



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2026 – 11:30 PM EDT

PDB ID : 4PKO / pdb_00004pko
Title : Crystal structure of the Football-shaped GroEL-GroES2-(ADPBeFx)₁₄ complex
Authors : Fei, X.; Ye, X.; Laronde-Leblanc, N.; Lorimer, G.H.
Deposited on : 2014-05-15
Resolution : 3.84 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

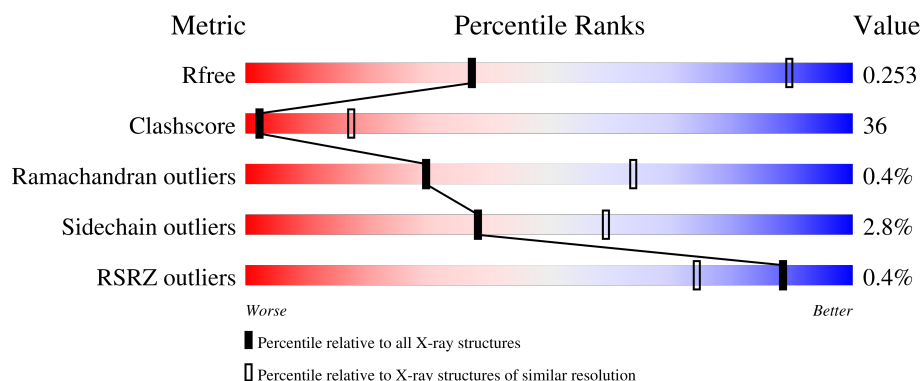
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)

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

Mol	Chain	Length	Quality of chain
1	A	548	
1	B	548	
1	C	548	
1	D	548	
1	E	548	

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Mol	Chain	Length	Quality of chain
1	F	548	%
1	G	548	%
1	H	548	%
1	I	548	%
1	J	548	%
1	K	548	%
1	L	548	%
1	M	548	%
1	N	548	%
2	1	97	%
2	2	97	%
2	O	97	%
2	P	97	%
2	Q	97	%
2	R	97	%
2	S	97	%
2	T	97	%
2	U	97	%
2	V	97	%
2	W	97	%
2	X	97	%
2	Y	97	%
2	Z	97	%

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	BEF	A	602	-	-	X	-
4	BEF	B	602	-	-	X	-
4	BEF	C	602	-	-	X	-
4	BEF	H	602	-	-	X	-
4	BEF	I	602	-	-	X	-
4	BEF	J	602	-	-	X	-
4	BEF	K	602	-	-	X	-
4	BEF	L	602	-	-	X	-
4	BEF	N	602	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 64559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

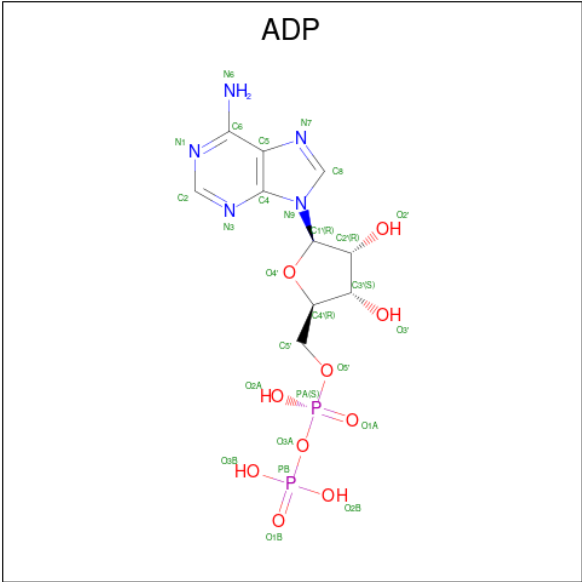
- Molecule 1 is a protein called 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	I	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	J	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	K	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	L	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	M	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	N	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			

- Molecule 2 is a protein called 10 kDa chaperonin.

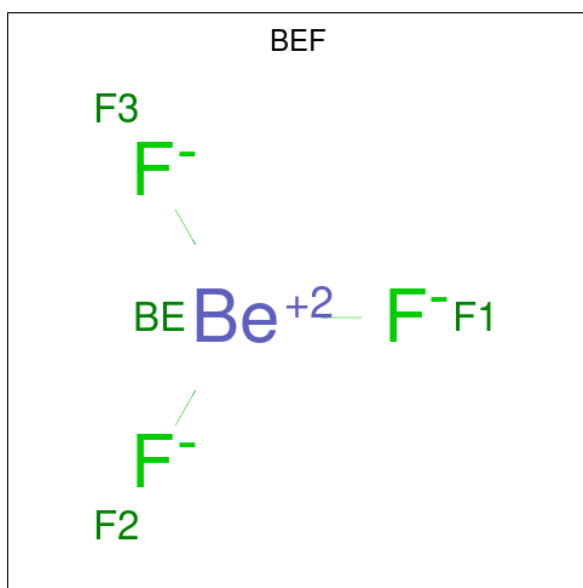
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	95	Total	C	N	O	S	0	0	0
			711	445	124	141	1			
2	P	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	Q	96	Total	C	N	O	S	0	0	0
			719	449	126	143	1			
2	R	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	S	96	Total	C	N	O	S	0	0	0
			719	449	126	143	1			
2	T	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	U	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	V	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	W	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	X	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	Y	96	Total	C	N	O	S	0	0	0
			722	451	126	143	2			
2	Z	95	Total	C	N	O	S	0	0	0
			713	446	125	140	2			
2	1	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	2	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	Be 1	F 3	0	0
4	B	1	Total 4	Be 1	F 3	0	0
4	C	1	Total 4	Be 1	F 3	0	0
4	D	1	Total 4	Be 1	F 3	0	0
4	E	1	Total 4	Be 1	F 3	0	0
4	F	1	Total 4	Be 1	F 3	0	0
4	G	1	Total 4	Be 1	F 3	0	0
4	H	1	Total 4	Be 1	F 3	0	0
4	I	1	Total 4	Be 1	F 3	0	0
4	J	1	Total 4	Be 1	F 3	0	0
4	K	1	Total 4	Be 1	F 3	0	0
4	L	1	Total 4	Be 1	F 3	0	0
4	M	1	Total 4	Be 1	F 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	N	1	Total	Be	F	0	0
			4	1	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		
5	I	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	K	1	Total	Mg	0	0
			1	1		
5	L	1	Total	Mg	0	0
			1	1		
5	M	1	Total	Mg	0	0
			1	1		
5	N	1	Total	Mg	0	0
			1	1		

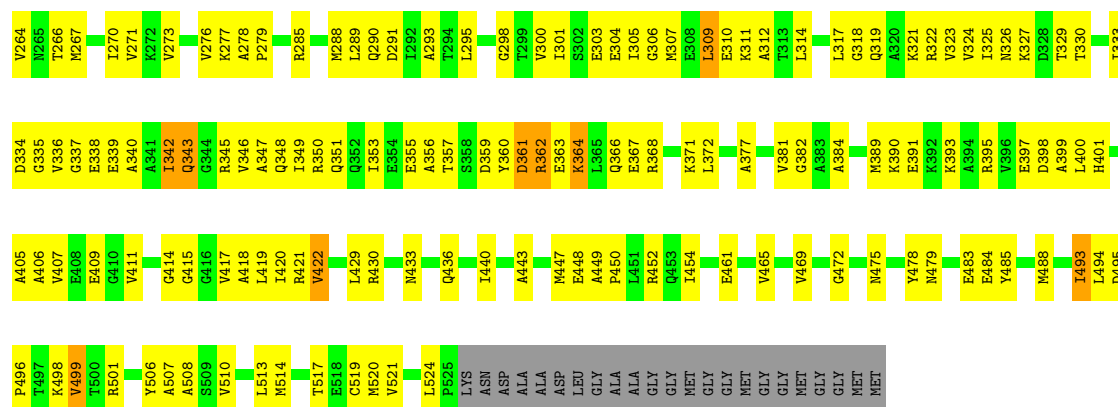
- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		
6	B	1	Total	K	0	0
			1	1		

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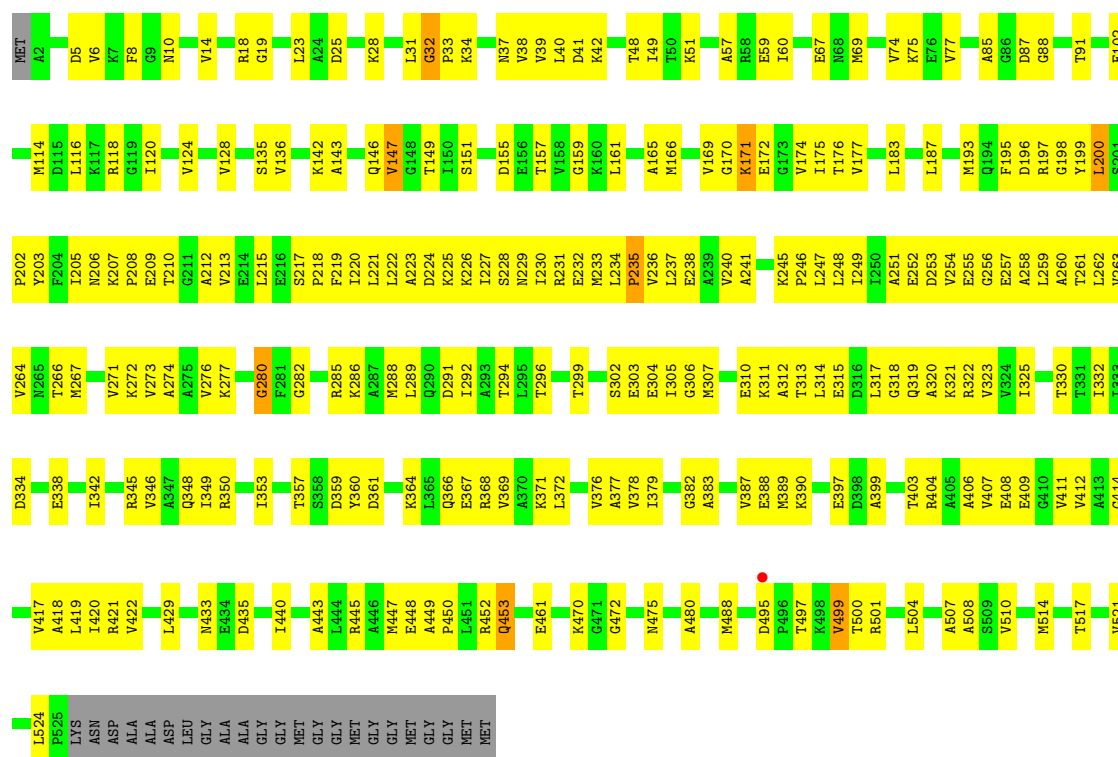
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0
6	E	1	Total 1	K 1	0	0
6	F	1	Total 1	K 1	0	0
6	G	1	Total 1	K 1	0	0
6	H	1	Total 1	K 1	0	0
6	I	1	Total 1	K 1	0	0
6	J	1	Total 1	K 1	0	0
6	K	1	Total 1	K 1	0	0
6	L	1	Total 1	K 1	0	0
6	M	1	Total 1	K 1	0	0
6	N	1	Total 1	K 1	0	0



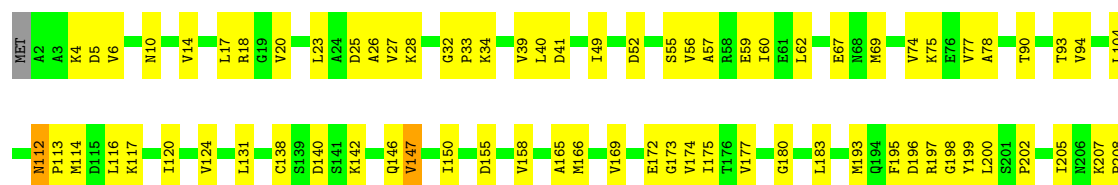
• Molecule 1: 60 kDa chaperonin

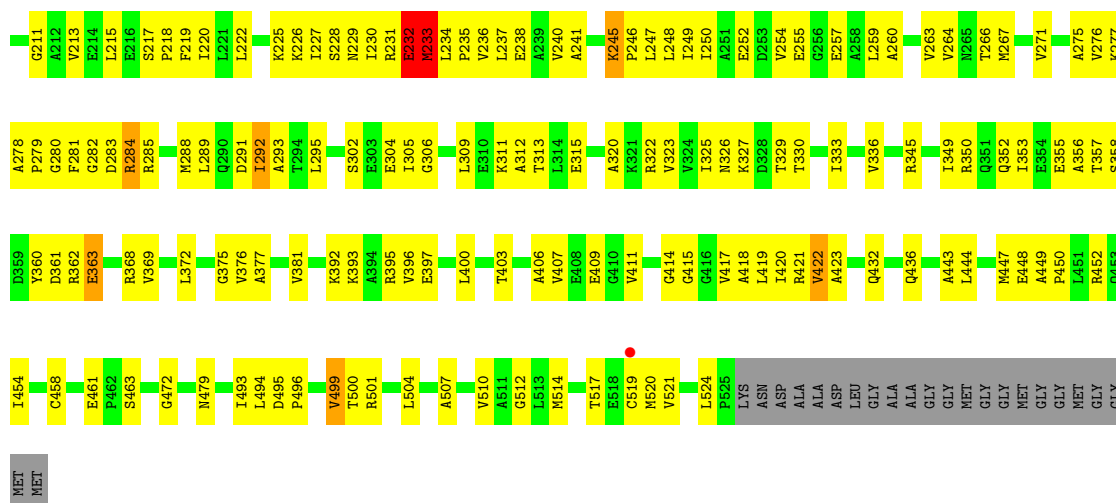
Chain C: 51% 43% • •



• Molecule 1: 60 kDa chaperonin

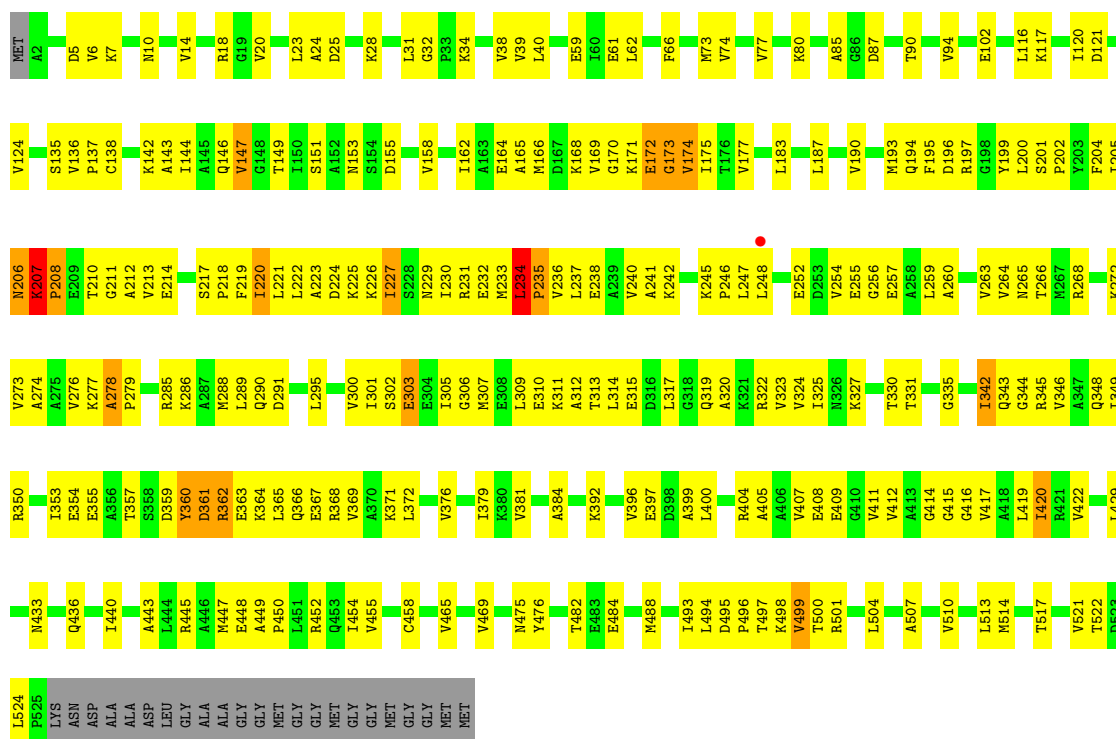
Chain D: 55% 39% • •





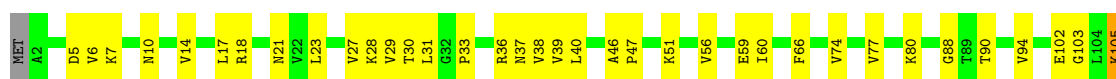
- Molecule 1: 60 kDa chaperonin

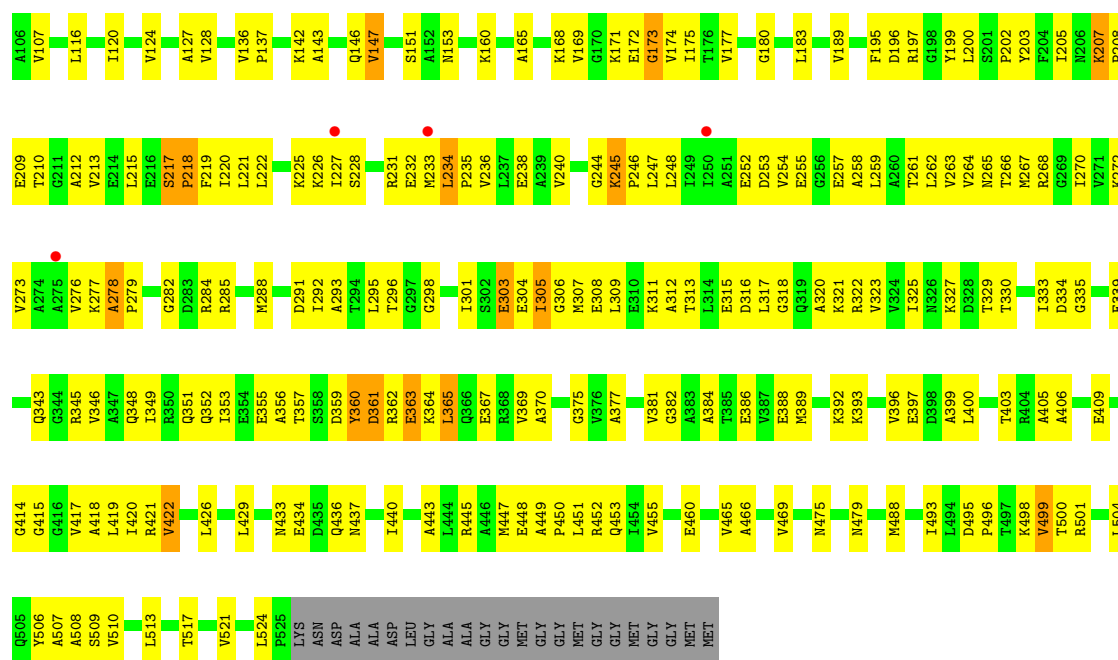
Chain E: 50% 42%



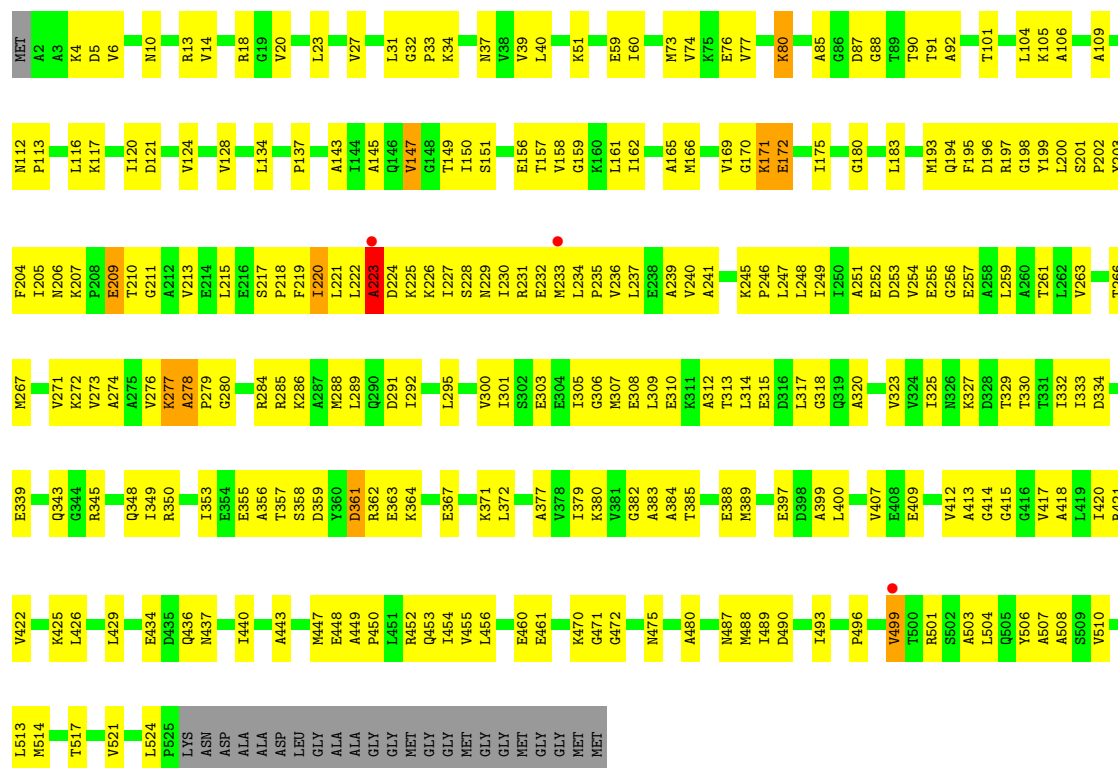
- Molecule 1: 60 kDa chaperonin

Chain F: 50% 42%



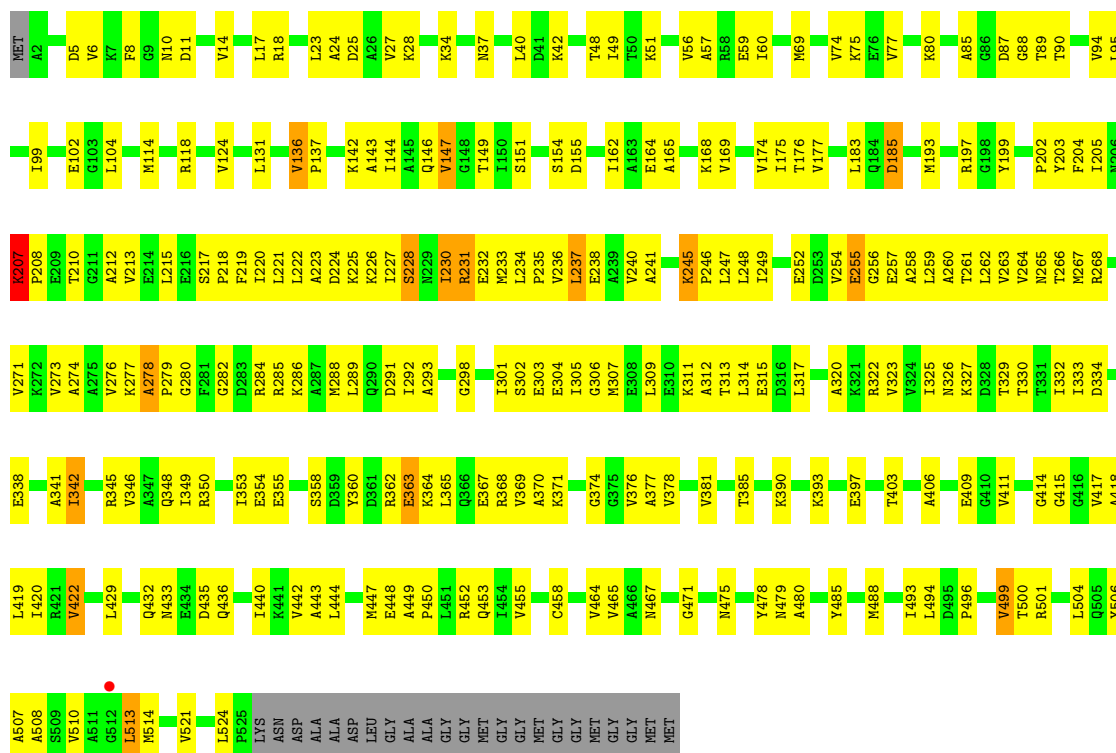


• Molecule 1: 60 kDa chaperonin

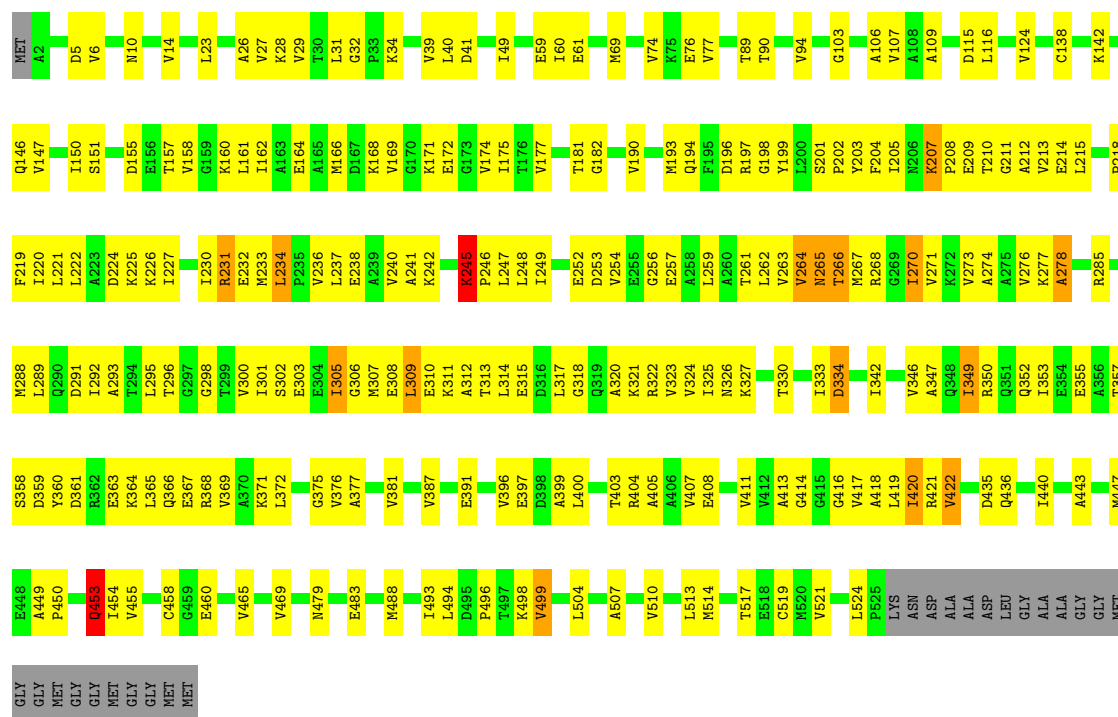


• Molecule 1: 60 kDa chaperonin



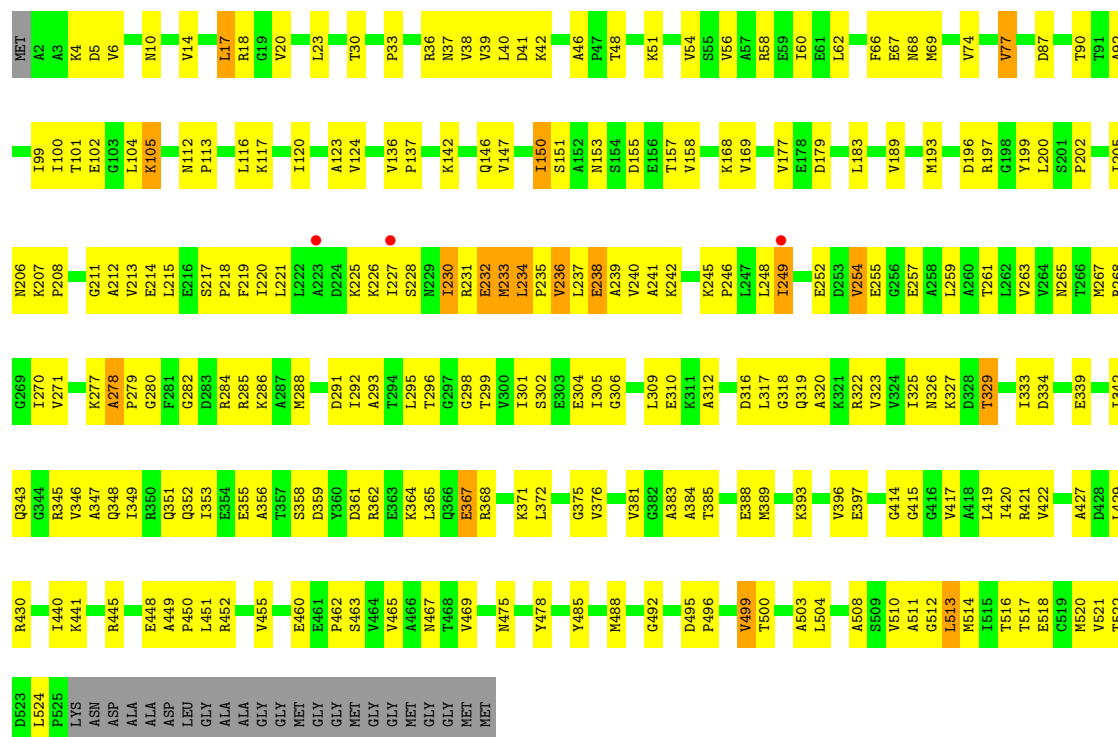


Chain J:

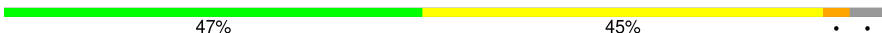


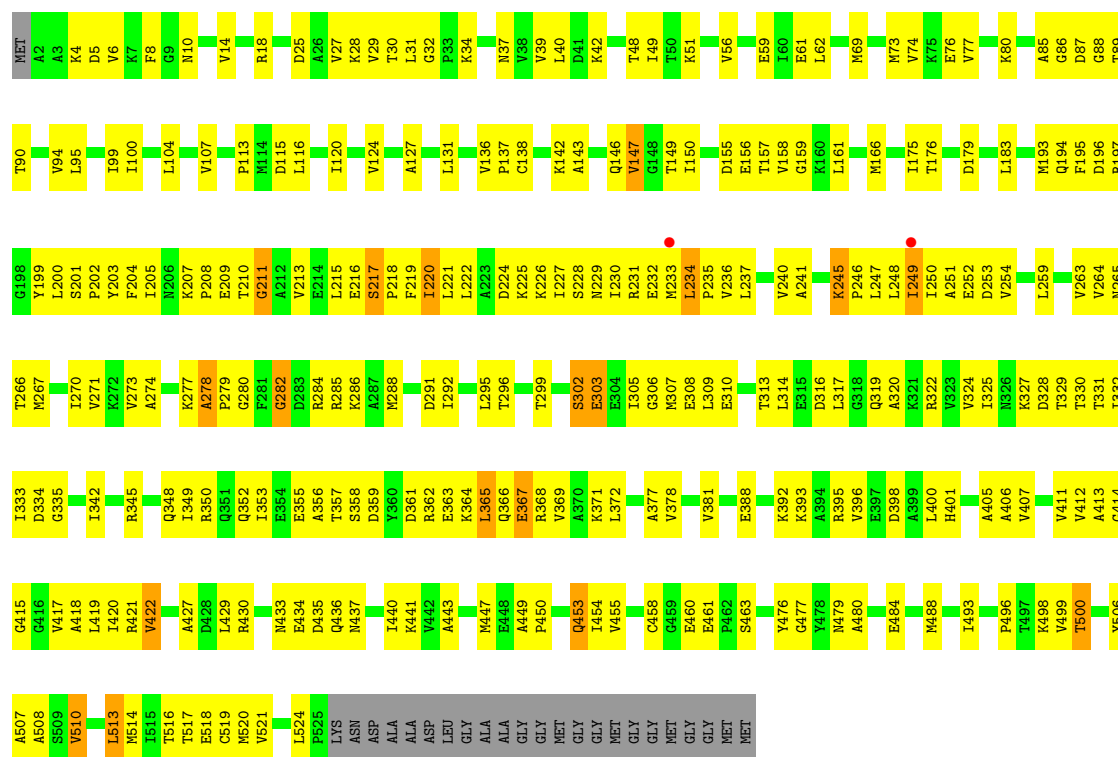
- Molecule 1: 60 kDa chaperonin

Chain K:



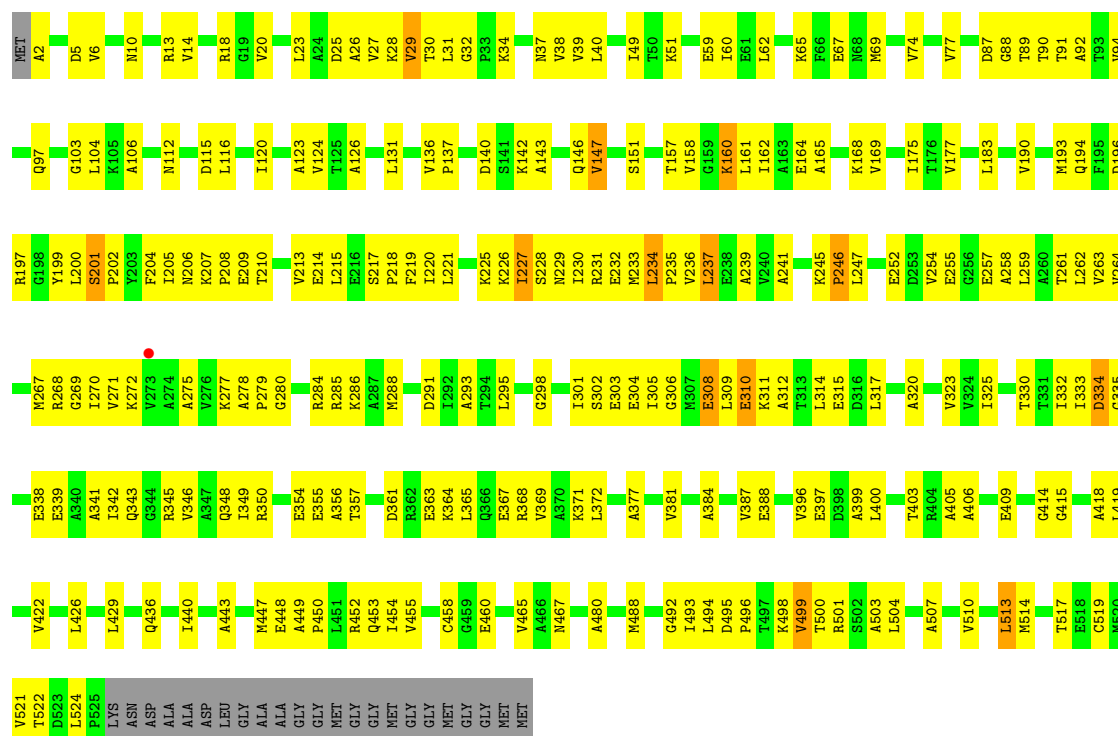
- Molecule 1: 60 kDa chaperonin

Chain L:  47% 45%

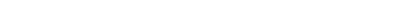


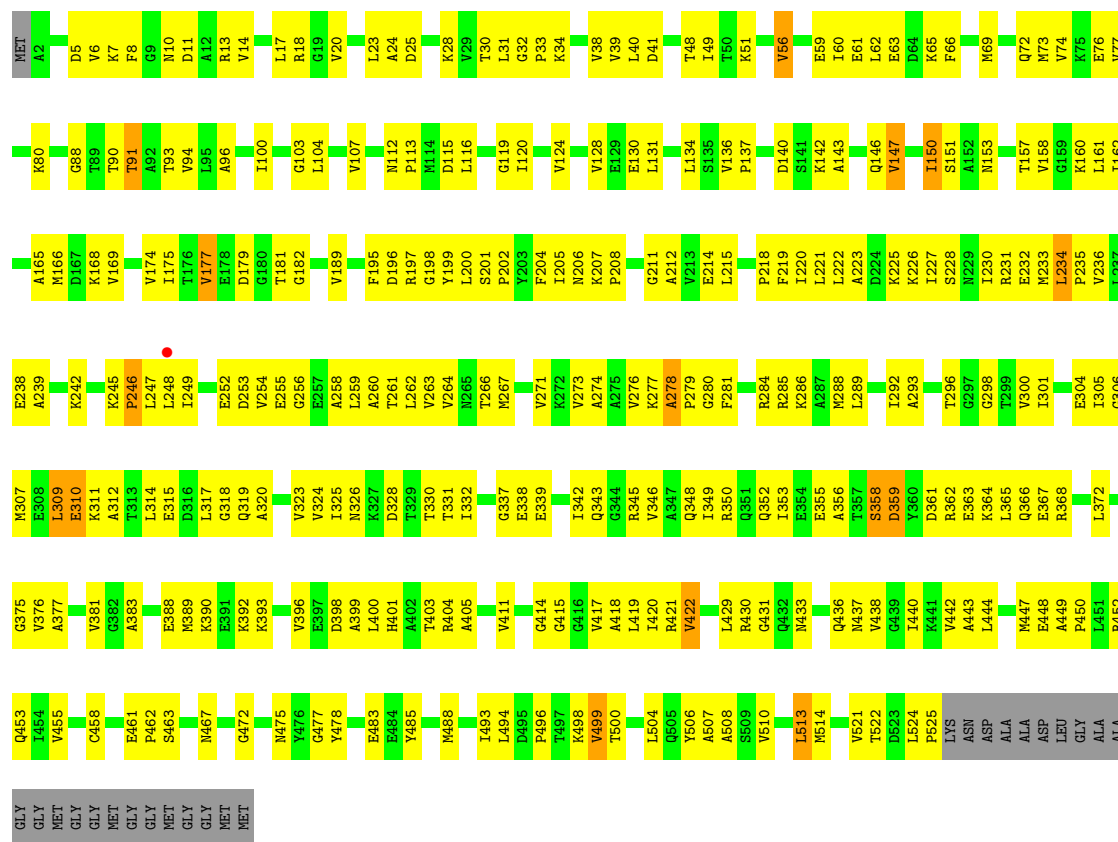
• Molecule 1: 60 kDa chaperonin

Chain M:  51% 42%



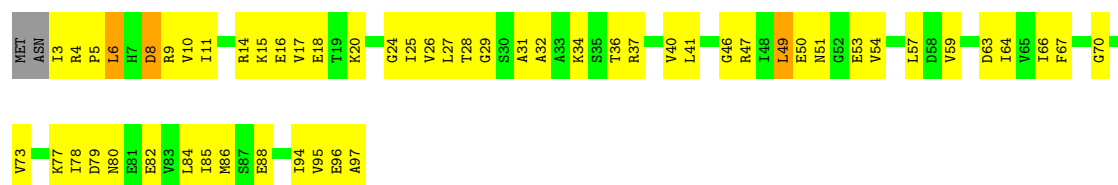
- Molecule 1: 60 kDa chaperonin

Chain N:  43% 49% . .

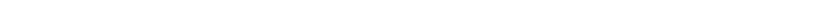


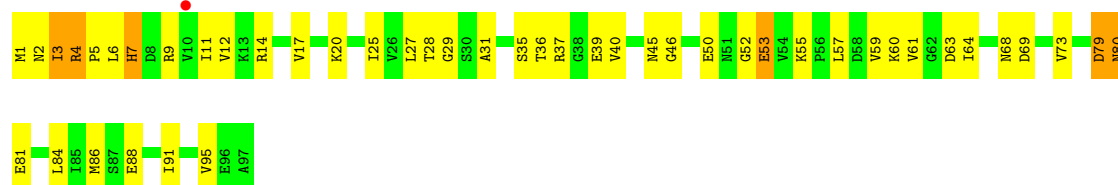
- Molecule 2: 10 kDa chaperonin

Chain 0: 41% 54% .

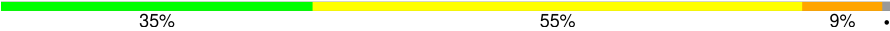


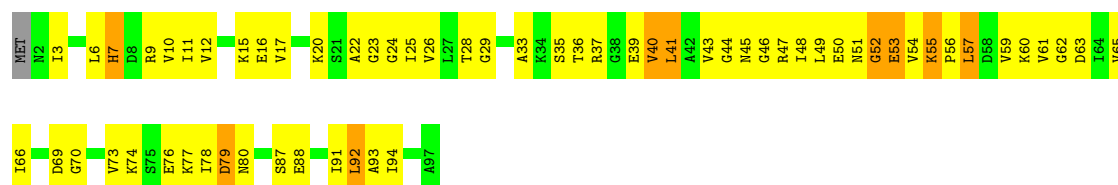
- Molecule 2: 10 kDa chaperonin

Chain P:  53% 41% 6%



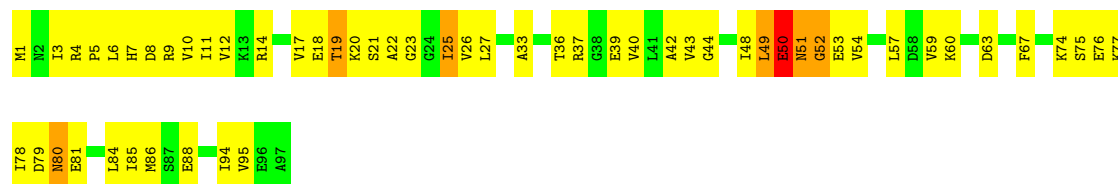
- Molecule 2: 10 kDa chaperonin

Chain Q: 



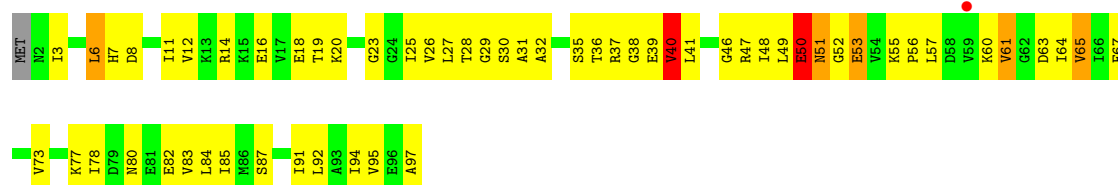
• Molecule 2: 10 kDa chaperonin

Chain R: 



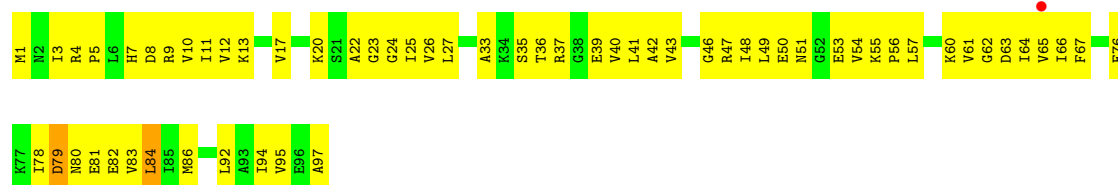
• Molecule 2: 10 kDa chaperonin

Chain S: 

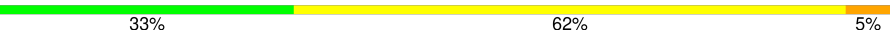


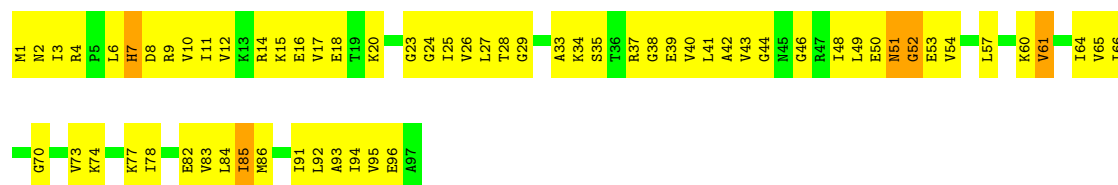
• Molecule 2: 10 kDa chaperonin

Chain T: 



• Molecule 2: 10 kDa chaperonin

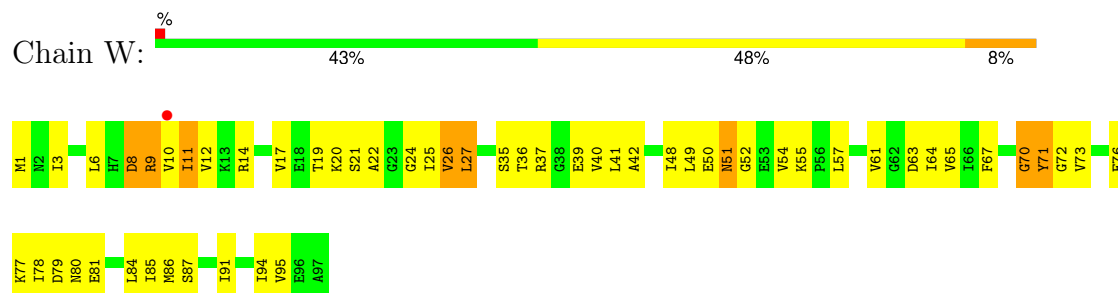
Chain U: 



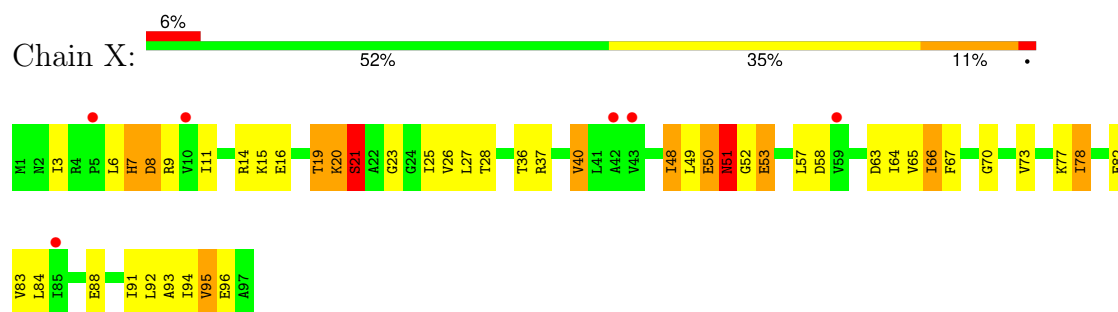
- Molecule 2: 10 kDa chaperonin



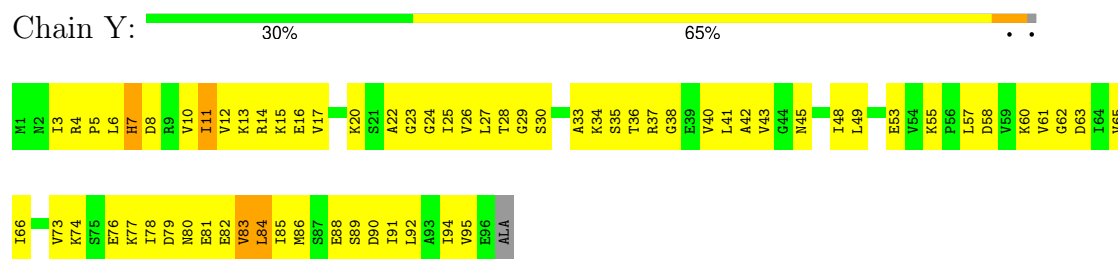
- Molecule 2: 10 kDa chaperonin



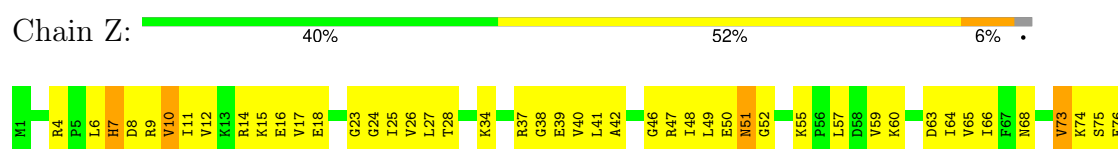
- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin

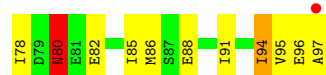


- Molecule 2: 10 kDa chaperonin





- Molecule 2: 10 kDa chaperonin



- Molecule 2: 10 kDa chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	169.79Å 174.49Å 410.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.90 – 3.84 90.90 – 3.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (90.90-3.84) 99.9 (90.90-3.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.183 , 0.248 0.189 , 0.253	Depositor DCC
R_{free} test set	1271 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	114.0	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 154.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.118 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	64559	wwPDB-VP
Average B, all atoms (Å ²)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, ADP, BEF

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	0.43	3/3883 (0.1%)	0.98	18/5243 (0.3%)
1	B	0.37	2/3883 (0.1%)	0.93	17/5243 (0.3%)
1	C	0.39	2/3883 (0.1%)	0.91	11/5243 (0.2%)
1	D	0.35	0/3883	0.90	10/5243 (0.2%)
1	E	0.46	3/3883 (0.1%)	1.00	27/5243 (0.5%)
1	F	0.35	1/3883 (0.0%)	0.93	16/5243 (0.3%)
1	G	0.38	2/3883 (0.1%)	0.92	16/5243 (0.3%)
1	H	0.33	0/3883	0.89	8/5243 (0.2%)
1	I	0.35	0/3883	0.89	4/5243 (0.1%)
1	J	0.38	1/3883 (0.0%)	0.98	20/5243 (0.4%)
1	K	0.37	1/3883 (0.0%)	0.94	15/5243 (0.3%)
1	L	0.36	0/3883	1.01	21/5243 (0.4%)
1	M	0.37	2/3883 (0.1%)	0.92	13/5243 (0.2%)
1	N	0.32	1/3883 (0.0%)	0.80	9/5243 (0.2%)
2	1	0.58	2/731 (0.3%)	1.19	8/983 (0.8%)
2	2	0.35	0/731	0.99	6/983 (0.6%)
2	O	0.34	0/715	0.95	1/962 (0.1%)
2	P	0.39	1/731 (0.1%)	0.98	7/983 (0.7%)
2	Q	0.37	0/723	1.06	7/973 (0.7%)
2	R	0.34	0/731	0.91	3/983 (0.3%)
2	S	0.42	0/723	0.91	1/973 (0.1%)
2	T	0.29	0/731	0.79	1/983 (0.1%)
2	U	0.39	0/731	0.84	1/983 (0.1%)
2	V	0.40	1/731 (0.1%)	1.17	12/983 (1.2%)
2	W	0.42	1/731 (0.1%)	1.05	6/983 (0.6%)
2	X	0.68	3/731 (0.4%)	1.41	12/983 (1.2%)
2	Y	0.36	0/726	1.07	7/976 (0.7%)
2	Z	0.36	0/717	0.82	1/964 (0.1%)
All	All	0.38	26/64545 (0.0%)	0.95	278/87097 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
2	1	0	2
2	S	0	1
All	All	0	5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	171	LYS	CA-C	12.52	1.69	1.52
1	C	171	LYS	CA-C	11.71	1.68	1.52
2	1	8	ASP	CA-C	11.02	1.67	1.52
2	X	51	ASN	CA-C	10.80	1.67	1.52
1	A	246	PRO	N-CD	-10.66	1.32	1.47
1	K	233	MET	CA-C	10.57	1.67	1.52
1	E	208	PRO	N-CD	-9.72	1.34	1.47
1	E	207	LYS	CA-C	9.35	1.64	1.52
1	A	309	LEU	CA-C	9.28	1.65	1.52
1	B	246	PRO	N-CD	-9.05	1.35	1.47
2	X	20	LYS	CA-C	8.74	1.64	1.52
1	J	265	ASN	CA-C	8.02	1.64	1.52
1	A	137	PRO	N-CD	7.57	1.58	1.47
1	G	171	LYS	CA-C	7.44	1.62	1.52
1	M	137	PRO	N-CD	6.95	1.57	1.47
2	W	71	TYR	CA-C	6.54	1.61	1.52
1	M	246	PRO	N-CD	-6.33	1.38	1.47
1	F	361	ASP	CA-C	6.24	1.61	1.52
1	G	137	PRO	N-CD	5.99	1.56	1.47
2	V	92	LEU	CA-C	5.75	1.60	1.52
1	B	245	LYS	CA-C	5.68	1.59	1.52
2	P	80	ASN	CA-C	5.53	1.61	1.52
1	N	246	PRO	N-CD	-5.27	1.40	1.47
2	1	51	ASN	N-CA	5.23	1.52	1.46
2	X	8	ASP	CA-C	5.06	1.60	1.52
1	C	235	PRO	N-CD	-5.01	1.40	1.47

All (278) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	21	SER	N-CA-C	16.75	146.49	110.80
1	A	310	GLU	N-CA-C	15.55	132.00	113.18
1	E	172	GLU	N-CA-C	14.12	129.96	113.01
2	X	7	HIS	CB-CA-C	-13.38	101.16	116.54
1	E	360	TYR	N-CA-C	12.48	126.30	111.82
1	C	172	GLU	N-CA-C	12.34	127.82	113.01
1	H	245	LYS	CA-C-N	12.03	131.94	120.03
1	H	245	LYS	C-N-CA	12.03	131.94	120.03
2	1	80	ASN	N-CA-C	11.80	127.67	111.74
2	X	9	ARG	N-CA-C	11.75	127.51	110.24
2	1	52	GLY	N-CA-C	11.73	140.97	113.18
1	J	264	VAL	N-CA-C	11.45	123.67	110.62
1	G	172	GLU	N-CA-C	11.34	126.91	113.18
2	X	21	SER	N-CA-CB	-11.34	91.32	110.49
1	K	232	GLU	N-CA-C	-10.54	98.95	112.23
2	1	9	ARG	N-CA-C	10.47	125.66	109.96
1	M	310	GLU	N-CA-C	10.43	125.79	113.18
1	E	171	LYS	N-CA-C	10.37	123.55	111.11
1	J	266	THR	N-CA-CB	10.37	125.65	110.20
1	B	246	PRO	N-CA-CB	-10.37	92.36	103.25
2	W	72	GLY	N-CA-C	-10.33	100.33	112.73
1	L	245	LYS	CA-C-N	10.17	130.28	120.31
1	L	245	LYS	C-N-CA	10.17	130.28	120.31
2	Y	84	LEU	N-CA-C	10.08	126.40	110.17
2	X	19	THR	CB-CA-C	9.84	127.64	111.41
2	X	8	ASP	CA-C-O	9.80	131.90	120.92
2	V	48	ILE	N-CA-C	9.77	122.01	107.75
1	E	171	LYS	CA-C-O	9.67	131.25	120.90
1	C	229	ASN	N-CA-C	9.65	121.75	111.03
1	J	266	THR	N-CA-C	-9.60	99.88	111.69
1	L	220	ILE	N-CA-C	9.60	121.61	108.17
2	V	55	LYS	CA-C-N	9.56	129.31	119.56
2	V	55	LYS	C-N-CA	9.56	129.31	119.56
1	K	233	MET	CA-C-O	9.45	130.84	120.63
1	J	265	ASN	N-CA-C	9.38	124.55	113.20
1	L	302	SER	N-CA-C	9.35	123.96	108.73
1	C	171	LYS	CA-C-O	9.28	130.83	120.90
1	F	362	ARG	N-CA-CB	9.27	124.02	110.20
1	D	245	LYS	CA-C-N	9.17	129.30	120.31
1	D	245	LYS	C-N-CA	9.17	129.30	120.31
1	C	171	LYS	N-CA-C	9.13	122.07	111.11
1	B	246	PRO	N-CA-C	9.01	131.03	112.47
2	2	80	ASN	N-CA-C	-8.82	98.73	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	201	SER	CA-C-N	8.63	128.28	119.56
1	L	201	SER	C-N-CA	8.63	128.28	119.56
1	E	362	ARG	N-CA-C	-8.59	101.91	111.28
2	V	93	ALA	N-CA-CB	-8.42	97.24	111.31
1	H	278	ALA	CA-C-N	8.23	128.18	119.05
1	H	278	ALA	C-N-CA	8.23	128.18	119.05
1	E	344	GLY	N-CA-C	-8.20	102.28	112.77
2	X	51	ASN	CA-C-O	8.15	132.16	120.51
1	A	310	GLU	N-CA-CB	-8.14	96.73	110.41
2	2	55	LYS	CA-C-N	8.08	128.13	119.89
2	2	55	LYS	C-N-CA	8.08	128.13	119.89
1	B	364	LYS	N-CA-C	8.07	122.95	113.18
1	K	46	ALA	CA-C-N	8.04	127.99	120.03
1	K	46	ALA	C-N-CA	8.04	127.99	120.03
1	K	238	GLU	N-CA-C	-8.01	102.50	111.71
1	B	244	GLY	N-CA-C	7.96	124.41	110.80
1	G	171	LYS	N-CA-C	7.95	120.64	111.11
1	L	249	ILE	N-CA-C	7.94	119.56	108.12
1	E	208	PRO	N-CA-C	7.94	128.82	112.47
1	F	234	LEU	N-CA-C	7.86	124.15	113.77
2	1	8	ASP	CA-C-O	7.86	131.75	120.51
1	A	245	LYS	CA-C-N	7.83	127.78	120.03
1	A	245	LYS	C-N-CA	7.83	127.78	120.03
1	K	233	MET	N-CA-C	7.74	120.70	111.33
2	Q	40	VAL	N-CA-C	7.73	118.50	110.62
2	X	7	HIS	N-CA-C	7.71	120.02	108.31
1	J	453	GLN	N-CA-C	7.66	119.71	111.36
1	J	265	ASN	CB-CA-C	-7.64	95.60	110.11
1	J	210	THR	N-CA-C	-7.62	103.56	112.86
1	G	278	ALA	CA-C-N	7.61	126.88	118.97
1	G	278	ALA	C-N-CA	7.61	126.88	118.97
1	L	367	GLU	N-CA-C	-7.61	102.93	111.07
2	W	71	TYR	CA-C-O	7.61	127.82	119.15
2	Q	55	LYS	CA-C-N	7.60	127.27	119.82
2	Q	55	LYS	C-N-CA	7.60	127.27	119.82
1	F	361	ASP	N-CA-C	7.59	122.54	113.28
1	N	32	GLY	CA-C-N	7.57	127.10	118.85
1	N	32	GLY	C-N-CA	7.57	127.10	118.85
1	A	278	ALA	CA-C-N	7.54	126.81	118.97
1	A	278	ALA	C-N-CA	7.54	126.81	118.97
2	W	70	GLY	N-CA-C	-7.53	102.42	112.81
2	O	59	VAL	N-CA-CB	7.40	118.78	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	LEU	N-CA-C	7.38	126.53	110.80
1	I	278	ALA	CA-C-N	7.34	126.60	118.97
1	I	278	ALA	C-N-CA	7.34	126.60	118.97
1	E	208	PRO	N-CA-CB	-7.30	95.58	103.25
1	F	278	ALA	CA-C-N	7.26	126.52	118.97
1	F	278	ALA	C-N-CA	7.26	126.52	118.97
1	L	217	SER	N-CA-C	7.23	125.78	109.81
1	F	362	ARG	N-CA-C	-7.17	102.87	111.69
1	M	227	ILE	N-CA-C	7.09	116.92	106.85
2	V	58	ASP	N-CA-C	7.08	120.93	111.30
1	J	201	SER	CA-C-N	7.07	126.70	119.56
1	J	201	SER	C-N-CA	7.07	126.70	119.56
1	M	308	GLU	N-CA-C	7.00	119.78	110.53
2	R	51	ASN	N-CA-CB	7.00	122.31	110.49
1	M	32	GLY	CA-C-N	6.94	126.55	119.19
1	M	32	GLY	C-N-CA	6.94	126.55	119.19
2	1	80	ASN	N-CA-CB	-6.92	101.68	112.13
1	F	361	ASP	CA-C-O	6.91	127.41	119.18
1	M	136	VAL	CA-C-N	6.89	126.86	119.76
1	M	136	VAL	C-N-CA	6.89	126.86	119.76
1	J	265	ASN	CA-C-O	6.87	128.12	119.12
2	P	79	ASP	CB-CA-C	6.86	122.83	112.06
1	D	112	ASN	CA-C-N	6.86	126.66	119.05
1	D	112	ASN	C-N-CA	6.86	126.66	119.05
1	F	303	GLU	N-CA-C	-6.85	104.89	113.18
1	J	278	ALA	CA-C-N	6.80	126.04	118.97
1	J	278	ALA	C-N-CA	6.80	126.04	118.97
1	A	217	SER	CA-C-N	6.77	128.31	119.84
1	A	217	SER	C-N-CA	6.77	128.31	119.84
1	L	484	GLU	N-CA-C	6.76	120.18	109.50
2	W	71	TYR	CB-CA-C	-6.75	97.91	109.65
1	J	32	GLY	CA-C-N	6.74	126.20	118.85
1	J	32	GLY	C-N-CA	6.74	126.20	118.85
1	F	361	ASP	CB-CA-C	-6.73	96.80	109.72
1	A	246	PRO	N-CA-CB	-6.72	96.32	103.38
1	E	362	ARG	N-CA-CB	6.70	119.97	110.12
1	K	278	ALA	CA-C-N	6.70	126.49	119.05
1	K	278	ALA	C-N-CA	6.70	126.49	119.05
1	B	362	ARG	N-CA-C	-6.70	103.79	112.23
1	B	364	LYS	N-CA-CB	-6.69	99.17	110.41
2	Y	83	VAL	N-CA-C	6.62	118.47	108.80
1	E	278	ALA	CA-C-N	6.61	125.84	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	278	ALA	C-N-CA	6.61	125.84	118.97
1	E	208	PRO	N-CD-CG	-6.60	93.30	103.20
1	A	154	SER	CB-CA-C	-6.58	102.39	111.73
1	B	86	GLY	N-CA-C	-6.55	105.47	114.64
1	J	249	ILE	N-CA-C	6.53	117.44	107.77
2	Z	7	HIS	CB-CA-C	-6.51	109.08	116.63
1	J	245	LYS	CA-C-N	6.50	126.46	120.03
1	J	245	LYS	C-N-CA	6.50	126.46	120.03
1	M	112	ASN	CA-C-N	6.45	126.21	119.05
1	M	112	ASN	C-N-CA	6.45	126.21	119.05
1	G	32	GLY	CA-C-N	6.42	125.99	119.19
1	G	32	GLY	C-N-CA	6.42	125.99	119.19
1	G	201	SER	CA-C-N	6.40	126.02	119.56
1	G	201	SER	C-N-CA	6.40	126.02	119.56
1	G	229	ASN	N-CA-C	6.40	119.07	111.71
1	I	227	ILE	N-CA-C	6.38	115.91	106.85
2	Y	53	GLU	CB-CA-C	-6.35	108.59	117.23
1	B	201	SER	CA-C-N	6.34	125.96	119.56
1	B	201	SER	C-N-CA	6.34	125.96	119.56
2	1	7	HIS	CB-CA-C	-6.31	97.86	110.42
1	A	246	PRO	CA-N-CD	6.29	120.81	112.00
1	G	171	LYS	CA-C-O	6.29	127.64	120.90
1	B	245	LYS	N-CA-C	6.29	123.70	109.81
1	B	32	GLY	CA-C-N	6.28	125.69	118.85
1	B	32	GLY	C-N-CA	6.28	125.69	118.85
1	K	249	ILE	N-CA-C	6.26	116.89	107.75
1	K	367	GLU	N-CA-C	6.24	117.74	111.07
1	M	310	GLU	N-CA-CB	-6.22	99.96	110.41
1	E	361	ASP	CA-C-O	6.20	125.95	119.14
1	A	308	GLU	N-CA-C	6.18	123.97	110.80
2	V	40	VAL	N-CA-C	6.18	116.92	110.62
1	F	360	TYR	N-CA-C	6.17	123.95	110.80
1	L	86	GLY	N-CA-C	-6.17	106.00	114.64
1	L	32	GLY	CA-C-N	6.16	125.57	118.85
1	L	32	GLY	C-N-CA	6.16	125.57	118.85
1	A	154	SER	N-CA-C	6.15	120.04	111.74
1	E	342	ILE	N-CA-C	6.14	116.26	110.30
1	J	210	THR	N-CA-CB	6.12	121.90	112.41
1	M	201	SER	CA-C-N	6.12	125.74	119.56
1	M	201	SER	C-N-CA	6.12	125.74	119.56
1	E	170	GLY	N-CA-C	6.11	123.58	112.58
2	V	91	ILE	N-CA-C	6.09	116.02	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	201	SER	CA-C-N	6.07	125.69	119.56
1	E	201	SER	C-N-CA	6.07	125.69	119.56
2	P	80	ASN	CA-C-O	6.05	127.46	120.32
1	B	361	ASP	N-CA-C	6.04	119.12	111.69
1	E	220	ILE	N-CA-C	6.00	116.58	108.17
1	A	180	GLY	N-CA-C	6.00	127.39	113.18
1	A	179	ASP	N-CA-C	5.99	118.94	110.50
1	A	172	GLU	N-CA-C	5.99	120.42	113.18
1	E	32	GLY	CA-C-N	5.98	125.53	119.19
1	E	32	GLY	C-N-CA	5.98	125.53	119.19
1	C	280	GLY	N-CA-C	5.96	121.03	112.81
1	C	282	GLY	N-CA-C	5.94	119.83	112.64
2	W	61	VAL	N-CA-C	5.93	116.71	109.30
2	X	50	GLU	N-CA-C	5.91	123.38	110.80
2	W	71	TYR	N-CA-C	5.90	120.64	113.38
2	R	52	GLY	N-CA-C	-5.89	106.05	115.66
1	F	173	GLY	N-CA-C	-5.89	103.53	111.54
2	Q	53	GLU	CB-CA-C	-5.88	108.11	116.34
2	2	79	ASP	N-CA-C	-5.87	103.82	111.74
1	L	282	GLY	N-CA-C	5.86	119.73	112.64
1	L	342	ILE	N-CA-C	5.85	115.98	110.30
2	P	81	GLU	N-CA-C	-5.85	99.65	109.07
2	X	50	GLU	CB-CA-C	-5.83	98.81	110.42
1	E	208	PRO	CA-N-CD	5.82	120.14	112.00
1	C	170	GLY	N-CA-C	5.81	123.04	112.58
1	C	461	GLU	CA-C-N	5.79	125.17	118.85
1	C	461	GLU	C-N-CA	5.79	125.17	118.85
2	Q	7	HIS	CB-CA-C	-5.79	109.91	116.63
2	X	53	GLU	CB-CA-C	-5.78	109.89	116.54
1	N	278	ALA	CA-C-N	5.76	124.97	118.97
1	N	278	ALA	C-N-CA	5.76	124.97	118.97
1	N	358	SER	CB-CA-C	-5.75	109.42	117.23
1	D	232	GLU	N-CA-CB	5.74	120.20	110.49
2	R	19	THR	CB-CA-C	-5.74	108.31	116.34
1	E	227	ILE	N-CA-C	5.72	114.97	106.85
2	P	81	GLU	N-CA-CB	5.69	119.50	110.57
2	Y	55	LYS	CA-C-N	5.67	125.86	120.31
2	Y	55	LYS	C-N-CA	5.67	125.86	120.31
1	L	500	THR	N-CA-C	5.67	117.53	111.36
1	H	207	LYS	CA-C-N	5.66	125.58	119.76
1	H	207	LYS	C-N-CA	5.66	125.58	119.76
1	H	230	ILE	N-CA-C	5.63	116.09	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	217	SER	CA-C-N	-5.63	112.81	119.84
1	F	217	SER	C-N-CA	-5.63	112.81	119.84
1	N	112	ASN	CA-C-N	5.62	125.29	119.05
1	N	112	ASN	C-N-CA	5.62	125.29	119.05
1	K	230	ILE	N-CA-C	5.62	116.50	107.73
1	N	359	ASP	N-CA-C	5.61	117.87	111.02
1	D	284	ARG	N-CA-C	-5.60	104.57	111.40
1	I	361	ASP	N-CA-C	-5.58	104.83	111.69
1	B	342	ILE	N-CA-C	5.58	115.71	110.30
1	J	313	THR	N-CA-C	-5.57	100.81	109.72
1	G	172	GLU	N-CA-CB	-5.57	101.06	110.41
2	1	7	HIS	N-CA-C	5.56	122.65	110.80
2	Q	41	LEU	CB-CA-C	-5.56	109.67	117.23
1	J	315	GLU	N-CA-C	-5.55	106.01	112.89
2	P	7	HIS	CB-CA-C	-5.53	109.71	117.23
1	K	234	LEU	N-CA-C	5.53	122.03	109.81
1	D	233	MET	N-CA-C	5.50	122.52	110.80
2	V	41	LEU	CB-CA-C	-5.49	109.77	117.23
2	V	7	HIS	CB-CA-C	-5.47	110.29	116.63
2	2	51	ASN	N-CA-C	-5.46	106.61	113.28
1	E	303	GLU	N-CA-C	-5.46	106.62	113.28
1	E	355	GLU	CB-CA-C	-5.46	109.29	115.79
1	B	112	ASN	CA-C-N	5.44	125.08	119.05
1	B	112	ASN	C-N-CA	5.44	125.08	119.05
1	E	206	ASN	CB-CA-C	-5.42	99.64	110.42
1	H	231	ARG	CB-CA-C	-5.41	110.31	116.54
1	G	382	GLY	N-CA-C	5.40	125.98	113.18
2	P	80	ASN	CB-CA-C	-5.39	102.57	111.36
1	D	336	VAL	N-CA-C	5.35	114.44	106.85
1	B	246	PRO	CA-N-CD	5.33	119.46	112.00
1	G	220	ILE	N-CA-C	5.32	115.61	108.17
1	E	172	GLU	N-CA-CB	-5.31	101.10	110.39
1	L	210	THR	N-CA-C	-5.28	106.68	113.23
2	Y	80	ASN	CB-CA-C	-5.28	110.05	117.23
1	D	32	GLY	CA-C-N	5.28	124.78	119.19
1	D	32	GLY	C-N-CA	5.28	124.78	119.19
2	V	46	GLY	N-CA-C	5.26	117.72	110.56
2	Q	23	GLY	N-CA-C	-5.26	108.74	115.42
1	L	303	GLU	N-CA-CB	5.26	118.39	110.30
2	V	92	LEU	N-CA-C	5.23	121.94	110.80
1	L	278	ALA	CA-C-N	5.22	124.39	118.97
1	L	278	ALA	C-N-CA	5.22	124.39	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	223	ALA	CA-C-N	5.21	131.08	121.70
1	G	223	ALA	C-N-CA	5.21	131.08	121.70
2	U	7	HIS	N-CA-C	5.20	118.57	111.39
1	L	211	GLY	N-CA-C	-5.19	106.90	114.90
2	T	80	ASN	CB-CA-C	-5.19	110.17	117.23
2	X	20	LYS	CA-C-O	5.19	127.94	120.51
2	Y	95	VAL	N-CA-C	5.17	116.26	109.58
1	A	311	LYS	N-CA-C	5.16	117.14	108.73
1	C	32	GLY	CA-C-N	5.16	124.66	119.19
1	C	32	GLY	C-N-CA	5.16	124.66	119.19
2	P	80	ASN	N-CA-C	5.15	119.14	112.86
2	V	58	ASP	N-CA-CB	-5.15	104.26	111.62
2	1	51	ASN	N-CA-CB	-5.14	101.81	110.49
1	K	342	ILE	N-CA-C	5.12	115.24	110.42
1	M	136	VAL	N-CA-C	5.12	119.93	108.88
1	N	361	ASP	N-CA-C	-5.10	107.06	113.28
1	E	173	GLY	N-CA-C	-5.08	105.58	112.14
1	K	236	VAL	N-CA-C	5.07	115.79	110.62
2	S	65	VAL	N-CA-C	5.07	117.31	108.95
1	G	170	GLY	N-CA-C	5.06	121.69	112.58
1	F	46	ALA	CA-C-N	5.05	125.33	119.92
1	F	46	ALA	C-N-CA	5.05	125.33	119.92
1	F	244	GLY	N-CA-C	5.01	123.53	114.46
1	K	254	VAL	N-CA-C	5.01	115.18	107.77
2	2	7	HIS	CB-CA-C	-5.01	110.42	117.23

