TYR:HA	1.70	0.57
2:E:185:GLY:O	2:E:252:ASN:ND2	2.38	0.57
2:E:339:GLN:HB3	2:E:417:PHE:CZ	2.40	0.57
2:E:372:LEU:CD2	2:E:412:TYR:HE1	2.12	0.57
1:I:493:ALA:O	1:I:497:ARG:HG3	2.04	0.57
1:J:260:GLY:HA3	1:J:333:ARG:HG3	1.87	0.57
1:K:79:ILE:HA	1:K:112:LEU:HD21	1.86	0.57
1:K:492:VAL:O	1:K:496:ILE:HG13	2.05	0.57
2:N:35:GLN:NE2	2:N:64:CYS:SG	2.78	0.57
1:C:257:VAL:HG21	1:C:310:GLY:HA3	1.85	0.57
2:D:18:VAL:HB	2:D:52:ALA:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:218:ALA:O	2:E:222:ILE:HG12	2.05	0.57
1:A:120:PHE:CE2	1:A:173:ILE:HD12	2.39	0.57
1:A:232:GLY:N	1:A:233:PRO:HD3	2.20	0.57
1:A:497:ARG:HA	1:A:501:LEU:HD12	1.86	0.57
1:C:234:PHE:HD1	1:C:234:PHE:H	1.50	0.57
2:E:57:PHE:HA	2:E:219:ILE:HD13	1.86	0.57
1:J:281:THR:HG23	1:J:283:GLU:H	1.68	0.57
2:L:141:LEU:HD13	2:L:147:LEU:HD22	1.86	0.57
1:B:254:VAL:HG13	1:B:327:MET:SD	2.45	0.57
1:C:168:THR:HG22	1:C:171:ASP:CG	2.26	0.57
1:J:262:ARG:HH21	2:M:350:ARG:NH1	2.03	0.57
1:J:392:PRO:HA	1:J:399:GLU:HG3	1.85	0.57
1:K:206:ASP:HB2	1:K:440:GLU:OE2	2.05	0.57
1:K:501:LEU:N	1:K:501:LEU:HD23	2.20	0.57
2:N:110:ASP:OD2	2:N:112:ASN:ND2	2.35	0.57
2:N:378:GLN:O	2:N:378:GLN:NE2	2.29	0.57
1:B:216:ILE:HD12	1:B:245:ILE:CD1	2.35	0.56
2:D:164:ILE:O	2:D:168:ALA:N	2.38	0.56
2:D:166:ARG:NH1	2:D:197:ASP:OD2	2.33	0.56
2:F:273:TYR:CD2	2:F:314:PRO:HG2	2.40	0.56
2:F:325:GLY:HA3	2:F:326:GLN:CG	2.28	0.56
1:I:209:MET:SD	1:I:385:THR:HG21	2.44	0.56
1:J:30:VAL:O	1:J:35:VAL:HG22	2.05	0.56
1:J:196:GLY:HA2	1:J:368:ARG:NH1	2.20	0.56
1:J:254:VAL:HB	1:J:289:THR:HG23	1.86	0.56
1:K:238:LYS:HG3	4:K:601:ANP:O2B	2.05	0.56
1:K:422:LYS:O	1:K:423:ARG:HB2	2.05	0.56
1:A:220:PHE:CZ	1:A:430:TRP:HA	2.40	0.56
1:C:262:ARG:NH1	4:C:601:ANP:O3G	2.29	0.56
2:D:29:LEU:HB2	2:D:73:LEU:CD1	2.29	0.56
2:D:177:PHE:O	2:D:206:ARG:NE	2.38	0.56
2:E:438:PRO:HG2	2:E:441:GLU:HB2	1.86	0.56
2:F:250:MET:HB2	2:F:304:LEU:HB3	1.85	0.56
4:J:601:ANP:HNB1	2:M:350:ARG:NH2	2.04	0.56
1:K:259:CYS:O	1:K:330:SER:N	2.32	0.56
2:N:132:ILE:HA	2:N:415:GLN:OE1	2.04	0.56
1:A:10:SER:CB	2:D:46:GLU:HG3	2.34	0.56
1:A:39:ILE:HG21	1:A:47:ALA:HB1	1.87	0.56
1:A:73:VAL:HG13	1:A:193:VAL:CG1	2.31	0.56
1:B:28:CYS:SG	1:B:49:ILE:HD13	2.45	0.56
1:B:356:ALA:HB1	2:F:258:ARG:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ASN:N	1:B:510:ASP:OD2	2.31	0.56
1:C:300:VAL:HG13	1:C:303:ARG:CD	2.35	0.56
2:D:270:ARG:HG2	2:D:271:ARG:HG2	1.87	0.56
2:D:326:GLN:C	2:D:347:SER:HB2	2.24	0.56
2:E:226:ARG:O	2:E:230:THR:OG1	2.23	0.56
2:E:443:LYS:NZ	2:E:443:LYS:HB2	2.20	0.56
2:F:138:LEU:HD13	2:F:344:VAL:HB	1.87	0.56
1:J:259:CYS:HA	1:J:294:ASN:CB	2.35	0.56
1:K:59:GLY:O	1:K:62:GLU:HB2	2.05	0.56
1:K:262:ARG:HH12	4:K:601:ANP:PG	2.27	0.56
1:K:500:TYR:HB3	1:K:501:LEU:HD23	1.85	0.56
2:L:6:ARG:CD	2:L:70:VAL:H	2.18	0.56
2:L:371:GLN:OE1	2:L:444:ARG:N	2.38	0.56
2:M:141:LEU:HD13	2:M:147:LEU:HB2	1.87	0.56
2:M:183:ALA:HB1	2:M:186:ILE:CD1	2.35	0.56
2:M:309:ASP:OD1	2:M:331:ARG:NH1	2.38	0.56
2:N:30:ILE:HG21	2:N:54:VAL:HG11	1.86	0.56
1:I:410:LYS:HB3	1:I:436:LEU:HB2	1.87	0.56
1:J:28:CYS:CB	1:J:66:SER:HA	2.35	0.56
1:J:114:HIS:ND1	1:J:170:ASP:OD1	2.38	0.56
1:J:333:ARG:HD2	2:M:278:TYR:CE1	2.41	0.56
1:K:120:PHE:CE2	1:K:137:GLY:HA3	2.40	0.56
1:K:213:GLN:H	1:K:216:ILE:CD1	2.18	0.56
1:K:260:GLY:HA3	1:K:333:ARG:CG	2.33	0.56
2:M:15:LEU:HD22	2:M:55:GLN:CB	2.31	0.56
1:A:113:ASP:OD1	1:A:116:LYS:N	2.38	0.56
1:B:425:PHE:HB3	1:B:426:PRO:HA	1.88	0.56
2:D:77:LEU:HB3	2:D:111:ILE:HD13	1.86	0.56
2:D:156:PRO:HD3	2:D:334:TYR:CD2	2.41	0.56
2:E:90:PHE:CD1	2:E:96:PRO:HG3	2.40	0.56
1:J:16:ALA:C	1:J:46:VAL:HG13	2.25	0.56
1:J:428:ILE:H	1:J:428:ILE:HD12	1.70	0.56
2:N:378:GLN:HA	2:N:381:GLN:HE22	1.70	0.56
1:C:203:LEU:HD21	1:C:373:ILE:HG13	1.87	0.56
1:C:259:CYS:SG	1:C:306:SER:OG	2.64	0.56
2:D:78:GLN:NE2	2:D:110:ASP:OD1	2.35	0.56
1:I:43:ARG:HA	1:I:43:ARG:NE	2.21	0.56
1:I:261:GLU:HB3	1:I:266:MET:HG2	1.87	0.56
1:J:378:ASP:N	1:J:378:ASP:OD1	2.39	0.56
1:K:499:ASP:N	1:K:499:ASP:OD1	2.38	0.56
2:L:166:ARG:HD2	2:L:201:THR:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:315:ILE:HB	2:M:316:PRO:HD3	1.88	0.56
1:A:114:HIS:O	1:A:168:THR:HB	2.06	0.56
1:B:221:PRO:HG2	1:B:441:VAL:HG21	1.87	0.56
1:B:437:TYR:O	1:B:441:VAL:HG23	2.05	0.56
1:C:324:VAL:O	1:C:384:ILE:HA	2.05	0.56
2:E:4:GLU:HA	2:E:71:ARG:HA	1.86	0.56
2:F:315:ILE:HB	2:F:316:PRO:HD3	1.87	0.56
1:I:23:CYS:SG	2:M:64:CYS:HB2	2.45	0.56
1:K:218:THR:HG21	1:K:500:TYR:CE1	2.41	0.56
2:L:184:ILE:HA	2:L:212:ASN:HB2	1.86	0.56
2:M:158:LYS:CD	2:M:158:LYS:H	2.17	0.56
2:N:35:GLN:HB3	2:N:67:ASN:HB2	1.88	0.56
2:N:144:GLY:HA2	2:N:298:VAL:O	2.05	0.56
2:N:213:LEU:HB2	2:N:216:ASP:OD1	2.04	0.56
1:B:28:CYS:HB3	1:B:66:SER:HA	1.87	0.56
1:C:199:ILE:HG21	1:C:372:VAL:HG21	1.86	0.56
1:I:204:ASN:ND2	2:M:192:GLU:HG3	2.19	0.56
1:J:12:PRO:HG3	1:J:344:ARG:CD	2.35	0.56
1:J:503:GLN:NE2	1:J:510:ASP:O	2.38	0.56
1:B:214:ARG:HD2	1:B:500:TYR:CE2	2.41	0.56
1:B:220:PHE:HZ	1:B:430:TRP:HA	1.70	0.56
1:C:230:VAL:HG22	1:C:413:TRP:HE3	1.70	0.56
1:K:16:ALA:O	1:K:46:VAL:HG13	2.06	0.56
2:M:446:LYS:O	2:M:450:LEU:HG	2.06	0.56
1:A:215:VAL:HA	1:A:219:PHE:CD2	2.40	0.56
1:B:378:ASP:N	1:B:378:ASP:OD1	2.38	0.56
2:F:158:LYS:HG2	2:F:190:GLU:HB3	1.88	0.56
1:I:412:PHE:CD2	1:I:433:SER:HA	2.41	0.56
1:J:374:ALA:N	1:J:380:ARG:O	2.35	0.56
1:K:319:ASP:O	1:K:380:ARG:NH1	2.38	0.56
2:L:16:MET:N	2:L:54:VAL:O	2.36	0.56
2:M:24:VAL:HG22	2:M:72:PHE:CE2	2.41	0.56
1:A:462:ARG:O	1:A:466:GLU:HB2	2.07	0.55
1:C:244:GLN:OE1	1:C:511:THR:OG1	2.24	0.55
2:D:58:GLU:OE1	2:D:58:GLU:N	2.34	0.55
2:E:149:VAL:HA	2:E:327:ILE:HB	1.88	0.55
2:F:171:LEU:H	2:F:171:LEU:HD12	1.72	0.55
1:I:355:PRO:HG2	1:I:358:LEU:HB2	1.88	0.55
2:M:21:VAL:HG13	2:M:24:VAL:HG21	1.87	0.55
2:N:129:GLN:NE2	2:N:422:THR:HA	2.19	0.55
1:B:482:LEU:HD22	1:B:490:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ILE:CG1	1:C:49:ILE:HG12	2.35	0.55
1:C:163:GLU:OE2	1:C:173:ILE:HB	2.07	0.55
2:D:86:ILE:HA	2:D:208:VAL:HG22	1.88	0.55
2:D:92:GLY:CA	2:D:224:THR:HG22	2.36	0.55
2:F:161:ALA:HB2	2:F:303:ILE:HD11	1.88	0.55
2:F:339:GLN:HA	2:F:341:PRO:N	2.21	0.55
1:A:215:VAL:O	1:A:219:PHE:HB2	2.06	0.55
2:D:184:ILE:O	2:D:252:ASN:ND2	2.34	0.55
2:D:226:ARG:HG2	2:D:284:LEU:HD21	1.87	0.55
1:J:218:THR:HG22	1:J:457:VAL:HG22	1.89	0.55
2:L:34:MET:SD	2:L:63:ILE:HG12	2.47	0.55
2:M:333:LEU:HD21	2:M:409:GLU:OE2	2.07	0.55
2:N:130:THR:HB	2:N:135:ILE:HB	1.89	0.55
2:N:180:VAL:HG22	2:N:208:VAL:HB	1.88	0.55
1:B:41:GLU:HA	2:F:12:VAL:CB	2.36	0.55
2:D:144:GLY:CA	2:D:289:GLY:HA2	2.37	0.55
2:D:325:GLY:CA	2:D:349:SER:HA	2.37	0.55
1:I:218:THR:HA	1:I:453:TRP:CZ2	2.42	0.55
1:K:85:ASP:OD2	1:K:89:ARG:HB2	2.06	0.55
1:K:218:THR:HB	1:K:453:TRP:HZ2	1.70	0.55
1:K:568:ALA:O	1:K:572:SER:OG	2.24	0.55
1:B:341:MET:O	1:B:345:LEU:HG	2.06	0.55
1:B:364:GLU:HG2	2:F:215:ASN:HA	1.87	0.55
1:B:494:LYS:HA	1:B:497:ARG:HD3	1.87	0.55
1:C:141:GLU:OE2	1:C:147:HIS:ND1	2.28	0.55
1:C:318:ARG:HD3	1:C:384:ILE:HD11	1.89	0.55
2:D:224:THR:OG1	2:D:225:PRO:HD3	2.07	0.55
1:I:41:GLU:HB2	1:I:48:SER:HB2	1.89	0.55
1:J:58:ILE:CG2	1:J:62:GLU:HG3	2.36	0.55
1:J:318:ARG:HD3	1:J:384:ILE:CD1	2.36	0.55
2:L:18:VAL:HG11	2:L:21:VAL:HG11	1.88	0.55
1:A:541:TYR:O	1:A:545:ILE:HG13	2.06	0.55
1:B:167:PHE:CD2	1:B:173:ILE:HG21	2.41	0.55
2:D:222:ILE:O	2:D:225:PRO:HD2	2.05	0.55
2:E:313:HIS:HB3	2:E:316:PRO:CD	2.36	0.55
2:F:161:ALA:HB1	2:F:246:ILE:HG21	1.88	0.55
1:I:84:PHE:HA	1:I:89:ARG:O	2.06	0.55
1:J:500:TYR:HE2	1:J:522:LEU:HD22	1.72	0.55
1:K:6:ILE:HG13	1:K:62:GLU:O	2.06	0.55
1:K:232:GLY:C	1:K:238:LYS:HD3	2.26	0.55
1:A:54:GLU:HB2	1:A:105:ARG:HH21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLU:O	1:A:128:THR:OG1	2.24	0.55
1:A:291:LEU:HD23	1:A:292:ILE:N	2.21	0.55
1:A:522:LEU:O	1:A:526:LEU:HG	2.06	0.55
1:B:494:LYS:HA	1:B:497:ARG:NH1	2.21	0.55
2:F:144:GLY:HA2	2:F:298:VAL:O	2.05	0.55
1:I:71:LEU:O	1:I:193:VAL:HG22	2.07	0.55
1:J:202:LYS:HE2	1:J:372:VAL:HG11	1.88	0.55
2:L:33:ARG:N	2:L:69:SER:O	2.25	0.55
2:N:224:THR:HB	2:N:225:PRO:HD3	1.87	0.55
1:A:83:MET:HE1	1:A:270:VAL:HG13	1.88	0.55
1:A:114:HIS:ND1	1:A:170:ASP:OD2	2.38	0.55
2:D:285:PHE:CE1	2:D:302:PRO:HB3	2.42	0.55
2:E:182:ALA:HB3	2:E:247:MET:HG3	1.88	0.55
1:I:177:GLU:HB2	1:I:182:LEU:CD2	2.37	0.55
1:K:144:ILE:HG13	1:K:145:ILE:HG13	1.88	0.55
2:N:288:ALA:HB1	2:N:298:VAL:O	2.06	0.55
1:A:224:LYS:NZ	1:A:250:ASP:OD1	2.36	0.55
1:A:264:ASN:HB2	2:D:351:LEU:HD13	1.88	0.55
2:F:158:LYS:H	2:F:158:LYS:HD2	1.71	0.55
1:J:43:ARG:HA	2:N:10:GLU:CB	2.36	0.55
1:J:71:LEU:O	1:J:193:VAL:HG22	2.06	0.55
1:J:230:VAL:N	1:J:231:PRO:HD3	2.22	0.55
1:K:423:ARG:HG3	2:N:373:PHE:CG	2.41	0.55
2:N:183:ALA:O	2:N:212:ASN:HB3	2.06	0.55
2:N:364:ASP:OD2	2:N:427:LEU:HD11	2.06	0.55
1:A:285:LEU:O	1:A:285:LEU:HD23	2.07	0.55
1:B:82:GLN:NE2	1:B:92:ASP:OD2	2.39	0.55
1:B:516:GLU:OE1	1:B:516:GLU:N	2.40	0.55
1:C:120:PHE:CE1	1:C:173:ILE:HD11	2.42	0.55
1:K:237:GLY:HA3	4:K:601:ANP:C8	2.36	0.55
1:K:290:VAL:HG11	1:K:313:ILE:HG21	1.87	0.55
2:L:148:PRO:O	2:L:327:ILE:N	2.36	0.55
2:L:222:ILE:CD1	2:L:260:ILE:HD11	2.37	0.55
2:N:328:ILE:HG13	2:N:346:PRO:CG	2.36	0.55
1:A:175:VAL:HG22	1:A:184:GLU:HG2	1.88	0.54
1:B:496:ILE:HG22	1:B:501:LEU:HD12	1.88	0.54
1:C:7:ILE:O	2:F:49:GLU:HA	2.07	0.54
1:C:31:GLY:HA2	1:C:62:GLU:HB3	1.89	0.54
1:C:80:ILE:HG23	1:C:290:VAL:HG22	1.89	0.54
1:I:177:GLU:CB	1:I:182:LEU:HD23	2.36	0.54
1:I:285:LEU:HD13	1:I:285:LEU:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:357:TYR:HB3	2:M:259:GLU:HG3	1.89	0.54
1:J:79:ILE:HG13	1:J:84:PHE:HZ	1.70	0.54
1:J:202:LYS:HB2	2:N:188:PHE:CZ	2.41	0.54
1:J:530:LYS:NZ	1:J:530:LYS:HB3	2.23	0.54
2:M:283:THR:O	2:M:287:ARG:HG2	2.07	0.54
2:N:339:GLN:O	2:N:414:ASN:HB3	2.07	0.54
2:N:347:SER:HB2	2:N:373:PHE:CE1	2.42	0.54
1:B:14:VAL:O	1:B:49:ILE:N	2.31	0.54
1:C:43:ARG:NH2	2:D:12:VAL:HG21	2.22	0.54
2:D:149:VAL:HA	2:D:327:ILE:HB	1.89	0.54
2:F:160:LEU:CD2	2:F:342:ILE:HD11	2.37	0.54
1:I:83:MET:SD	1:I:270:VAL:HG13	2.48	0.54
1:J:135:ILE:HA	1:J:149:ILE:O	2.07	0.54
1:J:338:LEU:HB3	1:J:355:PRO:HG3	1.89	0.54
2:N:181:PHE:HB3	2:N:209:MET:SD	2.47	0.54
1:A:202:LYS:HG3	1:A:372:VAL:CG1	2.35	0.54
1:A:254:VAL:N	1:A:289:THR:OG1	2.34	0.54
1:A:536:LEU:HG	1:A:545:ILE:HD12	1.88	0.54
1:B:11:GLY:N	1:B:12:PRO:HD2	2.22	0.54
1:B:230:VAL:HA	1:B:413:TRP:O	2.07	0.54
1:C:211:THR:HB	1:C:245:ILE:HD12	1.89	0.54
1:J:262:ARG:NH2	4:J:601:ANP:O2G	2.39	0.54
1:J:410:LYS:HD3	1:J:437:TYR:CE1	2.42	0.54
1:K:81:SER:OG	1:K:287:GLU:HA	2.06	0.54
1:K:514:SER:O	1:K:518:GLN:HG3	2.07	0.54
2:L:350:ARG:O	2:L:351:LEU:HD23	2.08	0.54
2:M:79:LEU:HB2	2:M:227:MET:HE1	1.88	0.54
2:M:178:ALA:HB3	2:M:243:VAL:HG22	1.89	0.54
1:A:75:LEU:O	1:A:189:GLN:N	2.26	0.54
1:B:7:ILE:O	2:E:48:GLN:HA	2.08	0.54
1:B:453:TRP:HZ3	1:B:519:PHE:HA	1.71	0.54
1:C:79:ILE:HA	1:C:112:LEU:HD21	1.89	0.54
2:D:249:ASP:OD1	2:D:304:LEU:HA	2.08	0.54
2:F:407:ARG:HB2	2:F:433:LEU:HD11	1.89	0.54
1:C:249:SER:HB3	1:C:251:VAL:HG22	1.88	0.54
2:D:15:LEU:HD11	2:D:263:ALA:HB1	1.89	0.54
2:E:372:LEU:HD21	2:E:412:TYR:CE1	2.25	0.54
2:E:405:ALA:O	2:E:409:GLU:HG3	2.08	0.54
2:F:421:ARG:CZ	2:F:429:LEU:HD13	2.38	0.54
1:I:25:GLN:HG3	2:M:61:SER:OG	2.07	0.54
1:J:14:VAL:HG23	1:J:51:VAL:CG2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:ARG:HD3	2:L:70:VAL:CA	2.37	0.54
2:L:349:SER:HB3	2:L:352:LYS:HZ2	1.73	0.54
2:N:44:VAL:HG22	2:N:54:VAL:CA	2.35	0.54
2:N:339:GLN:HA	2:N:341:PRO:HD3	1.89	0.54
1:B:220:PHE:CZ	1:B:430:TRP:HA	2.42	0.54
1:B:254:VAL:HA	1:B:325:ALA:O	2.07	0.54
2:D:158:LYS:HG3	2:D:194:PHE:CE1	2.42	0.54
2:E:438:PRO:HG2	2:E:441:GLU:CG	2.38	0.54
1:I:31:GLY:HA2	1:I:62:GLU:HB3	1.89	0.54
1:J:304:GLU:HG3	1:J:334:TRP:HE1	1.71	0.54
1:K:211:THR:CB	1:K:216:ILE:CD1	2.85	0.54
2:L:151:SER:OG	2:L:329:LEU:HD22	2.08	0.54
1:B:39:ILE:HG12	1:B:49:ILE:HG12	1.90	0.54
1:B:114:HIS:CD2	1:B:169:ILE:HD11	2.40	0.54
2:E:149:VAL:HB	2:E:303:ILE:HG12	1.88	0.54
2:F:26:TYR:CD1	2:F:27:GLU:N	2.75	0.54
2:F:233:GLU:HB3	2:F:237:TYR:CE1	2.42	0.54
1:J:352:GLU:CB	1:J:400:PRO:HG3	2.38	0.54
1:K:552:VAL:O	1:K:556:ILE:HG13	2.08	0.54
2:L:333:LEU:O	2:L:338:ILE:HB	2.08	0.54
2:M:439:ARG:NH2	2:M:450:LEU:HB2	2.22	0.54
2:N:339:GLN:HB3	2:N:417:PHE:CE2	2.42	0.54
1:A:424:HIS:CE1	1:A:501:LEU:HB3	2.43	0.54
1:A:503:GLN:NE2	1:A:510:ASP:O	2.35	0.54
1:B:392:PRO:HB2	1:B:396:ASP:O	2.08	0.54
1:C:297:ASN:ND2	2:F:115:VAL:HG13	2.23	0.54
2:D:45:LEU:HD13	2:D:264:ARG:HG2	1.90	0.54
2:D:273:TYR:CZ	2:D:313:HIS:HE1	2.26	0.54
2:E:313:HIS:CD2	2:E:314:PRO:HD2	2.43	0.54
2:F:44:VAL:CG2	2:F:54:VAL:HG12	2.25	0.54
1:J:262:ARG:HH21	2:M:350:ARG:HH12	1.54	0.54
1:K:2:GLN:HE22	1:K:20:SER:CB	2.21	0.54
1:K:144:ILE:HG21	1:K:281:THR:HB	1.90	0.54
1:K:295:THR:N	1:K:298:MET:HG3	2.22	0.54
2:L:222:ILE:HD13	2:L:260:ILE:HD11	1.90	0.54
1:B:225:GLY:HA2	1:B:384:ILE:O	2.08	0.54
1:B:278:ASP:O	1:B:282:GLY:HA3	2.07	0.54
2:D:213:LEU:O	2:D:216:ASP:HB2	2.08	0.54
2:D:345:LEU:N	2:D:346:PRO:HD2	2.23	0.54
2:E:212:ASN:OD1	2:E:221:ARG:HA	2.08	0.54
1:J:92:ASP:OD1	1:J:93:THR:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:41:GLU:OE1	2:L:12:VAL:HG22	2.08	0.54
1:K:326:ILE:HG23	1:K:386:ALA:HA	1.90	0.54
1:K:412:PHE:CD2	1:K:433:SER:HA	2.42	0.54
2:L:137:HIS:O	2:L:137:HIS:ND1	2.39	0.54
2:L:180:VAL:HB	2:L:245:VAL:HG22	1.90	0.54
2:M:48:GLN:HA	2:M:49:GLU:C	2.28	0.54
2:M:315:ILE:O	2:M:319:THR:OG1	2.23	0.54
2:M:318:LEU:O	2:M:321:TYR:HB2	2.08	0.54
2:N:408:PHE:CD2	2:N:413:VAL:HG23	2.43	0.54
1:A:263:GLY:O	1:A:267:THR:OG1	2.19	0.54
1:B:439:THR:O	1:B:443:ARG:NH2	2.41	0.54
2:E:32:VAL:HG22	2:E:70:VAL:HG22	1.89	0.54
2:E:309:ASP:OD2	2:E:331:ARG:NH1	2.41	0.54
1:I:415:LEU:CD2	1:I:428:ILE:HG12	2.37	0.54
1:J:202:LYS:NZ	1:J:367:GLU:O	2.28	0.54
1:J:324:VAL:O	1:J:384:ILE:HA	2.08	0.54
2:M:394:LEU:O	2:M:399:LYS:NZ	2.30	0.54
2:N:148:PRO:HG3	2:N:323:THR:CG2	2.37	0.54
1:A:16:ALA:O	1:A:46:VAL:HA	2.08	0.53
1:B:101:ASN:O	2:E:117:ASN:HB2	2.08	0.53
1:C:92:ASP:OD1	1:C:93:THR:N	2.41	0.53
1:C:300:VAL:CG1	1:C:303:ARG:HD2	2.38	0.53
2:D:138:LEU:HG	2:D:344:VAL:CG1	2.39	0.53
2:D:357:GLY:N	2:D:361:THR:OG1	2.41	0.53
2:F:16:MET:N	2:F:54:VAL:O	2.35	0.53
2:F:270:ARG:HG2	2:F:271:ARG:HG2	1.90	0.53
1:I:202:LYS:HG3	1:I:372:VAL:CG1	2.37	0.53
1:I:214:ARG:NH2	1:I:503:GLN:HG3	2.23	0.53
4:K:601:ANP:O3'	2:N:350:ARG:HA	2.08	0.53
2:L:170:VAL:HG11	2:L:173:SER:HB3	1.89	0.53
2:M:15:LEU:N	2:M:15:LEU:HD23	2.23	0.53
2:N:30:ILE:HG12	2:N:54:VAL:CB	2.37	0.53
2:N:283:THR:O	2:N:287:ARG:HG2	2.07	0.53
1:A:135:ILE:HD13	1:A:148:LYS:HD3	1.89	0.53
1:A:378:ASP:N	1:A:378:ASP:OD1	2.42	0.53
2:D:152:GLY:H	2:D:155:LEU:HD12	1.72	0.53
1:I:221:PRO:HB2	1:I:441:VAL:HG21	1.89	0.53
1:K:446:ASP:OD1	1:K:452:ASP:HA	2.08	0.53
1:K:498:GLU:HA	1:K:502:GLN:HG3	1.90	0.53
2:M:315:ILE:HB	2:M:316:PRO:CD	2.38	0.53
2:N:30:ILE:HG13	2:N:42:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:332:GLU:HA	2:N:335:LYS:HE3	1.89	0.53
1:I:24:ILE:HG13	2:M:11:VAL:HG11	1.89	0.53
1:I:120:PHE:CE2	1:I:122:ALA:HB2	2.44	0.53
1:J:94:PHE:O	1:J:98:THR:OG1	2.26	0.53
1:K:318:ARG:HD3	1:K:384:ILE:CD1	2.38	0.53
2:L:339:GLN:HA	2:L:341:PRO:HD3	1.90	0.53
2:M:261:SER:HB2	2:M:276:TYR:OH	2.09	0.53
2:D:362:ARG:HB2	2:D:427:LEU:HD13	1.90	0.53
1:J:38:GLU:HB2	1:J:50:GLN:HB2	1.90	0.53
1:K:484:ASP:HB3	1:K:542:PHE:HB2	1.91	0.53
2:L:6:ARG:NH1	2:L:69:SER:HA	2.23	0.53
2:N:57:PHE:O	2:N:217:PRO:HB3	2.08	0.53
1:B:238:LYS:HG2	1:B:415:LEU:HD13	1.89	0.53
1:C:144:ILE:HG23	1:C:145:ILE:HG12	1.90	0.53
2:F:315:ILE:HB	2:F:316:PRO:CD	2.39	0.53
2:L:153:SER:O	2:L:331:ARG:NH1	2.42	0.53
2:L:273:TYR:CE1	2:L:315:ILE:HG12	2.42	0.53
2:M:44:VAL:HG22	2:M:54:VAL:HG12	1.90	0.53
2:M:307:PRO:HG2	2:M:313:HIS:CD2	2.43	0.53
2:N:28:GLU:OE2	2:N:72:PHE:HB3	2.08	0.53
1:B:80:ILE:HD12	1:B:317:PHE:CZ	2.44	0.53
1:C:10:SER:CB	2:F:46:GLU:HG3	2.22	0.53
1:C:300:VAL:HG22	2:F:279:THR:HG21	1.90	0.53
2:F:309:ASP:OD2	2:F:331:ARG:NH1	2.42	0.53
2:F:325:GLY:N	2:F:350:ARG:HE	2.01	0.53
1:J:92:ASP:O	1:J:96:GLU:HG2	2.09	0.53
2:L:143:ARG:HD3	2:L:290:ARG:NH1	2.23	0.53
2:M:350:ARG:C	2:M:351:LEU:HD23	2.29	0.53
2:N:48:GLN:O	2:N:51:LYS:N	2.38	0.53
1:B:83:MET:HE1	2:E:119:ILE:CD1	2.39	0.53
1:C:329:ASP:OD1	1:C:330:SER:HB2	2.08	0.53
1:C:552:VAL:HG23	1:C:576:GLU:HG2	1.90	0.53
2:D:27:GLU:O	2:D:43:GLN:NE2	2.41	0.53
2:E:34:MET:HG3	2:E:38:GLU:HB3	1.90	0.53
2:F:149:VAL:HB	2:F:303:ILE:HG12	1.91	0.53
1:I:405:THR:O	1:I:409:VAL:HG22	2.08	0.53
1:J:463:ILE:HG22	1:J:493:ALA:HB2	1.91	0.53
1:K:213:GLN:CG	1:K:216:ILE:HD11	2.39	0.53
1:K:479:ILE:CG2	2:N:394:LEU:HA	2.38	0.53
4:K:601:ANP:C5'	2:N:350:ARG:HD3	2.21	0.53
2:N:148:PRO:HB2	2:N:150:PHE:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:446:ASP:CB	1:C:452:ASP:HA	2.39	0.53
2:E:5:TYR:O	2:E:70:VAL:N	2.30	0.53
2:E:91:ASP:OD1	2:E:95:ARG:HG3	2.09	0.53
2:E:148:PRO:O	2:E:327:ILE:HB	2.08	0.53
2:E:213:LEU:HB3	2:E:215:ASN:OD1	2.08	0.53
1:I:408:VAL:HG23	1:I:409:VAL:HG13	1.90	0.53
1:J:38:GLU:HG2	1:J:52:TYR:CZ	2.43	0.53
1:K:79:ILE:CA	1:K:112:LEU:HD21	2.38	0.53
1:K:260:GLY:CA	1:K:333:ARG:HG3	2.38	0.53
1:A:424:HIS:ND1	1:A:502:GLN:HG2	2.24	0.53
1:A:538:LEU:C	1:A:538:LEU:HD12	2.29	0.53
2:D:29:LEU:CB	2:D:73:LEU:HD21	2.39	0.53
2:E:329:LEU:HD22	2:E:341:PRO:O	2.08	0.53
2:E:338:ILE:HG22	2:E:414:ASN:HB3	1.91	0.53
1:I:19:MET:HE1	1:I:64:VAL:HB	1.90	0.53
1:J:149:ILE:HD13	1:J:149:ILE:N	2.23	0.53
1:J:236:ALA:HB1	1:J:415:LEU:HD12	1.90	0.53
1:J:300:VAL:CG2	2:M:279:THR:HG21	2.38	0.53
1:K:378:ASP:OD1	1:K:378:ASP:N	2.41	0.53
2:L:235:LEU:HA	2:L:239:LYS:HB2	1.90	0.53
2:M:135:ILE:O	2:M:140:THR:HA	2.09	0.53
2:N:13:GLY:O	2:N:60:THR:OG1	2.19	0.53
1:A:43:ARG:CG	1:A:46:VAL:HG13	2.39	0.53
1:A:177:GLU:HG3	1:A:182:LEU:HD23	1.91	0.53
2:D:212:ASN:OD1	2:D:221:ARG:HG3	2.09	0.53
2:E:26:TYR:CE2	2:E:27:GLU:HG3	2.44	0.53
2:E:127:PHE:HZ	2:E:136:ASP:CB	2.22	0.53
2:F:255:GLU:O	2:F:258:ARG:HG2	2.09	0.53
1:I:175:VAL:CG1	1:I:182:LEU:HD22	2.39	0.53
1:J:218:THR:HG1	1:J:500:TYR:HH	1.54	0.53
1:J:259:CYS:O	1:J:330:SER:N	2.37	0.53
1:K:51:VAL:HG21	1:K:55:THR:HG23	1.90	0.53
2:M:17:ALA:HA	2:M:53:MET:HA	1.91	0.53
2:M:270:ARG:O	2:M:271:ARG:HB2	2.09	0.53
2:M:446:LYS:HB3	2:M:448:ASP:OD1	2.08	0.53
1:A:425:PHE:O	1:A:503:GLN:N	2.22	0.52
1:B:515:ARG:HA	1:B:518:GLN:HG3	1.91	0.52
2:D:40:ARG:NH1	2:D:59:GLY:O	2.40	0.52
2:D:415:GLN:HB3	2:D:421:ARG:NH1	2.23	0.52
2:F:278:TYR:CE1	2:F:322:ILE:HG12	2.44	0.52
2:F:358:ALA:N	2:F:359:GLY:CA	2.69	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:50:GLN:HE21	1:J:345:LEU:CD1	2.22	0.52
1:K:214:ARG:NH1	1:K:499:ASP:O	2.42	0.52
2:L:9:LYS:HG3	2:L:19:GLU:CG	2.39	0.52
2:M:78:GLN:NE2	2:M:78:GLN:HA	2.24	0.52
2:M:82:SER:CB	2:M:103:ILE:HD11	2.09	0.52
1:A:120:PHE:HB2	1:A:187:MET:HE1	1.91	0.52
1:A:285:LEU:O	1:A:288:ARG:HG2	2.09	0.52
1:B:491:GLU:HG3	1:B:542:PHE:HZ	1.74	0.52
2:E:183:ALA:HB1	2:E:186:ILE:HD11	1.90	0.52
2:F:339:GLN:CA	2:F:341:PRO:HD3	2.38	0.52
1:I:208:PRO:HA	1:I:223:THR:HA	1.90	0.52
1:K:211:THR:OG1	1:K:216:ILE:HD12	2.09	0.52
2:L:257:LEU:HA	2:L:260:ILE:CD1	2.39	0.52
1:A:20:SER:HA	1:A:42:MET:CE	2.40	0.52
1:A:523:LYS:HA	1:A:523:LYS:HE3	1.92	0.52
1:B:29:LEU:HD23	1:B:65:ARG:HB2	1.90	0.52
2:D:220:GLU:O	2:D:224:THR:HG23	2.08	0.52
1:J:406:LEU:HD21	1:J:412:PHE:HB2	1.91	0.52
2:L:283:THR:HA	2:L:286:GLU:HB2	1.91	0.52
2:M:60:THR:OG1	2:M:63:ILE:HD12	2.09	0.52
2:M:82:SER:O	2:M:85:MET:HG3	2.09	0.52
2:M:147:LEU:O	2:M:302:PRO:HD2	2.09	0.52
2:N:67:ASN:OD1	2:N:67:ASN:N	2.42	0.52
1:A:140:ASP:OD1	1:A:146:GLN:HG3	2.09	0.52
1:A:323:ASP:OD1	1:A:383:SER:OG	2.28	0.52
1:A:445:MET:HG3	1:A:453:TRP:CE3	2.45	0.52
1:A:577:ILE:O	1:A:581:ILE:HG12	2.09	0.52
2:D:38:GLU:OE2	2:D:40:ARG:NE	2.33	0.52
2:E:56:ILE:HG22	2:E:59:GLY:H	1.75	0.52
2:E:423:ILE:O	2:E:427:LEU:HG	2.09	0.52
1:J:229:ALA:C	1:J:231:PRO:HD3	2.30	0.52
1:K:29:LEU:HB2	1:K:65:ARG:HE	1.74	0.52
2:L:30:ILE:HD12	2:L:30:ILE:O	2.10	0.52
2:M:235:LEU:HB2	2:M:243:VAL:HG21	1.91	0.52
2:M:388:VAL:HG13	2:M:389:LEU:HG	1.92	0.52
1:A:15:MET:HA	1:A:47:ALA:O	2.09	0.52
1:B:36:ILE:HD12	1:B:87:ILE:HD13	1.91	0.52
1:J:355:PRO:HG2	1:J:358:LEU:HB2	1.90	0.52
1:K:392:PRO:HB3	1:K:396:ASP:O	2.08	0.52
2:L:33:ARG:HB3	2:L:69:SER:OG	2.09	0.52
2:L:339:GLN:N	2:L:414:ASN:HD21	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:57:PHE:CE2	2:M:219:ILE:HG21	2.45	0.52
2:M:79:LEU:HB2	2:M:227:MET:HE3	1.92	0.52
2:N:347:SER:HB3	2:N:348:LEU:HA	1.91	0.52
1:A:43:ARG:HB3	1:A:44:GLN:CA	2.40	0.52
1:B:20:SER:HA	1:B:42:MET:HE2	1.91	0.52
1:B:251:VAL:HG21	1:B:325:ALA:HB3	1.90	0.52
1:B:547:GLU:HA	1:B:550:VAL:HG13	1.92	0.52
1:C:573:ILE:HG22	1:C:577:ILE:CD1	2.38	0.52
1:I:340:GLU:O	1:I:344:ARG:HG3	2.10	0.52
1:J:301:ALA:HB2	1:J:341:MET:HE2	1.91	0.52
1:K:59:GLY:HA3	2:N:25:LYS:HD3	1.92	0.52
1:K:500:TYR:HE2	1:K:522:LEU:CB	2.20	0.52
2:M:79:LEU:HD13	2:M:94:GLY:HA3	1.91	0.52
2:M:91:ASP:OD1	2:M:95:ARG:HG2	2.10	0.52
2:M:277:LEU:O	2:M:281:LEU:HB2	2.10	0.52
2:N:304:LEU:HD22	2:N:315:ILE:HG22	1.91	0.52
1:A:52:TYR:CB	1:A:299:PRO:HB3	2.40	0.52
1:C:71:LEU:HD23	1:C:193:VAL:HG21	1.91	0.52
1:C:331:THR:CG2	1:C:390:VAL:HG22	2.39	0.52
2:E:6:ARG:HA	2:E:69:SER:HA	1.92	0.52
2:F:142:VAL:HG21	2:F:351:LEU:HB3	1.90	0.52
1:I:43:ARG:HG2	1:I:46:VAL:HG13	1.91	0.52
1:I:139:VAL:O	1:I:147:HIS:HB3	2.09	0.52
1:J:84:PHE:O	1:J:292:ILE:HG23	2.09	0.52
1:K:32:ASP:H	1:K:62:GLU:HG2	1.74	0.52
2:L:79:LEU:HD13	2:L:227:MET:CE	2.40	0.52
2:L:120:ALA:O	2:L:292:ARG:HB2	2.10	0.52
2:M:231:ALA:O	2:M:235:LEU:HG	2.10	0.52
2:N:328:ILE:HG13	2:N:346:PRO:HG3	1.91	0.52
2:N:378:GLN:HB3	2:N:401:TYR:CD1	2.44	0.52
1:B:488:LEU:O	1:B:492:VAL:HG23	2.09	0.52
2:D:138:LEU:HG	2:D:344:VAL:CB	2.40	0.52
2:E:224:THR:HB	2:E:225:PRO:HD3	1.92	0.52
2:E:284:LEU:HD12	2:E:285:PHE:H	1.75	0.52
2:E:372:LEU:HD13	2:E:434:LEU:HG	1.91	0.52
2:F:65:LEU:N	2:F:65:LEU:HD23	2.24	0.52
2:F:215:ASN:OD1	2:F:215:ASN:N	2.40	0.52
1:I:42:MET:HG3	2:M:65:LEU:HD11	1.91	0.52
1:I:255:VAL:HG12	1:I:257:VAL:HG23	1.92	0.52
1:J:232:GLY:O	1:J:238:LYS:HD3	2.09	0.52
1:K:230:VAL:HG23	1:K:389:ALA:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:522:LEU:O	1:K:526:LEU:HB2	2.09	0.52
2:N:11:VAL:HG22	2:N:16:MET:HG3	1.92	0.52
1:A:75:LEU:HB3	1:A:316:TYR:CD2	2.44	0.52
1:B:230:VAL:HG13	1:B:413:TRP:O	2.10	0.52
1:B:339:ARG:NH2	2:E:275:GLY:O	2.43	0.52
1:C:367:GLU:HG2	2:D:215:ASN:ND2	2.24	0.52
1:C:412:PHE:CD2	1:C:433:SER:HA	2.45	0.52
2:E:6:ARG:CZ	2:L:290:ARG:HH21	2.23	0.52
2:E:132:ILE:HA	2:E:415:GLN:CD	2.30	0.52
2:F:324:GLU:HA	2:F:350:ARG:NE	2.24	0.52
1:J:83:MET:HE2	1:J:266:MET:HB3	1.92	0.52
1:J:148:LYS:C	1:J:149:ILE:HD13	2.30	0.52
1:J:210:ILE:O	1:J:210:ILE:HG13	2.10	0.52
1:J:231:PRO:HA	1:J:390:VAL:O	2.10	0.52
1:J:300:VAL:HG22	2:M:279:THR:HG21	1.91	0.52
1:K:444:TYR:HE2	1:K:515:ARG:HH12	1.58	0.52
2:L:18:VAL:O	2:L:51:LYS:HA	2.10	0.52
2:N:98:ASP:N	2:N:99:ASN:HA	2.25	0.52
2:N:269:GLY:N	2:N:273:TYR:O	2.31	0.52
1:A:225:GLY:HA2	1:A:384:ILE:O	2.09	0.52
1:A:315:GLU:HG2	1:A:318:ARG:HH21	1.74	0.52
1:A:330:SER:HB3	1:A:333:ARG:HG3	1.92	0.52
1:C:161:LYS:HE3	1:C:175:VAL:CG2	2.40	0.52
1:C:573:ILE:CG2	1:C:577:ILE:HD11	2.39	0.52
2:D:29:LEU:HD11	2:D:77:LEU:HA	1.91	0.52
2:D:184:ILE:HD13	2:D:225:PRO:HG3	1.92	0.52
2:E:30:ILE:HD11	2:E:42:GLY:HA3	1.92	0.52
1:I:33:LEU:H	1:I:33:LEU:HD12	1.75	0.52
1:J:19:MET:CE	1:J:64:VAL:HG11	2.40	0.52
1:J:144:ILE:HD11	1:J:288:ARG:HB3	1.92	0.52
2:M:147:LEU:HB3	2:M:301:ILE:HG12	1.90	0.52
1:A:120:PHE:HA	1:A:139:VAL:HG22	1.91	0.51
1:B:443:ARG:HB2	1:B:443:ARG:HH11	1.74	0.51
1:B:497:ARG:HA	1:B:501:LEU:CD1	2.40	0.51
1:C:552:VAL:CG2	1:C:576:GLU:HG2	2.41	0.51
2:D:33:ARG:N	2:D:69:SER:O	2.24	0.51
1:I:370:GLY:H	1:I:384:ILE:HB	1.75	0.51
1:J:494:LYS:O	1:J:498:GLU:HG2	2.10	0.51
1:K:213:GLN:HE22	1:K:244:GLN:HE21	1.57	0.51
1:K:234:PHE:HZ	2:N:311:LYS:HD2	1.75	0.51
1:K:262:ARG:CZ	2:N:350:ARG:HH12	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:222:ILE:HG23	2:L:253:TYR:CE1	2.44	0.51
1:A:261:GLU:CB	1:A:266:MET:HG2	2.40	0.51
1:A:340:GLU:HG3	2:D:276:TYR:HA	1.92	0.51
2:D:162:ALA:O	2:D:166:ARG:HG3	2.11	0.51
2:E:29:LEU:HD23	2:E:42:GLY:O	2.10	0.51
2:E:326:GLN:HB2	2:E:347:SER:HA	1.91	0.51
2:F:24:VAL:HG22	2:F:72:PHE:HE2	1.75	0.51
2:F:177:PHE:CE1	2:F:244:LEU:N	2.78	0.51
1:J:285:LEU:O	1:J:285:LEU:HD23	2.11	0.51
1:K:54:GLU:HB2	1:K:105:ARG:HD3	1.90	0.51
1:K:120:PHE:CZ	1:K:173:ILE:HD12	2.44	0.51
1:K:149:ILE:HD12	1:K:149:ILE:N	2.25	0.51
1:K:214:ARG:HH12	1:K:521:MET:HE1	1.75	0.51
1:K:215:VAL:HG23	1:K:216:ILE:N	2.25	0.51
1:K:503:GLN:NE2	1:K:510:ASP:O	2.33	0.51
2:M:437:LEU:HB2	2:M:442:LEU:HD21	1.93	0.51
2:N:4:GLU:HB3	2:N:71:ARG:CB	2.36	0.51
1:A:20:SER:HB3	1:A:45:ASP:HB3	1.92	0.51
1:B:39:ILE:HG12	1:B:49:ILE:HG23	1.91	0.51
1:C:169:ILE:HG23	1:C:187:MET:HB2	1.91	0.51
2:D:225:PRO:O	2:D:229:LEU:HG	2.11	0.51
2:D:315:ILE:O	2:D:319:THR:OG1	2.23	0.51
2:D:409:GLU:HA	2:D:413:VAL:CG2	2.40	0.51
2:F:26:TYR:HE1	2:F:45:LEU:HA	1.73	0.51
1:J:522:LEU:HG	1:J:526:LEU:HD11	1.93	0.51