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	50	GLU	Peptide
2	1	6	LEU	Peptide
1	A	179	ASP	Peptide
1	D	232	GLU	Peptide
2	S	50	GLU	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3855	0	3974	278	0
1	B	3855	0	3975	296	5
1	C	3855	0	3974	273	0
1	D	3855	0	3975	231	0
1	E	3855	0	3976	285	0
1	F	3855	0	3975	260	0
1	G	3855	0	3975	294	3
1	H	3855	0	3975	294	0
1	I	3855	0	3976	263	0
1	J	3855	0	3976	253	0
1	K	3855	0	3976	238	12
1	L	3855	0	3975	286	1
1	M	3855	0	3974	259	7
1	N	3855	0	3976	325	0
2	1	727	0	762	71	1
2	2	727	0	762	75	1
2	O	711	0	744	91	0
2	P	727	0	762	73	3
2	Q	719	0	750	74	0
2	R	727	0	762	108	0
2	S	719	0	750	88	0
2	T	727	0	762	80	1
2	U	727	0	762	107	0
2	V	727	0	762	92	0
2	W	727	0	762	82	0
2	X	727	0	762	68	0
2	Y	722	0	757	87	0
2	Z	713	0	751	92	0
3	A	27	0	12	1	0
3	B	27	0	12	5	0
3	C	27	0	12	4	0
3	D	27	0	12	4	0
3	E	27	0	12	4	0
3	F	27	0	12	4	0
3	G	27	0	12	5	0
3	H	27	0	12	2	0
3	I	27	0	12	3	0
3	J	27	0	12	1	0
3	K	27	0	12	4	0
3	L	27	0	12	2	0
3	M	27	0	12	4	0
3	N	27	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	0	2	0
4	B	4	0	0	3	0
4	C	4	0	0	4	0
4	D	4	0	0	1	0
4	E	4	0	0	1	0
4	F	4	0	0	1	0
4	G	4	0	0	1	0
4	H	4	0	0	4	0
4	I	4	0	0	4	0
4	J	4	0	0	2	0
4	K	4	0	0	2	0
4	L	4	0	0	2	0
4	M	4	0	0	1	0
4	N	4	0	0	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	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	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	64559	0	66430	4705	17

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 36.