1:K:508:ASP:N	1:K:508:ASP:OD1	2.43	0.51
2:L:31:GLU:O	2:L:70:VAL:HA	2.11	0.51
2:M:21:VAL:HG22	2:M:72:PHE:HZ	1.75	0.51
2:M:132:ILE:HG22	2:M:134:ALA:H	1.75	0.51
2:M:226:ARG:HH11	2:M:284:LEU:HD21	1.75	0.51
2:N:32:VAL:N	2:N:40:ARG:O	2.37	0.51
2:N:88:ARG:HH22	2:N:96:PRO:HB3	1.74	0.51
1:A:521:MET:CE	1:A:560:LYS:HB3	2.40	0.51
1:C:366:TYR:OH	1:C:388:SER:HB2	2.10	0.51
2:D:223:ALA:O	2:D:227:MET:HG3	2.10	0.51
2:E:325:GLY:N	2:E:350:ARG:HG2	2.26	0.51
1:I:20:SER:HB2	2:M:66:LYS:NZ	2.23	0.51
1:J:374:ALA:HB3	1:J:380:ARG:HG2	1.92	0.51
1:K:421:GLN:HB3	2:N:345:LEU:O	2.10	0.51
2:L:249:ASP:OD1	2:L:304:LEU:HA	2.11	0.51
2:N:44:VAL:HG21	2:N:54:VAL:HG12	1.85	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:338:ILE:HG22	2:N:414:ASN:HB2	1.93	0.51
1:C:149:ILE:HD12	1:C:149:ILE:N	2.22	0.51
1:C:278:ASP:HB3	1:C:281:THR:HG21	1.91	0.51
2:D:138:LEU:CG	2:D:344:VAL:HB	2.41	0.51
1:I:254:VAL:O	1:I:289:THR:HB	2.10	0.51
1:K:225:GLY:O	1:K:370:GLY:HA2	2.10	0.51
1:K:259:CYS:N	1:K:329:ASP:O	2.43	0.51
2:L:14:PRO:HB2	2:L:55:GLN:CG	2.38	0.51
2:M:21:VAL:CG1	2:M:24:VAL:HG21	2.40	0.51
2:M:88:ARG:NE	2:M:98:ASP:OD2	2.34	0.51
2:N:88:ARG:NH2	2:N:96:PRO:HB3	2.26	0.51
2:N:258:ARG:HD2	2:N:273:TYR:CE1	2.45	0.51
1:B:285:LEU:HD12	1:B:285:LEU:C	2.31	0.51
1:C:12:PRO:O	1:C:51:VAL:HG22	2.11	0.51
1:C:415:LEU:HD22	1:C:427:SER:O	2.09	0.51
1:C:423:ARG:NH1	2:F:348:LEU:HB2	2.26	0.51
2:F:338:ILE:O	2:F:341:PRO:HB3	2.11	0.51
1:J:236:ALA:CB	1:J:415:LEU:HD12	2.40	0.51
2:L:128:ILE:HD11	2:L:143:ARG:HA	1.92	0.51
1:C:295:THR:OG1	1:C:298:MET:SD	2.58	0.51
2:E:29:LEU:CD1	2:E:77:LEU:HG	2.36	0.51
2:E:93:LEU:HD12	2:E:95:ARG:CZ	2.40	0.51
1:I:199:ILE:HG21	1:I:372:VAL:HG21	1.93	0.51
1:I:232:GLY:HA3	1:I:415:LEU:HD12	1.92	0.51
1:I:439:THR:HG22	1:I:443:ARG:HH12	1.75	0.51
1:I:521:MET:O	1:I:525:ILE:HG13	2.11	0.51
1:K:41:GLU:HB2	2:L:12:VAL:HA	1.91	0.51
2:M:179:VAL:O	2:M:207:SER:HA	2.11	0.51
2:M:273:TYR:CD2	2:M:314:PRO:HG2	2.42	0.51
2:N:35:GLN:OE1	2:N:35:GLN:N	2.26	0.51
2:N:40:ARG:HD3	2:N:58:GLU:HB2	1.91	0.51
2:N:135:ILE:HA	2:N:139:ASN:HB2	1.92	0.51
1:A:497:ARG:CG	1:A:501:LEU:HD12	2.38	0.51
2:D:278:TYR:HE1	2:D:322:ILE:HG12	1.76	0.51
2:E:132:ILE:HD12	2:E:132:ILE:N	2.25	0.51
2:E:338:ILE:HG23	2:E:414:ASN:HB3	1.92	0.51
2:F:24:VAL:HG22	2:F:72:PHE:CE2	2.46	0.51
2:F:242:HIS:HA	2:F:297:SER:H	1.76	0.51
2:F:339:GLN:HB3	2:F:341:PRO:HD3	1.92	0.51
1:I:59:GLY:O	1:I:62:GLU:HG3	2.11	0.51
1:I:203:LEU:HD11	1:I:373:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:497:ARG:HA	1:I:501:LEU:CB	2.38	0.51
1:J:215:VAL:HG11	1:J:426:PRO:CG	2.40	0.51
1:J:419:LEU:HD23	1:J:422:LYS:HD2	1.93	0.51
1:K:191:TRP:HD1	1:K:312:THR:HG23	1.76	0.51
1:K:259:CYS:O	1:K:333:ARG:HG3	2.11	0.51
2:L:130:THR:H	2:L:136:ASP:CG	2.14	0.51
2:L:310:ASP:OD2	2:L:312:THR:OG1	2.29	0.51
2:L:329:LEU:HG	2:L:341:PRO:O	2.11	0.51
1:A:445:MET:O	1:A:449:LEU:HB2	2.10	0.51
1:A:484:ASP:OD2	1:A:484:ASP:N	2.43	0.51
1:B:214:ARG:HD2	1:B:500:TYR:HE2	1.76	0.51
1:B:252:ASP:OD2	1:B:252:ASP:N	2.43	0.51
1:C:75:LEU:O	1:C:189:GLN:N	2.43	0.51
1:C:233:PRO:HA	2:F:321:TYR:OH	2.11	0.51
2:E:149:VAL:HG22	2:E:327:ILE:HG21	1.92	0.51
2:E:283:THR:O	2:E:287:ARG:HG2	2.10	0.51
1:I:145:ILE:HG13	1:I:253:LEU:HD11	1.93	0.51
1:I:470:LEU:O	1:I:474:VAL:HG23	2.10	0.51
2:L:130:THR:N	2:L:136:ASP:OD2	2.44	0.51
2:L:151:SER:OG	2:L:157:HIS:HB3	2.11	0.51
2:M:304:LEU:HD22	2:M:315:ILE:HG22	1.92	0.51
2:N:248:THR:HB	2:N:303:ILE:HB	1.92	0.51
1:A:257:VAL:HG12	1:A:258:GLY:N	2.23	0.51
2:D:32:VAL:HG22	2:D:70:VAL:HG22	1.92	0.51
2:D:90:PHE:HA	2:D:96:PRO:HA	1.92	0.51
2:F:403:LYS:O	2:F:407:ARG:HG3	2.11	0.51
1:J:497:ARG:HA	1:J:501:LEU:CD1	2.41	0.51
1:K:202:LYS:HB3	2:L:188:PHE:CE2	2.46	0.51
1:K:233:PRO:CD	1:K:236:ALA:HB2	2.38	0.51
2:M:119:ILE:O	2:M:292:ARG:NH1	2.44	0.51
1:B:15:MET:HA	1:B:48:SER:HA	1.93	0.50
1:C:41:GLU:OE2	2:D:12:VAL:HG13	2.11	0.50
1:C:60:PRO:HD3	2:F:47:VAL:HG11	1.93	0.50
1:C:210:ILE:HD11	1:C:515:ARG:HH21	1.76	0.50
1:C:245:ILE:O	1:C:249:SER:OG	2.17	0.50
2:E:57:PHE:CE2	2:E:219:ILE:HG21	2.46	0.50
1:I:307:ILE:HB	1:I:365:TYR:CE1	2.45	0.50
1:J:247:LYS:HA	1:J:285:LEU:HD11	1.93	0.50
1:K:41:GLU:HB3	2:L:12:VAL:HA	1.93	0.50
2:L:345:LEU:HB2	2:L:346:PRO:CD	2.41	0.50
2:L:429:LEU:O	2:L:433:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ASN:O	1:A:275:GLU:HG2	2.11	0.50
1:B:292:ILE:HD11	1:B:313:ILE:HD12	1.92	0.50
1:B:406:LEU:HD21	1:B:412:PHE:CD1	2.47	0.50
2:F:133:SER:OG	2:F:426:THR:HG23	2.11	0.50
1:I:264:ASN:ND2	2:L:145:GLN:HA	2.25	0.50
1:J:188:MET:HG2	1:J:189:GLN:N	2.27	0.50
1:K:355:PRO:HG2	1:K:358:LEU:HB2	1.92	0.50
1:K:453:TRP:HZ3	1:K:519:PHE:HA	1.77	0.50
1:A:497:ARG:O	1:A:501:LEU:HB2	2.11	0.50
1:B:54:GLU:HB3	1:B:105:ARG:HH11	1.77	0.50
1:C:149:ILE:H	1:C:149:ILE:CD1	2.23	0.50
1:C:425:PHE:HB3	4:C:601:ANP:C6	2.41	0.50
2:E:152:GLY:O	2:E:155:LEU:HB2	2.11	0.50
2:F:126:GLU:H	2:F:142:VAL:CG1	2.25	0.50
2:F:126:GLU:H	2:F:142:VAL:HG12	1.76	0.50
2:F:133:SER:HB2	2:F:415:GLN:OE1	2.11	0.50
1:I:139:VAL:HG21	1:I:149:ILE:HD11	1.92	0.50
1:I:245:ILE:O	1:I:249:SER:OG	2.25	0.50
1:J:331:THR:HG21	1:J:388:SER:HB2	1.93	0.50
1:K:73:VAL:HG11	1:K:309:THR:HG23	1.93	0.50
2:L:185:GLY:O	2:L:252:ASN:ND2	2.44	0.50
2:M:124:PRO:HB3	2:M:143:ARG:O	2.12	0.50
1:A:485:ASN:OD1	1:A:533:ARG:NH1	2.44	0.50
1:A:532:ALA:O	1:A:536:LEU:HB2	2.11	0.50
1:B:429:ASN:O	1:B:433:SER:OG	2.26	0.50
1:C:521:MET:HE1	1:C:560:LYS:HB3	1.94	0.50
2:D:16:MET:N	2:D:54:VAL:O	2.39	0.50
2:D:159:GLU:O	2:D:163:GLN:HB2	2.12	0.50
2:D:235:LEU:HA	2:D:239:LYS:HB2	1.93	0.50
2:D:408:PHE:CD1	2:D:412:TYR:HB3	2.46	0.50
2:E:21:VAL:HG11	2:E:52:ALA:CB	2.29	0.50
1:I:479:ILE:HG13	1:I:480:ASP:N	2.26	0.50
1:J:390:VAL:O	1:J:392:PRO:HD3	2.11	0.50
1:K:87:ILE:HD11	1:K:89:ARG:NH2	2.26	0.50
1:K:269:VAL:HG11	1:K:291:LEU:HD21	1.93	0.50
2:L:251:THR:O	2:L:255:GLU:HG2	2.11	0.50
2:M:130:THR:OG1	2:M:135:ILE:HB	2.12	0.50
2:M:150:PHE:CZ	2:M:319:THR:HB	2.46	0.50
1:A:38:GLU:HB2	1:A:52:TYR:OH	2.11	0.50
1:A:208:PRO:CG	1:A:441:VAL:HG13	2.42	0.50
1:A:493:ALA:O	1:A:497:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:PHE:HA	1:B:426:PRO:C	2.32	0.50
1:K:28:CYS:SG	1:K:39:ILE:HD11	2.51	0.50
1:K:211:THR:CB	1:K:216:ILE:HD12	2.41	0.50
2:M:126:GLU:O	2:M:142:VAL:HG13	2.11	0.50
2:M:151:SER:O	2:M:305:THR:HA	2.12	0.50
1:A:266:MET:SD	1:A:293:ALA:HB1	2.52	0.50
1:B:119:TRP:HE1	1:B:121:GLU:HB2	1.76	0.50
1:B:173:ILE:HD13	1:B:173:ILE:H	1.77	0.50
1:B:285:LEU:CD1	1:B:288:ARG:CD	2.83	0.50
1:B:520:ASN:O	1:B:524:VAL:HG23	2.12	0.50
2:E:338:ILE:HG23	2:E:414:ASN:CB	2.42	0.50
1:I:460:GLY:O	1:I:464:LEU:HD12	2.11	0.50
1:J:273:PHE:HB2	1:J:274:PRO:HD3	1.94	0.50
1:K:176:ILE:N	1:K:183:LYS:O	2.41	0.50
1:K:222:VAL:HG22	1:K:413:TRP:HZ2	1.76	0.50
2:L:315:ILE:HB	2:L:316:PRO:HD3	1.93	0.50
2:L:339:GLN:HB2	2:L:417:PHE:CZ	2.46	0.50
2:N:256:ALA:O	2:N:260:ILE:HG12	2.11	0.50
1:A:218:THR:HA	1:A:453:TRP:CH2	2.47	0.50
1:A:257:VAL:O	1:A:328:ALA:HA	2.11	0.50
2:F:339:GLN:O	2:F:416:GLY:N	2.45	0.50
1:J:198:PRO:HB2	1:J:375:LEU:HD11	1.93	0.50
1:K:22:ALA:O	1:K:42:MET:SD	2.70	0.50
1:K:230:VAL:HG23	1:K:389:ALA:CA	2.41	0.50
1:B:83:MET:HE1	2:E:119:ILE:HD13	1.94	0.50
1:B:213:GLN:HG3	1:B:245:ILE:CD1	2.42	0.50
1:C:168:THR:HG22	1:C:171:ASP:OD2	2.12	0.50
1:C:185:LEU:O	1:C:185:LEU:HD12	2.12	0.50
1:C:331:THR:HG21	1:C:390:VAL:HG22	1.94	0.50
2:F:50:ASP:C	2:F:51:LYS:HG2	2.31	0.50
1:J:58:ILE:HG22	1:J:62:GLU:HG3	1.93	0.50
1:J:333:ARG:HD3	1:J:333:ARG:N	2.26	0.50
1:K:173:ILE:HD13	1:K:187:MET:HG2	1.94	0.50
1:K:225:GLY:HA3	1:K:371:ARG:N	2.27	0.50
1:K:314:ALA:HB1	1:K:324:VAL:HG11	1.93	0.50
2:L:40:ARG:NH1	2:L:59:GLY:O	2.45	0.50
2:L:269:GLY:N	2:L:273:TYR:O	2.44	0.50
2:M:219:ILE:O	2:M:223:ALA:N	2.45	0.50
2:N:329:LEU:HD22	2:N:341:PRO:O	2.12	0.50
1:A:18:ASN:N	1:A:45:ASP:OD1	2.43	0.50
1:B:504:ASN:OD1	1:B:506:PHE:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:ASN:HB3	2:D:349:SER:CB	2.41	0.50
2:D:270:ARG:NH1	2:D:270:ARG:HB3	2.27	0.50
1:I:169:ILE:O	1:I:186:THR:OG1	2.16	0.50
1:J:37:GLY:HA3	1:J:50:GLN:O	2.12	0.50
1:J:95:MET:SD	2:M:120:ALA:HB2	2.52	0.50
1:K:480:ASP:OD2	1:K:480:ASP:N	2.44	0.50
2:L:407:ARG:HD3	2:L:436:MET:HE2	1.94	0.50
2:M:88:ARG:NH2	2:M:100:GLY:O	2.45	0.50
2:N:347:SER:N	2:N:348:LEU:CA	2.75	0.50
1:C:54:GLU:O	1:C:105:ARG:NH1	2.45	0.49
1:C:73:VAL:HB	1:C:88:GLN:CD	2.31	0.49
2:F:434:LEU:HD13	2:F:434:LEU:H	1.77	0.49
1:I:13:LEU:HG	1:I:14:VAL:N	2.26	0.49
1:I:84:PHE:HB2	1:I:292:ILE:HD12	1.93	0.49
1:J:42:MET:HG3	2:N:65:LEU:HD11	1.92	0.49
1:K:197:ARG:NE	1:K:319:ASP:OD2	2.32	0.49
1:K:311:ILE:HB	1:K:365:TYR:HE1	1.76	0.49
2:L:183:ALA:HB1	2:L:186:ILE:CD1	2.41	0.49
1:B:41:GLU:OE2	1:B:43:ARG:NH1	2.36	0.49
1:B:226:GLY:H	1:B:385:THR:HG23	1.77	0.49
1:B:300:VAL:CG2	2:E:279:THR:HG21	2.42	0.49
1:C:79:ILE:HG13	1:C:84:PHE:CE2	2.47	0.49
2:D:32:VAL:HG21	2:D:56:ILE:HD11	1.94	0.49
2:E:146:LYS:HD2	2:E:323:THR:HA	1.94	0.49
2:F:47:VAL:HG23	2:F:52:ALA:CA	2.41	0.49
1:I:260:GLY:O	1:I:333:ARG:HG3	2.12	0.49
1:I:297:ASN:HB2	2:L:286:GLU:CG	2.40	0.49
1:J:318:ARG:CB	1:J:384:ILE:HD11	2.42	0.49
1:K:6:ILE:HG21	1:K:9:VAL:CG2	2.41	0.49
1:K:230:VAL:HG23	1:K:389:ALA:HB2	1.94	0.49
2:M:213:LEU:N	2:M:216:ASP:OD2	2.45	0.49
1:A:27:MET:CE	1:A:38:GLU:HG3	2.42	0.49
1:A:340:GLU:HG3	2:D:275:GLY:O	2.11	0.49
1:A:412:PHE:HD1	1:A:434:TYR:CE2	2.29	0.49
1:A:536:LEU:HD21	1:A:542:PHE:CA	2.41	0.49
1:B:301:ALA:HB2	1:B:341:MET:CE	2.41	0.49
1:B:440:GLU:C	1:B:443:ARG:HH22	2.15	0.49
1:C:130:VAL:HG22	1:C:157:GLY:O	2.12	0.49
2:E:122:ASP:OD1	2:E:123:TYR:N	2.45	0.49
2:E:379:GLY:HA3	2:E:405:ALA:HB2	1.93	0.49
1:J:423:ARG:HG2	2:M:348:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:114:HIS:ND1	1:K:169:ILE:HD11	2.27	0.49
1:K:523:LYS:O	1:K:527:THR:N	2.42	0.49
2:M:34:MET:HB2	2:M:40:ARG:NH2	2.23	0.49
2:M:285:PHE:HA	2:M:300:GLN:HE22	1.77	0.49
2:N:347:SER:N	2:N:348:LEU:HB2	2.27	0.49
1:A:86:GLY:N	1:A:294:ASN:HD21	2.10	0.49
1:B:284:SER:O	1:B:287:GLU:HB2	2.12	0.49
1:B:371:ARG:HG3	1:B:383:SER:HB3	1.94	0.49
1:C:6:ILE:HG21	1:C:9:VAL:HG22	1.93	0.49
1:C:27:MET:SD	1:C:36:ILE:HD11	2.52	0.49
1:C:238:LYS:NZ	4:C:601:ANP:O2B	2.34	0.49
1:C:240:VAL:O	1:C:244:GLN:HG2	2.12	0.49
1:C:315:GLU:OE1	1:C:368:ARG:NH2	2.42	0.49
1:C:408:VAL:HG23	1:C:409:VAL:HG13	1.93	0.49
1:C:414:GLY:C	1:C:415:LEU:HD23	2.33	0.49
1:C:425:PHE:HA	1:C:426:PRO:C	2.31	0.49
2:D:147:LEU:O	2:D:301:ILE:HA	2.12	0.49
2:F:150:PHE:HB3	2:F:306:MET:SD	2.52	0.49
2:F:198:PHE:CB	2:F:204:ILE:HB	2.19	0.49
1:J:8:LYS:O	1:J:14:VAL:HG13	2.12	0.49
1:J:28:CYS:HB3	1:J:66:SER:HA	1.93	0.49
1:J:102:PHE:HB3	2:M:114:GLU:HB3	1.93	0.49
1:J:269:VAL:HG11	1:J:291:LEU:HD21	1.94	0.49
1:J:352:GLU:HB3	1:J:400:PRO:HG3	1.94	0.49
1:K:202:LYS:HB3	2:L:188:PHE:CZ	2.47	0.49
1:K:202:LYS:HD3	2:L:188:PHE:CG	2.47	0.49
1:K:470:LEU:O	1:K:474:VAL:HG23	2.12	0.49
2:L:57:PHE:HB3	2:L:217:PRO:HG2	1.95	0.49
2:M:29:LEU:CD1	2:M:77:LEU:HA	2.42	0.49
2:M:60:THR:HA	2:M:63:ILE:HD12	1.93	0.49
2:M:93:LEU:HG	2:M:95:ARG:HH21	1.78	0.49
2:N:91:ASP:CB	2:N:95:ARG:HB2	2.42	0.49
2:N:129:GLN:HB3	2:N:169:THR:CB	2.42	0.49
1:A:28:CYS:SG	1:A:39:ILE:HD11	2.52	0.49
1:B:27:MET:SD	1:B:38:GLU:HG2	2.52	0.49
1:B:315:GLU:OE2	1:B:368:ARG:HB3	2.12	0.49
2:E:34:MET:HB2	2:E:36:ASN:OD1	2.12	0.49
2:E:93:LEU:HD12	2:E:95:ARG:NH1	2.27	0.49
2:E:281:LEU:HA	2:E:284:LEU:HD11	1.95	0.49
2:E:448:ASP:OD1	2:E:449:LEU:N	2.46	0.49
2:F:179:VAL:HG22	2:F:244:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:186:ILE:HB	2:F:190:GLU:OE1	2.12	0.49
2:F:326:GLN:HB2	2:F:348:LEU:N	2.27	0.49
1:I:213:GLN:NE2	1:I:244:GLN:HB3	2.28	0.49
1:I:262:ARG:NE	2:L:321:TYR:O	2.45	0.49
1:J:265:GLU:O	1:J:269:VAL:HG23	2.12	0.49
1:J:459:GLU:O	1:J:463:ILE:HG13	2.12	0.49
1:K:116:LYS:HD3	1:K:118:TRP:CZ2	2.48	0.49
1:K:247:LYS:HD2	1:K:276:LEU:HD13	1.94	0.49
2:L:206:ARG:O	2:L:206:ARG:HG2	2.12	0.49
2:N:129:GLN:HB3	2:N:169:THR:CA	2.42	0.49
1:A:43:ARG:HB3	1:A:44:GLN:C	2.33	0.49
1:B:56:SER:CA	2:E:26:TYR:HD2	2.26	0.49
1:B:85:ASP:OD1	1:B:89:ARG:N	2.27	0.49
2:E:76:PRO:O	2:E:78:GLN:HG3	2.13	0.49
2:E:183:ALA:O	2:E:212:ASN:HB2	2.12	0.49
2:E:324:GLU:HB2	2:E:350:ARG:O	2.13	0.49
2:F:428:ASP:O	2:F:432:GLU:HG3	2.12	0.49
1:I:91:LEU:HD12	1:I:91:LEU:N	2.25	0.49
1:I:144:ILE:HG21	1:I:288:ARG:HD3	1.94	0.49
1:I:266:MET:HE2	2:L:118:PRO:HB3	1.94	0.49
1:B:19:MET:N	1:B:45:ASP:O	2.25	0.49
1:B:30:VAL:O	1:B:35:VAL:HG22	2.13	0.49
2:D:57:PHE:HB3	2:D:217:PRO:HG2	1.94	0.49
2:D:132:ILE:HG22	2:D:134:ALA:N	2.27	0.49
1:J:285:LEU:O	1:J:288:ARG:HG3	2.12	0.49
1:K:5:LYS:HG3	1:K:61:GLY:CA	2.40	0.49
1:K:245:ILE:HG22	1:K:249:SER:OG	2.12	0.49
2:L:49:GLU:H	2:L:49:GLU:CD	2.16	0.49
2:L:60:THR:HA	2:L:63:ILE:HD12	1.94	0.49
2:M:183:ALA:HB1	2:M:186:ILE:HD11	1.95	0.49
1:A:130:VAL:HG22	1:A:157:GLY:H	1.77	0.49
1:A:498:GLU:HA	1:A:502:GLN:HG3	1.94	0.49
2:E:326:GLN:HG2	2:E:348:LEU:O	2.11	0.49
1:I:297:ASN:HB3	2:L:115:VAL:HG13	1.94	0.49
1:I:479:ILE:O	1:I:482:LEU:HG	2.12	0.49
1:I:550:VAL:O	1:I:554:GLU:HB2	2.12	0.49
1:J:75:LEU:HD13	1:J:316:TYR:HB2	1.94	0.49
1:K:16:ALA:O	1:K:46:VAL:HG22	2.13	0.49
2:L:10:GLU:H	2:L:17:ALA:HB3	1.76	0.49
2:N:117:ASN:HB3	2:N:120:ALA:HB3	1.95	0.49
2:N:183:ALA:CB	2:N:186:ILE:HD11	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:415:GLN:OE1	2:N:421:ARG:HD2	2.12	0.49
1:A:25:GLN:N	1:A:39:ILE:O	2.38	0.49
1:A:83:MET:CE	1:A:270:VAL:HG13	2.42	0.49
1:B:16:ALA:HB3	1:B:19:MET:HG3	1.95	0.49
1:B:20:SER:HB3	1:B:45:ASP:HA	1.94	0.49
1:B:225:GLY:O	1:B:370:GLY:HA2	2.12	0.49
1:C:225:GLY:HA2	1:C:384:ILE:O	2.13	0.49
2:D:178:ALA:O	2:D:243:VAL:HA	2.13	0.49
2:E:43:GLN:HB2	2:E:57:PHE:HE2	1.78	0.49
2:E:255:GLU:O	2:E:258:ARG:HG2	2.11	0.49
2:F:117:ASN:HB3	2:F:120:ALA:HB3	1.94	0.49
1:I:24:ILE:HG22	1:I:25:GLN:HG2	1.94	0.49
1:I:340:GLU:OE2	2:L:279:THR:OG1	2.25	0.49
1:J:425:PHE:HA	1:J:427:SER:N	2.28	0.49
1:K:237:GLY:HA2	4:K:601:ANP:PA	2.53	0.49
2:M:304:LEU:HD21	2:M:319:THR:OG1	2.12	0.49
2:N:235:LEU:HB2	2:N:243:VAL:HG21	1.95	0.49
1:A:97:VAL:HG11	1:A:109:LEU:HD21	1.95	0.49
1:B:49:ILE:HG22	1:B:50:GLN:O	2.12	0.49
1:B:238:LYS:HE2	1:B:391:SER:HB3	1.94	0.49
1:I:300:VAL:O	1:I:304:GLU:N	2.42	0.49
2:M:448:ASP:OD1	2:M:449:LEU:N	2.46	0.49
2:N:349:SER:HB3	2:N:352:LYS:CD	2.39	0.49
1:A:215:VAL:CG2	1:A:219:PHE:HD2	2.18	0.48
1:A:232:GLY:N	1:A:233:PRO:CD	2.76	0.48
1:A:516:GLU:HB2	1:A:567:LEU:HD21	1.95	0.48
1:B:330:SER:HB3	1:B:333:ARG:HG2	1.95	0.48
1:C:521:MET:O	1:C:525:ILE:HG13	2.13	0.48
2:D:77:LEU:HD21	2:D:93:LEU:HD22	1.94	0.48
1:J:177:GLU:HA	1:J:182:LEU:HA	1.95	0.48
1:J:202:LYS:HE2	1:J:372:VAL:CG1	2.43	0.48
1:A:39:ILE:HG12	1:A:49:ILE:HG12	1.94	0.48
1:A:120:PHE:HB2	1:A:187:MET:CE	2.43	0.48
1:A:159:VAL:HG22	1:A:176:ILE:CG1	2.40	0.48
1:A:251:VAL:HG21	1:A:325:ALA:CB	2.44	0.48
1:B:231:PRO:CD	1:B:412:PHE:HE1	2.26	0.48
1:B:253:LEU:HB2	1:B:324:VAL:HG22	1.94	0.48
1:B:258:GLY:O	1:B:294:ASN:N	2.38	0.48
1:C:211:THR:HG21	1:C:216:ILE:HG22	1.95	0.48
2:D:132:ILE:HG22	2:D:134:ALA:H	1.77	0.48
2:D:150:PHE:HB2	2:D:328:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:183:ALA:HB1	2:E:186:ILE:CD1	2.43	0.48
1:J:303:ARG:NH2	2:M:279:THR:HG22	2.28	0.48
1:K:38:GLU:N	1:K:50:GLN:O	2.37	0.48
1:K:121:GLU:HB3	1:K:138:TYR:CZ	2.49	0.48
1:K:400:PRO:O	1:K:404:ASN:ND2	2.28	0.48
2:L:81:VAL:HB	2:L:234:TYR:CD2	2.48	0.48
2:L:315:ILE:HB	2:L:316:PRO:CD	2.43	0.48
2:N:31:GLU:OE1	2:N:71:ARG:NH2	2.46	0.48
2:N:130:THR:HG21	2:N:135:ILE:HG22	1.94	0.48
2:N:346:PRO:N	2:N:347:SER:HA	2.27	0.48
1:A:130:VAL:CG2	1:A:157:GLY:H	2.26	0.48
2:D:29:LEU:HB2	2:D:73:LEU:HD21	1.95	0.48
2:E:81:VAL:HG11	2:E:234:TYR:CG	2.48	0.48
2:E:109:LEU:HD13	2:E:230:THR:HG22	1.94	0.48
2:E:235:LEU:O	2:E:239:LYS:HB2	2.13	0.48
2:F:235:LEU:O	2:F:240:GLY:N	2.47	0.48
1:I:318:ARG:HG3	1:I:384:ILE:CG1	2.33	0.48
1:K:30:VAL:HG13	1:K:64:VAL:HG22	1.95	0.48
1:K:245:ILE:O	1:K:249:SER:N	2.47	0.48
2:L:6:ARG:NH2	2:L:69:SER:CA	2.76	0.48
2:M:155:LEU:O	2:M:157:HIS:ND1	2.47	0.48
2:M:203:ALA:HA	2:M:206:ARG:NH1	2.28	0.48
2:N:346:PRO:C	2:N:348:LEU:HB2	2.33	0.48
2:N:347:SER:N	2:N:348:LEU:HA	2.27	0.48
1:A:396:ASP:N	1:A:396:ASP:OD2	2.47	0.48
1:B:265:GLU:O	1:B:269:VAL:HG23	2.13	0.48
1:B:270:VAL:O	1:B:274:PRO:HG2	2.13	0.48
1:B:297:ASN:ND2	2:E:115:VAL:HG13	2.27	0.48
1:B:311:ILE:HB	1:B:365:TYR:HE1	1.77	0.48
1:C:290:VAL:HG21	1:C:317:PHE:HE2	1.77	0.48
2:E:43:GLN:HB2	2:E:57:PHE:CE2	2.49	0.48
1:I:10:SER:HB3	1:I:13:LEU:O	2.13	0.48
2:L:140:THR:OG1	2:L:352:LYS:HB2	2.13	0.48
2:N:248:THR:HA	2:N:249:ASP:HA	1.56	0.48
1:A:497:ARG:HA	1:A:501:LEU:CB	2.40	0.48
1:B:14:VAL:HG21	1:B:51:VAL:HG21	1.95	0.48
1:B:231:PRO:HD2	1:B:413:TRP:O	2.14	0.48
1:C:33:LEU:H	1:C:33:LEU:HD12	1.78	0.48
1:C:121:GLU:HA	1:C:164:SER:OG	2.13	0.48
2:D:141:LEU:HD12	2:D:145:GLN:OE1	2.12	0.48
2:D:254:ALA:O	2:D:258:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:ARG:HD2	2:F:201:THR:HG21	1.96	0.48
2:F:345:LEU:N	2:F:346:PRO:HD2	2.28	0.48
1:I:231:PRO:HG3	1:I:412:PHE:CZ	2.49	0.48
1:I:254:VAL:HG22	1:I:325:ALA:HB3	1.96	0.48
1:J:242:GLN:OE1	1:J:329:ASP:HB2	2.13	0.48
1:K:191:TRP:CE3	1:K:192:PRO:HD2	2.49	0.48
2:L:32:VAL:HG13	2:L:70:VAL:HG22	1.96	0.48
2:L:88:ARG:NH1	2:L:101:PRO:O	2.46	0.48
2:L:146:LYS:HA	2:L:300:GLN:O	2.12	0.48
2:L:282:ALA:HA	2:L:322:ILE:HG21	1.96	0.48
2:M:15:LEU:HD23	2:M:55:GLN:HG3	1.94	0.48
1:B:517:LYS:HD3	1:B:564:GLU:OE2	2.13	0.48
1:C:133:GLY:O	1:C:380:ARG:NH1	2.40	0.48
2:D:390:GLY:HA2	2:D:391:GLU:HA	1.54	0.48
2:F:46:GLU:HG2	2:F:47:VAL:N	2.28	0.48
2:F:91:ASP:OD1	2:F:94:GLY:N	2.47	0.48
2:F:251:THR:HG22	2:F:315:ILE:HG21	1.96	0.48
1:K:132:ALA:O	1:K:375:LEU:HB3	2.14	0.48
2:L:349:SER:HB3	2:L:352:LYS:NZ	2.29	0.48
2:M:274:PRO:HB3	2:M:276:TYR:CE2	2.49	0.48
2:N:32:VAL:HG21	2:N:56:ILE:HD12	1.95	0.48
2:N:146:LYS:HG2	2:N:285:PHE:O	2.12	0.48
1:A:168:THR:OG1	1:A:171:ASP:OD2	2.23	0.48
1:B:27:MET:CE	1:B:52:TYR:HE2	2.27	0.48
1:C:237:GLY:O	1:C:241:VAL:HG23	2.14	0.48
2:D:30:ILE:N	2:D:42:GLY:O	2.41	0.48
2:D:222:ILE:HG22	2:D:226:ARG:HH21	1.78	0.48
2:F:26:TYR:O	2:F:27:GLU:HB2	2.14	0.48
2:F:150:PHE:O	2:F:329:LEU:HD12	2.14	0.48
1:K:8:LYS:CG	2:N:48:GLN:HB3	2.44	0.48
1:K:425:PHE:HA	1:K:426:PRO:C	2.33	0.48
2:L:219:ILE:HA	2:L:222:ILE:HD12	1.94	0.48
2:M:90:PHE:O	2:M:210:PHE:HA	2.14	0.48
2:M:180:VAL:HB	2:M:245:VAL:HG22	1.96	0.48
2:N:29:LEU:HD12	2:N:42:GLY:O	2.13	0.48
1:A:392:PRO:HB3	1:A:399:GLU:CD	2.34	0.48
1:A:531:GLU:HB3	1:A:581:ILE:HG13	1.95	0.48
1:B:12:PRO:HB2	1:B:344:ARG:HB3	1.95	0.48
1:C:14:VAL:HG23	1:C:51:VAL:HG13	1.95	0.48
1:C:568:ALA:O	1:C:570:ILE:HA	2.12	0.48
1:K:55:THR:O	2:N:26:TYR:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:257:LEU:HA	2:L:260:ILE:HD11	1.95	0.48
1:A:497:ARG:CA	1:A:501:LEU:HB2	2.40	0.48
1:B:190:LYS:HB2	1:B:190:LYS:NZ	2.28	0.48
1:B:196:GLY:HA2	1:B:368:ARG:CZ	2.43	0.48
1:B:443:ARG:O	1:B:447:GLN:HB2	2.14	0.48
1:C:11:GLY:O	1:C:55:THR:OG1	2.24	0.48
1:C:274:PRO:HA	1:C:284:SER:HB2	1.96	0.48
2:F:16:MET:HB2	2:F:54:VAL:CG2	2.37	0.48
2:F:33:ARG:HD2	2:F:71:ARG:HD3	1.96	0.48
1:I:6:ILE:CG1	1:I:64:VAL:HG22	2.44	0.48
1:K:199:ILE:HG21	1:K:372:VAL:HG21	1.95	0.48
1:K:231:PRO:CA	1:K:390:VAL:O	2.56	0.48
1:A:297:ASN:CG	2:D:286:GLU:HG3	2.34	0.48
1:B:120:PHE:HB2	1:B:187:MET:CE	2.43	0.48
1:C:85:ASP:OD1	1:C:89:ARG:N	2.46	0.48
1:C:120:PHE:CE2	1:C:137:GLY:HA3	2.49	0.48
2:D:88:ARG:HH12	2:D:102:GLU:CB	2.27	0.48
2:D:409:GLU:HA	2:D:413:VAL:HB	1.95	0.48
2:F:273:TYR:CE2	2:F:314:PRO:HG2	2.48	0.48
1:I:253:LEU:HG	1:I:317:PHE:CD1	2.49	0.48
1:J:339:ARG:HG3	1:J:353:GLY:O	2.14	0.48
1:J:513:THR:HG23	1:J:517:LYS:HG2	1.95	0.48
1:K:6:ILE:CG1	1:K:64:VAL:HG23	2.43	0.48
1:K:150:MET:HE3	1:K:320:MET:HG2	1.96	0.48
1:K:175:VAL:HA	1:K:184:GLU:HA	1.95	0.48
1:K:251:VAL:HG11	1:K:325:ALA:HB2	1.96	0.48
2:L:10:GLU:HA	2:L:65:LEU:HD23	1.96	0.48
2:L:92:GLY:O	2:L:227:MET:HE2	2.14	0.48
2:L:349:SER:C	2:L:352:LYS:HZ1	2.16	0.48
2:N:27:GLU:HA	2:N:27:GLU:OE2	2.13	0.48
2:N:34:MET:SD	2:N:63:ILE:HG12	2.53	0.48
2:N:185:GLY:CA	2:N:214:ALA:HA	2.41	0.48
1:B:352:GLU:CB	1:B:400:PRO:HG3	2.44	0.47
2:E:440:THR:O	2:E:443:LYS:HG3	2.14	0.47
2:F:282:ALA:HA	2:F:322:ILE:HG21	1.96	0.47
2:F:379:GLY:HA3	2:F:405:ALA:HB2	1.96	0.47
1:I:114:HIS:ND1	1:I:169:ILE:HD11	2.29	0.47
1:I:253:LEU:HD12	1:I:288:ARG:O	2.14	0.47
1:J:373:ILE:HD13	1:J:381:GLU:HB2	1.95	0.47
1:J:373:ILE:HD13	1:J:381:GLU:HG3	1.96	0.47
2:L:90:PHE:HE1	2:L:96:PRO:CB	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:334:TYR:HB2	2:L:341:PRO:HG3	1.96	0.47
2:M:15:LEU:HD22	2:M:55:GLN:HG3	1.97	0.47
2:M:21:VAL:HG13	2:M:24:VAL:CG2	2.44	0.47
2:N:126:GLU:HG2	2:N:143:ARG:HG3	1.94	0.47
2:N:352:LYS:H	2:N:352:LYS:HG2	1.36	0.47
1:B:304:GLU:HA	1:B:334:TRP:CD1	2.48	0.47
1:C:139:VAL:HG23	1:C:149:ILE:CD1	2.33	0.47
1:C:211:THR:HG21	1:C:216:ILE:HG21	1.96	0.47
2:D:249:ASP:HB3	2:D:252:ASN:ND2	2.28	0.47
1:I:43:ARG:CG	1:I:46:VAL:HG13	2.44	0.47
2:M:3:LYS:NZ	2:M:3:LYS:HB2	2.28	0.47
2:M:137:HIS:NE2	2:M:365:HIS:O	2.47	0.47
1:B:237:GLY:HA2	4:B:601:ANP:PA	2.54	0.47
1:C:205:PRO:HB2	1:C:224:LYS:O	2.14	0.47
1:C:253:LEU:O	1:C:325:ALA:N	2.46	0.47
2:D:132:ILE:HB	2:D:135:ILE:HG13	1.96	0.47
2:F:34:MET:HE2	2:F:38:GLU:HB3	1.96	0.47
1:K:2:GLN:OE1	1:K:20:SER:HB3	2.14	0.47
1:K:549:THR:O	1:K:553:ARG:HG3	2.14	0.47
2:M:28:GLU:O	2:M:44:VAL:HG23	2.15	0.47
2:M:324:GLU:C	2:M:350:ARG:HD2	2.34	0.47
2:N:34:MET:HG3	2:N:38:GLU:HB3	1.96	0.47
2:N:188:PHE:CZ	2:N:192:GLU:HG2	2.49	0.47
1:A:219:PHE:HE2	1:A:501:LEU:HD23	1.79	0.47
1:C:374:ALA:HB3	1:C:380:ARG:HG2	1.97	0.47
2:D:137:HIS:CE1	2:D:368:THR:HB	2.49	0.47
2:E:396:ASP:HA	2:E:399:LYS:HG3	1.94	0.47
2:F:30:ILE:HG22	2:F:72:PHE:CD1	2.50	0.47
2:F:155:LEU:HD13	2:F:329:LEU:HB3	1.97	0.47
2:F:273:TYR:HB3	2:F:277:LEU:HD22	1.95	0.47
2:F:439:ARG:CG	2:F:450:LEU:HD13	2.45	0.47
1:I:159:VAL:HA	1:I:176:ILE:HA	1.96	0.47
1:I:177:GLU:HG3	1:I:182:LEU:N	2.29	0.47
1:I:249:SER:HB3	1:I:251:VAL:HG22	1.95	0.47
1:I:253:LEU:HG	1:I:317:PHE:HD1	1.79	0.47
1:J:415:LEU:CD2	1:J:428:ILE:HG13	2.38	0.47
1:K:479:ILE:HG22	2:N:394:LEU:HA	1.95	0.47
2:L:128:ILE:HD13	2:L:177:PHE:CZ	2.50	0.47
2:N:137:HIS:HB3	2:N:412:TYR:OH	2.15	0.47
1:A:317:PHE:HA	1:A:320:MET:SD	2.54	0.47
1:B:179:GLU:OE2	1:B:180:GLN:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:ASN:ND2	2:D:189:GLU:HA	2.29	0.47
2:E:17:ALA:HA	2:E:52:ALA:O	2.15	0.47
2:E:326:GLN:N	2:E:348:LEU:O	2.47	0.47
2:F:229:LEU:HD22	2:F:300:GLN:OE1	2.14	0.47
1:I:343:GLY:HA3	2:L:275:GLY:HA3	1.97	0.47
2:M:91:ASP:CG	2:M:95:ARG:HG2	2.34	0.47
2:M:376:TYR:OH	2:M:409:GLU:OE2	2.32	0.47
1:B:11:GLY:N	1:B:12:PRO:CD	2.78	0.47
1:B:415:LEU:HG	1:B:428:ILE:HD13	1.96	0.47
1:C:378:ASP:OD1	1:C:378:ASP:N	2.46	0.47
1:C:524:VAL:HG13	1:C:573:ILE:HG21	1.94	0.47
2:D:231:ALA:O	2:D:235:LEU:HG	2.15	0.47
2:E:217:PRO:HD2	2:E:220:GLU:OE2	2.15	0.47
2:F:147:LEU:O	2:F:301:ILE:HA	2.14	0.47
1:I:73:VAL:CG1	1:I:309:THR:HG23	2.44	0.47
1:I:584:ILE:O	1:I:584:ILE:HG22	2.14	0.47
2:L:242:HIS:HD2	2:L:296:GLY:HA2	1.79	0.47
2:M:32:VAL:HG21	2:M:56:ILE:HD11	1.96	0.47
2:M:40:ARG:CG	2:M:56:ILE:HG21	2.44	0.47
2:N:340:PRO:HB3	2:N:417:PHE:CE1	2.49	0.47
1:A:7:ILE:O	2:D:49:GLU:HG2	2.14	0.47
1:A:39:ILE:HA	1:A:49:ILE:HA	1.97	0.47
1:A:225:GLY:HA3	1:A:370:GLY:HA2	1.96	0.47
1:A:274:PRO:HA	1:A:286:MET:HG2	1.97	0.47
1:B:16:ALA:O	1:B:46:VAL:HA	2.15	0.47
1:B:73:VAL:HG13	1:B:193:VAL:HG12	1.97	0.47
1:B:193:VAL:HG11	1:B:309:THR:HG22	1.96	0.47
1:B:244:GLN:OE1	1:B:511:THR:OG1	2.30	0.47
1:B:301:ALA:HB2	1:B:341:MET:HE1	1.96	0.47
1:B:362:LEU:HD13	1:B:405:THR:CG2	2.43	0.47
1:C:238:LYS:HG3	4:C:601:ANP:O2B	2.15	0.47
1:C:327:MET:HE3	1:C:387:ILE:HB	1.97	0.47
2:D:61:SER:O	2:D:63:ILE:HD12	2.15	0.47
2:D:132:ILE:HD11	2:D:163:GLN:NE2	2.30	0.47
2:D:141:LEU:HD22	2:D:147:LEU:CD2	2.41	0.47
2:D:152:GLY:N	2:D:155:LEU:HD12	2.28	0.47
2:E:95:ARG:HG2	2:E:95:ARG:HH11	1.78	0.47
2:E:423:ILE:HG13	2:E:427:LEU:HD11	1.97	0.47
2:F:111:ILE:HG13	2:F:112:ASN:N	2.29	0.47
2:F:157:HIS:CD2	2:F:158:LYS:HG3	2.50	0.47
2:F:413:VAL:HG12	2:F:414:ASN:CG	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:252:ASP:HB2	1:I:253:LEU:HD22	1.97	0.47
1:I:501:LEU:HD13	1:I:502:GLN:N	2.30	0.47
1:J:139:VAL:HG12	1:J:140:ASP:N	2.29	0.47
1:J:150:MET:CE	1:J:320:MET:HG2	2.45	0.47
1:J:225:GLY:O	1:J:370:GLY:HA2	2.15	0.47
2:L:147:LEU:HB3	2:L:301:ILE:HG12	1.96	0.47
2:L:158:LYS:HG3	2:L:194:PHE:CZ	2.49	0.47
2:M:146:LYS:HD3	2:M:285:PHE:O	2.15	0.47
1:A:308:TYR:O	1:A:312:THR:OG1	2.28	0.47
1:C:216:ILE:HD12	1:C:245:ILE:HD11	1.96	0.47
2:D:10:GLU:H	2:D:17:ALA:HB3	1.80	0.47
2:D:306:MET:CE	2:D:311:LYS:HA	2.44	0.47
2:E:86:ILE:HD13	2:E:208:VAL:CG2	2.44	0.47
1:I:6:ILE:CD1	1:I:30:VAL:HG13	2.45	0.47
1:I:134:ASP:O	1:I:151:VAL:HG23	2.15	0.47
1:I:425:PHE:HA	1:I:426:PRO:C	2.34	0.47
1:I:552:VAL:O	1:I:556:ILE:HG13	2.15	0.47
1:J:351:ASP:OD2	1:J:351:ASP:N	2.48	0.47
1:K:202:LYS:CG	1:K:372:VAL:HG12	2.42	0.47
1:K:259:CYS:SG	1:K:303:ARG:HB3	2.55	0.47
2:L:244:LEU:HA	2:L:299:THR:O	2.14	0.47
2:M:109:LEU:O	2:M:230:THR:HG21	2.15	0.47
2:M:137:HIS:HE1	2:M:368:THR:OG1	1.98	0.47
1:A:90:PRO:HD3	1:A:111:ALA:HA	1.96	0.47
1:A:436:LEU:HD12	1:A:436:LEU:H	1.80	0.47
1:A:521:MET:HE1	1:A:560:LYS:HB3	1.97	0.47
1:A:552:VAL:O	1:A:556:ILE:HG13	2.14	0.47
1:B:27:MET:HE1	1:B:52:TYR:HE2	1.80	0.47
2:E:163:GLN:O	2:E:167:GLN:HB2	2.13	0.47
2:F:163:GLN:HA	2:F:166:ARG:NH1	2.30	0.47
1:I:122:ALA:HA	1:I:137:GLY:HA3	1.97	0.47
1:I:340:GLU:OE1	2:L:278:TYR:HB3	2.15	0.47
1:J:74:GLU:HB2	1:J:111:ALA:HB3	1.97	0.47
1:J:84:PHE:O	1:J:293:ALA:N	2.47	0.47
1:K:6:ILE:HG21	1:K:9:VAL:HG23	1.97	0.47
1:K:18:ASN:ND2	1:K:18:ASN:O	2.44	0.47
1:K:507:ASP:HB3	1:K:510:ASP:HB3	1.96	0.47
2:M:16:MET:CE	2:M:32:VAL:HG21	2.45	0.47
2:M:324:GLU:CB	2:M:350:ARG:HB2	2.44	0.47
2:N:341:PRO:HD2	2:N:417:PHE:HZ	1.78	0.47
1:A:71:LEU:O	1:A:193:VAL:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:TRP:CZ3	1:A:279:PRO:HG2	2.50	0.47
1:C:7:ILE:HB	2:F:49:GLU:CB	2.45	0.47
1:C:102:PHE:HB3	2:F:114:GLU:HB2	1.97	0.47
2:D:32:VAL:HG22	2:D:70:VAL:HG13	1.97	0.47
2:D:148:PRO:HG2	2:D:325:GLY:O	2.15	0.47
2:E:78:GLN:HG2	2:E:110:ASP:HA	1.97	0.47
2:E:357:GLY:N	2:E:358:ALA:CA	2.77	0.47
1:I:262:ARG:O	1:I:266:MET:HB2	2.15	0.47
1:J:9:VAL:CG2	1:J:58:ILE:HB	2.21	0.47
1:J:364:GLU:HG2	2:N:215:ASN:HB2	1.96	0.47
1:K:33:LEU:HD22	1:K:106:GLY:HA3	1.97	0.47
1:K:188:MET:HE1	1:K:190:LYS:HG3	1.95	0.47
2:L:381:GLN:O	2:L:385:LEU:N	2.39	0.47
2:M:219:ILE:H	2:M:219:ILE:HD12	1.80	0.47
2:M:222:ILE:HG23	2:M:253:TYR:CE1	2.50	0.47
2:M:235:LEU:O	2:M:239:LYS:HB2	2.14	0.47
2:M:257:LEU:HD21	2:M:276:TYR:HE1	1.80	0.47
1:A:268:ASP:O	1:A:272:GLU:HB2	2.16	0.46
1:A:346:GLU:HG2	2:D:267:VAL:HB	1.97	0.46
1:C:7:ILE:HG23	1:C:17:GLU:HB2	1.97	0.46
1:C:44:GLN:CG	1:C:45:ASP:H	2.28	0.46
2:E:143:ARG:HH21	2:E:170:VAL:HG12	1.80	0.46
2:E:160:LEU:O	2:E:164:ILE:HG13	2.14	0.46
2:F:345:LEU:HA	2:F:373:PHE:CZ	2.50	0.46
1:J:114:HIS:O	1:J:168:THR:HB	2.15	0.46
1:J:232:GLY:CA	1:J:415:LEU:HG	2.44	0.46
1:J:371:ARG:HA	1:J:383:SER:HA	1.97	0.46
1:K:29:LEU:HB2	1:K:65:ARG:HG3	1.95	0.46
1:K:265:GLU:O	1:K:269:VAL:HG23	2.14	0.46
2:L:155:LEU:CD1	2:L:329:LEU:HB3	2.38	0.46
2:L:258:ARG:HD2	2:L:273:TYR:HD2	1.80	0.46
2:L:318:LEU:O	2:L:322:ILE:HG13	2.15	0.46
2:M:258:ARG:HH21	2:M:272:GLY:HA3	1.80	0.46
2:N:345:LEU:N	2:N:346:PRO:CD	2.78	0.46
1:A:262:ARG:NE	2:D:321:TYR:O	2.48	0.46
1:A:336:GLU:OE2	1:A:339:ARG:HD2	2.16	0.46
1:B:214:ARG:CB	1:B:500:TYR:CE2	2.95	0.46
1:B:251:VAL:HG21	1:B:325:ALA:CB	2.45	0.46
1:C:220:PHE:HB3	1:C:435:SER:HB2	1.96	0.46
1:C:243:HIS:O	1:C:247:LYS:HD2	2.15	0.46
2:F:88:ARG:NH2	2:F:98:ASP:OD1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:442:LEU:HD12	2:F:445:ILE:HD11	1.96	0.46
1:I:314:ALA:HB1	1:I:324:VAL:HG11	1.98	0.46
1:K:534:LYS:NZ	1:K:534:LYS:HB2	2.30	0.46
2:L:6:ARG:HE	2:L:8:ILE:CG1	2.28	0.46
2:L:44:VAL:HG13	2:L:53:MET:O	2.15	0.46
2:L:134:ALA:O	2:L:138:LEU:HB2	2.15	0.46
2:L:338:ILE:HG23	2:L:414:ASN:CG	2.35	0.46
2:M:16:MET:HE3	2:M:16:MET:HB2	1.69	0.46
1:C:256:TYR:HB3	1:C:291:LEU:HD12	1.96	0.46
1:C:405:THR:O	1:C:409:VAL:HG22	2.14	0.46
2:D:44:VAL:HG11	2:D:47:VAL:CG1	2.46	0.46
2:E:325:GLY:HA2	2:E:350:ARG:HG2	1.97	0.46
2:E:350:ARG:HA	2:E:351:LEU:HA	1.57	0.46
2:F:29:LEU:HD12	2:F:42:GLY:O	2.16	0.46
1:I:424:HIS:C	1:I:425:PHE:HD1	2.18	0.46
1:I:449:LEU:O	1:I:451:GLN:NE2	2.44	0.46
1:J:206:ASP:OD1	1:J:206:ASP:N	2.47	0.46
2:L:9:LYS:HD2	2:L:19:GLU:HG3	1.95	0.46
2:L:253:TYR:CE1	2:L:284:LEU:HD11	2.50	0.46
1:A:43:ARG:HB3	1:A:44:GLN:HA	1.95	0.46
1:A:86:GLY:H	1:A:294:ASN:ND2	2.11	0.46
1:B:102:PHE:HB3	2:E:114:GLU:HB3	1.97	0.46
1:B:496:ILE:HA	1:B:525:ILE:HD13	1.98	0.46
1:C:496:ILE:O	1:C:500:TYR:N	2.38	0.46
2:D:63:ILE:HG23	2:D:68:SER:OG	2.14	0.46
2:E:5:TYR:CZ	2:E:21:VAL:HG23	2.51	0.46
2:E:183:ALA:HB3	2:E:211:MET:HA	1.98	0.46
2:E:340:PRO:HD2	2:E:414:ASN:HA	1.97	0.46
1:I:307:ILE:HD11	1:I:334:TRP:CE2	2.51	0.46
1:I:463:ILE:HG22	1:I:493:ALA:HB2	1.97	0.46
2:M:226:ARG:NH1	2:M:284:LEU:HD21	2.30	0.46
2:M:324:GLU:HA	2:M:350:ARG:HH11	1.79	0.46
2:M:408:PHE:HD1	2:M:412:TYR:HB3	1.81	0.46
2:N:204:ILE:O	2:N:207:SER:OG	2.33	0.46
1:B:94:PHE:HZ	1:B:104:GLY:H	1.63	0.46
2:D:45:LEU:HB2	2:D:264:ARG:HD3	1.97	0.46
1:I:133:GLY:O	1:I:380:ARG:NH2	2.45	0.46
1:I:385:THR:H	1:I:385:THR:HG1	1.57	0.46
1:J:521:MET:HE1	1:J:560:LYS:HB3	1.97	0.46
2:M:133:SER:OG	2:M:412:TYR:O	2.33	0.46
1:B:92:ASP:OD1	1:B:93:THR:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:473:ILE:O	1:J:477:VAL:HG22	2.16	0.46
1:K:415:LEU:CD2	1:K:428:ILE:HG12	2.45	0.46
1:K:479:ILE:HA	1:K:482:LEU:HD13	1.97	0.46
2:L:127:PHE:CE1	2:L:140:THR:HB	2.51	0.46
2:L:345:LEU:N	2:L:346:PRO:HD2	2.30	0.46
2:N:26:TYR:O	2:N:27:GLU:HB2	2.15	0.46
2:N:88:ARG:HH22	2:N:96:PRO:CB	2.29	0.46
2:N:419:THR:HG22	2:N:421:ARG:HG3	1.97	0.46
1:A:39:ILE:CG1	1:A:49:ILE:HG12	2.45	0.46
1:A:466:GLU:O	1:A:470:LEU:HG	2.15	0.46
1:B:254:VAL:HG23	1:B:288:ARG:NH2	2.31	0.46
1:B:337:ALA:O	1:B:341:MET:HG2	2.15	0.46
1:C:232:GLY:O	1:C:392:PRO:HD2	2.14	0.46
2:D:32:VAL:HA	2:D:70:VAL:HA	1.98	0.46
1:I:478:GLY:O	1:I:481:SER:OG	2.16	0.46
1:J:137:GLY:O	1:J:149:ILE:HG12	2.15	0.46
1:K:213:GLN:HB2	1:K:216:ILE:HG12	1.95	0.46
1:K:329:ASP:HA	1:K:330:SER:HA	1.48	0.46
2:N:340:PRO:HD3	2:N:416:GLY:N	2.27	0.46
1:B:285:LEU:HD11	1:B:288:ARG:CD	2.43	0.46
1:C:26:ASP:O	1:C:39:ILE:HD12	2.16	0.46
1:C:318:ARG:CB	1:C:384:ILE:HD11	2.45	0.46
2:E:34:MET:HG2	2:E:38:GLU:O	2.16	0.46
1:I:42:MET:SD	1:I:47:ALA:HB2	2.56	0.46
1:I:120:PHE:CE1	1:I:173:ILE:HD12	2.51	0.46
1:J:5:LYS:HD2	1:J:61:GLY:HA2	1.97	0.46
1:J:251:VAL:HG21	1:J:325:ALA:CB	2.45	0.46
1:K:9:VAL:HG21	1:K:58:ILE:CG2	2.46	0.46
1:K:213:GLN:HG2	1:K:216:ILE:HD11	1.97	0.46
2:L:121:ARG:NH1	2:L:288:ALA:O	2.41	0.46
2:L:144:GLY:HA2	2:L:298:VAL:O	2.15	0.46
2:L:212:ASN:OD1	2:L:224:THR:OG1	2.12	0.46
2:M:239:LYS:HB2	2:M:241:MET:HG2	1.97	0.46
2:M:409:GLU:HA	2:M:413:VAL:CG2	2.46	0.46
2:N:32:VAL:O	2:N:40:ARG:N	2.44	0.46
2:N:336:SER:HB2	2:N:337:GLY:CA	2.41	0.46
2:N:381:GLN:HA	2:N:384:GLU:CG	2.46	0.46
1:B:42:MET:HE1	1:B:47:ALA:HB2	1.97	0.46
1:B:331:THR:HG23	1:B:390:VAL:HG22	1.97	0.46
1:B:437:TYR:OH	2:F:189:GLU:OE1	2.32	0.46
1:B:549:THR:O	1:B:552:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:601:ANP:O1A	4:B:601:ANP:N3B	2.49	0.46
4:B:601:ANP:O3'	2:E:350:ARG:HB2	2.16	0.46
1:C:161:LYS:HE3	1:C:175:VAL:HG23	1.98	0.46
1:C:234:PHE:CD1	1:C:234:PHE:N	2.80	0.46
2:D:93:LEU:HD21	2:D:220:GLU:HG2	1.98	0.46
2:D:313:HIS:CE1	2:D:314:PRO:HD2	2.51	0.46
2:E:225:PRO:O	2:E:229:LEU:HG	2.16	0.46
1:I:103:LEU:N	2:L:115:VAL:O	2.39	0.46
1:I:262:ARG:HD2	1:I:262:ARG:N	2.31	0.46
1:J:436:LEU:HD21	2:N:154:GLY:O	2.15	0.46
1:K:44:GLN:N	2:L:10:GLU:HG2	2.31	0.46
2:L:136:ASP:O	2:L:140:THR:HG22	2.16	0.46
2:L:430:GLY:O	2:L:434:LEU:HB2	2.15	0.46
2:M:30:ILE:HG21	2:M:54:VAL:HG11	1.98	0.46
2:M:222:ILE:HD11	2:M:257:LEU:HA	1.98	0.46
1:A:37:GLY:HA3	1:A:51:VAL:HG22	1.98	0.46
1:B:83:MET:HE2	1:B:291:LEU:CD2	2.45	0.46
1:B:200:LYS:NZ	1:B:379:GLN:OE1	2.49	0.46
2:D:282:ALA:HA	2:D:322:ILE:HG21	1.98	0.46
2:E:95:ARG:HG3	2:E:95:ARG:H	1.58	0.46
2:E:127:PHE:CE2	2:E:129:GLN:HA	2.51	0.46
1:I:91:LEU:HB2	2:L:119:ILE:HD13	1.98	0.46
1:J:73:VAL:HG11	1:J:309:THR:HG23	1.97	0.46
2:L:30:ILE:HG12	2:L:54:VAL:HB	1.97	0.46
2:M:351:LEU:HD23	2:M:351:LEU:N	2.31	0.46
2:N:88:ARG:NH2	2:N:100:GLY:H	2.14	0.46
2:N:151:SER:OG	2:N:155:LEU:HB2	2.15	0.46
2:N:336:SER:N	2:N:337:GLY:HA2	2.31	0.46
1:B:230:VAL:HG12	1:B:415:LEU:CD1	2.46	0.45
1:C:214:ARG:NH2	1:C:560:LYS:HB2	2.31	0.45
2:D:183:ALA:HB1	2:D:186:ILE:CD1	2.46	0.45
2:E:60:THR:HA	2:E:63:ILE:HD12	1.98	0.45
2:E:339:GLN:HA	2:E:341:PRO:HD3	1.98	0.45
1:I:83:MET:CE	2:L:119:ILE:CG2	2.90	0.45
1:I:214:ARG:HG2	1:I:513:THR:HB	1.97	0.45
1:I:220:PHE:HB3	1:I:413:TRP:HE1	1.80	0.45
2:M:102:GLU:CD	2:M:102:GLU:H	2.14	0.45
2:N:92:GLY:C	2:N:93:LEU:HD23	2.35	0.45
2:D:281:LEU:HD22	2:D:285:PHE:CE2	2.39	0.45
2:D:408:PHE:HE1	2:D:412:TYR:CD2	2.34	0.45
1:I:243:HIS:HB3	1:I:276:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:469:GLN:O	1:I:473:ILE:HG13	2.16	0.45
1:J:13:LEU:HD12	1:J:50:GLN:N	2.31	0.45
1:J:15:MET:HG2	1:J:48:SER:HA	1.99	0.45
1:J:16:ALA:O	1:J:46:VAL:HA	2.17	0.45
1:J:329:ASP:HA	1:J:330:SER:HA	1.50	0.45
1:J:419:LEU:HA	1:J:422:LYS:HD2	1.97	0.45
1:J:445:MET:SD	1:J:515:ARG:NH1	2.89	0.45
1:K:83:MET:SD	1:K:91:LEU:HD12	2.57	0.45
1:K:102:PHE:HB3	2:N:114:GLU:HB2	1.98	0.45
2:L:14:PRO:O	2:L:55:GLN:HA	2.16	0.45
2:L:149:VAL:HG22	2:L:327:ILE:HG13	1.97	0.45
2:L:264:ARG:HB3	2:L:266:GLU:HG3	1.98	0.45
2:N:29:LEU:O	2:N:73:LEU:HB2	2.15	0.45
2:N:85:MET:HG2	2:N:90:PHE:CZ	2.51	0.45
2:N:129:GLN:CB	2:N:169:THR:CB	2.94	0.45
1:A:307:ILE:HG13	1:A:308:TYR:N	2.30	0.45
1:B:15:MET:HG2	1:B:48:SER:OG	2.17	0.45
1:B:152:PRO:CD	1:B:185:LEU:HD22	2.46	0.45
1:B:214:ARG:HG3	1:B:500:TYR:O	2.15	0.45
1:C:230:VAL:CG2	1:C:413:TRP:HE3	2.30	0.45
1:C:247:LYS:HE2	1:C:276:LEU:CD1	2.46	0.45
1:C:257:VAL:HG22	1:C:292:ILE:HD13	1.98	0.45
2:D:21:VAL:HB	2:D:24:VAL:HG21	1.98	0.45
2:D:26:TYR:CE2	2:D:27:GLU:HG3	2.51	0.45
2:E:260:ILE:O	2:E:264:ARG:HG3	2.17	0.45
1:I:273:PHE:HB3	1:I:274:PRO:HD3	1.97	0.45
2:L:18:VAL:HG11	2:L:72:PHE:CZ	2.51	0.45
2:L:44:VAL:HG22	2:L:54:VAL:CG1	2.45	0.45
2:M:134:ALA:O	2:M:139:ASN:N	2.46	0.45
1:A:131:SER:N	1:A:134:ASP:OD2	2.36	0.45
1:A:220:PHE:CE1	1:A:433:SER:HB2	2.51	0.45
1:B:78:GLY:H	1:B:141:GLU:CD	2.20	0.45
1:B:412:PHE:O	1:B:433:SER:HB2	2.17	0.45
1:B:454:SER:O	1:B:458:THR:OG1	2.35	0.45
1:B:573:ILE:O	1:B:577:ILE:HG13	2.16	0.45
1:C:75:LEU:HD13	1:C:316:TYR:CG	2.51	0.45
1:C:237:GLY:HA2	4:C:601:ANP:O2A	2.16	0.45
1:C:246:ALA:HB1	1:C:254:VAL:HG11	1.98	0.45
1:C:300:VAL:HG13	1:C:303:ARG:NE	2.31	0.45
2:D:132:ILE:CG2	2:D:135:ILE:HG13	2.47	0.45
2:E:184:ILE:HD13	2:E:225:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:160:LEU:O	2:F:164:ILE:HG13	2.17	0.45
2:F:360:LYS:CB	2:F:361:THR:HA	2.46	0.45
1:J:237:GLY:HA2	4:J:601:ANP:O2A	2.16	0.45
1:K:123:THR:HG22	1:K:137:GLY:HA2	1.98	0.45
2:M:97:LYS:NZ	6:M:501:HOH:O	2.49	0.45
2:M:126:GLU:O	2:M:143:ARG:HG3	2.16	0.45
2:M:142:VAL:O	2:M:145:GLN:HB3	2.17	0.45
2:M:147:LEU:C	2:M:302:PRO:HD2	2.37	0.45
2:M:185:GLY:HA2	2:M:214:ALA:HA	1.99	0.45
1:A:300:VAL:HG21	1:A:341:MET:HG2	1.98	0.45
1:B:71:LEU:O	1:B:193:VAL:HG22	2.16	0.45
1:B:197:ARG:HA	1:B:198:PRO:HD3	1.85	0.45
1:B:329:ASP:HA	1:B:330:SER:HA	1.54	0.45
1:B:443:ARG:HB2	1:B:443:ARG:CZ	2.47	0.45
1:C:228:ALA:HA	1:C:411:VAL:HB	1.99	0.45
1:C:339:ARG:NH2	2:F:275:GLY:O	2.50	0.45
2:D:48:GLN:N	2:D:51:LYS:O	2.49	0.45
2:D:273:TYR:HD1	2:D:277:LEU:HD22	1.82	0.45
2:E:77:LEU:HB3	2:E:111:ILE:HD13	1.99	0.45
1:J:51:VAL:HG12	1:J:53:GLU:O	2.17	0.45
1:J:90:PRO:HG2	1:J:93:THR:HB	1.97	0.45
1:J:123:THR:HG22	1:J:137:GLY:HA2	1.99	0.45
1:J:290:VAL:HG11	1:J:313:ILE:HG21	1.99	0.45
1:J:509:VAL:HG11	1:J:561:TYR:O	2.17	0.45
1:K:29:LEU:CB	1:K:65:ARG:HE	2.30	0.45
1:K:191:TRP:CD2	1:K:192:PRO:HD2	2.51	0.45
2:L:160:LEU:O	2:L:164:ILE:HG13	2.17	0.45
2:L:215:ASN:OD1	2:L:215:ASN:N	2.44	0.45
2:M:34:MET:SD	2:M:63:ILE:HG12	2.56	0.45
2:M:150:PHE:HZ	2:M:319:THR:HB	1.81	0.45
2:N:143:ARG:HH22	2:N:242:HIS:CD2	2.34	0.45
1:A:43:ARG:HA	1:A:43:ARG:CZ	2.47	0.45
1:A:58:ILE:HG23	1:A:62:GLU:HG3	1.98	0.45
1:B:221:PRO:CB	1:B:441:VAL:HG11	2.46	0.45
1:B:492:VAL:O	1:B:496:ILE:HG13	2.16	0.45
1:C:44:GLN:HG3	1:C:45:ASP:H	1.81	0.45
1:C:240:VAL:HG23	4:C:601:ANP:O2A	2.17	0.45
2:E:184:ILE:CD1	2:E:225:PRO:HG3	2.47	0.45
2:E:313:HIS:HB3	2:E:316:PRO:HG3	1.99	0.45
2:F:248:THR:HA	2:F:249:ASP:HA	1.51	0.45
2:F:285:PHE:HB2	2:F:322:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:102:PHE:HD1	2:L:116:ILE:HG12	1.82	0.45
1:J:9:VAL:HG22	1:J:9:VAL:O	2.17	0.45
1:J:259:CYS:N	1:J:329:ASP:O	2.49	0.45
1:K:120:PHE:HE2	1:K:137:GLY:HA3	1.80	0.45
2:L:39:ILE:HD12	2:L:39:ILE:N	2.32	0.45
2:M:160:LEU:O	2:M:164:ILE:HG13	2.17	0.45
2:N:234:TYR:CD1	2:N:238:GLU:HG3	2.51	0.45
1:B:231:PRO:CG	1:B:412:PHE:HE1	2.30	0.45
1:C:41:GLU:CD	2:D:12:VAL:HG13	2.37	0.45
1:C:259:CYS:O	1:C:333:ARG:HG3	2.17	0.45
1:C:285:LEU:O	1:C:289:THR:OG1	2.27	0.45
1:C:462:ARG:O	1:C:466:GLU:HG3	2.17	0.45
2:D:151:SER:HB2	2:D:329:LEU:HD22	1.99	0.45
2:D:362:ARG:CB	2:D:427:LEU:HD13	2.45	0.45
2:E:315:ILE:N	2:E:316:PRO:HD2	2.32	0.45
1:I:304:GLU:O	1:I:334:TRP:NE1	2.49	0.45
1:J:3:ILE:HG23	1:J:64:VAL:O	2.16	0.45
1:J:19:MET:HG3	1:J:19:MET:O	2.17	0.45
1:J:78:GLY:H	1:J:141:GLU:CD	2.20	0.45
1:J:331:THR:HG22	1:J:389:ALA:O	2.17	0.45
1:K:406:LEU:HA	1:K:409:VAL:HG22	1.98	0.45
2:L:65:LEU:HD12	2:L:65:LEU:N	2.31	0.45
2:L:273:TYR:CD1	2:L:314:PRO:HB2	2.52	0.45
1:A:79:ILE:O	1:A:290:VAL:HG22	2.17	0.45
1:A:446:ASP:OD1	1:A:453:TRP:N	2.47	0.45
1:C:236:ALA:O	1:C:427:SER:OG	2.20	0.45
1:C:247:LYS:HE2	1:C:276:LEU:HD11	1.99	0.45
2:D:57:PHE:HB3	2:D:217:PRO:CG	2.47	0.45
2:D:236:ALA:O	2:D:296:GLY:HA3	2.17	0.45
2:E:273:TYR:CE1	2:E:315:ILE:HD11	2.52	0.45
1:J:428:ILE:HD12	1:J:428:ILE:N	2.31	0.45
1:K:220:PHE:HZ	1:K:430:TRP:CA	2.23	0.45
2:L:408:PHE:O	2:L:413:VAL:HG23	2.17	0.45
2:M:276:TYR:O	2:M:280:ASN:N	2.28	0.45
2:N:89:VAL:CG1	2:N:211:MET:HG2	2.47	0.45
2:N:319:THR:HG22	2:N:323:THR:HG21	1.99	0.45
1:A:82:GLN:NE2	1:A:93:THR:OG1	2.50	0.45
1:A:251:VAL:HG12	1:A:323:ASP:HB3	1.99	0.45
1:A:324:VAL:O	1:A:384:ILE:HA	2.17	0.45
1:B:82:GLN:HB3	1:B:84:PHE:CZ	2.51	0.45
1:C:157:GLY:HA3	1:C:177:GLU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:ARG:HD2	1:C:536:LEU:CD1	2.46	0.45
2:D:334:TYR:HB2	2:D:341:PRO:CB	2.46	0.45
2:F:148:PRO:HG3	2:F:323:THR:OG1	2.17	0.45
2:F:320:GLY:O	2:F:350:ARG:NH2	2.50	0.45
2:F:439:ARG:HD3	2:F:450:LEU:HD13	1.99	0.45
1:J:407:ARG:HG2	1:J:408:VAL:N	2.31	0.45
1:K:245:ILE:O	1:K:249:SER:OG	2.32	0.45
2:L:14:PRO:O	2:L:56:ILE:N	2.36	0.45
2:L:141:LEU:HD21	2:L:244:LEU:HD11	1.98	0.45
2:M:11:VAL:HG23	2:M:65:LEU:CD2	2.46	0.45
2:M:21:VAL:CG2	2:M:72:PHE:HZ	2.28	0.45
2:M:120:ALA:O	2:M:292:ARG:HB2	2.17	0.45
2:N:310:ASP:OD2	2:N:312:THR:OG1	2.26	0.45
1:B:36:ILE:CD1	1:B:87:ILE:HG21	2.47	0.45
1:B:199:ILE:HG21	1:B:372:VAL:HG21	1.99	0.45
1:C:214:ARG:HH22	1:C:560:LYS:HB2	1.82	0.45
1:C:278:ASP:HB3	1:C:281:THR:CG2	2.47	0.45
2:D:30:ILE:HD12	2:D:30:ILE:O	2.17	0.45
2:D:56:ILE:HG22	2:D:59:GLY:H	1.82	0.45
2:D:140:THR:HB	2:D:352:LYS:HA	1.99	0.45
2:E:6:ARG:NE	2:L:290:ARG:HH21	2.15	0.45
2:E:79:LEU:HD23	2:E:81:VAL:HG22	1.99	0.45
2:F:86:ILE:HB	2:F:206:ARG:O	2.17	0.45
2:F:213:LEU:HG	2:F:216:ASP:OD2	2.16	0.45
1:I:268:ASP:O	1:I:272:GLU:HB2	2.17	0.45
1:I:360:SER:O	1:I:364:GLU:HG3	2.16	0.45
1:K:18:ASN:HA	1:K:45:ASP:O	2.17	0.45
1:K:318:ARG:HD3	1:K:384:ILE:CG1	2.45	0.45
1:K:493:ALA:O	1:K:497:ARG:HG3	2.17	0.45
2:M:226:ARG:HD3	2:M:284:LEU:CD2	2.47	0.45
2:M:340:PRO:HA	2:M:341:PRO:HD3	1.90	0.45
1:A:188:MET:SD	1:A:190:LYS:HG3	2.57	0.44
1:B:85:ASP:OD2	1:B:89:ARG:HB2	2.17	0.44
1:B:261:GLU:OE2	1:B:330:SER:N	2.50	0.44
1:C:318:ARG:HB2	1:C:384:ILE:HD11	1.99	0.44
1:C:572:SER:O	1:C:575:GLU:N	2.49	0.44
2:D:29:LEU:CB	2:D:73:LEU:HD11	2.35	0.44
2:E:85:MET:HG2	2:E:90:PHE:CZ	2.52	0.44
2:E:178:ALA:HB3	2:E:243:VAL:HG22	1.99	0.44
1:I:158:THR:C	1:I:176:ILE:HG23	2.36	0.44
1:I:251:VAL:HG12	1:I:323:ASP:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:327:MET:HA	1:I:387:ILE:O	2.16	0.44
1:I:348:MET:HG3	2:M:265:ARG:HA	1.99	0.44
1:J:220:PHE:CZ	1:J:430:TRP:HA	2.40	0.44
1:J:234:PHE:HZ	2:M:311:LYS:CD	2.28	0.44
1:J:285:LEU:O	1:J:289:THR:OG1	2.35	0.44
1:K:292:ILE:HD12	1:K:292:ILE:N	2.32	0.44
2:L:415:GLN:HG2	2:L:421:ARG:HD2	1.99	0.44
2:M:85:MET:HG2	2:M:103:ILE:HD11	1.96	0.44
2:N:130:THR:CG2	2:N:135:ILE:HG22	2.46	0.44
1:A:73:VAL:HA	1:A:88:GLN:OE1	2.18	0.44
1:A:167:PHE:CD2	1:A:173:ILE:HG22	2.53	0.44
1:A:262:ARG:HG2	2:D:324:GLU:HG3	2.00	0.44
1:C:196:GLY:HA2	1:C:368:ARG:NH2	2.33	0.44
1:C:214:ARG:HB3	1:C:500:TYR:CD1	2.53	0.44
1:C:300:VAL:HG13	1:C:303:ARG:CZ	2.47	0.44
2:E:438:PRO:HG2	2:E:441:GLU:CB	2.47	0.44
2:F:133:SER:H	2:F:415:GLN:CD	2.19	0.44
2:F:177:PHE:HE1	2:F:243:VAL:C	2.20	0.44
1:I:348:MET:CG	2:M:265:ARG:HA	2.47	0.44
2:L:73:LEU:HD12	2:L:73:LEU:HA	1.74	0.44
2:M:24:VAL:HG22	2:M:72:PHE:CZ	2.53	0.44
2:M:158:LYS:H	2:M:158:LYS:HD3	1.82	0.44
2:M:371:GLN:NE2	2:M:442:LEU:HA	2.32	0.44
2:M:372:LEU:HD23	2:M:412:TYR:HE2	1.82	0.44
2:N:148:PRO:HG3	2:N:323:THR:CB	2.48	0.44
1:A:43:ARG:N	1:A:46:VAL:O	2.51	0.44
1:A:424:HIS:HE1	1:A:502:GLN:HG2	1.77	0.44
1:B:430:TRP:CD1	1:B:431:ILE:HG12	2.51	0.44
1:B:487:ARG:HA	1:B:490:LEU:HD12	1.99	0.44
2:D:291:ILE:HB	2:D:294:LEU:HD12	1.98	0.44
2:F:282:ALA:O	2:F:286:GLU:HG2	2.17	0.44
1:J:202:LYS:HB2	2:N:188:PHE:CE1	2.53	0.44
1:J:232:GLY:HA2	1:J:415:LEU:HG	1.98	0.44
2:L:173:SER:O	2:L:174:SER:HB3	2.18	0.44
2:L:183:ALA:O	2:L:212:ASN:N	2.47	0.44
2:M:40:ARG:NE	2:M:63:ILE:HD11	2.31	0.44
2:M:324:GLU:O	2:M:350:ARG:HD2	2.18	0.44
2:N:32:VAL:HB	2:N:40:ARG:HB3	1.99	0.44
1:A:81:SER:OG	1:A:287:GLU:HA	2.17	0.44
1:A:329:ASP:HA	1:A:330:SER:HA	1.51	0.44
2:E:235:LEU:HB2	2:E:243:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:307:PRO:HG3	2:F:313:HIS:CE1	2.52	0.44
1:I:3:ILE:HD12	1:I:3:ILE:N	2.33	0.44
1:I:424:HIS:NE2	1:I:501:LEU:HD22	2.33	0.44
1:J:36:ILE:HD12	1:J:87:ILE:HG22	1.99	0.44
1:J:37:GLY:HA2	1:J:52:TYR:H	1.83	0.44
1:K:52:TYR:O	1:K:299:PRO:HB3	2.17	0.44
1:K:214:ARG:HH22	1:K:560:LYS:HD3	1.82	0.44
2:L:29:LEU:HB3	2:L:73:LEU:HD23	1.98	0.44
2:L:87:GLY:HA3	2:L:205:ASP:HA	1.97	0.44
2:M:8:ILE:O	2:M:65:LEU:HB3	2.18	0.44
2:M:147:LEU:O	2:M:301:ILE:HG23	2.18	0.44
2:M:183:ALA:HB1	2:M:186:ILE:HD13	2.00	0.44
2:M:384:GLU:O	2:M:387:VAL:HG22	2.18	0.44
1:A:139:VAL:O	1:A:147:HIS:HB3	2.17	0.44
1:B:102:PHE:HB3	2:E:114:GLU:CB	2.48	0.44
1:B:549:THR:O	1:B:553:ARG:HG3	2.18	0.44
1:C:273:PHE:HE2	1:C:289:THR:HG21	1.82	0.44
2:D:157:HIS:HD2	2:D:158:LYS:N	2.15	0.44
2:D:176:ASP:HB3	2:D:206:ARG:CD	2.48	0.44
2:E:131:GLY:N	2:E:167:GLN:HB3	2.29	0.44
2:E:284:LEU:HD13	2:E:285:PHE:CD1	2.53	0.44
2:E:430:GLY:O	2:E:434:LEU:HB2	2.18	0.44
1:I:7:ILE:HB	2:L:49:GLU:HG2	1.98	0.44
1:I:43:ARG:HA	1:I:43:ARG:HE	1.82	0.44
1:I:94:PHE:CD1	1:I:109:LEU:HD12	2.52	0.44
1:I:257:VAL:HA	1:I:292:ILE:HB	2.00	0.44
1:J:532:ALA:O	1:J:536:LEU:HB2	2.17	0.44
1:K:36:ILE:HG22	1:K:53:GLU:OE2	2.18	0.44
1:K:405:THR:O	1:K:409:VAL:HG22	2.18	0.44
2:L:33:ARG:O	2:L:69:SER:N	2.46	0.44
2:L:270:ARG:HB3	2:L:270:ARG:HH11	1.82	0.44
2:N:213:LEU:HD12	2:N:213:LEU:N	2.30	0.44
1:A:43:ARG:N	1:A:44:GLN:HA	2.32	0.44
1:A:72:SER:HA	1:A:193:VAL:HG13	1.99	0.44
1:A:218:THR:HA	1:A:453:TRP:CZ2	2.52	0.44
1:A:315:GLU:HA	1:A:384:ILE:HD11	1.98	0.44
1:B:118:TRP:CZ3	1:B:141:GLU:HA	2.52	0.44
1:B:459:GLU:O	1:B:463:ILE:HG13	2.18	0.44
1:C:75:LEU:N	1:C:189:GLN:O	2.47	0.44
1:C:94:PHE:HZ	1:C:104:GLY:H	1.66	0.44
1:C:330:SER:HB3	1:C:333:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:57:PHE:HA	2:F:219:ILE:CB	2.48	0.44
2:F:251:THR:HG21	2:F:305:THR:O	2.17	0.44
2:F:282:ALA:HA	2:F:322:ILE:CG2	2.47	0.44
1:K:560:LYS:H	1:K:560:LYS:HG3	1.56	0.44
1:B:324:VAL:O	1:B:384:ILE:HA	2.18	0.44
1:B:521:MET:HE3	1:B:560:LYS:HB3	2.00	0.44
1:C:363:ALA:O	1:C:367:GLU:HB2	2.18	0.44
2:D:132:ILE:HD13	2:D:135:ILE:HD12	2.00	0.44
2:D:345:LEU:HD21	2:D:376:TYR:CE2	2.52	0.44
2:E:34:MET:CG	2:E:38:GLU:HB3	2.48	0.44
2:F:179:VAL:HG13	2:F:244:LEU:HD23	1.99	0.44
1:I:338:LEU:HD11	1:I:361:ARG:HG3	2.00	0.44
1:J:214:ARG:CD	1:J:513:THR:HG21	2.48	0.44
1:K:89:ARG:HD3	1:K:109:LEU:H	1.81	0.44
1:K:237:GLY:O	1:K:241:VAL:HG23	2.17	0.44
1:K:342:SER:HA	1:K:345:LEU:HD12	2.00	0.44
2:L:349:SER:CB	2:L:352:LYS:HZ2	2.31	0.44
2:N:427:LEU:O	2:N:427:LEU:HD13	2.17	0.44
1:A:82:GLN:HB3	1:A:84:PHE:CZ	2.53	0.44
1:A:285:LEU:CD2	1:A:288:ARG:HD3	2.47	0.44
1:B:12:PRO:CB	1:B:344:ARG:CD	2.90	0.44
1:B:126:GLU:OE2	1:B:161:LYS:HA	2.17	0.44
1:B:238:LYS:H	1:B:238:LYS:HG3	1.60	0.44
1:B:266:MET:CE	1:B:291:LEU:HD21	2.48	0.44
1:B:565:GLU:O	1:B:567:LEU:HD23	2.18	0.44
1:C:418:SER:O	1:C:422:LYS:HD2	2.17	0.44
2:E:162:ALA:O	2:E:166:ARG:HG3	2.18	0.44
2:F:175:ASP:HA	2:F:176:ASP:C	2.38	0.44
2:F:362:ARG:CB	2:F:427:LEU:HD21	2.48	0.44
1:I:120:PHE:CZ	1:I:173:ILE:HD12	2.52	0.44
1:J:29:LEU:H	1:J:29:LEU:HD22	1.83	0.44
1:J:232:GLY:C	1:J:238:LYS:HD3	2.38	0.44
2:L:137:HIS:HD2	2:L:426:THR:HG22	1.81	0.44
2:L:153:SER:HB3	2:L:331:ARG:NH2	2.32	0.44
2:L:404:PHE:HE1	2:L:434:LEU:HA	1.83	0.44
2:M:29:LEU:O	2:M:73:LEU:HB2	2.18	0.44
2:N:339:GLN:HA	2:N:341:PRO:CD	2.48	0.44
1:B:11:GLY:CA	1:B:55:THR:HG21	2.29	0.44
1:B:360:SER:O	1:B:364:GLU:HG3	2.17	0.44
1:C:39:ILE:HG23	1:C:48:SER:C	2.37	0.44
2:D:32:VAL:HG13	2:D:70:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:VAL:HG11	2:D:47:VAL:HG13	1.99	0.44
2:D:325:GLY:HA2	2:D:348:LEU:O	2.18	0.44
2:E:313:HIS:CG	2:E:314:PRO:HD2	2.53	0.44
2:F:325:GLY:HA2	2:F:326:GLN:HA	1.83	0.44
1:I:214:ARG:HG3	1:I:503:GLN:OE1	2.18	0.44
1:J:30:VAL:O	1:J:35:VAL:N	2.48	0.44
2:L:65:LEU:HD12	2:L:66:LYS:H	1.83	0.44
2:L:109:LEU:H	2:L:109:LEU:HD12	1.82	0.44
2:L:121:ARG:NH2	2:L:286:GLU:O	2.43	0.44
2:L:183:ALA:HA	2:L:248:THR:O	2.17	0.44
2:L:234:TYR:OH	2:L:239:LYS:NZ	2.36	0.44
2:L:412:TYR:C	2:L:412:TYR:CD2	2.91	0.44
2:M:48:GLN:CB	2:M:49:GLU:HA	2.47	0.44
2:N:34:MET:CG	2:N:38:GLU:HB3	2.47	0.44
2:N:155:LEU:CD1	2:N:329:LEU:HB2	2.48	0.44
1:A:42:MET:HG3	2:E:65:LEU:HD11	2.00	0.43
1:A:246:ALA:CB	1:A:254:VAL:HG11	2.48	0.43
1:A:255:VAL:HB	1:A:326:ILE:HA	2.00	0.43
1:A:273:PHE:HB3	1:A:274:PRO:HD3	1.99	0.43
1:B:406:LEU:HA	1:B:409:VAL:HG22	2.00	0.43
1:B:482:LEU:H	1:B:482:LEU:HD12	1.83	0.43
1:C:500:TYR:HD1	1:C:500:TYR:HA	1.72	0.43
2:E:20:LYS:HD3	2:L:292:ARG:NH1	2.33	0.43
2:E:134:ALA:HB2	2:E:412:TYR:O	2.18	0.43
2:F:258:ARG:HH21	2:F:272:GLY:CA	2.30	0.43
1:I:437:TYR:O	1:I:441:VAL:HG23	2.18	0.43
1:J:424:HIS:HE1	1:J:502:GLN:HB3	1.82	0.43
2:M:40:ARG:HD3	2:M:59:GLY:O	2.17	0.43
2:N:220:GLU:O	2:N:224:THR:OG1	2.27	0.43
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.84	0.43
1:B:246:ALA:HB2	1:B:327:MET:CG	2.48	0.43
2:D:345:LEU:HA	2:D:373:PHE:CZ	2.53	0.43
2:E:18:VAL:O	2:E:52:ALA:N	2.45	0.43
2:F:260:ILE:CG2	2:F:264:ARG:HH21	2.31	0.43
2:F:325:GLY:C	2:F:349:SER:HA	2.38	0.43
1:I:119:TRP:HA	1:I:119:TRP:CE3	2.54	0.43
1:I:402:THR:O	1:I:406:LEU:HG	2.18	0.43
1:J:35:VAL:CB	1:J:53:GLU:HB2	2.35	0.43
1:K:207:VAL:O	1:K:223:THR:HA	2.18	0.43
1:K:210:ILE:CG1	1:K:515:ARG:HH21	2.31	0.43
2:L:218:ALA:HA	2:L:221:ARG:HE	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:390:GLY:HA2	2:L:391:GLU:HA	1.70	0.43
2:L:405:ALA:O	2:L:409:GLU:HG3	2.18	0.43
2:M:251:THR:OG1	2:M:305:THR:N	2.39	0.43
2:M:372:LEU:HD12	2:M:372:LEU:HA	1.86	0.43
1:A:229:ALA:HA	1:A:388:SER:O	2.18	0.43
1:B:491:GLU:OE1	1:B:494:LYS:NZ	2.35	0.43
1:B:565:GLU:H	1:B:565:GLU:CD	2.10	0.43
2:D:124:PRO:HB2	2:D:142:VAL:HB	2.01	0.43
2:E:123:TYR:HA	2:E:124:PRO:HD3	1.89	0.43
2:E:178:ALA:O	2:E:243:VAL:HA	2.19	0.43
2:E:354:LYS:HA	2:E:355:GLY:HA2	1.50	0.43
2:E:423:ILE:HG23	2:E:424:THR:N	2.32	0.43
2:F:362:ARG:CB	2:F:365:HIS:HB2	2.48	0.43
2:L:158:LYS:HD3	2:L:190:GLU:HG2	2.00	0.43
2:M:218:ALA:O	2:M:222:ILE:HG13	2.19	0.43
1:A:202:LYS:HA	1:A:372:VAL:HG12	1.99	0.43
1:A:264:ASN:HD21	2:D:324:GLU:CD	2.19	0.43
1:A:529:GLY:O	1:A:533:ARG:HB2	2.18	0.43
1:C:424:HIS:NE2	1:C:501:LEU:O	2.52	0.43
2:D:73:LEU:HB2	2:D:75:HIS:CE1	2.53	0.43
2:E:33:ARG:HH12	2:E:71:ARG:HE	1.65	0.43
2:F:30:ILE:HG22	2:F:72:PHE:HD1	1.84	0.43
2:F:57:PHE:HB3	2:F:220:GLU:N	2.33	0.43
1:K:469:GLN:O	1:K:473:ILE:HG13	2.18	0.43
2:M:130:THR:HG21	2:M:135:ILE:CG2	2.41	0.43
2:M:229:LEU:HD22	2:M:287:ARG:HG3	1.99	0.43
2:N:328:ILE:CG1	2:N:346:PRO:HG2	2.48	0.43
1:A:98:THR:O	1:A:99:GLN:HB2	2.18	0.43
1:A:208:PRO:HG3	1:A:441:VAL:HG13	2.00	0.43
1:C:364:GLU:O	1:C:368:ARG:HG3	2.18	0.43
2:D:345:LEU:HD21	2:D:376:TYR:CD2	2.53	0.43
2:E:18:VAL:N	2:E:52:ALA:O	2.37	0.43
2:E:364:ASP:CB	2:E:449:LEU:HD22	2.49	0.43
2:F:258:ARG:NH2	2:F:272:GLY:HA3	2.33	0.43
2:F:313:HIS:CD2	2:F:314:PRO:HD2	2.54	0.43
1:I:124:ILE:O	1:I:162:ILE:HG21	2.18	0.43
1:K:278:ASP:HB3	1:K:281:THR:CG2	2.48	0.43
2:L:82:SER:O	2:L:85:MET:HG2	2.19	0.43
2:L:137:HIS:CD2	2:L:426:THR:HG22	2.53	0.43
2:L:364:ASP:HB2	2:L:431:TRP:HZ2	1.84	0.43
2:L:412:TYR:C	2:L:412:TYR:HD2	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:279:THR:O	2:M:283:THR:HG23	2.18	0.43
1:A:43:ARG:HG2	1:A:46:VAL:HG13	1.99	0.43
1:A:324:VAL:HG12	1:A:325:ALA:N	2.33	0.43
1:B:214:ARG:HB3	1:B:500:TYR:CZ	2.53	0.43
1:B:261:GLU:HG2	1:B:329:ASP:O	2.17	0.43
1:C:4:GLY:O	1:C:64:VAL:HG23	2.19	0.43
1:C:9:VAL:HG11	1:C:58:ILE:HB	2.01	0.43
1:C:20:SER:HB3	1:C:45:ASP:HA	2.01	0.43
1:C:242:GLN:OE1	1:C:329:ASP:HB2	2.19	0.43
2:D:148:PRO:HG3	2:D:323:THR:OG1	2.18	0.43
2:E:290:ARG:HG3	2:E:297:SER:HB3	2.01	0.43
2:F:124:PRO:HB2	2:F:142:VAL:HG11	1.96	0.43
2:F:197:ASP:O	2:F:201:THR:HG23	2.17	0.43
1:I:246:ALA:CB	1:I:254:VAL:HG11	2.48	0.43
1:I:262:ARG:HH12	2:L:350:ARG:CZ	2.31	0.43
1:J:41:GLU:CD	2:N:12:VAL:HG13	2.39	0.43
1:J:315:GLU:OE2	1:J:368:ARG:HB3	2.18	0.43