All (4705) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:95:VAL:HA	2:P:3:ILE:CG2	1.26	1.56
1:K:207:LYS:CG	1:K:208:PRO:HD3	1.46	1.42
2:O:95:VAL:CA	2:P:3:ILE:HG22	1.52	1.37
1:F:218:PRO:O	1:F:219:PHE:CD1	1.81	1.33
2:V:56:PRO:O	2:V:57:LEU:HG	1.26	1.32
2:R:6:LEU:HD21	2:R:7:HIS:CE1	1.65	1.30
1:L:208:PRO:O	1:L:209:GLU:CD	1.75	1.28
2:R:49:LEU:HD12	2:S:50:GLU:O	1.28	1.26
1:B:363:GLU:OE1	1:B:364:LYS:HG3	1.34	1.26
1:G:412:VAL:HG11	1:G:418:ALA:CB	1.64	1.24
2:U:48:ILE:O	2:U:49:LEU:HD12	1.12	1.24
2:O:96:GLU:O	2:P:1:MET:HA	1.22	1.23
2:R:49:LEU:HD12	2:S:50:GLU:C	1.62	1.22
2:Z:8:ASP:O	2:Z:57:LEU:HD21	1.39	1.22
1:L:208:PRO:C	1:L:209:GLU:OE1	1.83	1.20
1:G:412:VAL:CG1	1:G:418:ALA:HB2	1.70	1.20
2:R:6:LEU:CD2	2:R:7:HIS:ND1	2.06	1.19
1:G:205:ILE:HA	1:G:213:VAL:HG22	1.21	1.18
2:R:6:LEU:HD21	2:R:7:HIS:ND1	1.58	1.17
1:B:245:LYS:HB2	1:B:246:PRO:HD3	1.24	1.15
1:F:218:PRO:HB3	1:F:246:PRO:HG2	1.28	1.14
2:O:96:GLU:O	2:P:1:MET:CA	1.95	1.14
1:D:360:TYR:HA	1:D:363:GLU:HG3	1.27	1.14
1:G:412:VAL:HG11	1:G:418:ALA:HB1	1.26	1.13
2:T:20:LYS:HE2	2:T:22:ALA:HB3	1.23	1.12
1:F:233:MET:HG3	1:F:234:LEU:HD23	1.25	1.12
1:C:197:ARG:HG2	1:C:277:LYS:HB3	1.29	1.12
2:Y:12:VAL:HG12	2:Y:40:VAL:HA	1.32	1.12
1:K:207:LYS:HG2	1:K:208:PRO:HD3	1.29	1.11
2:U:48:ILE:O	2:U:49:LEU:CD1	1.98	1.11
1:C:6:VAL:HG12	1:C:521:VAL:HG22	1.33	1.11
1:K:207:LYS:HG3	1:K:208:PRO:CD	1.81	1.11
1:M:241:ALA:HA	1:M:271:VAL:HG11	1.30	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:20:LYS:HA	2:W:21:SER:HB3	1.14	1.11
2:O:95:VAL:CA	2:P:3:ILE:CG2	2.19	1.10
1:E:207:LYS:HB2	1:E:208:PRO:HD3	1.16	1.09
1:K:6:VAL:HG12	1:K:521:VAL:HG22	1.34	1.08
2:R:20:LYS:HA	2:R:21:SER:HB3	1.22	1.08
1:H:262:LEU:HD11	1:H:273:VAL:HG11	1.30	1.08
1:C:177:VAL:HG11	1:C:397:GLU:HG2	1.30	1.08
2:U:51:ASN:O	2:U:53:GLU:HG2	1.54	1.08
1:K:207:LYS:HG3	1:K:208:PRO:HD3	1.10	1.07
1:N:77:VAL:HG21	1:N:507:ALA:HA	1.32	1.06
1:L:245:LYS:HB3	1:L:246:PRO:HD2	1.36	1.06
1:H:238:GLU:HA	2:V:25:ILE:HD11	1.38	1.06
1:H:302:SER:HB2	1:H:305:ILE:HD13	1.35	1.06
2:S:49:LEU:CD2	2:T:48:ILE:HD12	1.85	1.05
2:P:64:ILE:HG23	2:P:95:VAL:HB	1.38	1.05
1:F:6:VAL:HG12	1:F:521:VAL:HG22	1.35	1.05
1:H:197:ARG:HG2	1:H:277:LYS:HB3	1.38	1.05
1:C:208:PRO:HB2	1:C:212:ALA:HB3	1.39	1.04
1:J:205:ILE:HA	1:J:213:VAL:HG22	1.34	1.04
1:L:412:VAL:CG1	1:L:418:ALA:HB2	1.88	1.03
2:S:49:LEU:HD22	2:T:48:ILE:HD12	1.11	1.03
1:G:412:VAL:CG1	1:G:418:ALA:CB	2.33	1.03
1:I:166:MET:HE1	1:I:407:VAL:HG21	1.41	1.03
2:S:8:ASP:HB3	2:S:47:ARG:HB3	1.38	1.03
1:A:236:VAL:HG21	1:A:312:ALA:HB3	1.40	1.03
1:D:232:GLU:HG2	1:D:309:LEU:HD23	1.40	1.02
1:E:205:ILE:HA	1:E:213:VAL:HG22	1.41	1.02
1:G:412:VAL:HG12	1:G:418:ALA:HB2	1.36	1.02
2:R:50:GLU:OE1	2:R:50:GLU:N	1.90	1.02
1:H:221:LEU:HD13	1:H:317:LEU:HD21	1.37	1.02
1:N:228:SER:HB3	1:N:255:GLU:HB2	1.38	1.02
1:L:412:VAL:HG11	1:L:418:ALA:CB	1.89	1.01
2:1:37:ARG:HH22	2:2:78:ILE:HG23	1.23	1.01
1:L:412:VAL:HG11	1:L:418:ALA:HB1	1.43	1.01
2:X:50:GLU:O	2:X:51:ASN:CG	2.04	1.01
2:1:49:LEU:HD12	2:1:50:GLU:O	1.61	1.01
2:S:49:LEU:HD22	2:T:48:ILE:CD1	1.89	1.01
1:E:207:LYS:CB	1:E:208:PRO:HD3	1.81	1.00
1:L:230:ILE:HG21	1:L:309:LEU:HD21	1.43	1.00
2:T:12:VAL:HG12	2:T:40:VAL:HG23	1.44	1.00
1:L:367:GLU:HG2	1:L:371:LYS:HE2	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:49:LEU:H	2:2:52:GLY:HA2	1.26	1.00
2:S:67:PHE:HA	2:S:92:LEU:HD13	1.40	1.00
2:T:97:ALA:HB2	2:U:1:MET:HA	1.43	1.00
2:Z:95:VAL:HA	2:1:3:ILE:HG22	1.44	1.00
1:E:166:MET:HE1	1:E:407:VAL:HG21	1.44	1.00
1:L:412:VAL:HG12	1:L:418:ALA:HB2	1.40	1.00
1:B:222:LEU:HD22	1:B:300:VAL:HG22	1.44	0.99
1:M:291:ASP:HB3	1:M:372:LEU:HD21	1.43	0.99
1:M:325:ILE:HG13	1:M:330:THR:HG23	1.42	0.99
1:A:309:LEU:HD12	1:A:310:GLU:H	1.26	0.99
2:2:65:VAL:HG12	2:2:94:ILE:HG22	1.42	0.99
1:C:236:VAL:HG21	1:C:312:ALA:HB3	1.39	0.99
2:O:8:ASP:HB2	2:O:57:LEU:HD11	1.44	0.99
2:R:36:THR:HG23	2:R:37:ARG:HG3	1.45	0.99
1:C:226:LYS:HG2	1:C:252:GLU:HG2	1.39	0.99
1:H:322:ARG:HB3	1:H:333:ILE:HD12	1.41	0.99
2:O:50:GLU:O	2:U:50:GLU:HG3	1.63	0.99
1:K:208:PRO:HB2	1:K:212:ALA:HB3	1.45	0.99
1:H:350:ARG:HD3	1:H:353:ILE:HD12	1.44	0.99
1:K:207:LYS:CG	1:K:208:PRO:CD	2.38	0.99
1:G:221:LEU:HD13	1:G:249:ILE:HD13	1.45	0.99
1:K:234:LEU:O	1:K:237:LEU:HG	1.63	0.98
1:M:177:VAL:HG11	1:M:397:GLU:HG2	1.42	0.98
1:N:284:ARG:HG2	1:N:288:MET:HE2	1.41	0.98
1:N:477:GLY:HA3	1:N:488:MET:HE2	1.41	0.98
2:R:3:ILE:HD11	2:R:11:ILE:HD12	1.44	0.98
1:E:234:LEU:HD23	1:E:235:PRO:HD3	1.44	0.98
1:G:230:ILE:HG21	1:G:309:LEU:HD21	1.46	0.98
1:J:265:ASN:HB2	1:J:270:ILE:HB	1.45	0.97
2:R:48:ILE:HA	2:R:54:VAL:HG12	1.46	0.97
1:D:166:MET:HE1	1:D:407:VAL:HG21	1.46	0.97
1:F:225:LYS:HG2	1:F:309:LEU:HD21	1.46	0.97
1:E:205:ILE:HD13	1:E:211:GLY:HA2	1.47	0.97
1:H:6:VAL:HG12	1:H:521:VAL:HG22	1.44	0.97
1:N:150:ILE:HD11	1:N:493:ILE:HG22	1.44	0.96
2:R:8:ASP:O	2:R:57:LEU:HD11	1.63	0.96
2:S:64:ILE:HG23	2:S:95:VAL:HG13	1.46	0.96
1:M:233:MET:HE3	1:M:237:LEU:HD23	1.48	0.96
1:B:230:ILE:HG21	1:B:309:LEU:HD13	1.48	0.96
2:X:37:ARG:HG2	2:X:66:ILE:HG23	1.48	0.96
1:B:363:GLU:OE1	1:B:364:LYS:CG	2.13	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:208:PRO:HB2	1:L:209:GLU:OE1	1.64	0.96
2:X:65:VAL:HG12	2:X:94:ILE:HG22	1.44	0.96
2:Z:93:ALA:HB2	2:1:5:PRO:HA	1.46	0.96
1:F:199:TYR:HA	1:F:276:VAL:HG12	1.46	0.95
1:H:305:ILE:HG23	1:I:267:MET:HE1	1.46	0.95
2:O:95:VAL:HG22	2:P:3:ILE:HG21	1.48	0.95
1:A:309:LEU:HD12	1:A:310:GLU:N	1.82	0.95
1:J:322:ARG:HB3	1:J:333:ILE:HD12	1.47	0.95
1:K:177:VAL:HG11	1:K:397:GLU:HG2	1.48	0.95
2:R:49:LEU:HD11	2:S:50:GLU:HA	1.49	0.95
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.48	0.94
1:G:172:GLU:N	1:G:172:GLU:OE1	2.00	0.94
2:Z:8:ASP:OD1	2:Z:9:ARG:N	2.00	0.94
1:F:357:THR:HG21	1:F:361:ASP:OD2	1.68	0.94
1:J:231:ARG:HD2	1:J:257:GLU:OE1	1.68	0.94
1:K:284:ARG:HD3	1:K:364:LYS:HE3	1.48	0.94
1:K:302:SER:HB2	1:K:305:ILE:HD13	1.50	0.94
2:U:49:LEU:HB3	2:U:50:GLU:OE1	1.67	0.94
1:D:230:ILE:O	1:D:231:ARG:HG2	1.68	0.93
2:O:64:ILE:HG23	2:O:95:VAL:HB	1.48	0.93
2:X:67:PHE:HA	2:X:92:LEU:HD13	1.48	0.93
1:H:367:GLU:HG2	1:H:371:LYS:HE2	1.48	0.93
1:J:367:GLU:HG2	1:J:371:LYS:HE2	1.51	0.93
1:N:247:LEU:HG	1:N:249:ILE:HD11	1.50	0.93
2:U:49:LEU:C	2:U:50:GLU:OE1	2.10	0.93
1:B:6:VAL:HG12	1:B:521:VAL:HG22	1.50	0.93
1:A:306:GLY:HA3	1:B:264:VAL:HG21	1.51	0.93
1:G:226:LYS:HB3	1:G:253:ASP:HB2	1.51	0.93
1:L:208:PRO:O	1:L:209:GLU:OE1	1.78	0.93
1:N:411:VAL:HG21	1:N:494:LEU:HD23	1.50	0.93
2:R:6:LEU:HD23	2:R:7:HIS:CG	2.03	0.93
1:B:245:LYS:CB	1:B:246:PRO:HD3	1.95	0.92
2:R:48:ILE:HG12	2:R:54:VAL:HG11	1.51	0.92
1:G:230:ILE:HD13	1:G:309:LEU:HD22	1.51	0.92
1:I:205:ILE:HA	1:I:213:VAL:HG22	1.50	0.92
1:I:199:TYR:HE2	1:I:202:PRO:HA	1.34	0.92
2:R:49:LEU:CD1	2:S:50:GLU:C	2.42	0.92
1:E:248:LEU:HD22	1:E:323:VAL:HG11	1.52	0.92
1:L:6:VAL:HG12	1:L:521:VAL:HG22	1.51	0.92
2:V:25:ILE:HG13	2:V:26:VAL:HG23	1.51	0.92
1:L:219:PHE:HA	1:L:317:LEU:HD21	1.48	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:34:LYS:HE3	2:Z:76:GLU:HA	1.52	0.92
1:B:305:ILE:HG22	1:B:306:GLY:H	1.34	0.92
1:K:349:ILE:HD12	1:K:352:GLN:HB2	1.51	0.92
2:O:8:ASP:HA	2:O:57:LEU:HD21	1.50	0.91
1:A:276:VAL:HG11	1:A:325:ILE:HG21	1.52	0.91
1:M:6:VAL:HG12	1:M:521:VAL:HG22	1.53	0.91
2:W:1:MET:HE2	2:W:79:ASP:HB3	1.51	0.91
1:C:321:LYS:HB2	1:C:334:ASP:HB3	1.52	0.91
1:B:325:ILE:HG13	1:B:330:THR:HG23	1.51	0.91
1:G:358:SER:HA	1:G:362:ARG:HE	1.35	0.91
2:R:49:LEU:CD1	2:S:50:GLU:O	2.18	0.91
2:1:64:ILE:HG23	2:1:95:VAL:HB	1.51	0.91
1:G:284:ARG:HG2	1:G:288:MET:HE2	1.53	0.91
2:R:49:LEU:CD1	2:S:50:GLU:HA	2.01	0.91
1:D:228:SER:HA	1:D:255:GLU:HB2	1.52	0.91
2:W:9:ARG:HG2	2:W:9:ARG:HH11	1.36	0.91
1:L:40:LEU:HD13	1:L:59:GLU:HG3	1.52	0.90
1:J:305:ILE:HG23	1:J:307:MET:H	1.34	0.90
2:R:6:LEU:CD2	2:R:7:HIS:CG	2.55	0.90
1:J:214:GLU:HG2	1:J:324:VAL:HG22	1.49	0.90
1:H:207:LYS:HB3	1:H:208:PRO:HD3	1.51	0.90
1:A:6:VAL:HG12	1:A:521:VAL:HG22	1.50	0.90
1:F:220:ILE:HG13	1:F:296:THR:HG21	1.51	0.90
1:C:420:ILE:HD11	1:C:470:LYS:HG3	1.53	0.90
2:U:15:LYS:HG2	2:U:38:GLY:HA2	1.51	0.90
1:N:225:LYS:HB3	1:N:231:ARG:HH21	1.37	0.90
1:K:221:LEU:HD13	1:K:317:LEU:HD21	1.53	0.90
1:G:222:LEU:HD22	1:G:300:VAL:HG22	1.52	0.89
2:V:11:ILE:HG22	2:V:85:ILE:HG12	1.55	0.89
1:L:412:VAL:CG1	1:L:418:ALA:CB	2.48	0.89
1:H:278:ALA:HB3	1:H:285:ARG:HD2	1.51	0.89
1:G:5:ASP:HB2	1:G:524:LEU:HD23	1.55	0.89
1:G:240:VAL:HG11	1:G:247:LEU:HD21	1.54	0.89
1:N:325:ILE:HG13	1:N:330:THR:HG23	1.53	0.89
2:Z:15:LYS:HG2	2:Z:38:GLY:HA2	1.54	0.88
1:N:6:VAL:HG12	1:N:521:VAL:HG22	1.54	0.88
1:M:405:ALA:HB1	1:M:498:LYS:HB3	1.56	0.88
2:1:17:VAL:HG23	2:1:34:LYS:HA	1.53	0.88
2:V:57:LEU:HD13	2:V:88:GLU:HG3	1.56	0.88
2:1:65:VAL:HG12	2:1:94:ILE:HG22	1.55	0.88
1:E:221:LEU:HD21	1:E:301:ILE:HD12	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:HD13	1:A:59:GLU:HG3	1.56	0.87
1:A:177:VAL:HG21	1:A:397:GLU:HG2	1.53	0.87
1:F:205:ILE:HA	1:F:213:VAL:HG22	1.56	0.87
1:G:77:VAL:HG21	1:G:507:ALA:HA	1.54	0.87
2:Y:65:VAL:HG12	2:Y:94:ILE:HG22	1.56	0.87
1:H:302:SER:CB	1:H:305:ILE:HD13	2.03	0.87
1:K:518:GLU:HB3	1:L:29:VAL:HG11	1.55	0.87
2:W:20:LYS:HA	2:W:21:SER:CB	1.99	0.87
2:S:40:VAL:HG12	2:S:41:LEU:H	1.40	0.87
2:W:17:VAL:HG23	2:W:19:THR:H	1.39	0.87
1:C:171:LYS:HD2	1:C:407:VAL:HG11	1.56	0.87
1:E:183:LEU:HD22	1:E:384:ALA:HA	1.55	0.86
1:E:234:LEU:HD23	1:E:235:PRO:CD	2.04	0.86
1:H:77:VAL:HG21	1:H:507:ALA:HA	1.56	0.86
2:Q:37:ARG:HG2	2:Q:66:ILE:HG12	1.58	0.86
1:C:197:ARG:HE	1:C:277:LYS:HD2	1.39	0.86
1:D:420:ILE:CD1	1:D:448:GLU:HG2	2.06	0.86
2:1:95:VAL:HG22	2:2:3:ILE:HG21	1.57	0.86
1:D:420:ILE:HD13	1:D:448:GLU:HG2	1.56	0.86
2:1:49:LEU:CD1	2:1:50:GLU:O	2.23	0.86
1:I:40:LEU:HD13	1:I:59:GLU:HG3	1.58	0.86
1:A:353:ILE:HG12	1:A:365:LEU:HD13	1.56	0.86
1:N:77:VAL:HB	1:N:510:VAL:HG21	1.56	0.86
1:N:288:MET:HG2	1:N:368:ARG:HD3	1.57	0.86
1:A:245:LYS:HB3	1:A:246:PRO:CD	2.05	0.86
1:A:325:ILE:HG13	1:A:330:THR:HG23	1.57	0.86
1:B:228:SER:HB3	1:B:255:GLU:HG2	1.56	0.86
1:C:232:GLU:HG3	1:C:310:GLU:HG3	1.56	0.85
1:F:236:VAL:HG11	1:F:312:ALA:HB3	1.56	0.85
1:F:284:ARG:HD3	1:F:364:LYS:HE2	1.57	0.85
1:E:5:ASP:HB2	1:E:524:LEU:HD23	1.58	0.85
1:F:305:ILE:HG22	1:F:306:GLY:H	1.40	0.85
1:B:230:ILE:CG2	1:B:309:LEU:HD13	2.06	0.85
1:M:305:ILE:HG22	1:M:306:GLY:H	1.38	0.85
2:R:78:ILE:HG13	2:R:79:ASP:H	1.38	0.85
2:T:17:VAL:HG23	2:T:33:ALA:HB2	1.58	0.85
1:M:197:ARG:HD2	1:M:277:LYS:HB2	1.58	0.85
1:M:429:LEU:HG	1:M:440:ILE:HD13	1.59	0.85
1:G:455:VAL:HG13	1:G:460:GLU:HB2	1.57	0.85
1:M:234:LEU:HB3	1:M:235:PRO:HD2	1.56	0.85
2:Y:11:ILE:HG22	2:Y:85:ILE:HB	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:193:MET:HE1	1:I:292:ILE:CG1	2.07	0.85
1:D:305:ILE:HG22	1:D:306:GLY:H	1.41	0.85
1:H:197:ARG:CG	1:H:277:LYS:HB3	2.06	0.85
1:E:234:LEU:O	1:E:236:VAL:N	2.10	0.84
1:I:197:ARG:NH1	1:I:277:LYS:HD2	1.92	0.84
1:B:276:VAL:HG21	1:B:325:ILE:HG21	1.59	0.84
1:D:205:ILE:HA	1:D:213:VAL:HG22	1.59	0.84
1:E:229:ASN:OD1	1:E:230:ILE:HD12	1.77	0.84
2:W:55:LYS:HE3	2:X:53:GLU:HG2	1.57	0.84
1:B:77:VAL:HG21	1:B:507:ALA:HA	1.60	0.84
1:H:326:ASN:HB3	1:H:329:THR:HG22	1.57	0.84
1:I:252:GLU:HG3	1:I:285:ARG:NH1	1.92	0.84
1:J:278:ALA:HB1	1:J:285:ARG:HD2	1.60	0.84
1:K:455:VAL:HG13	1:K:460:GLU:HB2	1.59	0.84
1:M:279:PRO:HG2	1:M:285:ARG:HA	1.57	0.84
1:F:245:LYS:HB3	1:F:246:PRO:HD2	1.60	0.84
2:2:49:LEU:N	2:2:52:GLY:HA2	1.93	0.84
1:B:240:VAL:HG11	1:B:247:LEU:HD23	1.60	0.84
1:F:77:VAL:HB	1:F:510:VAL:HG21	1.59	0.83
1:G:40:LEU:HD13	1:G:59:GLU:HG3	1.60	0.83
1:J:357:THR:HG21	1:J:361:ASP:HB2	1.59	0.83
1:B:351:GLN:HG2	1:C:210:THR:HG23	1.60	0.83
1:G:223:ALA:HB2	1:G:251:ALA:HA	1.58	0.83
1:L:284:ARG:HG2	1:L:288:MET:HE2	1.58	0.83
2:V:1:MET:N	2:2:97:ALA:O	2.11	0.83
1:J:314:LEU:HD23	1:J:314:LEU:O	1.77	0.83
1:A:181:THR:HG21	1:A:380:LYS:HD3	1.58	0.83
1:B:301:ILE:HG12	1:B:307:MET:CE	2.08	0.83
2:Q:50:GLU:CD	2:Q:51:ASN:H	1.85	0.83
1:C:236:VAL:CG2	1:C:312:ALA:HB3	2.07	0.83
1:I:193:MET:HE1	1:I:292:ILE:HG12	1.61	0.83
1:J:166:MET:HE1	1:J:407:VAL:HG21	1.59	0.83
1:N:419:LEU:HD21	1:N:500:THR:HG23	1.60	0.83
1:L:205:ILE:HD13	1:L:211:GLY:HA2	1.60	0.83
2:2:78:ILE:H	2:2:78:ILE:HD12	1.44	0.83
2:V:50:GLU:HG3	2:W:50:GLU:HB3	1.61	0.83
1:C:225:LYS:HG3	1:C:303:GLU:HG3	1.60	0.83
1:D:278:ALA:HB1	1:D:285:ARG:HG3	1.60	0.83
1:F:221:LEU:HD13	1:F:317:LEU:HD21	1.61	0.82
1:N:245:LYS:HB3	1:N:246:PRO:HD2	1.60	0.82
1:J:162:ILE:HG21	1:J:403:THR:HG21	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:50:GLU:O	2:1:51:ASN:OD1	1.96	0.82
1:N:305:ILE:HG22	1:N:306:GLY:H	1.44	0.82
1:B:278:ALA:CB	1:B:285:ARG:HD2	2.10	0.82
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.62	0.82
1:L:357:THR:HG21	1:L:361:ASP:HB2	1.59	0.82
1:N:228:SER:HA	1:N:258:ALA:HB2	1.59	0.82
2:Y:34:LYS:HD2	2:Z:76:GLU:HG2	1.62	0.82
1:M:234:LEU:HB3	1:M:235:PRO:CD	2.10	0.82
2:R:19:THR:HG21	2:R:33:ALA:HB1	1.61	0.81
2:W:78:ILE:HG13	2:W:79:ASP:H	1.44	0.81
1:A:147:VAL:HG12	1:A:494:LEU:HB2	1.60	0.81
1:B:233:MET:C	1:B:235:PRO:HD2	2.05	0.81
1:H:367:GLU:CG	1:H:371:LYS:HE2	2.09	0.81
2:P:17:VAL:HG12	2:P:35:SER:HB2	1.61	0.81
2:R:49:LEU:CD1	2:S:50:GLU:CA	2.58	0.81
2:V:50:GLU:O	2:V:51:ASN:ND2	2.12	0.81
2:Y:40:VAL:HG13	2:Y:62:GLY:H	1.45	0.81
1:L:218:PRO:HA	1:L:219:PHE:HB2	1.62	0.81
1:N:261:THR:HB	2:2:29:GLY:H	1.43	0.81
1:B:222:LEU:HD13	1:B:300:VAL:HA	1.61	0.81
1:D:279:PRO:HB2	1:D:288:MET:HE3	1.63	0.81
2:R:12:VAL:HG12	2:R:40:VAL:HA	1.63	0.81
2:W:12:VAL:HG12	2:W:40:VAL:HA	1.63	0.81
1:F:233:MET:CG	1:F:234:LEU:HD23	2.06	0.81
2:R:59:VAL:HG22	2:R:94:ILE:HD11	1.62	0.81
1:H:174:VAL:HG23	1:H:376:VAL:HG13	1.62	0.81
1:J:204:PHE:CZ	1:J:262:LEU:HD22	2.16	0.81
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.63	0.81
2:S:8:ASP:OD1	2:S:87:SER:OG	1.97	0.81
1:F:321:LYS:HB2	1:F:334:ASP:HB3	1.63	0.81
1:K:205:ILE:HA	1:K:213:VAL:HG22	1.60	0.81
1:N:252:GLU:HA	1:N:285:ARG:HH12	1.46	0.81
2:Z:93:ALA:CB	2:1:5:PRO:HA	2.10	0.81
1:H:305:ILE:HG22	1:H:306:GLY:H	1.45	0.81
2:O:6:LEU:CD1	2:U:93:ALA:HA	2.10	0.81
1:C:241:ALA:HA	1:C:271:VAL:HG11	1.62	0.81
1:K:353:ILE:HA	1:K:365:LEU:HD13	1.63	0.81
1:M:267:MET:HE2	1:M:267:MET:HA	1.62	0.81
1:K:205:ILE:HD13	1:K:211:GLY:HA2	1.61	0.80
1:C:174:VAL:HG13	1:C:376:VAL:HG13	1.62	0.80
1:E:240:VAL:CG1	1:E:247:LEU:HD21	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.62	0.80
1:L:218:PRO:HG2	1:L:220:ILE:HD11	1.63	0.80
2:X:92:LEU:HB3	2:Y:85:ILE:HD13	1.61	0.80
2:V:20:LYS:HG3	2:V:28:THR:HG23	1.63	0.80
1:G:230:ILE:CG2	1:G:309:LEU:HD11	2.11	0.80
1:F:308:GLU:HB2	1:F:311:LYS:HB3	1.63	0.80
1:G:254:VAL:HG12	1:G:259:LEU:HG	1.63	0.80
2:W:10:VAL:HG21	2:W:91:ILE:HD11	1.62	0.80
2:X:58:ASP:OD2	2:Y:7:HIS:ND1	2.14	0.80
1:B:270:ILE:HG12	2:P:25:ILE:HD13	1.62	0.80
1:D:360:TYR:CA	1:D:363:GLU:HG3	2.09	0.80
1:B:166:MET:HE1	1:B:407:VAL:HG21	1.63	0.80
1:K:305:ILE:HG22	1:K:306:GLY:H	1.45	0.80
1:N:352:GLN:HB3	1:N:365:LEU:HD11	1.63	0.80
2:U:48:ILE:C	2:U:49:LEU:HD12	2.05	0.80
1:A:267:MET:HE2	1:A:267:MET:HA	1.64	0.80
1:N:31:LEU:HD23	1:N:453:GLN:HB3	1.63	0.80
1:J:208:PRO:HB2	1:J:212:ALA:HB3	1.63	0.80
2:V:4:ARG:HD2	2:2:94:ILE:HD11	1.63	0.80
1:D:237:LEU:HD22	2:R:27:LEU:HD11	1.63	0.79
1:B:234:LEU:HA	1:B:237:LEU:HD13	1.64	0.79
2:O:96:GLU:C	2:P:1:MET:HA	2.06	0.79
2:O:97:ALA:HB2	2:P:1:MET:H1	1.47	0.79
2:R:20:LYS:HA	2:R:21:SER:CB	2.03	0.79
2:W:36:THR:HG23	2:W:37:ARG:HG3	1.65	0.79
1:H:305:ILE:HG23	1:I:267:MET:CE	2.12	0.79
1:N:228:SER:CB	1:N:255:GLU:HB2	2.13	0.79
1:G:230:ILE:HG21	1:G:309:LEU:HD11	1.64	0.79
1:B:199:TYR:CE1	1:B:202:PRO:HA	2.18	0.79
1:F:168:LYS:HG2	1:F:189:VAL:HG11	1.62	0.79
1:A:267:MET:HG3	1:G:305:ILE:HG12	1.65	0.79
1:G:6:VAL:HG12	1:G:521:VAL:HG22	1.65	0.79
1:H:278:ALA:CB	1:H:285:ARG:HD2	2.12	0.79
1:I:241:ALA:HB1	2:W:25:ILE:HD13	1.65	0.79
1:J:270:ILE:HG21	2:X:27:LEU:CD2	2.12	0.79
1:M:303:GLU:HG3	1:M:309:LEU:HD11	1.65	0.79
2:1:37:ARG:HH22	2:2:78:ILE:CG2	1.96	0.79
2:1:37:ARG:NH2	2:2:78:ILE:HG23	1.98	0.79
1:F:74:VAL:O	1:F:77:VAL:HG12	1.83	0.79
1:L:208:PRO:CB	1:L:209:GLU:OE1	2.30	0.79
1:M:233:MET:HB2	1:M:237:LEU:HD21	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:199:TYR:CE1	1:N:202:PRO:HA	2.18	0.79
1:J:325:ILE:HG13	1:J:330:THR:HG23	1.64	0.78
1:K:381:VAL:HG22	1:K:396:VAL:HG21	1.65	0.78
1:N:234:LEU:HD12	1:N:234:LEU:H	1.46	0.78
1:B:305:ILE:HD12	1:C:263:VAL:HG11	1.65	0.78
1:E:183:LEU:CD2	1:E:384:ALA:HA	2.13	0.78
1:G:204:PHE:CD2	1:G:274:ALA:HA	2.17	0.78
1:J:230:ILE:HG13	1:J:231:ARG:H	1.46	0.78
1:J:349:ILE:HD12	1:J:369:VAL:HG22	1.64	0.78
1:L:306:GLY:O	1:L:307:MET:HG3	1.82	0.78
1:L:479:ASN:HD22	1:L:493:ILE:HD11	1.46	0.78
1:M:5:ASP:HB2	1:M:524:LEU:CD2	2.14	0.78
2:R:49:LEU:HD22	2:R:50:GLU:OE1	1.83	0.78
1:E:208:PRO:HB2	1:E:212:ALA:HB3	1.66	0.78
1:E:240:VAL:HG11	1:E:247:LEU:HD21	1.66	0.78
1:F:320:ALA:HA	1:F:335:GLY:HA2	1.65	0.78
1:F:325:ILE:HG13	1:F:330:THR:HG23	1.66	0.78
1:H:307:MET:HG2	1:H:311:LYS:HZ2	1.49	0.78
2:P:57:LEU:HD13	2:P:88:GLU:HB2	1.65	0.78
2:T:92:LEU:HD23	2:U:85:ILE:HD13	1.65	0.78
1:N:77:VAL:CG2	1:N:507:ALA:HA	2.12	0.78
2:U:49:LEU:O	2:U:50:GLU:CD	2.26	0.78
2:T:12:VAL:HB	2:T:39:GLU:O	1.84	0.78
1:F:420:ILE:HD12	1:F:451:LEU:HD13	1.66	0.78
1:G:246:PRO:HA	1:G:272:LYS:O	1.84	0.78
1:H:40:LEU:HD13	1:H:59:GLU:HG3	1.66	0.78
1:I:74:VAL:O	1:I:77:VAL:HG12	1.83	0.78
1:K:215:LEU:HB2	1:K:323:VAL:HG22	1.65	0.78
1:C:177:VAL:HG11	1:C:397:GLU:CG	2.12	0.78
1:E:301:ILE:HG12	1:E:307:MET:HE1	1.65	0.78
1:F:278:ALA:HB1	1:F:279:PRO:HD2	1.65	0.78
1:G:205:ILE:HD13	1:G:211:GLY:HA2	1.66	0.78
1:H:238:GLU:HA	2:V:25:ILE:CD1	2.14	0.77
1:L:207:LYS:HG2	1:L:208:PRO:HD2	1.66	0.77
1:E:5:ASP:HB2	1:E:524:LEU:CD2	2.14	0.77
1:E:214:GLU:HG2	1:E:324:VAL:HG22	1.63	0.77
1:G:200:LEU:HD11	1:G:277:LYS:HB2	1.66	0.77
1:J:322:ARG:HB3	1:J:333:ILE:CD1	2.15	0.77
1:N:175:ILE:HG12	1:N:377:ALA:HB3	1.66	0.77
1:F:218:PRO:HB3	1:F:246:PRO:CG	2.11	0.77
1:G:306:GLY:O	1:G:307:MET:HG3	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:349:ILE:HD12	1:H:369:VAL:HG22	1.65	0.77
1:N:40:LEU:HD21	1:N:56:VAL:HG22	1.66	0.77
1:A:188:ASP:HB2	1:A:378:VAL:HG23	1.64	0.77
1:C:231:ARG:HD3	1:C:258:ALA:HA	1.67	0.77
1:C:254:VAL:HG12	1:C:259:LEU:HG	1.67	0.77
1:E:301:ILE:HG12	1:E:307:MET:CE	2.14	0.77
1:F:5:ASP:HB2	1:F:524:LEU:CD2	2.13	0.77
1:H:245:LYS:HB3	1:H:246:PRO:HD2	1.64	0.77
1:M:199:TYR:CE1	1:M:202:PRO:HA	2.19	0.77
2:U:51:ASN:O	2:U:53:GLU:N	2.17	0.77
1:A:245:LYS:HB3	1:A:246:PRO:HD2	1.65	0.77
1:K:268:ARG:HG3	2:Y:27:LEU:HD21	1.64	0.77
1:H:354:GLU:O	1:H:355:GLU:HG3	1.84	0.77
1:F:221:LEU:HD13	1:F:317:LEU:CD2	2.14	0.77
1:D:229:ASN:OD1	1:D:230:ILE:N	2.17	0.77
1:G:209:GLU:HG2	1:G:210:THR:H	1.49	0.77
1:E:174:VAL:HG22	1:E:376:VAL:HG13	1.67	0.77
1:G:232:GLU:HG3	1:G:310:GLU:OE2	1.85	0.77
2:R:8:ASP:O	2:R:57:LEU:CD1	2.32	0.76
1:B:236:VAL:HG21	1:B:312:ALA:HB3	1.67	0.76
1:H:74:VAL:O	1:H:77:VAL:HG12	1.85	0.76
1:H:385:THR:HG22	1:N:80:LYS:HG2	1.66	0.76
1:L:479:ASN:ND2	1:L:493:ILE:HD11	2.00	0.76
2:S:12:VAL:HG22	2:S:40:VAL:HG13	1.66	0.76
1:I:228:SER:HB3	1:I:255:GLU:HB2	1.67	0.76
1:L:355:GLU:HG3	1:L:356:ALA:H	1.51	0.76
2:O:5:PRO:HA	2:U:93:ALA:CB	2.15	0.76
2:R:17:VAL:HG23	2:R:19:THR:H	1.51	0.76
2:X:64:ILE:HG23	2:X:95:VAL:HG13	1.67	0.76
1:B:291:ASP:HB3	1:B:372:LEU:HD21	1.67	0.76
1:J:270:ILE:HG21	2:X:27:LEU:HD23	1.67	0.76
1:L:226:LYS:N	1:L:252:GLU:HB3	2.00	0.76
1:M:5:ASP:HB2	1:M:524:LEU:HD21	1.67	0.76
1:F:218:PRO:CB	1:F:246:PRO:HG2	2.12	0.76
2:R:21:SER:N	2:R:27:LEU:O	2.15	0.76
2:R:49:LEU:O	2:R:51:ASN:N	2.18	0.76
2:2:73:VAL:HG22	2:2:86:MET:HB3	1.68	0.76
1:A:77:VAL:HG21	1:A:507:ALA:HA	1.68	0.76
1:E:195:PHE:CE1	1:E:330:THR:HB	2.20	0.76
2:Q:6:LEU:HD13	2:Q:7:HIS:HD2	1.51	0.76
1:A:200:LEU:HD11	1:A:277:LYS:HB2	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASP:OD2	1:C:368:ARG:HD3	1.86	0.76
2:O:5:PRO:HA	2:U:93:ALA:HB2	1.66	0.76
2:V:56:PRO:C	2:V:57:LEU:HG	2.10	0.76
2:W:20:LYS:CA	2:W:21:SER:HB3	2.07	0.76
1:K:291:ASP:HB2	1:K:372:LEU:HD21	1.66	0.76
2:Z:65:VAL:CG1	2:Z:94:ILE:HG22	2.16	0.76
1:N:77:VAL:HG21	1:N:507:ALA:CA	2.15	0.75
2:P:80:ASN:OD1	2:P:80:ASN:O	2.05	0.75
1:D:350:ARG:HD2	1:D:353:ILE:HD12	1.67	0.75
1:F:218:PRO:O	1:F:219:PHE:CG	2.38	0.75
2:V:6:LEU:HD21	2:2:91:ILE:HG22	1.67	0.75
1:C:23:LEU:HD23	1:C:60:ILE:HB	1.69	0.75
1:C:291:ASP:O	1:C:345:ARG:NH1	2.19	0.75
1:F:419:LEU:HD11	1:F:500:THR:HG23	1.68	0.75
1:G:230:ILE:HD13	1:G:309:LEU:CD2	2.17	0.75
2:S:12:VAL:HG13	2:S:40:VAL:HA	1.68	0.75
1:B:215:LEU:HD12	1:B:248:LEU:HD21	1.66	0.75
1:H:233:MET:HE1	1:H:237:LEU:HD12	1.67	0.75
1:L:367:GLU:CG	1:L:371:LYS:HE2	2.16	0.75
1:L:381:VAL:HG11	1:L:392:LYS:HB3	1.67	0.75
1:B:307:MET:HG2	1:B:311:LYS:HZ2	1.52	0.75
1:C:166:MET:HE1	1:C:407:VAL:HG21	1.69	0.75
1:C:367:GLU:CG	1:C:371:LYS:HE2	2.17	0.75
1:I:236:VAL:CG2	1:I:312:ALA:HB3	2.17	0.75
1:C:350:ARG:HH12	1:C:369:VAL:HG11	1.50	0.75
1:E:245:LYS:HE2	1:E:246:PRO:HD2	1.67	0.75
1:G:239:ALA:HB1	1:G:314:LEU:HD13	1.68	0.75
1:M:177:VAL:CG1	1:M:397:GLU:HG2	2.14	0.75
2:U:49:LEU:CB	2:U:50:GLU:OE1	2.35	0.75
1:E:276:VAL:HG11	1:E:325:ILE:HG21	1.67	0.75
1:F:220:ILE:N	1:F:318:GLY:O	2.19	0.75
1:J:245:LYS:HB3	1:J:246:PRO:HD2	1.68	0.75
1:E:200:LEU:HD11	1:E:277:LYS:HB2	1.67	0.75
1:M:302:SER:HB2	1:M:305:ILE:HD13	1.66	0.75
1:F:360:TYR:HA	1:F:363:GLU:HG3	1.68	0.74
1:J:357:THR:CG2	1:J:361:ASP:HB2	2.16	0.74
2:Z:65:VAL:HG12	2:Z:94:ILE:HG22	1.68	0.74
1:H:175:ILE:HG12	1:H:377:ALA:HB3	1.67	0.74
1:H:241:ALA:HB3	2:V:25:ILE:HD12	1.67	0.74
1:M:91:THR:OG1	3:M:601:ADP:O3B	2.05	0.74
1:I:151:SER:HB3	1:I:399:ALA:HA	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:234:LEU:HD23	2:Z:23:GLY:HA3	1.69	0.74
1:N:219:PHE:HB3	1:N:317:LEU:HB3	1.70	0.74
2:O:95:VAL:HA	2:P:3:ILE:HG21	1.58	0.74
2:S:50:GLU:CG	2:S:51:ASN:H	2.01	0.74
1:F:77:VAL:HG21	1:F:507:ALA:HA	1.66	0.74
1:F:420:ILE:HD11	1:F:451:LEU:HB3	1.69	0.74
1:I:199:TYR:CE2	1:I:202:PRO:HA	2.19	0.74
1:K:302:SER:CB	1:K:305:ILE:HD13	2.15	0.74
1:E:229:ASN:OD1	1:E:230:ILE:CD1	2.35	0.74
2:T:49:LEU:HD13	2:U:50:GLU:H	1.51	0.74
1:D:417:VAL:HA	1:D:420:ILE:HG22	1.70	0.74
1:G:230:ILE:HG21	1:G:309:LEU:CD2	2.17	0.74
1:L:175:ILE:HG12	1:L:377:ALA:HB3	1.70	0.74
1:L:230:ILE:HG12	1:L:309:LEU:HD21	1.68	0.74
1:M:241:ALA:CA	1:M:271:VAL:HG11	2.16	0.74
2:V:69:ASP:CB	2:V:73:VAL:HG11	2.18	0.74
1:B:231:ARG:HH22	2:P:31:ALA:HB2	1.52	0.74
1:J:266:THR:HG22	1:J:273:VAL:H	1.52	0.74
1:C:195:PHE:CE1	1:C:330:THR:HB	2.23	0.74
1:C:345:ARG:O	1:C:348:GLN:HG3	1.86	0.74
1:E:232:GLU:O	1:E:234:LEU:N	2.20	0.74
1:F:247:LEU:HB2	1:F:273:VAL:HG13	1.69	0.74
1:J:6:VAL:HG12	1:J:521:VAL:HG22	1.70	0.74
1:A:166:MET:HE1	1:A:407:VAL:HG21	1.69	0.74
1:E:151:SER:HB3	1:E:399:ALA:HA	1.69	0.74
1:B:231:ARG:HH12	2:P:31:ALA:HB2	1.52	0.74
1:C:207:LYS:HB3	1:C:208:PRO:HD3	1.68	0.74
1:F:305:ILE:HG22	1:F:306:GLY:N	2.02	0.74
1:G:5:ASP:HB2	1:G:524:LEU:CD2	2.18	0.73
1:G:350:ARG:HD3	1:G:353:ILE:HD12	1.70	0.73
1:B:301:ILE:HG12	1:B:307:MET:HE2	1.68	0.73
1:H:220:ILE:HG22	1:H:222:LEU:HD11	1.69	0.73
1:H:236:VAL:CG2	1:H:312:ALA:HB3	2.18	0.73
1:L:234:LEU:H	1:L:234:LEU:HD12	1.52	0.73
1:M:338:GLU:HG2	1:M:341:ALA:H	1.53	0.73
1:N:222:LEU:HD22	1:N:300:VAL:HG22	1.70	0.73
1:B:307:MET:HG2	1:B:311:LYS:NZ	2.03	0.73
1:E:199:TYR:HA	1:E:276:VAL:HG12	1.69	0.73
2:V:56:PRO:O	2:V:57:LEU:CG	2.22	0.73
1:D:215:LEU:HB2	1:D:323:VAL:CG2	2.19	0.73
1:B:230:ILE:HD11	1:B:232:GLU:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:124:VAL:HG21	1:K:508:ALA:HB1	1.68	0.73
1:N:381:VAL:HG22	1:N:396:VAL:HG21	1.71	0.73
2:Y:60:LYS:HE3	2:Y:61:VAL:HG22	1.70	0.73
1:C:313:THR:HB	1:C:315:GLU:HG3	1.71	0.73
1:C:6:VAL:CG1	1:C:521:VAL:HG22	2.15	0.73
1:I:305:ILE:HG22	1:I:306:GLY:H	1.52	0.73
1:B:278:ALA:HB1	1:B:285:ARG:HD2	1.69	0.73
1:C:294:THR:OG1	1:C:345:ARG:NH1	2.22	0.73
1:C:367:GLU:HG2	1:C:371:LYS:HE2	1.70	0.73
1:H:276:VAL:CG1	1:H:325:ILE:HD13	2.19	0.73
1:H:305:ILE:HG22	1:H:306:GLY:N	2.04	0.73
1:M:519:CYS:HB3	1:N:38:VAL:HG13	1.70	0.73
1:N:5:ASP:HB2	1:N:524:LEU:HD21	1.70	0.73
1:K:309:LEU:HD12	1:K:310:GLU:N	2.04	0.73
2:W:9:ARG:HG2	2:W:9:ARG:NH1	2.02	0.73
1:E:194:GLN:HG2	1:E:331:THR:HG23	1.71	0.73
1:C:305:ILE:HG22	1:C:306:GLY:H	1.52	0.72
1:G:240:VAL:CG1	1:G:247:LEU:HD21	2.19	0.72
1:K:228:SER:HB3	1:K:255:GLU:HB2	1.71	0.72
1:L:203:TYR:HB3	1:L:267:MET:HE2	1.71	0.72
2:W:55:LYS:HE3	2:X:53:GLU:CG	2.19	0.72
2:Q:17:VAL:HG12	2:Q:35:SER:H	1.52	0.72
2:Q:69:ASP:HB2	2:Q:73:VAL:HG11	1.70	0.72
2:Z:55:LYS:HE2	2:1:48:ILE:HD11	1.71	0.72
1:I:196:ASP:O	1:I:196:ASP:OD1	2.06	0.72
2:T:51:ASN:O	2:T:51:ASN:OD1	2.07	0.72
1:F:225:LYS:CG	1:F:309:LEU:HD21	2.19	0.72
1:J:74:VAL:O	1:J:77:VAL:HG12	1.89	0.72
1:K:215:LEU:HB2	1:K:323:VAL:CG2	2.18	0.72
2:O:95:VAL:CG2	2:P:3:ILE:HG21	2.19	0.72
2:T:20:LYS:HB3	2:T:26:VAL:O	1.88	0.72
1:A:181:THR:CG2	1:A:380:LYS:HD3	2.19	0.72
1:A:223:ALA:HB3	1:A:251:ALA:HB2	1.71	0.72
1:C:420:ILE:HD11	1:C:470:LYS:CG	2.19	0.72
1:D:205:ILE:HD13	1:D:211:GLY:HA2	1.72	0.72
1:E:219:PHE:HB3	1:E:317:LEU:HB3	1.70	0.72
1:L:31:LEU:HD23	1:L:453:GLN:HB3	1.70	0.72
2:W:49:LEU:HB2	2:W:52:GLY:HA3	1.70	0.72
1:A:232:GLU:HG3	1:A:234:LEU:HD23	1.71	0.72
1:B:488:MET:CE	1:B:493:ILE:HD12	2.19	0.72
1:D:349:ILE:HA	1:D:352:GLN:HG3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:ASP:HB2	1:F:524:LEU:HD23	1.71	0.72
2:S:14:ARG:HE	2:S:35:SER:HB2	1.55	0.72
1:E:230:ILE:HG12	1:E:309:LEU:HD13	1.71	0.72
1:J:28:LYS:HG2	1:J:94:VAL:HG22	1.70	0.72
1:L:455:VAL:HG13	1:L:460:GLU:HB2	1.71	0.72
1:N:236:VAL:HG22	1:N:312:ALA:HB3	1.69	0.72
1:E:6:VAL:HG12	1:E:521:VAL:HG22	1.71	0.72
1:F:199:TYR:HA	1:F:276:VAL:CG1	2.18	0.72
1:I:429:LEU:HG	1:I:440:ILE:HD13	1.71	0.72
2:V:69:ASP:HB2	2:V:73:VAL:HG11	1.70	0.72
1:B:350:ARG:HD3	1:B:353:ILE:HD12	1.72	0.72
1:D:419:LEU:HD21	1:D:500:THR:HG23	1.71	0.72
1:F:177:VAL:HG11	1:F:397:GLU:HG2	1.71	0.72
2:W:14:ARG:HD3	2:W:35:SER:HB3	1.72	0.72
1:E:429:LEU:HG	1:E:440:ILE:HD13	1.72	0.71
1:G:417:VAL:HA	1:G:420:ILE:HG22	1.71	0.71
1:J:203:TYR:CD2	1:J:263:VAL:HG13	2.25	0.71
1:K:345:ARG:HD2	1:K:348:GLN:NE2	2.05	0.71
1:N:207:LYS:HB3	1:N:208:PRO:HD3	1.72	0.71
2:T:97:ALA:CB	2:U:1:MET:HA	2.19	0.71
1:A:362:ARG:HA	1:A:365:LEU:HD23	1.72	0.71
1:D:199:TYR:CE1	1:D:202:PRO:HA	2.25	0.71
1:D:215:LEU:HB2	1:D:323:VAL:HG22	1.72	0.71
1:N:225:LYS:HB3	1:N:231:ARG:NH2	2.04	0.71
1:N:227:ILE:HG23	1:N:231:ARG:HB2	1.69	0.71
2:R:67:PHE:HB2	2:R:86:MET:HE1	1.71	0.71
2:U:64:ILE:HG23	2:U:95:VAL:CG2	2.20	0.71
2:2:79:ASP:O	2:2:80:ASN:C	2.32	0.71
1:B:321:LYS:HB2	1:B:334:ASP:HB2	1.72	0.71
1:D:415:GLY:N	3:D:601:ADP:O2'	2.20	0.71
1:L:221:LEU:HD11	1:L:249:ILE:HG23	1.71	0.71
1:N:284:ARG:HD3	1:N:364:LYS:HE2	1.71	0.71
2:U:10:VAL:HG11	2:U:91:ILE:HD11	1.72	0.71
1:C:321:LYS:CB	1:C:334:ASP:HB3	2.20	0.71
1:E:197:ARG:HG2	1:E:279:PRO:HA	1.72	0.71
1:G:248:LEU:CD2	1:G:325:ILE:HD11	2.20	0.71
1:H:5:ASP:HB2	1:H:524:LEU:CD2	2.19	0.71
2:1:17:VAL:CG2	2:1:34:LYS:HA	2.21	0.71
1:M:206:ASN:ND2	1:M:214:GLU:O	2.23	0.71
2:2:14:ARG:NH1	2:2:84:LEU:HD21	2.05	0.71
1:C:238:GLU:HG2	2:Q:25:ILE:HG12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:305:ILE:CG2	1:I:267:MET:HE1	2.19	0.71
2:Q:15:LYS:HB3	2:Q:16:GLU:CD	2.16	0.71
1:K:23:LEU:HD23	1:K:60:ILE:HB	1.69	0.71
1:A:74:VAL:O	1:A:77:VAL:HG12	1.90	0.71
1:M:305:ILE:HG22	1:M:306:GLY:N	2.05	0.71
1:N:136:VAL:HG13	1:N:137:PRO:HD2	1.72	0.71
2:S:20:LYS:NZ	2:S:27:LEU:O	2.23	0.71
2:X:36:THR:HG23	2:X:37:ARG:HG3	1.73	0.71
2:2:78:ILE:HD12	2:2:78:ILE:N	2.03	0.71
1:E:206:ASN:OD1	1:E:207:LYS:HG2	1.91	0.71
1:F:40:LEU:HD13	1:F:59:GLU:HG3	1.71	0.71
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.73	0.71
1:K:305:ILE:HG22	1:K:306:GLY:N	2.06	0.71
1:M:200:LEU:HD22	1:M:254:VAL:HB	1.73	0.71
1:G:205:ILE:HA	1:G:213:VAL:CG2	2.12	0.71
1:I:252:GLU:HG3	1:I:285:ARG:HH11	1.53	0.71
1:I:449:ALA:HB3	1:I:450:PRO:HD3	1.71	0.71
1:K:193:MET:SD	1:K:371:LYS:HB3	2.31	0.71
1:N:420:ILE:HG22	1:N:448:GLU:HA	1.71	0.71
1:F:232:GLU:OE1	1:F:232:GLU:N	2.23	0.70
2:W:50:GLU:O	2:W:51:ASN:ND2	2.25	0.70
2:Z:46:GLY:HA2	2:Z:57:LEU:CD1	2.21	0.70
1:H:204:PHE:CD2	1:H:274:ALA:HA	2.27	0.70
1:L:230:ILE:CG2	1:L:309:LEU:HD21	2.20	0.70
2:O:36:THR:HB	2:O:67:PHE:O	1.91	0.70
2:V:57:LEU:HB2	2:V:88:GLU:OE2	1.91	0.70
2:2:12:VAL:HG22	2:2:40:VAL:HA	1.72	0.70
1:C:253:ASP:OD1	1:C:277:LYS:HE2	1.90	0.70
1:D:305:ILE:HG22	1:D:306:GLY:N	2.06	0.70
1:F:418:ALA:O	1:F:422:VAL:HG13	1.92	0.70
1:K:305:ILE:HG23	1:L:264:VAL:HG22	1.72	0.70
1:B:305:ILE:HG22	1:B:306:GLY:N	2.06	0.70
1:C:219:PHE:HE2	1:C:245:LYS:HB2	1.55	0.70
1:G:412:VAL:HG12	1:G:413:ALA:N	2.05	0.70
1:N:239:ALA:HB1	1:N:314:LEU:HD11	1.73	0.70
1:C:197:ARG:CG	1:C:277:LYS:HB3	2.15	0.70
1:F:301:ILE:HG23	1:F:307:MET:HB3	1.72	0.70
1:L:219:PHE:CA	1:L:317:LEU:HD21	2.22	0.70
2:Q:79:ASP:O	2:Q:80:ASN:ND2	2.24	0.70
1:C:305:ILE:HG22	1:C:306:GLY:N	2.06	0.70
1:F:282:GLY:HA2	1:F:285:ARG:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:LYS:CG	1:H:303:GLU:HG3	2.21	0.70
2:Q:12:VAL:HG23	2:Q:39:GLU:O	1.90	0.70
1:C:232:GLU:CG	1:C:310:GLU:HG3	2.20	0.70
1:E:219:PHE:HB3	1:E:317:LEU:HD13	1.73	0.70
1:E:230:ILE:HG21	1:E:309:LEU:HB3	1.72	0.70
1:E:307:MET:HE3	1:E:311:LYS:NZ	2.07	0.70
1:I:302:SER:CB	1:I:305:ILE:HD13	2.22	0.70
1:N:197:ARG:HG2	1:N:277:LYS:HB3	1.73	0.70
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.72	0.70
1:L:322:ARG:HB3	1:L:333:ILE:HD12	1.72	0.70
1:N:34:LYS:NZ	1:N:483:GLU:OE2	2.24	0.70
2:S:50:GLU:HG2	2:S:51:ASN:H	1.55	0.70
1:A:271:VAL:HG11	2:O:25:ILE:HD13	1.72	0.70
1:B:197:ARG:HE	1:B:277:LYS:HD3	1.55	0.70
2:Q:60:LYS:NZ	2:Q:63:ASP:HB3	2.06	0.70
2:W:17:VAL:HG23	2:W:19:THR:N	2.07	0.70
2:Y:74:LYS:NZ	2:Y:76:GLU:OE2	2.25	0.70
1:E:25:ASP:HA	1:E:28:LYS:HE2	1.74	0.70
1:F:301:ILE:HG23	1:F:307:MET:CB	2.21	0.70
2:Z:55:LYS:HE2	2:1:48:ILE:CD1	2.22	0.70
1:C:196:ASP:O	1:C:197:ARG:NH1	2.25	0.69
1:E:222:LEU:HD22	1:E:289:LEU:HD22	1.72	0.69
1:H:5:ASP:HB2	1:H:524:LEU:HD23	1.74	0.69
2:V:20:LYS:NZ	2:V:33:ALA:O	2.24	0.69
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.73	0.69
1:C:91:THR:N	4:C:602:BEF:F3	2.08	0.69
1:G:247:LEU:HB2	1:G:273:VAL:HG13	1.74	0.69
1:H:177:VAL:HG11	1:H:397:GLU:HG2	1.74	0.69
1:C:304:GLU:C	1:C:305:ILE:HD12	2.16	0.69
1:J:204:PHE:HE1	1:J:263:VAL:HA	1.58	0.69
2:O:6:LEU:HD12	2:U:93:ALA:HA	1.74	0.69
1:B:74:VAL:O	1:B:77:VAL:HG12	1.91	0.69
1:C:325:ILE:HG12	1:C:330:THR:HG23	1.73	0.69
1:J:213:VAL:O	1:J:324:VAL:HA	1.92	0.69
1:J:233:MET:SD	1:J:309:LEU:O	2.50	0.69
2:O:18:GLU:HB3	2:O:28:THR:HB	1.73	0.69
1:A:179:ASP:OD1	1:A:393:LYS:HD3	1.92	0.69
1:B:219:PHE:HB3	1:B:317:LEU:HD13	1.72	0.69
1:L:89:THR:N	4:L:602:BEF:F2	2.14	0.69
2:X:57:LEU:HD12	2:X:57:LEU:H	1.57	0.69
1:F:238:GLU:HG3	2:T:23:GLY:HA3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:PHE:HA	1:G:318:GLY:O	1.92	0.69
1:H:205:ILE:HA	1:H:213:VAL:HG12	1.74	0.69
1:H:479:ASN:ND2	1:H:493:ILE:HD11	2.08	0.69
1:J:288:MET:HE3	1:J:368:ARG:HG3	1.74	0.69
1:N:197:ARG:HH11	1:N:198:GLY:H	1.40	0.69
2:R:12:VAL:HG12	2:R:40:VAL:HG13	1.73	0.69
1:A:310:GLU:H	1:A:310:GLU:CD	2.01	0.69
1:A:355:GLU:HG3	1:A:356:ALA:H	1.57	0.69
1:G:219:PHE:HE2	1:G:245:LYS:HB2	1.57	0.69
1:I:415:GLY:N	3:I:601:ADP:O2'	2.20	0.69
1:K:74:VAL:O	1:K:77:VAL:HG13	1.93	0.69
1:L:418:ALA:O	1:L:422:VAL:HG13	1.93	0.69
1:N:262:LEU:HD11	1:N:273:VAL:HB	1.74	0.69
2:Q:20:LYS:NZ	2:Q:33:ALA:O	2.25	0.69
2:X:70:GLY:O	2:X:73:VAL:HG12	1.93	0.69
1:C:223:ALA:CB	1:C:227:ILE:HD11	2.22	0.69
1:C:232:GLU:OE1	1:C:232:GLU:N	2.22	0.69
1:F:124:VAL:HG13	1:F:504:LEU:CD1	2.22	0.69
1:H:267:MET:HE2	1:H:267:MET:HA	1.72	0.69
1:J:177:VAL:HG11	1:J:397:GLU:HG2	1.73	0.69
1:J:496:PRO:HG2	1:J:499:VAL:CG1	2.23	0.69
1:K:199:TYR:HE1	1:K:202:PRO:HA	1.57	0.69
1:L:208:PRO:O	1:L:209:GLU:CG	2.41	0.69
1:M:405:ALA:CB	1:M:498:LYS:HD3	2.22	0.69
2:Q:92:LEU:HD23	2:Q:92:LEU:H	1.54	0.69
2:U:64:ILE:HG23	2:U:95:VAL:HG23	1.74	0.69
2:1:95:VAL:HG13	2:2:3:ILE:HG22	1.74	0.69
2:1:95:VAL:HA	2:2:3:ILE:HG22	1.73	0.69
1:D:418:ALA:O	1:D:422:VAL:HG13	1.92	0.69
1:G:226:LYS:CB	1:G:253:ASP:HB2	2.23	0.69
1:H:233:MET:CE	1:H:237:LEU:HD12	2.22	0.69
1:H:350:ARG:HA	1:H:353:ILE:HD12	1.73	0.69
1:L:204:PHE:CD2	1:L:274:ALA:HA	2.28	0.69
2:R:49:LEU:HD11	2:S:50:GLU:CA	2.22	0.69
2:T:11:ILE:HD11	2:T:42:ALA:HB3	1.75	0.69
1:A:234:LEU:HA	1:A:237:LEU:HB3	1.75	0.69
1:E:513:LEU:HD11	1:F:388:GLU:HA	1.75	0.69
1:F:218:PRO:O	1:F:219:PHE:CE1	2.44	0.69
1:G:280:GLY:O	1:G:285:ARG:NE	2.22	0.69
1:I:238:GLU:HG2	2:W:27:LEU:CD1	2.23	0.69
1:K:234:LEU:HB3	1:K:235:PRO:HD3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:291:ASP:HB2	1:L:372:LEU:HD21	1.74	0.69
1:M:278:ALA:HB1	1:M:279:PRO:HD2	1.74	0.69
2:R:6:LEU:HD21	2:R:7:HIS:CG	2.25	0.69
2:T:55:LYS:HG2	2:U:48:ILE:CD1	2.22	0.69
2:X:93:ALA:CB	2:Y:5:PRO:HA	2.23	0.69
1:D:289:LEU:O	1:D:293:ALA:N	2.26	0.68
1:F:172:GLU:O	1:F:370:ALA:HB2	1.93	0.68
1:F:320:ALA:HB1	1:F:334:ASP:O	1.93	0.68
1:G:203:TYR:HB3	1:G:267:MET:HE2	1.75	0.68
1:G:358:SER:HA	1:G:362:ARG:NE	2.07	0.68
1:I:241:ALA:CB	2:W:25:ILE:HD13	2.23	0.68
1:A:236:VAL:CG2	1:A:312:ALA:HB3	2.21	0.68
1:A:254:VAL:HG12	1:A:259:LEU:HB2	1.74	0.68
1:D:226:LYS:HB3	1:D:252:GLU:HG2	1.75	0.68
1:F:238:GLU:HG3	2:T:23:GLY:CA	2.24	0.68
1:G:350:ARG:HD3	1:G:353:ILE:CD1	2.22	0.68
1:I:5:ASP:HB2	1:I:524:LEU:HD23	1.74	0.68
1:K:449:ALA:HB3	1:K:450:PRO:HD3	1.74	0.68
1:L:74:VAL:O	1:L:77:VAL:HG12	1.94	0.68
1:M:231:ARG:HH21	1:M:257:GLU:HB3	1.58	0.68
1:N:429:LEU:O	1:N:430:ARG:NH1	2.25	0.68
2:X:23:GLY:O	2:X:26:VAL:HG12	1.92	0.68
2:X:50:GLU:O	2:X:50:GLU:CD	2.36	0.68
2:1:17:VAL:HA	2:1:35:SER:H	1.57	0.68
1:A:199:TYR:CE1	1:A:202:PRO:HA	2.28	0.68
1:C:74:VAL:O	1:C:77:VAL:HG12	1.92	0.68
1:D:226:LYS:HA	1:D:252:GLU:HB3	1.75	0.68
1:D:302:SER:OG	1:D:305:ILE:HD13	1.92	0.68
1:E:74:VAL:O	1:E:77:VAL:HG12	1.93	0.68
1:H:234:LEU:CD2	2:V:22:ALA:HB1	2.23	0.68
1:K:18:ARG:HB3	1:K:18:ARG:NH1	2.07	0.68
1:K:237:LEU:HD12	1:K:238:GLU:N	2.08	0.68
1:L:245:LYS:HB3	1:L:246:PRO:CD	2.20	0.68
1:N:254:VAL:HG12	1:N:259:LEU:HG	1.75	0.68
2:T:53:GLU:CD	2:T:54:VAL:H	2.00	0.68
2:U:51:ASN:C	2:U:53:GLU:H	2.01	0.68
2:V:1:MET:O	2:V:1:MET:HG2	1.93	0.68
2:Z:64:ILE:HG23	2:Z:95:VAL:HG22	1.74	0.68
1:A:420:ILE:HD13	1:A:451:LEU:HD13	1.74	0.68
1:B:367:GLU:HG2	1:B:371:LYS:HE2	1.73	0.68
1:D:138:CYS:HB2	1:D:411:VAL:HG13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:THR:CG2	1:D:361:ASP:HB2	2.23	0.68
1:M:23:LEU:HD22	1:M:74:VAL:HG23	1.75	0.68
1:B:175:ILE:CD1	1:B:377:ALA:HB3	2.23	0.68
1:E:411:VAL:HG21	1:E:494:LEU:HD23	1.75	0.68
1:G:241:ALA:HA	1:G:271:VAL:HG11	1.75	0.68
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.75	0.68
1:D:5:ASP:HB2	1:D:524:LEU:CD2	2.23	0.68
1:G:241:ALA:HA	1:G:271:VAL:CG1	2.23	0.68
1:H:25:ASP:HA	1:H:28:LYS:HE2	1.75	0.68
1:L:149:THR:HG23	1:L:159:GLY:HA3	1.76	0.68
1:N:25:ASP:HA	1:N:28:LYS:HE2	1.76	0.68
1:D:217:SER:HA	1:D:320:ALA:O	1.94	0.68
1:M:357:THR:HG21	1:M:361:ASP:HB3	1.75	0.68
2:U:40:VAL:HG12	2:U:41:LEU:H	1.58	0.68
1:B:288:MET:HG2	1:B:368:ARG:HG3	1.74	0.68
1:D:226:LYS:CA	1:D:252:GLU:HB3	2.23	0.68
1:F:304:GLU:HB3	1:F:305:ILE:HD12	1.75	0.68
2:U:3:ILE:HD13	2:U:78:ILE:HD13	1.76	0.68
2:U:51:ASN:C	2:U:53:GLU:N	2.49	0.68
2:W:3:ILE:HD11	2:W:11:ILE:HD12	1.76	0.68
1:F:90:THR:N	3:F:601:ADP:O2B	2.26	0.68
1:F:127:ALA:CA	1:F:426:LEU:HD11	2.24	0.68
1:I:174:VAL:HG21	1:I:367:GLU:HA	1.75	0.68
1:K:263:VAL:CG1	1:K:267:MET:HE3	2.23	0.68
1:K:268:ARG:HG3	2:Y:27:LEU:CD2	2.23	0.68
1:L:254:VAL:HG12	1:L:259:LEU:HG	1.76	0.68
2:Z:46:GLY:HA2	2:Z:57:LEU:HD12	1.76	0.68
1:B:175:ILE:HD13	1:B:377:ALA:HB3	1.76	0.68
1:C:231:ARG:HH12	1:C:234:LEU:HD21	1.58	0.68
1:E:197:ARG:NH1	1:E:279:PRO:O	2.28	0.68
1:E:234:LEU:O	1:E:235:PRO:C	2.37	0.68
1:H:124:VAL:HG13	1:H:504:LEU:HD12	1.76	0.68
1:H:193:MET:SD	1:H:371:LYS:HB3	2.34	0.68
1:J:479:ASN:ND2	1:J:493:ILE:HD11	2.09	0.68
1:M:177:VAL:HG11	1:M:397:GLU:CG	2.23	0.68
1:A:291:ASP:OD1	1:A:345:ARG:NH2	2.24	0.67
1:A:308:GLU:CD	1:A:311:LYS:HB2	2.20	0.67
1:A:362:ARG:HA	1:A:365:LEU:CD2	2.24	0.67
1:B:301:ILE:HG12	1:B:307:MET:HE1	1.75	0.67
1:C:226:LYS:HG2	1:C:252:GLU:CG	2.19	0.67
1:D:74:VAL:O	1:D:77:VAL:HG12	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:291:ASP:OD1	1:H:345:ARG:NH2	2.20	0.67
3:J:601:ADP:O3B	4:J:602:BEF:F1	2.02	0.67
1:N:488:MET:SD	1:N:493:ILE:HD11	2.35	0.67
2:U:37:ARG:HG2	2:U:66:ILE:HG12	1.76	0.67
2:Y:20:LYS:HB3	2:Y:26:VAL:O	1.94	0.67
1:E:207:LYS:HB2	1:E:208:PRO:CD	2.10	0.67
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.75	0.67
1:J:151:SER:HB3	1:J:399:ALA:HA	1.76	0.67
1:K:208:PRO:HB2	1:K:212:ALA:CB	2.23	0.67
1:K:355:GLU:HG3	1:K:356:ALA:H	1.58	0.67
2:W:11:ILE:CG2	2:W:42:ALA:HB3	2.24	0.67
1:B:349:ILE:CD1	1:B:368:ARG:HD2	2.25	0.67
1:I:90:THR:N	4:I:602:BEF:F2	2.17	0.67
1:M:124:VAL:HG13	1:M:504:LEU:CD1	2.24	0.67
1:N:247:LEU:HG	1:N:249:ILE:CD1	2.23	0.67
2:V:12:VAL:HG23	2:V:39:GLU:O	1.94	0.67
2:V:49:LEU:CD1	2:W:50:GLU:HG3	2.24	0.67
2:Z:50:GLU:HG2	2:Z:50:GLU:O	1.92	0.67
2:Z:93:ALA:HA	2:1:5:PRO:O	1.95	0.67
1:F:6:VAL:CG1	1:F:521:VAL:HG22	2.19	0.67
1:H:304:GLU:C	1:H:305:ILE:HD12	2.20	0.67
1:M:305:ILE:CG2	1:M:306:GLY:H	2.08	0.67
2:X:16:GLU:HG2	2:X:19:THR:HB	1.75	0.67
2:2:17:VAL:HG23	2:2:18:GLU:HG3	1.77	0.67
1:A:234:LEU:HG	1:A:235:PRO:HD3	1.77	0.67
1:E:222:LEU:HD21	1:E:289:LEU:HB3	1.76	0.67
1:F:233:MET:HG3	1:F:234:LEU:CD2	2.14	0.67
1:L:449:ALA:HB3	1:L:450:PRO:HD3	1.77	0.67
1:M:279:PRO:HB2	1:M:288:MET:HE3	1.76	0.67
1:N:278:ALA:HB3	1:N:285:ARG:CZ	2.24	0.67
2:Q:43:VAL:HG21	2:Q:57:LEU:HD11	1.77	0.67
2:X:91:ILE:HB	2:Y:6:LEU:HD22	1.75	0.67
1:A:165:ALA:O	1:A:169:VAL:HG22	1.95	0.67
1:A:349:ILE:HD13	1:A:368:ARG:HD2	1.76	0.67
1:I:227:ILE:HG23	1:I:230:ILE:HB	1.76	0.67
1:M:418:ALA:O	1:M:422:VAL:HG13	1.95	0.67
2:U:50:GLU:HG2	2:U:50:GLU:O	1.94	0.67
1:B:357:THR:HG21	1:B:361:ASP:HB2	1.77	0.67
1:D:357:THR:HB	1:D:361:ASP:CB	2.25	0.67
1:F:254:VAL:HG12	1:F:259:LEU:HG	1.75	0.67
1:G:277:LYS:HG3	1:G:278:ALA:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:338:GLU:O	1:H:342:ILE:HD13	1.94	0.67
1:M:239:ALA:HB1	1:M:314:LEU:HD23	1.77	0.67
1:M:246:PRO:HA	1:M:272:LYS:O	1.95	0.67
2:S:12:VAL:HG13	2:S:40:VAL:H	1.60	0.67
2:X:20:LYS:HB3	2:X:28:THR:OG1	1.94	0.67
1:J:357:THR:CB	1:J:361:ASP:HB2	2.25	0.67
1:K:419:LEU:HD11	1:K:500:THR:HG23	1.77	0.67
1:L:412:VAL:HG12	1:L:413:ALA:N	2.10	0.67
1:N:147:VAL:CG2	1:N:403:THR:HG22	2.24	0.67
2:1:50:GLU:O	2:1:51:ASN:CG	2.37	0.67
1:K:5:ASP:HB2	1:K:524:LEU:HD23	1.76	0.67
1:C:219:PHE:HA	1:C:318:GLY:O	1.95	0.67
1:C:323:VAL:HG12	1:C:332:ILE:HG12	1.77	0.67
1:C:429:LEU:HG	1:C:440:ILE:HD13	1.76	0.67
1:E:124:VAL:HG13	1:E:504:LEU:CD1	2.24	0.67
1:H:234:LEU:N	1:H:235:PRO:HD2	2.10	0.67
1:L:415:GLY:N	3:L:601:ADP:O2'	2.27	0.67
1:N:218:PRO:HG3	1:N:323:VAL:CG2	2.25	0.67
1:B:411:VAL:HG21	1:B:494:LEU:HD23	1.76	0.66
1:C:135:SER:HB2	1:C:497:THR:HG21	1.78	0.66
1:I:149:THR:HG21	1:I:156:GLU:HG2	1.76	0.66
1:M:231:ARG:HD3	1:M:261:THR:HG21	1.76	0.66
1:M:513:LEU:HD22	1:N:49:ILE:HG21	1.77	0.66
1:D:234:LEU:N	1:D:235:PRO:HD2	2.10	0.66
1:F:339:GLU:O	1:F:343:GLN:HB2	1.95	0.66
1:I:367:GLU:HG2	1:I:371:LYS:HE2	1.75	0.66
1:J:264:VAL:O	1:J:268:ARG:HG2	1.95	0.66
1:K:168:LYS:HG2	1:K:189:VAL:HG11	1.77	0.66
2:O:6:LEU:HD12	2:O:6:LEU:N	2.10	0.66
1:A:216:GLU:O	1:A:245:LYS:HE2	1.96	0.66
1:F:220:ILE:HG13	1:F:296:THR:CG2	2.25	0.66
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.76	0.66
1:I:231:ARG:HD3	1:I:257:GLU:OE2	1.95	0.66
1:K:270:ILE:H	1:K:270:ILE:HD12	1.58	0.66
2:R:20:LYS:HB2	2:R:22:ALA:N	2.10	0.66
1:B:13:ARG:HD2	1:B:104:LEU:HD22	1.75	0.66
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.76	0.66
1:G:172:GLU:N	1:G:172:GLU:CD	2.53	0.66
1:G:203:TYR:HB3	1:G:267:MET:CE	2.26	0.66
1:K:146:GLN:OE1	1:K:492:GLY:HA2	1.95	0.66
1:M:443:ALA:O	1:M:447:MET:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:53:GLU:CG	2:T:54:VAL:H	2.08	0.66
1:D:449:ALA:HB3	1:D:450:PRO:HD3	1.76	0.66
1:L:208:PRO:C	1:L:209:GLU:CD	2.46	0.66
2:X:77:LYS:HD3	2:X:82:GLU:HA	1.77	0.66
2:Z:57:LEU:HD12	2:Z:57:LEU:H	1.59	0.66
1:A:291:ASP:HB3	1:A:372:LEU:HD21	1.78	0.66
1:A:388:GLU:HA	1:G:513:LEU:CD1	2.26	0.66
1:K:197:ARG:NH1	1:K:277:LYS:HD2	2.11	0.66
1:M:309:LEU:HB2	1:M:310:GLU:OE1	1.95	0.66
1:C:234:LEU:N	1:C:235:PRO:HD2	2.10	0.66
1:C:302:SER:OG	1:C:305:ILE:HD13	1.95	0.66
1:C:305:ILE:CG2	1:C:306:GLY:H	2.08	0.66
1:H:226:LYS:HG2	1:H:252:GLU:HG2	1.78	0.66
1:I:305:ILE:HG22	1:I:306:GLY:N	2.11	0.66
1:M:199:TYR:HE1	1:M:202:PRO:HA	1.59	0.66
1:B:147:VAL:HG12	1:B:494:LEU:HB2	1.76	0.66
1:G:359:ASP:O	1:G:363:GLU:HG2	1.95	0.66
1:J:254:VAL:HG12	1:J:259:LEU:HG	1.78	0.66
1:J:419:LEU:O	1:J:422:VAL:HG22	1.96	0.66
1:L:218:PRO:HB2	1:L:219:PHE:C	2.19	0.66
1:N:5:ASP:HB2	1:N:524:LEU:CD2	2.25	0.66
2:U:49:LEU:C	2:U:50:GLU:CD	2.62	0.66
1:E:208:PRO:HG2	1:E:214:GLU:HG3	1.78	0.66
1:F:203:TYR:HD2	1:F:263:VAL:HG11	1.61	0.66
1:H:236:VAL:HG21	1:H:312:ALA:HB3	1.78	0.66
1:I:200:LEU:HD13	1:I:275:ALA:O	1.95	0.66
1:J:253:ASP:OD1	1:J:277:LYS:NZ	2.23	0.66
2:Q:50:GLU:CG	2:Q:51:ASN:H	2.07	0.66
2:S:36:THR:HG23	2:S:37:ARG:HG3	1.77	0.66
2:V:49:LEU:HD22	2:V:50:GLU:H	1.59	0.66
1:A:305:ILE:HG12	1:A:306:GLY:H	1.60	0.66
1:C:517:THR:HG23	1:D:39:VAL:HG23	1.77	0.66
1:E:102:GLU:OE1	1:E:445:ARG:NH1	2.28	0.66
1:J:31:LEU:HD23	1:J:453:GLN:HB3	1.77	0.66
1:J:349:ILE:O	1:J:353:ILE:HG13	1.96	0.66
1:M:231:ARG:NH2	1:M:257:GLU:HB3	2.10	0.66
1:F:226:LYS:HA	1:F:252:GLU:HB3	1.77	0.65
1:G:195:PHE:CE1	1:G:330:THR:HB	2.30	0.65
1:G:417:VAL:HA	1:G:420:ILE:CG2	2.26	0.65
1:H:225:LYS:HG3	1:H:303:GLU:HG3	1.78	0.65
1:H:241:ALA:HB3	2:V:25:ILE:CD1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:ILE:HG22	1:J:318:GLY:CA	2.26	0.65
1:J:278:ALA:CB	1:J:285:ARG:HD2	2.25	0.65
1:M:268:ARG:HB2	1:M:269:GLY:HA2	1.78	0.65
1:C:233:MET:C	1:C:235:PRO:HD2	2.20	0.65
1:D:254:VAL:HG12	1:D:259:LEU:HG	1.77	0.65
1:F:18:ARG:HB3	1:F:18:ARG:NH1	2.12	0.65
1:H:305:ILE:CG2	1:H:306:GLY:H	2.09	0.65
1:K:230:ILE:HG22	1:K:233:MET:H	1.61	0.65
2:U:57:LEU:HD12	2:U:57:LEU:H	1.61	0.65
2:Y:15:LYS:CD	2:Y:37:ARG:HB3	2.25	0.65
1:A:202:PRO:O	1:A:205:ILE:HG12	1.96	0.65
1:A:479:ASN:ND2	1:A:493:ILE:HD11	2.11	0.65
1:B:254:VAL:HG12	1:B:259:LEU:HG	1.79	0.65
1:C:357:THR:CG2	1:C:361:ASP:HB2	2.27	0.65
1:G:209:GLU:CG	1:G:210:THR:H	2.09	0.65
1:G:222:LEU:HD23	1:G:289:LEU:HD22	1.77	0.65
1:G:240:VAL:HG11	1:G:247:LEU:CD2	2.26	0.65
1:L:204:PHE:CE2	1:L:274:ALA:HA	2.31	0.65
1:N:218:PRO:HG3	1:N:323:VAL:HG22	1.77	0.65
1:N:233:MET:O	1:N:236:VAL:N	2.28	0.65
1:B:351:GLN:CG	1:C:210:THR:HG23	2.24	0.65
1:F:219:PHE:CE2	1:F:240:VAL:HG13	2.31	0.65
1:L:496:PRO:HG2	1:L:499:VAL:CG2	2.26	0.65
1:B:40:LEU:HD13	1:B:59:GLU:HG3	1.77	0.65
1:C:345:ARG:HA	1:C:348:GLN:HG2	1.78	0.65
1:G:339:GLU:O	1:G:343:GLN:HB2	1.96	0.65
1:H:197:ARG:HG2	1:H:277:LYS:CB	2.22	0.65
1:K:254:VAL:HG12	1:K:259:LEU:HG	1.77	0.65
1:M:40:LEU:HD13	1:M:59:GLU:HG3	1.78	0.65
2:T:20:LYS:HE2	2:T:22:ALA:CB	2.14	0.65
2:W:26:VAL:O	2:W:27:LEU:HB2	1.96	0.65
1:A:276:VAL:CG1	1:A:325:ILE:HG21	2.26	0.65
1:D:358:SER:O	1:D:362:ARG:HG3	1.96	0.65
1:I:31:LEU:HD23	1:I:453:GLN:HB3	1.77	0.65
1:L:367:GLU:O	1:L:371:LYS:HG3	1.97	0.65
1:M:228:SER:O	1:M:231:ARG:HB3	1.96	0.65
1:N:301:ILE:HG12	1:N:307:MET:HE1	1.78	0.65
2:X:65:VAL:CG1	2:X:94:ILE:HG22	2.21	0.65
1:A:39:VAL:HG23	1:G:517:THR:HG23	1.79	0.65
1:A:199:TYR:HA	1:A:276:VAL:HG12	1.79	0.65
1:C:448:GLU:O	1:C:452:ARG:HG2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:ALA:O	1:D:447:MET:HG3	1.97	0.65
1:F:207:LYS:HB3	1:F:208:PRO:HD3	1.79	0.65
1:L:218:PRO:HG2	1:L:220:ILE:CD1	2.26	0.65
1:M:291:ASP:OD2	1:M:368:ARG:HD3	1.96	0.65
1:N:231:ARG:HD3	1:N:309:LEU:HB3	1.77	0.65
2:O:5:PRO:C	2:O:6:LEU:HD12	2.22	0.65
1:A:247:LEU:HG	1:A:273:VAL:CG1	2.26	0.65
1:A:252:GLU:HA	1:A:285:ARG:HH11	1.61	0.65
1:C:224:ASP:OD1	1:C:286:LYS:HD3	1.97	0.65
1:E:278:ALA:CB	1:E:285:ARG:HD2	2.26	0.65
1:F:228:SER:CB	1:F:255:GLU:HB2	2.27	0.65
1:H:232:GLU:C	1:H:234:LEU:HD12	2.22	0.65
1:K:252:GLU:HG3	1:K:285:ARG:NH1	2.10	0.65
2:R:12:VAL:HG11	2:R:40:VAL:HG22	1.79	0.65
2:Z:95:VAL:CA	2:1:3:ILE:HG22	2.23	0.65
1:A:245:LYS:CB	1:A:246:PRO:HD3	2.26	0.65
1:C:302:SER:CB	1:C:305:ILE:HD13	2.27	0.65
1:D:218:PRO:HA	1:D:246:PRO:HG2	1.77	0.65
1:G:325:ILE:HG12	1:G:330:THR:HG23	1.79	0.65
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.79	0.65
1:I:197:ARG:HH11	1:I:277:LYS:HD2	1.62	0.65
1:I:228:SER:HB3	1:I:255:GLU:CB	2.27	0.65
1:M:87:ASP:OD2	1:M:151:SER:OG	2.14	0.65
1:M:233:MET:HB3	1:M:236:VAL:CG2	2.27	0.65
2:U:16:GLU:OE1	2:U:16:GLU:N	2.30	0.65
2:W:40:VAL:HB	2:W:63:ASP:H	1.62	0.65
1:B:136:VAL:CG2	1:B:137:PRO:HD2	2.26	0.65
1:B:207:LYS:HB3	1:B:208:PRO:HD3	1.79	0.65
1:B:219:PHE:HA	1:B:318:GLY:O	1.96	0.65
1:K:305:ILE:CG2	1:K:306:GLY:H	2.10	0.65
2:T:20:LYS:CE	2:T:22:ALA:HB3	2.15	0.65
1:A:320:ALA:HA	1:A:335:GLY:HA2	1.78	0.64
1:G:355:GLU:HG3	1:G:356:ALA:H	1.62	0.64
1:J:196:ASP:O	1:J:197:ARG:HG2	1.97	0.64
1:J:420:ILE:HD11	1:J:469:VAL:HG12	1.79	0.64
1:K:219:PHE:CZ	1:K:245:LYS:HG3	2.31	0.64
1:N:420:ILE:CG2	1:N:448:GLU:HA	2.27	0.64
2:V:86:MET:HG3	2:V:91:ILE:HD11	1.77	0.64
1:A:241:ALA:CB	1:A:271:VAL:HG12	2.28	0.64
1:D:200:LEU:CD1	1:D:276:VAL:HA	2.26	0.64
1:F:288:MET:HA	1:F:291:ASP:OD2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:VAL:HG13	1:G:504:LEU:CD1	2.27	0.64
1:H:350:ARG:HD3	1:H:353:ILE:CD1	2.23	0.64
2:O:73:VAL:HG12	2:O:86:MET:HB3	1.78	0.64
2:W:64:ILE:CG2	2:W:95:VAL:HB	2.27	0.64
1:A:416:GLY:O	1:A:420:ILE:HD12	1.97	0.64
1:B:305:ILE:CG2	1:B:306:GLY:H	2.09	0.64
1:C:5:ASP:HB2	1:C:524:LEU:HD23	1.80	0.64
1:G:161:LEU:HD23	1:G:379:ILE:HD11	1.79	0.64
1:I:102:GLU:OE1	1:I:445:ARG:NH1	2.31	0.64
1:I:349:ILE:HG23	1:I:365:LEU:HD11	1.79	0.64
1:L:124:VAL:HG21	1:L:508:ALA:CB	2.27	0.64
1:L:364:LYS:O	1:L:367:GLU:HB3	1.97	0.64
2:R:3:ILE:HD11	2:R:11:ILE:CD1	2.23	0.64
2:W:8:ASP:O	2:W:57:LEU:HD11	1.97	0.64
1:J:231:ARG:CD	1:J:257:GLU:OE1	2.43	0.64
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.79	0.64
2:S:67:PHE:CA	2:S:92:LEU:HD13	2.24	0.64
1:C:217:SER:HA	1:C:320:ALA:O	1.98	0.64
1:G:230:ILE:HG22	1:G:232:GLU:HG2	1.77	0.64
1:G:240:VAL:HG11	1:G:247:LEU:HD11	1.78	0.64
1:J:301:ILE:HG12	1:J:307:MET:CE	2.28	0.64
1:K:199:TYR:CE1	1:K:202:PRO:HA	2.33	0.64
1:M:74:VAL:O	1:M:77:VAL:HG12	1.97	0.64
2:Q:78:ILE:HG13	2:Q:79:ASP:OD2	1.97	0.64
2:R:78:ILE:HG13	2:R:79:ASP:N	2.12	0.64
1:B:34:LYS:NZ	1:B:483:GLU:OE2	2.30	0.64
1:E:302:SER:O	1:E:305:ILE:HG22	1.97	0.64
1:F:23:LEU:HD23	1:F:60:ILE:HB	1.80	0.64
1:F:169:VAL:HB	1:F:375:GLY:O	1.97	0.64
1:H:177:VAL:HG11	1:H:397:GLU:CG	2.28	0.64
1:H:208:PRO:HB2	1:H:212:ALA:HB3	1.80	0.64
1:I:450:PRO:O	1:I:454:ILE:HG13	1.98	0.64
1:L:510:VAL:O	1:L:514:MET:HB2	1.97	0.64
1:N:201:SER:HB3	1:N:204:PHE:CZ	2.32	0.64
1:C:69:MET:SD	1:D:41:ASP:HB2	2.38	0.64
1:E:77:VAL:HG21	1:E:507:ALA:HA	1.80	0.64
1:F:349:ILE:HG21	1:F:369:VAL:HG22	1.80	0.64
1:G:284:ARG:HD3	1:G:364:LYS:HE2	1.79	0.64
1:I:311:LYS:HB3	1:I:311:LYS:NZ	2.12	0.64
1:J:230:ILE:HG21	1:J:309:LEU:HD13	1.80	0.64
1:L:282:GLY:HA2	1:L:285:ARG:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:64:ILE:H	2:T:64:ILE:HD12	1.63	0.64
2:2:17:VAL:HA	2:2:35:SER:HB2	1.79	0.64
1:B:77:VAL:HB	1:B:510:VAL:HG21	1.80	0.64
1:D:177:VAL:CG2	1:D:393:LYS:HG3	2.27	0.64
1:D:304:GLU:C	1:D:305:ILE:HD12	2.22	0.64
1:E:196:ASP:O	1:E:197:ARG:HG2	1.98	0.64
1:H:77:VAL:HB	1:H:510:VAL:HG21	1.79	0.64
1:K:124:VAL:HG21	1:K:508:ALA:CB	2.26	0.64
1:M:197:ARG:CD	1:M:277:LYS:HB2	2.28	0.64
1:M:455:VAL:HG13	1:M:460:GLU:HB2	1.79	0.64
2:T:92:LEU:CD2	2:U:85:ILE:HD13	2.27	0.64
1:A:147:VAL:HG12	1:A:494:LEU:CB	2.28	0.64
1:B:263:VAL:O	1:B:267:MET:HG2	1.97	0.64
1:I:291:ASP:OD1	1:I:345:ARG:NH2	2.28	0.64
1:L:320:ALA:HA	1:L:335:GLY:HA2	1.80	0.64
1:M:293:ALA:O	1:M:298:GLY:N	2.29	0.64
1:A:268:ARG:N	1:A:269:GLY:HA2	2.13	0.63
1:C:174:VAL:CG1	1:C:376:VAL:HG13	2.27	0.63
1:C:225:LYS:CG	1:C:303:GLU:HG3	2.28	0.63
1:E:136:VAL:CG2	1:E:137:PRO:HD2	2.28	0.63
1:I:417:VAL:HA	1:I:420:ILE:HG22	1.79	0.63
1:J:124:VAL:HG13	1:J:504:LEU:CD1	2.28	0.63
1:K:420:ILE:HD12	1:K:451:LEU:HD13	1.79	0.63
1:L:232:GLU:HB2	1:L:234:LEU:HD13	1.80	0.63
2:Q:40:VAL:HG11	2:Q:61:VAL:HA	1.79	0.63
1:H:406:ALA:HB1	1:H:411:VAL:HG12	1.79	0.63
1:J:449:ALA:HB3	1:J:450:PRO:HD3	1.80	0.63
1:J:496:PRO:HG2	1:J:499:VAL:HG13	1.80	0.63
1:K:221:LEU:HD13	1:K:317:LEU:CD2	2.27	0.63
1:M:225:LYS:HD3	1:M:303:GLU:OE1	1.97	0.63
2:T:7:HIS:HB2	2:T:46:GLY:O	1.98	0.63
1:E:205:ILE:HA	1:E:213:VAL:CG2	2.23	0.63
1:E:219:PHE:CB	1:E:317:LEU:HD13	2.29	0.63
1:I:397:GLU:O	1:I:401:HIS:ND1	2.30	0.63
1:J:321:LYS:HD2	1:J:334:ASP:HB2	1.78	0.63
2:R:6:LEU:HD23	2:R:7:HIS:ND1	1.97	0.63
1:A:276:VAL:HG11	1:A:325:ILE:CG2	2.27	0.63
1:B:245:LYS:HB2	1:B:246:PRO:CD	2.15	0.63
1:D:313:THR:CG2	1:D:315:GLU:HG2	2.28	0.63
3:G:601:ADP:O3B	4:G:602:BEF:F1	2.06	0.63
1:J:202:PRO:O	1:J:205:ILE:HG13	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:168:LYS:HG2	1:K:189:VAL:HG21	1.80	0.63
1:L:85:ALA:HB1	1:L:499:VAL:HG22	1.79	0.63
1:L:350:ARG:HD3	1:L:353:ILE:CD1	2.28	0.63
1:N:168:LYS:HD3	1:N:189:VAL:HG11	1.80	0.63
2:V:11:ILE:HD12	2:V:11:ILE:O	1.98	0.63
1:B:349:ILE:HD11	1:B:368:ARG:HD2	1.78	0.63
1:D:177:VAL:HG22	1:D:393:LYS:HG3	1.80	0.63
1:E:234:LEU:HD23	1:E:235:PRO:N	2.12	0.63
1:E:365:LEU:O	1:E:369:VAL:HG23	1.99	0.63
1:K:218:PRO:HA	1:K:246:PRO:HG2	1.81	0.63
1:L:299:THR:N	1:L:316:ASP:O	2.23	0.63
1:N:124:VAL:O	1:N:128:VAL:HG23	1.99	0.63
1:N:405:ALA:HB1	1:N:498:LYS:HB3	1.81	0.63
2:W:67:PHE:HB2	2:W:86:MET:HE1	1.81	0.63
2:Z:47:ARG:CD	2:Z:49:LEU:HD12	2.28	0.63
1:A:308:GLU:HG2	1:A:311:LYS:HB2	1.81	0.63
1:I:205:ILE:HG21	1:I:211:GLY:HA2	1.80	0.63
1:J:301:ILE:HA	1:J:307:MET:CE	2.29	0.63
1:L:455:VAL:CG1	1:L:460:GLU:HB2	2.29	0.63
1:M:279:PRO:HG2	1:M:285:ARG:CA	2.27	0.63
2:U:48:ILE:HG13	2:U:53:GLU:HA	1.81	0.63
1:B:128:VAL:HG12	1:B:132:LYS:HE2	1.81	0.63
1:H:234:LEU:HD12	1:H:234:LEU:H	1.64	0.63
1:I:288:MET:HG3	1:I:368:ARG:CZ	2.28	0.63
1:C:37:ASN:OD1	1:C:51:LYS:HB2	1.99	0.63
1:C:77:VAL:HG21	1:C:507:ALA:HA	1.81	0.63
1:D:357:THR:HB	1:D:361:ASP:HB2	1.81	0.63
1:H:89:THR:N	4:H:602:BEF:F3	2.22	0.63
1:I:18:ARG:NH1	1:I:18:ARG:HB3	2.14	0.63
1:A:271:VAL:O	1:A:273:VAL:HG23	1.98	0.63
1:E:226:LYS:HG2	1:E:252:GLU:OE1	1.99	0.63
1:E:230:ILE:HG23	1:E:310:GLU:OE2	1.99	0.63
1:F:209:GLU:HG3	1:F:210:THR:H	1.63	0.63
1:G:350:ARG:HH11	1:G:353:ILE:HD11	1.63	0.63
1:M:310:GLU:CD	1:M:310:GLU:N	2.57	0.63
2:O:94:ILE:HD11	2:P:4:ARG:HB2	1.81	0.63
2:U:48:ILE:HA	2:U:53:GLU:O	1.99	0.63
1:H:349:ILE:O	1:H:353:ILE:HG13	1.98	0.62
1:I:392:LYS:O	1:I:396:VAL:HG23	1.99	0.62
1:N:6:VAL:CG1	1:N:521:VAL:HG22	2.29	0.62
1:B:293:ALA:O	1:B:298:GLY:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ALA:HB3	1:C:389:MET:SD	2.39	0.62
1:D:496:PRO:HG2	1:D:499:VAL:CG1	2.27	0.62
1:K:228:SER:OG	1:K:255:GLU:OE2	2.17	0.62
1:L:247:LEU:HD13	1:L:248:LEU:N	2.14	0.62
2:Q:69:ASP:CB	2:Q:73:VAL:HG11	2.29	0.62
2:R:8:ASP:OD1	2:R:9:ARG:HG3	1.98	0.62
2:W:95:VAL:HA	2:X:3:ILE:HG22	1.80	0.62
2:Y:15:LYS:HD3	2:Y:37:ARG:HB3	1.81	0.62
2:Y:58:ASP:O	2:Y:58:ASP:OD1	2.17	0.62
1:A:496:PRO:HG2	1:A:499:VAL:CG1	2.29	0.62
1:B:322:ARG:HB3	1:B:333:ILE:HD12	1.81	0.62
1:D:237:LEU:HD21	2:R:27:LEU:HD21	1.80	0.62
3:F:601:ADP:O3B	4:F:602:BEF:F2	2.08	0.62
1:I:200:LEU:CD1	1:I:276:VAL:HA	2.30	0.62
1:I:302:SER:HB2	1:I:305:ILE:HD13	1.82	0.62
1:J:5:ASP:HB2	1:J:524:LEU:CD2	2.29	0.62
1:L:77:VAL:HB	1:L:510:VAL:HG21	1.81	0.62
2:Y:20:LYS:HE2	2:Y:22:ALA:HB3	1.82	0.62
1:C:124:VAL:HG21	1:C:508:ALA:CB	2.29	0.62
1:G:10:ASN:O	1:G:14:VAL:HG23	1.99	0.62
1:G:77:VAL:HB	1:G:510:VAL:HG21	1.79	0.62
1:G:88:GLY:N	3:G:601:ADP:O1B	2.32	0.62
1:K:448:GLU:O	1:K:452:ARG:HG2	1.99	0.62
1:A:5:ASP:HB2	1:A:524:LEU:HD21	1.82	0.62
1:B:304:GLU:O	1:B:305:ILE:HD13	2.00	0.62
1:F:215:LEU:HB2	1:F:323:VAL:CG2	2.30	0.62
1:G:345:ARG:O	1:G:349:ILE:HG13	2.00	0.62
1:I:194:GLN:NE2	1:I:329:THR:HG21	2.14	0.62
1:I:280:GLY:O	1:I:285:ARG:NE	2.24	0.62
1:L:433:ASN:HD21	1:L:435:ASP:HB2	1.64	0.62
2:O:53:GLU:HG3	2:O:54:VAL:H	1.62	0.62
1:A:418:ALA:O	1:A:422:VAL:HG13	2.00	0.62
1:D:175:ILE:HA	1:D:377:ALA:O	2.00	0.62
1:E:285:ARG:O	1:E:289:LEU:HG	1.99	0.62
1:F:270:ILE:HD13	2:T:26:VAL:HA	1.82	0.62
1:L:6:VAL:CG1	1:L:521:VAL:HG22	2.25	0.62
1:N:443:ALA:O	1:N:447:MET:HG3	1.99	0.62
1:A:245:LYS:CB	1:A:246:PRO:CD	2.67	0.62
1:D:177:VAL:HG11	1:D:397:GLU:HG2	1.81	0.62
1:E:302:SER:HB2	1:E:305:ILE:CG2	2.30	0.62
1:E:419:LEU:HD11	1:E:500:THR:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:GLU:HG2	1:G:371:LYS:HE2	1.80	0.62
1:H:276:VAL:HG11	1:H:325:ILE:HD13	1.82	0.62
1:M:409:GLU:OE2	1:M:501:ARG:NH2	2.32	0.62
2:T:67:PHE:HB2	2:T:86:MET:HE1	1.80	0.62
1:A:365:LEU:O	1:A:369:VAL:HG23	2.00	0.62
1:F:31:LEU:HD23	1:F:453:GLN:HB3	1.82	0.62
1:F:443:ALA:O	1:F:447:MET:HG3	2.00	0.62
1:I:69:MET:SD	1:J:41:ASP:HB2	2.40	0.62
1:K:62:LEU:HD23	1:K:67:GLU:HB3	1.81	0.62
1:K:280:GLY:O	1:K:285:ARG:HB3	1.99	0.62
1:B:198:GLY:O	1:B:276:VAL:HG13	1.99	0.62
1:C:231:ARG:NH1	1:C:234:LEU:HD21	2.14	0.62
1:E:136:VAL:HG22	1:E:137:PRO:HD2	1.82	0.62
1:E:225:LYS:HG2	1:E:226:LYS:N	2.15	0.62
1:E:291:ASP:OD2	1:E:368:ARG:HD3	2.00	0.62
1:F:513:LEU:HD11	1:G:388:GLU:HA	1.80	0.62
1:J:89:THR:N	4:J:602:BEF:F1	2.19	0.62
1:E:222:LEU:HD22	1:E:289:LEU:HD13	1.81	0.62
1:H:232:GLU:HG3	1:H:233:MET:N	2.14	0.62
1:I:224:ASP:OD1	1:I:286:LYS:HE3	1.99	0.62
2:S:14:ARG:HG2	2:S:35:SER:HB3	1.80	0.62
1:B:429:LEU:HG	1:B:440:ILE:HD13	1.81	0.61
1:C:142:LYS:O	1:C:146:GLN:HG3	2.00	0.61
1:D:479:ASN:ND2	1:D:493:ILE:HD11	2.15	0.61
1:E:247:LEU:HB2	1:E:273:VAL:HG13	1.81	0.61
1:G:231:ARG:HG2	1:G:257:GLU:OE1	2.00	0.61
1:H:234:LEU:HD23	2:V:22:ALA:HB1	1.82	0.61
1:I:363:GLU:OE1	1:I:364:LYS:HG2	2.00	0.61
1:K:296:THR:OG1	1:K:318:GLY:HA3	2.00	0.61
1:K:381:VAL:CG2	1:K:396:VAL:HG21	2.30	0.61
1:M:233:MET:HB2	1:M:237:LEU:CD2	2.30	0.61
1:M:302:SER:CB	1:M:305:ILE:HD13	2.30	0.61
1:N:222:LEU:HD22	1:N:293:ALA:HB2	1.82	0.61
2:T:55:LYS:HD2	2:T:56:PRO:HD2	1.80	0.61
2:W:70:GLY:O	2:W:73:VAL:HG12	2.00	0.61
1:A:388:GLU:HA	1:G:513:LEU:HD11	1.81	0.61
1:B:142:LYS:O	1:B:146:GLN:HG3	2.00	0.61
1:D:142:LYS:O	1:D:146:GLN:HG3	1.99	0.61
1:D:241:ALA:HB2	1:D:271:VAL:HG11	1.83	0.61
1:D:263:VAL:CG1	1:D:267:MET:HE3	2.30	0.61
1:E:234:LEU:O	1:E:237:LEU:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:223:ALA:HA	1:H:301:ILE:HB	1.81	0.61
1:I:225:LYS:HG3	1:I:226:LYS:H	1.65	0.61
1:K:228:SER:CB	1:K:255:GLU:HB2	2.30	0.61
1:N:346:VAL:HG22	1:N:372:LEU:CD1	2.31	0.61
2:T:94:ILE:HD11	2:U:4:ARG:HD2	1.81	0.61
2:V:74:LYS:NZ	2:2:68:ASN:HB3	2.15	0.61
2:1:66:ILE:HG21	2:2:76:GLU:HG3	1.82	0.61
1:A:193:MET:HB3	1:A:332:ILE:HB	1.82	0.61
1:B:357:THR:CG2	1:B:361:ASP:HB2	2.30	0.61
1:C:48:THR:HG22	1:C:390:LYS:NZ	2.14	0.61
1:E:364:LYS:HD2	1:E:367:GLU:HB3	1.82	0.61
1:G:74:VAL:O	1:G:77:VAL:HG12	1.99	0.61
1:G:364:LYS:O	1:G:367:GLU:HB3	2.01	0.61
1:N:381:VAL:CG2	1:N:396:VAL:HG21	2.30	0.61
2:Q:3:ILE:HD11	2:Q:78:ILE:HD13	1.83	0.61
2:U:12:VAL:HG23	2:U:40:VAL:HA	1.80	0.61
1:B:443:ALA:O	1:B:447:MET:HG3	1.99	0.61
1:C:248:LEU:HD23	1:C:249:ILE:N	2.16	0.61
1:J:215:LEU:HB2	1:J:323:VAL:HG22	1.83	0.61
2:P:5:PRO:HD3	2:P:11:ILE:HD12	1.82	0.61
2:W:49:LEU:HB2	2:W:52:GLY:CA	2.29	0.61
1:C:218:PRO:HA	1:C:246:PRO:O	1.99	0.61
1:E:172:GLU:HB3	1:E:366:GLN:OE1	2.01	0.61
1:F:225:LYS:HG2	1:F:309:LEU:CD2	2.26	0.61
1:I:280:GLY:H	1:I:285:ARG:HB3	1.65	0.61
1:J:218:PRO:HD2	1:J:320:ALA:O	2.00	0.61
1:K:518:GLU:CB	1:L:29:VAL:HG11	2.28	0.61
1:M:34:LYS:HD2	1:M:458:CYS:SG	2.40	0.61
1:M:304:GLU:C	1:M:305:ILE:HD12	2.26	0.61
2:O:49:LEU:HD13	2:O:50:GLU:H	1.63	0.61
2:O:97:ALA:HB2	2:P:1:MET:N	2.15	0.61
1:B:234:LEU:N	1:B:235:PRO:HD2	2.15	0.61
1:E:165:ALA:O	1:E:169:VAL:HG22	2.01	0.61
1:H:48:THR:HG22	1:H:390:LYS:NZ	2.15	0.61
1:H:358:SER:HA	1:H:362:ARG:CZ	2.30	0.61
1:N:252:GLU:HA	1:N:285:ARG:NH1	2.15	0.61
1:N:307:MET:HG2	1:N:311:LYS:HZ2	1.65	0.61
1:A:195:PHE:O	1:A:329:THR:HG23	2.01	0.61
1:B:475:ASN:O	1:B:488:MET:HG2	2.00	0.61
1:C:345:ARG:O	1:C:349:ILE:HG13	2.00	0.61
1:D:218:PRO:HD2	1:D:320:ALA:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:THR:HG23	1:E:39:VAL:HG23	1.83	0.61
1:E:225:LYS:NZ	1:E:230:ILE:HD11	2.16	0.61
1:F:80:LYS:HD2	1:F:506:TYR:CZ	2.36	0.61
1:H:227:ILE:HA	1:H:230:ILE:CG2	2.30	0.61
1:I:20:VAL:HG13	1:I:74:VAL:HG11	1.82	0.61
1:I:225:LYS:HD2	1:I:252:GLU:OE2	2.01	0.61
1:I:517:THR:HG23	1:J:39:VAL:HG23	1.81	0.61
1:J:416:GLY:O	1:J:420:ILE:HG23	2.00	0.61
1:M:354:GLU:N	1:M:354:GLU:OE2	2.33	0.61
2:Y:40:VAL:HG13	2:Y:62:GLY:N	2.12	0.61
1:D:381:VAL:HG11	1:D:392:LYS:HB3	1.82	0.61
1:F:175:ILE:HA	1:F:377:ALA:O	2.00	0.61
1:H:218:PRO:HD2	1:H:320:ALA:O	2.01	0.61
1:H:258:ALA:O	1:H:262:LEU:HB2	2.00	0.61
1:I:227:ILE:HA	1:I:230:ILE:HD13	1.83	0.61
1:K:231:ARG:HD2	1:K:261:THR:HG21	1.82	0.61
1:L:443:ALA:O	1:L:447:MET:HG3	2.00	0.61
1:N:325:ILE:CG1	1:N:330:THR:HG23	2.29	0.61
2:R:12:VAL:CG1	2:R:40:VAL:HG22	2.30	0.61
2:V:57:LEU:HD12	2:V:59:VAL:HG13	1.83	0.61
2:Y:86:MET:HE3	2:Y:90:ASP:HB2	1.82	0.61
2:1:58:ASP:O	2:1:58:ASP:OD1	2.18	0.61
1:G:215:LEU:HB3	1:G:246:PRO:HB2	1.83	0.61
1:H:143:ALA:O	1:H:147:VAL:HG13	2.00	0.61
1:J:207:LYS:HB3	1:J:208:PRO:HD3	1.83	0.61
1:K:92:ALA:HB2	1:K:503:ALA:HB1	1.82	0.61
2:T:49:LEU:HD23	2:T:50:GLU:HG3	1.83	0.61
1:B:278:ALA:HB3	1:B:285:ARG:HD2	1.80	0.61
1:G:234:LEU:H	1:G:234:LEU:HD12	1.64	0.61
1:H:136:VAL:HG23	1:H:137:PRO:HD2	1.81	0.61
1:J:350:ARG:HD3	1:J:353:ILE:CD1	2.31	0.61
1:L:131:LEU:HD23	1:L:422:VAL:HG11	1.83	0.61
1:L:218:PRO:CA	1:L:219:PHE:HB2	2.31	0.61
1:L:280:GLY:H	1:L:285:ARG:HB3	1.66	0.61
1:M:13:ARG:HD2	1:M:104:LEU:HD22	1.83	0.61
2:Y:7:HIS:HD2	2:Y:7:HIS:O	1.84	0.61
1:A:40:LEU:HD21	1:A:56:VAL:HG22	1.83	0.60
1:I:238:GLU:HG2	2:W:27:LEU:HD11	1.82	0.60
1:J:225:LYS:HG2	1:J:226:LYS:N	2.16	0.60
1:L:240:VAL:HG11	1:L:247:LEU:HB2	1.81	0.60
1:M:208:PRO:HG3	1:M:214:GLU:CD	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:11:ILE:HG23	2:R:42:ALA:H	1.64	0.60
2:Y:20:LYS:HB2	2:Y:28:THR:HG23	1.83	0.60
1:B:222:LEU:CD2	1:B:300:VAL:HG22	2.24	0.60
1:E:405:ALA:HB1	1:E:498:LYS:HB3	1.82	0.60
1:J:411:VAL:HG21	1:J:494:LEU:HD23	1.81	0.60
1:K:237:LEU:HD12	1:K:237:LEU:C	2.26	0.60
1:K:293:ALA:O	1:K:298:GLY:N	2.34	0.60
2:S:73:VAL:HA	2:S:85:ILE:O	2.01	0.60
1:D:237:LEU:CD2	2:R:27:LEU:HD21	2.31	0.60
1:D:360:TYR:HA	1:D:363:GLU:CG	2.17	0.60
1:G:134:LEU:HD11	1:G:425:LYS:NZ	2.16	0.60
1:G:418:ALA:O	1:G:422:VAL:HG13	2.01	0.60
1:H:313:THR:CG2	1:H:315:GLU:HG3	2.32	0.60
1:J:204:PHE:CD2	1:J:274:ALA:HA	2.36	0.60
1:B:448:GLU:O	1:B:452:ARG:HG2	2.01	0.60
1:E:10:ASN:O	1:E:14:VAL:HG23	2.01	0.60
1:F:200:LEU:HD22	1:F:254:VAL:HB	1.83	0.60
1:H:307:MET:HG2	1:H:311:LYS:NZ	2.17	0.60
1:L:205:ILE:CD1	1:L:211:GLY:HA2	2.30	0.60
2:R:25:ILE:HD12	2:R:25:ILE:O	2.01	0.60
2:R:25:ILE:HG22	2:R:26:VAL:HG22	1.83	0.60
1:A:233:MET:C	1:A:235:PRO:HD2	2.27	0.60
1:B:321:LYS:CB	1:B:334:ASP:HB2	2.31	0.60
1:C:183:LEU:HA	1:C:382:GLY:O	2.00	0.60
1:E:314:LEU:HD12	1:E:315:GLU:N	2.17	0.60
1:G:230:ILE:HG21	1:G:309:LEU:CD1	2.31	0.60
1:J:363:GLU:HG3	1:J:364:LYS:H	1.65	0.60
1:K:33:PRO:HA	1:K:153:ASN:OD1	2.01	0.60
1:L:513:LEU:HD22	1:M:49:ILE:HG21	1.83	0.60
1:N:247:LEU:CG	1:N:249:ILE:HD11	2.28	0.60
2:2:49:LEU:C	2:2:52:GLY:H	2.09	0.60
1:A:18:ARG:NH1	1:A:18:ARG:HB3	2.17	0.60
1:A:308:GLU:CG	1:A:311:LYS:HB2	2.31	0.60
1:E:177:VAL:HG11	1:E:397:GLU:CG	2.31	0.60
1:F:361:ASP:O	1:F:365:LEU:HB2	2.01	0.60
1:G:77:VAL:CG2	1:G:507:ALA:HA	2.29	0.60
1:J:157:THR:O	1:J:161:LEU:HD13	2.01	0.60
1:L:230:ILE:HG21	1:L:309:LEU:CD2	2.27	0.60
2:O:97:ALA:HB2	2:P:1:MET:HB2	1.82	0.60
2:U:40:VAL:HG12	2:U:41:LEU:N	2.16	0.60
2:Y:14:ARG:HD2	2:Y:84:LEU:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:16:GLU:OE1	2:Y:16:GLU:N	2.28	0.60
1:B:305:ILE:HD11	1:C:203:TYR:HE2	1.66	0.60
1:C:5:ASP:HB2	1:C:524:LEU:CD2	2.32	0.60
1:C:40:LEU:HD13	1:C:59:GLU:HG3	1.82	0.60
1:C:200:LEU:HB3	1:C:259:LEU:HD11	1.83	0.60
1:C:245:LYS:HE2	1:C:246:PRO:HD2	1.83	0.60
1:D:18:ARG:NH1	1:D:18:ARG:HB3	2.17	0.60
1:G:124:VAL:HG21	1:G:508:ALA:CB	2.32	0.60
1:H:199:TYR:CE1	1:H:202:PRO:HA	2.37	0.60
1:I:207:LYS:HB3	1:I:208:PRO:HD3	1.84	0.60
1:K:168:LYS:CG	1:K:189:VAL:HG11	2.32	0.60
2:S:12:VAL:HG13	2:S:40:VAL:CA	2.32	0.60
2:U:14:ARG:CZ	2:U:34:LYS:HD3	2.31	0.60
1:B:218:PRO:HA	1:B:246:PRO:O	2.02	0.60
1:C:314:LEU:HD12	1:C:315:GLU:N	2.17	0.60
1:D:5:ASP:HB2	1:D:524:LEU:HD23	1.83	0.60
1:D:305:ILE:CG2	1:D:306:GLY:H	2.12	0.60
1:E:361:ASP:OD1	1:E:362:ARG:N	2.35	0.60
1:H:345:ARG:O	1:H:348:GLN:HG3	2.00	0.60
1:J:443:ALA:O	1:J:447:MET:HG3	2.01	0.60
1:N:346:VAL:HG12	1:N:350:ARG:HH12	1.66	0.60
2:O:96:GLU:O	2:P:1:MET:CB	2.49	0.60
2:V:57:LEU:C	2:V:58:ASP:CG	2.70	0.60
2:Z:15:LYS:HB2	2:Z:37:ARG:O	2.02	0.60
2:2:69:ASP:OD1	2:2:69:ASP:N	2.34	0.60
1:A:455:VAL:HG13	1:A:460:GLU:HB2	1.83	0.60
1:B:168:LYS:HD3	1:B:189:VAL:HG21	1.84	0.60
1:G:236:VAL:HG22	1:G:312:ALA:HB3	1.82	0.60
1:N:228:SER:HA	1:N:258:ALA:CB	2.31	0.60
1:N:236:VAL:HG22	1:N:312:ALA:CB	2.32	0.60
2:Z:10:VAL:HG23	2:Z:42:ALA:O	2.02	0.60
1:C:18:ARG:HB3	1:C:18:ARG:NH1	2.17	0.60
1:D:77:VAL:HG21	1:D:507:ALA:HA	1.84	0.60
1:F:355:GLU:HG3	1:F:356:ALA:H	1.65	0.60
1:G:165:ALA:O	1:G:169:VAL:HG22	2.01	0.60
1:J:164:GLU:O	1:J:168:LYS:HG2	2.01	0.60
1:J:174:VAL:HG13	1:J:376:VAL:HG13	1.84	0.60
1:J:247:LEU:HD13	1:J:248:LEU:N	2.17	0.60
1:J:405:ALA:HB1	1:J:498:LYS:HB3	1.83	0.60
1:N:231:ARG:C	1:N:232:GLU:HG2	2.26	0.60
2:Q:25:ILE:HG13	2:Q:26:VAL:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:77:LYS:NZ	2:Q:80:ASN:HA	2.17	0.60
2:Z:17:VAL:HG13	2:Z:18:GLU:CD	2.27	0.60
2:1:95:VAL:HG22	2:2:3:ILE:CG2	2.30	0.60
1:D:198:GLY:O	1:D:276:VAL:HG23	2.02	0.59
1:H:69:MET:SD	1:I:41:ASP:HB2	2.42	0.59
1:I:205:ILE:HA	1:I:213:VAL:CG2	2.28	0.59
1:J:40:LEU:HD13	1:J:59:GLU:HG3	1.82	0.59
1:J:77:VAL:HG21	1:J:507:ALA:HA	1.84	0.59
1:L:208:PRO:CA	1:L:209:GLU:OE1	2.50	0.59
1:L:225:LYS:C	1:L:252:GLU:HB3	2.27	0.59
2:T:36:THR:C	2:T:37:ARG:HD2	2.27	0.59
2:Y:5:PRO:HD3	2:Y:42:ALA:CB	2.32	0.59
1:C:199:TYR:CE1	1:C:202:PRO:HA	2.37	0.59
1:E:205:ILE:CD1	1:E:211:GLY:HA2	2.28	0.59
1:E:305:ILE:HG12	1:E:306:GLY:H	1.67	0.59
1:G:171:LYS:HB2	1:G:172:GLU:OE1	2.02	0.59
1:G:219:PHE:CZ	1:G:245:LYS:HD2	2.37	0.59
1:G:220:ILE:C	1:G:221:LEU:HD12	2.27	0.59
1:G:291:ASP:OD1	1:G:292:ILE:N	2.35	0.59
1:I:57:ALA:O	1:I:75:LYS:HE2	2.03	0.59
1:I:124:VAL:HG22	1:I:504:LEU:HD11	1.84	0.59
1:M:302:SER:OG	1:M:305:ILE:HB	2.02	0.59
1:N:349:ILE:O	1:N:353:ILE:HG13	2.02	0.59
2:W:48:ILE:HD13	2:W:54:VAL:HG12	1.84	0.59
2:Y:11:ILE:CG1	2:Y:42:ALA:HB3	2.32	0.59
1:B:42:LYS:HE2	1:B:48:THR:CG2	2.32	0.59
1:F:27:VAL:O	1:F:30:THR:HG22	2.02	0.59
1:F:127:ALA:HA	1:F:426:LEU:HD11	1.83	0.59
1:F:284:ARG:CD	1:F:364:LYS:HE2	2.32	0.59
1:J:381:VAL:HG22	1:J:396:VAL:HG21	1.85	0.59
1:L:131:LEU:CD2	1:L:422:VAL:HG11	2.32	0.59
1:M:355:GLU:HG2	1:M:356:ALA:H	1.67	0.59
2:W:10:VAL:CG2	2:W:91:ILE:HD11	2.33	0.59
1:B:180:GLY:HA3	1:B:382:GLY:HA2	1.83	0.59
1:E:450:PRO:O	1:E:454:ILE:HG13	2.03	0.59
1:F:177:VAL:HG11	1:F:397:GLU:CG	2.32	0.59
1:H:226:LYS:HE2	1:H:252:GLU:HG2	1.84	0.59
1:J:303:GLU:OE2	1:J:309:LEU:HD11	2.03	0.59
1:K:6:VAL:CG1	1:K:521:VAL:HG22	2.20	0.59
1:L:219:PHE:HA	1:L:317:LEU:HD11	1.83	0.59
1:N:368:ARG:O	1:N:372:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:77:LYS:HZ1	2:Q:80:ASN:HA	1.65	0.59
1:A:236:VAL:HG22	1:A:312:ALA:O	2.01	0.59
1:B:351:GLN:HG2	1:C:210:THR:CG2	2.29	0.59
1:E:236:VAL:CG2	1:E:312:ALA:HB3	2.32	0.59
1:M:239:ALA:HB1	1:M:314:LEU:HB3	1.83	0.59
1:N:143:ALA:O	1:N:147:VAL:HG13	2.03	0.59
2:R:8:ASP:C	2:R:57:LEU:HD11	2.27	0.59
2:X:20:LYS:CB	2:X:28:THR:OG1	2.50	0.59
2:Y:10:VAL:HG13	2:Y:42:ALA:O	2.02	0.59
1:C:32:GLY:N	3:C:601:ADP:O2A	2.35	0.59
1:E:266:THR:HG22	1:E:273:VAL:H	1.67	0.59
1:K:263:VAL:HG12	1:K:267:MET:HE3	1.83	0.59
1:K:304:GLU:C	1:K:305:ILE:HD12	2.27	0.59
1:N:288:MET:HG2	1:N:368:ARG:CD	2.32	0.59
2:U:50:GLU:C	2:U:52:GLY:H	2.11	0.59
2:Y:10:VAL:HG22	2:Y:43:VAL:HA	1.83	0.59
2:Y:12:VAL:HG12	2:Y:40:VAL:CA	2.20	0.59
2:Z:85:ILE:HD12	2:Z:85:ILE:O	2.02	0.59
1:A:216:GLU:O	1:A:245:LYS:CE	2.51	0.59
1:D:325:ILE:HG13	1:D:330:THR:HG23	1.85	0.59
1:G:305:ILE:HG22	1:G:306:GLY:N	2.18	0.59
1:H:34:LYS:HD2	1:H:458:CYS:SG	2.42	0.59
1:K:5:ASP:N	1:K:522:THR:O	2.36	0.59
1:K:124:VAL:HG13	1:K:504:LEU:CD1	2.32	0.59
1:L:88:GLY:N	3:L:601:ADP:O1B	2.33	0.59
1:M:517:THR:HG23	1:N:39:VAL:HG23	1.85	0.59
1:N:346:VAL:HG22	1:N:372:LEU:HD12	1.84	0.59
2:P:17:VAL:HG12	2:P:35:SER:CB	2.31	0.59
2:R:51:ASN:OD1	2:R:52:GLY:N	2.36	0.59
2:V:15:LYS:HB3	2:V:16:GLU:CD	2.27	0.59
2:X:50:GLU:O	2:X:50:GLU:CG	2.46	0.59
2:Y:11:ILE:HG22	2:Y:85:ILE:CB	2.31	0.59
2:1:78:ILE:HG13	2:1:78:ILE:O	2.01	0.59
1:H:124:VAL:HG13	1:H:504:LEU:CD1	2.32	0.59
1:I:258:ALA:HA	1:I:261:THR:HG22	1.84	0.59
1:J:224:ASP:OD2	1:J:302:SER:HB3	2.02	0.59
2:R:19:THR:CG2	2:R:33:ALA:HB1	2.30	0.59
2:T:12:VAL:HG12	2:T:40:VAL:CG2	2.25	0.59
2:W:20:LYS:HB3	2:W:22:ALA:N	2.17	0.59
1:C:232:GLU:H	1:C:232:GLU:CD	2.09	0.59
1:G:455:VAL:CG1	1:G:460:GLU:HB2	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:SER:HA	1:H:320:ALA:O	2.02	0.59
1:H:418:ALA:O	1:H:422:VAL:HG13	2.03	0.59
1:I:124:VAL:HG13	1:I:504:LEU:HD12	1.84	0.59
1:N:199:TYR:HE2	1:N:326:ASN:HA	1.68	0.59
2:P:1:MET:O	2:P:1:MET:HG2	2.02	0.59
1:A:182:GLY:C	1:A:184:GLN:H	2.11	0.59
1:B:236:VAL:CG2	1:B:312:ALA:HB3	2.33	0.59
1:D:114:MET:HE2	1:E:153:ASN:ND2	2.18	0.59
1:D:291:ASP:HB3	1:D:372:LEU:HD21	1.84	0.59
1:F:311:LYS:NZ	1:F:313:THR:OG1	2.35	0.59
1:N:418:ALA:O	1:N:422:VAL:HG13	2.03	0.59
1:A:320:ALA:HB1	1:A:334:ASP:O	2.02	0.58
1:B:222:LEU:HD23	1:B:289:LEU:HB3	1.84	0.58
1:C:276:VAL:HG21	1:C:330:THR:OG1	2.03	0.58
1:C:419:LEU:HD21	1:C:500:THR:HG23	1.85	0.58
1:F:205:ILE:HA	1:F:213:VAL:CG2	2.31	0.58
1:I:5:ASP:HB2	1:I:524:LEU:CD2	2.32	0.58
1:M:142:LYS:HE2	1:M:146:GLN:HE22	1.68	0.58
1:N:288:MET:CG	1:N:368:ARG:HD3	2.29	0.58
1:N:449:ALA:HB3	1:N:450:PRO:HD3	1.83	0.58
2:V:40:VAL:CG1	2:V:62:GLY:H	2.16	0.58
2:X:92:LEU:HB3	2:Y:85:ILE:CD1	2.31	0.58
1:A:358:SER:O	1:A:362:ARG:HB2	2.02	0.58
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.85	0.58
1:C:219:PHE:HB3	1:C:317:LEU:HB3	1.84	0.58
1:C:350:ARG:HA	1:C:353:ILE:HD12	1.86	0.58
1:I:10:ASN:O	1:I:14:VAL:HG23	2.02	0.58
1:I:285:ARG:HG3	1:I:286:LYS:N	2.18	0.58
2:O:11:ILE:HG12	2:O:85:ILE:HG12	1.85	0.58
2:W:1:MET:CE	2:W:79:ASP:HB3	2.28	0.58
1:A:250:ILE:O	1:A:250:ILE:HG22	2.03	0.58
1:B:205:ILE:HA	1:B:213:VAL:HG22	1.85	0.58
1:B:218:PRO:HG3	1:B:323:VAL:CG1	2.34	0.58
1:E:225:LYS:HG2	1:E:226:LYS:H	1.68	0.58
1:F:351:GLN:HG2	1:G:210:THR:HA	1.85	0.58
1:H:257:GLU:O	1:H:261:THR:HG22	2.03	0.58
1:I:236:VAL:HG21	1:I:312:ALA:HB3	1.83	0.58
1:J:305:ILE:HG12	1:J:306:GLY:H	1.67	0.58
1:K:339:GLU:O	1:K:343:GLN:HB2	2.04	0.58
2:V:57:LEU:CD1	2:V:59:VAL:HG13	2.33	0.58
1:A:134:LEU:HD23	1:A:134:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:GLU:N	1:A:304:GLU:OE1	2.36	0.58
1:A:429:LEU:HG	1:A:440:ILE:HD13	1.85	0.58
1:B:231:ARG:NH1	2:P:31:ALA:HB2	2.18	0.58
1:E:359:ASP:OD1	1:E:362:ARG:NH2	2.36	0.58
1:G:510:VAL:O	1:G:514:MET:HB2	2.03	0.58
1:H:162:ILE:HG21	1:H:403:THR:HG21	1.86	0.58
1:H:293:ALA:O	1:H:298:GLY:N	2.35	0.58
1:L:291:ASP:OD1	1:L:292:ILE:HG13	2.04	0.58
2:O:46:GLY:HA2	2:O:57:LEU:HD22	1.86	0.58
2:T:48:ILE:HA	2:T:53:GLU:O	2.02	0.58
2:T:67:PHE:CB	2:T:86:MET:HE1	2.32	0.58
1:A:306:GLY:HA3	1:B:264:VAL:CG2	2.31	0.58
1:B:172:GLU:OE1	1:B:172:GLU:N	2.36	0.58
1:B:270:ILE:HG23	1:B:271:VAL:H	1.66	0.58
1:C:215:LEU:HD11	1:C:274:ALA:HB3	1.84	0.58
1:D:193:MET:HE2	1:D:292:ILE:HG13	1.86	0.58
1:D:280:GLY:O	1:D:285:ARG:HB2	2.02	0.58
1:D:349:ILE:HA	1:D:352:GLN:CG	2.33	0.58
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.85	0.58
1:F:225:LYS:HB2	1:F:303:GLU:CD	2.29	0.58
1:G:205:ILE:CA	1:G:213:VAL:HG22	2.14	0.58
1:J:285:ARG:O	1:J:289:LEU:HG	2.04	0.58
1:L:124:VAL:HG21	1:L:508:ALA:HB1	1.85	0.58
1:M:409:GLU:CD	1:M:501:ARG:HH21	2.10	0.58
1:N:201:SER:HB3	1:N:204:PHE:CE2	2.38	0.58
2:Q:57:LEU:HD13	2:Q:59:VAL:HG22	1.84	0.58
2:R:36:THR:HG23	2:R:37:ARG:CG	2.26	0.58
2:S:23:GLY:O	2:S:26:VAL:HG12	2.04	0.58
1:B:234:LEU:HD23	1:B:235:PRO:HD3	1.84	0.58
1:F:232:GLU:O	1:F:235:PRO:HD2	2.04	0.58
1:G:248:LEU:HD23	1:G:325:ILE:HD11	1.85	0.58
1:G:412:VAL:CG1	1:G:413:ALA:N	2.66	0.58
1:J:513:LEU:HD11	1:K:388:GLU:HA	1.86	0.58
1:K:238:GLU:HG3	2:Y:23:GLY:HA3	1.85	0.58
1:N:352:GLN:CB	1:N:365:LEU:HD11	2.33	0.58
1:N:496:PRO:HG2	1:N:499:VAL:CG1	2.34	0.58
2:S:55:LYS:HD2	2:S:56:PRO:HD2	1.84	0.58
2:U:43:VAL:HG23	2:U:57:LEU:HD22	1.84	0.58
2:U:51:ASN:O	2:U:52:GLY:C	2.46	0.58
2:X:93:ALA:HB2	2:Y:5:PRO:HA	1.86	0.58
1:H:220:ILE:O	1:H:317:LEU:HD22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:GLU:OE1	1:H:285:ARG:NH2	2.36	0.58
1:I:322:ARG:HG2	1:I:323:VAL:N	2.19	0.58
1:L:225:LYS:HB2	1:L:303:GLU:CD	2.28	0.58