1:J:392:PRO:HG3	1:J:402:THR:OG1	2.19	0.43
1:K:209:MET:N	1:K:222:VAL:O	2.37	0.43
1:K:351:ASP:OD2	1:K:351:ASP:N	2.50	0.43
2:L:21:VAL:HG21	2:L:52:ALA:HB2	2.00	0.43
2:M:21:VAL:HG22	2:M:72:PHE:CZ	2.53	0.43
2:N:45:LEU:HD22	2:N:46:GLU:H	1.83	0.43
2:N:242:HIS:HA	2:N:297:SER:H	1.84	0.43
2:N:381:GLN:HA	2:N:384:GLU:HG3	2.01	0.43
1:A:85:ASP:OD2	1:A:88:GLN:N	2.51	0.43
1:B:79:ILE:HB	1:B:112:LEU:CD1	2.48	0.43
1:B:191:TRP:CG	1:B:192:PRO:HD2	2.53	0.43
1:B:266:MET:HE3	1:B:291:LEU:HD21	2.01	0.43
1:B:425:PHE:HB2	4:B:601:ANP:N6	2.33	0.43
2:D:48:GLN:CB	2:D:51:LYS:HG2	2.47	0.43
2:D:129:GLN:O	2:D:168:ALA:HA	2.19	0.43
2:E:167:GLN:HG3	2:E:420:ASN:CB	2.48	0.43
2:F:437:LEU:HD23	2:F:441:GLU:OE2	2.19	0.43
1:I:33:LEU:HD12	1:I:33:LEU:N	2.34	0.43
1:J:50:GLN:HE21	1:J:345:LEU:HD11	1.83	0.43
1:J:79:ILE:HG13	1:J:84:PHE:CE2	2.54	0.43
1:J:295:THR:O	1:J:298:MET:HB2	2.18	0.43
1:J:362:LEU:O	1:J:366:TYR:HD2	2.02	0.43
1:K:41:GLU:O	1:K:47:ALA:HB1	2.19	0.43
2:L:6:ARG:NH2	2:L:6:ARG:CB	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:113:GLY:HA3	2:M:287:ARG:NH1	2.33	0.43
2:M:130:THR:HB	2:M:135:ILE:HD12	2.01	0.43
2:N:130:THR:HG21	2:N:135:ILE:C	2.39	0.43
2:N:213:LEU:H	2:N:213:LEU:CD1	2.30	0.43
1:A:198:PRO:HB2	1:A:375:LEU:HD11	2.01	0.43
1:A:297:ASN:ND2	2:D:115:VAL:HG13	2.33	0.43
1:A:352:GLU:HB2	1:A:400:PRO:HG2	2.00	0.43
1:B:29:LEU:HD12	1:B:34:GLY:O	2.17	0.43
1:B:215:VAL:HG11	1:B:426:PRO:HG2	1.99	0.43
1:B:229:ALA:HA	1:B:388:SER:O	2.19	0.43
1:B:258:GLY:HA3	1:B:266:MET:SD	2.59	0.43
1:C:62:GLU:OE2	2:F:25:LYS:NZ	2.34	0.43
1:C:256:TYR:CD1	1:C:327:MET:HB2	2.53	0.43
2:D:131:GLY:C	2:D:132:ILE:HD12	2.39	0.43
2:D:232:ALA:HB1	2:D:243:VAL:HG11	2.00	0.43
2:D:313:HIS:CG	2:D:314:PRO:HD2	2.54	0.43
2:E:285:PHE:CE2	2:E:319:THR:HG23	2.54	0.43
2:E:338:ILE:HG23	2:E:414:ASN:OD1	2.19	0.43
1:I:16:ALA:HB1	1:I:64:VAL:HG21	2.01	0.43
1:I:185:LEU:N	1:I:185:LEU:HD23	2.34	0.43
1:I:295:THR:H	1:I:298:MET:CG	2.26	0.43
1:J:401:VAL:O	1:J:405:THR:OG1	2.28	0.43
1:J:498:GLU:O	1:J:502:GLN:HB2	2.19	0.43
1:K:9:VAL:HG21	1:K:58:ILE:HG21	2.01	0.43
1:K:131:SER:N	1:K:134:ASP:OD2	2.32	0.43
2:M:11:VAL:HG23	2:M:65:LEU:HD23	2.00	0.43
2:M:147:LEU:O	2:M:301:ILE:HA	2.18	0.43
2:N:126:GLU:CG	2:N:143:ARG:HG3	2.49	0.43
2:N:186:ILE:H	2:N:186:ILE:HG12	1.64	0.43
2:N:403:LYS:O	2:N:407:ARG:HG3	2.17	0.43
1:A:188:MET:HB3	1:A:188:MET:HE3	1.78	0.43
1:A:405:THR:O	1:A:409:VAL:HG22	2.19	0.43
1:B:209:MET:HG2	1:B:210:ILE:N	2.33	0.43
1:B:237:GLY:N	4:B:601:ANP:O3A	2.47	0.43
1:B:292:ILE:HD12	1:B:292:ILE:N	2.34	0.43
1:C:39:ILE:HG23	1:C:48:SER:O	2.19	0.43
1:C:292:ILE:HD12	1:C:292:ILE:N	2.33	0.43
2:E:306:MET:HG2	2:E:310:ASP:O	2.17	0.43
1:I:145:ILE:HG13	1:I:253:LEU:CD1	2.48	0.43
1:I:263:GLY:O	1:I:267:THR:OG1	2.28	0.43
1:J:199:ILE:HG21	1:J:372:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:332:SER:HG	1:K:391:SER:H	1.65	0.43
1:A:84:PHE:CE2	1:A:290:VAL:HG13	2.54	0.43
1:A:426:PRO:HD2	1:A:501:LEU:O	2.19	0.43
1:A:532:ALA:O	1:A:536:LEU:N	2.50	0.43
1:B:315:GLU:OE2	1:B:368:ARG:NE	2.52	0.43
2:D:163:GLN:HG3	2:D:417:PHE:HD1	1.83	0.43
2:E:434:LEU:HD22	2:E:442:LEU:HD22	2.00	0.43
2:F:175:ASP:N	2:F:176:ASP:CB	2.82	0.43
1:I:83:MET:HE3	2:L:119:ILE:CG2	2.40	0.43
1:I:254:VAL:H	1:I:289:THR:CG2	2.27	0.43
1:J:37:GLY:N	1:J:52:TYR:HD1	2.16	0.43
1:J:88:GLN:OE1	1:J:111:ALA:HB1	2.19	0.43
1:J:406:LEU:HD21	1:J:412:PHE:CG	2.54	0.43
1:K:237:GLY:N	4:K:601:ANP:O3A	2.49	0.43
2:M:128:ILE:HG13	2:M:143:ARG:CG	2.24	0.43
2:N:7:THR:O	2:N:19:GLU:HG2	2.19	0.43
2:N:29:LEU:HD13	2:N:77:LEU:HB3	2.00	0.43
2:N:130:THR:O	2:N:132:ILE:HD12	2.19	0.43
2:N:156:PRO:HD3	2:N:334:TYR:CE1	2.54	0.43
2:N:199:ARG:HA	2:N:204:ILE:HG21	2.01	0.43
2:N:362:ARG:O	2:N:365:HIS:HB3	2.18	0.43
1:A:219:PHE:HE2	1:A:501:LEU:CD2	2.32	0.42
2:D:16:MET:HB2	2:D:54:VAL:HG22	2.01	0.42
2:D:159:GLU:HB3	2:D:417:PHE:CG	2.54	0.42
2:D:224:THR:HG1	2:D:225:PRO:HD3	1.83	0.42
2:D:408:PHE:O	2:D:413:VAL:HG23	2.19	0.42
2:F:45:LEU:H	2:F:45:LEU:HG	1.55	0.42
2:F:86:ILE:CA	2:F:208:VAL:HG22	2.48	0.42
1:I:136:ILE:CG1	1:I:137:GLY:N	2.81	0.42
1:J:211:THR:HB	1:J:245:ILE:CD1	2.49	0.42
1:K:24:ILE:HG21	2:L:60:THR:HG23	2.01	0.42
1:K:41:GLU:CD	2:L:12:VAL:HG22	2.38	0.42
2:L:90:PHE:CD1	2:L:96:PRO:HA	2.54	0.42
2:L:224:THR:HB	2:L:225:PRO:HD3	2.00	0.42
2:M:186:ILE:HD12	2:M:191:ALA:HA	2.01	0.42
2:M:213:LEU:HB3	2:M:215:ASN:OD1	2.19	0.42
2:N:92:GLY:HA3	2:N:220:GLU:OE1	2.18	0.42
2:N:251:THR:HG23	2:N:315:ILE:HG13	2.01	0.42
1:A:238:LYS:HE2	1:A:238:LYS:HB3	1.93	0.42
1:A:256:TYR:HB3	1:A:291:LEU:HG	2.01	0.42
1:B:153:ASN:HB2	1:B:191:TRP:HZ3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:LEU:HB3	1:B:355:PRO:HG3	2.01	0.42
1:C:461:MET:O	1:C:465:GLN:HG3	2.19	0.42
2:D:130:THR:HG23	2:D:141:LEU:HD23	2.01	0.42
2:D:282:ALA:HA	2:D:322:ILE:HD13	2.01	0.42
2:E:151:SER:O	2:E:305:THR:HA	2.19	0.42
2:E:345:LEU:HB2	2:E:346:PRO:CD	2.47	0.42
2:F:21:VAL:HB	2:F:24:VAL:HG21	2.00	0.42
2:F:66:LYS:HB3	2:F:66:LYS:HE3	1.77	0.42
2:F:212:ASN:OD1	2:F:221:ARG:HG2	2.19	0.42
1:I:173:ILE:HG22	6:I:601:HOH:O	2.18	0.42
1:I:424:HIS:O	1:I:424:HIS:CG	2.71	0.42
1:I:492:VAL:O	1:I:496:ILE:HG13	2.20	0.42
1:J:73:VAL:HG23	1:J:73:VAL:O	2.20	0.42
1:K:311:ILE:O	1:K:315:GLU:HG3	2.19	0.42
1:K:338:LEU:HB3	1:K:355:PRO:HG3	2.00	0.42
1:K:402:THR:O	1:K:406:LEU:HG	2.18	0.42
2:L:6:ARG:NE	2:L:8:ILE:HG13	2.29	0.42
2:L:151:SER:CB	2:L:157:HIS:HB3	2.49	0.42
2:M:31:GLU:HB3	2:M:71:ARG:HB2	2.01	0.42
2:N:139:ASN:HA	2:N:349:SER:HB2	2.00	0.42
2:N:180:VAL:N	2:N:244:LEU:O	2.35	0.42
2:N:277:LEU:HD23	2:N:318:LEU:HD12	2.01	0.42
1:C:210:ILE:HD11	1:C:515:ARG:NH2	2.34	0.42
1:C:237:GLY:HA2	4:C:601:ANP:PA	2.59	0.42
1:C:257:VAL:HG11	1:C:306:SER:O	2.20	0.42
2:E:45:LEU:HD13	2:E:45:LEU:N	2.35	0.42
2:E:372:LEU:HD12	2:E:404:PHE:HZ	1.84	0.42
2:F:77:LEU:O	2:F:111:ILE:HG23	2.19	0.42
2:F:445:ILE:HD13	2:F:445:ILE:H	1.83	0.42
1:I:222:VAL:HB	1:I:411:VAL:HG21	2.00	0.42
1:J:33:LEU:HD13	1:J:105:ARG:HB2	2.02	0.42
1:K:58:ILE:O	2:N:25:LYS:HA	2.19	0.42
1:K:59:GLY:CA	2:N:25:LYS:HD3	2.50	0.42
1:K:197:ARG:HA	1:K:198:PRO:HD3	1.86	0.42
2:L:97:LYS:HE2	2:L:97:LYS:HB3	1.71	0.42
2:N:34:MET:CE	2:N:63:ILE:HG12	2.49	0.42
1:A:262:ARG:HG2	2:D:322:ILE:O	2.19	0.42
1:A:406:LEU:HA	1:A:409:VAL:HG22	2.00	0.42
1:A:425:PHE:N	1:A:425:PHE:CD1	2.88	0.42
1:B:83:MET:CE	2:E:119:ILE:HD11	2.50	0.42
2:D:135:ILE:O	2:D:135:ILE:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:157:HIS:HD2	2:D:158:LYS:H	1.68	0.42
2:F:358:ALA:HA	2:F:363:GLU:HA	2.00	0.42
1:I:206:ASP:N	1:I:206:ASP:OD2	2.52	0.42
1:K:507:ASP:HB3	1:K:510:ASP:CB	2.49	0.42
2:L:141:LEU:HD13	2:L:147:LEU:HB2	2.01	0.42
2:M:26:TYR:O	2:M:27:GLU:HB2	2.18	0.42
2:M:91:ASP:OD2	2:M:93:LEU:HB2	2.20	0.42
2:M:219:ILE:HD11	2:M:260:ILE:HD12	2.00	0.42
2:M:285:PHE:CE1	2:M:302:PRO:HB3	2.54	0.42
2:N:45:LEU:HD22	2:N:45:LEU:N	2.34	0.42
2:N:199:ARG:HA	2:N:204:ILE:CG2	2.49	0.42
2:N:378:GLN:CA	2:N:381:GLN:HE22	2.32	0.42
1:B:215:VAL:CG1	1:B:426:PRO:HG2	2.49	0.42
1:B:326:ILE:O	1:B:386:ALA:HA	2.19	0.42
1:C:351:ASP:O	1:C:352:GLU:HB2	2.20	0.42
1:C:562:ILE:H	1:C:562:ILE:HD12	1.84	0.42
2:D:29:LEU:HB3	2:D:73:LEU:HD21	2.02	0.42
2:E:318:LEU:O	2:E:322:ILE:HG13	2.19	0.42
2:F:32:VAL:HG21	2:F:56:ILE:HD12	2.01	0.42
2:F:139:ASN:HB3	2:F:349:SER:HB3	2.01	0.42
2:F:161:ALA:HB2	2:F:303:ILE:CD1	2.49	0.42
2:F:342:ILE:HG22	2:F:343:ASP:O	2.20	0.42
1:I:80:ILE:HG22	1:I:81:SER:H	1.84	0.42
1:I:155:ILE:HD12	1:I:183:LYS:HG2	2.01	0.42
1:J:47:ALA:O	1:J:49:ILE:HG13	2.20	0.42
1:J:190:LYS:HB2	1:J:190:LYS:NZ	2.34	0.42
1:J:311:ILE:HG23	1:J:368:ARG:HH21	1.84	0.42
1:J:415:LEU:HD23	1:J:415:LEU:H	1.83	0.42
1:K:33:LEU:CD2	1:K:106:GLY:HA3	2.49	0.42
1:K:54:GLU:CB	1:K:105:ARG:HD3	2.48	0.42
2:L:376:TYR:CD1	2:L:408:PHE:HD2	2.37	0.42
2:M:15:LEU:HD22	2:M:55:GLN:CG	2.50	0.42
2:M:396:ASP:HA	2:M:399:LYS:HG3	2.01	0.42
2:M:446:LYS:HA	2:M:446:LYS:CE	2.38	0.42
2:N:129:GLN:HE22	2:N:422:THR:CA	2.26	0.42
2:N:409:GLU:HA	2:N:413:VAL:CB	2.49	0.42
1:B:56:SER:HA	2:E:26:TYR:HD2	1.84	0.42
1:B:238:LYS:HG2	1:B:415:LEU:CD1	2.50	0.42
1:B:505:ALA:O	1:B:511:THR:HB	2.20	0.42
1:C:19:MET:HE2	1:C:64:VAL:HG12	2.01	0.42
1:C:329:ASP:HA	1:C:330:SER:HA	1.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:86:ILE:CG2	2:F:208:VAL:HG22	2.46	0.42
2:F:229:LEU:O	2:F:233:GLU:N	2.40	0.42
1:J:292:ILE:HD12	1:J:292:ILE:N	2.35	0.42
1:J:352:GLU:HB2	1:J:400:PRO:HG3	2.02	0.42
1:K:278:ASP:CG	1:K:279:PRO:HD2	2.40	0.42
2:L:34:MET:HB3	2:L:36:ASN:OD1	2.19	0.42
2:L:76:PRO:O	2:L:78:GLN:HG3	2.20	0.42
2:M:29:LEU:HD11	2:M:77:LEU:HD23	2.02	0.42
1:A:20:SER:HB3	1:A:45:ASP:CB	2.49	0.42
1:A:35:VAL:HB	1:A:53:GLU:HB2	2.02	0.42
1:B:27:MET:SD	1:B:71:LEU:HB2	2.59	0.42
1:B:309:THR:O	1:B:313:ILE:HG13	2.19	0.42
1:B:564:GLU:N	1:B:565:GLU:OE1	2.52	0.42
1:C:80:ILE:HG13	1:C:141:GLU:OE1	2.20	0.42
1:C:399:GLU:HA	1:C:400:PRO:HD3	1.90	0.42
2:D:39:ILE:HD12	2:D:39:ILE:N	2.34	0.42
2:E:77:LEU:O	2:E:111:ILE:HG23	2.20	0.42
2:E:112:ASN:O	2:E:287:ARG:NH1	2.53	0.42
1:I:251:VAL:HG11	1:I:385:THR:OG1	2.20	0.42
1:J:456:MET:HB3	1:J:526:LEU:HD11	2.01	0.42
1:J:543:ASN:OD1	1:J:543:ASN:N	2.52	0.42
1:K:209:MET:HE2	1:K:211:THR:HG23	2.01	0.42
1:K:504:ASN:N	1:K:510:ASP:OD2	2.39	0.42
2:L:44:VAL:HG11	2:L:47:VAL:HG12	2.02	0.42
2:L:129:GLN:O	2:L:168:ALA:HA	2.20	0.42
2:M:124:PRO:HG2	2:M:351:LEU:CD1	2.49	0.42
2:M:219:ILE:HD12	2:M:219:ILE:N	2.35	0.42
2:M:306:MET:HA	2:M:307:PRO:HD3	1.76	0.42
2:M:372:LEU:CD2	2:M:412:TYR:HE2	2.33	0.42
2:N:278:TYR:CE1	2:N:322:ILE:HG12	2.54	0.42
1:B:1:MET:HG2	1:B:2:GLN:H	1.85	0.42
1:B:29:LEU:O	1:B:64:VAL:HG13	2.20	0.42
1:B:499:ASP:CG	1:B:556:ILE:HG22	2.41	0.42
1:C:237:GLY:HA2	4:C:601:ANP:H8	2.01	0.42
2:D:30:ILE:HG13	2:D:42:GLY:O	2.18	0.42
2:D:343:ASP:HB3	2:D:346:PRO:CD	2.49	0.42
2:E:273:TYR:OH	2:E:315:ILE:HD11	2.19	0.42
1:J:394:GLY:N	2:M:317:ASP:OD2	2.35	0.42
1:J:467:GLU:OE2	1:J:497:ARG:NH1	2.53	0.42
1:J:470:LEU:O	1:J:474:VAL:HG23	2.20	0.42
1:K:29:LEU:O	1:K:65:ARG:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:349:PRO:HB2	1:K:353:GLY:HA2	2.02	0.42
2:L:8:ILE:HA	2:L:17:ALA:O	2.20	0.42
2:M:29:LEU:HD11	2:M:77:LEU:HA	2.02	0.42
2:N:134:ALA:O	2:N:139:ASN:N	2.52	0.42
2:N:345:LEU:HA	2:N:345:LEU:HD12	1.75	0.42
1:A:130:VAL:HG11	1:A:176:ILE:HD13	2.01	0.42
1:A:254:VAL:C	1:A:289:THR:HG21	2.40	0.42
1:A:331:THR:HG21	1:A:388:SER:HB3	2.02	0.42
1:C:257:VAL:HG13	1:C:292:ILE:HB	2.01	0.42
2:D:117:ASN:HB3	2:D:120:ALA:HB3	2.02	0.42
2:D:331:ARG:O	2:D:335:LYS:HB2	2.20	0.42
2:F:35:GLN:H	2:F:35:GLN:CD	2.23	0.42
1:I:295:THR:O	1:I:303:ARG:HD3	2.19	0.42
1:J:83:MET:SD	1:J:293:ALA:HB2	2.60	0.42
1:K:2:GLN:HE22	1:K:20:SER:HB3	1.85	0.42
1:K:341:MET:O	1:K:345:LEU:HG	2.19	0.42
2:L:286:GLU:OE2	2:L:286:GLU:HA	2.19	0.42
2:L:379:GLY:HA3	2:L:405:ALA:HB2	2.02	0.42
2:M:113:GLY:HA3	2:M:287:ARG:HH12	1.85	0.42
2:M:217:PRO:HB2	2:M:220:GLU:HG3	2.01	0.42
1:A:424:HIS:NE2	1:A:501:LEU:HB3	2.35	0.42
1:B:18:ASN:HA	1:B:45:ASP:HB2	2.02	0.42
1:B:120:PHE:N	1:B:165:GLY:O	2.47	0.42
1:B:254:VAL:CG2	1:B:288:ARG:NH2	2.82	0.42
1:C:54:GLU:HB2	1:C:105:ARG:CD	2.50	0.42
1:C:126:GLU:HG3	1:C:162:ILE:HG22	2.02	0.42
1:J:49:ILE:HG22	1:J:50:GLN:O	2.20	0.42
1:J:230:VAL:HG23	1:J:389:ALA:HA	2.02	0.42
1:J:241:VAL:O	1:J:245:ILE:HG12	2.20	0.42
1:K:218:THR:HG23	1:K:219:PHE:CD2	2.54	0.42
1:K:262:ARG:NH2	2:N:350:ARG:NH1	2.67	0.42
2:L:156:PRO:HG3	2:L:334:TYR:CE1	2.55	0.42
2:M:325:GLY:HA3	2:M:348:LEU:O	2.20	0.42
2:N:193:PHE:O	2:N:197:ASP:HB2	2.19	0.42
1:A:449:LEU:O	1:A:450:GLN:HB2	2.20	0.41
1:B:473:ILE:O	1:B:477:VAL:HG22	2.19	0.41
1:C:135:ILE:HA	1:C:135:ILE:HD13	1.62	0.41
2:D:155:LEU:HD21	2:D:331:ARG:HG2	2.01	0.41
2:F:210:PHE:CD2	2:F:228:ALA:HA	2.54	0.41
1:I:262:ARG:HD3	1:I:265:GLU:OE1	2.20	0.41
1:K:78:GLY:H	1:K:141:GLU:CD	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:167:PHE:HD2	1:K:173:ILE:HG22	1.85	0.41
1:K:247:LYS:HD2	1:K:276:LEU:CD1	2.50	0.41
2:L:21:VAL:CG2	2:L:24:VAL:HG21	2.49	0.41
2:L:148:PRO:HG3	2:L:323:THR:OG1	2.19	0.41
2:L:350:ARG:C	2:L:351:LEU:HD23	2.41	0.41
2:N:130:THR:CB	2:N:135:ILE:HB	2.49	0.41
2:N:328:ILE:HB	2:N:346:PRO:HG2	2.02	0.41
1:A:52:TYR:CD2	1:A:299:PRO:HB3	2.55	0.41
1:A:255:VAL:N	1:A:325:ALA:O	2.41	0.41
1:B:114:HIS:HA	1:B:169:ILE:HG12	2.01	0.41
1:C:79:ILE:HG13	1:C:84:PHE:CZ	2.55	0.41
2:D:182:ALA:HB2	2:D:228:ALA:HB2	2.02	0.41
2:E:91:ASP:OD1	2:E:94:GLY:N	2.53	0.41
2:E:163:GLN:NE2	2:E:416:GLY:O	2.46	0.41
2:E:328:ILE:HG13	2:E:346:PRO:HB2	2.01	0.41
2:E:422:THR:OG1	2:E:425:GLU:HG3	2.19	0.41
1:I:39:ILE:CG2	1:I:47:ALA:HB1	2.49	0.41
1:I:499:ASP:OD2	1:I:525:ILE:HG12	2.20	0.41
1:J:357:TYR:HB3	2:N:259:GLU:CD	2.40	0.41
1:K:56:SER:HB2	2:N:27:GLU:HG3	2.02	0.41
1:K:232:GLY:N	1:K:238:LYS:HD3	2.33	0.41
1:K:488:LEU:O	1:K:492:VAL:HG23	2.20	0.41
2:M:345:LEU:HG	2:M:373:PHE:HE2	1.85	0.41
2:N:326:GLN:HE21	2:N:326:GLN:HB2	1.56	0.41
1:A:251:VAL:O	1:A:288:ARG:NH2	2.53	0.41
1:B:211:THR:HB	1:B:245:ILE:HD12	2.03	0.41
1:C:6:ILE:HA	1:C:16:ALA:HA	2.03	0.41
1:C:15:MET:HA	1:C:47:ALA:O	2.20	0.41
1:C:120:PHE:HE2	1:C:137:GLY:HA3	1.85	0.41
2:D:82:SER:HB2	2:D:104:LEU:CB	2.50	0.41
2:D:88:ARG:NH1	2:D:102:GLU:CB	2.83	0.41
2:D:279:THR:O	2:D:283:THR:OG1	2.37	0.41
2:E:132:ILE:H	2:E:132:ILE:CD1	2.30	0.41
2:F:386:ALA:O	2:F:390:GLY:N	2.53	0.41
1:I:221:PRO:O	1:I:437:TYR:HB2	2.20	0.41
1:J:191:TRP:CD2	1:J:192:PRO:HD2	2.55	0.41
1:J:197:ARG:HH11	1:J:316:TYR:HA	1.84	0.41
1:J:262:ARG:NH2	2:M:350:ARG:NH1	2.67	0.41
1:J:304:GLU:HG3	1:J:334:TRP:NE1	2.35	0.41
1:K:215:VAL:HG22	1:K:426:PRO:HG2	2.02	0.41
2:L:147:LEU:O	2:L:301:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:40:ARG:HG3	2:N:58:GLU:OE1	2.20	0.41
1:B:214:ARG:NH2	1:B:510:ASP:OD1	2.53	0.41
1:B:233:PRO:HG3	1:B:417:SER:CB	2.47	0.41
1:C:173:ILE:O	1:C:173:ILE:HG13	2.21	0.41
1:C:191:TRP:CD2	1:C:192:PRO:HD2	2.56	0.41
1:C:348:MET:CG	2:D:265:ARG:HA	2.47	0.41
1:C:560:LYS:H	1:C:560:LYS:HG3	1.58	0.41
2:D:34:MET:CG	2:D:63:ILE:HG13	2.51	0.41
2:D:35:GLN:CD	2:D:35:GLN:H	2.23	0.41
2:D:206:ARG:O	2:D:206:ARG:HG2	2.21	0.41
2:F:332:GLU:HA	2:F:335:LYS:HG2	2.02	0.41
1:I:36:ILE:H	1:I:36:ILE:HD12	1.84	0.41
1:I:167:PHE:HB2	6:I:601:HOH:O	2.20	0.41
1:I:262:ARG:O	1:I:266:MET:N	2.38	0.41
1:I:501:LEU:HD13	1:I:501:LEU:C	2.41	0.41
1:J:573:ILE:O	1:J:577:ILE:HG13	2.21	0.41
1:K:415:LEU:HD21	1:K:428:ILE:HG12	2.02	0.41
1:K:494:LYS:HA	1:K:497:ARG:HD3	2.01	0.41
2:M:60:THR:HA	2:M:63:ILE:CD1	2.50	0.41
2:M:273:TYR:HA	2:M:274:PRO:HD3	1.89	0.41
2:N:218:ALA:HA	2:N:221:ARG:HG3	2.01	0.41
2:N:307:PRO:HB2	2:N:313:HIS:CD2	2.55	0.41
2:N:343:ASP:O	2:N:346:PRO:HD2	2.20	0.41
1:A:243:HIS:O	1:A:247:LYS:HG2	2.19	0.41
1:A:301:ALA:O	1:A:305:ALA:N	2.43	0.41
1:B:72:SER:HA	1:B:193:VAL:HG13	2.03	0.41
1:B:75:LEU:O	1:B:188:MET:HA	2.20	0.41
2:D:248:THR:HA	2:D:249:ASP:HA	1.73	0.41
2:E:191:ALA:O	2:E:195:MET:HG3	2.19	0.41
2:F:151:SER:HB2	2:F:157:HIS:HB3	2.02	0.41
1:I:231:PRO:HD2	1:I:414:GLY:HA2	2.03	0.41
1:I:504:ASN:OD1	1:I:506:PHE:HB2	2.20	0.41
1:J:150:MET:HE2	1:J:320:MET:CA	2.49	0.41
1:J:220:PHE:CZ	1:J:433:SER:HB2	2.55	0.41
1:J:424:HIS:O	1:J:427:SER:HB3	2.21	0.41
1:K:214:ARG:HH21	1:K:503:GLN:HG3	1.86	0.41
1:K:273:PHE:HB2	1:K:274:PRO:HD3	2.01	0.41
2:L:225:PRO:O	2:L:229:LEU:HG	2.20	0.41
2:M:148:PRO:HA	2:M:302:PRO:HG2	2.03	0.41
2:M:335:LYS:HE2	2:M:335:LYS:HB3	1.89	0.41
2:N:29:LEU:HD23	2:N:73:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:89:VAL:HG22	2:N:209:MET:CB	2.50	0.41
1:A:219:PHE:CE2	1:A:501:LEU:CD2	3.03	0.41
1:B:116:LYS:HG2	1:B:118:TRP:NE1	2.35	0.41
1:C:202:LYS:HG3	1:C:372:VAL:CG1	2.38	0.41
1:C:311:ILE:HB	1:C:365:TYR:HE1	1.85	0.41
1:C:318:ARG:NH2	1:C:319:ASP:OD1	2.39	0.41
2:E:213:LEU:HB2	2:E:216:ASP:OD1	2.20	0.41
2:F:42:GLY:HA2	2:F:57:PHE:CE2	2.56	0.41
2:F:264:ARG:HD2	2:F:266:GLU:OE2	2.21	0.41
2:F:442:LEU:HD23	2:F:442:LEU:N	2.35	0.41
1:J:114:HIS:HA	1:J:169:ILE:HG12	2.03	0.41
1:J:144:ILE:HG13	1:J:145:ILE:N	2.36	0.41
1:J:296:SER:CA	1:J:303:ARG:HH21	2.28	0.41
1:J:523:LYS:HA	1:J:526:LEU:HD12	2.03	0.41
1:J:562:ILE:HB	1:J:570:ILE:HD11	2.02	0.41
2:M:411:GLU:OE1	2:M:411:GLU:N	2.53	0.41
1:A:219:PHE:CE2	1:A:501:LEU:HD21	2.56	0.41
1:A:246:ALA:HB1	1:A:254:VAL:HG11	2.01	0.41
1:B:56:SER:N	2:E:26:TYR:HD2	2.19	0.41
1:B:167:PHE:CE2	1:B:173:ILE:HG21	2.56	0.41
1:B:273:PHE:N	1:B:274:PRO:CD	2.83	0.41
1:C:265:GLU:O	1:C:269:VAL:HG23	2.21	0.41
1:C:534:LYS:O	1:C:538:LEU:HG	2.21	0.41
2:D:151:SER:OG	2:D:155:LEU:HB2	2.20	0.41
2:E:73:LEU:HD13	2:E:75:HIS:ND1	2.36	0.41
2:E:82:SER:HB2	2:E:103:ILE:HD11	2.02	0.41
2:E:122:ASP:N	2:E:290:ARG:O	2.39	0.41
2:E:166:ARG:HD3	2:E:197:ASP:OD2	2.19	0.41
2:F:431:TRP:CH2	2:F:445:ILE:HG21	2.56	0.41
1:J:574:ASN:OD1	1:J:574:ASN:N	2.54	0.41
1:K:211:THR:O	1:K:245:ILE:HD13	2.20	0.41
1:K:225:GLY:HA2	1:K:384:ILE:O	2.21	0.41
1:K:233:PRO:CD	1:K:415:LEU:HB2	2.48	0.41
1:K:311:ILE:HB	1:K:365:TYR:CE1	2.54	0.41
1:K:315:GLU:HA	1:K:384:ILE:HD11	2.02	0.41
2:N:98:ASP:CG	2:N:99:ASN:HA	2.40	0.41
2:N:129:GLN:H	2:N:169:THR:C	2.24	0.41
1:A:83:MET:HE3	1:A:83:MET:HB3	1.82	0.41
1:B:6:ILE:O	1:B:60:PRO:HA	2.20	0.41
1:B:27:MET:C	1:B:67:THR:HG1	2.24	0.41
1:B:513:THR:HG22	1:B:518:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:GLN:OE1	1:C:111:ALA:HB1	2.20	0.41
1:C:238:LYS:HE2	1:C:238:LYS:HB2	1.92	0.41
1:C:278:ASP:O	1:C:281:THR:OG1	2.26	0.41
1:C:541:TYR:HB2	1:C:544:GLU:HG3	2.01	0.41
2:D:21:VAL:HB	2:D:24:VAL:CG2	2.51	0.41
2:D:87:GLY:HA2	2:D:204:ILE:O	2.21	0.41
2:D:128:ILE:HD11	2:D:143:ARG:CA	2.40	0.41
2:D:177:PHE:CE2	2:D:242:HIS:HB3	2.56	0.41
2:E:244:LEU:HD12	2:E:299:THR:HB	2.02	0.41
2:F:141:LEU:HD12	2:F:147:LEU:HB2	2.03	0.41
2:F:313:HIS:HA	2:F:314:PRO:HD3	1.93	0.41
2:F:339:GLN:O	2:F:414:ASN:HB3	2.20	0.41
1:I:11:GLY:HA2	1:I:55:THR:OG1	2.21	0.41
1:I:94:PHE:HA	1:I:109:LEU:HD12	2.02	0.41
1:I:311:ILE:O	1:I:315:GLU:HG3	2.21	0.41
1:I:412:PHE:HB2	1:I:434:TYR:CE2	2.55	0.41
1:K:6:ILE:HG12	1:K:64:VAL:HG23	2.02	0.41
1:K:196:GLY:HA2	1:K:368:ARG:NH2	2.36	0.41
1:K:219:PHE:CE1	1:K:457:VAL:HG13	2.56	0.41
1:K:219:PHE:CE1	1:K:461:MET:HG2	2.56	0.41
2:M:151:SER:OG	2:M:157:HIS:HB3	2.21	0.41
2:N:111:ILE:HB	2:N:226:ARG:HB3	2.02	0.41
1:A:176:ILE:N	1:A:183:LYS:O	2.50	0.41
1:A:425:PHE:N	1:A:425:PHE:HD1	2.18	0.41
1:B:500:TYR:HD2	1:B:500:TYR:HA	1.69	0.41
1:C:39:ILE:HG13	1:C:49:ILE:HG23	2.03	0.41
4:C:601:ANP:HNB1	2:F:350:ARG:NH1	2.17	0.41
2:D:124:PRO:HB3	2:D:143:ARG:O	2.20	0.41
2:D:281:LEU:HD23	2:D:281:LEU:HA	1.97	0.41
2:E:256:ALA:O	2:E:260:ILE:HG12	2.20	0.41
2:E:339:GLN:HB3	2:E:417:PHE:CE1	2.56	0.41
2:E:345:LEU:N	2:E:346:PRO:HD2	2.36	0.41
2:E:431:TRP:HZ3	2:E:450:LEU:HD23	1.86	0.41
2:F:183:ALA:HB1	2:F:186:ILE:CD1	2.49	0.41
2:F:389:LEU:CB	2:F:393:ALA:HB3	2.50	0.41
2:F:450:LEU:H	2:F:450:LEU:HG	1.61	0.41
1:I:126:GLU:HG2	1:I:162:ILE:HG22	2.03	0.41
1:I:152:PRO:HG3	6:I:602:HOH:O	2.20	0.41
1:J:237:GLY:O	1:J:241:VAL:HG23	2.21	0.41
1:J:268:ASP:HB2	2:M:123:TYR:CE1	2.56	0.41
1:J:270:VAL:O	1:J:274:PRO:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:373:ILE:HD13	1:J:381:GLU:CG	2.51	0.41
1:K:1:MET:HB3	1:K:2:GLN:H	1.65	0.41
1:K:24:ILE:HG23	1:K:40:ILE:O	2.21	0.41
1:K:29:LEU:CD1	1:K:65:ARG:HH21	2.34	0.41
2:L:170:VAL:HG13	2:L:173:SER:HB3	2.03	0.41
2:L:183:ALA:O	2:L:212:ASN:HB2	2.20	0.41
2:M:65:LEU:H	2:M:65:LEU:CD1	2.25	0.41
2:M:117:ASN:HB3	2:M:120:ALA:HB3	2.02	0.41
2:M:345:LEU:N	2:M:346:PRO:HD2	2.36	0.41
2:N:128:ILE:HD11	2:N:143:ARG:CA	2.50	0.41
2:N:265:ARG:HB2	2:N:265:ARG:HH11	1.85	0.41
2:N:319:THR:HG22	2:N:323:THR:CG2	2.51	0.41
2:N:427:LEU:HA	2:N:427:LEU:HD22	1.82	0.41
1:A:10:SER:CB	2:D:46:GLU:HB2	2.50	0.41
1:A:236:ALA:HB1	1:A:415:LEU:HB3	2.02	0.41
1:A:339:ARG:HD3	2:D:270:ARG:HH12	1.86	0.41
1:B:44:GLN:HG3	2:F:9:LYS:O	2.21	0.41
1:C:401:VAL:O	1:C:405:THR:N	2.47	0.41
1:C:541:TYR:O	1:C:545:ILE:HG13	2.21	0.41
2:D:26:TYR:HE1	2:D:45:LEU:HA	1.86	0.41
2:E:24:VAL:O	2:E:25:LYS:HD3	2.21	0.41
2:E:35:GLN:H	2:E:35:GLN:CD	2.21	0.41
1:J:152:PRO:HA	1:J:153:ASN:HA	1.37	0.41
1:K:318:ARG:CD	1:K:384:ILE:HG13	2.48	0.41
2:L:180:VAL:O	2:L:245:VAL:HG13	2.21	0.41
2:L:180:VAL:HG13	2:L:208:VAL:HB	2.02	0.41
2:M:16:MET:O	2:M:54:VAL:N	2.34	0.41
2:M:234:TYR:CD1	2:M:238:GLU:HG3	2.56	0.41
2:N:188:PHE:O	2:N:192:GLU:HB2	2.21	0.41
1:A:27:MET:HE1	1:A:38:GLU:HG3	2.03	0.40
1:A:230:VAL:HG22	1:A:413:TRP:HE3	1.85	0.40
4:C:601:ANP:H8	4:C:601:ANP:O5'	2.20	0.40
2:D:158:LYS:HG3	2:D:194:PHE:CZ	2.56	0.40
2:D:403:LYS:HA	2:D:403:LYS:HD2	1.94	0.40
2:E:315:ILE:H	2:E:315:ILE:HG13	1.63	0.40
2:E:434:LEU:HD22	2:E:442:LEU:CD2	2.51	0.40
2:F:151:SER:CA	2:F:329:LEU:HD12	2.47	0.40
1:I:227:ALA:HB3	1:I:409:VAL:HG12	2.03	0.40
1:I:324:VAL:O	1:I:385:THR:N	2.33	0.40
1:J:214:ARG:HD3	1:J:513:THR:HG21	2.02	0.40
1:J:406:LEU:CD2	1:J:412:PHE:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:520:ASN:O	1:J:524:VAL:HG23	2.21	0.40
2:L:116:ILE:HG21	2:L:291:ILE:HD12	2.02	0.40
2:L:156:PRO:HD3	2:L:334:TYR:CD1	2.56	0.40
2:L:281:LEU:HD23	2:L:281:LEU:HA	1.90	0.40
2:N:32:VAL:HG21	2:N:56:ILE:CD1	2.51	0.40
1:A:85:ASP:OD2	1:A:87:ILE:HG13	2.22	0.40
1:A:294:ASN:HB3	1:A:298:MET:HG3	2.04	0.40
1:A:354:TYR:HB3	1:A:358:LEU:HD22	2.04	0.40
1:B:497:ARG:CA	1:B:501:LEU:HD13	2.52	0.40
1:C:4:GLY:O	1:C:64:VAL:N	2.53	0.40
1:C:205:PRO:HB3	1:C:371:ARG:CB	2.52	0.40
1:C:507:ASP:OD2	1:C:510:ASP:N	2.54	0.40
2:D:44:VAL:HG13	2:D:53:MET:O	2.21	0.40
2:D:147:LEU:HA	2:D:148:PRO:HD3	1.83	0.40
2:E:117:ASN:HA	2:E:118:PRO:HD3	1.98	0.40
2:F:159:GLU:HG3	2:F:193:PHE:CZ	2.56	0.40
1:I:73:VAL:HG11	1:I:309:THR:HG23	2.02	0.40
1:K:38:GLU:OE2	1:K:52:TYR:OH	2.34	0.40
1:K:363:ALA:O	1:K:367:GLU:HB2	2.20	0.40
1:K:479:ILE:HG21	2:N:394:LEU:HA	2.03	0.40
1:K:500:TYR:CE2	1:K:522:LEU:HD13	2.56	0.40
2:N:49:GLU:HA	2:N:50:ASP:HA	1.67	0.40
2:N:150:PHE:N	2:N:150:PHE:CD1	2.90	0.40
2:N:184:ILE:HD12	2:N:184:ILE:N	2.37	0.40
2:N:267:VAL:HA	2:N:268:PRO:HD3	1.95	0.40
1:A:80:ILE:HA	1:A:290:VAL:HG22	2.03	0.40
1:A:88:GLN:HG2	1:A:88:GLN:O	2.21	0.40
1:A:112:LEU:HD12	1:A:188:MET:HG2	2.03	0.40
1:A:459:GLU:OE2	1:A:462:ARG:NH2	2.46	0.40
1:B:79:ILE:HG13	1:B:112:LEU:HD21	2.03	0.40
1:B:221:PRO:CG	1:B:441:VAL:HG21	2.51	0.40
1:C:308:TYR:O	1:C:312:THR:OG1	2.35	0.40
2:D:345:LEU:HA	2:D:373:PHE:CE1	2.56	0.40
2:E:146:LYS:HE2	2:E:324:GLU:HG2	2.03	0.40
2:F:339:GLN:HB3	2:F:340:PRO:HA	2.03	0.40
1:I:76:GLY:H	1:I:112:LEU:CD1	2.34	0.40
1:I:122:ALA:HB1	1:I:162:ILE:HD11	2.03	0.40
1:I:449:LEU:O	1:I:450:GLN:HB2	2.20	0.40
1:K:351:ASP:OD2	2:L:258:ARG:NH2	2.54	0.40
2:L:82:SER:H	2:L:85:MET:HE3	1.86	0.40
2:M:130:THR:CB	2:M:135:ILE:HB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:44:VAL:HG22	2:N:54:VAL:HG12	1.93	0.40
2:N:160:LEU:O	2:N:164:ILE:HG13	2.21	0.40
2:N:318:LEU:HD23	2:N:318:LEU:HA	1.93	0.40
1:A:259:CYS:HA	1:A:260:GLY:HA2	1.76	0.40
1:B:208:PRO:HD2	1:B:444:TYR:CD2	2.56	0.40
1:B:262:ARG:NH2	4:B:601:ANP:O3G	2.39	0.40
1:C:36:ILE:CD1	1:C:87:ILE:HG23	2.52	0.40
2:D:307:PRO:HG2	2:D:313:HIS:CE1	2.57	0.40
2:D:313:HIS:O	2:D:317:ASP:HB2	2.21	0.40
2:D:343:ASP:HB3	2:D:346:PRO:CG	2.52	0.40
1:I:244:GLN:OE1	1:I:248:TRP:NE1	2.38	0.40
1:J:58:ILE:HG23	1:J:62:GLU:HG3	2.02	0.40
1:J:84:PHE:O	1:J:292:ILE:HA	2.21	0.40
1:K:73:VAL:HG13	1:K:193:VAL:HG12	2.04	0.40
1:K:238:LYS:NZ	4:K:601:ANP:O2B	2.42	0.40
2:N:158:LYS:HB2	2:N:158:LYS:HE3	1.80	0.40
2:N:354:LYS:HD3	2:N:354:LYS:HA	1.84	0.40
1:B:79:ILE:HB	1:B:112:LEU:HD13	2.04	0.40
1:B:482:LEU:HD23	1:B:486:ASP:HB3	2.04	0.40
1:C:533:ARG:HD2	1:C:536:LEU:HD11	2.02	0.40
2:D:225:PRO:CB	2:D:284:LEU:HD13	2.52	0.40
2:D:340:PRO:HA	2:D:341:PRO:HD3	1.87	0.40
2:D:351:LEU:HB3	2:D:354:LYS:HD2	2.02	0.40
2:D:362:ARG:O	2:D:365:HIS:HB2	2.20	0.40
2:E:34:MET:N	2:E:38:GLU:O	2.41	0.40
2:E:155:LEU:O	2:E:157:HIS:ND1	2.54	0.40
2:F:143:ARG:CZ	2:F:170:VAL:HG21	2.51	0.40
2:F:285:PHE:HB2	2:F:322:ILE:CG2	2.52	0.40
2:F:357:GLY:C	2:F:359:GLY:HA3	2.40	0.40
1:I:113:ASP:OD2	1:I:116:LYS:N	2.51	0.40
1:I:247:LYS:HG3	1:I:248:TRP:N	2.36	0.40
1:J:233:PRO:HD3	1:J:415:LEU:O	2.21	0.40
1:J:358:LEU:O	1:J:362:LEU:HG	2.20	0.40
1:K:125:GLU:O	1:K:128:THR:OG1	2.39	0.40
1:K:232:GLY:H	1:K:238:LYS:CD	2.34	0.40
2:L:362:ARG:O	2:L:365:HIS:HB3	2.21	0.40
2:N:347:SER:H	2:N:348:LEU:HA	1.86	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	582/600 (97%)	579 (100%)	3 (0%)	0	100	100
1	B	582/600 (97%)	570 (98%)	12 (2%)	0	100	100
1	C	582/600 (97%)	569 (98%)	13 (2%)	0	100	100
1	I	579/600 (96%)	570 (98%)	9 (2%)	0	100	100
1	J	582/600 (97%)	572 (98%)	10 (2%)	0	100	100
1	K	582/600 (97%)	572 (98%)	10 (2%)	0	100	100
2	D	443/465 (95%)	441 (100%)	1 (0%)	1 (0%)	47	78
2	E	451/465 (97%)	447 (99%)	4 (1%)	0	100	100
2	F	443/465 (95%)	438 (99%)	5 (1%)	0	100	100
2	L	443/465 (95%)	435 (98%)	8 (2%)	0	100	100
2	M	451/465 (97%)	441 (98%)	10 (2%)	0	100	100
2	N	427/465 (92%)	411 (96%)	16 (4%)	0	100	100
All	All	6147/6390 (96%)	6045 (98%)	101 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	105	PRO

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	471/511 (92%)	430 (91%)	41 (9%)	10	35
1	B	465/511 (91%)	418 (90%)	47 (10%)	7	28
1	C	420/511 (82%)	375 (89%)	45 (11%)	6	25
1	I	430/511 (84%)	391 (91%)	39 (9%)	9	32
1	J	461/511 (90%)	416 (90%)	45 (10%)	8	29
1	K	467/511 (91%)	423 (91%)	44 (9%)	8	31
2	D	337/387 (87%)	301 (89%)	36 (11%)	6	25
2	E	329/387 (85%)	294 (89%)	35 (11%)	6	25
2	F	317/387 (82%)	275 (87%)	42 (13%)	4	16
2	L	354/387 (92%)	309 (87%)	45 (13%)	4	18
2	M	323/387 (84%)	282 (87%)	41 (13%)	4	18
2	N	300/387 (78%)	251 (84%)	49 (16%)	2	10
All	All	4674/5388 (87%)	4165 (89%)	509 (11%)	6	24

All (509) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	19	MET
1	A	32	ASP
1	A	46	VAL
1	A	52	TYR
1	A	65	ARG
1	A	67	THR
1	A	80	ILE
1	A	83	MET
1	A	87	ILE
1	A	89	ARG
1	A	98	THR
1	A	105	ARG
1	A	128	THR
1	A	129	GLU
1	A	161	LYS
1	A	171	ASP
1	A	178	THR
1	A	179	GLU
1	A	185	LEU
1	A	186	THR
1	A	247	LYS