2:Q:60:LYS:HZ2	2:Q:63:ASP:HB3	1.69	0.58
2:V:50:GLU:CG	2:W:50:GLU:HB3	2.29	0.58
2:2:64:ILE:HG23	2:2:95:VAL:HB	1.86	0.58
1:A:199:TYR:CZ	1:A:205:ILE:HD11	2.39	0.58
1:A:517:THR:HG23	1:B:39:VAL:HG23	1.85	0.58
1:E:278:ALA:HB3	1:E:285:ARG:HD2	1.86	0.58
1:F:322:ARG:HG2	1:F:323:VAL:N	2.19	0.58
1:I:357:THR:HB	1:I:361:ASP:HB2	1.85	0.58
1:I:417:VAL:HA	1:I:420:ILE:CG2	2.33	0.58
1:L:392:LYS:HD2	1:L:395:ARG:HH21	1.69	0.58
1:M:169:VAL:HG11	1:M:377:ALA:HB2	1.86	0.58
1:M:233:MET:HE3	1:M:237:LEU:CD2	2.29	0.58
2:Q:94:ILE:HD11	2:R:4:ARG:NH2	2.19	0.58
1:B:228:SER:CB	1:B:255:GLU:HG2	2.30	0.58
1:B:231:ARG:NH2	2:P:31:ALA:HB2	2.18	0.58
1:B:496:PRO:HG2	1:B:499:VAL:CG1	2.33	0.58
1:E:342:ILE:O	1:E:346:VAL:HG23	2.03	0.58
1:F:226:LYS:HB3	1:F:252:GLU:HG2	1.85	0.58
1:F:414:GLY:HA2	1:F:495:ASP:OD2	2.04	0.58
1:G:87:ASP:OD2	1:G:151:SER:OG	2.20	0.58
1:H:207:LYS:CB	1:H:208:PRO:HD3	2.28	0.58
1:H:370:ALA:O	1:H:374:GLY:N	2.37	0.58
1:J:517:THR:HG23	1:K:39:VAL:HG23	1.84	0.58
1:K:231:ARG:HD3	1:K:257:GLU:OE2	2.03	0.58
1:N:30:THR:HB	1:N:51:LYS:HG3	1.86	0.58
2:S:14:ARG:HG2	2:S:35:SER:CB	2.33	0.58
2:T:17:VAL:HG23	2:T:33:ALA:CB	2.30	0.58
2:X:83:VAL:C	2:X:84:LEU:HD12	2.27	0.58
1:A:206:ASN:ND2	1:A:214:GLU:O	2.36	0.58
1:B:193:MET:SD	1:B:371:LYS:HB3	2.43	0.58
1:C:349:ILE:O	1:C:353:ILE:HG13	2.04	0.58
1:G:415:GLY:N	3:G:601:ADP:O2'	2.30	0.58
1:H:230:ILE:HB	1:H:309:LEU:HD13	1.85	0.58
1:H:338:GLU:HG2	1:H:341:ALA:H	1.69	0.58
1:I:124:VAL:HG13	1:I:504:LEU:CD1	2.34	0.58
1:K:4:LYS:HG3	1:L:59:GLU:O	2.04	0.58
1:K:510:VAL:O	1:K:514:MET:HB2	2.03	0.58
1:N:276:VAL:HG11	1:N:325:ILE:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:285:ARG:HG3	1:N:286:LYS:N	2.19	0.58
2:U:48:ILE:C	2:U:49:LEU:CD1	2.71	0.58
2:X:94:ILE:CD1	2:X:96:GLU:HG3	2.34	0.58
1:E:174:VAL:HG22	1:E:376:VAL:CG1	2.33	0.57
1:F:180:GLY:HA3	1:F:382:GLY:HA2	1.86	0.57
1:I:304:GLU:C	1:I:305:ILE:HD12	2.28	0.57
1:J:199:TYR:HD2	1:J:325:ILE:HG22	1.69	0.57
1:L:291:ASP:OD1	1:L:292:ILE:N	2.37	0.57
1:M:345:ARG:O	1:M:348:GLN:HG3	2.03	0.57
1:N:355:GLU:HG3	1:N:356:ALA:H	1.69	0.57
2:X:15:LYS:HG3	2:X:16:GLU:OE1	2.03	0.57
2:2:52:GLY:HA3	2:2:53:GLU:HB3	1.85	0.57
1:E:245:LYS:HE2	1:E:245:LYS:HA	1.85	0.57
1:E:290:GLN:HG2	1:E:300:VAL:HG21	1.85	0.57
1:F:419:LEU:H	1:F:419:LEU:HD12	1.68	0.57
1:G:313:THR:CG2	1:G:315:GLU:HG2	2.34	0.57
1:I:233:MET:C	1:I:235:PRO:HD2	2.29	0.57
1:K:205:ILE:HA	1:K:213:VAL:CG2	2.33	0.57
1:K:322:ARG:HB3	1:K:333:ILE:CG2	2.34	0.57
1:L:237:LEU:HD22	2:Z:26:VAL:HG21	1.85	0.57
2:Q:92:LEU:HD23	2:Q:92:LEU:N	2.18	0.57
2:S:12:VAL:HG13	2:S:40:VAL:N	2.19	0.57
2:U:46:GLY:HA2	2:U:57:LEU:HD12	1.85	0.57
1:E:219:PHE:HB2	1:E:247:LEU:CD1	2.34	0.57
1:I:142:LYS:HE2	1:I:146:GLN:NE2	2.18	0.57
1:I:169:VAL:HG23	1:I:173:GLY:HA3	1.85	0.57
1:J:311:LYS:O	1:J:311:LYS:HD3	2.04	0.57
1:K:455:VAL:HG11	1:K:462:PRO:HA	1.85	0.57
1:L:368:ARG:O	1:L:372:LEU:HG	2.05	0.57
2:V:12:VAL:CG1	2:V:86:MET:HE3	2.34	0.57
1:B:88:GLY:HA2	3:B:601:ADP:O2B	2.03	0.57
3:B:601:ADP:O3B	4:B:602:BEF:F2	2.13	0.57
1:H:304:GLU:OE1	1:H:304:GLU:N	2.37	0.57
1:H:360:TYR:HA	1:H:363:GLU:HG3	1.85	0.57
1:H:448:GLU:O	1:H:452:ARG:HG2	2.05	0.57
1:J:76:GLU:OE2	1:K:385:THR:HB	2.04	0.57
1:J:220:ILE:HG22	1:J:318:GLY:C	2.30	0.57
1:J:225:LYS:HD2	1:J:309:LEU:HD21	1.85	0.57
1:N:221:LEU:HD13	1:N:317:LEU:CD2	2.35	0.57
1:N:279:PRO:HB2	1:N:288:MET:HE3	1.85	0.57
2:R:6:LEU:CD2	2:R:7:HIS:HD1	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:13:LYS:HD2	2:T:81:GLU:OE1	2.04	0.57
1:D:230:ILE:O	1:D:231:ARG:CG	2.48	0.57
1:F:218:PRO:C	1:F:219:PHE:CD1	2.75	0.57
1:H:210:THR:O	1:H:326:ASN:ND2	2.37	0.57
1:H:232:GLU:CD	1:H:234:LEU:HD13	2.29	0.57
1:I:241:ALA:HB2	1:I:271:VAL:CG1	2.35	0.57
1:L:228:SER:O	1:L:231:ARG:HG3	2.03	0.57
1:M:254:VAL:HG21	1:M:275:ALA:HB1	1.86	0.57
2:Z:25:ILE:H	2:Z:25:ILE:HD12	1.69	0.57
2:Z:40:VAL:HG21	2:Z:59:VAL:CG1	2.35	0.57
1:A:5:ASP:HB2	1:A:524:LEU:CD2	2.34	0.57
1:A:25:ASP:HA	1:A:28:LYS:HE2	1.87	0.57
1:B:221:LEU:HD23	1:B:222:LEU:N	2.20	0.57
1:D:40:LEU:HD13	1:D:59:GLU:HG3	1.86	0.57
1:D:231:ARG:O	1:D:233:MET:HG2	2.04	0.57
1:D:279:PRO:CB	1:D:288:MET:HE3	2.34	0.57
1:E:350:ARG:HD3	1:E:353:ILE:HD12	1.86	0.57
1:F:199:TYR:CE1	1:F:202:PRO:HA	2.40	0.57
1:F:406:ALA:HB2	1:F:496:PRO:HB3	1.85	0.57
1:F:409:GLU:OE2	1:F:501:ARG:NH2	2.29	0.57
1:H:124:VAL:HG21	1:H:508:ALA:CB	2.35	0.57
1:I:193:MET:CE	1:I:292:ILE:HG12	2.31	0.57
1:M:308:GLU:HB2	1:M:311:LYS:HB3	1.84	0.57
1:N:147:VAL:HG23	1:N:403:THR:HG22	1.87	0.57
1:N:165:ALA:O	1:N:169:VAL:HG22	2.03	0.57
2:U:10:VAL:HG23	2:U:42:ALA:O	2.04	0.57
2:X:40:VAL:HG12	2:X:63:ASP:O	2.04	0.57
2:X:50:GLU:O	2:X:51:ASN:ND2	2.38	0.57
1:C:227:ILE:HG12	1:C:251:ALA:HB1	1.85	0.57
1:C:240:VAL:HG11	1:C:247:LEU:HD23	1.86	0.57
1:C:345:ARG:HA	1:C:348:GLN:CG	2.34	0.57
1:C:350:ARG:NH1	1:C:369:VAL:HG11	2.20	0.57
1:E:222:LEU:CD2	1:E:289:LEU:HD22	2.35	0.57
1:G:218:PRO:HG3	1:G:323:VAL:HG13	1.86	0.57
1:K:236:VAL:HG21	1:K:310:GLU:O	2.05	0.57
1:L:10:ASN:O	1:L:14:VAL:HG23	2.04	0.57
1:L:194:GLN:O	1:L:371:LYS:NZ	2.30	0.57
1:L:296:THR:O	1:L:319:GLN:N	2.36	0.57
1:L:517:THR:HG23	1:M:39:VAL:HG23	1.86	0.57
1:N:381:VAL:HG11	1:N:392:LYS:HB3	1.87	0.57
2:Q:40:VAL:CG1	2:Q:61:VAL:HA	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:49:LEU:HB2	2:2:52:GLY:CA	2.35	0.57
1:B:418:ALA:O	1:B:422:VAL:HG13	2.05	0.57
1:C:42:LYS:HE2	1:C:48:THR:CG2	2.35	0.57
1:E:311:LYS:O	1:E:311:LYS:HD3	2.04	0.57
1:G:453:GLN:NE2	1:G:456:LEU:HD23	2.20	0.57
1:I:305:ILE:CG2	1:I:306:GLY:H	2.17	0.57
1:L:225:LYS:HG3	1:L:226:LYS:N	2.20	0.57
1:N:363:GLU:HG3	1:N:364:LYS:H	1.68	0.57
2:Y:36:THR:O	2:Y:66:ILE:HG12	2.05	0.57
1:A:393:LYS:O	1:A:397:GLU:HG3	2.05	0.57
1:B:169:VAL:CG1	1:B:173:GLY:HA3	2.35	0.57
1:C:220:ILE:HG22	1:C:222:LEU:HD11	1.87	0.57
1:E:24:ALA:O	1:E:28:LYS:HG3	2.05	0.57
1:G:305:ILE:HG22	1:G:306:GLY:H	1.70	0.57
1:H:204:PHE:CE2	1:H:274:ALA:HA	2.39	0.57
1:H:230:ILE:HG12	1:H:309:LEU:HB3	1.87	0.57
1:J:414:GLY:O	1:J:417:VAL:HG12	2.05	0.57
1:M:227:ILE:HD12	1:M:227:ILE:N	2.20	0.57
2:R:48:ILE:CA	2:R:54:VAL:HG12	2.28	0.57
2:T:20:LYS:HB3	2:T:27:LEU:HA	1.87	0.57
2:Z:60:LYS:HB3	2:Z:63:ASP:CG	2.30	0.57
2:2:65:VAL:HG12	2:2:94:ILE:CG2	2.25	0.57
1:A:245:LYS:HE3	1:A:246:PRO:HD3	1.87	0.57
1:F:200:LEU:HD13	1:F:276:VAL:HA	1.86	0.57
1:H:18:ARG:HB3	1:H:18:ARG:NH1	2.20	0.57
1:H:231:ARG:HE	1:H:257:GLU:HG3	1.70	0.57
1:I:152:ALA:HB2	1:I:399:ALA:HB2	1.86	0.57
1:J:166:MET:HE2	1:J:171:LYS:HG2	1.87	0.57
1:M:305:ILE:HD12	1:M:305:ILE:N	2.20	0.57
1:N:136:VAL:CG1	1:N:137:PRO:HD2	2.35	0.57
2:S:50:GLU:CD	2:S:51:ASN:H	2.12	0.57
1:A:177:VAL:HG11	1:A:396:VAL:HG12	1.87	0.56
1:B:208:PRO:HB2	1:B:212:ALA:HB3	1.86	0.56
1:B:415:GLY:N	3:B:601:ADP:O2'	2.26	0.56
1:E:234:LEU:CG	1:E:235:PRO:N	2.67	0.56
1:G:149:THR:HG23	1:G:159:GLY:HA3	1.86	0.56
1:G:219:PHE:HB2	1:G:247:LEU:CD1	2.34	0.56
1:G:256:GLY:HA2	1:G:259:LEU:HB2	1.86	0.56
1:I:169:VAL:CG2	1:I:173:GLY:HA3	2.34	0.56
1:J:363:GLU:HG3	1:J:364:LYS:N	2.20	0.56
1:K:215:LEU:HD12	1:K:323:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:49:LEU:HD22	2:U:50:GLU:HA	1.86	0.56
2:T:65:VAL:HG12	2:T:94:ILE:HG22	1.87	0.56
1:B:276:VAL:CG2	1:B:325:ILE:HG21	2.34	0.56
1:C:165:ALA:O	1:C:169:VAL:HG22	2.05	0.56
1:C:443:ALA:O	1:C:447:MET:HG3	2.05	0.56
1:E:302:SER:HB2	1:E:305:ILE:HG22	1.86	0.56
1:G:77:VAL:HG21	1:G:507:ALA:CA	2.33	0.56
1:J:39:VAL:HG22	1:J:49:ILE:HG12	1.87	0.56
1:J:181:THR:HG23	1:J:182:GLY:H	1.70	0.56
1:K:230:ILE:HG21	1:K:233:MET:HG3	1.86	0.56
1:K:252:GLU:HG3	1:K:285:ARG:HH12	1.71	0.56
1:L:355:GLU:HG3	1:L:356:ALA:N	2.18	0.56
1:N:168:LYS:HD3	1:N:189:VAL:HG21	1.87	0.56
1:N:345:ARG:O	1:N:348:GLN:HG3	2.05	0.56
1:N:346:VAL:O	1:N:349:ILE:HG22	2.06	0.56
2:O:37:ARG:HG2	2:O:66:ILE:HG12	1.86	0.56
2:O:57:LEU:HD22	2:O:57:LEU:H	1.70	0.56
2:O:67:PHE:CE2	2:O:86:MET:HE1	2.40	0.56
2:W:17:VAL:HG23	2:W:19:THR:HA	1.87	0.56
1:A:314:LEU:HD12	1:A:315:GLU:N	2.20	0.56
1:B:177:VAL:HG21	1:B:397:GLU:HG2	1.85	0.56
1:B:231:ARG:HD2	1:B:258:ALA:HA	1.87	0.56
1:B:510:VAL:O	1:B:514:MET:HB2	2.05	0.56
1:C:349:ILE:HD13	1:C:368:ARG:HD2	1.88	0.56
1:D:236:VAL:O	1:D:240:VAL:HG23	2.05	0.56
1:E:222:LEU:HD13	1:E:289:LEU:HD13	1.88	0.56
1:E:248:LEU:HD13	1:E:323:VAL:HG21	1.88	0.56
1:F:219:PHE:HE2	1:F:240:VAL:HG13	1.69	0.56
1:G:18:ARG:NH1	1:G:18:ARG:HB3	2.21	0.56
1:G:224:ASP:OD1	1:G:286:LYS:HG2	2.05	0.56
1:G:225:LYS:HG3	1:G:226:LYS:H	1.70	0.56
1:H:263:VAL:O	1:H:267:MET:HG2	2.05	0.56
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.86	0.56
1:I:418:ALA:O	1:I:422:VAL:HG13	2.06	0.56
1:M:23:LEU:HD12	1:M:60:ILE:HB	1.87	0.56
1:N:225:LYS:HG3	1:N:226:LYS:N	2.20	0.56
2:R:20:LYS:CA	2:R:21:SER:HB3	2.15	0.56
2:X:48:ILE:H	2:X:48:ILE:HD12	1.69	0.56
1:B:305:ILE:HD11	1:C:203:TYR:CE2	2.41	0.56
1:E:77:VAL:HB	1:E:510:VAL:HG21	1.88	0.56
1:E:177:VAL:HG11	1:E:397:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:359:ASP:O	1:E:363:GLU:HG3	2.05	0.56
1:H:276:VAL:HG13	1:H:325:ILE:HD13	1.87	0.56
1:H:302:SER:HB2	1:H:305:ILE:CD1	2.24	0.56
1:J:5:ASP:HB2	1:J:524:LEU:HD23	1.87	0.56
1:L:27:VAL:CG1	1:L:90:THR:HG23	2.35	0.56
2:V:49:LEU:HD13	2:V:50:GLU:N	2.20	0.56
2:V:60:LYS:HG3	2:V:63:ASP:CG	2.30	0.56
2:X:77:LYS:HE3	2:X:82:GLU:HB2	1.87	0.56
1:A:174:VAL:HG13	1:A:370:ALA:CB	2.34	0.56
1:A:353:ILE:HA	1:A:365:LEU:HD22	1.87	0.56
1:A:420:ILE:HD11	1:A:451:LEU:HB2	1.88	0.56
1:B:355:GLU:HG3	1:B:356:ALA:H	1.70	0.56
1:C:102:GLU:OE1	1:C:445:ARG:NH1	2.36	0.56
1:C:368:ARG:O	1:C:372:LEU:HG	2.06	0.56
1:D:23:LEU:HD23	1:D:60:ILE:HB	1.88	0.56
1:E:234:LEU:CD2	1:E:235:PRO:HD3	2.29	0.56
1:F:258:ALA:O	1:F:262:LEU:HB2	2.05	0.56
1:G:225:LYS:HD3	1:G:303:GLU:OE1	2.06	0.56
1:H:236:VAL:HG22	1:H:312:ALA:HB3	1.86	0.56
1:I:230:ILE:H	1:I:230:ILE:HD12	1.69	0.56
1:J:307:MET:HG2	1:J:311:LYS:NZ	2.20	0.56
1:L:18:ARG:NH1	1:L:18:ARG:HB3	2.21	0.56
1:N:130:GLU:O	1:N:134:LEU:HD13	2.06	0.56
1:N:284:ARG:CD	1:N:364:LYS:HE2	2.34	0.56
2:O:8:ASP:CA	2:O:57:LEU:HD21	2.31	0.56
2:U:23:GLY:O	2:U:26:VAL:HG12	2.05	0.56
2:V:57:LEU:HD11	2:V:59:VAL:HG22	1.87	0.56
2:V:74:LYS:HZ3	2:2:68:ASN:HB3	1.69	0.56
2:Y:92:LEU:HD23	2:Z:85:ILE:CD1	2.35	0.56
2:2:59:VAL:HG11	2:2:91:ILE:HD12	1.88	0.56
1:A:234:LEU:HG	1:A:235:PRO:CD	2.35	0.56
1:A:241:ALA:HB1	1:A:271:VAL:HG12	1.88	0.56
1:B:48:THR:HG22	1:B:390:LYS:NZ	2.19	0.56
1:B:250:ILE:HG22	1:B:278:ALA:HB2	1.87	0.56
1:H:165:ALA:O	1:H:169:VAL:HG22	2.06	0.56
1:H:225:LYS:HG2	1:H:303:GLU:HG3	1.87	0.56
1:H:323:VAL:HG12	1:H:332:ILE:HG12	1.88	0.56
1:I:326:ASN:HD21	1:I:329:THR:HB	1.71	0.56
1:M:18:ARG:HB3	1:M:18:ARG:NH1	2.20	0.56
1:M:448:GLU:O	1:M:452:ARG:HG3	2.06	0.56
1:N:214:GLU:HG2	1:N:324:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:222:LEU:HB2	1:N:300:VAL:HA	1.85	0.56
1:N:231:ARG:HB3	1:N:233:MET:HG3	1.88	0.56
2:R:6:LEU:CD2	2:R:7:HIS:CE1	2.55	0.56
2:Y:20:LYS:HE2	2:Y:22:ALA:CB	2.36	0.56
2:1:95:VAL:HA	2:2:3:ILE:CG2	2.36	0.56
2:2:53:GLU:OE2	2:2:54:VAL:HG23	2.06	0.56
1:C:25:ASP:HA	1:C:28:LYS:HE2	1.86	0.56
1:E:231:ARG:HD3	1:E:257:GLU:OE2	2.06	0.56
1:E:345:ARG:O	1:E:348:GLN:HG3	2.06	0.56
1:H:260:ALA:O	1:H:264:VAL:HG23	2.06	0.56
1:J:175:ILE:HG12	1:J:377:ALA:HB3	1.87	0.56
1:J:230:ILE:O	1:J:232:GLU:N	2.39	0.56
1:K:225:LYS:HG3	1:K:226:LYS:H	1.71	0.56
1:N:77:VAL:HB	1:N:510:VAL:CG2	2.32	0.56
1:A:114:MET:HE2	1:B:153:ASN:ND2	2.21	0.56
1:A:199:TYR:HB3	1:A:276:VAL:HG12	1.87	0.56
1:A:266:THR:O	1:A:269:GLY:HA3	2.05	0.56
1:C:87:ASP:OD2	1:C:151:SER:OG	2.16	0.56
1:C:203:TYR:HB3	1:C:267:MET:CE	2.36	0.56
1:H:231:ARG:HE	1:H:257:GLU:CG	2.19	0.56
1:K:230:ILE:CG2	1:K:233:MET:HG3	2.36	0.56
2:O:96:GLU:HB3	2:P:2:ASN:H	1.70	0.56
2:R:6:LEU:HD23	2:R:7:HIS:CB	2.35	0.56
2:R:95:VAL:HG22	2:S:3:ILE:HG21	1.88	0.56
2:1:64:ILE:CG2	2:1:95:VAL:HB	2.31	0.56
1:F:127:ALA:N	1:F:426:LEU:HD11	2.21	0.56
1:G:215:LEU:HD22	1:G:246:PRO:CB	2.35	0.56
1:G:333:ILE:O	1:G:334:ASP:HB2	2.06	0.56
1:H:230:ILE:HD13	1:H:309:LEU:HB2	1.87	0.56
1:J:227:ILE:N	1:J:227:ILE:HD12	2.20	0.56
1:K:77:VAL:HG12	1:K:510:VAL:HG21	1.88	0.56
1:M:151:SER:HB3	1:M:399:ALA:HA	1.86	0.56
1:M:263:VAL:O	1:M:267:MET:HG2	2.06	0.56
2:P:73:VAL:HG22	2:P:86:MET:HB3	1.88	0.56
2:T:36:THR:O	2:T:66:ILE:HG12	2.06	0.56
2:Y:7:HIS:O	2:Y:8:ASP:HB3	2.04	0.56
2:Y:36:THR:HG22	2:Y:37:ARG:NH1	2.21	0.56
1:A:236:VAL:O	1:A:240:VAL:HG23	2.06	0.56
1:A:280:GLY:O	1:A:285:ARG:NE	2.39	0.56
1:B:128:VAL:CG1	1:B:132:LYS:HE2	2.34	0.56
1:I:230:ILE:C	1:I:232:GLU:H	2.12	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:308:GLU:HB3	1:J:311:LYS:HB3	1.87	0.56
1:K:90:THR:OG1	3:K:601:ADP:O2B	2.21	0.56
2:R:8:ASP:OD1	2:R:9:ARG:N	2.38	0.56
2:S:57:LEU:H	2:S:57:LEU:HD12	1.69	0.56
2:Z:47:ARG:HD3	2:Z:49:LEU:HD12	1.88	0.56
2:1:66:ILE:HD12	2:2:3:ILE:CD1	2.35	0.56
1:A:6:VAL:CG1	1:A:521:VAL:HG22	2.31	0.55
1:D:10:ASN:O	1:D:14:VAL:HG23	2.05	0.55
1:D:230:ILE:O	1:D:230:ILE:HG23	2.06	0.55
1:F:345:ARG:O	1:F:348:GLN:HG3	2.06	0.55
1:G:183:LEU:HD12	1:G:384:ALA:HB2	1.89	0.55
1:G:280:GLY:H	1:G:285:ARG:HB3	1.71	0.55
1:L:237:LEU:HD22	2:Z:26:VAL:CG2	2.36	0.55
1:L:417:VAL:HG21	1:L:477:GLY:HA3	1.87	0.55
2:U:15:LYS:HB2	2:U:37:ARG:O	2.06	0.55
2:W:77:LYS:HG3	2:W:81:GLU:O	2.06	0.55
2:2:57:LEU:HD13	2:2:88:GLU:HB2	1.88	0.55
1:A:176:THR:OG1	1:A:378:VAL:HG12	2.06	0.55
1:A:270:ILE:HG22	1:A:271:VAL:N	2.20	0.55
1:A:301:ILE:CD1	1:A:312:ALA:HB2	2.35	0.55
1:B:359:ASP:O	1:B:360:TYR:HB2	2.05	0.55
1:C:57:ALA:O	1:C:75:LYS:HE2	2.06	0.55
1:D:496:PRO:HG2	1:D:499:VAL:HG11	1.88	0.55
1:E:260:ALA:HB3	2:S:30:SER:HB3	1.87	0.55
1:E:368:ARG:O	1:E:372:LEU:HG	2.07	0.55
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.88	0.55
1:G:134:LEU:HD11	1:G:425:LYS:HZ1	1.69	0.55
1:G:291:ASP:HB2	1:G:372:LEU:HD21	1.87	0.55
1:G:461:GLU:OE2	1:I:452:ARG:NH2	2.38	0.55
1:I:381:VAL:HG11	1:I:392:LYS:HB3	1.86	0.55
1:N:227:ILE:HG23	1:N:231:ARG:CB	2.37	0.55
1:N:475:ASN:O	1:N:488:MET:HG2	2.06	0.55
2:O:95:VAL:HA	2:P:3:ILE:HG22	0.59	0.55
2:V:49:LEU:HD13	2:V:50:GLU:CB	2.37	0.55
2:Y:40:VAL:HG12	2:Y:63:ASP:O	2.07	0.55
1:B:510:VAL:HG12	1:C:387:VAL:HG21	1.88	0.55
1:D:90:THR:O	1:D:94:VAL:HG23	2.07	0.55
1:E:325:ILE:HD12	1:E:325:ILE:N	2.21	0.55
1:F:33:PRO:HA	1:F:153:ASN:OD1	2.07	0.55
1:G:228:SER:O	1:G:231:ARG:HG3	2.07	0.55
1:I:73:MET:HE1	1:J:387:VAL:HG11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:349:ILE:O	1:L:353:ILE:HG13	2.06	0.55
1:L:479:ASN:HD22	1:L:493:ILE:CD1	2.15	0.55
1:N:158:VAL:O	1:N:162:ILE:HG13	2.06	0.55
1:C:10:ASN:O	1:C:14:VAL:HG23	2.06	0.55
1:C:245:LYS:HE2	1:C:245:LYS:HA	1.87	0.55
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.88	0.55
1:F:31:LEU:CD2	1:F:453:GLN:HB3	2.36	0.55
1:H:449:ALA:HB3	1:H:450:PRO:HD3	1.87	0.55
1:I:147:VAL:HG22	1:I:403:THR:HG22	1.87	0.55
1:J:420:ILE:HD11	1:J:469:VAL:CG1	2.35	0.55
1:M:131:LEU:CD2	1:M:422:VAL:HG11	2.36	0.55
1:M:197:ARG:HD2	1:M:277:LYS:CB	2.34	0.55
2:O:10:VAL:N	2:O:86:MET:O	2.36	0.55
2:T:40:VAL:CG1	2:T:62:GLY:H	2.19	0.55
2:T:64:ILE:HD12	2:T:64:ILE:N	2.21	0.55
2:Y:36:THR:C	2:Y:37:ARG:HD2	2.30	0.55
1:A:31:LEU:HD23	1:A:453:GLN:HB3	1.88	0.55
1:A:199:TYR:HE1	1:A:202:PRO:HA	1.71	0.55
1:C:238:GLU:HG2	2:Q:25:ILE:CG1	2.35	0.55
1:G:223:ALA:HB2	1:G:251:ALA:CA	2.32	0.55
1:L:230:ILE:HG12	1:L:309:LEU:CD2	2.36	0.55
2:R:17:VAL:HG23	2:R:19:THR:N	2.19	0.55
2:R:20:LYS:HB2	2:R:22:ALA:CB	2.36	0.55
2:Z:16:GLU:OE1	2:Z:16:GLU:N	2.39	0.55
1:B:232:GLU:O	1:B:234:LEU:HD23	2.06	0.55
1:B:307:MET:HE3	1:B:311:LYS:HZ2	1.72	0.55
1:C:231:ARG:CD	1:C:261:THR:HG21	2.36	0.55
1:D:463:SER:HB2	1:L:463:SER:HB2	1.89	0.55
1:E:420:ILE:HD11	1:E:469:VAL:HG12	1.87	0.55
1:F:124:VAL:HG13	1:F:504:LEU:HD12	1.88	0.55
1:I:404:ARG:O	1:I:408:GLU:HG2	2.06	0.55
1:J:124:VAL:HG13	1:J:504:LEU:HD12	1.88	0.55
1:J:174:VAL:O	1:J:376:VAL:HG13	2.07	0.55
1:J:367:GLU:O	1:J:371:LYS:HG3	2.07	0.55
1:L:5:ASP:HB2	1:L:524:LEU:HD23	1.88	0.55
1:L:219:PHE:HA	1:L:317:LEU:CD2	2.29	0.55
1:M:165:ALA:O	1:M:169:VAL:HG22	2.06	0.55
1:N:222:LEU:CD2	1:N:300:VAL:HG22	2.36	0.55
2:Y:17:VAL:HG23	2:Y:33:ALA:CB	2.37	0.55
1:A:245:LYS:HE3	1:A:246:PRO:CD	2.36	0.55
1:A:365:LEU:HD12	1:A:366:GLN:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLY:N	1:B:381:VAL:O	2.39	0.55
3:B:601:ADP:O3A	4:B:602:BEF:F3	2.15	0.55
1:C:176:THR:OG1	1:C:378:VAL:HG22	2.05	0.55
1:C:203:TYR:HD2	1:C:263:VAL:HG11	1.72	0.55
1:D:5:ASP:HB2	1:D:524:LEU:HD21	1.88	0.55
1:D:355:GLU:HG3	1:D:356:ALA:H	1.71	0.55
1:G:101:THR:O	1:G:105:LYS:HG3	2.05	0.55
1:I:265:ASN:OD1	2:W:27:LEU:HA	2.06	0.55
1:J:205:ILE:HD13	1:J:211:GLY:HA2	1.88	0.55
1:J:218:PRO:HA	1:J:246:PRO:HG2	1.88	0.55
1:J:236:VAL:CG1	1:J:312:ALA:HB3	2.37	0.55
1:K:219:PHE:HD2	1:K:240:VAL:HG13	1.71	0.55
1:K:325:ILE:HD12	1:K:325:ILE:N	2.21	0.55
1:L:352:GLN:HE21	1:M:209:GLU:CD	2.15	0.55
2:T:48:ILE:HG22	2:T:53:GLU:O	2.07	0.55
2:1:80:ASN:OD1	2:1:80:ASN:N	2.39	0.55
1:A:309:LEU:CD1	1:A:310:GLU:H	2.09	0.55
1:A:420:ILE:HD11	1:A:451:LEU:CB	2.36	0.55
1:A:455:VAL:CG1	1:A:460:GLU:HB2	2.37	0.55
1:B:346:VAL:O	1:B:349:ILE:HG22	2.07	0.55
1:B:517:THR:HG23	1:C:39:VAL:HG23	1.88	0.55
1:C:383:ALA:CB	1:C:389:MET:HA	2.36	0.55
1:D:199:TYR:HE1	1:D:202:PRO:HA	1.70	0.55
1:E:219:PHE:HE1	1:E:319:GLN:HG2	1.71	0.55
1:E:238:GLU:HA	1:E:241:ALA:HB3	1.88	0.55
1:F:349:ILE:O	1:F:353:ILE:N	2.40	0.55
1:F:414:GLY:HA2	1:F:495:ASP:CG	2.32	0.55
1:H:203:TYR:CE2	1:N:305:ILE:HD11	2.41	0.55
1:H:230:ILE:HG23	1:H:231:ARG:N	2.22	0.55
1:A:199:TYR:CA	1:A:276:VAL:HG12	2.37	0.55
1:F:171:LYS:O	1:F:171:LYS:HD2	2.07	0.55
1:F:226:LYS:CA	1:F:252:GLU:HB3	2.36	0.55
1:H:314:LEU:HD12	1:H:315:GLU:N	2.22	0.55
1:J:303:GLU:CD	1:J:309:LEU:HD21	2.32	0.55
1:K:513:LEU:O	1:K:516:THR:OG1	2.24	0.55
1:M:280:GLY:O	1:M:285:ARG:HB3	2.07	0.55
1:N:231:ARG:O	1:N:232:GLU:HG2	2.07	0.55
2:S:40:VAL:HG12	2:S:41:LEU:N	2.18	0.55
2:V:17:VAL:HA	2:V:35:SER:HB2	1.87	0.55
2:V:48:ILE:HG13	2:V:54:VAL:HG12	1.87	0.55
1:A:223:ALA:HB3	1:A:251:ALA:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:PRO:HG2	1:B:214:GLU:HG3	1.89	0.55
1:C:226:LYS:CG	1:C:252:GLU:HG2	2.25	0.55
1:C:364:LYS:HA	1:C:367:GLU:HB3	1.88	0.55
1:C:418:ALA:O	1:C:422:VAL:HG13	2.06	0.55
1:G:252:GLU:HG3	1:G:285:ARG:NH1	2.21	0.55
1:G:313:THR:HB	1:G:315:GLU:HG2	1.89	0.55
1:H:142:LYS:O	1:H:146:GLN:HG3	2.07	0.55
1:H:305:ILE:CG2	1:H:306:GLY:N	2.69	0.55
1:J:23:LEU:HD23	1:J:60:ILE:CB	2.37	0.55
1:J:270:ILE:HG21	2:X:27:LEU:HD22	1.89	0.55
1:L:234:LEU:H	1:L:234:LEU:CD1	2.18	0.55
1:L:412:VAL:CG1	1:L:413:ALA:N	2.69	0.55
1:M:25:ASP:HA	1:M:28:LYS:HE2	1.88	0.55
2:P:3:ILE:H	2:P:3:ILE:HD12	1.71	0.55
2:R:10:VAL:HG13	2:R:57:LEU:HD13	1.88	0.55
1:B:398:ASP:OD2	4:B:602:BEF:F1	2.14	0.54
1:E:40:LEU:HD13	1:E:59:GLU:HG3	1.88	0.54
1:E:302:SER:HB2	1:E:305:ILE:HB	1.89	0.54
1:H:232:GLU:HG3	1:H:233:MET:H	1.72	0.54
1:K:219:PHE:CD1	1:K:319:GLN:HG3	2.41	0.54
1:K:219:PHE:HD1	1:K:319:GLN:HG3	1.72	0.54
1:L:215:LEU:O	1:L:322:ARG:HG3	2.07	0.54
1:L:227:ILE:N	1:L:227:ILE:HD12	2.22	0.54
1:N:293:ALA:HB1	1:N:298:GLY:O	2.08	0.54
2:S:16:GLU:HG3	2:S:19:THR:CG2	2.37	0.54
2:V:15:LYS:HB3	2:V:16:GLU:OE2	2.06	0.54
2:Z:7:HIS:C	2:Z:46:GLY:O	2.50	0.54
2:Z:40:VAL:HG21	2:Z:59:VAL:HG11	1.88	0.54
1:B:241:ALA:HA	1:B:271:VAL:HG11	1.89	0.54
1:B:461:GLU:OE1	1:N:463:SER:OG	2.24	0.54
1:D:245:LYS:HB3	1:D:246:PRO:HD2	1.88	0.54
1:E:18:ARG:HB3	1:E:18:ARG:NH1	2.22	0.54
1:E:320:ALA:HA	1:E:335:GLY:HA2	1.89	0.54
1:E:325:ILE:HG13	1:E:330:THR:HG23	1.90	0.54
1:E:443:ALA:O	1:E:447:MET:HG3	2.06	0.54
1:G:206:ASN:OD1	1:G:207:LYS:HG3	2.06	0.54
1:J:357:THR:HB	1:J:361:ASP:CB	2.38	0.54
1:K:217:SER:O	1:K:245:LYS:HD2	2.07	0.54
1:C:266:THR:HG22	1:C:273:VAL:H	1.73	0.54
1:E:236:VAL:HG21	1:E:312:ALA:HB3	1.90	0.54
1:E:237:LEU:O	1:E:241:ALA:N	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:ILE:O	1:F:353:ILE:HG13	2.07	0.54
1:L:204:PHE:CE1	1:L:266:THR:HG21	2.42	0.54
1:L:414:GLY:HA3	1:L:493:ILE:HG22	1.89	0.54
1:M:142:LYS:HE2	1:M:146:GLN:NE2	2.22	0.54
1:N:151:SER:HB3	1:N:399:ALA:HA	1.89	0.54
2:U:25:ILE:HD12	2:U:25:ILE:N	2.22	0.54
2:U:73:VAL:HG12	2:U:86:MET:CB	2.37	0.54
2:V:43:VAL:HG22	2:V:44:GLY:N	2.22	0.54
2:V:78:ILE:HG13	2:V:79:ASP:OD2	2.07	0.54
1:A:122:LYS:HE2	1:A:429:LEU:HD11	1.89	0.54
1:D:169:VAL:HG23	1:D:173:GLY:HA3	1.88	0.54
1:D:172:GLU:OE1	1:D:172:GLU:N	2.30	0.54
1:G:448:GLU:O	1:G:452:ARG:HG2	2.07	0.54
1:J:265:ASN:C	1:J:265:ASN:OD1	2.51	0.54
1:L:429:LEU:HD12	1:L:430:ARG:H	1.72	0.54
1:N:8:PHE:O	1:N:11:ASP:HB3	2.07	0.54
1:N:363:GLU:O	1:N:367:GLU:HG3	2.08	0.54
2:S:20:LYS:HE3	2:S:29:GLY:N	2.22	0.54
2:U:65:VAL:HG12	2:U:94:ILE:HB	1.88	0.54
1:A:248:LEU:HD13	1:A:249:ILE:N	2.22	0.54
1:B:351:GLN:HG2	1:C:210:THR:HA	1.89	0.54
1:C:232:GLU:C	1:C:234:LEU:H	2.16	0.54
1:D:230:ILE:HB	1:D:257:GLU:OE1	2.08	0.54
1:H:443:ALA:O	1:H:447:MET:HG3	2.07	0.54
1:J:234:LEU:HD11	2:X:26:VAL:HA	1.88	0.54
1:L:279:PRO:HD2	1:L:285:ARG:HB2	1.89	0.54
1:M:201:SER:HB2	1:M:259:LEU:HD11	1.89	0.54
1:N:174:VAL:HB	1:N:376:VAL:HG13	1.89	0.54
1:N:234:LEU:N	1:N:235:PRO:HD2	2.22	0.54
2:Q:57:LEU:CD1	2:Q:59:VAL:HG22	2.37	0.54
2:S:48:ILE:HG13	2:S:52:GLY:H	1.73	0.54
2:V:78:ILE:HD13	2:2:37:ARG:HH12	1.72	0.54
2:Y:20:LYS:CE	2:Y:22:ALA:HB3	2.38	0.54
1:C:218:PRO:HD2	1:C:320:ALA:O	2.07	0.54
1:E:404:ARG:O	1:E:408:GLU:HG2	2.08	0.54
1:F:305:ILE:HD12	1:F:305:ILE:N	2.22	0.54
1:G:23:LEU:HD23	1:G:60:ILE:HB	1.89	0.54
1:G:228:SER:HB3	1:G:255:GLU:HG2	1.89	0.54
1:L:350:ARG:HD3	1:L:353:ILE:HD12	1.87	0.54
1:L:366:GLN:HA	1:L:369:VAL:HB	1.88	0.54
1:M:89:THR:OG1	4:M:602:BEF:F3	2.13	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:248:LEU:HD13	1:N:249:ILE:N	2.22	0.54
1:N:259:LEU:CD2	1:N:262:LEU:HD23	2.38	0.54
2:W:11:ILE:HB	2:W:85:ILE:CD1	2.38	0.54
2:Y:35:SER:OG	2:Y:37:ARG:O	2.25	0.54
1:A:183:LEU:HD22	1:A:384:ALA:HA	1.89	0.54
1:B:136:VAL:CG2	1:B:137:PRO:CD	2.86	0.54
1:B:311:LYS:O	1:B:311:LYS:HD3	2.08	0.54
1:D:236:VAL:CG2	1:D:312:ALA:HB3	2.37	0.54
1:E:227:ILE:HD12	1:E:227:ILE:N	2.23	0.54
1:H:215:LEU:HB2	1:H:323:VAL:HG22	1.89	0.54
1:I:6:VAL:HG22	1:I:521:VAL:HG22	1.89	0.54
1:I:284:ARG:HD2	1:I:364:LYS:NZ	2.22	0.54
1:N:254:VAL:CG1	1:N:259:LEU:HG	2.38	0.54
1:N:438:VAL:O	1:N:442:VAL:HG23	2.08	0.54
1:B:218:PRO:HG3	1:B:323:VAL:CG2	2.37	0.54
1:D:305:ILE:HD12	1:D:305:ILE:N	2.23	0.54
1:D:326:ASN:OD1	1:D:329:THR:HB	2.07	0.54
1:E:183:LEU:HD22	1:E:384:ALA:CA	2.33	0.54
1:F:77:VAL:CG2	1:F:507:ALA:HA	2.38	0.54
1:G:227:ILE:N	1:G:227:ILE:HD12	2.22	0.54
1:H:237:LEU:HD21	1:H:271:VAL:HG21	1.90	0.54
1:J:222:LEU:HD22	1:J:300:VAL:HG22	1.90	0.54
1:J:357:THR:HB	1:J:361:ASP:HB2	1.89	0.54
1:K:368:ARG:O	1:K:372:LEU:HG	2.08	0.54
1:K:517:THR:HG23	1:L:39:VAL:HG23	1.90	0.54
1:L:302:SER:CB	1:L:305:ILE:HB	2.38	0.54
1:L:309:LEU:HD23	1:L:309:LEU:H	1.73	0.54
1:N:177:VAL:HG22	1:N:393:LYS:HG3	1.89	0.54
2:Q:56:PRO:C	2:Q:57:LEU:HG	2.33	0.54
2:V:12:VAL:HG13	2:V:86:MET:HE3	1.89	0.54
2:Y:7:HIS:O	2:Y:7:HIS:CD2	2.61	0.54
2:Z:25:ILE:HD12	2:Z:25:ILE:N	2.23	0.54
1:A:232:GLU:CG	1:A:234:LEU:HD23	2.37	0.54
1:A:306:GLY:CA	1:B:264:VAL:HG21	2.32	0.54
1:F:293:ALA:O	1:F:298:GLY:N	2.40	0.54
1:H:221:LEU:CD1	1:H:317:LEU:HD21	2.25	0.54
1:J:199:TYR:HE2	1:J:326:ASN:HA	1.73	0.54
1:L:488:MET:HE3	1:L:493:ILE:HG21	1.88	0.54
1:M:496:PRO:HG2	1:M:499:VAL:CG1	2.38	0.54
1:N:34:LYS:HD2	1:N:458:CYS:SG	2.48	0.54
1:N:448:GLU:O	1:N:452:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:73:VAL:HG11	2:P:84:LEU:HD23	1.90	0.54
2:Z:14:ARG:NH2	2:Z:34:LYS:HD3	2.23	0.54
1:A:227:ILE:HD12	1:A:227:ILE:N	2.23	0.54
1:A:247:LEU:HG	1:A:273:VAL:HG13	1.89	0.54
1:B:136:VAL:HG23	1:B:137:PRO:HD2	1.90	0.54
1:C:203:TYR:HB3	1:C:267:MET:HE2	1.89	0.54
1:C:227:ILE:HG22	1:C:227:ILE:O	2.08	0.54
1:D:219:PHE:O	1:D:247:LEU:HD12	2.08	0.54
1:D:417:VAL:HA	1:D:420:ILE:CG2	2.37	0.54
1:K:196:ASP:O	1:K:197:ARG:HG2	2.07	0.54
1:K:225:LYS:HD2	1:K:252:GLU:OE1	2.08	0.54
1:K:322:ARG:HB3	1:K:333:ILE:HG22	1.89	0.54
1:L:230:ILE:CG1	1:L:309:LEU:HD21	2.36	0.54
1:M:151:SER:CB	1:M:399:ALA:HA	2.38	0.54
2:Q:36:THR:HG23	2:Q:37:ARG:HG3	1.90	0.54
2:S:6:LEU:HD12	2:S:6:LEU:O	2.08	0.54
2:U:14:ARG:NH1	2:U:84:LEU:HD21	2.22	0.54
2:2:17:VAL:CA	2:2:35:SER:HB2	2.38	0.54
1:A:252:GLU:HA	1:A:285:ARG:NH1	2.23	0.53
1:B:215:LEU:HB3	1:B:246:PRO:HB2	1.90	0.53
1:C:311:LYS:O	1:C:311:LYS:HD3	2.07	0.53
1:D:199:TYR:OH	1:D:327:LYS:HG3	2.08	0.53
1:D:266:THR:HG22	1:D:271:VAL:O	2.08	0.53
1:F:220:ILE:HB	1:F:318:GLY:C	2.32	0.53
1:F:386:GLU:O	1:F:389:MET:HB3	2.08	0.53
1:G:223:ALA:CB	1:G:224:ASP:C	2.81	0.53
1:G:224:ASP:O	1:G:252:GLU:HB2	2.08	0.53
1:H:302:SER:OG	1:H:305:ILE:HB	2.08	0.53
1:H:406:ALA:HB1	1:H:411:VAL:CG1	2.37	0.53
1:I:513:LEU:O	1:I:516:THR:OG1	2.23	0.53
1:J:496:PRO:HG2	1:J:499:VAL:HG11	1.90	0.53
1:K:18:ARG:HB3	1:K:18:ARG:HH11	1.72	0.53
1:M:5:ASP:HB2	1:M:524:LEU:HD23	1.87	0.53
1:M:34:LYS:HE3	1:M:480:ALA:O	2.08	0.53
1:M:269:GLY:C	1:M:271:VAL:H	2.16	0.53
1:N:40:LEU:HD13	1:N:59:GLU:HG3	1.90	0.53
2:O:94:ILE:O	2:P:3:ILE:HG22	2.08	0.53
2:Y:48:ILE:HD12	2:Y:48:ILE:N	2.23	0.53
1:A:92:ALA:HB2	1:A:503:ALA:HB1	1.90	0.53
1:B:136:VAL:HG22	1:B:137:PRO:HD2	1.88	0.53
1:H:220:ILE:HG22	1:H:222:LEU:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:261:THR:O	1:K:265:ASN:ND2	2.40	0.53
1:K:465:VAL:O	1:K:469:VAL:HG23	2.09	0.53
2:Q:12:VAL:HG23	2:Q:39:GLU:C	2.34	0.53
2:Y:7:HIS:HA	2:Y:45:ASN:H	1.73	0.53
1:A:301:ILE:HD11	1:A:312:ALA:HB2	1.89	0.53
1:C:230:ILE:HB	1:C:232:GLU:OE1	2.08	0.53
1:C:232:GLU:HG3	1:C:310:GLU:CG	2.34	0.53
1:E:227:ILE:HG23	1:E:230:ILE:HB	1.89	0.53
1:I:49:ILE:HD12	1:I:49:ILE:N	2.22	0.53
1:J:256:GLY:HA2	1:J:259:LEU:HB2	1.89	0.53
1:K:268:ARG:HB2	1:K:270:ILE:CD1	2.39	0.53
1:K:302:SER:OG	1:K:305:ILE:HB	2.08	0.53
1:L:406:ALA:HB2	1:L:496:PRO:HB3	1.90	0.53
1:M:77:VAL:HG21	1:M:507:ALA:HA	1.90	0.53
1:M:333:ILE:O	1:M:334:ASP:HB2	2.08	0.53
1:M:357:THR:CG2	1:M:361:ASP:HB3	2.38	0.53
1:N:219:PHE:HA	1:N:318:GLY:O	2.08	0.53
2:Q:17:VAL:HA	2:Q:35:SER:HB2	1.91	0.53
2:R:6:LEU:HD23	2:R:6:LEU:C	2.33	0.53
2:W:1:MET:HE2	2:W:79:ASP:CB	2.32	0.53
2:1:97:ALA:HA	2:2:1:MET:SD	2.48	0.53
1:C:157:THR:O	1:C:161:LEU:HB2	2.08	0.53
1:D:4:LYS:HG3	1:E:59:GLU:O	2.08	0.53
1:F:208:PRO:HB2	1:F:212:ALA:HB3	1.89	0.53
1:I:90:THR:OG1	4:I:602:BEF:F1	2.10	0.53
1:J:23:LEU:HD23	1:J:60:ILE:HB	1.90	0.53
1:L:233:MET:HE2	1:L:236:VAL:HB	1.89	0.53
1:L:417:VAL:HA	1:L:420:ILE:HG22	1.89	0.53
1:M:142:LYS:O	1:M:146:GLN:HG3	2.07	0.53
1:M:450:PRO:O	1:M:454:ILE:HG13	2.07	0.53
2:Y:5:PRO:CD	2:Y:42:ALA:HB1	2.38	0.53
1:A:321:LYS:HB2	1:A:334:ASP:HB3	1.89	0.53
1:A:496:PRO:HG2	1:A:499:VAL:HG13	1.90	0.53
1:B:177:VAL:HG21	1:B:397:GLU:CG	2.38	0.53
1:C:305:ILE:CG2	1:C:306:GLY:N	2.68	0.53
1:D:222:LEU:N	1:D:222:LEU:HD12	2.24	0.53
1:D:232:GLU:HG3	1:D:233:MET:H	1.73	0.53
1:G:202:PRO:O	1:G:205:ILE:HG13	2.08	0.53
1:H:440:ILE:O	1:H:444:LEU:HG	2.08	0.53
1:I:177:VAL:HG11	1:I:397:GLU:CG	2.39	0.53
1:J:350:ARG:HD3	1:J:353:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:102:GLU:HG3	1:K:445:ARG:HD2	1.90	0.53
1:K:208:PRO:HG2	1:K:214:GLU:HG3	1.89	0.53
1:K:236:VAL:O	1:K:239:ALA:HB3	2.09	0.53
3:N:601:ADP:O3B	4:N:602:BEF:F3	2.17	0.53
2:Z:46:GLY:HA2	2:Z:57:LEU:HD11	1.91	0.53
2:Z:74:LYS:HE2	2:Z:75:SER:O	2.07	0.53
1:A:230:ILE:HG23	1:A:309:LEU:HD13	1.90	0.53
1:A:362:ARG:O	1:A:365:LEU:HG	2.08	0.53
1:B:270:ILE:HG23	1:B:271:VAL:N	2.23	0.53
1:F:233:MET:CG	1:F:234:LEU:CD2	2.80	0.53
1:F:360:TYR:HA	1:F:363:GLU:CG	2.37	0.53
1:G:199:TYR:CE2	1:G:327:LYS:HA	2.44	0.53
1:G:225:LYS:HG3	1:G:226:LYS:N	2.23	0.53
1:H:175:ILE:HA	1:H:377:ALA:O	2.08	0.53
1:M:69:MET:SD	1:N:41:ASP:HB2	2.48	0.53
2:R:12:VAL:HG12	2:R:40:VAL:CA	2.34	0.53
2:T:92:LEU:HA	2:U:9:ARG:HD2	1.90	0.53
2:W:9:ARG:HA	2:W:87:SER:HA	1.91	0.53
2:W:17:VAL:HG23	2:W:19:THR:CA	2.39	0.53
2:X:37:ARG:CG	2:X:66:ILE:HG23	2.30	0.53
1:D:25:ASP:HA	1:D:28:LYS:HE2	1.91	0.53
1:E:208:PRO:HB2	1:E:212:ALA:CB	2.36	0.53
1:F:142:LYS:O	1:F:146:GLN:HG3	2.08	0.53
1:F:455:VAL:HG13	1:F:460:GLU:HB2	1.90	0.53
1:G:223:ALA:HB3	1:G:224:ASP:C	2.33	0.53
1:H:301:ILE:HD13	1:H:307:MET:HE2	1.91	0.53
1:I:456:LEU:HD13	1:I:462:PRO:HG3	1.90	0.53
1:J:138:CYS:HB2	1:J:411:VAL:HG13	1.90	0.53
1:K:280:GLY:O	1:K:285:ARG:NE	2.41	0.53
1:L:69:MET:HE2	1:L:520:MET:HE3	1.90	0.53
1:L:232:GLU:HB2	1:L:234:LEU:CD1	2.38	0.53
2:O:28:THR:HG22	2:O:29:GLY:O	2.09	0.53
2:U:11:ILE:CG2	2:U:42:ALA:HB3	2.39	0.53
2:W:19:THR:HG22	2:W:20:LYS:H	1.73	0.53
1:A:10:ASN:O	1:A:14:VAL:HG23	2.09	0.53
1:F:124:VAL:HG22	1:F:504:LEU:HD11	1.91	0.53
1:F:496:PRO:HG2	1:F:499:VAL:CG1	2.38	0.53
1:G:117:LYS:NZ	1:G:121:ASP:OD2	2.36	0.53
1:G:218:PRO:HA	1:G:246:PRO:O	2.09	0.53
1:G:291:ASP:OD1	1:G:292:ILE:HG13	2.08	0.53
1:H:42:LYS:HE2	1:H:48:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:305:ILE:HD12	1:H:305:ILE:N	2.23	0.53
1:J:368:ARG:O	1:J:372:LEU:HG	2.08	0.53
1:K:383:ALA:HB3	1:K:389:MET:HE2	1.90	0.53
2:V:77:LYS:NZ	2:V:80:ASN:HA	2.24	0.53
1:A:307:MET:C	1:A:308:GLU:HG3	2.34	0.53
1:D:392:LYS:O	1:D:396:VAL:HG23	2.09	0.53
1:E:124:VAL:HG13	1:E:504:LEU:HD12	1.89	0.53
1:E:234:LEU:HD11	1:E:238:GLU:OE1	2.08	0.53
1:H:346:VAL:HG13	1:H:369:VAL:HG13	1.91	0.53
1:I:355:GLU:HG3	1:I:356:ALA:H	1.74	0.53
1:J:174:VAL:HG12	1:J:376:VAL:HG22	1.91	0.53
1:J:181:THR:HG23	1:J:182:GLY:N	2.24	0.53
1:J:352:GLN:HA	1:J:355:GLU:HG2	1.90	0.53
1:K:227:ILE:HD12	1:K:233:MET:SD	2.49	0.53
1:L:95:LEU:O	1:L:99:ILE:HG13	2.09	0.53
1:N:74:VAL:O	1:N:77:VAL:HG12	2.09	0.53
1:N:230:ILE:O	1:N:309:LEU:HD22	2.09	0.53
2:P:3:ILE:HD12	2:P:3:ILE:O	2.08	0.53
2:R:48:ILE:HG12	2:R:54:VAL:CG1	2.32	0.53
1:A:220:ILE:HG13	1:A:296:THR:HG21	1.89	0.53
1:D:175:ILE:HG12	1:D:377:ALA:HB3	1.90	0.53
1:D:357:THR:CB	1:D:361:ASP:HB2	2.38	0.53
1:F:183:LEU:CD2	1:F:384:ALA:HA	2.39	0.53
1:F:479:ASN:ND2	1:F:493:ILE:HD11	2.24	0.53
1:H:215:LEU:O	1:H:322:ARG:HA	2.09	0.53
1:I:217:SER:N	1:I:218:PRO:HD3	2.24	0.53
1:J:203:TYR:OH	1:J:267:MET:HB2	2.08	0.53
1:N:227:ILE:HD12	1:N:227:ILE:N	2.24	0.53
2:P:37:ARG:NH2	2:Q:77:LYS:O	2.42	0.53
1:A:197:ARG:HG3	1:A:278:ALA:C	2.34	0.52
1:A:256:GLY:O	1:A:260:ALA:N	2.40	0.52
1:A:309:LEU:HD12	1:A:310:GLU:HB3	1.91	0.52
1:C:124:VAL:HG13	1:C:504:LEU:CD1	2.38	0.52
3:C:601:ADP:O2B	4:C:602:BEF:F1	2.17	0.52
1:D:368:ARG:O	1:D:372:LEU:HG	2.09	0.52
1:E:208:PRO:HG2	1:E:214:GLU:CG	2.38	0.52
1:G:13:ARG:HD2	1:G:104:LEU:HD22	1.90	0.52
1:J:193:MET:HE2	1:J:292:ILE:HG12	1.91	0.52
1:K:10:ASN:O	1:K:14:VAL:HG23	2.09	0.52
1:L:381:VAL:CG1	1:L:392:LYS:HB3	2.37	0.52
1:M:241:ALA:HA	1:M:271:VAL:CG1	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:124:VAL:HG21	1:N:508:ALA:CB	2.39	0.52
1:A:219:PHE:HB3	1:A:317:LEU:HD13	1.92	0.52
1:B:263:VAL:HG13	1:B:267:MET:HE2	1.90	0.52
1:C:510:VAL:O	1:C:514:MET:HB2	2.09	0.52
1:D:417:VAL:CA	1:D:420:ILE:HG22	2.37	0.52
1:G:349:ILE:O	1:G:353:ILE:HG13	2.10	0.52
1:H:221:LEU:HD13	1:H:317:LEU:CD2	2.26	0.52
1:I:218:PRO:HB3	1:I:246:PRO:HG2	1.90	0.52
1:L:305:ILE:HG22	1:L:306:GLY:H	1.75	0.52
1:N:496:PRO:HG2	1:N:499:VAL:HG11	1.92	0.52
2:1:96:GLU:O	2:2:1:MET:HB2	2.09	0.52
1:B:5:ASP:HB2	1:B:524:LEU:HD23	1.92	0.52
1:B:218:PRO:HG3	1:B:323:VAL:HG13	1.91	0.52
1:E:225:LYS:HZ1	1:E:230:ILE:HD11	1.74	0.52
1:E:448:GLU:O	1:E:452:ARG:HG2	2.10	0.52
1:G:422:VAL:O	1:G:426:LEU:HG	2.09	0.52
1:H:48:THR:HG22	1:H:390:LYS:HZ2	1.74	0.52
1:H:252:GLU:O	1:H:277:LYS:HG3	2.09	0.52
3:H:601:ADP:O3B	4:H:602:BEF:F3	2.18	0.52
1:K:280:GLY:C	1:K:285:ARG:HB3	2.33	0.52
1:M:25:ASP:OD1	1:M:97:GLN:NE2	2.43	0.52
1:M:219:PHE:O	1:M:247:LEU:HD12	2.10	0.52
2:T:40:VAL:HG22	2:T:41:LEU:N	2.24	0.52
2:Z:57:LEU:HD12	2:Z:57:LEU:N	2.24	0.52
2:1:17:VAL:HA	2:1:35:SER:N	2.24	0.52
1:A:346:VAL:O	1:A:350:ARG:HG2	2.08	0.52
1:A:364:LYS:HA	1:A:367:GLU:HB3	1.90	0.52
1:C:124:VAL:O	1:C:128:VAL:HG23	2.09	0.52
1:D:40:LEU:HD21	1:D:56:VAL:HG22	1.92	0.52
1:D:421:ARG:NH1	1:D:472:GLY:O	2.42	0.52
1:E:169:VAL:CG2	1:E:173:GLY:HA3	2.40	0.52
1:F:266:THR:CG2	1:F:273:VAL:H	2.23	0.52
1:F:313:THR:HG22	1:F:315:GLU:H	1.74	0.52
1:G:37:ASN:OD1	1:G:51:LYS:HB2	2.09	0.52
1:G:218:PRO:HG3	1:G:323:VAL:CG1	2.40	0.52
1:J:225:LYS:HG2	1:J:226:LYS:H	1.73	0.52
1:L:40:LEU:HD21	1:L:56:VAL:HG22	1.90	0.52
1:L:233:MET:C	1:L:235:PRO:HD2	2.35	0.52
1:L:305:ILE:HG22	1:L:306:GLY:N	2.24	0.52
1:N:305:ILE:HG22	1:N:306:GLY:N	2.21	0.52
2:T:35:SER:OG	2:T:37:ARG:O	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:36:THR:HB	2:1:67:PHE:O	2.10	0.52
1:A:34:LYS:HE3	1:A:480:ALA:O	2.09	0.52
1:A:419:LEU:HD21	1:A:500:THR:HG23	1.91	0.52
1:D:260:ALA:O	1:D:264:VAL:HG23	2.09	0.52
1:E:90:THR:HB	3:E:601:ADP:O2B	2.10	0.52
1:E:365:LEU:HD23	1:E:369:VAL:HG23	1.89	0.52
1:F:225:LYS:CB	1:F:309:LEU:HD21	2.39	0.52
1:F:349:ILE:HD11	1:F:365:LEU:HD23	1.90	0.52
1:F:517:THR:HG23	1:G:39:VAL:HG23	1.91	0.52
1:I:124:VAL:HG21	1:I:508:ALA:CB	2.39	0.52
1:I:419:LEU:HD21	1:I:500:THR:HG23	1.91	0.52
1:J:245:LYS:CB	1:J:246:PRO:HD2	2.38	0.52
1:J:455:VAL:HG21	1:J:465:VAL:HG11	1.90	0.52
1:L:40:LEU:HD13	1:L:59:GLU:CG	2.33	0.52
1:L:305:ILE:HA	1:M:264:VAL:HG12	1.92	0.52
1:L:363:GLU:HA	1:L:366:GLN:OE1	2.08	0.52
1:M:157:THR:O	1:M:161:LEU:HB2	2.09	0.52
1:M:252:GLU:HA	1:M:285:ARG:NH1	2.25	0.52
1:M:519:CYS:CB	1:N:38:VAL:HG13	2.39	0.52
1:N:242:LYS:C	1:N:242:LYS:HD3	2.35	0.52
1:N:510:VAL:O	1:N:514:MET:HB2	2.09	0.52
2:1:70:GLY:O	2:1:73:VAL:HG22	2.10	0.52
1:E:219:PHE:HB2	1:E:247:LEU:HD12	1.92	0.52
1:G:228:SER:HB3	1:G:255:GLU:CG	2.39	0.52
1:H:230:ILE:HG23	1:H:231:ARG:H	1.75	0.52
1:I:225:LYS:HG3	1:I:226:LYS:N	2.25	0.52
1:I:239:ALA:HB1	1:I:314:LEU:HD21	1.92	0.52
1:N:266:THR:HA	1:N:271:VAL:O	2.10	0.52
2:Y:15:LYS:HB2	2:Y:38:GLY:HA2	1.91	0.52
1:A:387:VAL:HG13	1:G:76:GLU:OE1	2.09	0.52
1:B:247:LEU:C	1:B:247:LEU:HD12	2.35	0.52
1:C:149:THR:OG1	1:C:159:GLY:HA3	2.08	0.52
1:C:305:ILE:HG13	1:D:267:MET:HE1	1.90	0.52
1:C:412:VAL:HG13	1:C:497:THR:OG1	2.08	0.52
1:E:223:ALA:O	1:E:224:ASP:HB2	2.09	0.52
1:G:27:VAL:CG1	1:G:90:THR:HG23	2.29	0.52
1:G:225:LYS:HB2	1:G:303:GLU:CD	2.35	0.52
1:G:358:SER:HA	1:G:362:ARG:HH21	1.74	0.52
1:H:114:MET:HE2	1:I:153:ASN:ND2	2.25	0.52
1:H:280:GLY:C	1:H:285:ARG:HB2	2.35	0.52
1:H:325:ILE:HG12	1:H:330:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:279:PRO:HB2	1:I:288:MET:HE3	1.92	0.52
1:K:218:PRO:HD2	1:K:320:ALA:O	2.09	0.52
1:L:519:CYS:HB3	1:M:38:VAL:HG22	1.91	0.52
1:M:449:ALA:HB3	1:M:450:PRO:HD3	1.91	0.52
1:N:256:GLY:O	1:N:260:ALA:N	2.43	0.52
1:N:447:MET:HE2	1:N:504:LEU:HD21	1.90	0.52
2:X:94:ILE:HD12	2:X:96:GLU:HG3	1.91	0.52
2:Z:93:ALA:CA	2:1:5:PRO:HA	2.39	0.52
1:A:463:SER:HB3	1:H:464:VAL:HG23	1.91	0.52
1:B:77:VAL:CG2	1:B:507:ALA:HA	2.35	0.52
1:M:261:THR:O	1:M:264:VAL:HG22	2.10	0.52
1:N:48:THR:HG22	1:N:390:LYS:NZ	2.24	0.52
1:N:363:GLU:HG3	1:N:364:LYS:N	2.25	0.52
2:R:20:LYS:HB2	2:R:22:ALA:H	1.75	0.52
2:S:12:VAL:HA	2:S:40:VAL:HA	1.92	0.52
2:S:46:GLY:HA2	2:S:57:LEU:CD1	2.40	0.52
2:V:88:GLU:HA	2:V:91:ILE:HD13	1.91	0.52
1:B:351:GLN:HG2	1:C:210:THR:CB	2.40	0.52
1:C:124:VAL:HG21	1:C:508:ALA:HB1	1.92	0.52
1:D:350:ARG:HD2	1:D:353:ILE:CD1	2.38	0.52
1:E:214:GLU:HA	1:E:323:VAL:O	2.10	0.52
1:F:28:LYS:HG2	1:F:94:VAL:HG22	1.92	0.52
1:G:199:TYR:HE1	1:G:202:PRO:HB3	1.75	0.52
1:I:396:VAL:O	1:I:400:LEU:HB2	2.10	0.52
1:J:236:VAL:HG11	1:J:312:ALA:HB3	1.92	0.52
1:K:116:LEU:O	1:K:120:ILE:HG13	2.10	0.52
1:L:39:VAL:HG22	1:L:49:ILE:HG12	1.92	0.52
1:M:325:ILE:CG1	1:M:330:THR:HG23	2.29	0.52
2:Q:94:ILE:HG13	2:Q:94:ILE:O	2.10	0.52
2:W:71:TYR:C	2:W:71:TYR:CD1	2.88	0.52
1:E:415:GLY:N	3:E:601:ADP:O2'	2.34	0.52
1:F:509:SER:OG	1:G:385:THR:HG22	2.10	0.52
1:G:221:LEU:HD12	1:G:221:LEU:N	2.25	0.52
1:L:77:VAL:HG21	1:L:507:ALA:HA	1.92	0.52
1:L:221:LEU:O	1:L:221:LEU:HD12	2.10	0.52
1:M:147:VAL:HG12	1:M:494:LEU:HD12	1.91	0.52
1:M:201:SER:HB3	1:M:204:PHE:CZ	2.44	0.52
1:M:510:VAL:O	1:M:514:MET:HB2	2.10	0.52
2:U:39:GLU:HA	2:U:64:ILE:HA	1.91	0.52
1:A:254:VAL:HG11	1:A:259:LEU:HD13	1.92	0.51
1:D:200:LEU:HD13	1:D:276:VAL:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:PHE:HD2	1:D:240:VAL:HG22	1.75	0.51
1:E:222:LEU:HD12	1:E:222:LEU:O	2.10	0.51
1:F:291:ASP:OD1	1:F:292:ILE:N	2.43	0.51
1:H:177:VAL:CG1	1:H:397:GLU:HG2	2.39	0.51
1:K:197:ARG:HH12	1:K:277:LYS:HD2	1.75	0.51
1:L:195:PHE:O	1:L:329:THR:OG1	2.29	0.51
1:M:116:LEU:O	1:M:120:ILE:HG13	2.09	0.51
1:M:415:GLY:N	3:M:601:ADP:O2'	2.41	0.51
1:N:61:GLU:C	1:N:62:LEU:HD12	2.35	0.51
2:O:49:LEU:CD1	2:O:50:GLU:H	2.22	0.51
2:Q:51:ASN:O	2:Q:53:GLU:N	2.43	0.51
2:U:85:ILE:HD12	2:U:85:ILE:O	2.10	0.51
1:B:85:ALA:O	1:B:401:HIS:HB3	2.11	0.51
1:B:270:ILE:HG12	2:P:25:ILE:CD1	2.38	0.51
1:B:493:ILE:C	1:B:494:LEU:HD12	2.35	0.51
1:C:255:GLU:OE1	1:C:255:GLU:N	2.42	0.51
1:D:34:LYS:HD2	1:D:458:CYS:SG	2.50	0.51
1:H:220:ILE:N	1:H:220:ILE:HD12	2.25	0.51
1:H:227:ILE:HA	1:H:230:ILE:HG22	1.93	0.51
1:I:115:ASP:O	1:I:436:GLN:HG2	2.10	0.51
1:J:103:GLY:O	1:J:107:VAL:HG23	2.10	0.51
1:J:265:ASN:OD1	1:J:266:THR:N	2.44	0.51
1:J:419:LEU:HD12	1:J:419:LEU:H	1.74	0.51
1:K:5:ASP:HB2	1:K:524:LEU:CD2	2.38	0.51
1:L:136:VAL:CG2	1:L:137:PRO:HD2	2.40	0.51
1:L:229:ASN:OD1	1:L:230:ILE:HD12	2.09	0.51
1:M:325:ILE:HD12	1:M:325:ILE:N	2.24	0.51
2:O:64:ILE:CG2	2:O:95:VAL:HB	2.30	0.51
2:Q:45:ASN:OD1	2:Q:46:GLY:N	2.42	0.51
2:R:11:ILE:CG2	2:R:42:ALA:HB3	2.40	0.51
2:R:67:PHE:CB	2:R:86:MET:HE1	2.39	0.51
2:U:10:VAL:HG11	2:U:91:ILE:CD1	2.39	0.51
2:Y:40:VAL:HG11	2:Y:60:LYS:O	2.11	0.51
1:A:450:PRO:O	1:A:454:ILE:HG13	2.10	0.51
1:B:221:LEU:HD23	1:B:221:LEU:C	2.34	0.51
1:B:255:GLU:HB3	1:B:257:GLU:OE1	2.09	0.51
1:C:302:SER:HB2	1:C:305:ILE:HD13	1.92	0.51
1:E:199:TYR:CA	1:E:276:VAL:HG12	2.37	0.51
1:F:245:LYS:CB	1:F:246:PRO:HD2	2.35	0.51
1:G:221:LEU:HD13	1:G:249:ILE:CD1	2.30	0.51
1:I:228:SER:CB	1:I:255:GLU:HB2	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:169:VAL:HB	1:J:375:GLY:O	2.10	0.51
1:J:199:TYR:HA	1:J:276:VAL:HG12	1.91	0.51
1:J:305:ILE:HG23	1:J:306:GLY:N	2.25	0.51
1:J:350:ARG:HA	1:J:353:ILE:CD1	2.40	0.51
1:L:4:LYS:HG3	1:M:59:GLU:O	2.10	0.51
1:L:247:LEU:HD22	1:L:248:LEU:H	1.74	0.51
1:M:88:GLY:HA2	3:M:601:ADP:PB	2.49	0.51
1:M:199:TYR:HD2	1:M:325:ILE:HG22	1.75	0.51
1:N:10:ASN:O	1:N:14:VAL:HG23	2.11	0.51
1:N:197:ARG:HG2	1:N:277:LYS:CB	2.39	0.51
2:Q:48:ILE:HD12	2:Q:48:ILE:N	2.25	0.51
2:R:51:ASN:C	2:R:53:GLU:H	2.17	0.51
2:T:13:LYS:HG3	2:T:83:VAL:HG12	1.91	0.51
2:X:27:LEU:C	2:X:27:LEU:HD12	2.35	0.51
2:Z:50:GLU:O	2:Z:51:ASN:OD1	2.29	0.51
2:2:49:LEU:HB2	2:2:52:GLY:HA2	1.92	0.51
1:A:291:ASP:HB3	1:A:372:LEU:CD2	2.40	0.51
1:B:285:ARG:O	1:B:289:LEU:HG	2.10	0.51
1:C:285:ARG:HG3	1:C:286:LYS:N	2.25	0.51
1:C:350:ARG:HH12	1:C:369:VAL:CG1	2.19	0.51
1:D:69:MET:HE2	1:D:520:MET:HE3	1.93	0.51
1:D:381:VAL:HG13	1:D:392:LYS:HG2	1.90	0.51
1:E:256:GLY:HA2	1:E:259:LEU:HD12	1.91	0.51
1:E:419:LEU:O	1:E:422:VAL:HG22	2.11	0.51
1:G:215:LEU:HB2	1:G:323:VAL:CG2	2.40	0.51
1:I:414:GLY:HA2	1:I:495:ASP:OD2	2.11	0.51
1:M:10:ASN:O	1:M:14:VAL:HG23	2.11	0.51
1:N:199:TYR:HE1	1:N:202:PRO:HA	1.69	0.51
1:N:222:LEU:HD12	1:N:222:LEU:N	2.26	0.51
1:N:493:ILE:C	1:N:494:LEU:HD12	2.35	0.51
2:S:20:LYS:HE3	2:S:29:GLY:H	1.75	0.51
2:V:11:ILE:O	2:V:41:LEU:HB2	2.10	0.51
2:1:6:LEU:HB3	2:1:7:HIS:HB2	1.91	0.51
2:2:68:ASN:N	2:2:68:ASN:OD1	2.42	0.51
1:A:199:TYR:OH	1:A:205:ILE:HD11	2.10	0.51
1:A:216:GLU:HB2	1:A:245:LYS:NZ	2.26	0.51
1:B:319:GLN:O	1:B:336:VAL:HG23	2.11	0.51
1:D:392:LYS:HD2	1:D:395:ARG:NH2	2.25	0.51
1:D:450:PRO:O	1:D:454:ILE:HG13	2.11	0.51
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.92	0.51
1:E:199:TYR:OH	1:E:327:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:MET:HE3	1:E:311:LYS:HZ2	1.75	0.51
1:J:226:LYS:HB2	1:J:252:GLU:CD	2.35	0.51
1:J:519:CYS:HB3	1:K:38:VAL:HG22	1.90	0.51
1:K:305:ILE:HD12	1:K:305:ILE:N	2.25	0.51
1:M:37:ASN:OD1	1:M:51:LYS:HB2	2.09	0.51
1:M:405:ALA:HB1	1:M:498:LYS:HD3	1.92	0.51
1:M:414:GLY:HA2	1:M:495:ASP:OD2	2.09	0.51
2:P:12:VAL:HG13	2:P:39:GLU:O	2.10	0.51
2:R:48:ILE:HG23	2:R:54:VAL:CG1	2.41	0.51
2:S:25:ILE:N	2:S:25:ILE:HD12	2.25	0.51
2:W:20:LYS:NZ	2:X:77:LYS:HB2	2.26	0.51
2:Y:15:LYS:HD2	2:Y:37:ARG:HB3	1.91	0.51
2:Y:17:VAL:HG23	2:Y:33:ALA:HB3	1.92	0.51
1:A:231:ARG:HB3	1:A:258:ALA:HB1	1.92	0.51
1:B:90:THR:HB	3:B:601:ADP:O1B	2.11	0.51
1:B:230:ILE:HG23	1:B:230:ILE:O	2.11	0.51
1:B:342:ILE:O	1:B:346:VAL:HG23	2.11	0.51
1:B:393:LYS:O	1:B:397:GLU:HG3	2.11	0.51
1:E:278:ALA:HB1	1:E:285:ARG:HD2	1.91	0.51
1:F:245:LYS:HB3	1:F:246:PRO:CD	2.36	0.51
1:G:223:ALA:HB3	1:G:224:ASP:CA	2.40	0.51
1:H:176:THR:OG1	1:H:378:VAL:HG22	2.10	0.51
1:H:496:PRO:HG2	1:H:499:VAL:CG1	2.39	0.51
1:J:220:ILE:HG21	1:J:296:THR:OG1	2.10	0.51
1:M:175:ILE:HA	1:M:377:ALA:O	2.10	0.51
1:N:13:ARG:HD3	1:N:104:LEU:HD22	1.93	0.51
2:P:17:VAL:HG12	2:P:35:SER:CA	2.41	0.51
2:Q:11:ILE:O	2:Q:41:LEU:HB2	2.10	0.51
2:R:20:LYS:HB2	2:R:22:ALA:HB3	1.92	0.51
2:R:77:LYS:HG3	2:R:81:GLU:O	2.11	0.51
2:U:83:VAL:C	2:U:84:LEU:HD12	2.35	0.51
2:Z:14:ARG:NH1	2:Z:84:LEU:HD21	2.25	0.51
2:Z:92:LEU:HD22	2:1:9:ARG:HD3	1.93	0.51
1:B:228:SER:HA	1:B:255:GLU:HB2	1.92	0.51
1:C:205:ILE:HA	1:C:213:VAL:HG22	1.91	0.51
1:F:40:LEU:HD21	1:F:56:VAL:HG22	1.93	0.51
1:I:311:LYS:HB3	1:I:311:LYS:HZ2	1.76	0.51
1:J:34:LYS:NZ	1:J:483:GLU:OE2	2.38	0.51
1:K:42:LYS:HE2	1:K:48:THR:OG1	2.11	0.51
1:L:357:THR:HG22	1:L:359:ASP:HB2	1.91	0.51
1:M:218:PRO:HD2	1:M:320:ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:223:ALA:HA	1:N:301:ILE:O	2.11	0.51
2:U:83:VAL:HG12	2:U:84:LEU:N	2.25	0.51
2:V:6:LEU:HD11	2:2:91:ILE:O	2.11	0.51
2:V:49:LEU:HD12	2:W:50:GLU:HG3	1.92	0.51
2:W:6:LEU:HD23	2:W:6:LEU:C	2.36	0.51
2:1:57:LEU:HD22	2:1:57:LEU:H	1.76	0.51
1:A:77:VAL:HB	1:A:510:VAL:HG21	1.93	0.51
1:A:291:ASP:OD2	1:A:368:ARG:HD3	2.11	0.51
1:A:355:GLU:HG3	1:A:356:ALA:N	2.26	0.51
1:B:42:LYS:HE2	1:B:48:THR:HG21	1.92	0.51
1:F:17:LEU:HG	1:F:21:ASN:ND2	2.25	0.51
1:F:234:LEU:HB2	1:F:235:PRO:HD3	1.91	0.51
1:H:207:LYS:HB3	1:H:208:PRO:CD	2.33	0.51
1:H:241:ALA:CB	2:V:25:ILE:HD12	2.38	0.51
1:I:199:TYR:HA	1:I:276:VAL:HG12	1.93	0.51
1:I:220:ILE:HD12	1:I:220:ILE:N	2.25	0.51
1:I:234:LEU:N	1:I:235:PRO:HD2	2.25	0.51
1:I:237:LEU:HD23	2:W:27:LEU:CD2	2.40	0.51
1:N:227:ILE:HG23	1:N:231:ARG:CG	2.40	0.51
1:N:309:LEU:HD12	1:N:310:GLU:N	2.26	0.51
2:S:50:GLU:CG	2:S:51:ASN:N	2.65	0.51
2:T:12:VAL:HA	2:T:40:VAL:HA	1.91	0.51
2:W:78:ILE:HG13	2:W:79:ASP:N	2.20	0.51
1:B:103:GLY:O	1:B:107:VAL:HG23	2.10	0.51
1:B:406:ALA:HB2	1:B:496:PRO:HB3	1.92	0.51
1:G:223:ALA:HB3	1:G:224:ASP:HA	1.93	0.51
1:H:88:GLY:N	4:H:602:BEF:F3	2.34	0.51
1:I:237:LEU:HD23	2:W:27:LEU:HD22	1.93	0.51
1:L:149:THR:HG22	1:L:155:ASP:O	2.10	0.51
1:M:309:LEU:CB	1:M:310:GLU:OE1	2.58	0.51
1:N:115:ASP:O	1:N:436:GLN:HG2	2.11	0.51
1:N:233:MET:HB3	1:N:236:VAL:HB	1.93	0.51
2:Q:43:VAL:HG22	2:Q:44:GLY:O	2.10	0.51
2:T:37:ARG:HH12	2:U:78:ILE:HG22	1.76	0.51
2:U:50:GLU:O	2:U:52:GLY:N	2.44	0.51
1:A:174:VAL:HG13	1:A:370:ALA:HB1	1.92	0.51
1:A:247:LEU:HG	1:A:273:VAL:HG11	1.92	0.51
1:A:278:ALA:HB3	1:A:285:ARG:NE	2.26	0.51
1:A:309:LEU:HD12	1:A:310:GLU:CB	2.37	0.51
1:B:348:GLN:HA	1:C:209:GLU:HG2	1.93	0.51
1:B:465:VAL:O	1:B:469:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:GLU:O	1:C:342:ILE:HD13	2.11	0.51
1:D:90:THR:HB	3:D:601:ADP:O2B	2.11	0.51
1:G:228:SER:HB3	1:G:255:GLU:CD	2.35	0.51
1:H:282:GLY:HA2	1:H:285:ARG:HH21	1.77	0.51
1:H:406:ALA:HB2	1:H:496:PRO:HB3	1.93	0.51
1:J:404:ARG:O	1:J:408:GLU:HG2	2.11	0.51
1:L:107:VAL:HG13	1:L:113:PRO:HG3	1.92	0.51
1:M:200:LEU:CD2	1:M:254:VAL:H	2.24	0.51
1:M:200:LEU:HD11	1:M:277:LYS:CG	2.41	0.51
1:M:205:ILE:HA	1:M:213:VAL:HG22	1.93	0.51
1:M:323:VAL:HG12	1:M:332:ILE:HG12	1.93	0.51
1:N:177:VAL:CG2	1:N:396:VAL:HG11	2.42	0.51
2:O:95:VAL:CB	2:P:3:ILE:CG2	2.87	0.51
2:R:95:VAL:HA	2:S:3:ILE:HG22	1.92	0.51
2:W:84:LEU:O	2:W:84:LEU:HD12	2.10	0.51
2:X:25:ILE:N	2:X:25:ILE:HD12	2.26	0.51
2:1:14:ARG:NH2	2:1:69:ASP:OD2	2.44	0.51
2:1:65:VAL:HG12	2:1:94:ILE:CG2	2.35	0.51
1:C:233:MET:HE3	1:C:237:LEU:HD12	1.93	0.50
1:E:218:PRO:HA	1:E:246:PRO:O	2.11	0.50
1:E:248:LEU:HD22	1:E:323:VAL:CG1	2.34	0.50
1:F:102:GLU:OE1	1:F:445:ARG:NH1	2.39	0.50
1:F:405:ALA:HB1	1:F:498:LYS:HD3	1.92	0.50
1:F:419:LEU:HD11	1:F:500:THR:CG2	2.39	0.50
1:G:73:MET:HB3	1:G:514:MET:HE2	1.93	0.50
1:H:232:GLU:CG	1:H:233:MET:H	2.22	0.50
1:H:510:VAL:O	1:H:514:MET:HB2	2.11	0.50
1:I:496:PRO:O	1:I:499:VAL:HG22	2.11	0.50
1:J:231:ARG:HH21	1:J:261:THR:HG21	1.76	0.50
1:K:77:VAL:CG1	1:K:510:VAL:HG21	2.41	0.50
1:K:102:GLU:OE1	1:K:445:ARG:NH1	2.41	0.50
1:M:197:ARG:CG	1:M:277:LYS:HB2	2.41	0.50
1:M:215:LEU:HD22	1:M:246:PRO:HB3	1.93	0.50
1:N:247:LEU:HB3	1:N:273:VAL:HG13	1.93	0.50
2:Q:65:VAL:HG12	2:Q:94:ILE:HG22	1.93	0.50
2:Y:5:PRO:HD3	2:Y:42:ALA:HB1	1.93	0.50
1:C:197:ARG:NE	1:C:277:LYS:HD2	2.18	0.50
1:C:208:PRO:HB2	1:C:212:ALA:CB	2.26	0.50
1:C:219:PHE:H	1:C:247:LEU:HA	1.75	0.50
1:D:288:MET:HG3	1:D:368:ARG:HE	1.75	0.50
1:D:381:VAL:HG13	1:D:392:LYS:CG	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:VAL:CG1	1:D:392:LYS:HB3	2.41	0.50
1:E:20:VAL:HG13	1:E:74:VAL:HG11	1.93	0.50
1:E:245:LYS:HE2	1:E:246:PRO:CD	2.38	0.50
1:G:199:TYR:HE2	1:G:327:LYS:HG3	1.74	0.50
1:J:230:ILE:C	1:J:231:ARG:HG2	2.36	0.50
1:J:233:MET:O	1:J:236:VAL:N	2.42	0.50
1:L:247:LEU:HD13	1:L:247:LEU:C	2.36	0.50
1:L:248:LEU:HD13	1:L:249:ILE:N	2.25	0.50
1:L:295:LEU:C	1:L:295:LEU:HD23	2.36	0.50
1:M:225:LYS:HG3	1:M:226:LYS:N	2.26	0.50
1:N:220:ILE:N	1:N:220:ILE:HD12	2.27	0.50
2:V:57:LEU:CD1	2:V:59:VAL:HG22	2.41	0.50
2:X:57:LEU:HD23	2:X:88:GLU:HB2	1.93	0.50
1:A:279:PRO:HB2	1:A:288:MET:HE1	1.93	0.50
1:B:200:LEU:HD11	1:B:277:LYS:HB2	1.94	0.50
1:B:496:PRO:HG2	1:B:499:VAL:HG13	1.94	0.50
1:E:117:LYS:NZ	1:E:121:ASP:OD2	2.43	0.50
1:E:138:CYS:SG	1:E:144:ILE:HD13	2.51	0.50
1:E:219:PHE:CE1	1:E:319:GLN:HG2	2.46	0.50
1:E:455:VAL:HG21	1:E:465:VAL:HG11	1.93	0.50
1:F:225:LYS:HB2	1:F:303:GLU:OE2	2.10	0.50
1:F:353:ILE:HD11	1:F:369:VAL:HG21	1.93	0.50
1:H:87:ASP:OD2	1:H:151:SER:OG	2.27	0.50
1:I:177:VAL:HG11	1:I:397:GLU:HG3	1.93	0.50
1:I:305:ILE:HD12	1:I:305:ILE:N	2.27	0.50
1:I:405:ALA:HB1	1:I:498:LYS:HB3	1.92	0.50
1:I:409:GLU:CD	1:I:501:ARG:HH21	2.18	0.50
1:L:350:ARG:HD3	1:L:353:ILE:HD11	1.92	0.50
1:L:429:LEU:HD12	1:L:430:ARG:N	2.26	0.50
1:L:436:GLN:O	1:L:440:ILE:HG13	2.11	0.50
1:M:367:GLU:HG2	1:M:371:LYS:NZ	2.25	0.50
1:N:415:GLY:N	3:N:601:ADP:O2'	2.29	0.50
2:O:17:VAL:HG23	2:O:34:LYS:HA	1.94	0.50
2:Q:60:LYS:HZ1	2:Q:63:ASP:HB3	1.75	0.50
1:A:267:MET:HG3	1:G:305:ILE:CG1	2.37	0.50
1:A:478:TYR:HD1	1:A:485:TYR:CE1	2.30	0.50
1:C:256:GLY:HA2	1:C:259:LEU:HB2	1.92	0.50
1:D:228:SER:OG	1:D:255:GLU:HG2	2.12	0.50
1:D:349:ILE:O	1:D:353:ILE:HG13	2.11	0.50
1:E:116:LEU:O	1:E:120:ILE:HG13	2.11	0.50
1:J:172:GLU:HB3	1:J:366:GLN:OE1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:241:ALA:HA	1:J:271:VAL:CG1	2.42	0.50
1:J:450:PRO:O	1:J:454:ILE:HG13	2.10	0.50
1:K:220:ILE:N	1:K:220:ILE:HD12	2.27	0.50
1:M:268:ARG:N	1:M:269:GLY:HA2	2.26	0.50
1:N:90:THR:HB	3:N:601:ADP:O2B	2.12	0.50
1:B:6:VAL:CG1	1:B:521:VAL:HG22	2.34	0.50
1:B:218:PRO:CB	1:B:248:LEU:HD23	2.41	0.50
1:C:8:PHE:HE1	1:D:26:ALA:HA	1.77	0.50
3:D:601:ADP:O3B	4:D:602:BEF:F3	2.19	0.50
1:E:7:LYS:HG3	1:E:66:PHE:CE2	2.46	0.50
1:G:247:LEU:HD23	1:G:273:VAL:HG22	1.93	0.50
1:H:367:GLU:O	1:H:371:LYS:HG3	2.12	0.50
1:I:488:MET:HE3	1:I:493:ILE:HG21	1.94	0.50
1:K:343:GLN:HA	1:K:346:VAL:HG22	1.93	0.50
1:L:166:MET:HE1	1:L:407:VAL:HG21	1.92	0.50
1:L:213:VAL:O	1:L:324:VAL:HA	2.12	0.50
1:M:284:ARG:HG2	1:M:288:MET:HE2	1.94	0.50
2:Q:50:GLU:CG	2:Q:51:ASN:N	2.74	0.50
2:T:53:GLU:CG	2:T:54:VAL:N	2.75	0.50
2:1:18:GLU:HB3	2:1:28:THR:HB	1.93	0.50
1:A:220:ILE:HG22	1:A:222:LEU:HD11	1.93	0.50
1:A:234:LEU:O	1:A:238:GLU:N	2.34	0.50
1:C:367:GLU:O	1:C:371:LYS:HG3	2.12	0.50
1:D:357:THR:HB	1:D:361:ASP:CG	2.37	0.50
1:F:348:GLN:OE1	1:F:352:GLN:NE2	2.44	0.50
1:G:450:PRO:O	1:G:454:ILE:HG13	2.12	0.50
1:H:149:THR:HG23	1:H:155:ASP:C	2.37	0.50
1:H:174:VAL:CG2	1:H:376:VAL:HG22	2.41	0.50
1:I:240:VAL:HG12	1:I:245:LYS:O	2.11	0.50
1:I:347:ALA:O	1:I:350:ARG:HB2	2.12	0.50
1:J:238:GLU:HG3	1:J:242:LYS:HZ1	1.76	0.50
1:J:381:VAL:CG2	1:J:396:VAL:HG21	2.42	0.50
1:L:179:ASP:OD1	1:L:393:LYS:HD2	2.11	0.50
1:N:398:ASP:OD2	4:N:602:BEF:F1	2.20	0.50
2:V:49:LEU:HD13	2:V:50:GLU:HB2	1.94	0.50
2:2:28:THR:HG22	2:2:29:GLY:O	2.12	0.50
1:D:200:LEU:HD13	1:D:275:ALA:O	2.11	0.50
1:E:28:LYS:HG2	1:E:94:VAL:HG22	1.93	0.50
1:E:409:GLU:CD	1:E:501:ARG:HH21	2.18	0.50
1:F:392:LYS:O	1:F:396:VAL:HG23	2.11	0.50
1:G:221:LEU:HD11	1:G:317:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:LEU:HD13	1:H:104:LEU:HD12	1.94	0.50
1:H:233:MET:HG2	1:H:233:MET:O	2.10	0.50
1:I:313:THR:HG22	1:I:314:LEU:N	2.27	0.50
1:K:23:LEU:CD2	1:K:60:ILE:HB	2.41	0.50
1:K:207:LYS:HG2	1:K:208:PRO:CD	2.21	0.50
1:K:414:GLY:HA2	1:K:495:ASP:OD2	2.12	0.50
1:M:124:VAL:HG13	1:M:504:LEU:HD12	1.92	0.50
1:N:197:ARG:CG	1:N:277:LYS:HB3	2.41	0.50
2:P:25:ILE:C	2:P:25:ILE:HD12	2.36	0.50
2:1:91:ILE:HG22	2:2:6:LEU:HD12	1.92	0.50
1:A:215:LEU:HB2	1:A:323:VAL:CG2	2.42	0.50
1:B:285:ARG:NH1	1:B:289:LEU:HD11	2.27	0.50
1:E:291:ASP:OD1	1:E:345:ARG:NH2	2.39	0.50
1:F:168:LYS:CG	1:F:189:VAL:HG11	2.36	0.50
1:G:215:LEU:HD22	1:G:246:PRO:HB2	1.93	0.50
1:H:14:VAL:O	1:H:18:ARG:HG3	2.11	0.50
1:H:183:LEU:N	1:H:183:LEU:HD12	2.27	0.50
1:H:415:GLY:N	3:H:601:ADP:O2'	2.39	0.50
1:I:157:THR:O	1:I:161:LEU:HD13	2.11	0.50
1:J:234:LEU:HA	1:J:237:LEU:HB3	1.94	0.50
1:K:17:LEU:HD13	1:K:104:LEU:HD12	1.94	0.50
1:K:359:ASP:C	1:K:361:ASP:H	2.19	0.50
1:L:204:PHE:C	1:L:213:VAL:HG22	2.37	0.50
1:L:216:GLU:CD	1:L:217:SER:N	2.70	0.50
1:M:175:ILE:HG12	1:M:377:ALA:HB3	1.93	0.50
1:M:409:GLU:OE1	1:M:498:LYS:HA	2.12	0.50
1:N:197:ARG:HG2	1:N:277:LYS:N	2.27	0.50
1:N:208:PRO:HB2	1:N:212:ALA:HB3	1.94	0.50
2:S:50:GLU:HG2	2:S:51:ASN:N	2.20	0.50
1:C:246:PRO:HA	1:C:272:LYS:O	2.12	0.50
1:D:313:THR:HG21	1:D:315:GLU:HG2	1.93	0.50
1:E:142:LYS:O	1:E:146:GLN:HG3	2.11	0.50
1:H:232:GLU:HA	1:H:234:LEU:CD1	2.42	0.50
1:H:248:LEU:HD13	1:H:249:ILE:N	2.26	0.50
1:H:333:ILE:O	1:H:334:ASP:HB2	2.11	0.50
1:I:359:ASP:O	1:I:360:TYR:HB3	2.11	0.50
1:J:360:TYR:O	1:J:363:GLU:HG2	2.12	0.50
1:K:155:ASP:OD1	1:K:157:THR:OG1	2.20	0.50
1:L:405:ALA:HB1	1:L:498:LYS:HD3	1.94	0.50
1:L:417:VAL:O	1:L:421:ARG:HB2	2.12	0.50
1:M:233:MET:O	1:M:234:LEU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:261:THR:HB	2:2:29:GLY:N	2.21	0.50
1:N:342:ILE:O	1:N:346:VAL:HG23	2.12	0.50
2:O:95:VAL:CA	2:P:3:ILE:HG21	2.28	0.50
2:O:97:ALA:HB2	2:P:1:MET:CB	2.42	0.50
2:S:39:GLU:O	2:S:39:GLU:HG2	2.11	0.50
2:1:57:LEU:HD22	2:1:57:LEU:N	2.27	0.50
1:A:40:LEU:HD11	1:A:56:VAL:HA	1.93	0.49
1:A:191:GLU:OE1	1:A:191:GLU:N	2.36	0.49
1:B:234:LEU:O	1:B:237:LEU:N	2.40	0.49
1:B:479:ASN:HB3	1:B:484:GLU:O	2.12	0.49
1:D:6:VAL:HG22	1:D:521:VAL:HG22	1.94	0.49
1:E:254:VAL:HG12	1:E:259:LEU:HG	1.93	0.49
1:F:195:PHE:CE1	1:F:330:THR:HB	2.46	0.49
1:F:420:ILE:HD11	1:F:451:LEU:CB	2.39	0.49
1:G:31:LEU:HD12	3:G:601:ADP:O2A	2.11	0.49
1:G:409:GLU:OE2	1:G:501:ARG:NH2	2.27	0.49
1:G:496:PRO:HG2	1:G:499:VAL:CG1	2.42	0.49
1:H:241:ALA:HA	1:H:271:VAL:HG11	1.94	0.49
1:M:339:GLU:O	1:M:343:GLN:HB2	2.12	0.49
1:N:88:GLY:N	4:N:602:BEF:F3	2.34	0.49
2:O:17:VAL:HB	2:O:34:LYS:HE3	1.94	0.49
2:U:78:ILE:HD12	2:U:78:ILE:C	2.37	0.49
1:A:456:LEU:HD23	1:A:456:LEU:O	2.11	0.49
1:B:336:VAL:O	1:B:336:VAL:HG12	2.12	0.49
1:D:345:ARG:O	1:D:349:ILE:HG13	2.11	0.49
1:D:414:GLY:HA2	1:D:495:ASP:OD2	2.13	0.49
1:G:91:THR:OG1	3:G:601:ADP:O2B	2.29	0.49
1:H:149:THR:HG22	1:H:154:SER:HA	1.94	0.49
1:K:101:THR:O	1:K:105:LYS:HG2	2.11	0.49
1:K:232:GLU:O	1:K:235:PRO:HD2	2.12	0.49
1:K:248:LEU:HD13	1:K:248:LEU:C	2.37	0.49
2:U:2:ASN:C	2:U:3:ILE:HD12	2.37	0.49
2:Y:34:LYS:CE	2:Z:76:GLU:HA	2.34	0.49
1:A:90:THR:O	1:A:94:VAL:HG23	2.12	0.49
1:A:231:ARG:HD2	1:A:261:THR:HG21	1.94	0.49
1:B:247:LEU:C	1:B:248:LEU:HD22	2.37	0.49
1:B:414:GLY:HA2	1:B:495:ASP:OD2	2.12	0.49
1:E:345:ARG:O	1:E:349:ILE:HG13	2.12	0.49
1:H:5:ASP:HB2	1:H:524:LEU:HD21	1.92	0.49
1:J:350:ARG:HD3	1:J:353:ILE:HD11	1.93	0.49
1:K:20:VAL:HG13	1:K:74:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:205:ILE:CD1	1:K:211:GLY:HA2	2.37	0.49
1:K:415:GLY:N	3:K:601:ADP:O2'	2.32	0.49
1:M:364:LYS:HD3	1:M:364:LYS:C	2.37	0.49
1:N:524:LEU:CD2	1:N:525:PRO:HD2	2.42	0.49
2:P:36:THR:HG21	2:Q:76:GLU:OE2	2.12	0.49
2:S:64:ILE:HG23	2:S:95:VAL:CG1	2.32	0.49
1:B:197:ARG:NE	1:B:277:LYS:HD3	2.25	0.49
1:C:218:PRO:HG3	1:C:323:VAL:HG13	1.94	0.49
1:C:238:GLU:O	2:Q:25:ILE:HD11	2.12	0.49
1:D:230:ILE:C	1:D:231:ARG:HG2	2.33	0.49
1:D:409:GLU:OE2	1:D:501:ARG:NH2	2.28	0.49
3:E:601:ADP:O3B	4:E:602:BEF:F1	2.21	0.49
1:G:6:VAL:CG1	1:G:521:VAL:HG22	2.39	0.49
1:I:193:MET:HE1	1:I:292:ILE:HG13	1.93	0.49
1:K:299:THR:N	1:K:316:ASP:O	2.41	0.49
1:K:333:ILE:O	1:K:334:ASP:HB2	2.11	0.49
1:M:268:ARG:CB	1:M:269:GLY:HA2	2.41	0.49
1:N:181:THR:OG1	1:N:182:GLY:N	2.46	0.49
2:O:4:ARG:CD	2:U:96:GLU:HG3	2.41	0.49
2:P:40:VAL:HG23	2:P:63:ASP:O	2.12	0.49
2:Q:56:PRO:O	2:Q:57:LEU:HG	2.12	0.49
2:V:57:LEU:HD12	2:V:57:LEU:C	2.38	0.49
2:W:8:ASP:OD2	2:W:8:ASP:N	2.42	0.49
1:B:10:ASN:O	1:B:14:VAL:HG23	2.12	0.49
1:B:227:ILE:O	1:B:227:ILE:HG22	2.13	0.49
1:B:488:MET:HE3	1:B:493:ILE:HD12	1.95	0.49
1:C:49:ILE:N	1:C:49:ILE:HD12	2.27	0.49
1:C:116:LEU:O	1:C:120:ILE:HG13	2.13	0.49
1:C:276:VAL:HG11	1:C:330:THR:HG21	1.94	0.49
1:E:493:ILE:C	1:E:494:LEU:HD12	2.38	0.49
1:F:233:MET:HG3	1:F:234:LEU:N	2.27	0.49
1:I:149:THR:HG23	1:I:155:ASP:C	2.38	0.49
1:I:234:LEU:HD12	1:I:234:LEU:H	1.77	0.49
1:I:420:ILE:HD11	1:I:470:LYS:HG3	1.93	0.49
1:J:171:LYS:HD3	1:J:407:VAL:CG1	2.43	0.49
1:J:493:ILE:C	1:J:494:LEU:HD12	2.38	0.49
1:K:415:GLY:O	1:K:451:LEU:HD12	2.12	0.49
1:L:29:VAL:O	1:L:29:VAL:HG12	2.12	0.49
1:L:34:LYS:HE3	1:L:480:ALA:O	2.13	0.49
1:L:200:LEU:HD11	1:L:277:LYS:HB2	1.94	0.49
1:N:284:ARG:HG2	1:N:288:MET:CE	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:285:ARG:O	1:N:289:LEU:N	2.45	0.49
2:O:70:GLY:O	2:O:73:VAL:HG22	2.12	0.49
2:Q:41:LEU:O	2:Q:61:VAL:HG13	2.12	0.49
2:W:50:GLU:C	2:W:52:GLY:H	2.21	0.49
1:A:92:ALA:HB2	1:A:503:ALA:CB	2.42	0.49
1:A:175:ILE:HD12	1:A:175:ILE:N	2.28	0.49
1:C:342:ILE:N	1:C:342:ILE:HD12	2.28	0.49
1:F:263:VAL:HG13	1:F:267:MET:HE3	1.94	0.49
1:F:295:LEU:HD23	1:F:295:LEU:C	2.37	0.49
1:F:305:ILE:CG2	1:F:306:GLY:H	2.14	0.49
1:G:355:GLU:HG3	1:G:356:ALA:N	2.27	0.49
1:G:417:VAL:CA	1:G:420:ILE:HG22	2.40	0.49
1:I:25:ASP:HA	1:I:28:LYS:HE2	1.95	0.49
1:I:258:ALA:HA	1:I:261:THR:CG2	2.42	0.49
1:I:338:GLU:O	1:I:342:ILE:HG13	2.13	0.49
1:J:240:VAL:HA	1:J:314:LEU:HD12	1.93	0.49
1:K:196:ASP:OD1	1:K:196:ASP:N	2.45	0.49
1:M:31:LEU:HD23	1:M:453:GLN:HB3	1.95	0.49
1:M:301:ILE:HD11	1:M:312:ALA:HB2	1.95	0.49
1:N:63:GLU:OE1	1:N:63:GLU:N	2.27	0.49
1:N:88:GLY:N	3:N:601:ADP:O3B	2.39	0.49
2:P:14:ARG:NH2	2:P:69:ASP:OD2	2.45	0.49
2:T:12:VAL:HG23	2:T:84:LEU:CD1	2.43	0.49
2:U:74:LYS:HB3	2:U:85:ILE:HD11	1.94	0.49
2:V:88:GLU:HA	2:V:91:ILE:CD1	2.43	0.49
2:1:3:ILE:HD12	2:1:3:ILE:O	2.12	0.49
2:1:77:LYS:HG2	2:1:82:GLU:HA	1.94	0.49
1:A:182:GLY:O	1:A:183:LEU:HB2	2.11	0.49
1:B:220:ILE:HD12	1:B:220:ILE:N	2.27	0.49
1:D:169:VAL:HB	1:D:375:GLY:O	2.12	0.49
1:G:197:ARG:HG3	1:G:278:ALA:O	2.13	0.49
1:G:199:TYR:CE1	1:G:202:PRO:HA	2.47	0.49
1:G:301:ILE:HG23	1:G:307:MET:HB3	1.94	0.49
1:H:174:VAL:HG22	1:H:376:VAL:HG22	1.94	0.49
1:H:293:ALA:HB1	1:H:298:GLY:O	2.12	0.49
1:I:326:ASN:ND2	1:I:329:THR:HB	2.27	0.49
1:L:325:ILE:HG12	1:L:330:THR:HG23	1.93	0.49
1:L:353:ILE:O	1:L:362:ARG:HD2	2.13	0.49
1:M:220:ILE:HD12	1:M:220:ILE:N	2.28	0.49
1:N:219:PHE:O	1:N:247:LEU:HD12	2.13	0.49
1:N:315:GLU:OE1	1:N:315:GLU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:346:VAL:HG12	1:N:350:ARG:NH1	2.26	0.49
1:N:383:ALA:HB3	1:N:389:MET:HE2	1.94	0.49
2:S:25:ILE:O	2:S:25:ILE:HG22	2.12	0.49
2:T:43:VAL:CG1	2:T:57:LEU:HD12	2.43	0.49
2:Y:78:ILE:HG13	2:Y:79:ASP:H	1.77	0.49
1:F:253:ASP:HA	1:F:277:LYS:HB3	1.95	0.49
1:H:183:LEU:HD12	1:H:183:LEU:H	1.77	0.49
1:H:322:ARG:HB3	1:H:333:ILE:CD1	2.28	0.49
1:L:138:CYS:HB2	1:L:411:VAL:HG13	1.93	0.49
1:L:219:PHE:CE2	1:L:245:LYS:HB2	2.48	0.49
1:L:220:ILE:O	1:L:317:LEU:HG	2.13	0.49
1:M:320:ALA:HA	1:M:335:GLY:HA2	1.95	0.49
1:M:346:VAL:O	1:M:350:ARG:HG2	2.13	0.49
1:N:249:ILE:N	1:N:249:ILE:HD12	2.28	0.49
1:N:259:LEU:HD23	1:N:262:LEU:HD23	1.93	0.49
2:X:16:GLU:CG	2:X:19:THR:HB	2.43	0.49
2:2:49:LEU:CA	2:2:52:GLY:HA2	2.43	0.49
1:B:218:PRO:HB2	1:B:248:LEU:HD23	1.94	0.49
1:C:34:LYS:HE3	1:C:480:ALA:O	2.13	0.49
1:E:496:PRO:HG2	1:E:499:VAL:CG2	2.43	0.49
1:F:325:ILE:CG1	1:F:330:THR:HG23	2.40	0.49
1:G:223:ALA:HB1	1:G:225:LYS:N	2.27	0.49
1:G:443:ALA:O	1:G:447:MET:HG3	2.12	0.49
1:H:147:VAL:HG12	1:H:494:LEU:HB2	1.94	0.49
1:H:285:ARG:O	1:H:289:LEU:HG	2.13	0.49
1:I:455:VAL:HG13	1:I:460:GLU:HB2	1.95	0.49
1:K:155:ASP:CG	1:K:158:VAL:HG23	2.38	0.49
1:K:225:LYS:HG3	1:K:226:LYS:N	2.28	0.49
1:K:358:SER:HA	1:K:362:ARG:HH21	1.78	0.49
1:L:230:ILE:HD12	1:L:230:ILE:H	1.78	0.49
1:L:247:LEU:HD12	1:L:249:ILE:HD11	1.94	0.49
1:N:231:ARG:O	1:N:309:LEU:HD13	2.13	0.49
1:N:284:ARG:CZ	1:N:364:LYS:HE2	2.42	0.49
2:P:5:PRO:HD3	2:P:11:ILE:CD1	2.43	0.49
2:P:20:LYS:HA	2:P:27:LEU:HG	1.95	0.49
2:U:46:GLY:HA2	2:U:57:LEU:CD1	2.42	0.49
2:V:86:MET:CG	2:V:91:ILE:HD11	2.42	0.49
2:2:84:LEU:HD12	2:2:84:LEU:N	2.28	0.49
1:B:322:ARG:HG2	1:B:323:VAL:N	2.27	0.49
1:B:367:GLU:O	1:B:371:LYS:HG3	2.13	0.49
1:D:282:GLY:O	1:D:283:ASP:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:LYS:N	1:E:208:PRO:CD	2.67	0.49
1:F:40:LEU:HD11	1:F:56:VAL:HA	1.95	0.49
1:H:230:ILE:HB	1:H:309:LEU:CD1	2.43	0.49
1:H:349:ILE:CD1	1:H:369:VAL:HG22	2.40	0.49
1:I:41:ASP:O	1:I:42:LYS:HD2	2.13	0.49
1:I:486:GLY:HA3	1:I:491:MET:HE3	1.94	0.49
1:J:301:ILE:HA	1:J:307:MET:HE1	1.94	0.49
1:L:302:SER:HB3	1:L:305:ILE:HB	1.95	0.49
1:M:20:VAL:HG13	1:M:74:VAL:HG11	1.95	0.49
1:N:80:LYS:HG3	1:N:506:TYR:CZ	2.48	0.49
1:N:337:GLY:O	1:N:338:GLU:HG2	2.12	0.49
1:N:365:LEU:HD23	1:N:365:LEU:O	2.12	0.49
2:T:11:ILE:HG13	2:T:42:ALA:H	1.77	0.49
2:1:15:LYS:O	2:1:16:GLU:HB2	2.13	0.49
1:D:155:ASP:CG	1:D:158:VAL:HG23	2.38	0.48
1:D:226:LYS:N	1:D:252:GLU:HB3	2.27	0.48
1:E:227:ILE:HA	1:E:230:ILE:HD13	1.95	0.48
1:F:196:ASP:O	1:F:197:ARG:HG2	2.13	0.48
1:F:220:ILE:HB	1:F:318:GLY:CA	2.43	0.48
1:F:240:VAL:HG11	1:F:247:LEU:HD11	1.94	0.48
1:H:221:LEU:HA	1:H:317:LEU:HD22	1.95	0.48
1:H:350:ARG:O	1:H:353:ILE:HB	2.12	0.48
3:I:601:ADP:O3B	4:I:602:BEF:F3	2.20	0.48
1:K:291:ASP:HB2	1:K:372:LEU:CD2	2.41	0.48
1:L:116:LEU:O	1:L:120:ILE:HG13	2.12	0.48
1:L:219:PHE:CE1	1:L:240:VAL:HG22	2.47	0.48
1:L:398:ASP:OD2	4:L:602:BEF:F3	2.21	0.48
1:N:228:SER:CA	1:N:258:ALA:HB2	2.37	0.48
1:N:248:LEU:C	1:N:249:ILE:HD12	2.38	0.48
1:N:284:ARG:NE	1:N:364:LYS:HE2	2.28	0.48
1:N:320:ALA:HB1	1:N:332:ILE:HG23	1.95	0.48
2:Q:59:VAL:O	2:Q:59:VAL:HG23	2.13	0.48
1:A:164:GLU:O	1:A:168:LYS:HB2	2.13	0.48
1:A:452:ARG:NH2	1:A:463:SER:HA	2.28	0.48
1:C:42:LYS:HE2	1:C:48:THR:HG21	1.93	0.48
1:D:417:VAL:O	1:D:420:ILE:HG22	2.13	0.48
1:E:151:SER:CB	1:E:399:ALA:HA	2.39	0.48
1:F:5:ASP:HB2	1:F:524:LEU:HD21	1.93	0.48
1:F:174:VAL:HG11	1:F:367:GLU:HA	1.95	0.48
1:G:34:LYS:HE3	1:G:480:ALA:O	2.13	0.48
1:G:222:LEU:HD22	1:G:300:VAL:CG2	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:ALA:O	1:I:28:LYS:HG3	2.12	0.48
1:I:266:THR:HG22	1:I:271:VAL:O	2.13	0.48
1:J:166:MET:CE	1:J:171:LYS:HG2	2.43	0.48
1:K:221:LEU:HB2	1:K:317:LEU:HD22	1.95	0.48
1:K:255:GLU:OE2	1:K:255:GLU:N	2.46	0.48
1:K:355:GLU:HG3	1:K:356:ALA:N	2.28	0.48
1:L:143:ALA:O	1:L:147:VAL:HG12	2.13	0.48
2:S:16:GLU:HG3	2:S:19:THR:HG23	1.95	0.48
2:T:5:PRO:HB3	2:T:11:ILE:HG23	1.94	0.48
2:T:7:HIS:O	2:T:8:ASP:HB3	2.13	0.48
2:Z:89:SER:O	2:1:9:ARG:NH2	2.46	0.48
2:2:12:VAL:HG13	2:2:39:GLU:O	2.13	0.48
1:B:155:ASP:CG	1:B:158:VAL:HG23	2.38	0.48
1:B:325:ILE:CG1	1:B:330:THR:HG23	2.34	0.48
1:B:346:VAL:O	1:B:350:ARG:HG2	2.12	0.48
1:D:180:GLY:N	1:D:381:VAL:O	2.46	0.48
1:D:448:GLU:O	1:D:452:ARG:HG3	2.13	0.48
1:E:136:VAL:CG2	1:E:137:PRO:CD	2.91	0.48
1:E:236:VAL:O	1:E:240:VAL:HG23	2.13	0.48
1:F:151:SER:HB3	1:F:399:ALA:HA	1.95	0.48
1:F:346:VAL:O	1:F:349:ILE:HG22	2.13	0.48
1:G:183:LEU:HD12	1:G:384:ALA:CB	2.43	0.48
1:G:414:GLY:HA3	1:G:493:ILE:HG22	1.96	0.48
1:H:57:ALA:O	1:H:75:LYS:HE2	2.13	0.48
1:I:510:VAL:O	1:I:514:MET:HE3	2.14	0.48
1:M:419:LEU:HD21	1:M:500:THR:HG23	1.94	0.48
1:N:113:PRO:HA	1:N:116:LEU:HD12	1.95	0.48
2:U:50:GLU:C	2:U:52:GLY:N	2.71	0.48
1:B:510:VAL:O	1:B:514:MET:HE3	2.13	0.48
1:C:23:LEU:C	1:C:23:LEU:HD13	2.38	0.48
1:C:232:GLU:HG3	1:C:310:GLU:OE2	2.13	0.48
1:D:174:VAL:HG23	1:D:376:VAL:HG13	1.96	0.48
1:F:147:VAL:CG2	1:F:403:THR:HG22	2.43	0.48
1:G:357:THR:HG22	1:G:359:ASP:HB2	1.96	0.48
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.95	0.48
1:H:226:LYS:HG2	1:H:252:GLU:HB3	1.94	0.48
1:I:138:CYS:SG	1:I:144:ILE:HD13	2.53	0.48
1:J:77:VAL:CG2	1:J:507:ALA:HA	2.43	0.48
1:K:87:ASP:OD2	1:K:151:SER:OG	2.24	0.48
1:L:234:LEU:N	1:L:235:PRO:HD2	2.28	0.48
1:N:293:ALA:O	1:N:298:GLY:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:47:ARG:NH1	2:Q:47:ARG:HB2	2.28	0.48
2:V:47:ARG:O	2:V:54:VAL:HA	2.13	0.48
2:X:67:PHE:CA	2:X:92:LEU:HD13	2.33	0.48
2:Y:48:ILE:HG22	2:Y:48:ILE:O	2.14	0.48
2:2:7:HIS:O	2:2:44:GLY:HA3	2.13	0.48
1:A:218:PRO:HD2	1:A:320:ALA:O	2.13	0.48
1:A:496:PRO:HG2	1:A:499:VAL:HG11	1.95	0.48
1:E:197:ARG:HG3	1:E:278:ALA:O	2.13	0.48
1:E:234:LEU:CD2	1:E:235:PRO:N	2.77	0.48
1:F:88:GLY:N	3:F:601:ADP:O1B	2.38	0.48
1:F:136:VAL:HG12	1:F:137:PRO:HD2	1.96	0.48
1:F:217:SER:HA	1:F:320:ALA:O	2.13	0.48
1:G:237:LEU:HD22	2:U:26:VAL:CG2	2.43	0.48
1:G:345:ARG:O	1:G:348:GLN:HG3	2.13	0.48
1:H:227:ILE:HG22	1:H:227:ILE:O	2.14	0.48
1:I:197:ARG:NH1	1:I:277:LYS:CD	2.72	0.48
1:I:285:ARG:HG3	1:I:286:LYS:HG3	1.95	0.48
1:K:320:ALA:HB1	1:K:334:ASP:O	2.13	0.48
1:K:463:SER:O	1:K:467:ASN:HB2	2.14	0.48
1:K:478:TYR:HD1	1:K:485:TYR:CE1	2.32	0.48
1:M:131:LEU:HD23	1:M:422:VAL:HG11	1.94	0.48
1:N:147:VAL:HG22	1:N:403:THR:HG22	1.95	0.48
2:O:5:PRO:CA	2:U:93:ALA:HB2	2.40	0.48
2:S:7:HIS:HA	2:S:46:GLY:O	2.14	0.48
2:Y:92:LEU:HD23	2:Z:85:ILE:HD13	1.93	0.48
2:1:67:PHE:CD2	2:1:86:MET:HE1	2.49	0.48
1:B:276:VAL:HG21	1:B:325:ILE:CG2	2.38	0.48
1:E:219:PHE:HB3	1:E:317:LEU:CD1	2.43	0.48
1:G:240:VAL:HG11	1:G:247:LEU:CD1	2.43	0.48
1:G:333:ILE:O	1:G:333:ILE:HG22	2.14	0.48
1:I:228:SER:H	1:I:230:ILE:CD1	2.27	0.48
1:I:284:ARG:HD2	1:I:364:LYS:HZ1	1.78	0.48
1:I:320:ALA:HA	1:I:335:GLY:HA2	1.94	0.48
1:J:230:ILE:HG13	1:J:231:ARG:N	2.22	0.48
1:K:231:ARG:O	1:K:234:LEU:HB3	2.13	0.48
1:K:414:GLY:O	1:K:417:VAL:HG12	2.14	0.48
1:L:396:VAL:O	1:L:400:LEU:HB2	2.13	0.48
1:M:405:ALA:HB2	1:M:498:LYS:HD3	1.94	0.48
1:N:150:ILE:HG22	1:N:151:SER:N	2.28	0.48
1:N:222:LEU:CD2	1:N:293:ALA:HB2	2.42	0.48
2:O:96:GLU:O	2:P:1:MET:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:11:ILE:O	2:2:41:LEU:HB2	2.14	0.48
1:A:200:LEU:HD21	1:A:253:ASP:OD1	2.13	0.48
1:A:228:SER:O	1:A:258:ALA:HB2	2.14	0.48
1:B:199:TYR:HE1	1:B:202:PRO:HA	1.74	0.48
1:E:202:PRO:O	1:E:205:ILE:HG13	2.14	0.48
1:F:231:ARG:HB2	1:F:234:LEU:HD12	1.94	0.48
1:F:448:GLU:O	1:F:452:ARG:HG2	2.14	0.48
1:F:475:ASN:O	1:F:488:MET:HG2	2.12	0.48
1:G:215:LEU:HD22	1:G:246:PRO:HB3	1.95	0.48
1:L:85:ALA:O	1:L:401:HIS:HB3	2.14	0.48
1:L:218:PRO:HB2	1:L:219:PHE:O	2.13	0.48
1:N:339:GLU:OE1	1:N:339:GLU:N	2.47	0.48
2:T:48:ILE:HG22	2:T:53:GLU:C	2.39	0.48
2:V:37:ARG:HG2	2:V:66:ILE:HG12	1.95	0.48
2:V:40:VAL:HG11	2:V:63:ASP:OD1	2.13	0.48
2:Z:23:GLY:O	2:Z:26:VAL:HG12	2.13	0.48
1:A:196:ASP:O	1:A:197:ARG:HG2	2.14	0.48
1:B:337:GLY:O	1:B:338:GLU:HG2	2.13	0.48
1:C:259:LEU:O	1:C:263:VAL:N	2.42	0.48
1:C:357:THR:HB	1:C:361:ASP:CB	2.44	0.48
1:D:228:SER:CA	1:D:255:GLU:HB2	2.34	0.48
1:H:80:LYS:HG2	1:I:385:THR:HG22	1.95	0.48
1:H:124:VAL:HG22	1:H:504:LEU:HD11	1.95	0.48
1:I:4:LYS:HG3	1:J:59:GLU:O	2.13	0.48
1:I:193:MET:HG3	1:I:371:LYS:HB3	1.96	0.48
1:I:199:TYR:HB3	1:I:325:ILE:HG21	1.95	0.48
1:K:23:LEU:C	1:K:23:LEU:HD13	2.39	0.48
1:B:305:ILE:HD12	1:C:263:VAL:CG1	2.41	0.48
1:C:215:LEU:HB2	1:C:323:VAL:CG2	2.43	0.48
1:C:364:LYS:O	1:C:367:GLU:HB3	2.14	0.48
1:C:417:VAL:HA	1:C:420:ILE:HG22	1.96	0.48
1:E:240:VAL:HG12	1:E:247:LEU:HD21	1.92	0.48
1:F:165:ALA:O	1:F:169:VAL:HG22	2.13	0.48
1:G:195:PHE:O	1:G:329:THR:HG23	2.12	0.48
1:J:10:ASN:O	1:J:14:VAL:HG23	2.13	0.48
1:J:214:GLU:HA	1:J:323:VAL:O	2.13	0.48
1:K:345:ARG:O	1:K:348:GLN:HG2	2.14	0.48
1:K:419:LEU:O	1:K:422:VAL:HG22	2.14	0.48
1:L:136:VAL:HG22	1:L:137:PRO:HD2	1.95	0.48
1:M:160:LYS:O	1:M:164:GLU:HG3	2.14	0.48
1:N:175:ILE:HA	1:N:377:ALA:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:78:ILE:HD12	2:O:79:ASP:OD1	2.14	0.48
2:V:15:LYS:HA	2:V:16:GLU:HA	1.59	0.48
2:V:80:ASN:ND2	2:V:80:ASN:O	2.47	0.48
2:X:15:LYS:HB2	2:X:37:ARG:O	2.14	0.48
1:A:89:THR:N	4:A:602:BEF:F1	2.37	0.48
1:A:234:LEU:HB2	2:O:26:VAL:HG21	1.95	0.48
1:A:234:LEU:N	1:A:235:PRO:HD2	2.28	0.48
1:A:345:ARG:O	1:A:348:GLN:HG3	2.13	0.48
1:C:228:SER:HB3	1:C:255:GLU:OE1	2.14	0.48
1:D:62:LEU:HD23	1:D:67:GLU:HB3	1.95	0.48
1:D:291:ASP:OD1	1:D:345:ARG:NH2	2.36	0.48
1:E:66:PHE:CE1	1:E:522:THR:HG22	2.49	0.48
1:H:89:THR:OG1	4:H:602:BEF:F2	2.22	0.48
1:H:230:ILE:CD1	1:H:309:LEU:HB2	2.44	0.48
1:I:199:TYR:CE1	1:I:327:LYS:HA	2.49	0.48
1:I:217:SER:O	1:I:245:LYS:HD3	2.14	0.48
1:K:117:LYS:HG3	1:K:512:GLY:C	2.39	0.48
1:M:225:LYS:HD3	1:M:303:GLU:CD	2.38	0.48
1:N:304:GLU:O	1:N:305:ILE:HD13	2.13	0.48
2:W:12:VAL:HA	2:W:41:LEU:HD13	1.96	0.48
2:1:7:HIS:O	2:1:8:ASP:HB3	2.14	0.48
1:A:224:ASP:OD2	1:A:302:SER:HB3	2.14	0.47
1:A:348:GLN:OE1	1:A:352:GLN:NE2	2.47	0.47
1:C:48:THR:HG22	1:C:390:LYS:HZ1	1.78	0.47
1:C:114:MET:HG3	1:C:118:ARG:NH1	2.29	0.47
1:D:417:VAL:C	1:D:420:ILE:HG22	2.39	0.47
1:E:417:VAL:HG21	1:E:476:TYR:O	2.13	0.47
1:E:433:ASN:OD1	1:E:436:GLN:HG3	2.13	0.47
1:F:227:ILE:O	1:F:254:VAL:HA	2.13	0.47
1:G:252:GLU:HA	1:G:285:ARG:NH1	2.29	0.47
1:H:267:MET:HE2	1:H:267:MET:CA	2.44	0.47
1:J:488:MET:HE3	1:J:493:ILE:HG21	1.95	0.47
1:K:429:LEU:HG	1:K:440:ILE:HD13	1.95	0.47
1:L:196:ASP:O	1:L:197:ARG:HG2	2.14	0.47
1:M:190:VAL:HG11	1:M:194:GLN:CD	2.39	0.47
1:N:199:TYR:CE2	1:N:326:ASN:HA	2.49	0.47
1:N:288:MET:O	1:N:292:ILE:HG13	2.14	0.47
1:N:440:ILE:O	1:N:444:LEU:HG	2.14	0.47
2:O:96:GLU:O	2:O:97:ALA:CB	2.61	0.47
2:W:17:VAL:C	2:W:19:THR:H	2.21	0.47
1:B:69:MET:SD	1:C:41:ASP:HB2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:GLU:CD	1:C:501:ARG:HH21	2.21	0.47
1:D:220:ILE:HD12	1:D:220:ILE:N	2.29	0.47
1:D:238:GLU:OE2	2:R:23:GLY:N	2.34	0.47
1:E:23:LEU:C	1:E:23:LEU:HD13	2.38	0.47
1:E:175:ILE:HD12	1:E:400:LEU:HD21	1.96	0.47
1:E:230:ILE:O	1:E:230:ILE:HG22	2.14	0.47
1:E:234:LEU:HG	1:E:235:PRO:N	2.28	0.47
1:E:302:SER:HB2	1:E:305:ILE:CB	2.44	0.47
1:F:263:VAL:O	1:F:267:MET:HG3	2.14	0.47
1:I:222:LEU:HD23	1:I:250:ILE:HB	1.96	0.47
1:I:278:ALA:HB1	1:I:279:PRO:CD	2.43	0.47
1:I:325:ILE:N	1:I:325:ILE:HD12	2.29	0.47
1:I:326:ASN:OD1	1:I:329:THR:HB	2.13	0.47
1:L:433:ASN:ND2	1:L:435:ASP:HB2	2.29	0.47
1:M:126:ALA:HB1	1:M:426:LEU:HD22	1.96	0.47
1:M:305:ILE:CG2	1:M:306:GLY:N	2.72	0.47
1:N:307:MET:HG2	1:N:311:LYS:NZ	2.27	0.47
2:P:52:GLY:HA3	2:P:53:GLU:HA	1.60	0.47
1:A:152:ALA:HB2	1:A:399:ALA:HB2	1.96	0.47
1:B:169:VAL:HG13	1:B:173:GLY:HA3	1.95	0.47
1:B:339:GLU:OE1	1:B:339:GLU:N	2.48	0.47
1:C:219:PHE:CE2	1:C:245:LYS:HB2	2.43	0.47
1:C:223:ALA:HB1	1:C:227:ILE:HD11	1.94	0.47
1:C:305:ILE:HD12	1:C:305:ILE:N	2.28	0.47
1:D:226:LYS:HB3	1:D:252:GLU:CG	2.43	0.47
1:D:279:PRO:HB2	1:D:288:MET:CE	2.41	0.47
1:E:307:MET:HE3	1:E:311:LYS:HZ3	1.77	0.47
1:H:49:ILE:N	1:H:49:ILE:HD12	2.29	0.47
1:H:102:GLU:HB2	1:H:442:VAL:HG13	1.96	0.47
1:H:311:LYS:O	1:H:311:LYS:HD3	2.14	0.47
1:J:268:ARG:HB2	1:J:270:ILE:HG12	1.96	0.47
1:L:278:ALA:HB1	1:L:285:ARG:HB2	1.96	0.47
1:N:177:VAL:HG21	1:N:396:VAL:HG11	1.96	0.47
2:P:45:ASN:OD1	2:P:46:GLY:N	2.47	0.47
2:V:6:LEU:HD12	2:V:6:LEU:O	2.14	0.47
2:W:49:LEU:HD12	2:W:52:GLY:HA3	1.96	0.47
2:Z:11:ILE:CG1	2:Z:83:VAL:HG11	2.44	0.47
2:2:17:VAL:HG23	2:2:18:GLU:CG	2.43	0.47
1:A:295:LEU:C	1:A:295:LEU:HD23	2.40	0.47
1:B:149:THR:HG23	1:B:155:ASP:C	2.39	0.47
1:D:39:VAL:HG22	1:D:49:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LEU:CD2	1:D:422:VAL:HG11	2.43	0.47
1:D:147:VAL:CG2	1:D:403:THR:HG22	2.44	0.47
1:D:169:VAL:CG2	1:D:173:GLY:HA3	2.44	0.47
1:E:217:SER:HA	1:E:320:ALA:O	2.15	0.47
1:E:224:ASP:OD2	1:E:286:LYS:HE2	2.14	0.47
1:F:257:GLU:O	1:F:261:THR:HG22	2.14	0.47
1:G:195:PHE:CD1	1:G:195:PHE:C	2.93	0.47
1:H:417:VAL:O	1:H:420:ILE:HG22	2.14	0.47
1:I:117:LYS:HG3	1:I:512:GLY:C	2.39	0.47
1:I:197:ARG:HD3	1:I:197:ARG:HA	1.73	0.47
1:I:255:GLU:OE1	1:I:255:GLU:HA	2.14	0.47
1:K:305:ILE:CG2	1:K:306:GLY:N	2.72	0.47
1:L:365:LEU:O	1:L:369:VAL:HG23	2.14	0.47
1:M:123:ALA:HB2	1:M:440:ILE:HG23	1.96	0.47
1:N:169:VAL:HB	1:N:375:GLY:O	2.14	0.47
1:N:177:VAL:CG2	1:N:393:LYS:HG3	2.44	0.47