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Mol	Chain	Res	Type
1	A	264	ASN
1	A	265	GLU
1	A	268	ASP
1	A	304	GLU
1	A	331	THR
1	A	338	LEU
1	A	352	GLU
1	A	378	ASP
1	A	396	ASP
1	A	399	GLU
1	A	416	ASP
1	A	439	THR
1	A	448	ILE
1	A	449	LEU
1	A	514	SER
1	A	523	LYS
1	A	530	LYS
1	A	541	TYR
1	A	549	THR
1	B	3	ILE
1	B	21	GLU
1	B	25	GLN
1	B	38	GLU
1	B	54	GLU
1	B	67	THR
1	B	72	SER
1	B	80	ILE
1	B	140	ASP
1	B	141	GLU
1	B	143	LYS
1	B	147	HIS
1	B	148	LYS
1	B	150	MET
1	B	173	ILE
1	B	179	GLU
1	B	183	LYS
1	B	185	LEU
1	B	214	ARG
1	B	238	LYS
1	B	252	ASP
1	B	253	LEU
1	B	285	LEU

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Mol	Chain	Res	Type
1	B	288	ARG
1	B	291	LEU
1	B	295	THR
1	B	297	ASN
1	B	319	ASP
1	B	327	MET
1	B	344	ARG
1	B	378	ASP
1	B	385	THR
1	B	415	LEU
1	B	424	HIS
1	B	443	ARG
1	B	458	THR
1	B	476	LEU
1	B	489	THR
1	B	494	LYS
1	B	498	GLU
1	B	499	ASP
1	B	500	TYR
1	B	501	LEU
1	B	503	GLN
1	B	508	ASP
1	B	536	LEU
1	B	567	LEU
1	C	13	LEU
1	C	15	MET
1	C	25	GLN
1	C	39	ILE
1	C	40	ILE
1	C	53	GLU
1	C	65	ARG
1	C	82	GLN
1	C	87	ILE
1	C	88	GLN
1	C	89	ARG
1	C	124	ILE
1	C	128	THR
1	C	135	ILE
1	C	150	MET
1	C	161	LYS
1	C	163	GLU
1	C	167	PHE

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Mol	Chain	Res	Type
1	C	173	ILE
1	C	195	ARG
1	C	199	ILE
1	C	203	LEU
1	C	218	THR
1	C	224	LYS
1	C	234	PHE
1	C	252	ASP
1	C	253	LEU
1	C	259	CYS
1	C	273	PHE
1	C	276	LEU
1	C	278	ASP
1	C	285	LEU
1	C	288	ARG
1	C	297	ASN
1	C	331	THR
1	C	332	SER
1	C	378	ASP
1	C	390	VAL
1	C	399	GLU
1	C	500	TYR
1	C	536	LEU
1	C	547	GLU
1	C	554	GLU
1	C	560	LYS
1	C	580	THR
2	D	5	TYR
2	D	34	MET
2	D	43	GLN
2	D	45	LEU
2	D	49	GLU
2	D	51	LYS
2	D	65	LEU
2	D	69	SER
2	D	73	LEU
2	D	77	LEU
2	D	138	LEU
2	D	143	ARG
2	D	157	HIS
2	D	163	GLN
2	D	176	ASP

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Mol	Chain	Res	Type
2	D	177	PHE
2	D	239	LYS
2	D	279	THR
2	D	280	ASN
2	D	283	THR
2	D	324	GLU
2	D	330	THR
2	D	332	GLU
2	D	335	LYS
2	D	339	GLN
2	D	343	ASP
2	D	345	LEU
2	D	348	LEU
2	D	360	LYS
2	D	362	ARG
2	D	370	ASN
2	D	401	TYR
2	D	414	ASN
2	D	415	GLN
2	D	432	GLU
2	D	442	LEU
2	E	6	ARG
2	E	33	ARG
2	E	43	GLN
2	E	45	LEU
2	E	77	LEU
2	E	79	LEU
2	E	82	SER
2	E	86	ILE
2	E	90	PHE
2	E	95	ARG
2	E	103	ILE
2	E	104	LEU
2	E	109	LEU
2	E	123	TYR
2	E	129	GLN
2	E	153	SER
2	E	158	LYS
2	E	167	GLN
2	E	170	VAL
2	E	176	ASP
2	E	187	THR

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Mol	Chain	Res	Type
2	E	212	ASN
2	E	215	ASN
2	E	230	THR
2	E	284	LEU
2	E	290	ARG
2	E	295	LYS
2	E	335	LYS
2	E	339	GLN
2	E	412	TYR
2	E	419	THR
2	E	421	ARG
2	E	434	LEU
2	E	443	LYS
2	E	444	ARG
2	F	9	LYS
2	F	31	GLU
2	F	44	VAL
2	F	45	LEU
2	F	50	ASP
2	F	60	THR
2	F	61	SER
2	F	65	LEU
2	F	71	ARG
2	F	73	LEU
2	F	86	ILE
2	F	97	LYS
2	F	133	SER
2	F	136	ASP
2	F	142	VAL
2	F	147	LEU
2	F	171	LEU
2	F	177	PHE
2	F	187	THR
2	F	190	GLU
2	F	207	SER
2	F	208	VAL
2	F	213	LEU
2	F	226	ARG
2	F	257	LEU
2	F	292	ARG
2	F	305	THR
2	F	308	GLU

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Mol	Chain	Res	Type
2	F	330	THR
2	F	335	LYS
2	F	338	ILE
2	F	339	GLN
2	F	348	LEU
2	F	352	LYS
2	F	427	LEU
2	F	429	LEU
2	F	433	LEU
2	F	434	LEU
2	F	437	LEU
2	F	442	LEU
2	F	445	ILE
2	F	450	LEU
1	I	13	LEU
1	I	14	VAL
1	I	46	VAL
1	I	65	ARG
1	I	80	ILE
1	I	81	SER
1	I	94	PHE
1	I	103	LEU
1	I	115	GLU
1	I	124	ILE
1	I	128	THR
1	I	130	VAL
1	I	131	SER
1	I	140	ASP
1	I	143	LYS
1	I	167	PHE
1	I	185	LEU
1	I	186	THR
1	I	201	GLN
1	I	209	MET
1	I	244	GLN
1	I	272	GLU
1	I	331	THR
1	I	338	LEU
1	I	351	ASP
1	I	385	THR
1	I	424	HIS
1	I	452	ASP

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Mol	Chain	Res	Type
1	I	454	SER
1	I	461	MET
1	I	464	LEU
1	I	475	ARG
1	I	495	SER
1	I	500	TYR
1	I	501	LEU
1	I	502	GLN
1	I	525	ILE
1	I	527	THR
1	I	554	GLU
1	J	1	MET
1	J	13	LEU
1	J	36	ILE
1	J	53	GLU
1	J	85	ASP
1	J	87	ILE
1	J	88	GLN
1	J	94	PHE
1	J	98	THR
1	J	148	LYS
1	J	155	ILE
1	J	174	CYS
1	J	215	VAL
1	J	217	ASP
1	J	230	VAL
1	J	238	LYS
1	J	250	ASP
1	J	276	LEU
1	J	288	ARG
1	J	289	THR
1	J	294	ASN
1	J	295	THR
1	J	297	ASN
1	J	298	MET
1	J	326	ILE
1	J	327	MET
1	J	351	ASP
1	J	378	ASP
1	J	391	SER
1	J	405	THR
1	J	407	ARG

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Mol	Chain	Res	Type
1	J	415	LEU
1	J	416	ASP
1	J	479	ILE
1	J	499	ASP
1	J	500	TYR
1	J	512	PHE
1	J	527	THR
1	J	528	PHE
1	J	530	LYS
1	J	533	ARG
1	J	536	LEU
1	J	541	TYR
1	J	543	ASN
1	J	544	GLU
1	K	13	LEU
1	K	15	MET
1	K	20	SER
1	K	23	CYS
1	K	25	GLN
1	K	40	ILE
1	K	41	GLU
1	K	55	THR
1	K	62	GLU
1	K	65	ARG
1	K	84	PHE
1	K	108	GLN
1	K	128	THR
1	K	140	ASP
1	K	150	MET
1	K	158	THR
1	K	161	LYS
1	K	163	GLU
1	K	188	MET
1	K	189	GLN
1	K	211	THR
1	K	216	ILE
1	K	222	VAL
1	K	253	LEU
1	K	259	CYS
1	K	270	VAL
1	K	295	THR
1	K	298	MET

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Mol	Chain	Res	Type
1	K	346	GLU
1	K	351	ASP
1	K	378	ASP
1	K	380	ARG
1	K	385	THR
1	K	391	SER
1	K	423	ARG
1	K	480	ASP
1	K	499	ASP
1	K	500	TYR
1	K	508	ASP
1	K	512	PHE
1	K	524	VAL
1	K	538	LEU
1	K	560	LYS
1	K	572	SER
2	L	6	ARG
2	L	10	GLU
2	L	34	MET
2	L	38	GLU
2	L	45	LEU
2	L	48	GLN
2	L	55	GLN
2	L	65	LEU
2	L	73	LEU
2	L	86	ILE
2	L	109	LEU
2	L	128	ILE
2	L	130	THR
2	L	151	SER
2	L	153	SER
2	L	171	LEU
2	L	177	PHE
2	L	201	THR
2	L	212	ASN
2	L	215	ASN
2	L	219	ILE
2	L	244	LEU
2	L	257	LEU
2	L	260	ILE
2	L	271	ARG
2	L	279	THR

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Mol	Chain	Res	Type
2	L	283	THR
2	L	287	ARG
2	L	309	ASP
2	L	315	ILE
2	L	350	ARG
2	L	352	LYS
2	L	368	THR
2	L	372	LEU
2	L	378	GLN
2	L	380	LYS
2	L	385	LEU
2	L	403	LYS
2	L	412	TYR
2	L	414	ASN
2	L	424	THR
2	L	427	LEU
2	L	433	LEU
2	L	434	LEU
2	L	439	ARG
2	M	10	GLU
2	M	15	LEU
2	M	16	MET
2	M	21	VAL
2	M	43	GLN
2	M	45	LEU
2	M	54	VAL
2	M	67	ASN
2	M	73	LEU
2	M	77	LEU
2	M	78	GLN
2	M	84	ASP
2	M	86	ILE
2	M	93	LEU
2	M	95	ARG
2	M	102	GLU
2	M	130	THR
2	M	136	ASP
2	M	137	HIS
2	M	146	LYS
2	M	151	SER
2	M	158	LYS
2	M	163	GLN

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Mol	Chain	Res	Type
2	M	170	VAL
2	M	215	ASN
2	M	226	ARG
2	M	230	THR
2	M	251	THR
2	M	270	ARG
2	M	281	LEU
2	M	292	ARG
2	M	305	THR
2	M	306	MET
2	M	319	THR
2	M	351	LEU
2	M	368	THR
2	M	373	PHE
2	M	396	ASP
2	M	444	ARG
2	M	445	ILE
2	M	446	LYS
2	N	4	GLU
2	N	5	TYR
2	N	26	TYR
2	N	31	GLU
2	N	45	LEU
2	N	48	GLN
2	N	51	LYS
2	N	61	SER
2	N	65	LEU
2	N	67	ASN
2	N	73	LEU
2	N	77	LEU
2	N	85	MET
2	N	98	ASP
2	N	104	LEU
2	N	110	ASP
2	N	122	ASP
2	N	123	TYR
2	N	125	ASP
2	N	126	GLU
2	N	186	ILE
2	N	187	THR
2	N	192	GLU
2	N	197	ASP

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Mol	Chain	Res	Type
2	N	207	SER
2	N	219	ILE
2	N	221	ARG
2	N	264	ARG
2	N	265	ARG
2	N	270	ARG
2	N	280	ASN
2	N	305	THR
2	N	319	THR
2	N	326	GLN
2	N	338	ILE
2	N	345	LEU
2	N	349	SER
2	N	352	LYS
2	N	353	ASP
2	N	373	PHE
2	N	378	GLN
2	N	381	GLN
2	N	384	GLU
2	N	385	LEU
2	N	392	SER
2	N	403	LYS
2	N	407	ARG
2	N	421	ARG
2	N	427	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	B	503	GLN
2	D	157	HIS
2	D	215	ASN
2	D	313	HIS
2	E	55	GLN
1	I	213	GLN
1	J	50	GLN
1	J	213	GLN
1	J	244	GLN
1	K	18	ASN
1	K	213	GLN
2	L	163	GLN

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Mol	Chain	Res	Type
2	N	129	GLN
2	N	365	HIS
2	N	414	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z  > 2$
4	ANP	C	601	5	29,33,33	1.07	4 (13%)	31,52,52	1.33	4 (12%)
4	ANP	B	601	5	29,33,33	1.10	4 (13%)	31,52,52	1.24	3 (9%)
4	ANP	J	601	5	29,33,33	1.11	4 (13%)	31,52,52	1.20	4 (12%)
4	ANP	K	601	5	29,33,33	1.09	4 (13%)	31,52,52	1.09	2 (6%)
3	GOL	A	601	-	5,5,5	0.37	0	5,5,5	0.15	0

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
4	ANP	C	601	5	-	1/14/38/38	0/3/3/3
4	ANP	B	601	5	-	3/14/38/38	0/3/3/3
4	ANP	J	601	5	-	5/14/38/38	0/3/3/3
4	ANP	K	601	5	-	3/14/38/38	0/3/3/3
3	GOL	A	601	-	-	2/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	601	ANP	PG-N3B	2.75	1.70	1.63
4	C	601	ANP	PG-N3B	2.52	1.69	1.63
4	C	601	ANP	PG-O1G	2.51	1.50	1.46
4	B	601	ANP	PB-O3A	-2.48	1.55	1.59
4	K	601	ANP	PG-O1G	2.47	1.50	1.46
4	B	601	ANP	PG-O1G	2.45	1.50	1.46
4	B	601	ANP	PG-N3B	2.42	1.69	1.63
4	K	601	ANP	PB-O3A	-2.41	1.56	1.59
4	J	601	ANP	PB-O3A	-2.41	1.56	1.59
4	K	601	ANP	PG-N3B	2.41	1.69	1.63
4	B	601	ANP	PB-O1B	2.38	1.49	1.46
4	K	601	ANP	PB-O1B	2.37	1.49	1.46
4	J	601	ANP	PG-O1G	2.27	1.49	1.46
4	J	601	ANP	PB-O1B	2.27	1.49	1.46
4	C	601	ANP	PB-O3A	-2.18	1.56	1.59
4	C	601	ANP	PB-O1B	2.10	1.49	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	601	ANP	PB-O3A-PA	-3.59	119.98	132.62
4	B	601	ANP	PB-O3A-PA	-3.58	119.99	132.62
4	C	601	ANP	PB-O3A-PA	-3.57	120.03	132.62
4	J	601	ANP	PB-O3A-PA	-3.29	121.04	132.62
4	C	601	ANP	C3'-C2'-C1'	3.12	105.68	100.98
4	J	601	ANP	C3'-C2'-C1'	3.02	105.52	100.98
4	B	601	ANP	C3'-C2'-C1'	2.99	105.48	100.98
4	J	601	ANP	O2G-PG-O1G	-2.35	107.55	113.45
4	J	601	ANP	C5-C6-N6	2.32	123.87	120.35
4	B	601	ANP	C5-C6-N6	2.28	123.82	120.35
4	K	601	ANP	C5-C6-N6	2.28	123.81	120.35
4	C	601	ANP	C5-C6-N6	2.23	123.75	120.35
4	C	601	ANP	C4-C5-N7	2.13	111.61	109.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

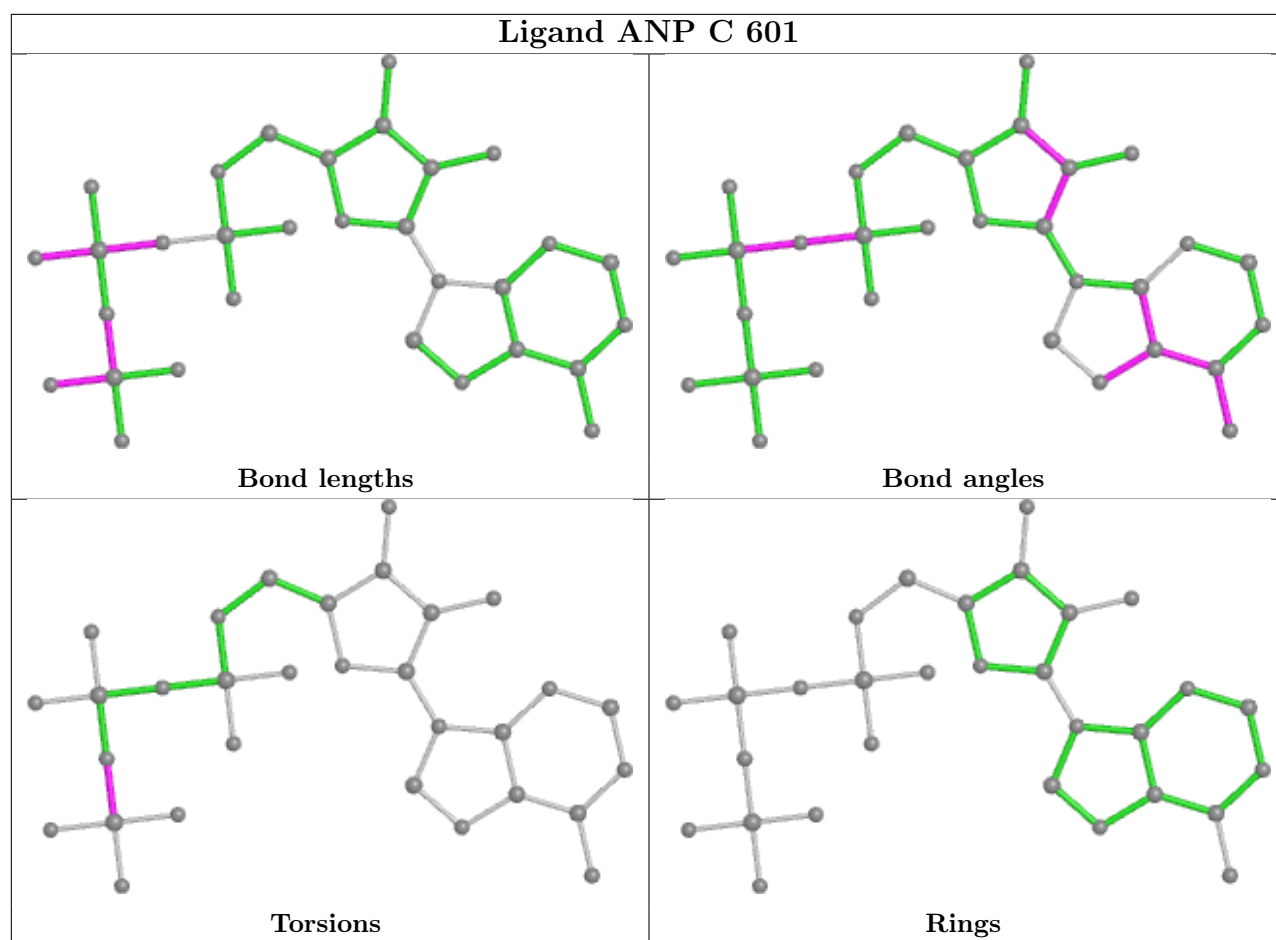
Mol	Chain	Res	Type	Atoms
3	A	601	GOL	C1-C2-C3-O3
3	A	601	GOL	O2-C2-C3-O3
4	B	601	ANP	PB-N3B-PG-O1G
4	B	601	ANP	PG-N3B-PB-O1B
4	B	601	ANP	PG-N3B-PB-O3A
4	C	601	ANP	PB-N3B-PG-O1G
4	J	601	ANP	PB-N3B-PG-O1G
4	J	601	ANP	C5'-O5'-PA-O3A
4	K	601	ANP	PB-N3B-PG-O1G
4	J	601	ANP	O4'-C4'-C5'-O5'
4	K	601	ANP	O4'-C4'-C5'-O5'
4	J	601	ANP	PG-N3B-PB-O1B
4	K	601	ANP	C3'-C4'-C5'-O5'
4	J	601	ANP	C5'-O5'-PA-O1A

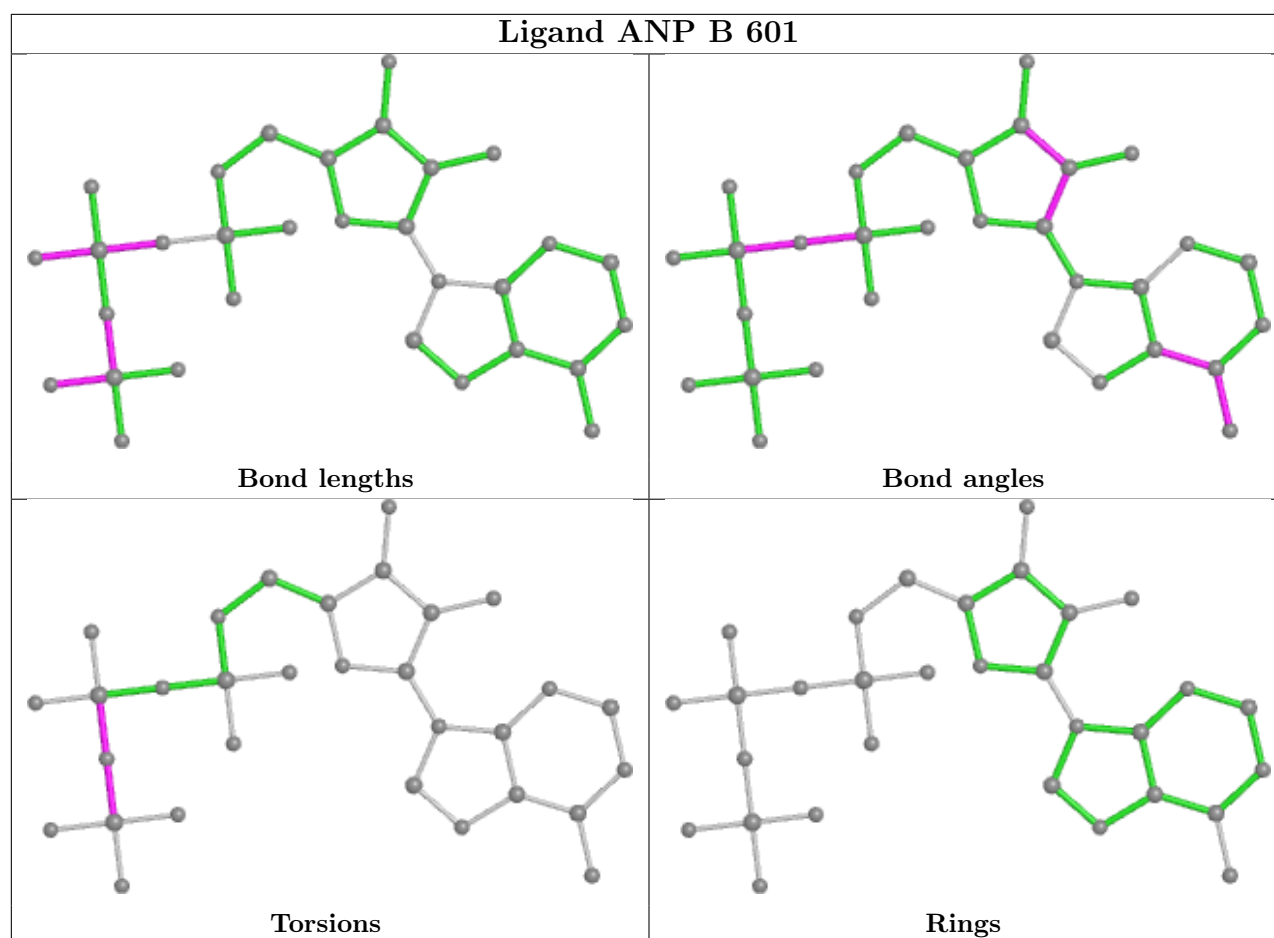
There are no ring outliers.