1:N:197:ARG:CD	1:N:277:LYS:HB3	2.45	0.47
1:N:276:VAL:CG1	1:N:325:ILE:HG21	2.45	0.47
1:N:325:ILE:N	1:N:325:ILE:HD12	2.28	0.47
1:N:392:LYS:O	1:N:396:VAL:HG23	2.13	0.47
2:T:60:LYS:HB3	2:T:63:ASP:OD1	2.13	0.47
2:Z:27:LEU:HD23	2:Z:28:THR:N	2.29	0.47
2:2:12:VAL:HG13	2:2:39:GLU:N	2.29	0.47
1:A:322:ARG:HG2	1:A:323:VAL:N	2.29	0.47
1:D:496:PRO:HG2	1:D:499:VAL:HG13	1.95	0.47
1:E:190:VAL:HG11	1:E:194:GLN:CD	2.39	0.47
1:E:343:GLN:HA	1:E:346:VAL:HB	1.96	0.47
1:F:10:ASN:O	1:F:14:VAL:HG23	2.14	0.47
1:F:124:VAL:HG21	1:F:508:ALA:CB	2.45	0.47
1:F:177:VAL:CG2	1:F:393:LYS:HG3	2.45	0.47
1:F:452:ARG:HH21	1:F:466:ALA:CB	2.27	0.47
1:G:257:GLU:O	1:G:261:THR:HG22	2.13	0.47
1:H:364:LYS:HA	1:H:367:GLU:HB3	1.96	0.47
1:I:124:VAL:HG21	1:I:508:ALA:HB2	1.94	0.47
1:I:510:VAL:O	1:I:514:MET:HB2	2.14	0.47
1:M:288:MET:HG3	1:M:364:LYS:NZ	2.29	0.47
1:M:381:VAL:HG22	1:M:396:VAL:HG21	1.97	0.47
1:N:286:LYS:NZ	1:N:304:GLU:OE1	2.34	0.47
2:R:60:LYS:HG3	2:R:63:ASP:OD1	2.14	0.47
2:V:37:ARG:HH21	2:W:76:GLU:HG3	1.79	0.47
2:X:50:GLU:O	2:X:51:ASN:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:MET:HE1	1:B:493:ILE:HD12	1.96	0.47
1:C:198:GLY:O	1:C:276:VAL:HG23	2.14	0.47
1:C:345:ARG:NH2	1:C:372:LEU:HD22	2.30	0.47
1:D:20:VAL:HG13	1:D:74:VAL:HG11	1.97	0.47
1:D:280:GLY:O	1:D:285:ARG:NH1	2.48	0.47
1:D:349:ILE:HD12	1:D:369:VAL:HG22	1.97	0.47
1:F:209:GLU:CG	1:F:210:THR:H	2.26	0.47
1:F:360:TYR:CA	1:F:363:GLU:HG3	2.41	0.47
1:F:455:VAL:CG1	1:F:460:GLU:HB2	2.45	0.47
1:H:236:VAL:O	1:H:240:VAL:HG23	2.14	0.47
1:I:355:GLU:HG3	1:I:356:ALA:N	2.29	0.47
1:J:219:PHE:HB3	1:J:317:LEU:HD13	1.95	0.47
1:K:326:ASN:HD21	1:K:329:THR:HG22	1.80	0.47
1:M:88:GLY:HA2	3:M:601:ADP:O3B	2.13	0.47
1:M:357:THR:HB	1:M:361:ASP:CG	2.39	0.47
1:N:14:VAL:O	1:N:18:ARG:HG3	2.15	0.47
2:O:31:ALA:O	2:O:32:ALA:HB3	2.14	0.47
2:T:60:LYS:CG	2:T:61:VAL:H	2.28	0.47
1:A:188:ASP:HB2	1:A:378:VAL:CG2	2.41	0.47
1:A:197:ARG:HG3	1:A:278:ALA:O	2.15	0.47
1:A:270:ILE:HG22	1:A:271:VAL:HG13	1.97	0.47
1:A:313:THR:O	1:A:316:ASP:HB2	2.15	0.47
1:A:333:ILE:O	1:A:334:ASP:HB2	2.14	0.47
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.44	0.47
1:B:310:GLU:OE1	1:B:310:GLU:N	2.47	0.47
1:B:417:VAL:HA	1:B:420:ILE:HG22	1.96	0.47
1:B:519:CYS:HB3	1:C:38:VAL:HG22	1.96	0.47
1:D:165:ALA:O	1:D:169:VAL:HG22	2.14	0.47
1:E:194:GLN:CG	1:E:331:THR:HG23	2.41	0.47
1:E:301:ILE:HG12	1:E:307:MET:HE2	1.93	0.47
1:E:350:ARG:HD3	1:E:353:ILE:CD1	2.45	0.47
1:F:169:VAL:CG2	1:F:173:GLY:HA3	2.45	0.47
1:F:496:PRO:HG2	1:F:499:VAL:HG13	1.97	0.47
1:G:196:ASP:O	1:G:197:ARG:HG2	2.15	0.47
1:G:219:PHE:HB3	1:G:317:LEU:HB3	1.97	0.47
1:G:412:VAL:CG1	1:G:413:ALA:H	2.27	0.47
1:I:346:VAL:O	1:I:350:ARG:HG2	2.14	0.47
1:J:23:LEU:C	1:J:23:LEU:HD13	2.39	0.47
1:J:399:ALA:O	1:J:403:THR:HG23	2.15	0.47
1:J:455:VAL:HG13	1:J:460:GLU:HB2	1.96	0.47
1:K:293:ALA:HB1	1:K:298:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:327:LYS:HD3	1:K:327:LYS:H	1.80	0.47
1:L:76:GLU:O	1:L:80:LYS:HB2	2.15	0.47
1:M:205:ILE:HG22	1:M:206:ASN:O	2.15	0.47
1:N:76:GLU:O	1:N:80:LYS:N	2.45	0.47
1:N:227:ILE:CG1	1:N:231:ARG:HG3	2.44	0.47
2:O:57:LEU:HD12	2:O:88:GLU:CB	2.44	0.47
2:Q:40:VAL:CG1	2:Q:62:GLY:H	2.27	0.47
2:R:36:THR:C	2:R:37:ARG:HG3	2.40	0.47
2:S:18:GLU:HG3	2:S:32:ALA:HB2	1.97	0.47
2:S:48:ILE:HG13	2:S:53:GLU:H	1.79	0.47
2:T:10:VAL:N	2:T:86:MET:O	2.40	0.47
2:U:6:LEU:HD12	2:U:7:HIS:HB2	1.97	0.47
2:V:5:PRO:HG2	2:V:43:VAL:C	2.40	0.47
2:V:50:GLU:HG2	2:2:50:GLU:OE1	2.14	0.47
2:Y:13:LYS:HD2	2:Y:81:GLU:OE1	2.15	0.47
1:A:62:LEU:HD23	1:A:67:GLU:HB3	1.96	0.47
1:C:261:THR:HB	2:Q:29:GLY:O	2.14	0.47
1:D:200:LEU:HD11	1:D:277:LYS:N	2.30	0.47
1:D:327:LYS:H	1:D:327:LYS:HD3	1.80	0.47
1:E:238:GLU:CD	2:S:25:ILE:HD13	2.39	0.47
1:F:220:ILE:HG22	1:F:222:LEU:HD11	1.97	0.47
1:G:234:LEU:HD23	2:U:23:GLY:HA3	1.96	0.47
1:J:364:LYS:NZ	1:J:367:GLU:OE2	2.42	0.47
1:K:100:ILE:O	1:K:104:LEU:HG	2.14	0.47
1:K:421:ARG:HD3	1:K:421:ARG:HA	1.77	0.47
1:L:458:CYS:SG	1:L:480:ALA:HB1	2.55	0.47
1:M:221:LEU:HD11	1:M:301:ILE:HD12	1.96	0.47
1:M:280:GLY:H	1:M:285:ARG:HB3	1.80	0.47
1:N:13:ARG:HG2	1:N:104:LEU:HD13	1.97	0.47
1:N:278:ALA:HB1	1:N:279:PRO:HD2	1.96	0.47
1:N:431:GLY:N	1:N:437:ASN:OD1	2.32	0.47
2:R:12:VAL:HG12	2:R:40:VAL:CG1	2.42	0.47
2:T:53:GLU:CD	2:T:54:VAL:HG22	2.40	0.47
2:Z:15:LYS:NZ	2:Z:64:ILE:HD12	2.29	0.47
2:Z:17:VAL:HG22	2:Z:18:GLU:N	2.30	0.47
2:Z:84:LEU:N	2:Z:84:LEU:HD12	2.29	0.47
2:1:57:LEU:HD12	2:1:88:GLU:CD	2.40	0.47
1:C:175:ILE:HA	1:C:377:ALA:O	2.15	0.47
1:C:404:ARG:O	1:C:408:GLU:HG2	2.15	0.47
1:C:406:ALA:HB1	1:C:411:VAL:CG1	2.45	0.47
1:H:245:LYS:CB	1:H:246:PRO:HD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:ASP:N	1:I:522:THR:O	2.46	0.47
1:I:124:VAL:HG22	1:I:504:LEU:CD1	2.44	0.47
1:L:155:ASP:CG	1:L:158:VAL:HG23	2.40	0.47
1:L:331:THR:HG22	1:L:332:ILE:N	2.30	0.47
1:N:414:GLY:O	1:N:417:VAL:HG12	2.15	0.47
1:N:429:LEU:HG	1:N:440:ILE:HD13	1.97	0.47
2:O:77:LYS:HE2	2:O:82:GLU:HB2	1.97	0.47
2:U:20:LYS:HB3	2:U:27:LEU:HD12	1.96	0.47
2:Y:73:VAL:HG22	2:Y:86:MET:HB3	1.96	0.47
1:A:85:ALA:O	1:A:401:HIS:HB3	2.14	0.47
1:B:13:ARG:CD	1:B:104:LEU:HD22	2.42	0.47
1:F:220:ILE:HG13	1:F:296:THR:CB	2.44	0.47
1:F:231:ARG:O	1:F:234:LEU:HG	2.15	0.47
1:F:282:GLY:CA	1:F:285:ARG:HG2	2.42	0.47
1:F:291:ASP:OD1	1:F:292:ILE:HG13	2.15	0.47
1:F:419:LEU:HD12	1:F:419:LEU:N	2.30	0.47
1:G:436:GLN:O	1:G:440:ILE:HG13	2.14	0.47
1:I:77:VAL:HB	1:I:510:VAL:HG21	1.96	0.47
1:L:115:ASP:O	1:L:436:GLN:HG2	2.14	0.47
1:L:450:PRO:O	1:L:454:ILE:HG13	2.15	0.47
1:N:204:PHE:CE2	1:N:274:ALA:HA	2.50	0.47
2:Q:49:LEU:C	2:Q:49:LEU:HD12	2.40	0.47
2:V:49:LEU:HD22	2:V:50:GLU:N	2.28	0.47
2:Z:92:LEU:HD13	2:1:85:ILE:HG21	1.96	0.47
1:A:143:ALA:O	1:A:147:VAL:HG13	2.14	0.46
1:A:266:THR:HG22	1:A:273:VAL:H	1.80	0.46
1:B:213:VAL:O	1:B:324:VAL:HA	2.15	0.46
1:F:301:ILE:HD11	1:F:316:ASP:OD2	2.15	0.46
1:G:306:GLY:O	1:G:307:MET:CG	2.60	0.46
1:G:367:GLU:O	1:G:371:LYS:HG3	2.15	0.46
1:H:234:LEU:HD21	2:V:22:ALA:HB1	1.96	0.46
1:H:429:LEU:HG	1:H:440:ILE:HD13	1.96	0.46
1:I:217:SER:N	1:I:218:PRO:CD	2.78	0.46
1:I:237:LEU:CD2	2:W:27:LEU:CD2	2.93	0.46
1:I:487:ASN:HB3	1:I:490:ASP:HB2	1.96	0.46
1:M:207:LYS:N	1:M:208:PRO:HD2	2.30	0.46
1:M:219:PHE:HB3	1:M:317:LEU:HD13	1.97	0.46
1:N:478:TYR:HD1	1:N:485:TYR:CE1	2.32	0.46
2:O:80:ASN:ND2	2:U:24:GLY:H	2.14	0.46
2:V:36:THR:HG21	2:W:76:GLU:OE1	2.15	0.46
1:B:180:GLY:HA3	1:B:382:GLY:CA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:LEU:HD11	1:E:277:LYS:CB	2.42	0.46
1:E:204:PHE:CD2	1:E:274:ALA:HA	2.51	0.46
1:H:278:ALA:HB1	1:H:279:PRO:HD2	1.97	0.46
1:H:354:GLU:C	1:H:355:GLU:HG3	2.40	0.46
1:H:455:VAL:HG21	1:H:465:VAL:HG11	1.97	0.46
1:I:18:ARG:HB3	1:I:18:ARG:HH11	1.80	0.46
1:J:215:LEU:HB2	1:J:323:VAL:CG2	2.44	0.46
1:J:295:LEU:HD23	1:J:295:LEU:C	2.41	0.46
1:J:510:VAL:O	1:J:514:MET:HB2	2.15	0.46
1:M:230:ILE:H	1:M:230:ILE:HD12	1.80	0.46
1:M:293:ALA:HB1	1:M:298:GLY:O	2.15	0.46
1:N:221:LEU:HD13	1:N:317:LEU:HD21	1.97	0.46
1:N:222:LEU:HD22	1:N:300:VAL:CG2	2.44	0.46
1:N:226:LYS:HE3	1:N:253:ASP:HB3	1.98	0.46
1:N:455:VAL:HG11	1:N:462:PRO:HA	1.97	0.46
2:S:60:LYS:HB2	2:S:63:ASP:OD2	2.15	0.46
1:B:218:PRO:HG3	1:B:323:VAL:HG22	1.96	0.46
1:C:357:THR:HG22	1:C:357:THR:O	2.16	0.46
1:H:34:LYS:HE3	1:H:480:ALA:O	2.15	0.46
1:H:232:GLU:CG	1:H:233:MET:N	2.76	0.46
1:I:180:GLY:HA2	1:I:380:LYS:HB3	1.97	0.46
1:I:347:ALA:HA	1:I:350:ARG:HG3	1.97	0.46
1:J:23:LEU:CD2	1:J:60:ILE:HG13	2.46	0.46
1:J:34:LYS:HD2	1:J:458:CYS:SG	2.55	0.46
1:J:198:GLY:HA3	1:J:327:LYS:O	2.16	0.46
1:J:291:ASP:HB3	1:J:372:LEU:HD21	1.98	0.46
1:K:248:LEU:HD13	1:K:249:ILE:N	2.30	0.46
1:K:513:LEU:CD2	1:L:49:ILE:HG21	2.45	0.46
1:L:193:MET:SD	1:L:371:LYS:HB3	2.56	0.46
1:L:285:ARG:HG3	1:L:286:LYS:N	2.30	0.46
1:M:2:ALA:O	1:N:61:GLU:HB3	2.15	0.46
1:M:151:SER:OG	1:M:399:ALA:HA	2.14	0.46
1:N:66:PHE:CE1	1:N:522:THR:HG22	2.51	0.46
1:N:96:ALA:O	1:N:100:ILE:HG13	2.15	0.46
1:N:161:LEU:HD12	1:N:161:LEU:HA	1.84	0.46
2:R:17:VAL:HG23	2:R:19:THR:HA	1.97	0.46
2:S:64:ILE:CG2	2:S:95:VAL:HG13	2.32	0.46
2:Z:23:GLY:H	2:1:80:ASN:HB3	1.80	0.46
1:B:130:GLU:O	1:B:134:LEU:HD13	2.15	0.46
1:B:226:LYS:HE3	1:B:253:ASP:HB3	1.96	0.46
1:B:419:LEU:O	1:B:422:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:VAL:O	1:D:267:MET:HG3	2.16	0.46
1:E:177:VAL:HG23	1:E:381:VAL:CG2	2.46	0.46
1:F:327:LYS:HD3	1:F:327:LYS:H	1.80	0.46
1:G:143:ALA:O	1:G:147:VAL:HG13	2.16	0.46
1:G:210:THR:O	1:G:210:THR:HG22	2.14	0.46
1:H:419:LEU:O	1:H:422:VAL:HG22	2.16	0.46
1:I:278:ALA:HB1	1:I:279:PRO:HD2	1.96	0.46
1:J:209:GLU:C	1:J:211:GLY:N	2.73	0.46
1:J:350:ARG:HA	1:J:353:ILE:HD12	1.96	0.46
1:K:288:MET:O	1:K:292:ILE:HG13	2.15	0.46
1:L:218:PRO:O	1:L:319:GLN:HG2	2.14	0.46
1:L:510:VAL:O	1:L:514:MET:HE3	2.15	0.46
1:M:349:ILE:HG21	1:M:369:VAL:HG22	1.97	0.46
1:N:150:ILE:HD11	1:N:493:ILE:CG2	2.31	0.46
1:N:273:VAL:HG12	1:N:274:ALA:N	2.31	0.46
2:P:59:VAL:HG11	2:P:91:ILE:HD12	1.97	0.46
2:W:36:THR:C	2:W:37:ARG:HG3	2.39	0.46
2:Y:78:ILE:HG13	2:Y:79:ASP:OD1	2.15	0.46
1:A:193:MET:SD	1:A:371:LYS:HB3	2.56	0.46
1:A:327:LYS:H	1:A:327:LYS:HD3	1.81	0.46
1:C:23:LEU:CD2	1:C:60:ILE:HB	2.43	0.46
1:D:57:ALA:O	1:D:75:LYS:HE2	2.16	0.46
1:E:232:GLU:C	1:E:234:LEU:N	2.74	0.46
1:E:234:LEU:N	1:E:235:PRO:HD2	2.31	0.46
1:E:234:LEU:C	1:E:236:VAL:N	2.72	0.46
1:F:465:VAL:O	1:F:469:VAL:HG23	2.15	0.46
1:G:237:LEU:HD23	1:G:237:LEU:C	2.41	0.46
1:H:77:VAL:HG21	1:H:507:ALA:CA	2.36	0.46
1:H:95:LEU:O	1:H:99:ILE:HG13	2.15	0.46
1:I:215:LEU:HB2	1:I:323:VAL:CG2	2.46	0.46
1:I:233:MET:CB	1:I:309:LEU:HD21	2.45	0.46
1:J:237:LEU:HD23	1:J:237:LEU:C	2.41	0.46
1:L:234:LEU:HD23	2:Z:23:GLY:CA	2.44	0.46
1:L:237:LEU:HD23	1:L:237:LEU:C	2.40	0.46
1:M:147:VAL:HG12	1:M:494:LEU:CD1	2.46	0.46
1:M:232:GLU:OE1	1:M:232:GLU:N	2.39	0.46
1:N:296:THR:HG22	1:N:320:ALA:HB2	1.98	0.46
2:R:25:ILE:HA	2:R:26:VAL:HG22	1.96	0.46
2:X:6:LEU:HD12	2:X:6:LEU:O	2.15	0.46
2:X:20:LYS:HG3	2:X:21:SER:H	1.80	0.46
2:Y:11:ILE:CG2	2:Y:85:ILE:HB	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:40:VAL:HG23	2:2:63:ASP:O	2.16	0.46
1:B:169:VAL:HG13	1:B:169:VAL:O	2.15	0.46
1:E:223:ALA:HA	1:E:301:ILE:O	2.15	0.46
1:F:215:LEU:HB2	1:F:323:VAL:HG22	1.97	0.46
1:G:116:LEU:O	1:G:120:ILE:HG13	2.16	0.46
1:H:185:ASP:OD1	1:H:185:ASP:N	2.49	0.46
1:H:234:LEU:H	1:H:234:LEU:CD1	2.28	0.46
1:H:256:GLY:O	1:H:260:ALA:N	2.40	0.46
1:H:278:ALA:HB1	1:H:279:PRO:CD	2.46	0.46
1:K:179:ASP:OD1	1:K:393:LYS:HD3	2.14	0.46
2:O:17:VAL:HB	2:O:34:LYS:CE	2.46	0.46
2:Q:40:VAL:HG11	2:Q:60:LYS:O	2.16	0.46
2:S:97:ALA:HA	2:T:1:MET:HG3	1.97	0.46
2:U:57:LEU:HD12	2:U:57:LEU:N	2.29	0.46
2:Y:24:GLY:HA2	2:Y:25:ILE:HA	1.43	0.46
1:A:197:ARG:HG2	1:A:279:PRO:HA	1.97	0.46
1:G:219:PHE:HB2	1:G:247:LEU:HD12	1.98	0.46
1:G:252:GLU:HA	1:G:285:ARG:HH11	1.81	0.46
1:I:513:LEU:HD21	1:J:391:GLU:HG2	1.98	0.46
1:J:465:VAL:O	1:J:469:VAL:HG23	2.16	0.46
1:M:91:THR:HG23	1:M:450:PRO:HB3	1.98	0.46
1:M:233:MET:HB3	1:M:236:VAL:HG21	1.97	0.46
2:O:4:ARG:HD3	2:U:96:GLU:HG3	1.97	0.46
2:Q:9:ARG:HA	2:Q:87:SER:HA	1.98	0.46
2:U:83:VAL:HG12	2:U:84:LEU:H	1.80	0.46
1:A:59:GLU:O	1:G:4:LYS:HG3	2.16	0.46
1:A:415:GLY:N	3:A:601:ADP:O2'	2.44	0.46
1:B:4:LYS:HG3	1:C:59:GLU:O	2.16	0.46
1:C:220:ILE:N	1:C:220:ILE:HD12	2.31	0.46
1:I:259:LEU:O	1:I:263:VAL:HG23	2.16	0.46
1:I:381:VAL:CG1	1:I:392:LYS:HB3	2.45	0.46
1:L:200:LEU:CD2	1:L:254:VAL:HB	2.46	0.46
1:M:91:THR:CG2	1:M:450:PRO:HB3	2.46	0.46
1:M:200:LEU:HD11	1:M:277:LYS:HG3	1.98	0.46
1:M:314:LEU:HD12	1:M:315:GLU:N	2.31	0.46
1:N:10:ASN:HA	1:N:13:ARG:HB3	1.96	0.46
1:N:231:ARG:HD3	1:N:231:ARG:HA	1.74	0.46
2:O:14:ARG:HE	2:O:84:LEU:HD11	1.81	0.46
2:O:15:LYS:O	2:O:16:GLU:HB2	2.15	0.46
2:R:12:VAL:CG1	2:R:40:VAL:HA	2.40	0.46
2:S:3:ILE:C	2:S:3:ILE:HD12	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:40:VAL:HG13	2:T:62:GLY:H	1.80	0.46
2:U:14:ARG:HG2	2:U:35:SER:OG	2.15	0.46
2:V:94:ILE:O	2:V:94:ILE:HG13	2.16	0.46
2:1:49:LEU:HD12	2:1:49:LEU:C	2.40	0.46
1:A:38:VAL:HB	1:A:56:VAL:HG21	1.98	0.46
1:B:409:GLU:CD	1:B:501:ARG:HH21	2.24	0.46
1:C:219:PHE:HB3	1:C:317:LEU:HD13	1.97	0.46
1:E:164:GLU:O	1:E:168:LYS:HG2	2.16	0.46
1:H:197:ARG:CD	1:H:277:LYS:HB3	2.45	0.46
1:I:241:ALA:HB2	1:I:271:VAL:HG11	1.98	0.46
1:J:27:VAL:CG1	1:J:90:THR:HG23	2.40	0.46
1:J:204:PHE:CE1	1:J:263:VAL:HA	2.44	0.46
1:J:346:VAL:O	1:J:350:ARG:HG2	2.16	0.46
1:K:288:MET:HG3	1:K:368:ARG:NE	2.31	0.46
1:L:249:ILE:HD12	1:L:274:ALA:O	2.15	0.46
1:L:263:VAL:O	1:L:267:MET:HG2	2.16	0.46
1:N:74:VAL:HG13	1:N:514:MET:SD	2.56	0.46
1:N:358:SER:HA	1:N:362:ARG:NH2	2.31	0.46
2:O:16:GLU:HB3	2:O:17:VAL:H	1.61	0.46
2:R:12:VAL:HB	2:R:39:GLU:O	2.16	0.46
2:S:57:LEU:HD12	2:S:57:LEU:N	2.31	0.46
2:U:38:GLY:O	2:U:65:VAL:N	2.28	0.46
2:U:60:LYS:HG2	2:U:61:VAL:H	1.80	0.46
2:V:70:GLY:O	2:V:73:VAL:HG12	2.16	0.46
2:X:8:ASP:O	2:X:57:LEU:HD21	2.16	0.46
2:2:17:VAL:HG11	2:2:34:LYS:HD3	1.97	0.46
1:A:199:TYR:CB	1:A:276:VAL:HG12	2.46	0.46
1:B:225:LYS:HB2	1:B:303:GLU:HG3	1.98	0.46
1:C:259:LEU:O	1:C:263:VAL:HG23	2.15	0.46
1:C:342:ILE:O	1:C:346:VAL:HG23	2.16	0.46
1:E:187:LEU:HD13	1:E:379:ILE:HG12	1.97	0.46
1:G:171:LYS:HD3	1:G:407:VAL:HG11	1.98	0.46
1:H:69:MET:CE	1:I:39:VAL:HG12	2.46	0.46
1:H:409:GLU:CD	1:H:501:ARG:HH21	2.24	0.46
1:I:2:ALA:N	1:J:61:GLU:OE1	2.48	0.46
1:I:233:MET:HB3	1:I:309:LEU:CD2	2.46	0.46
1:I:252:GLU:O	1:I:277:LYS:HG3	2.15	0.46
1:K:112:ASN:HA	1:K:113:PRO:HD3	1.85	0.46
1:N:77:VAL:CG2	1:N:507:ALA:CA	2.86	0.46
1:N:421:ARG:NH1	1:N:472:GLY:O	2.44	0.46
2:P:14:ARG:NH1	2:P:84:LEU:HD21	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:41:LEU:O	2:Q:61:VAL:HG22	2.16	0.46
2:S:40:VAL:HG23	2:S:63:ASP:O	2.16	0.46
2:T:24:GLY:HA2	2:T:25:ILE:HA	1.37	0.46
2:X:49:LEU:O	2:X:52:GLY:N	2.48	0.46
2:Z:64:ILE:CG2	2:Z:95:VAL:HG22	2.42	0.46
2:1:95:VAL:CA	2:2:3:ILE:HG22	2.46	0.46
1:C:350:ARG:HA	1:C:353:ILE:CD1	2.45	0.45
1:D:229:ASN:CG	1:D:230:ILE:H	2.12	0.45
1:E:255:GLU:N	1:E:255:GLU:OE1	2.49	0.45
1:E:364:LYS:O	1:E:367:GLU:HB3	2.16	0.45
1:F:325:ILE:N	1:F:325:ILE:HD12	2.31	0.45
1:H:291:ASP:OD2	1:H:368:ARG:HD3	2.16	0.45
1:J:245:LYS:HB3	1:J:245:LYS:HE2	1.60	0.45
1:L:488:MET:HE3	1:L:493:ILE:CG2	2.47	0.45
1:M:215:LEU:HD22	1:M:246:PRO:CB	2.46	0.45
1:M:234:LEU:CB	1:M:235:PRO:CD	2.84	0.45
1:M:488:MET:HE3	1:M:493:ILE:HG21	1.97	0.45
1:N:91:THR:OG1	3:N:601:ADP:O2B	2.31	0.45
1:N:116:LEU:O	1:N:120:ILE:HG13	2.16	0.45
1:N:221:LEU:HD13	1:N:317:LEU:HD23	1.97	0.45
2:Q:55:LYS:HE3	2:R:52:GLY:HA2	1.98	0.45
2:R:7:HIS:O	2:R:44:GLY:HA3	2.16	0.45
2:X:66:ILE:HG21	2:Y:76:GLU:HG3	1.96	0.45
2:Z:48:ILE:HG13	2:Z:52:GLY:O	2.17	0.45
1:D:237:LEU:HD22	2:R:27:LEU:CD1	2.42	0.45
1:D:510:VAL:O	1:D:514:MET:HB2	2.17	0.45
1:E:219:PHE:HB3	1:E:317:LEU:CB	2.41	0.45
1:E:264:VAL:O	1:E:268:ARG:HG2	2.17	0.45
1:E:265:ASN:OD1	2:S:27:LEU:HD22	2.16	0.45
1:F:322:ARG:HG2	1:F:323:VAL:H	1.81	0.45
1:G:151:SER:HB3	1:G:399:ALA:HA	1.99	0.45
1:J:230:ILE:O	1:J:231:ARG:HG2	2.16	0.45
1:J:291:ASP:OD2	1:J:368:ARG:HD3	2.17	0.45
1:J:305:ILE:CG2	1:J:307:MET:H	2.18	0.45
1:J:314:LEU:HD23	1:J:314:LEU:C	2.40	0.45
1:J:325:ILE:CG1	1:J:330:THR:HG23	2.40	0.45
1:K:40:LEU:HD11	1:K:56:VAL:HA	1.97	0.45
1:M:231:ARG:HB3	1:M:258:ALA:HB2	1.98	0.45
2:T:78:ILE:HG13	2:T:79:ASP:N	2.31	0.45
2:U:6:LEU:HD12	2:U:6:LEU:C	2.41	0.45
2:U:11:ILE:HG23	2:U:42:ALA:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:5:PRO:HD3	2:Y:42:ALA:HB3	1.98	0.45
2:1:41:LEU:O	2:1:61:VAL:HG13	2.16	0.45
1:A:205:ILE:HA	1:A:213:VAL:HG22	1.98	0.45
1:A:230:ILE:HG22	1:A:230:ILE:O	2.16	0.45
1:B:197:ARG:HH21	1:B:277:LYS:HD3	1.82	0.45
1:D:254:VAL:CG1	1:D:259:LEU:HG	2.46	0.45
1:E:220:ILE:HD12	1:E:220:ILE:O	2.16	0.45
1:F:175:ILE:HB	1:F:400:LEU:HD11	1.98	0.45
1:F:228:SER:HB2	1:F:255:GLU:HB2	1.98	0.45
1:G:295:LEU:HD23	1:G:295:LEU:C	2.41	0.45
1:H:40:LEU:HD11	1:H:56:VAL:HA	1.97	0.45
1:H:210:THR:O	1:H:210:THR:HG22	2.16	0.45
1:H:266:THR:HG22	1:H:273:VAL:H	1.82	0.45
1:I:62:LEU:HD23	1:I:67:GLU:HB3	1.99	0.45
1:J:162:ILE:O	1:J:166:MET:HG3	2.16	0.45
1:J:208:PRO:HG2	1:J:214:GLU:HG3	1.97	0.45
1:L:225:LYS:CG	1:L:226:LYS:N	2.79	0.45
2:S:16:GLU:CG	2:S:19:THR:HG23	2.46	0.45
2:Y:13:LYS:HG3	2:Y:83:VAL:HG12	1.99	0.45
1:A:227:ILE:CG2	1:A:231:ARG:HA	2.47	0.45
1:B:513:LEU:HD11	1:C:388:GLU:HA	1.98	0.45
1:C:88:GLY:N	4:C:602:BEF:F2	2.36	0.45
1:C:263:VAL:O	1:C:267:MET:HG2	2.16	0.45
1:E:200:LEU:HD22	1:E:254:VAL:HB	1.99	0.45
1:E:226:LYS:HE2	1:E:255:GLU:OE2	2.15	0.45
1:G:157:THR:O	1:G:161:LEU:HB2	2.15	0.45
1:G:358:SER:CA	1:G:362:ARG:HE	2.18	0.45
1:I:207:LYS:N	1:I:208:PRO:CD	2.80	0.45
1:I:239:ALA:CB	1:I:314:LEU:HD21	2.47	0.45
1:K:169:VAL:HB	1:K:375:GLY:O	2.17	0.45
1:K:475:ASN:O	1:K:488:MET:HG2	2.16	0.45
1:L:221:LEU:HG	1:L:248:LEU:O	2.16	0.45
1:L:241:ALA:HA	1:L:271:VAL:CG1	2.46	0.45
1:L:433:ASN:OD1	1:L:436:GLN:HG3	2.16	0.45
1:M:229:ASN:C	1:M:231:ARG:H	2.22	0.45
1:M:496:PRO:O	1:M:499:VAL:HG22	2.17	0.45
1:N:358:SER:OG	1:N:359:ASP:N	2.49	0.45
1:N:510:VAL:O	1:N:514:MET:HE3	2.16	0.45
2:O:15:LYS:HG2	2:O:37:ARG:O	2.17	0.45
2:U:73:VAL:HG12	2:U:86:MET:HB2	1.98	0.45
2:X:14:ARG:HG3	2:X:84:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:25:ILE:O	2:X:25:ILE:HG22	2.16	0.45
2:Y:49:LEU:HD23	2:Y:49:LEU:C	2.42	0.45
1:A:207:LYS:HB3	1:A:208:PRO:HD3	1.99	0.45
1:B:239:ALA:CB	1:B:314:LEU:HD11	2.46	0.45
1:B:337:GLY:C	1:B:338:GLU:HG2	2.41	0.45
1:E:322:ARG:HG2	1:E:323:VAL:N	2.31	0.45
1:H:77:VAL:HG23	1:H:506:TYR:C	2.41	0.45
1:I:152:ALA:HB2	1:I:399:ALA:CB	2.44	0.45
1:J:142:LYS:O	1:J:146:GLN:HG3	2.16	0.45
1:J:227:ILE:HD12	1:J:227:ILE:H	1.80	0.45
1:K:54:VAL:HG22	1:K:58:ARG:HE	1.81	0.45
1:K:217:SER:HA	1:K:320:ALA:O	2.17	0.45
1:L:149:THR:CG2	1:L:156:GLU:HA	2.47	0.45
1:N:69:MET:O	1:N:73:MET:HG3	2.16	0.45
2:Q:88:GLU:HA	2:Q:91:ILE:HG22	1.98	0.45
2:T:48:ILE:O	2:T:48:ILE:HG13	2.16	0.45
2:V:57:LEU:O	2:V:59:VAL:HG13	2.17	0.45
2:Z:11:ILE:O	2:Z:41:LEU:HB2	2.17	0.45
1:A:419:LEU:HD22	1:A:419:LEU:H	1.82	0.45
1:B:338:GLU:HG3	1:B:340:ALA:H	1.82	0.45
1:D:423:ALA:HA	1:D:444:LEU:HD22	1.99	0.45
1:E:34:LYS:HD2	1:E:458:CYS:SG	2.57	0.45
1:H:224:ASP:OD1	1:H:286:LYS:HG3	2.17	0.45
1:I:295:LEU:C	1:I:295:LEU:HD23	2.41	0.45
1:J:293:ALA:O	1:J:298:GLY:N	2.49	0.45
1:K:361:ASP:O	1:K:365:LEU:HG	2.17	0.45
1:L:392:LYS:O	1:L:396:VAL:HG23	2.16	0.45
1:M:92:ALA:HB2	1:M:503:ALA:HB1	1.97	0.45
2:O:51:ASN:ND2	2:P:50:GLU:O	2.49	0.45
2:P:55:LYS:HD2	2:P:55:LYS:HA	1.75	0.45
2:U:28:THR:HG22	2:U:29:GLY:O	2.17	0.45
2:W:50:GLU:OE1	2:W:50:GLU:N	2.50	0.45
1:A:222:LEU:N	1:A:222:LEU:HD12	2.32	0.45
1:A:443:ALA:O	1:A:447:MET:HG3	2.17	0.45
1:B:23:LEU:HD23	1:B:60:ILE:HB	1.99	0.45
1:D:78:ALA:HB2	1:D:93:THR:OG1	2.17	0.45
1:D:177:VAL:HG21	1:D:393:LYS:HG3	1.96	0.45
1:E:73:MET:HG3	1:F:47:PRO:HG2	1.98	0.45
1:E:360:TYR:O	1:E:360:TYR:CG	2.70	0.45
1:F:400:LEU:HD23	1:F:400:LEU:C	2.41	0.45
1:H:268:ARG:HD2	1:H:268:ARG:HA	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:432:GLN:HB2	1:H:436:GLN:OE1	2.17	0.45
1:J:240:VAL:HA	1:J:314:LEU:CD1	2.47	0.45
1:J:488:MET:HE3	1:J:493:ILE:CG2	2.47	0.45
1:K:208:PRO:CB	1:K:212:ALA:HB3	2.32	0.45
1:L:237:LEU:HD23	1:L:237:LEU:O	2.17	0.45
1:L:434:GLU:O	1:L:437:ASN:HB2	2.16	0.45
1:M:164:GLU:O	1:M:168:LYS:HB2	2.17	0.45
1:N:227:ILE:HG12	1:N:231:ARG:HG3	1.98	0.45
1:N:419:LEU:O	1:N:422:VAL:HG22	2.17	0.45
2:T:23:GLY:O	2:T:26:VAL:HG12	2.17	0.45
2:U:49:LEU:O	2:U:50:GLU:CG	2.64	0.45
2:X:16:GLU:HG2	2:X:16:GLU:O	2.16	0.45
1:A:278:ALA:HB3	1:A:285:ARG:HD3	1.99	0.45
1:A:518:GLU:HB2	1:B:36:ARG:HB2	1.99	0.45
1:B:222:LEU:N	1:B:222:LEU:HD12	2.32	0.45
1:D:124:VAL:HG13	1:D:504:LEU:CD1	2.47	0.45
1:E:31:LEU:HA	3:E:601:ADP:O2A	2.16	0.45
1:E:414:GLY:HA2	1:E:495:ASP:OD2	2.17	0.45
1:F:264:VAL:O	1:F:268:ARG:HG2	2.17	0.45
1:F:301:ILE:HG12	1:F:307:MET:HG3	1.99	0.45
1:F:304:GLU:CB	1:F:305:ILE:HD12	2.43	0.45
1:F:381:VAL:HG21	1:F:392:LYS:HG3	1.99	0.45
1:G:288:MET:O	1:G:292:ILE:HG13	2.17	0.45
1:G:313:THR:HB	1:G:315:GLU:CG	2.47	0.45
1:G:409:GLU:CD	1:G:501:ARG:HH21	2.20	0.45
1:H:228:SER:HB2	1:H:255:GLU:OE1	2.17	0.45
1:H:414:GLY:O	1:H:417:VAL:HG12	2.17	0.45
1:H:419:LEU:H	1:H:419:LEU:HD22	1.81	0.45
1:I:307:MET:O	1:I:307:MET:HG3	2.17	0.45
1:L:28:LYS:HG2	1:L:94:VAL:HG22	1.99	0.45
1:L:333:ILE:O	1:L:334:ASP:HB2	2.15	0.45
1:L:488:MET:CE	1:L:493:ILE:HG21	2.47	0.45
1:M:200:LEU:CD2	1:M:254:VAL:HB	2.44	0.45
1:M:349:ILE:HG21	1:M:369:VAL:CG2	2.47	0.45
2:Q:15:LYS:HB3	2:Q:16:GLU:OE2	2.17	0.45
2:S:82:GLU:O	2:S:82:GLU:HG2	2.15	0.45
2:U:43:VAL:HG22	2:U:44:GLY:N	2.32	0.45
2:Y:57:LEU:HD13	2:Y:88:GLU:HB2	1.99	0.45
2:Z:39:GLU:HA	2:Z:64:ILE:HA	1.99	0.45
1:A:359:ASP:O	1:A:360:TYR:HB2	2.17	0.45
1:G:220:ILE:HD12	1:G:220:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:LEU:CD2	1:G:300:VAL:HG22	2.37	0.45
1:G:266:THR:CG2	1:G:273:VAL:HB	2.47	0.45
1:H:42:LYS:HE2	1:H:48:THR:CG2	2.47	0.45
1:H:203:TYR:HE2	1:N:305:ILE:HD11	1.81	0.45
1:H:363:GLU:O	1:H:367:GLU:HB2	2.17	0.45
1:K:259:LEU:O	1:K:263:VAL:HG23	2.17	0.45
1:L:25:ASP:OD1	1:L:28:LYS:HE2	2.16	0.45
1:L:230:ILE:O	1:L:232:GLU:HG2	2.16	0.45
1:L:320:ALA:HB1	1:L:334:ASP:O	2.17	0.45
1:L:361:ASP:O	1:L:365:LEU:HD13	2.17	0.45
1:N:74:VAL:CG1	1:N:514:MET:HE1	2.46	0.45
1:N:307:MET:HE3	1:N:311:LYS:NZ	2.32	0.45
2:X:94:ILE:HD11	2:Y:4:ARG:HD3	1.98	0.45
2:1:31:ALA:O	2:1:32:ALA:HB3	2.17	0.45
1:A:359:ASP:CG	1:A:360:TYR:H	2.24	0.45
1:B:18:ARG:NH1	1:B:18:ARG:HB3	2.32	0.45
1:B:48:THR:HG22	1:B:390:LYS:HZ1	1.80	0.45
1:B:262:LEU:O	1:B:266:THR:HG23	2.16	0.45
1:C:226:LYS:HA	1:C:252:GLU:HB3	1.99	0.45
1:C:226:LYS:HE2	1:C:252:GLU:HG2	1.99	0.45
1:E:230:ILE:HD12	1:E:230:ILE:H	1.82	0.45
1:E:237:LEU:HD23	1:E:237:LEU:C	2.42	0.45
1:E:295:LEU:HD23	1:E:295:LEU:C	2.42	0.45
1:G:429:LEU:HG	1:G:440:ILE:HD13	1.98	0.45
1:H:10:ASN:O	1:H:14:VAL:HG23	2.16	0.45
1:I:321:LYS:HD2	1:I:334:ASP:OD2	2.16	0.45
1:J:365:LEU:O	1:J:369:VAL:HG23	2.17	0.45
3:K:601:ADP:O3B	4:K:602:BEF:F1	2.25	0.45
1:L:282:GLY:CA	1:L:285:ARG:HG2	2.45	0.45
1:M:228:SER:HB3	1:M:255:GLU:HB3	1.99	0.45
1:M:236:VAL:CG1	1:M:312:ALA:HB3	2.46	0.45
1:N:331:THR:HG22	1:N:332:ILE:N	2.32	0.45
2:R:11:ILE:HB	2:R:85:ILE:CD1	2.46	0.45
2:R:12:VAL:HG23	2:R:84:LEU:HD11	1.99	0.45
2:S:12:VAL:CG1	2:S:40:VAL:HA	2.43	0.45
2:Z:15:LYS:HZ2	2:Z:64:ILE:HD12	1.82	0.45
1:A:174:VAL:HG23	1:A:376:VAL:HG13	1.99	0.44
1:B:232:GLU:O	1:B:232:GLU:HG2	2.17	0.44
1:D:77:VAL:HB	1:D:510:VAL:HG21	1.98	0.44
1:D:278:ALA:CB	1:D:285:ARG:HG3	2.37	0.44
1:E:496:PRO:O	1:E:499:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:510:VAL:O	1:E:514:MET:HB2	2.17	0.44
1:H:238:GLU:HG2	2:V:25:ILE:HG12	1.99	0.44
1:I:202:PRO:O	1:I:205:ILE:HG13	2.17	0.44
1:I:294:THR:OG1	1:I:345:ARG:HG3	2.17	0.44
1:J:175:ILE:HA	1:J:377:ALA:O	2.17	0.44
1:J:197:ARG:HD3	1:J:197:ARG:HA	1.79	0.44
1:L:345:ARG:O	1:L:348:GLN:HG3	2.17	0.44
1:M:196:ASP:O	1:M:197:ARG:HG2	2.18	0.44
1:M:367:GLU:HG2	1:M:371:LYS:HZ1	1.82	0.44
2:O:57:LEU:HD22	2:O:57:LEU:N	2.32	0.44
2:P:20:LYS:HG2	2:P:27:LEU:HD23	1.99	0.44
2:S:6:LEU:HD12	2:S:6:LEU:H	1.81	0.44
1:A:247:LEU:CD1	1:A:249:ILE:HD11	2.47	0.44
1:A:271:VAL:HG11	2:O:25:ILE:CD1	2.45	0.44
1:B:86:GLY:HA3	1:B:401:HIS:ND1	2.31	0.44
1:B:124:VAL:HG21	1:B:508:ALA:CB	2.47	0.44
1:B:232:GLU:C	1:B:234:LEU:H	2.25	0.44
1:C:196:ASP:OD1	1:C:196:ASP:N	2.48	0.44
1:F:245:LYS:CB	1:F:246:PRO:CD	2.94	0.44
1:F:259:LEU:O	1:F:263:VAL:HG23	2.17	0.44
1:G:196:ASP:OD1	1:G:196:ASP:N	2.50	0.44
1:G:358:SER:HA	1:G:362:ARG:NH2	2.32	0.44
1:H:226:LYS:HG2	1:H:252:GLU:CG	2.46	0.44
1:H:248:LEU:HD13	1:H:248:LEU:C	2.42	0.44
1:I:31:LEU:CD2	1:I:453:GLN:HB3	2.45	0.44
1:I:204:PHE:CE1	1:I:263:VAL:HG22	2.51	0.44
1:I:230:ILE:HG22	1:I:230:ILE:O	2.17	0.44
1:K:37:ASN:OD1	1:K:51:LYS:HB2	2.17	0.44
1:M:259:LEU:O	1:M:262:LEU:HB3	2.17	0.44
1:N:196:ASP:OD1	1:N:196:ASP:N	2.48	0.44
2:O:25:ILE:C	2:O:25:ILE:HD12	2.42	0.44
2:S:38:GLY:O	2:S:64:ILE:HA	2.18	0.44
2:U:15:LYS:HD3	2:U:15:LYS:HA	1.69	0.44
2:Z:47:ARG:NE	2:Z:49:LEU:HD12	2.32	0.44
1:A:278:ALA:HB3	1:A:285:ARG:CD	2.47	0.44
1:A:329:THR:CG2	1:A:330:THR:N	2.80	0.44
1:B:245:LYS:N	1:B:246:PRO:HD2	2.32	0.44
1:C:221:LEU:HB2	1:C:317:LEU:CD2	2.47	0.44
1:G:33:PRO:CG	1:G:480:ALA:HB3	2.47	0.44
1:I:210:THR:O	1:I:210:THR:HG22	2.16	0.44
1:J:69:MET:SD	1:K:41:ASP:HB2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:325:ILE:HD12	1:J:325:ILE:N	2.32	0.44
1:J:353:ILE:HG12	1:J:365:LEU:CD2	2.46	0.44
1:K:302:SER:HB2	1:K:305:ILE:CD1	2.36	0.44
1:L:217:SER:O	1:L:245:LYS:HE3	2.16	0.44
1:L:253:ASP:OD1	1:L:277:LYS:HE2	2.17	0.44
1:M:147:VAL:HG22	1:M:403:THR:HG22	1.99	0.44
1:M:234:LEU:O	1:M:237:LEU:HG	2.17	0.44
1:M:236:VAL:HG11	1:M:312:ALA:HB3	1.99	0.44
2:O:6:LEU:HD11	2:U:94:ILE:H	1.81	0.44
2:Z:6:LEU:HD12	2:Z:6:LEU:O	2.16	0.44
2:Z:27:LEU:HD23	2:Z:27:LEU:C	2.42	0.44
1:B:325:ILE:HD12	1:B:325:ILE:N	2.33	0.44
1:C:177:VAL:CG1	1:C:397:GLU:HG2	2.22	0.44
1:C:419:LEU:HD22	1:C:419:LEU:N	2.32	0.44
1:D:419:LEU:HD22	1:D:419:LEU:H	1.83	0.44
1:E:193:MET:HE3	1:E:195:PHE:HD2	1.83	0.44
1:E:197:ARG:CG	1:E:279:PRO:HA	2.45	0.44
1:F:222:LEU:HD12	1:F:222:LEU:N	2.33	0.44
1:F:329:THR:CG2	1:F:330:THR:N	2.80	0.44
1:I:176:THR:OG1	1:I:378:VAL:HG22	2.18	0.44
1:I:367:GLU:CG	1:I:371:LYS:HE2	2.46	0.44
1:K:168:LYS:HG2	1:K:189:VAL:CG1	2.45	0.44
1:K:207:LYS:HG3	1:K:208:PRO:N	2.30	0.44
1:M:365:LEU:O	1:M:369:VAL:HG23	2.17	0.44
1:N:220:ILE:O	1:N:317:LEU:HA	2.17	0.44
1:N:307:MET:HE3	1:N:311:LYS:HZ2	1.83	0.44
2:O:6:LEU:CD1	2:O:6:LEU:N	2.80	0.44
2:V:40:VAL:HG11	2:V:60:LYS:O	2.17	0.44
2:Y:15:LYS:HD3	2:Y:37:ARG:CB	2.46	0.44
2:Z:17:VAL:HG13	2:Z:18:GLU:OE2	2.17	0.44
1:B:215:LEU:CD1	1:B:248:LEU:HD21	2.44	0.44
1:B:421:ARG:NH1	1:B:472:GLY:O	2.50	0.44
1:B:429:LEU:HD12	1:B:430:ARG:N	2.32	0.44
1:D:196:ASP:O	1:D:197:ARG:HG2	2.16	0.44
1:D:263:VAL:HG13	1:D:267:MET:HE3	1.98	0.44
1:G:198:GLY:O	1:G:276:VAL:HG23	2.17	0.44
1:G:226:LYS:HE2	1:G:253:ASP:HB2	1.98	0.44
1:L:200:LEU:HD22	1:L:254:VAL:HB	2.00	0.44
1:N:311:LYS:O	1:N:311:LYS:HD3	2.17	0.44
2:R:3:ILE:C	2:R:3:ILE:HD12	2.43	0.44
2:V:14:ARG:NE	2:V:84:LEU:HD21	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:9:ARG:H	2:W:9:ARG:HG3	1.58	0.44
2:Z:15:LYS:HD2	2:Z:16:GLU:OE1	2.18	0.44
1:A:305:ILE:HG23	1:A:306:GLY:N	2.32	0.44
1:B:69:MET:HE2	1:B:520:MET:HE3	2.00	0.44
1:B:236:VAL:O	1:B:240:VAL:HG23	2.17	0.44
1:B:391:GLU:OE2	1:B:395:ARG:NE	2.43	0.44
1:C:260:ALA:O	1:C:264:VAL:HG23	2.18	0.44
1:D:236:VAL:HG22	1:D:312:ALA:HB3	1.99	0.44
1:D:240:VAL:HG12	1:D:245:LYS:O	2.17	0.44
1:D:295:LEU:C	1:D:295:LEU:HD23	2.42	0.44
1:E:143:ALA:O	1:E:147:VAL:HG13	2.17	0.44
1:E:367:GLU:O	1:E:371:LYS:HG3	2.17	0.44
1:E:517:THR:HG23	1:F:39:VAL:HG23	1.99	0.44
1:G:285:ARG:HG3	1:G:286:LYS:N	2.33	0.44
1:G:361:ASP:OD1	1:G:361:ASP:N	2.51	0.44
1:H:199:TYR:CD1	1:H:202:PRO:HA	2.53	0.44
1:I:280:GLY:O	1:I:285:ARG:HB3	2.17	0.44
1:J:190:VAL:HG13	1:J:194:GLN:CD	2.43	0.44
1:J:222:LEU:HD12	1:J:222:LEU:N	2.32	0.44
1:M:221:LEU:HB2	1:M:317:LEU:CD2	2.47	0.44
1:N:24:ALA:O	1:N:28:LYS:HG3	2.17	0.44
2:O:40:VAL:HG23	2:O:63:ASP:O	2.17	0.44
2:Z:47:ARG:HG3	2:Z:49:LEU:HG	2.00	0.44
1:A:34:LYS:HD2	1:A:458:CYS:SG	2.58	0.44
1:B:77:VAL:HG21	1:B:507:ALA:CA	2.39	0.44
1:B:205:ILE:HD12	1:B:211:GLY:HA2	2.00	0.44
1:B:429:LEU:HD12	1:B:430:ARG:H	1.82	0.44
1:F:414:GLY:O	1:F:417:VAL:HG12	2.17	0.44
1:H:222:LEU:HD12	1:H:222:LEU:N	2.32	0.44
1:I:417:VAL:CA	1:I:420:ILE:HG22	2.46	0.44
1:J:421:ARG:HD3	1:J:421:ARG:HA	1.68	0.44
1:K:353:ILE:HG12	1:K:365:LEU:HB3	2.00	0.44
1:L:248:LEU:HD13	1:L:248:LEU:C	2.42	0.44
1:L:412:VAL:CG1	1:L:413:ALA:H	2.31	0.44
1:M:200:LEU:HD22	1:M:254:VAL:CB	2.46	0.44
1:M:400:LEU:HD13	1:M:400:LEU:C	2.43	0.44
1:N:142:LYS:O	1:N:146:GLN:HG3	2.17	0.44
1:N:400:LEU:C	1:N:400:LEU:HD13	2.42	0.44
2:P:57:LEU:HD22	2:P:88:GLU:CD	2.43	0.44
2:U:17:VAL:HG22	2:U:18:GLU:N	2.31	0.44
2:Z:6:LEU:O	2:Z:9:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:17:VAL:CG1	2:2:35:SER:H	2.31	0.44
1:A:195:PHE:CE1	1:A:330:THR:HB	2.53	0.44
1:A:367:GLU:HG3	1:A:371:LYS:NZ	2.33	0.44
1:A:475:ASN:O	1:A:488:MET:HG2	2.17	0.44
1:B:73:MET:SD	1:C:49:ILE:HD11	2.57	0.44
1:B:305:ILE:CD1	1:C:203:TYR:HE2	2.31	0.44
1:B:305:ILE:CD1	1:C:263:VAL:HG11	2.44	0.44
1:B:307:MET:HE3	1:B:311:LYS:NZ	2.33	0.44
1:B:478:TYR:HD1	1:B:485:TYR:CE1	2.35	0.44
1:C:143:ALA:O	1:C:147:VAL:HG13	2.18	0.44
1:C:215:LEU:HD22	1:C:246:PRO:HB2	2.00	0.44
1:D:254:VAL:HB	1:D:259:LEU:HD21	1.99	0.44
1:D:326:ASN:ND2	1:D:329:THR:H	2.15	0.44
1:D:329:THR:CG2	1:D:330:THR:N	2.81	0.44
1:D:393:LYS:O	1:D:397:GLU:HG3	2.17	0.44
1:E:232:GLU:C	1:E:234:LEU:H	2.25	0.44
1:E:248:LEU:CD2	1:E:323:VAL:HG11	2.36	0.44
1:G:124:VAL:O	1:G:128:VAL:HG23	2.17	0.44
1:H:365:LEU:O	1:H:369:VAL:HG23	2.18	0.44
1:J:116:LEU:HD23	1:J:435:ASP:O	2.18	0.44
1:K:371:LYS:HE2	1:K:376:VAL:HG21	2.00	0.44
1:L:271:VAL:O	1:L:273:VAL:HG23	2.16	0.44
1:M:90:THR:O	1:M:94:VAL:HG23	2.17	0.44
2:O:94:ILE:HG13	2:P:4:ARG:O	2.17	0.44
2:R:57:LEU:HD22	2:R:88:GLU:HB2	2.00	0.44
2:R:80:ASN:OD1	2:R:81:GLU:HG3	2.18	0.44
1:A:392:LYS:O	1:A:396:VAL:HG23	2.17	0.44
1:B:136:VAL:HG22	1:B:137:PRO:CD	2.48	0.44
1:B:450:PRO:O	1:B:454:ILE:HG13	2.18	0.44
1:C:200:LEU:HB3	1:C:259:LEU:CD1	2.48	0.44
1:D:234:LEU:N	1:D:235:PRO:CD	2.80	0.44
1:E:361:ASP:O	1:E:365:LEU:HB2	2.18	0.44
1:F:183:LEU:HD22	1:F:384:ALA:HA	2.00	0.44
1:H:114:MET:HG3	1:H:118:ARG:NH1	2.33	0.44
1:K:268:ARG:HB2	1:K:270:ILE:HD12	1.99	0.44
1:L:127:ALA:O	1:L:131:LEU:HG	2.17	0.44
1:L:282:GLY:HA2	1:L:285:ARG:CG	2.47	0.44
1:M:364:LYS:HZ3	1:M:368:ARG:HE	1.66	0.44
1:N:259:LEU:HA	1:N:262:LEU:HB3	2.00	0.44
2:R:25:ILE:HA	2:R:26:VAL:CG2	2.48	0.44
2:S:41:LEU:O	2:S:61:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:50:GLU:OE1	2:U:50:GLU:N	2.49	0.44
2:Y:7:HIS:O	2:Y:8:ASP:CB	2.66	0.44
1:A:147:VAL:CG1	1:A:494:LEU:HD12	2.48	0.43
1:A:205:ILE:HG22	1:A:206:ASN:O	2.18	0.43
1:A:213:VAL:HB	1:A:325:ILE:HB	2.00	0.43
1:B:496:PRO:HG2	1:B:499:VAL:HG11	1.99	0.43
1:C:218:PRO:O	1:C:319:GLN:HA	2.18	0.43
1:F:177:VAL:HG22	1:F:393:LYS:HG3	1.99	0.43
1:G:323:VAL:HG12	1:G:332:ILE:HG12	1.99	0.43
1:I:295:LEU:HD23	1:I:295:LEU:O	2.18	0.43
1:J:23:LEU:HD22	1:J:60:ILE:HG13	1.98	0.43
1:J:265:ASN:CB	1:J:270:ILE:HB	2.32	0.43
1:J:350:ARG:HA	1:J:353:ILE:HG13	2.00	0.43
1:K:197:ARG:HD3	1:K:197:ARG:HA	1.82	0.43
1:L:225:LYS:HD3	1:L:303:GLU:OE1	2.18	0.43
1:L:230:ILE:O	1:L:231:ARG:HB2	2.17	0.43
1:M:200:LEU:HD11	1:M:277:LYS:HG2	2.00	0.43
1:N:157:THR:O	1:N:161:LEU:HB2	2.18	0.43
1:N:233:MET:C	1:N:235:PRO:HD2	2.43	0.43
2:Q:40:VAL:HG21	2:Q:60:LYS:O	2.17	0.43
2:U:3:ILE:CD1	2:U:78:ILE:HD13	2.46	0.43
2:Y:91:ILE:HG22	2:Z:6:LEU:HD21	2.00	0.43
1:B:96:ALA:O	1:B:100:ILE:HG13	2.19	0.43
1:B:198:GLY:HA3	1:B:327:LYS:O	2.18	0.43
1:B:368:ARG:O	1:B:372:LEU:HG	2.18	0.43
1:C:231:ARG:HH12	1:C:234:LEU:CD2	2.29	0.43
1:C:364:LYS:HA	1:C:367:GLU:CB	2.48	0.43
1:E:149:THR:HG23	1:E:155:ASP:C	2.43	0.43
1:G:158:VAL:O	1:G:162:ILE:HG13	2.18	0.43
1:G:313:THR:CB	1:G:315:GLU:HG2	2.49	0.43
1:H:77:VAL:CG2	1:H:507:ALA:HA	2.39	0.43
1:H:207:LYS:N	1:H:208:PRO:CD	2.81	0.43
1:I:230:ILE:C	1:I:232:GLU:N	2.76	0.43
1:I:367:GLU:O	1:I:371:LYS:HG3	2.17	0.43
1:J:358:SER:OG	1:J:359:ASP:N	2.50	0.43
1:K:99:ILE:CG2	1:K:511:ALA:HB1	2.47	0.43
1:K:213:VAL:HB	1:K:325:ILE:HB	1.99	0.43
1:K:232:GLU:OE1	1:K:232:GLU:N	2.50	0.43
1:K:285:ARG:HG3	1:K:286:LYS:N	2.32	0.43
1:M:217:SER:N	1:M:218:PRO:HD3	2.33	0.43
1:M:267:MET:HA	1:M:267:MET:CE	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:285:ARG:HG3	1:M:286:LYS:N	2.34	0.43
1:A:95:LEU:O	1:A:99:ILE:HG13	2.17	0.43
1:A:267:MET:HE2	1:A:267:MET:CA	2.41	0.43
1:D:400:LEU:HD13	1:D:400:LEU:C	2.43	0.43
1:E:136:VAL:HG22	1:E:137:PRO:CD	2.48	0.43
1:F:393:LYS:O	1:F:397:GLU:HG3	2.18	0.43
1:F:421:ARG:HD3	1:F:421:ARG:HA	1.75	0.43
1:G:209:GLU:CG	1:G:210:THR:N	2.79	0.43
1:G:223:ALA:HB1	1:G:225:LYS:O	2.19	0.43
1:H:25:ASP:OD1	1:H:28:LYS:HE2	2.19	0.43
1:I:213:VAL:HB	1:I:325:ILE:HB	2.01	0.43
1:I:219:PHE:HD1	1:I:319:GLN:HG2	1.84	0.43
1:I:401:HIS:O	1:I:404:ARG:HB2	2.19	0.43
1:I:496:PRO:HG2	1:I:499:VAL:CG1	2.48	0.43
1:J:155:ASP:CG	1:J:158:VAL:HG23	2.43	0.43
1:J:208:PRO:HG2	1:J:214:GLU:CG	2.49	0.43
1:J:238:GLU:HG3	1:J:242:LYS:NZ	2.34	0.43
1:K:218:PRO:CA	1:K:246:PRO:HG2	2.47	0.43
1:L:510:VAL:HG12	1:M:387:VAL:HG21	2.00	0.43
1:N:197:ARG:HG2	1:N:277:LYS:CA	2.48	0.43
1:N:199:TYR:CD1	1:N:202:PRO:HA	2.52	0.43
1:N:200:LEU:HD12	1:N:200:LEU:N	2.33	0.43
2:P:28:THR:HG22	2:P:29:GLY:O	2.18	0.43
2:Q:50:GLU:HB3	2:Q:52:GLY:H	1.83	0.43
2:Q:92:LEU:O	2:R:6:LEU:HB3	2.18	0.43
2:T:60:LYS:HG3	2:T:61:VAL:H	1.82	0.43
2:U:65:VAL:CG1	2:U:94:ILE:HG22	2.48	0.43
2:X:73:VAL:CG2	2:X:84:LEU:HB3	2.48	0.43
2:1:25:ILE:C	2:1:25:ILE:HD12	2.43	0.43
1:B:219:PHE:HB3	1:B:317:LEU:HB3	2.00	0.43
1:B:367:GLU:CG	1:B:371:LYS:HE2	2.43	0.43
1:C:421:ARG:NH1	1:C:472:GLY:O	2.50	0.43
1:H:147:VAL:HG23	1:H:403:THR:HG22	1.99	0.43
1:H:220:ILE:CG2	1:H:222:LEU:HD11	2.44	0.43
1:H:234:LEU:N	1:H:235:PRO:CD	2.80	0.43
1:I:23:LEU:HD23	1:I:60:ILE:HB	2.00	0.43
1:J:232:GLU:O	1:J:310:GLU:HG3	2.18	0.43
1:K:168:LYS:HG2	1:K:189:VAL:CG2	2.48	0.43
1:K:496:PRO:HG2	1:K:499:VAL:CG2	2.49	0.43
1:L:496:PRO:HG2	1:L:499:VAL:HG21	1.97	0.43
1:M:65:LYS:HB3	1:M:522:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:177:VAL:HG23	1:M:381:VAL:HG23	2.00	0.43
1:N:225:LYS:CG	1:N:226:LYS:N	2.81	0.43
2:Q:54:VAL:O	2:Q:54:VAL:HG23	2.17	0.43
2:Q:94:ILE:HD11	2:R:4:ARG:HH21	1.83	0.43
2:U:77:LYS:HG2	2:U:82:GLU:HA	2.00	0.43
2:V:40:VAL:HG13	2:V:41:LEU:N	2.33	0.43
2:V:78:ILE:HD13	2:2:37:ARG:HH22	1.83	0.43
2:Y:11:ILE:HG12	2:Y:42:ALA:HB3	2.01	0.43
1:B:278:ALA:HB1	1:B:279:PRO:HD2	1.99	0.43
1:C:248:LEU:HD23	1:C:248:LEU:C	2.43	0.43
1:C:359:ASP:O	1:C:360:TYR:HB3	2.18	0.43
1:D:198:GLY:HA3	1:D:327:LYS:O	2.17	0.43
1:D:233:MET:HB3	1:D:309:LEU:CD2	2.48	0.43
1:E:392:LYS:O	1:E:396:VAL:HG23	2.18	0.43
1:F:160:LYS:HD2	1:F:160:LYS:HA	1.82	0.43
1:G:106:ALA:O	1:G:109:ALA:HB3	2.19	0.43
1:H:228:SER:HA	1:H:255:GLU:HB2	2.00	0.43
1:H:381:VAL:HG21	1:H:393:LYS:HA	2.00	0.43
1:I:302:SER:OG	1:I:305:ILE:HD13	2.18	0.43
1:I:368:ARG:O	1:I:372:LEU:HG	2.19	0.43
1:M:115:ASP:O	1:M:436:GLN:HG2	2.18	0.43
1:M:143:ALA:O	1:M:147:VAL:HG13	2.18	0.43
1:M:419:LEU:N	1:M:419:LEU:HD22	2.34	0.43
2:Q:88:GLU:OE2	2:R:7:HIS:HE1	2.00	0.43
2:R:5:PRO:HB2	2:R:9:ARG:O	2.18	0.43
2:R:12:VAL:CG2	2:R:84:LEU:HD11	2.48	0.43
2:R:76:GLU:HG3	2:R:77:LYS:N	2.33	0.43
2:S:11:ILE:CG1	2:S:83:VAL:HG11	2.48	0.43
2:X:36:THR:OG1	2:Y:76:GLU:OE2	2.28	0.43
2:1:66:ILE:HD12	2:2:3:ILE:HD12	2.00	0.43
2:2:27:LEU:HD12	2:2:27:LEU:N	2.34	0.43
1:A:227:ILE:HD12	1:A:227:ILE:H	1.83	0.43
1:C:205:ILE:HG12	1:C:206:ASN:O	2.18	0.43
1:C:232:GLU:C	1:C:234:LEU:N	2.75	0.43
1:C:256:GLY:O	1:C:260:ALA:N	2.35	0.43
3:C:601:ADP:O3B	4:C:602:BEF:F2	2.26	0.43
1:D:112:ASN:HA	1:D:113:PRO:HD3	1.80	0.43
1:E:87:ASP:OD2	1:E:151:SER:OG	2.29	0.43
1:E:136:VAL:HG23	1:E:137:PRO:HD2	2.00	0.43
1:E:158:VAL:O	1:E:162:ILE:HG13	2.19	0.43
1:F:23:LEU:HD13	1:F:23:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:THR:HG22	1:G:156:GLU:HA	1.99	0.43
1:G:193:MET:HE2	1:G:292:ILE:HG12	2.00	0.43
1:G:255:GLU:OE1	1:G:255:GLU:N	2.50	0.43
1:G:263:VAL:O	1:G:267:MET:HG2	2.19	0.43
1:I:200:LEU:CD2	1:I:254:VAL:HB	2.49	0.43
1:I:221:LEU:HD11	1:I:301:ILE:HD12	1.99	0.43
1:I:230:ILE:HD12	1:I:230:ILE:N	2.34	0.43
1:J:26:ALA:O	1:J:29:VAL:HG22	2.19	0.43
1:J:455:VAL:CG2	1:J:465:VAL:HG11	2.48	0.43
1:L:37:ASN:OD1	1:L:51:LYS:HB2	2.18	0.43
1:M:455:VAL:HG21	1:M:465:VAL:HG11	2.01	0.43
2:O:96:GLU:HB2	2:P:2:ASN:O	2.19	0.43
2:R:74:LYS:HD2	2:R:75:SER:H	1.84	0.43
2:T:78:ILE:HG13	2:T:79:ASP:H	1.84	0.43
2:V:2:ASN:ND2	2:V:2:ASN:C	2.73	0.43
2:W:12:VAL:HB	2:W:39:GLU:O	2.18	0.43
2:W:19:THR:HG22	2:W:20:LYS:N	2.33	0.43
2:Z:8:ASP:OD1	2:Z:9:ARG:CA	2.66	0.43
2:Z:94:ILE:O	2:Z:94:ILE:HG13	2.19	0.43
1:B:171:LYS:HA	1:B:171:LYS:HD2	1.70	0.43
1:B:326:ASN:ND2	1:B:329:THR:O	2.51	0.43
1:C:215:LEU:HB2	1:C:323:VAL:HG22	2.00	0.43
1:C:220:ILE:HD13	1:C:296:THR:HB	2.00	0.43
1:D:17:LEU:HD13	1:D:104:LEU:HD12	2.00	0.43
1:E:400:LEU:HD13	1:E:400:LEU:C	2.43	0.43
1:F:124:VAL:O	1:F:128:VAL:HG23	2.19	0.43
1:G:112:ASN:HA	1:G:113:PRO:HD3	1.89	0.43
1:G:180:GLY:HA2	1:G:380:LYS:HG2	2.01	0.43
1:G:233:MET:C	1:G:235:PRO:HD2	2.44	0.43
1:H:40:LEU:HD13	1:H:59:GLU:CG	2.42	0.43
1:H:513:LEU:CD2	1:I:49:ILE:HG21	2.49	0.43
1:I:112:ASN:HA	1:I:113:PRO:HD3	1.84	0.43
1:I:415:GLY:O	1:I:451:LEU:HD23	2.17	0.43
1:K:282:GLY:HA2	1:K:285:ARG:CD	2.48	0.43
1:K:301:ILE:HD11	1:K:312:ALA:HB2	2.01	0.43
1:M:146:GLN:OE1	1:M:492:GLY:HA2	2.19	0.43
1:N:195:PHE:CZ	1:N:330:THR:HB	2.54	0.43
1:N:205:ILE:HD12	1:N:211:GLY:HA2	2.00	0.43
1:N:524:LEU:HD22	1:N:525:PRO:HD2	2.01	0.43
2:O:80:ASN:CG	2:U:23:GLY:H	2.26	0.43
2:O:97:ALA:CB	2:P:1:MET:HB2	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:6:LEU:O	2:P:9:ARG:HD2	2.19	0.43
2:X:64:ILE:CG2	2:X:95:VAL:HG13	2.44	0.43
2:Z:95:VAL:HG12	2:1:3:ILE:HG21	1.99	0.43
1:B:362:ARG:HB3	1:B:366:GLN:NE2	2.33	0.43
1:C:203:TYR:HD2	1:C:263:VAL:CG1	2.31	0.43
1:C:230:ILE:HG22	1:C:232:GLU:HB3	2.01	0.43
1:C:247:LEU:CD1	1:C:249:ILE:HG12	2.49	0.43
1:C:285:ARG:O	1:C:289:LEU:N	2.52	0.43
1:E:475:ASN:O	1:E:488:MET:HG2	2.18	0.43
1:E:510:VAL:O	1:E:514:MET:HE3	2.18	0.43
1:I:420:ILE:HD11	1:I:470:LYS:CG	2.49	0.43
1:J:301:ILE:HG12	1:J:307:MET:HE1	1.99	0.43
1:J:322:ARG:CB	1:J:333:ILE:HD12	2.34	0.43
1:J:342:ILE:O	1:J:346:VAL:HG23	2.19	0.43
1:K:30:THR:HA	1:K:36:ARG:O	2.19	0.43
1:K:200:LEU:HD22	1:K:254:VAL:HB	2.00	0.43
1:M:30:THR:HB	1:M:51:LYS:HG3	2.01	0.43
1:N:103:GLY:O	1:N:107:VAL:HG23	2.19	0.43
2:V:14:ARG:O	2:V:14:ARG:HG3	2.18	0.43
2:2:49:LEU:H	2:2:52:GLY:CA	2.12	0.43
1:A:138:CYS:HB2	1:A:411:VAL:HG13	2.01	0.43
1:A:322:ARG:HD2	1:A:333:ILE:HD12	2.01	0.43
1:A:438:VAL:O	1:A:442:VAL:HG23	2.19	0.43
1:A:504:LEU:C	1:A:504:LEU:HD13	2.44	0.43
1:A:519:CYS:HB3	1:B:38:VAL:HG22	2.01	0.43
1:B:205:ILE:HG12	1:B:206:ASN:O	2.19	0.43
1:C:31:LEU:HD23	1:C:453:GLN:HB3	2.00	0.43
1:C:257:GLU:O	1:C:261:THR:HG22	2.18	0.43
1:D:69:MET:HE3	1:E:39:VAL:HG12	2.01	0.43
1:D:116:LEU:O	1:D:120:ILE:HG13	2.19	0.43
1:D:421:ARG:HA	1:D:421:ARG:HD3	1.76	0.43
1:E:231:ARG:NH1	2:S:31:ALA:O	2.49	0.43
1:F:103:GLY:O	1:F:107:VAL:HG23	2.19	0.43
1:H:207:LYS:HB2	1:H:207:LYS:HE3	1.82	0.43
1:H:226:LYS:HG2	1:H:252:GLU:CB	2.49	0.43
1:J:230:ILE:C	1:J:232:GLU:H	2.26	0.43
1:J:488:MET:CE	1:J:493:ILE:HG21	2.49	0.43
1:L:30:THR:HB	1:L:51:LYS:HG3	2.01	0.43
1:L:100:ILE:O	1:L:104:LEU:HG	2.18	0.43
1:L:176:THR:OG1	1:L:378:VAL:HG22	2.19	0.43
1:L:358:SER:HA	1:L:362:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:197:ARG:HD3	1:M:197:ARG:HA	1.86	0.43
1:M:339:GLU:HA	1:M:342:ILE:HB	2.01	0.43
1:N:215:LEU:O	1:N:218:PRO:HD3	2.19	0.43
1:N:401:HIS:O	1:N:404:ARG:HB2	2.19	0.43
2:R:84:LEU:O	2:R:84:LEU:HD12	2.19	0.43
2:S:46:GLY:HA2	2:S:57:LEU:HD11	2.00	0.43
2:X:94:ILE:HD11	2:Y:4:ARG:CG	2.49	0.43
2:Z:8:ASP:O	2:Z:57:LEU:CD2	2.34	0.43
1:A:199:TYR:HD2	1:A:325:ILE:HG22	1.83	0.43
1:A:247:LEU:O	1:A:273:VAL:HG13	2.19	0.43
1:A:267:MET:HA	1:A:267:MET:CE	2.41	0.43
1:A:268:ARG:N	1:A:269:GLY:CA	2.81	0.43
1:B:405:ALA:HB1	1:B:498:LYS:HD3	2.01	0.43
1:B:488:MET:O	1:B:493:ILE:HG13	2.19	0.43
1:C:14:VAL:O	1:C:18:ARG:HG3	2.19	0.43
1:D:140:ASP:OD2	1:D:142:LYS:HB3	2.18	0.43
1:D:225:LYS:HG3	1:D:226:LYS:N	2.33	0.43
1:F:359:ASP:O	1:F:360:TYR:HB3	2.19	0.43
1:G:234:LEU:N	1:G:235:PRO:HD2	2.34	0.43
1:H:232:GLU:O	1:H:234:LEU:HD12	2.18	0.43
1:J:271:VAL:O	1:J:273:VAL:HG23	2.18	0.43
1:K:349:ILE:HD12	1:K:352:GLN:CB	2.36	0.43
1:L:28:LYS:HD2	1:L:453:GLN:CD	2.44	0.43
1:M:448:GLU:OE1	1:M:452:ARG:NH1	2.52	0.43
1:N:461:GLU:HA	1:N:462:PRO:HD3	1.77	0.43
2:P:3:ILE:HD12	2:P:3:ILE:N	2.29	0.43
2:Q:6:LEU:HD13	2:Q:7:HIS:CD2	2.41	0.43
2:S:97:ALA:O	2:T:1:MET:HA	2.18	0.43
2:U:84:LEU:HD12	2:U:84:LEU:N	2.34	0.43
2:1:94:ILE:O	2:2:3:ILE:HB	2.18	0.43
1:A:310:GLU:HG2	1:A:311:LYS:HG3	2.01	0.42
1:B:347:ALA:O	1:B:350:ARG:HB2	2.19	0.42
1:C:187:LEU:HD13	1:C:379:ILE:HG12	2.01	0.42
1:D:248:LEU:HD13	1:D:249:ILE:N	2.33	0.42
1:F:105:LYS:HD3	1:F:105:LYS:HA	1.66	0.42
1:F:228:SER:O	1:F:258:ALA:HB2	2.19	0.42
1:G:239:ALA:CB	1:G:314:LEU:HD13	2.45	0.42
1:H:210:THR:HG22	1:H:326:ASN:HD21	1.84	0.42
1:H:232:GLU:O	1:H:233:MET:HB3	2.18	0.42
1:H:254:VAL:HG12	1:H:259:LEU:HG	2.00	0.42
1:I:228:SER:HB3	1:I:255:GLU:CG	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:455:VAL:HG21	1:I:465:VAL:HG11	2.01	0.42
1:J:400:LEU:HD13	1:J:400:LEU:C	2.44	0.42
1:K:199:TYR:OH	1:K:327:LYS:HG3	2.19	0.42
1:L:265:ASN:OD1	1:L:270:ILE:HD12	2.20	0.42
1:M:165:ALA:HB1	1:M:175:ILE:HD13	2.00	0.42
1:M:231:ARG:HH11	2:1:29:GLY:HA3	1.84	0.42
1:N:337:GLY:C	1:N:338:GLU:HG2	2.44	0.42
1:N:346:VAL:CG1	1:N:350:ARG:HH12	2.32	0.42
2:Q:40:VAL:HG13	2:Q:41:LEU:N	2.34	0.42
2:S:49:LEU:H	2:S:52:GLY:HA3	1.83	0.42
2:V:4:ARG:HB3	2:2:94:ILE:HG13	2.00	0.42
2:Z:50:GLU:O	2:Z:51:ASN:CG	2.62	0.42
1:B:197:ARG:HH11	1:B:198:GLY:H	1.67	0.42
1:B:314:LEU:N	1:B:314:LEU:HD12	2.34	0.42
1:D:207:LYS:N	1:D:208:PRO:CD	2.82	0.42
1:D:230:ILE:C	1:D:232:GLU:H	2.26	0.42
1:E:225:LYS:HD2	1:E:303:GLU:OE1	2.19	0.42
1:E:234:LEU:CD1	1:E:238:GLU:OE1	2.67	0.42
1:F:433:ASN:OD1	1:F:436:GLN:HG3	2.19	0.42
1:G:209:GLU:HG2	1:G:210:THR:N	2.25	0.42
1:G:217:SER:HA	1:G:320:ALA:O	2.19	0.42
1:H:233:MET:HE3	1:H:237:LEU:HB2	2.01	0.42
1:I:162:ILE:HG21	1:I:403:THR:HG21	2.01	0.42
1:I:231:ARG:HD3	1:I:257:GLU:CD	2.43	0.42
1:J:77:VAL:HB	1:J:510:VAL:HG21	1.99	0.42
1:J:106:ALA:O	1:J:109:ALA:HB3	2.19	0.42
1:J:417:VAL:HG11	1:J:488:MET:HG3	2.01	0.42
1:K:136:VAL:HG13	1:K:137:PRO:HD2	2.01	0.42
1:K:347:ALA:O	1:K:351:GLN:NE2	2.39	0.42
1:L:357:THR:HG21	1:L:361:ASP:CB	2.40	0.42
1:N:18:ARG:HB3	1:N:18:ARG:NH1	2.35	0.42
2:R:19:THR:HG21	2:R:33:ALA:CB	2.42	0.42
2:Z:65:VAL:HA	2:Z:94:ILE:HA	2.02	0.42
1:A:325:ILE:N	1:A:325:ILE:HD12	2.34	0.42
1:B:295:LEU:HD23	1:B:295:LEU:C	2.44	0.42
1:E:61:GLU:C	1:E:62:LEU:HD12	2.45	0.42
1:E:238:GLU:O	1:E:242:LYS:HG3	2.18	0.42
1:E:412:VAL:HG13	1:E:497:THR:OG1	2.19	0.42
1:E:416:GLY:O	1:E:420:ILE:HG23	2.18	0.42
1:G:247:LEU:HD22	1:G:247:LEU:N	2.34	0.42
1:G:475:ASN:HB3	1:G:489:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:90:THR:O	1:H:94:VAL:HG23	2.19	0.42
1:H:349:ILE:O	1:H:353:ILE:N	2.51	0.42
1:K:228:SER:OG	1:K:255:GLU:HB2	2.19	0.42
1:L:229:ASN:CG	1:L:230:ILE:HD12	2.44	0.42
1:N:319:GLN:OE1	1:N:319:GLN:N	2.53	0.42
1:N:326:ASN:OD1	1:N:328:ASP:HB2	2.19	0.42
2:P:1:MET:HE1	2:P:79:ASP:N	2.34	0.42
2:R:8:ASP:HA	2:R:57:LEU:HD21	2.01	0.42
2:S:14:ARG:CZ	2:S:84:LEU:HD21	2.49	0.42
2:S:36:THR:HG23	2:S:37:ARG:CG	2.44	0.42
2:Z:57:LEU:CD1	2:Z:57:LEU:H	2.29	0.42
1:A:18:ARG:HB3	1:A:18:ARG:HH11	1.83	0.42
1:B:221:LEU:HD22	1:B:249:ILE:HG23	2.01	0.42
1:C:253:ASP:OD1	1:C:277:LYS:CE	2.64	0.42
1:D:117:LYS:HG3	1:D:512:GLY:C	2.45	0.42
1:D:219:PHE:CD2	1:D:240:VAL:HG22	2.54	0.42
1:E:504:LEU:HD13	1:E:504:LEU:C	2.43	0.42
1:J:301:ILE:HA	1:J:307:MET:HE2	2.02	0.42
1:K:367:GLU:O	1:K:371:LYS:HG2	2.20	0.42
1:L:77:VAL:HG21	1:L:507:ALA:CA	2.49	0.42
1:M:193:MET:SD	1:M:371:LYS:HB3	2.59	0.42
2:Q:92:LEU:HG	2:Q:93:ALA:H	1.85	0.42
2:U:12:VAL:CG1	2:U:86:MET:HE3	2.48	0.42
2:V:40:VAL:HG13	2:V:62:GLY:H	1.84	0.42
2:X:48:ILE:HD12	2:X:48:ILE:N	2.34	0.42
2:Z:12:VAL:HG23	2:Z:39:GLU:O	2.19	0.42
2:Z:74:LYS:HG3	2:Z:76:GLU:HG3	2.01	0.42
2:2:49:LEU:HB2	2:2:52:GLY:C	2.45	0.42
2:2:54:VAL:HG12	2:2:56:PRO:HD3	2.01	0.42
1:A:177:VAL:HG21	1:A:397:GLU:CG	2.39	0.42
1:A:421:ARG:HD3	1:A:421:ARG:HA	1.77	0.42
1:B:421:ARG:HA	1:B:421:ARG:HD3	1.85	0.42
1:C:175:ILE:N	1:C:175:ILE:HD12	2.34	0.42
1:C:195:PHE:CD1	1:C:195:PHE:C	2.97	0.42
1:F:23:LEU:HD23	1:F:60:ILE:CB	2.48	0.42
1:F:127:ALA:HB2	1:F:426:LEU:HD12	2.01	0.42
1:F:240:VAL:HG11	1:F:247:LEU:CD1	2.49	0.42
1:F:266:THR:HG22	1:F:273:VAL:H	1.84	0.42
1:G:207:LYS:O	1:G:209:GLU:N	2.42	0.42
1:G:276:VAL:HG22	1:G:277:LYS:N	2.34	0.42
1:H:69:MET:HE3	1:I:39:VAL:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:278:ALA:HB3	1:H:285:ARG:CD	2.36	0.42
1:I:515:ILE:C	1:I:515:ILE:HD12	2.43	0.42
1:K:105:LYS:HD3	1:K:105:LYS:HA	1.72	0.42
1:M:23:LEU:O	1:M:27:VAL:HG23	2.19	0.42
1:N:20:VAL:HG11	1:N:100:ILE:HD12	2.00	0.42
1:N:151:SER:CB	1:N:399:ALA:HA	2.50	0.42
1:N:168:LYS:CD	1:N:189:VAL:HG21	2.49	0.42
2:V:86:MET:SD	2:V:91:ILE:HD11	2.59	0.42
2:X:7:HIS:O	2:X:8:ASP:C	2.61	0.42
2:Z:27:LEU:HD23	2:Z:28:THR:C	2.44	0.42
1:A:307:MET:C	1:A:308:GLU:CG	2.91	0.42
1:A:339:GLU:N	1:A:339:GLU:OE1	2.53	0.42
1:D:305:ILE:HG23	1:E:263:VAL:HG11	2.01	0.42
1:F:18:ARG:HB3	1:F:18:ARG:HH11	1.80	0.42
1:F:127:ALA:HB2	1:F:426:LEU:CD1	2.49	0.42
1:F:218:PRO:HB2	1:F:246:PRO:C	2.44	0.42
1:G:488:MET:HE3	1:G:493:ILE:CG2	2.49	0.42
1:H:475:ASN:O	1:H:488:MET:HG2	2.19	0.42
1:H:478:TYR:HD1	1:H:485:TYR:CD1	2.37	0.42
1:I:197:ARG:HH12	1:I:277:LYS:HD2	1.78	0.42
1:I:232:GLU:C	1:I:234:LEU:H	2.27	0.42
1:I:302:SER:OG	1:I:305:ILE:HB	2.20	0.42
1:J:175:ILE:HG23	1:J:377:ALA:O	2.19	0.42
1:L:232:GLU:HG3	1:L:310:GLU:OE2	2.19	0.42
1:N:263:VAL:O	1:N:267:MET:HG2	2.18	0.42
2:O:67:PHE:CD2	2:O:86:MET:HE1	2.53	0.42
2:U:54:VAL:O	2:U:54:VAL:HG23	2.19	0.42
2:U:65:VAL:HB	2:U:94:ILE:HG22	2.01	0.42
2:Y:11:ILE:HD11	2:Y:42:ALA:HB3	2.01	0.42
2:2:49:LEU:CB	2:2:52:GLY:HA2	2.49	0.42
1:A:20:VAL:HG13	1:A:74:VAL:HG11	2.01	0.42
1:A:230:ILE:HD12	1:A:230:ILE:H	1.85	0.42
1:A:365:LEU:HD12	1:A:365:LEU:C	2.45	0.42
1:B:266:THR:CG2	1:B:273:VAL:HB	2.50	0.42
1:B:290:GLN:HG3	1:B:345:ARG:NH2	2.34	0.42
1:C:151:SER:HB3	1:C:399:ALA:HA	2.01	0.42
1:C:234:LEU:N	1:C:235:PRO:CD	2.81	0.42
1:D:33:PRO:HG3	3:D:601:ADP:C6	2.54	0.42
1:D:114:MET:HE2	1:E:153:ASN:HD21	1.84	0.42
1:D:282:GLY:HA2	1:D:285:ARG:NH2	2.35	0.42
1:D:311:LYS:HE2	1:D:311:LYS:HB3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:PRO:HA	1:E:272:LYS:O	2.18	0.42
1:F:265:ASN:OD1	2:T:26:VAL:HG23	2.19	0.42
1:F:434:GLU:O	1:F:437:ASN:HB2	2.20	0.42
1:H:164:GLU:O	1:H:168:LYS:HG3	2.20	0.42
1:I:402:ALA:HB1	1:I:496:PRO:HG3	2.01	0.42
1:L:8:PHE:CE2	1:M:26:ALA:HA	2.55	0.42
1:L:157:THR:O	1:L:161:LEU:HB2	2.19	0.42
1:L:327:LYS:HG3	1:L:328:ASP:OD1	2.20	0.42
1:L:427:ALA:O	1:L:441:LYS:NZ	2.53	0.42
1:M:310:GLU:OE1	1:M:310:GLU:N	2.52	0.42
1:M:363:GLU:HG3	1:M:364:LYS:N	2.34	0.42
1:N:150:ILE:CD1	1:N:493:ILE:HA	2.49	0.42
2:O:20:LYS:HB3	2:O:27:LEU:HD12	2.01	0.42
2:O:95:VAL:CB	2:P:3:ILE:HG21	2.49	0.42
2:P:3:ILE:C	2:P:3:ILE:CD1	2.92	0.42
2:P:60:LYS:HG2	2:P:61:VAL:H	1.84	0.42
2:Q:22:ALA:C	2:Q:24:GLY:H	2.26	0.42
2:R:12:VAL:HG12	2:R:40:VAL:CB	2.49	0.42
2:R:43:VAL:HG23	2:R:57:LEU:HD12	2.01	0.42
2:U:6:LEU:O	2:U:9:ARG:HG2	2.20	0.42
2:Y:20:LYS:HB2	2:Y:28:THR:CG2	2.47	0.42
2:Y:77:LYS:HE2	2:Y:82:GLU:OE1	2.20	0.42
1:C:226:LYS:HG2	1:C:252:GLU:CB	2.50	0.42
1:C:258:ALA:O	1:C:262:LEU:HB2	2.20	0.42
1:D:138:CYS:HB2	1:D:411:VAL:CG1	2.48	0.42
1:D:218:PRO:CA	1:D:246:PRO:HG2	2.47	0.42
1:D:519:CYS:HB3	1:E:38:VAL:HG22	2.01	0.42
1:E:365:LEU:HD23	1:E:369:VAL:CG2	2.48	0.42
1:G:175:ILE:HA	1:G:377:ALA:O	2.19	0.42
1:H:136:VAL:HG23	1:H:137:PRO:CD	2.49	0.42
1:I:142:LYS:HE2	1:I:146:GLN:HE22	1.81	0.42
1:K:17:LEU:CD1	1:K:104:LEU:HD12	2.49	0.42
1:K:38:VAL:HB	1:K:56:VAL:HG21	2.01	0.42
1:M:196:ASP:OD1	1:M:196:ASP:N	2.52	0.42
1:M:288:MET:HG3	1:M:364:LYS:HZ3	1.85	0.42
1:N:362:ARG:O	1:N:366:GLN:HB2	2.20	0.42
2:P:27:LEU:HD12	2:P:27:LEU:N	2.34	0.42
2:X:93:ALA:HB1	2:Y:5:PRO:HA	2.00	0.42
1:A:219:PHE:HA	1:A:318:GLY:O	2.19	0.42
1:B:231:ARG:CD	1:B:258:ALA:HA	2.48	0.42
1:C:288:MET:O	1:C:292:ILE:HG13	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:THR:HG22	1:C:361:ASP:HB2	2.00	0.42
1:D:147:VAL:HG21	1:D:403:THR:HA	2.01	0.42
1:D:504:LEU:C	1:D:504:LEU:HD13	2.44	0.42
1:E:238:GLU:O	1:E:242:LYS:N	2.47	0.42
1:E:349:ILE:CG2	1:E:365:LEU:HD21	2.50	0.42
1:F:174:VAL:CG1	1:F:367:GLU:HA	2.49	0.42
1:G:219:PHE:HE2	1:G:245:LYS:CB	2.30	0.42
1:G:383:ALA:HB3	1:G:389:MET:HA	2.02	0.42
1:G:496:PRO:HG2	1:G:499:VAL:CG2	2.50	0.42
1:H:37:ASN:OD1	1:H:51:LYS:HB2	2.20	0.42
1:I:143:ALA:O	1:I:147:VAL:HG13	2.20	0.42
1:L:42:LYS:HE2	1:L:48:THR:HB	2.01	0.42
1:L:199:TYR:CE1	1:L:202:PRO:HA	2.54	0.42
1:L:421:ARG:HD3	1:L:421:ARG:HA	1.93	0.42
1:L:513:LEU:CD1	1:M:388:GLU:HA	2.50	0.42
1:L:513:LEU:O	1:L:516:THR:OG1	2.36	0.42
1:M:228:SER:HB3	1:M:255:GLU:CB	2.50	0.42
1:N:477:GLY:CA	1:N:488:MET:HE2	2.31	0.42
1:N:496:PRO:HG2	1:N:499:VAL:HG13	2.00	0.42
2:O:5:PRO:HA	2:U:93:ALA:CA	2.49	0.42
2:S:78:ILE:CG2	2:S:83:VAL:HG21	2.50	0.42
2:V:6:LEU:CD2	2:2:91:ILE:HG22	2.43	0.42
2:1:5:PRO:HB3	2:1:11:ILE:HD11	2.01	0.42
1:A:245:LYS:HB3	1:A:246:PRO:HD3	1.85	0.42
1:A:252:GLU:O	1:A:285:ARG:NH1	2.53	0.42
1:B:234:LEU:HD23	1:B:235:PRO:CD	2.47	0.42
1:B:414:GLY:O	1:B:417:VAL:HG12	2.19	0.42
1:C:359:ASP:C	1:C:361:ASP:H	2.28	0.42
1:C:419:LEU:HD22	1:C:419:LEU:H	1.84	0.42
1:C:433:ASN:OD1	1:C:435:ASP:HB2	2.20	0.42
1:F:210:THR:O	1:F:210:THR:HG22	2.19	0.42
1:F:270:ILE:HD13	2:T:25:ILE:O	2.20	0.42
1:H:49:ILE:HG21	1:N:513:LEU:HD22	2.02	0.42
1:H:183:LEU:H	1:H:183:LEU:CD1	2.32	0.42
1:H:233:MET:C	1:H:235:PRO:HD2	2.44	0.42
1:H:322:ARG:HG2	1:H:323:VAL:N	2.35	0.42
1:I:236:VAL:O	1:I:240:VAL:HG23	2.20	0.42
1:J:115:ASP:O	1:J:436:GLN:HG2	2.20	0.42
1:K:343:GLN:HA	1:K:346:VAL:CG2	2.50	0.42
1:N:40:LEU:HD21	1:N:56:VAL:CG2	2.42	0.42
1:N:131:LEU:HD23	1:N:131:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:17:VAL:CG2	2:O:18:GLU:HG3	2.50	0.42
2:R:18:GLU:O	2:R:19:THR:OG1	2.33	0.42
2:Y:29:GLY:HA2	2:Y:30:SER:HA	1.74	0.42
2:Z:24:GLY:H	2:1:80:ASN:ND2	2.18	0.42
2:2:55:LYS:HG3	2:2:55:LYS:O	2.19	0.42
1:A:241:ALA:CB	1:A:271:VAL:CG1	2.97	0.41
1:B:510:VAL:HG12	1:C:387:VAL:CG2	2.50	0.41
1:C:322:ARG:HG2	1:C:323:VAL:N	2.35	0.41
1:E:124:VAL:HG22	1:E:504:LEU:HD11	2.02	0.41
1:E:206:ASN:OD1	1:E:207:LYS:N	2.43	0.41
1:E:295:LEU:HD23	1:E:295:LEU:O	2.20	0.41
1:F:322:ARG:HB3	1:F:333:ILE:CG2	2.50	0.41
1:H:8:PHE:O	1:H:11:ASP:HB3	2.19	0.41
1:H:219:PHE:O	1:H:247:LEU:HG	2.20	0.41
1:H:271:VAL:O	1:H:273:VAL:HG23	2.20	0.41
1:H:345:ARG:O	1:H:349:ILE:HG13	2.20	0.41
1:I:194:GLN:HG3	1:I:330:THR:O	2.20	0.41
1:I:419:LEU:O	1:I:422:VAL:HG22	2.20	0.41
1:J:230:ILE:O	1:J:231:ARG:CG	2.68	0.41
1:J:314:LEU:O	1:J:314:LEU:CD2	2.60	0.41
1:K:295:LEU:HD23	1:K:295:LEU:O	2.19	0.41
1:L:313:THR:HG22	1:L:314:LEU:N	2.35	0.41
1:M:303:GLU:O	1:M:303:GLU:HG2	2.20	0.41
1:N:225:LYS:HG3	1:N:226:LYS:H	1.83	0.41
2:O:9:ARG:HD3	2:U:92:LEU:HD22	2.02	0.41
2:S:16:GLU:CG	2:S:19:THR:CG2	2.98	0.41
2:S:20:LYS:NZ	2:S:26:VAL:HG22	2.34	0.41
2:S:73:VAL:CG2	2:S:84:LEU:HB3	2.49	0.41
2:V:13:LYS:HB2	2:V:41:LEU:HD11	2.02	0.41
2:V:49:LEU:HD13	2:V:49:LEU:C	2.45	0.41
2:W:3:ILE:C	2:W:3:ILE:HD12	2.45	0.41
2:W:9:ARG:NH1	2:W:9:ARG:CG	2.73	0.41
2:W:37:ARG:CZ	2:X:78:ILE:HD11	2.50	0.41
2:1:16:GLU:HB3	2:1:17:VAL:H	1.54	0.41
2:1:95:VAL:HG13	2:2:3:ILE:CG2	2.46	0.41
1:A:147:VAL:HG12	1:A:494:LEU:HD12	2.02	0.41
1:C:323:VAL:CG1	1:C:332:ILE:HG12	2.48	0.41
1:D:432:GLN:HB2	1:D:436:GLN:OE1	2.19	0.41
1:E:195:PHE:CZ	1:E:330:THR:HB	2.55	0.41
1:F:151:SER:CB	1:F:399:ALA:HA	2.49	0.41
1:G:234:LEU:H	1:G:234:LEU:CD1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:VAL:CG2	1:H:376:VAL:HG13	2.42	0.41
1:H:288:MET:HA	1:H:291:ASP:OD2	2.21	0.41
1:I:114:MET:HG3	1:I:118:ARG:NH1	2.35	0.41
1:I:178:GLU:OE1	1:I:378:VAL:HG11	2.20	0.41
1:I:230:ILE:O	1:I:232:GLU:N	2.52	0.41
1:J:413:ALA:O	1:J:418:ALA:HB2	2.20	0.41
1:K:90:THR:HG23	4:K:602:BEF:F1	2.10	0.41
1:L:224:ASP:OD2	1:L:286:LYS:HE2	2.19	0.41
1:L:506:TYR:O	1:L:510:VAL:HG22	2.20	0.41
1:M:190:VAL:HG11	1:M:194:GLN:NE2	2.35	0.41
1:M:333:ILE:O	1:M:333:ILE:HG22	2.19	0.41
1:N:239:ALA:HB1	1:N:314:LEU:CD1	2.46	0.41
2:W:24:GLY:O	2:W:25:ILE:HG22	2.20	0.41
2:Y:86:MET:HE3	2:Y:90:ASP:CB	2.50	0.41
2:Z:68:ASN:HD21	2:1:74:LYS:HE2	1.86	0.41
2:1:76:GLU:HG3	2:1:77:LYS:N	2.35	0.41
1:A:386:GLU:HB3	1:G:76:GLU:OE2	2.20	0.41
1:B:295:LEU:HD23	1:B:335:GLY:HA3	2.02	0.41
1:C:33:PRO:CG	1:C:480:ALA:HB3	2.50	0.41
1:C:33:PRO:HG3	3:C:601:ADP:C6	2.55	0.41
1:C:149:THR:HG23	1:C:155:ASP:C	2.46	0.41
1:C:247:LEU:C	1:C:247:LEU:HD12	2.46	0.41
1:D:281:PHE:O	1:D:284:ARG:HB2	2.20	0.41
1:E:197:ARG:HG3	1:E:278:ALA:C	2.45	0.41
1:F:143:ALA:O	1:F:146:GLN:HB2	2.20	0.41
1:G:194:GLN:NE2	1:G:329:THR:HG21	2.34	0.41
1:G:223:ALA:CB	1:G:224:ASP:CA	2.98	0.41
1:H:225:LYS:HD3	1:H:225:LYS:HA	1.62	0.41
1:H:265:ASN:OD1	2:V:26:VAL:HG13	2.21	0.41
1:I:219:PHE:CD1	1:I:319:GLN:HG2	2.55	0.41
1:J:221:LEU:HD13	1:J:317:LEU:CD2	2.50	0.41
1:J:288:MET:O	1:J:288:MET:HG3	2.20	0.41
1:K:242:LYS:O	1:K:242:LYS:HD3	2.20	0.41
1:K:305:ILE:CG2	1:L:264:VAL:HG22	2.47	0.41
1:L:31:LEU:CD2	1:L:453:GLN:HB3	2.44	0.41
1:L:225:LYS:HD2	1:L:226:LYS:H	1.83	0.41
1:L:227:ILE:HD12	1:L:227:ILE:H	1.84	0.41
1:N:7:LYS:HG3	1:N:66:PHE:CE2	2.55	0.41
1:N:162:ILE:O	1:N:166:MET:N	2.49	0.41
1:N:263:VAL:CG1	1:N:267:MET:HE2	2.50	0.41
2:O:96:GLU:OE1	2:P:1:MET:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:12:VAL:HG23	2:Z:39:GLU:C	2.46	0.41
2:Z:59:VAL:HG21	2:Z:91:ILE:HG21	2.02	0.41
2:1:55:LYS:HA	2:1:56:PRO:HD2	1.88	0.41
2:1:95:VAL:CG1	2:2:3:ILE:HG22	2.48	0.41
1:A:160:LYS:HA	1:A:160:LYS:HD2	1.89	0.41
1:A:181:THR:HG21	1:A:380:LYS:CD	2.41	0.41
1:F:7:LYS:HD2	1:F:66:PHE:CE2	2.55	0.41
1:F:219:PHE:O	1:F:248:LEU:HB3	2.20	0.41
1:G:266:THR:HG22	1:G:273:VAL:H	1.85	0.41
1:G:421:ARG:HD3	1:G:421:ARG:HA	1.90	0.41
1:I:174:VAL:HG21	1:I:367:GLU:CA	2.48	0.41
1:I:364:LYS:HB3	1:I:364:LYS:HE2	1.90	0.41
1:I:451:LEU:HD13	1:I:451:LEU:C	2.46	0.41
1:L:136:VAL:CG2	1:L:137:PRO:CD	2.98	0.41
1:L:216:GLU:OE1	1:L:245:LYS:HD2	2.21	0.41
1:M:103:GLY:O	1:M:106:ALA:HB3	2.19	0.41
1:M:140:ASP:OD1	1:M:143:ALA:N	2.49	0.41
1:N:72:GLN:HE21	1:N:72:GLN:HB3	1.63	0.41
2:O:94:ILE:C	2:P:3:ILE:HG22	2.46	0.41
2:U:70:GLY:O	2:U:73:VAL:HG22	2.21	0.41
2:W:79:ASP:O	2:W:80:ASN:OD1	2.38	0.41
2:Y:36:THR:O	2:Y:36:THR:HG22	2.20	0.41
1:A:49:ILE:HD11	1:G:73:MET:SD	2.60	0.41
1:A:124:VAL:HG22	1:A:504:LEU:HD11	2.03	0.41
1:B:149:THR:HG23	1:B:155:ASP:O	2.20	0.41
1:B:183:LEU:CD2	1:B:384:ALA:HA	2.50	0.41
1:B:210:THR:HG22	1:B:210:THR:O	2.20	0.41
1:B:233:MET:HE3	1:B:309:LEU:O	2.21	0.41
1:E:135:SER:HB2	1:E:497:THR:HG21	2.03	0.41
1:F:349:ILE:HG21	1:F:369:VAL:CG2	2.49	0.41
1:G:18:ARG:HB3	1:G:18:ARG:HH11	1.86	0.41
1:G:314:LEU:HD12	1:G:314:LEU:HA	1.95	0.41
1:G:487:ASN:HB3	1:G:490:ASP:HB2	2.03	0.41
1:H:326:ASN:CG	1:H:327:LYS:H	2.28	0.41
1:J:151:SER:CB	1:J:399:ALA:HA	2.48	0.41
1:K:69:MET:HE2	1:K:520:MET:HE3	2.03	0.41
1:L:61:GLU:C	1:L:62:LEU:HD12	2.45	0.41
1:L:222:LEU:N	1:L:222:LEU:HD12	2.35	0.41
1:M:158:VAL:O	1:M:162:ILE:HG13	2.20	0.41
1:N:278:ALA:HB1	1:N:279:PRO:CD	2.50	0.41
2:R:14:ARG:HB3	2:R:84:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:14:ARG:HE	2:R:84:LEU:CD2	2.34	0.41
2:R:50:GLU:N	2:R:50:GLU:CD	2.73	0.41
2:S:6:LEU:HD12	2:S:6:LEU:C	2.45	0.41
2:S:48:ILE:HG13	2:S:53:GLU:N	2.35	0.41
2:S:94:ILE:HD13	2:T:4:ARG:HH21	1.85	0.41
2:T:43:VAL:HG13	2:T:57:LEU:HD12	2.02	0.41
2:T:76:GLU:O	2:T:82:GLU:HB2	2.21	0.41
2:W:25:ILE:O	2:W:25:ILE:HG23	2.20	0.41
1:A:87:ASP:OD1	4:A:602:BEF:F2	2.29	0.41
1:A:231:ARG:HB3	1:A:258:ALA:CB	2.51	0.41
1:A:307:MET:O	1:A:308:GLU:HG3	2.20	0.41
1:B:250:ILE:HG23	1:B:278:ALA:HA	2.03	0.41
1:B:325:ILE:HG23	1:B:330:THR:OG1	2.19	0.41
1:C:399:ALA:O	1:C:403:THR:HG23	2.20	0.41
1:C:475:ASN:O	1:C:488:MET:HG2	2.21	0.41
1:D:313:THR:HG22	1:D:315:GLU:H	1.85	0.41
1:E:222:LEU:CD2	1:E:289:LEU:HD13	2.49	0.41
1:F:37:ASN:OD1	1:F:51:LYS:HB2	2.20	0.41
1:F:225:LYS:HB2	1:F:303:GLU:OE1	2.20	0.41
1:F:415:GLY:N	3:F:601:ADP:O2'	2.51	0.41
1:G:145:ALA:O	1:G:149:THR:HG23	2.21	0.41
1:G:222:LEU:HD23	1:G:289:LEU:HB3	2.03	0.41
1:G:278:ALA:HA	1:G:279:PRO:HD3	1.86	0.41
1:G:305:ILE:CG2	1:G:306:GLY:N	2.83	0.41
1:H:218:PRO:HA	1:H:246:PRO:HG2	2.03	0.41
1:H:222:LEU:HD21	1:H:292:ILE:CG2	2.51	0.41
1:I:305:ILE:CG2	1:I:306:GLY:N	2.76	0.41
1:J:307:MET:HG2	1:J:311:LYS:HZ2	1.83	0.41
1:L:142:LYS:O	1:L:146:GLN:HG3	2.21	0.41
1:L:216:GLU:CD	1:L:217:SER:H	2.29	0.41
1:M:221:LEU:HB2	1:M:317:LEU:HD22	2.02	0.41
1:N:23:LEU:HD23	1:N:60:ILE:HB	2.01	0.41
1:N:33:PRO:HA	1:N:153:ASN:OD1	2.21	0.41
1:N:160:LYS:HA	1:N:160:LYS:HD2	1.89	0.41
1:N:285:ARG:O	1:N:289:LEU:HG	2.21	0.41
2:Q:3:ILE:HD11	2:Q:78:ILE:CD1	2.50	0.41
2:T:64:ILE:HB	2:T:95:VAL:HG13	2.02	0.41
2:W:17:VAL:C	2:W:19:THR:N	2.78	0.41
2:W:40:VAL:C	2:W:41:LEU:HD12	2.45	0.41
2:W:65:VAL:HG12	2:W:94:ILE:HG12	2.03	0.41
1:A:238:GLU:CD	2:O:24:GLY:HA3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLU:O	1:A:367:GLU:HB2	2.21	0.41
1:C:210:THR:O	1:C:210:THR:HG22	2.21	0.41
1:D:52:ASP:O	1:D:55:SER:HB2	2.20	0.41
1:D:305:ILE:CG2	1:D:306:GLY:N	2.74	0.41
1:E:207:LYS:N	1:E:208:PRO:HD2	2.35	0.41
1:F:333:ILE:O	1:F:334:ASP:HB2	2.21	0.41
1:G:166:MET:HE2	1:G:166:MET:HB3	1.89	0.41
1:G:420:ILE:HD11	1:G:470:LYS:HG3	2.03	0.41
1:H:23:LEU:HD23	1:H:60:ILE:HB	2.02	0.41
1:I:340:ALA:O	1:I:344:GLY:N	2.54	0.41
1:J:291:ASP:HB3	1:J:372:LEU:CD2	2.50	0.41
1:J:347:ALA:HA	1:J:350:ARG:CG	2.51	0.41
1:J:419:LEU:HD12	1:J:419:LEU:N	2.34	0.41
1:M:183:LEU:HD22	1:M:384:ALA:HA	2.03	0.41
1:N:77:VAL:HG23	1:N:506:TYR:C	2.45	0.41
1:N:228:SER:O	1:N:258:ALA:HB2	2.21	0.41
1:N:284:ARG:NH2	1:N:364:LYS:HG3	2.35	0.41
1:N:324:VAL:C	1:N:325:ILE:HD12	2.46	0.41
1:N:355:GLU:HG3	1:N:356:ALA:N	2.32	0.41
2:T:5:PRO:HD3	2:T:11:ILE:CD1	2.51	0.41
2:Z:17:VAL:O	2:Z:18:GLU:HG2	2.21	0.41
1:A:278:ALA:HB3	1:A:285:ARG:CZ	2.50	0.41
1:A:326:ASN:ND2	1:A:329:THR:O	2.54	0.41
1:B:77:VAL:HG23	1:B:506:TYR:C	2.46	0.41
1:B:264:VAL:O	1:B:267:MET:HB2	2.21	0.41
1:C:193:MET:HE2	1:C:292:ILE:HG12	2.02	0.41
1:D:77:VAL:HG21	1:D:507:ALA:CA	2.49	0.41
1:D:197:ARG:HA	1:D:197:ARG:HD3	1.88	0.41
1:D:259:LEU:O	1:D:263:VAL:HG23	2.21	0.41
1:D:322:ARG:HD2	1:D:333:ILE:HD12	2.03	0.41
1:F:200:LEU:HD12	1:F:200:LEU:N	2.36	0.41
1:G:350:ARG:HD3	1:G:353:ILE:HD11	2.01	0.41
1:G:434:GLU:HA	1:G:437:ASN:HB2	2.02	0.41
1:H:144:ILE:O	1:H:147:VAL:HG22	2.21	0.41
1:H:197:ARG:HD3	1:H:197:ARG:HA	1.94	0.41
1:H:467:ASN:O	1:H:471:GLY:N	2.51	0.41
3:I:601:ADP:O2B	4:I:602:BEF:F2	2.28	0.41
1:J:205:ILE:HA	1:J:213:VAL:CG2	2.25	0.41
1:K:66:PHE:CE1	1:K:522:THR:HG22	2.55	0.41
1:K:183:LEU:HD21	1:K:384:ALA:HA	2.03	0.41
1:L:196:ASP:OD1	1:L:196:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:219:PHE:CD1	1:L:240:VAL:HG22	2.56	0.41
1:M:295:LEU:HD23	1:M:295:LEU:C	2.45	0.41
1:M:306:GLY:HA3	1:N:264:VAL:HG21	2.03	0.41
1:N:230:ILE:HD11	1:N:231:ARG:HG2	2.03	0.41
1:N:234:LEU:H	1:N:234:LEU:CD1	2.22	0.41
1:N:261:THR:CB	2:2:29:GLY:H	2.24	0.41
2:O:3:ILE:N	2:U:95:VAL:HA	2.36	0.41
2:S:12:VAL:HG22	2:S:40:VAL:HA	2.03	0.41
2:S:65:VAL:HG21	2:S:91:ILE:HD12	2.02	0.41
2:U:17:VAL:HG23	2:U:33:ALA:O	2.20	0.41
2:W:37:ARG:NH2	2:X:78:ILE:HD11	2.35	0.41
2:Y:13:LYS:HB2	2:Y:41:LEU:HD11	2.02	0.41
2:Y:27:LEU:C	2:Y:27:LEU:HD12	2.46	0.41
1:B:197:ARG:HG2	1:B:277:LYS:O	2.20	0.41
1:B:219:PHE:CB	1:B:317:LEU:HD13	2.45	0.41
1:B:263:VAL:CG1	1:B:267:MET:HE2	2.50	0.41
1:B:343:GLN:HA	1:B:346:VAL:HB	2.02	0.41
1:C:124:VAL:HG21	1:C:508:ALA:HB2	2.03	0.41
1:C:183:LEU:HD12	1:C:183:LEU:N	2.36	0.41
1:C:254:VAL:CG1	1:C:259:LEU:HG	2.44	0.41
1:C:276:VAL:HG22	1:C:277:LYS:N	2.35	0.41
1:C:280:GLY:C	1:C:285:ARG:HB3	2.46	0.41
1:C:299:THR:HG21	1:C:307:MET:HE1	2.03	0.41
1:C:414:GLY:O	1:C:417:VAL:HG12	2.21	0.41
1:D:248:LEU:CD1	1:D:250:ILE:HG13	2.51	0.41
1:D:305:ILE:CG2	1:E:263:VAL:HG11	2.50	0.41
1:D:419:LEU:HB3	1:D:447:MET:HB3	2.03	0.41
1:E:5:ASP:HB2	1:E:524:LEU:HD21	1.99	0.41
1:E:210:THR:HG22	1:E:210:THR:O	2.21	0.41
1:E:327:LYS:H	1:E:327:LYS:HD3	1.86	0.41
1:E:400:LEU:HD13	1:E:400:LEU:O	2.21	0.41
1:G:92:ALA:HB2	1:G:503:ALA:CB	2.50	0.41
1:G:221:LEU:HD22	1:G:249:ILE:HD12	2.02	0.41
1:G:230:ILE:CG2	1:G:309:LEU:HD21	2.33	0.41
1:G:400:LEU:HD13	1:G:400:LEU:C	2.46	0.41
1:H:284:ARG:HD3	1:H:284:ARG:HA	1.83	0.41
1:I:218:PRO:HD2	1:I:320:ALA:O	2.21	0.41
1:J:171:LYS:HD3	1:J:407:VAL:HG11	2.02	0.41
1:J:349:ILE:HG22	1:J:365:LEU:HD21	2.01	0.41
1:K:23:LEU:HD23	1:K:60:ILE:CB	2.44	0.41
1:K:123:ALA:HB2	1:K:440:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:215:LEU:HD12	1:K:323:VAL:CG2	2.50	0.41
1:K:278:ALA:HB1	1:K:279:PRO:HD2	2.02	0.41
1:K:296:THR:CB	1:K:318:GLY:HA3	2.51	0.41
1:K:455:VAL:CG1	1:K:460:GLU:HB2	2.40	0.41
1:L:349:ILE:O	1:L:353:ILE:N	2.53	0.41
1:L:350:ARG:HA	1:L:353:ILE:CD1	2.51	0.41
1:M:62:LEU:HD23	1:M:67:GLU:HB3	2.02	0.41
1:M:183:LEU:CD2	1:M:384:ALA:HA	2.50	0.41
1:M:210:THR:HG22	1:M:210:THR:O	2.20	0.41
1:M:363:GLU:HG3	1:M:364:LYS:H	1.86	0.41
1:M:406:ALA:HB2	1:M:496:PRO:HB3	2.02	0.41
1:N:61:GLU:O	1:N:62:LEU:HD12	2.21	0.41
1:N:215:LEU:HB2	1:N:323:VAL:CG2	2.50	0.41
1:N:325:ILE:HG22	1:N:326:ASN:N	2.35	0.41
1:N:388:GLU:O	1:N:392:LYS:HB2	2.20	0.41
2:O:77:LYS:HG2	2:O:82:GLU:HA	2.02	0.41
2:P:68:ASN:HB3	2:Q:74:LYS:NZ	2.36	0.41
2:Q:43:VAL:CG2	2:Q:57:LEU:HD11	2.48	0.41
2:Q:70:GLY:O	2:Q:73:VAL:HG12	2.19	0.41
2:Q:88:GLU:O	2:Q:88:GLU:HG2	2.21	0.41
2:R:17:VAL:C	2:R:19:THR:H	2.27	0.41
2:T:5:PRO:HB2	2:T:9:ARG:O	2.21	0.41
2:U:49:LEU:CA	2:U:50:GLU:OE1	2.69	0.41
2:V:86:MET:SD	2:V:91:ILE:HG13	2.61	0.41
2:W:11:ILE:HG21	2:W:42:ALA:HB3	2.02	0.41
2:W:64:ILE:HG21	2:W:95:VAL:HB	2.01	0.41
2:X:58:ASP:OD2	2:Y:7:HIS:CE1	2.73	0.41
2:Y:78:ILE:HG13	2:Y:79:ASP:N	2.36	0.41
2:Z:47:ARG:HE	2:Z:49:LEU:HD12	1.86	0.41
2:Z:47:ARG:CG	2:Z:49:LEU:HG	2.51	0.41
2:Z:73:VAL:HG12	2:Z:86:MET:HB3	2.02	0.41
2:2:17:VAL:HG12	2:2:35:SER:H	1.86	0.41
2:2:51:ASN:O	2:2:51:ASN:OD1	2.39	0.41
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.45	0.41
1:A:247:LEU:C	1:A:247:LEU:HD12	2.46	0.41
1:A:321:LYS:HD2	1:A:334:ASP:OD2	2.20	0.41
1:B:112:ASN:HA	1:B:113:PRO:HD3	1.85	0.41
1:B:151:SER:HB3	1:B:399:ALA:HA	2.03	0.41
1:B:180:GLY:H	1:B:389:MET:CE	2.33	0.41
1:B:222:LEU:HD21	1:B:293:ALA:HB2	2.02	0.41
1:B:400:LEU:C	1:B:400:LEU:HD13	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:LEU:HD12	1:B:494:LEU:N	2.36	0.41
1:C:406:ALA:HB1	1:C:411:VAL:HG12	2.03	0.41
1:D:291:ASP:HB3	1:D:372:LEU:HD11	2.03	0.41
1:E:195:PHE:CD1	1:E:195:PHE:C	2.98	0.41
1:E:221:LEU:HB2	1:E:317:LEU:CD2	2.51	0.41
1:E:496:PRO:HG2	1:E:499:VAL:CG1	2.50	0.41
1:F:18:ARG:HB3	1:F:18:ARG:CZ	2.51	0.41
1:F:29:VAL:O	1:F:36:ARG:N	2.43	0.41
1:F:452:ARG:HH21	1:F:466:ALA:HB3	1.86	0.41
1:F:513:LEU:CD1	1:G:388:GLU:HA	2.48	0.41
1:G:307:MET:O	1:G:308:GLU:HG2	2.21	0.41
1:I:188:ASP:O	1:I:377:ALA:HA	2.21	0.41
1:J:147:VAL:HG21	1:J:403:THR:HA	2.03	0.41
1:K:62:LEU:HB2	1:K:68:ASN:HA	2.03	0.41
1:K:150:ILE:HG22	1:K:151:SER:N	2.36	0.41
1:K:427:ALA:O	1:K:441:LYS:NZ	2.43	0.41
1:L:419:LEU:HD11	1:L:500:THR:HG23	2.02	0.41
1:L:518:GLU:HB3	1:M:29:VAL:HG21	2.02	0.41
1:M:202:PRO:O	1:M:205:ILE:HG12	2.20	0.41
1:N:65:LYS:O	1:N:69:MET:HG3	2.21	0.41
1:N:140:ASP:OD2	1:N:142:LYS:HB3	2.21	0.41
1:N:179:ASP:HA	1:N:389:MET:SD	2.61	0.41
2:P:17:VAL:HG12	2:P:35:SER:N	2.36	0.41
2:T:12:VAL:HG23	2:T:84:LEU:HD12	2.02	0.41
2:V:2:ASN:HD22	2:V:2:ASN:H	1.69	0.41
2:W:11:ILE:HB	2:W:85:ILE:HD13	2.03	0.41
2:Y:92:LEU:O	2:Z:9:ARG:HD2	2.21	0.41
1:B:23:LEU:HD13	1:B:23:LEU:C	2.46	0.40
1:B:129:GLU:OE2	1:B:132:LYS:HD2	2.21	0.40
1:B:433:ASN:OD1	1:B:436:GLN:HG3	2.21	0.40
1:C:19:GLY:HA3	1:C:67:GLU:O	2.21	0.40
1:D:183:LEU:HD12	1:D:183:LEU:N	2.36	0.40
1:D:406:ALA:HB2	1:D:496:PRO:HB3	2.03	0.40
1:E:199:TYR:CB	1:E:276:VAL:HG12	2.51	0.40
1:E:247:LEU:HD22	1:E:247:LEU:N	2.36	0.40
1:E:494:LEU:HD12	1:E:494:LEU:N	2.35	0.40
1:F:236:VAL:HG11	1:F:312:ALA:CB	2.38	0.40
1:F:263:VAL:CG1	1:F:267:MET:HE3	2.51	0.40
1:F:420:ILE:HG12	1:F:448:GLU:HA	2.03	0.40
1:G:420:ILE:HD11	1:G:470:LYS:CG	2.51	0.40
1:H:24:ALA:O	1:H:28:LYS:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:245:LYS:CB	1:H:246:PRO:CD	3.00	0.40
1:H:301:ILE:HD13	1:H:307:MET:CE	2.51	0.40
1:J:5:ASP:HB2	1:J:524:LEU:HD21	2.02	0.40
1:K:241:ALA:HB2	1:K:271:VAL:HG11	2.03	0.40
1:M:226:LYS:HG2	1:M:252:GLU:HG2	2.02	0.40
1:M:267:MET:HE2	1:M:267:MET:CA	2.43	0.40
1:N:234:LEU:O	1:N:238:GLU:HG3	2.21	0.40
2:P:17:VAL:CG1	2:P:35:SER:HB2	2.43	0.40
2:2:10:VAL:HG12	2:2:11:ILE:N	2.36	0.40
1:A:25:ASP:OD1	1:A:28:LYS:HE2	2.21	0.40
1:A:77:VAL:HG21	1:A:507:ALA:CA	2.47	0.40
1:A:272:LYS:HG3	1:A:272:LYS:O	2.21	0.40
1:C:313:THR:HG22	1:C:314:LEU:N	2.36	0.40
1:E:346:VAL:O	1:E:350:ARG:HG2	2.21	0.40
1:E:482:THR:OG1	1:E:484:GLU:HG2	2.21	0.40
1:F:116:LEU:O	1:F:120:ILE:HG13	2.21	0.40
1:G:20:VAL:HG13	1:G:74:VAL:HG11	2.03	0.40
1:G:80:LYS:HD2	1:G:506:TYR:CZ	2.56	0.40
1:G:309:LEU:HD23	1:G:310:GLU:H	1.85	0.40
1:G:383:ALA:CB	1:G:389:MET:HA	2.51	0.40
1:G:417:VAL:O	1:G:421:ARG:HB2	2.21	0.40
1:H:358:SER:HA	1:H:362:ARG:NE	2.36	0.40
1:I:116:LEU:O	1:I:120:ILE:HG13	2.22	0.40
1:I:288:MET:HG3	1:I:368:ARG:NH1	2.35	0.40
1:J:23:LEU:HD23	1:J:60:ILE:HG21	2.03	0.40
1:J:160:LYS:HD2	1:J:160:LYS:HA	1.81	0.40
1:K:30:THR:OG1	1:K:90:THR:HG21	2.21	0.40
1:K:142:LYS:O	1:K:146:GLN:HG3	2.21	0.40
1:L:73:MET:HB3	1:L:514:MET:HE2	2.02	0.40
1:N:433:ASN:OD1	1:N:436:GLN:HG3	2.21	0.40
1:N:524:LEU:HD23	1:N:524:LEU:HA	1.91	0.40
2:Q:10:VAL:HG22	2:Q:11:ILE:N	2.36	0.40
2:Q:43:VAL:HG22	2:Q:44:GLY:N	2.36	0.40
2:S:77:LYS:HD3	2:S:82:GLU:HA	2.03	0.40
2:T:92:LEU:CA	2:U:9:ARG:HD2	2.50	0.40
2:U:6:LEU:CD1	2:U:7:HIS:HB2	2.51	0.40
2:X:50:GLU:C	2:X:51:ASN:CG	2.86	0.40
1:A:49:ILE:O	1:A:391:GLU:HB2	2.21	0.40
1:B:131:LEU:CD2	1:B:422:VAL:HG11	2.51	0.40
1:B:160:LYS:O	1:B:164:GLU:HG3	2.21	0.40
1:B:208:PRO:HG2	1:B:214:GLU:CD	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:LEU:CD1	1:C:388:GLU:HA	2.51	0.40
1:D:195:PHE:CE1	1:D:330:THR:HB	2.56	0.40
1:D:278:ALA:HB3	1:D:285:ARG:CD	2.50	0.40
1:E:288:MET:HA	1:E:291:ASP:OD2	2.21	0.40
1:E:419:LEU:HB3	1:E:447:MET:HB3	2.02	0.40
1:F:282:GLY:HA2	1:F:285:ARG:CG	2.47	0.40
1:G:226:LYS:HD3	1:G:255:GLU:OE2	2.21	0.40
1:G:289:LEU:HA	1:G:289:LEU:HD23	1.83	0.40
1:I:233:MET:CB	1:I:309:LEU:CD2	3.00	0.40
1:I:241:ALA:HB1	2:W:25:ILE:CD1	2.43	0.40
1:L:250:ILE:HG22	1:L:251:ALA:N	2.35	0.40
1:L:307:MET:O	1:L:308:GLU:HG2	2.21	0.40
1:N:119:GLY:O	1:N:440:ILE:HG12	2.21	0.40
2:O:17:VAL:HG22	2:O:18:GLU:HG3	2.02	0.40
2:O:40:VAL:HG12	2:O:41:LEU:N	2.37	0.40
2:S:27:LEU:HD12	2:S:28:THR:O	2.21	0.40
2:T:8:ASP:HB2	2:T:47:ARG:HB3	2.03	0.40
2:V:11:ILE:HG13	2:V:42:ALA:O	2.22	0.40
2:Z:49:LEU:O	2:Z:52:GLY:N	2.49	0.40
2:1:6:LEU:HD23	2:1:6:LEU:HA	1.79	0.40
1:A:238:GLU:OE2	2:O:24:GLY:HA3	2.21	0.40
1:B:231:ARG:HH22	2:P:31:ALA:CB	2.27	0.40
1:B:406:ALA:CA	1:B:496:PRO:HB3	2.51	0.40
1:C:236:VAL:O	1:C:240:VAL:HG23	2.21	0.40
1:D:69:MET:CE	1:E:39:VAL:HG12	2.52	0.40
1:D:146:GLN:HB2	1:D:494:LEU:HD12	2.04	0.40
1:E:238:GLU:OE1	2:S:25:ILE:HD13	2.20	0.40
1:E:247:LEU:HD23	1:E:273:VAL:HG22	2.02	0.40
1:E:357:THR:HG22	1:E:357:THR:O	2.21	0.40
1:F:38:VAL:HB	1:F:56:VAL:CG2	2.52	0.40
1:G:124:VAL:HG13	1:G:504:LEU:HD12	2.02	0.40
1:G:236:VAL:CG2	1:G:312:ALA:HB3	2.50	0.40
1:H:131:LEU:HD13	1:H:500:THR:HG22	2.04	0.40
1:H:433:ASN:OD1	1:H:435:ASP:HB2	2.22	0.40
1:I:123:ALA:HB2	1:I:440:ILE:HG23	2.04	0.40
1:I:200:LEU:HD13	1:I:276:VAL:HA	2.03	0.40
1:I:263:VAL:O	1:I:267:MET:HG3	2.20	0.40
1:J:238:GLU:OE1	2:X:25:ILE:HD13	2.21	0.40
1:K:322:ARG:HB3	1:K:333:ILE:HG21	2.01	0.40
1:L:30:THR:O	1:L:51:LYS:HE2	2.21	0.40
1:L:388:GLU:O	1:L:392:LYS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:92:ALA:HB2	1:M:503:ALA:CB	2.51	0.40
1:N:13:ARG:CD	1:N:104:LEU:HD22	2.50	0.40
1:N:280:GLY:O	1:N:285:ARG:HB3	2.22	0.40
2:R:17:VAL:HG23	2:R:19:THR:CA	2.52	0.40
2:R:36:THR:CG2	2:R:37:ARG:HG3	2.34	0.40
2:X:3:ILE:O	2:X:3:ILE:HD12	2.22	0.40
2:Z:37:ARG:HG2	2:Z:66:ILE:HG12	2.02	0.40
2:Z:48:ILE:O	2:Z:48:ILE:HG23	2.21	0.40
1:A:112:ASN:HA	1:A:113:PRO:HD3	1.89	0.40
1:A:182:GLY:C	1:A:184:GLN:N	2.78	0.40
1:A:205:ILE:HD12	1:A:211:GLY:C	2.47	0.40
1:B:15:LYS:O	1:B:67:GLU:HG2	2.22	0.40
1:B:113:PRO:O	1:B:116:LEU:HB2	2.21	0.40
1:C:236:VAL:HG22	1:C:312:ALA:O	2.22	0.40
1:D:166:MET:CE	1:D:407:VAL:HG21	2.35	0.40
1:E:313:THR:HG22	1:E:314:LEU:N	2.37	0.40
1:F:304:GLU:C	1:F:305:ILE:HD12	2.46	0.40
1:F:429:LEU:HG	1:F:440:ILE:HD13	2.04	0.40
1:G:197:ARG:HA	1:G:197:ARG:HD3	1.93	0.40
1:G:305:ILE:CG2	1:G:306:GLY:H	2.35	0.40
1:G:488:MET:HE3	1:G:493:ILE:HG21	2.02	0.40
1:I:178:GLU:CD	1:I:378:VAL:HG11	2.46	0.40
1:I:295:LEU:HD12	1:I:372:LEU:HD23	2.02	0.40
1:I:421:ARG:NH1	1:I:472:GLY:O	2.54	0.40
1:J:436:GLN:O	1:J:440:ILE:HG13	2.21	0.40
1:K:51:LYS:NZ	3:K:601:ADP:O2A	2.47	0.40
1:L:87:ASP:O	1:L:499:VAL:HG13	2.21	0.40
1:L:279:PRO:HB2	1:L:288:MET:HE3	2.03	0.40
1:L:381:VAL:HG22	1:L:396:VAL:HG21	2.02	0.40
1:M:295:LEU:HD23	1:M:295:LEU:O	2.22	0.40
1:N:20:VAL:HG13	1:N:74:VAL:HG21	2.04	0.40
1:N:143:ALA:O	1:N:146:GLN:HB2	2.21	0.40
1:N:281:PHE:O	1:N:284:ARG:N	2.55	0.40
2:O:47:ARG:O	2:O:54:VAL:HA	2.20	0.40
2:P:7:HIS:HA	2:P:45:ASN:OD1	2.22	0.40
2:T:92:LEU:N	2:T:92:LEU:HD12	2.36	0.40
2:U:65:VAL:HG12	2:U:94:ILE:CG2	2.52	0.40
2:V:37:ARG:HH21	2:W:76:GLU:CG	2.34	0.40
2:Y:92:LEU:HD23	2:Z:85:ILE:HD11	2.03	0.40

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLU:OE2	1:K:207:LYS:NZ[1_545]	0.50	1.70
1:K:430:ARG:CG	1:M:245:LYS:NZ[4_565]	0.86	1.34
1:B:339:GLU:CD	1:K:207:LYS:NZ[1_545]	1.06	1.14
1:K:430:ARG:CB	1:M:245:LYS:NZ[4_565]	1.09	1.11
1:G:471:GLY:C	2:P:2:ASN:ND2[3_554]	1.53	0.67
1:B:339:GLU:OE2	1:K:207:LYS:CE[1_545]	1.58	0.62
1:K:430:ARG:CA	1:M:245:LYS:NZ[4_565]	1.76	0.44
1:K:430:ARG:CG	1:M:245:LYS:CE[4_565]	1.78	0.42
1:G:472:GLY:N	2:P:2:ASN:ND2[3_554]	1.79	0.41
1:G:471:GLY:O	2:P:2:ASN:ND2[3_554]	1.84	0.36
1:K:430:ARG:CD	1:M:245:LYS:NZ[4_565]	1.86	0.34
1:L:476:TYR:OH	2:2:79:ASP:OD2[4_565]	1.95	0.25
1:K:430:ARG:CB	1:M:245:LYS:CE[4_565]	2.03	0.17
1:B:339:GLU:CG	1:K:207:LYS:NZ[1_545]	2.06	0.14
2:T:53:GLU:OE1	2:1:53:GLU:OE2[1_645]	2.09	0.11
1:B:339:GLU:OE1	1:K:207:LYS:NZ[1_545]	2.11	0.09
1:K:430:ARG:N	1:M:245:LYS:CE[4_565]	2.17	0.03