4 monomers are involved in 46 short contacts:

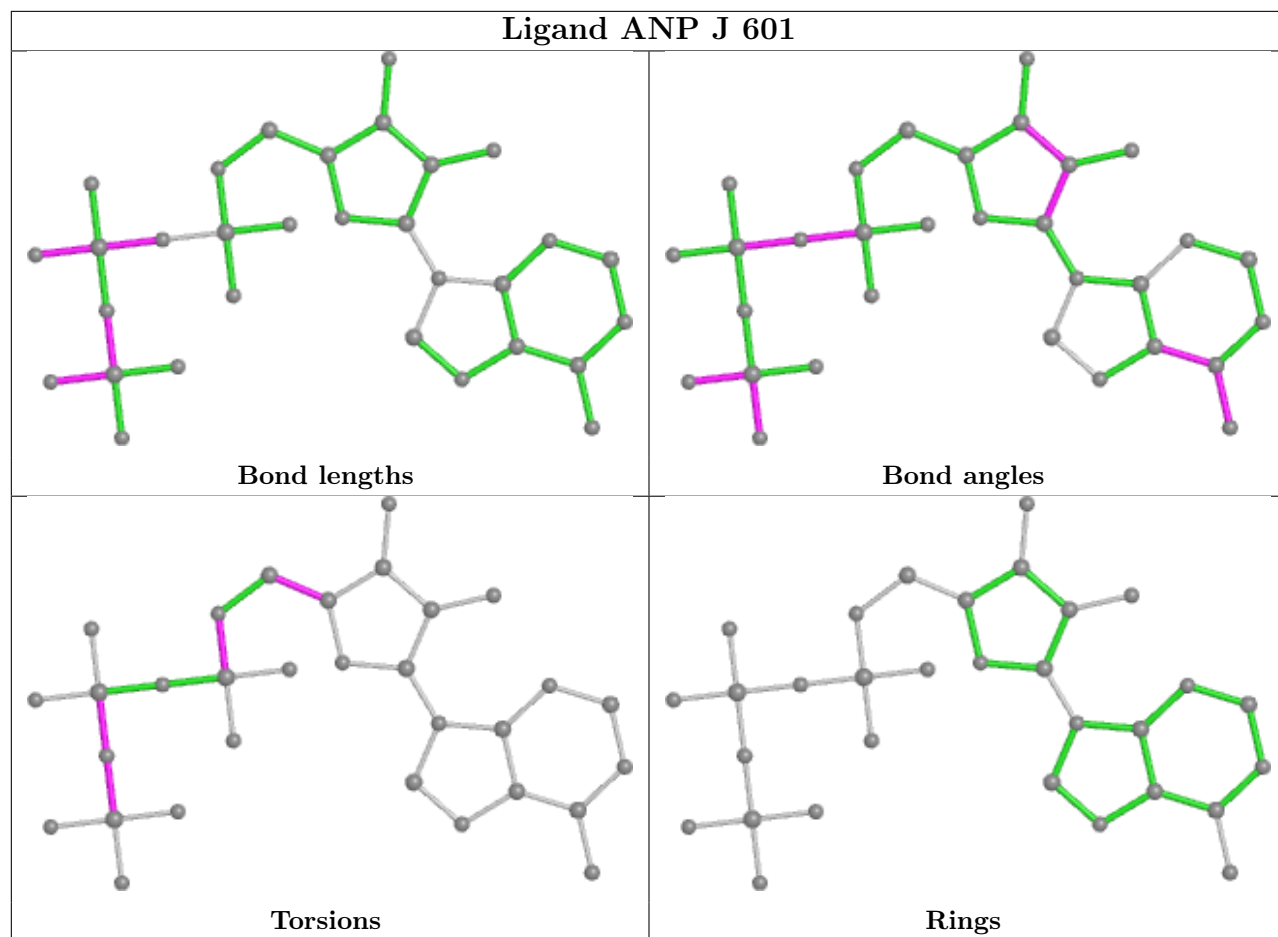
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	ANP	14	0
4	B	601	ANP	9	0
4	J	601	ANP	7	0
4	K	601	ANP	16	0

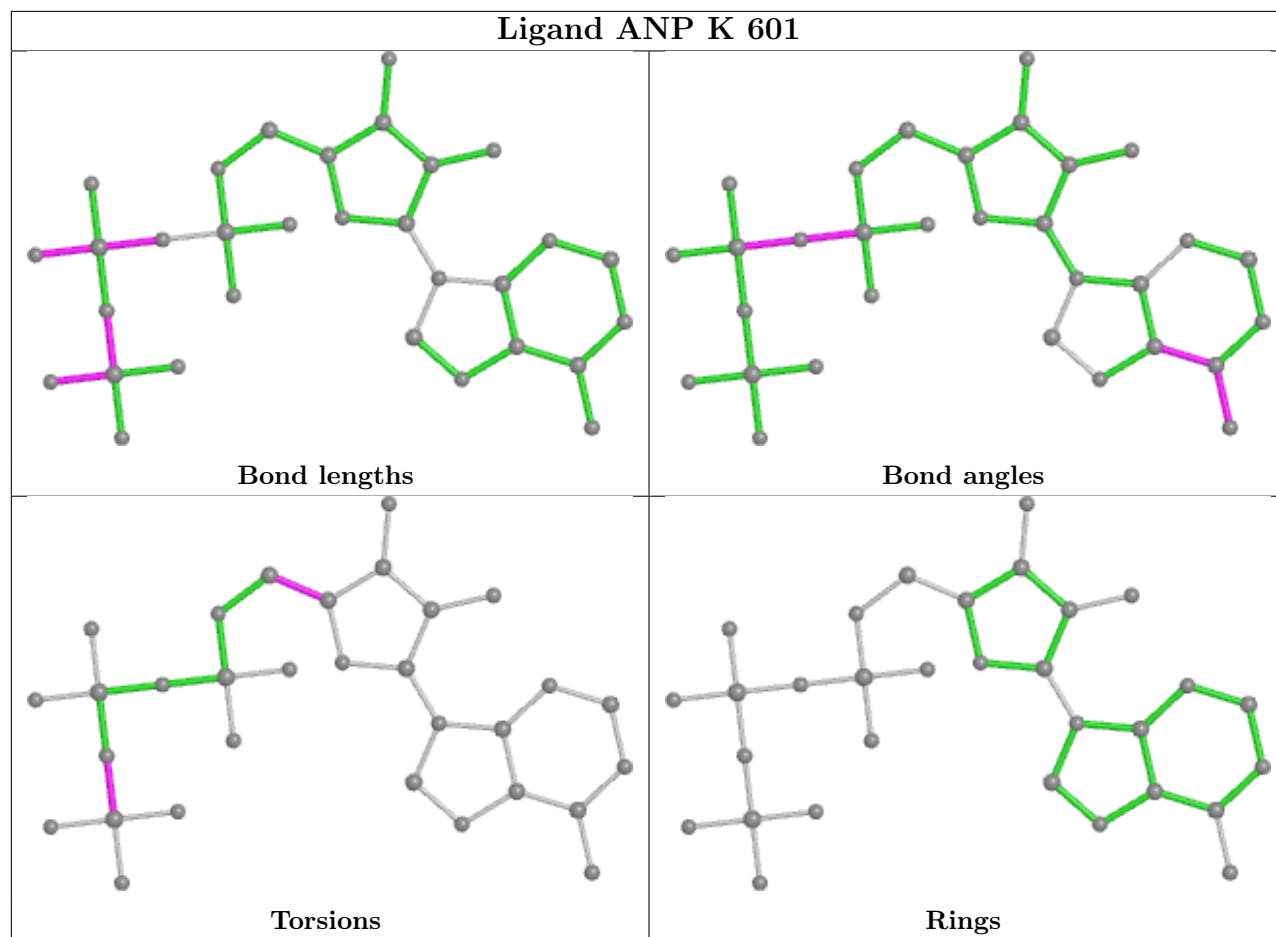
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





## Ligand ANP J 601





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	584/600 (97%)	0.52	29 (4%)	28 32	42, 77, 103, 125	0
1	B	584/600 (97%)	0.53	40 (6%)	17 21	37, 72, 98, 116	0
1	C	584/600 (97%)	0.61	49 (8%)	11 13	39, 80, 129, 154	0
1	I	583/600 (97%)	0.42	31 (5%)	26 30	38, 72, 100, 125	0
1	J	584/600 (97%)	0.68	47 (8%)	12 14	66, 92, 117, 151	0
1	K	584/600 (97%)	0.50	44 (7%)	14 17	34, 69, 105, 178	0
2	D	447/465 (96%)	0.64	36 (8%)	12 14	45, 78, 112, 131	0
2	E	453/465 (97%)	0.49	18 (3%)	38 41	49, 73, 107, 135	0
2	F	445/465 (95%)	0.81	47 (10%)	6 8	44, 75, 121, 154	0
2	L	447/465 (96%)	0.62	35 (7%)	13 16	37, 70, 122, 153	0
2	M	453/465 (97%)	0.78	47 (10%)	6 8	52, 90, 130, 150	0
2	N	429/465 (92%)	0.85	56 (13%)	3 4	51, 93, 128, 168	0
All	All	6177/6390 (96%)	0.61	479 (7%)	13 16	34, 78, 117, 178	0

All (479) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	389	LEU	8.5
2	F	386	ALA	7.3
2	F	445	ILE	6.7
2	D	102	GLU	6.7
1	K	567	LEU	6.4
2	F	52	ALA	6.3
1	C	181	GLY	6.3
2	N	172	ASP	6.2
2	F	438	PRO	6.1
1	I	395	GLY	6.1
1	K	280	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	12	PRO	6.0
2	F	382	ALA	5.7
1	I	396	ASP	5.5
1	K	61	GLY	5.5
2	M	73	LEU	5.5
2	N	176	ASP	5.4
2	N	386	ALA	5.4
1	K	571	SER	5.4
1	B	279	PRO	5.1
1	B	342	SER	5.0
2	D	384	GLU	5.0
1	A	181	GLY	4.9
2	F	392	SER	4.7
1	J	385	THR	4.7
2	D	103	ILE	4.7
2	D	390	GLY	4.6
1	B	13	LEU	4.6
2	N	104	LEU	4.6
1	B	206	ASP	4.6
2	N	60	THR	4.6
1	J	35	VAL	4.6
2	N	31	GLU	4.6
2	F	92	GLY	4.5
1	I	480	ASP	4.5
2	M	99	ASN	4.5
1	K	283	GLU	4.4
2	F	442	LEU	4.4
2	L	377	ALA	4.4
2	F	440	THR	4.4
2	L	388	VAL	4.3
2	F	443	LYS	4.3
2	M	297	SER	4.3
1	C	106	GLY	4.3
2	N	54	VAL	4.3
1	K	76	GLY	4.2
2	D	70	VAL	4.2
2	F	391	GLU	4.2
1	A	396	ASP	4.2
2	L	393	ALA	4.1
1	B	539	GLY	4.1
2	E	354	LYS	4.1
1	A	52	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
2	M	402	ALA	4.1
2	D	5	TYR	4.0
2	D	77	LEU	4.0
2	L	62	GLY	4.0
1	J	131	SER	4.0
2	N	359	GLY	4.0
2	D	73	LEU	4.0
2	D	45	LEU	3.9
2	N	391	GLU	3.9
2	E	142	VAL	3.9
1	C	410	LYS	3.9
2	F	11	VAL	3.9
2	D	393	ALA	3.9
1	B	376	GLY	3.9
1	K	5	LYS	3.9
1	K	284	SER	3.8
2	L	364	ASP	3.8
2	N	171	LEU	3.8
1	K	232	GLY	3.7
2	M	174	SER	3.7
1	I	398	SER	3.7
1	C	539	GLY	3.7
1	C	163	GLU	3.6
1	A	508	ASP	3.6
2	M	45	LEU	3.6
2	F	439	ARG	3.6
1	J	9	VAL	3.6
2	E	337	GLY	3.6
2	F	131	GLY	3.6
1	J	129	GLU	3.5
1	C	279	PRO	3.5
1	K	282	GLY	3.5
1	K	278	ASP	3.5
2	N	18	VAL	3.5
2	D	130	THR	3.5
1	I	577	ILE	3.5
1	A	180	GLN	3.5
1	C	139	VAL	3.5
1	K	19	MET	3.5
2	N	379	GLY	3.5
2	F	200	GLN	3.4
1	C	545	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	215	VAL	3.4
2	D	140	THR	3.4
1	K	77	PRO	3.4
2	N	340	PRO	3.4
2	D	440	THR	3.4
2	L	130	THR	3.4
2	N	395	SER	3.4
1	J	38	GLU	3.4
1	A	484	ASP	3.4
1	C	9	VAL	3.4
2	F	60	THR	3.4
1	A	154	GLY	3.4
2	L	57	PHE	3.3
1	C	280	ASN	3.3
1	I	235	GLY	3.3
2	N	341	PRO	3.3
2	N	103	ILE	3.3
1	C	180	GLN	3.3
2	N	347	SER	3.3
1	C	278	ASP	3.3
1	B	40	ILE	3.3
1	K	162	ILE	3.3
1	I	76	GLY	3.3
2	E	134	ALA	3.3
2	D	388	VAL	3.3
1	K	279	PRO	3.2
1	K	31	GLY	3.2
2	M	182	ALA	3.2
1	K	41	GLU	3.2
1	K	281	THR	3.2
1	J	107	VAL	3.2
1	B	157	GLY	3.2
2	D	170	VAL	3.2
2	N	358	ALA	3.2
1	C	551	ALA	3.2
2	M	32	VAL	3.2
1	A	537	SER	3.2
2	F	371	GLN	3.2
1	C	495	SER	3.1
1	I	10	SER	3.1
1	J	381	GLU	3.1
2	F	448	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	162	ILE	3.1
2	F	387	VAL	3.1
2	F	358	ALA	3.1
2	N	69	SER	3.1
2	L	68	SER	3.1
1	C	167	PHE	3.1
2	D	32	VAL	3.1
2	L	432	GLU	3.1
1	J	42	MET	3.1
1	B	377	SER	3.0
2	L	11	VAL	3.0
2	F	435	ALA	3.0
1	A	40	ILE	3.0
1	K	136	ILE	3.0
2	M	390	GLY	3.0
1	I	502	GLN	3.0
1	J	423	ARG	3.0
1	J	18	ASN	3.0
2	N	389	LEU	3.0
1	B	280	ASN	2.9
2	F	349	SER	2.9
2	N	13	GLY	2.9
2	M	179	VAL	2.9
2	M	395	SER	2.9
2	N	55	GLN	2.9
2	F	176	ASP	2.9
2	L	125	ASP	2.9
1	I	423	ARG	2.9
1	J	232	GLY	2.9
1	A	162	ILE	2.9
2	E	43	GLN	2.9
2	M	43	GLN	2.9
2	L	80	GLY	2.9
1	K	568	ALA	2.9
2	D	420	ASN	2.9
1	C	67	THR	2.9
2	M	72	PHE	2.9
1	C	569	LYS	2.8
2	M	106	GLU	2.8
2	M	237	TYR	2.8
2	N	175	ASP	2.8
1	J	313	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	N	74	GLY	2.8
1	K	570	ILE	2.8
1	B	504	ASN	2.8
1	A	231	PRO	2.8
2	M	67	ASN	2.8
1	J	156	LYS	2.8
2	F	355	GLY	2.8
2	M	164	ILE	2.8
1	B	51	VAL	2.8
2	L	36	ASN	2.8
1	A	219	PHE	2.8
1	B	343	GLY	2.7
1	A	155	ILE	2.7
2	N	412	TYR	2.7
1	C	499	ASP	2.7
2	L	154	GLY	2.7
2	N	378	GLN	2.7
1	I	421	GLN	2.7
1	J	373	ILE	2.7
2	M	397	ILE	2.7
1	B	449	LEU	2.7
2	M	450	LEU	2.7
2	L	392	SER	2.7
1	J	168	THR	2.7
2	L	425	GLU	2.7
2	M	68	SER	2.7
2	F	90	PHE	2.7
1	A	103	LEU	2.6
1	C	209	MET	2.6
1	C	253	LEU	2.6
1	J	10	SER	2.6
2	F	325	GLY	2.6
2	N	364	ASP	2.6
1	I	264	ASN	2.6
1	C	87	ILE	2.6
1	B	10	SER	2.6
2	F	422	THR	2.6
2	L	360	LYS	2.6
1	B	249	SER	2.6
2	F	138	LEU	2.6
2	L	385	LEU	2.6
1	J	22	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	M	7	THR	2.6
1	C	40	ILE	2.6
1	J	571	SER	2.6
1	I	259	CYS	2.6
1	A	448	ILE	2.6
2	N	251	THR	2.6
1	K	22	ALA	2.5
2	N	170	VAL	2.5
1	J	173	ILE	2.5
1	J	279	PRO	2.5
2	N	89	VAL	2.5
1	A	449	LEU	2.5
2	M	8	ILE	2.5
2	F	139	ASN	2.5
2	N	183	ALA	2.5
2	E	390	GLY	2.5
1	J	531	GLU	2.5
1	B	16	ALA	2.5
1	K	51	VAL	2.5
2	M	6	ARG	2.5
1	K	63	PRO	2.5
1	J	3	ILE	2.5
1	K	385	THR	2.5
1	K	59	GLY	2.5
1	C	25	GLN	2.5
1	C	7	ILE	2.5
1	J	106	GLY	2.5
2	D	237	TYR	2.5
2	L	302	PRO	2.5
2	N	85	MET	2.5
2	E	93	LEU	2.5
2	N	329	LEU	2.5
1	I	40	ILE	2.5
1	I	481	SER	2.5
2	M	365	HIS	2.5
1	A	43	ARG	2.5
1	K	28	CYS	2.5
2	M	209	MET	2.5
1	A	291	LEU	2.5
1	J	538	LEU	2.4
2	F	326	GLN	2.4
2	L	145	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	121	GLU	2.4
2	N	164	ILE	2.4
1	C	51	VAL	2.4
1	C	174	CYS	2.4
1	J	233	PRO	2.4
2	E	413	VAL	2.4
2	N	42	GLY	2.4
2	L	194	PHE	2.4
1	C	186	THR	2.4
2	F	140	THR	2.4
1	K	46	VAL	2.4
2	N	52	ALA	2.4
2	N	56	ILE	2.4
2	M	161	ALA	2.4
1	C	281	THR	2.4
1	B	322	TYR	2.4
1	I	23	CYS	2.4
1	C	123	THR	2.4
2	L	7	THR	2.4
2	D	392	SER	2.4
1	A	539	GLY	2.4
2	M	388	VAL	2.4
2	M	181	PHE	2.4
2	M	147	LEU	2.4
2	D	180	VAL	2.4
1	K	34	GLY	2.4
1	C	41	GLU	2.4
1	I	211	THR	2.4
1	I	501	LEU	2.4
1	B	45	ASP	2.3
1	K	86	GLY	2.3
2	D	205	ASP	2.3
2	E	175	ASP	2.3
2	F	367	ALA	2.3
2	F	433	LEU	2.3
2	M	128	ILE	2.3
1	B	346	GLU	2.3
1	C	283	GLU	2.3
2	F	103	ILE	2.3
2	N	196	GLU	2.3
2	M	39	ILE	2.3
2	N	40	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	211	MET	2.3
1	J	379	GLN	2.3
2	N	7	THR	2.3
2	D	56	ILE	2.3
1	B	231	PRO	2.3
2	N	404	PHE	2.3
2	F	10	GLU	2.3
1	K	233	PRO	2.3
2	D	105	PRO	2.3
2	N	152	GLY	2.3
2	N	46	GLU	2.3
1	C	160	GLN	2.3
1	A	501	LEU	2.3
2	M	94	GLY	2.3
1	I	579	GLU	2.3
1	B	253	LEU	2.3
1	C	385	THR	2.3
1	I	313	ILE	2.3
1	J	294	ASN	2.3
2	N	303	ILE	2.3
2	D	202	GLY	2.3
2	F	13	GLY	2.3
2	F	16	MET	2.3
1	B	503	GLN	2.3
1	B	4	GLY	2.3
1	C	158	THR	2.3
1	C	206	ASP	2.3
2	F	170	VAL	2.3
2	D	106	GLU	2.3
2	E	437	LEU	2.3
1	B	146	GLN	2.3
2	L	365	HIS	2.3
1	A	106	GLY	2.3
1	J	287	GLU	2.3
2	F	348	LEU	2.3
2	M	341	PRO	2.3
1	K	277	ILE	2.3
2	E	178	ALA	2.3
1	K	62	GLU	2.2
2	D	57	PHE	2.2
2	F	204	ILE	2.2
2	F	216	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	346	GLU	2.2
2	N	382	ALA	2.2
2	M	364	ASP	2.2
1	J	524	VAL	2.2
2	M	243	VAL	2.2
2	N	385	LEU	2.2
2	L	177	PHE	2.2
1	B	35	VAL	2.2
1	C	323	ASP	2.2
1	K	32	ASP	2.2
2	F	19	GLU	2.2
2	L	9	LYS	2.2
2	M	29	LEU	2.2
1	J	30	VAL	2.2
2	D	30	ILE	2.2
1	C	287	GLU	2.2
1	K	287	GLU	2.2
1	B	274	PRO	2.2
2	L	142	VAL	2.2
1	A	25	GLN	2.2
2	D	288	ALA	2.2
1	K	211	THR	2.2
2	M	361	THR	2.2
2	M	71	ARG	2.2
1	B	175	VAL	2.2
1	I	177	GLU	2.2
2	L	340	PRO	2.2
1	J	8	LYS	2.2
2	E	99	ASN	2.2
2	F	54	VAL	2.2
1	J	65	ARG	2.2
1	J	528	PHE	2.2
2	L	8	ILE	2.2
1	I	11	GLY	2.2
2	N	165	ALA	2.2
2	N	200	GLN	2.2
2	L	249	ASP	2.2
1	B	509	VAL	2.2
1	C	150	MET	2.2
1	K	7	ILE	2.2
2	E	279	THR	2.2
2	M	276	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	306	SER	2.2
2	E	127	PHE	2.2
1	B	179	GLU	2.2
2	D	50	ASP	2.2
2	N	142	VAL	2.2
2	E	356	THR	2.2
2	F	359	GLY	2.2
1	C	369	SER	2.1
1	C	162	ILE	2.1
1	C	179	GLU	2.1
2	L	148	PRO	2.1
2	F	53	MET	2.1
2	D	147	LEU	2.1
2	E	389	LEU	2.1
2	M	178	ALA	2.1
2	M	127	PHE	2.1
1	J	579	GLU	2.1
2	L	153	SER	2.1
1	C	574	ASN	2.1
1	K	55	THR	2.1
2	N	418	TYR	2.1
1	J	160	GLN	2.1
2	D	24	VAL	2.1
2	M	81	VAL	2.1
1	J	226	GLY	2.1
1	J	377	SER	2.1
1	I	499	ASP	2.1
2	L	394	LEU	2.1
1	B	229	ALA	2.1
1	C	572	SER	2.1
1	B	512	PHE	2.1
2	E	375	ALA	2.1
2	L	6	ARG	2.1
1	I	385	THR	2.1
1	A	298	MET	2.1
1	K	37	GLY	2.1
1	J	325	ALA	2.1
1	C	153	ASN	2.1
2	L	152	GLY	2.1
1	C	290	VAL	2.1
1	I	473	ILE	2.1
2	D	137	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	485	ASN	2.1
1	A	322	TYR	2.1
2	F	197	ASP	2.1
2	D	65	LEU	2.1
1	B	211	THR	2.1
1	A	578	LYS	2.1
1	K	305	ALA	2.1
1	C	550	VAL	2.1
2	M	107	LYS	2.1
1	B	28	CYS	2.1
2	N	339	GLN	2.1
2	N	408	PHE	2.1
1	A	261	GLU	2.1
2	N	383	LYS	2.1
1	K	500	TYR	2.1
1	B	140	ASP	2.1
2	M	175	ASP	2.1
1	K	531	GLU	2.0
1	B	325	ALA	2.0
1	I	153	ASN	2.0
1	C	173	ILE	2.0
2	D	337	GLY	2.0
1	J	249	SER	2.0
2	L	353	ASP	2.0
2	N	43	GLN	2.0
1	J	554	GLU	2.0
1	C	152	PRO	2.0
1	K	60	PRO	2.0
1	B	44	GLN	2.0
1	B	275	GLU	2.0
2	D	386	ALA	2.0
1	J	421	GLN	2.0
1	K	10	SER	2.0
2	N	132	ILE	2.0
2	E	96	PRO	2.0
1	B	15	MET	2.0
1	J	186	THR	2.0
2	M	10	GLU	2.0
1	A	250	ASP	2.0
1	A	559	SER	2.0
1	C	185	LEU	2.0
2	D	69	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	N	264	ARG	2.0
1	I	19	MET	2.0
1	I	186	THR	2.0
2	M	130	THR	2.0
1	I	51	VAL	2.0
1	J	73	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

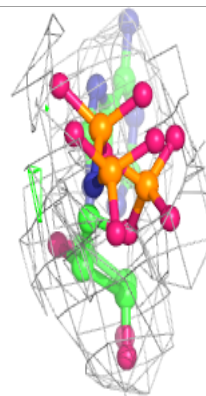
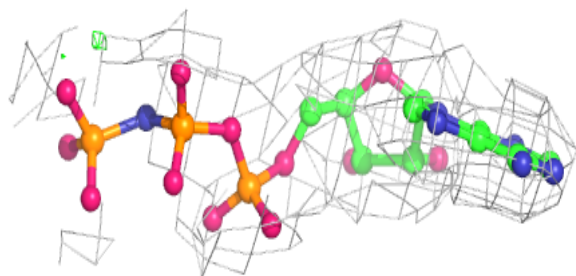
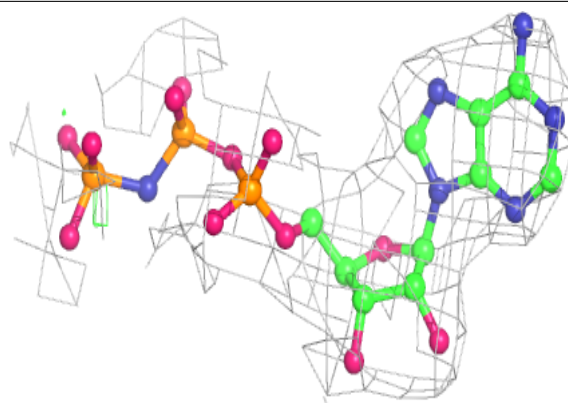
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	C	602	1/1	0.75	0.26	49,49,49,49	0
3	GOL	A	601	6/6	0.82	0.19	11,13,16,16	0
4	ANP	J	601	31/31	0.94	0.15	29,47,58,71	0
4	ANP	K	601	31/31	0.94	0.18	29,45,69,85	0
4	ANP	C	601	31/31	0.94	0.22	28,34,99,113	0
4	ANP	B	601	31/31	0.95	0.16	19,28,45,45	0
5	MG	J	602	1/1	0.96	0.09	26,26,26,26	0
5	MG	B	602	1/1	0.97	0.14	8,8,8,8	0
5	MG	K	602	1/1	0.97	0.13	27,27,27,27	0

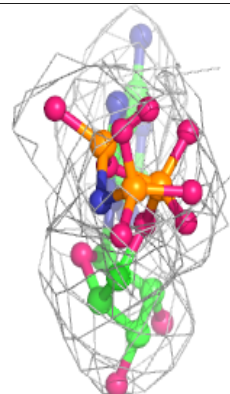
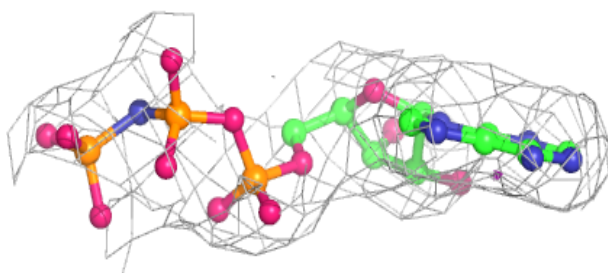
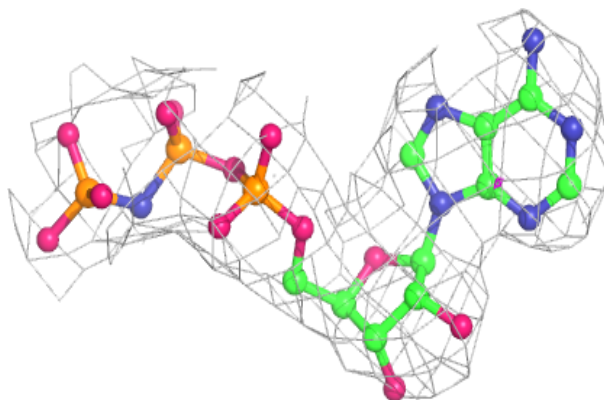
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ANP J 601:**

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

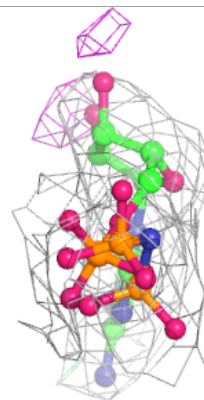
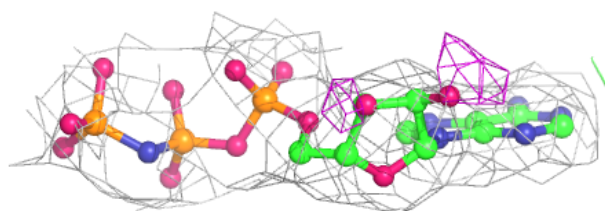
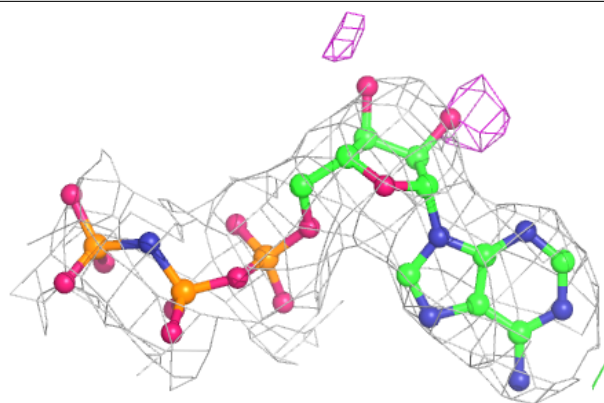
**Electron density around ANP K 601:**

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

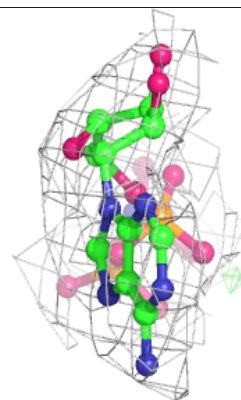
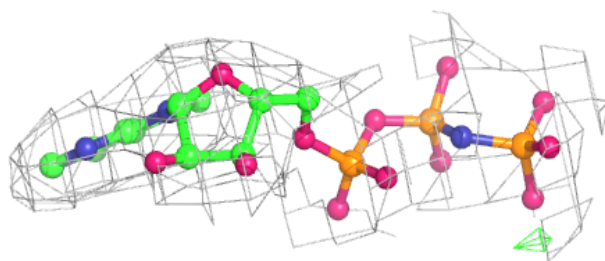
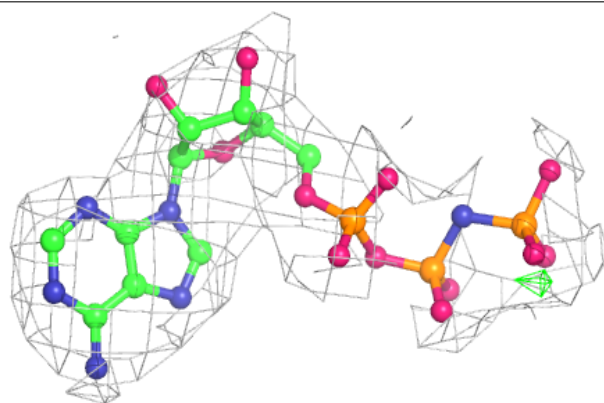


**Electron density around ANP C 601:**

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

**Electron density around ANP B 601:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.