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	522/548 (95%)	496 (95%)	23 (4%)	3 (1%)	21	55
1	B	522/548 (95%)	499 (96%)	21 (4%)	2 (0%)	30	64
1	C	522/548 (95%)	509 (98%)	13 (2%)	0	100	100
1	D	522/548 (95%)	502 (96%)	19 (4%)	1 (0%)	43	74
1	E	522/548 (95%)	500 (96%)	18 (3%)	4 (1%)	16	50
1	F	522/548 (95%)	504 (97%)	16 (3%)	2 (0%)	30	64
1	G	522/548 (95%)	508 (97%)	12 (2%)	2 (0%)	30	64
1	H	522/548 (95%)	502 (96%)	19 (4%)	1 (0%)	43	74
1	I	522/548 (95%)	507 (97%)	14 (3%)	1 (0%)	43	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	522/548 (95%)	503 (96%)	17 (3%)	2 (0%)	30	64
1	K	522/548 (95%)	507 (97%)	15 (3%)	0	100	100
1	L	522/548 (95%)	504 (97%)	18 (3%)	0	100	100
1	M	522/548 (95%)	503 (96%)	16 (3%)	3 (1%)	21	55
1	N	522/548 (95%)	503 (96%)	19 (4%)	0	100	100
2	1	95/97 (98%)	87 (92%)	4 (4%)	4 (4%)	2	20
2	2	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	11	43
2	O	93/97 (96%)	89 (96%)	4 (4%)	0	100	100
2	P	95/97 (98%)	86 (90%)	9 (10%)	0	100	100
2	Q	94/97 (97%)	84 (89%)	9 (10%)	1 (1%)	11	43
2	R	95/97 (98%)	88 (93%)	6 (6%)	1 (1%)	11	43
2	S	94/97 (97%)	83 (88%)	10 (11%)	1 (1%)	11	43
2	T	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
2	U	95/97 (98%)	85 (90%)	8 (8%)	2 (2%)	5	32
2	V	95/97 (98%)	89 (94%)	5 (5%)	1 (1%)	11	43
2	W	95/97 (98%)	84 (88%)	10 (10%)	1 (1%)	11	43
2	X	95/97 (98%)	87 (92%)	6 (6%)	2 (2%)	5	32
2	Y	94/97 (97%)	90 (96%)	4 (4%)	0	100	100
2	Z	93/97 (96%)	89 (96%)	4 (4%)	0	100	100
All	All	8631/9030 (96%)	8265 (96%)	331 (4%)	35 (0%)	30	64

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	233	MET
1	E	233	MET
1	E	234	LEU
1	M	270	ILE
2	R	50	GLU
2	S	40	VAL
1	A	270	ILE
1	B	228	SER
1	H	228	SER
1	I	231	ARG
2	X	21	SER

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Mol	Chain	Res	Type
2	X	51	ASN
2	1	6	LEU
2	1	7	HIS
1	B	245	LYS
1	E	235	PRO
1	F	305	ILE
1	G	209	GLU
2	Q	52	GLY
2	U	51	ASN
1	A	271	VAL
1	A	309	LEU
1	F	218	PRO
1	G	223	ALA
1	J	231	ARG
2	U	52	GLY
2	W	26	VAL
2	2	54	VAL
1	M	234	LEU
1	M	334	ASP
2	1	5	PRO
1	E	207	LYS
1	J	270	ILE
2	V	92	LEU
2	1	8	ASP

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	404/415 (97%)	398 (98%)	6 (2%)	57	69
1	B	404/415 (97%)	396 (98%)	8 (2%)	48	65
1	C	404/415 (97%)	397 (98%)	7 (2%)	53	68
1	D	404/415 (97%)	396 (98%)	8 (2%)	48	65
1	E	404/415 (97%)	397 (98%)	7 (2%)	53	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	404/415 (97%)	395 (98%)	9 (2%)	45	64
1	G	404/415 (97%)	397 (98%)	7 (2%)	53	68
1	H	404/415 (97%)	392 (97%)	12 (3%)	36	57
1	I	404/415 (97%)	396 (98%)	8 (2%)	48	65
1	J	404/415 (97%)	392 (97%)	12 (3%)	36	57
1	K	404/415 (97%)	395 (98%)	9 (2%)	45	64
1	L	404/415 (97%)	394 (98%)	10 (2%)	42	62
1	M	404/415 (97%)	397 (98%)	7 (2%)	53	68
1	N	404/415 (97%)	387 (96%)	17 (4%)	26	51
2	1	80/80 (100%)	76 (95%)	4 (5%)	22	47
2	2	80/80 (100%)	75 (94%)	5 (6%)	16	43
2	O	78/80 (98%)	75 (96%)	3 (4%)	29	53
2	P	80/80 (100%)	77 (96%)	3 (4%)	29	53
2	Q	79/80 (99%)	75 (95%)	4 (5%)	21	47
2	R	80/80 (100%)	75 (94%)	5 (6%)	16	43
2	S	79/80 (99%)	72 (91%)	7 (9%)	9	32
2	T	80/80 (100%)	77 (96%)	3 (4%)	29	53
2	U	80/80 (100%)	77 (96%)	3 (4%)	29	53
2	V	80/80 (100%)	75 (94%)	5 (6%)	16	43
2	W	80/80 (100%)	75 (94%)	5 (6%)	16	43
2	X	80/80 (100%)	73 (91%)	7 (9%)	9	33
2	Y	80/80 (100%)	76 (95%)	4 (5%)	22	47
2	Z	79/80 (99%)	73 (92%)	6 (8%)	12	38
All	All	6771/6930 (98%)	6580 (97%)	191 (3%)	38	59

All (191) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	147	VAL
1	A	305	ILE
1	A	308	GLU
1	A	422	VAL
1	A	499	VAL

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Mol	Chain	Res	Type
1	B	147	VAL
1	B	150	ILE
1	B	169	VAL
1	B	309	LEU
1	B	343	GLN
1	B	422	VAL
1	B	493	ILE
1	B	499	VAL
1	C	136	VAL
1	C	147	VAL
1	C	200	LEU
1	C	366	GLN
1	C	453	GLN
1	C	495	ASP
1	C	499	VAL
1	D	147	VAL
1	D	150	ILE
1	D	227	ILE
1	D	292	ILE
1	D	363	GLU
1	D	422	VAL
1	D	461	GLU
1	D	499	VAL
1	E	80	LYS
1	E	147	VAL
1	E	174	VAL
1	E	234	LEU
1	E	354	GLU
1	E	420	ILE
1	E	499	VAL
1	F	105	LYS
1	F	147	VAL
1	F	207	LYS
1	F	245	LYS
1	F	272	LYS
1	F	363	GLU
1	F	365	LEU
1	F	422	VAL
1	F	499	VAL
1	G	80	LYS
1	G	147	VAL
1	G	150	ILE

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Mol	Chain	Res	Type
1	G	277	LYS
1	G	361	ASP
1	G	397	GLU
1	G	499	VAL
1	H	136	VAL
1	H	147	VAL
1	H	185	ASP
1	H	207	LYS
1	H	237	LEU
1	H	255	GLU
1	H	342	ILE
1	H	363	GLU
1	H	422	VAL
1	H	453	GLN
1	H	499	VAL
1	H	513	LEU
1	I	74	VAL
1	I	136	VAL
1	I	147	VAL
1	I	150	ILE
1	I	308	GLU
1	I	343	GLN
1	I	499	VAL
1	I	513	LEU
1	J	150	ILE
1	J	207	LYS
1	J	234	LEU
1	J	245	LYS
1	J	305	ILE
1	J	309	LEU
1	J	334	ASP
1	J	349	ILE
1	J	420	ILE
1	J	422	VAL
1	J	453	GLN
1	J	499	VAL
1	K	17	LEU
1	K	77	VAL
1	K	105	LYS
1	K	147	VAL
1	K	150	ILE
1	K	206	ASN

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Mol	Chain	Res	Type
1	K	329	THR
1	K	499	VAL
1	K	513	LEU
1	L	147	VAL
1	L	150	ILE
1	L	183	LEU
1	L	234	LEU
1	L	365	LEU
1	L	422	VAL
1	L	453	GLN
1	L	461	GLU
1	L	510	VAL
1	L	513	LEU
1	M	29	VAL
1	M	147	VAL
1	M	160	LYS
1	M	237	LEU
1	M	467	ASN
1	M	499	VAL
1	M	513	LEU
1	N	17	LEU
1	N	56	VAL
1	N	91	THR
1	N	93	THR
1	N	94	VAL
1	N	147	VAL
1	N	150	ILE
1	N	177	VAL
1	N	206	ASN
1	N	234	LEU
1	N	309	LEU
1	N	310	GLU
1	N	343	GLN
1	N	422	VAL
1	N	467	ASN
1	N	499	VAL
1	N	513	LEU
2	O	6	LEU
2	O	8	ASP
2	O	49	LEU
2	P	3	ILE
2	P	4	ARG

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Mol	Chain	Res	Type
2	P	53	GLU
2	Q	28	THR
2	Q	57	LEU
2	Q	79	ASP
2	Q	92	LEU
2	R	1	MET
2	R	25	ILE
2	R	49	LEU
2	R	50	GLU
2	R	80	ASN
2	S	6	LEU
2	S	40	VAL
2	S	50	GLU
2	S	51	ASN
2	S	53	GLU
2	S	61	VAL
2	S	80	ASN
2	T	3	ILE
2	T	79	ASP
2	T	84	LEU
2	U	8	ASP
2	U	61	VAL
2	U	85	ILE
2	V	2	ASN
2	V	12	VAL
2	V	58	ASP
2	V	59	VAL
2	V	88	GLU
2	W	8	ASP
2	W	9	ARG
2	W	11	ILE
2	W	27	LEU
2	W	51	ASN
2	X	11	ILE
2	X	21	SER
2	X	40	VAL
2	X	48	ILE
2	X	66	ILE
2	X	78	ILE
2	X	95	VAL
2	Y	3	ILE
2	Y	7	HIS

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Mol	Chain	Res	Type
2	Y	11	ILE
2	Y	89	SER
2	Z	4	ARG
2	Z	10	VAL
2	Z	51	ASN
2	Z	73	VAL
2	Z	85	ILE
2	Z	95	VAL
2	1	3	ILE
2	1	7	HIS
2	1	80	ASN
2	1	94	ILE
2	2	17	VAL
2	2	43	VAL
2	2	45	ASN
2	2	68	ASN
2	2	78	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	B	82	ASN
1	B	366	GLN
1	C	351	GLN
1	D	265	ASN
1	E	319	GLN
1	E	343	GLN
1	E	351	GLN
1	F	68	ASN
1	F	348	GLN
1	F	352	GLN
1	F	366	GLN
1	G	82	ASN
1	G	146	GLN
1	G	453	GLN
1	G	457	ASN
1	H	82	ASN
1	H	146	GLN
1	H	194	GLN
1	H	351	GLN
1	H	467	ASN

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Mol	Chain	Res	Type
1	I	10	ASN
1	I	194	GLN
1	I	343	GLN
1	J	146	GLN
1	J	453	GLN
1	J	505	GLN
1	K	401	HIS
1	K	475	ASN
1	L	82	ASN
1	L	453	GLN
1	L	505	GLN
1	M	10	ASN
1	M	194	GLN
1	M	467	ASN
1	N	10	ASN
1	N	475	ASN
2	O	7	HIS
2	T	51	ASN
2	U	45	ASN
2	V	2	ASN
2	1	7	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 28 are monoatomic - leaving 28 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
3	ADP	I	601	5,6	28,29,29	1.35	5 (17%)	43,45,45	1.87	10 (23%)
3	ADP	J	601	5,6	28,29,29	1.43	5 (17%)	43,45,45	1.93	12 (27%)
4	BEF	G	602	-	0,3,3	-	-	-	-	-
3	ADP	N	601	5,6	28,29,29	1.41	5 (17%)	43,45,45	1.87	11 (25%)
4	BEF	F	602	-	0,3,3	-	-	-	-	-
3	ADP	F	601	5,6	28,29,29	1.38	4 (14%)	43,45,45	1.87	11 (25%)
4	BEF	H	602	-	0,3,3	-	-	-	-	-
3	ADP	B	601	5,6	28,29,29	1.44	6 (21%)	43,45,45	1.86	9 (20%)
4	BEF	M	602	-	0,3,3	-	-	-	-	-
3	ADP	A	601	5,4,6	28,29,29	1.44	5 (17%)	43,45,45	1.89	11 (25%)
4	BEF	E	602	-	0,3,3	-	-	-	-	-
3	ADP	E	601	5,6	28,29,29	1.40	5 (17%)	43,45,45	1.92	11 (25%)
4	BEF	B	602	-	0,3,3	-	-	-	-	-
4	BEF	L	602	-	0,3,3	-	-	-	-	-
4	BEF	D	602	-	0,3,3	-	-	-	-	-
3	ADP	C	601	5,6	28,29,29	1.41	5 (17%)	43,45,45	1.90	8 (18%)
4	BEF	C	602	-	0,3,3	-	-	-	-	-
4	BEF	I	602	-	0,3,3	-	-	-	-	-
4	BEF	J	602	-	0,3,3	-	-	-	-	-
3	ADP	M	601	5,6	28,29,29	1.41	5 (17%)	43,45,45	1.88	10 (23%)
4	BEF	A	602	3	0,3,3	-	-	-	-	-
3	ADP	D	601	5,6	28,29,29	1.41	6 (21%)	43,45,45	1.90	11 (25%)
3	ADP	K	601	5,6	28,29,29	1.38	4 (14%)	43,45,45	1.86	11 (25%)
3	ADP	H	601	5,6	28,29,29	1.40	5 (17%)	43,45,45	1.89	11 (25%)
4	BEF	N	602	-	0,3,3	-	-	-	-	-
3	ADP	G	601	5,6	28,29,29	1.45	5 (17%)	43,45,45	1.91	10 (23%)
3	ADP	L	601	5,6	28,29,29	1.37	4 (14%)	43,45,45	1.93	12 (27%)
4	BEF	K	602	-	0,3,3	-	-	-	-	-

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
3	ADP	I	601	5,6	-	4/16/32/32	0/3/3/3
3	ADP	B	601	5,6	-	1/16/32/32	0/3/3/3
3	ADP	J	601	5,6	-	6/16/32/32	0/3/3/3
3	ADP	H	601	5,6	-	6/16/32/32	0/3/3/3
3	ADP	A	601	5,4,6	-	1/16/32/32	0/3/3/3
3	ADP	N	601	5,6	-	8/16/32/32	0/3/3/3
3	ADP	G	601	5,6	-	4/16/32/32	0/3/3/3
3	ADP	E	601	5,6	-	3/16/32/32	0/3/3/3
3	ADP	M	601	5,6	-	7/16/32/32	0/3/3/3
3	ADP	L	601	5,6	-	1/16/32/32	0/3/3/3
3	ADP	D	601	5,6	-	6/16/32/32	0/3/3/3
3	ADP	C	601	5,6	-	5/16/32/32	0/3/3/3
3	ADP	K	601	5,6	-	5/16/32/32	0/3/3/3
3	ADP	F	601	5,6	-	3/16/32/32	0/3/3/3

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	ADP	C5-C4	4.65	1.47	1.39
3	H	601	ADP	C5-C4	4.57	1.47	1.39
3	B	601	ADP	C5-C4	4.54	1.47	1.39
3	N	601	ADP	C5-C4	4.53	1.47	1.39
3	A	601	ADP	C5-C4	4.50	1.47	1.39
3	J	601	ADP	C5-C4	4.49	1.47	1.39
3	G	601	ADP	C5-C4	4.49	1.47	1.39
3	E	601	ADP	C5-C4	4.48	1.47	1.39
3	L	601	ADP	C5-C4	4.47	1.47	1.39
3	F	601	ADP	C5-C4	4.47	1.47	1.39
3	K	601	ADP	C5-C4	4.41	1.46	1.39
3	M	601	ADP	C5-C4	4.40	1.46	1.39
3	I	601	ADP	C5-C4	4.39	1.46	1.39
3	D	601	ADP	C5-C4	4.35	1.46	1.39
3	G	601	ADP	PA-O3A	2.90	1.62	1.59
3	B	601	ADP	C5-C6	2.85	1.48	1.41
3	J	601	ADP	C5-C6	2.84	1.48	1.41
3	H	601	ADP	C5-C6	2.80	1.48	1.41
3	N	601	ADP	C5-C6	2.79	1.48	1.41
3	G	601	ADP	C5-C6	2.76	1.48	1.41
3	M	601	ADP	C5-C6	2.73	1.48	1.41
3	D	601	ADP	C5-C6	2.70	1.48	1.41
3	E	601	ADP	C5-C6	2.69	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	601	ADP	C5-C6	2.69	1.48	1.41
3	A	601	ADP	C5-C6	2.68	1.48	1.41
3	K	601	ADP	C5-C6	2.67	1.48	1.41
3	L	601	ADP	C5-C6	2.64	1.48	1.41
3	A	601	ADP	PA-O3A	2.64	1.62	1.59
3	C	601	ADP	C5-C6	2.63	1.48	1.41
3	I	601	ADP	C5-C6	2.56	1.48	1.41
3	H	601	ADP	C8-N7	2.51	1.36	1.31
3	B	601	ADP	C8-N7	2.49	1.36	1.31
3	D	601	ADP	C8-N7	2.47	1.36	1.31
3	J	601	ADP	C8-N7	2.47	1.36	1.31
3	L	601	ADP	C8-N7	2.39	1.36	1.31
3	E	601	ADP	C8-N7	2.38	1.36	1.31
3	G	601	ADP	C8-N7	2.38	1.36	1.31
3	N	601	ADP	C8-N7	2.36	1.36	1.31
3	I	601	ADP	C8-N7	2.36	1.36	1.31
3	K	601	ADP	C8-N7	2.35	1.36	1.31
3	F	601	ADP	C5-N7	-2.35	1.34	1.39
3	M	601	ADP	C8-N7	2.35	1.36	1.31
3	A	601	ADP	C8-N7	2.34	1.36	1.31
3	B	601	ADP	PA-O3A	2.34	1.62	1.59
3	C	601	ADP	C5-N7	-2.32	1.34	1.39
3	C	601	ADP	C8-N7	2.31	1.36	1.31
3	I	601	ADP	C5-N7	-2.27	1.34	1.39
3	K	601	ADP	C5-N7	-2.27	1.34	1.39
3	F	601	ADP	C8-N7	2.25	1.36	1.31
3	J	601	ADP	PA-O3A	2.25	1.61	1.59
3	D	601	ADP	C4-N9	-2.24	1.33	1.37
3	L	601	ADP	C5-N7	-2.22	1.35	1.39
3	A	601	ADP	C5-N7	-2.22	1.35	1.39
3	M	601	ADP	C5-N7	-2.20	1.35	1.39
3	D	601	ADP	PA-O3A	2.20	1.61	1.59
3	N	601	ADP	C5-N7	-2.19	1.35	1.39
3	J	601	ADP	C4-N9	-2.16	1.33	1.37
3	D	601	ADP	C5-N7	-2.15	1.35	1.39
3	H	601	ADP	C4-N9	-2.14	1.33	1.37
3	I	601	ADP	C4-N9	-2.14	1.33	1.37
3	E	601	ADP	C5-N7	-2.14	1.35	1.39
3	C	601	ADP	PA-O3A	2.13	1.61	1.59
3	G	601	ADP	C5-N7	-2.13	1.35	1.39
3	E	601	ADP	PA-O3A	2.13	1.61	1.59
3	B	601	ADP	C5-N7	-2.11	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	601	ADP	C4-N9	-2.11	1.33	1.37
3	N	601	ADP	C4-N9	-2.07	1.33	1.37
3	H	601	ADP	C5-N7	-2.04	1.35	1.39
3	B	601	ADP	C4-N9	-2.01	1.33	1.37

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	ADP	C5-C4-N3	-6.14	118.26	126.72
3	G	601	ADP	C5-C4-N3	-5.77	118.78	126.72
3	A	601	ADP	C5-C4-N3	-5.65	118.94	126.72
3	N	601	ADP	C5-C4-N3	-5.55	119.08	126.72
3	M	601	ADP	C5-C4-N3	-5.55	119.08	126.72
3	K	601	ADP	C5-C4-N3	-5.54	119.08	126.72
3	F	601	ADP	C5-C4-N3	-5.53	119.10	126.72
3	B	601	ADP	C5-C4-N3	-5.53	119.10	126.72
3	L	601	ADP	C5-C4-N3	-5.53	119.11	126.72
3	E	601	ADP	C5-C4-N3	-5.51	119.14	126.72
3	I	601	ADP	C5-C4-N3	-5.35	119.34	126.72
3	D	601	ADP	C5-C4-N3	-5.21	119.55	126.72
3	H	601	ADP	C5-C4-N3	-5.18	119.58	126.72
3	J	601	ADP	C5-C4-N3	-5.14	119.64	126.72
3	C	601	ADP	N3-C4-N9	4.93	135.55	127.17
3	G	601	ADP	N3-C4-N9	4.74	135.22	127.17
3	L	601	ADP	N3-C4-N9	4.59	134.98	127.17
3	A	601	ADP	N3-C4-N9	4.56	134.93	127.17
3	I	601	ADP	N3-C4-N9	4.54	134.89	127.17
3	F	601	ADP	N3-C4-N9	4.47	134.77	127.17
3	E	601	ADP	N3-C4-N9	4.44	134.71	127.17
3	K	601	ADP	N3-C4-N9	4.42	134.68	127.17
3	N	601	ADP	N3-C4-N9	4.38	134.61	127.17
3	M	601	ADP	N3-C4-N9	4.35	134.56	127.17
3	B	601	ADP	N3-C4-N9	4.19	134.29	127.17
3	D	601	ADP	N3-C4-N9	4.16	134.24	127.17
3	H	601	ADP	N3-C4-N9	4.01	133.99	127.17
3	G	601	ADP	C2-N3-C4	3.95	121.47	111.83
3	J	601	ADP	N3-C4-N9	3.92	133.83	127.17
3	F	601	ADP	C2-N3-C4	3.91	121.39	111.83
3	F	601	ADP	N3-C2-N1	-3.90	122.68	128.58
3	E	601	ADP	N3-C2-N1	-3.89	122.70	128.58
3	E	601	ADP	C2-N3-C4	3.89	121.32	111.83
3	J	601	ADP	C4-C5-N7	-3.87	106.15	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	ADP	C2-N3-C4	3.87	121.29	111.83
3	B	601	ADP	C4-C5-N7	-3.86	106.17	110.58
3	G	601	ADP	N3-C2-N1	-3.84	122.77	128.58
3	L	601	ADP	N3-C2-N1	-3.83	122.78	128.58
3	L	601	ADP	C2-N3-C4	3.83	121.19	111.83
3	A	601	ADP	C2-N3-C4	3.82	121.17	111.83
3	M	601	ADP	C2-N3-C4	3.81	121.14	111.83
3	K	601	ADP	C2-N3-C4	3.81	121.13	111.83
3	B	601	ADP	C2-N3-C4	3.79	121.09	111.83
3	H	601	ADP	C2-N3-C4	3.78	121.07	111.83
3	N	601	ADP	C2-N3-C4	3.78	121.06	111.83
3	D	601	ADP	N3-C2-N1	-3.77	122.88	128.58
3	H	601	ADP	N3-C2-N1	-3.76	122.89	128.58
3	J	601	ADP	C2-N3-C4	3.74	120.95	111.83
3	N	601	ADP	C4-C5-N7	-3.72	106.32	110.58
3	D	601	ADP	C2-N3-C4	3.72	120.92	111.83
3	K	601	ADP	N3-C2-N1	-3.72	122.95	128.58
3	H	601	ADP	C4-C5-N7	-3.72	106.33	110.58
3	I	601	ADP	C4-N9-C8	3.71	109.63	105.74
3	J	601	ADP	N3-C2-N1	-3.68	123.00	128.58
3	A	601	ADP	N3-C2-N1	-3.67	123.03	128.58
3	M	601	ADP	C4-C5-N7	-3.65	106.41	110.58
3	N	601	ADP	N3-C2-N1	-3.64	123.07	128.58
3	M	601	ADP	N3-C2-N1	-3.64	123.08	128.58
3	I	601	ADP	C2-N3-C4	3.61	120.66	111.83
3	D	601	ADP	C4-C5-N7	-3.55	106.53	110.58
3	I	601	ADP	N3-C2-N1	-3.54	123.22	128.58
3	A	601	ADP	C4-C5-N7	-3.53	106.55	110.58
3	D	601	ADP	C4-N9-C8	3.53	109.44	105.74
3	B	601	ADP	N3-C2-N1	-3.51	123.26	128.58
3	C	601	ADP	N3-C2-N1	-3.48	123.31	128.58
3	L	601	ADP	C4-N9-C8	3.43	109.34	105.74
3	K	601	ADP	C4-C5-N7	-3.43	106.66	110.58
3	C	601	ADP	C4-C5-N7	-3.42	106.67	110.58
3	G	601	ADP	C4-C5-N7	-3.40	106.69	110.58
3	E	601	ADP	C4-C5-N7	-3.39	106.70	110.58
3	F	601	ADP	C4-C5-N7	-3.35	106.75	110.58
3	L	601	ADP	C4-C5-N7	-3.32	106.78	110.58
3	J	601	ADP	C4-N9-C8	3.31	109.22	105.74
3	H	601	ADP	C4-N9-C8	3.27	109.17	105.74
3	I	601	ADP	C4-C5-N7	-3.27	106.84	110.58
3	G	601	ADP	C4-N9-C8	3.24	109.14	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	601	ADP	C4-N9-C8	3.23	109.13	105.74
3	A	601	ADP	C4-N9-C8	3.20	109.09	105.74
3	M	601	ADP	C4-N9-C8	3.13	109.02	105.74
3	E	601	ADP	C4-N9-C8	3.09	108.98	105.74
3	K	601	ADP	C4-N9-C8	3.05	108.94	105.74
3	F	601	ADP	C4-N9-C8	3.03	108.92	105.74
3	B	601	ADP	C4-N9-C8	3.00	108.89	105.74
3	J	601	ADP	C5-N7-C8	2.91	108.02	103.45
3	N	601	ADP	C5-N7-C8	2.86	107.94	103.45
3	B	601	ADP	C5-N7-C8	2.86	107.94	103.45
3	G	601	ADP	C5-N7-C8	2.81	107.86	103.45
3	H	601	ADP	C5-N7-C8	2.81	107.86	103.45
3	L	601	ADP	C5-N7-C8	2.78	107.81	103.45
3	J	601	ADP	C6-C5-N7	2.77	137.42	132.09
3	F	601	ADP	C5-N7-C8	2.75	107.77	103.45
3	D	601	ADP	C5-N7-C8	2.75	107.77	103.45
3	A	601	ADP	C5-N7-C8	2.74	107.76	103.45
3	I	601	ADP	N9-C8-N7	-2.74	110.04	113.94
3	D	601	ADP	N9-C8-N7	-2.74	110.05	113.94
3	I	601	ADP	C5-N7-C8	2.72	107.72	103.45
3	J	601	ADP	N9-C8-N7	-2.72	110.08	113.94
3	K	601	ADP	C5-N7-C8	2.70	107.70	103.45
3	M	601	ADP	C5-N7-C8	2.70	107.70	103.45
3	C	601	ADP	C5-N7-C8	2.70	107.69	103.45
3	E	601	ADP	C5-N7-C8	2.69	107.69	103.45
3	C	601	ADP	C4-N9-C8	2.67	108.54	105.74
3	L	601	ADP	N9-C8-N7	-2.67	110.15	113.94
3	H	601	ADP	C6-C5-N7	2.66	137.21	132.09
3	H	601	ADP	N9-C8-N7	-2.63	110.21	113.94
3	N	601	ADP	N9-C8-N7	-2.57	110.29	113.94
3	G	601	ADP	N9-C8-N7	-2.56	110.30	113.94
3	B	601	ADP	C6-C5-N7	2.52	136.95	132.09
3	B	601	ADP	N9-C8-N7	-2.49	110.40	113.94
3	F	601	ADP	N9-C8-N7	-2.47	110.43	113.94
3	D	601	ADP	C6-C5-N7	2.45	136.82	132.09
3	K	601	ADP	N9-C8-N7	-2.45	110.46	113.94
3	A	601	ADP	N9-C8-N7	-2.44	110.47	113.94
3	E	601	ADP	N9-C8-N7	-2.44	110.48	113.94
3	M	601	ADP	N9-C8-N7	-2.41	110.52	113.94
3	M	601	ADP	C6-C5-N7	2.35	136.62	132.09
3	H	601	ADP	C3'-C2'-C1'	2.35	105.91	101.46
3	N	601	ADP	C6-C5-N7	2.35	136.61	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	601	ADP	C3'-C2'-C1'	2.32	105.86	101.46
3	E	601	ADP	C6-C5-N7	2.29	136.51	132.09
3	J	601	ADP	O2A-PA-O3A	2.26	113.38	107.27
3	A	601	ADP	C3'-C2'-C1'	2.25	105.72	101.46
3	F	601	ADP	C6-C5-N7	2.25	136.43	132.09
3	F	601	ADP	O3B-PB-O2B	2.24	116.20	107.80
3	J	601	ADP	C3'-C2'-C1'	2.24	105.70	101.46
3	A	601	ADP	C6-C5-N7	2.21	136.34	132.09
3	K	601	ADP	C6-C5-N7	2.18	136.30	132.09
3	J	601	ADP	C2-N1-C6	2.18	122.31	118.73
3	L	601	ADP	O3B-PB-O2B	2.18	115.96	107.80
3	H	601	ADP	C2-N1-C6	2.17	122.30	118.73
3	G	601	ADP	C6-C5-N7	2.16	136.26	132.09
3	D	601	ADP	C2-N1-C6	2.16	122.28	118.73
3	E	601	ADP	C2-N1-C6	2.16	122.28	118.73
3	L	601	ADP	C6-C5-N7	2.15	136.24	132.09
3	C	601	ADP	N9-C8-N7	-2.14	110.90	113.94
3	F	601	ADP	C2-N1-C6	2.13	122.23	118.73
3	L	601	ADP	C2-N1-C6	2.13	122.23	118.73
3	K	601	ADP	C3'-C2'-C1'	2.12	105.48	101.46
3	L	601	ADP	C3'-C2'-C1'	2.11	105.45	101.46
3	N	601	ADP	C3'-C2'-C1'	2.10	105.44	101.46
3	N	601	ADP	C2-N1-C6	2.10	122.18	118.73
3	I	601	ADP	C6-C5-N7	2.09	136.11	132.09
3	K	601	ADP	C2-N1-C6	2.07	122.14	118.73
3	M	601	ADP	O3B-PB-O2B	2.07	115.56	107.80
3	D	601	ADP	C3'-C2'-C1'	2.06	105.36	101.46
3	G	601	ADP	C2-N1-C6	2.05	122.10	118.73
3	I	601	ADP	C2-N1-C6	2.04	122.08	118.73
3	A	601	ADP	C2-N1-C6	2.02	122.04	118.73

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	601	ADP	C5'-O5'-PA-O2A
3	C	601	ADP	C5'-O5'-PA-O3A
3	D	601	ADP	C5'-O5'-PA-O2A
3	D	601	ADP	C5'-O5'-PA-O3A
3	F	601	ADP	C3'-C4'-C5'-O5'
3	G	601	ADP	C5'-O5'-PA-O1A
3	G	601	ADP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	H	601	ADP	C5'-O5'-PA-O1A
3	H	601	ADP	C5'-O5'-PA-O2A
3	H	601	ADP	C5'-O5'-PA-O3A
3	I	601	ADP	C5'-O5'-PA-O2A
3	J	601	ADP	PA-O3A-PB-O2B
3	J	601	ADP	C5'-O5'-PA-O1A
3	J	601	ADP	C5'-O5'-PA-O2A
3	J	601	ADP	C5'-O5'-PA-O3A
3	K	601	ADP	C5'-O5'-PA-O2A
3	K	601	ADP	C5'-O5'-PA-O3A
3	K	601	ADP	C3'-C4'-C5'-O5'
3	M	601	ADP	PA-O3A-PB-O2B
3	M	601	ADP	PB-O3A-PA-O5'
3	M	601	ADP	C5'-O5'-PA-O3A
3	N	601	ADP	PB-O3A-PA-O5'
3	N	601	ADP	C5'-O5'-PA-O2A
3	N	601	ADP	C5'-O5'-PA-O3A
3	I	601	ADP	C3'-C4'-C5'-O5'
3	N	601	ADP	O4'-C4'-C5'-O5'
3	C	601	ADP	C3'-C4'-C5'-O5'
3	F	601	ADP	O4'-C4'-C5'-O5'
3	I	601	ADP	O4'-C4'-C5'-O5'
3	K	601	ADP	O4'-C4'-C5'-O5'
3	N	601	ADP	C3'-C4'-C5'-O5'
3	D	601	ADP	O4'-C4'-C5'-O5'
3	D	601	ADP	C3'-C4'-C5'-O5'
3	M	601	ADP	O4'-C4'-C5'-O5'
3	M	601	ADP	C3'-C4'-C5'-O5'
3	L	601	ADP	C3'-C4'-C5'-O5'
3	G	601	ADP	PA-O3A-PB-O1B
3	C	601	ADP	O4'-C4'-C5'-O5'
3	D	601	ADP	PB-O3A-PA-O5'
3	E	601	ADP	PB-O3A-PA-O5'
3	I	601	ADP	PB-O3A-PA-O5'
3	N	601	ADP	PA-O3A-PB-O1B
3	K	601	ADP	PA-O3A-PB-O2B
3	H	601	ADP	PB-O3A-PA-O2A
3	B	601	ADP	C5'-O5'-PA-O1A
3	M	601	ADP	C5'-O5'-PA-O1A
3	M	601	ADP	PA-O3A-PB-O1B
3	G	601	ADP	PB-O3A-PA-O2A
3	H	601	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	F	601	ADP	C4'-C5'-O5'-PA
3	D	601	ADP	PB-O3A-PA-O1A
3	E	601	ADP	PB-O3A-PA-O1A
3	J	601	ADP	PA-O3A-PB-O1B
3	N	601	ADP	PA-O3A-PB-O2B
3	N	601	ADP	PA-O3A-PB-O3B
3	E	601	ADP	O4'-C4'-C5'-O5'
3	A	601	ADP	PB-O3A-PA-O1A
3	H	601	ADP	PB-O3A-PA-O1A
3	C	601	ADP	PB-O3A-PA-O2A
3	J	601	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

28 monomers are involved in 65 short contacts:

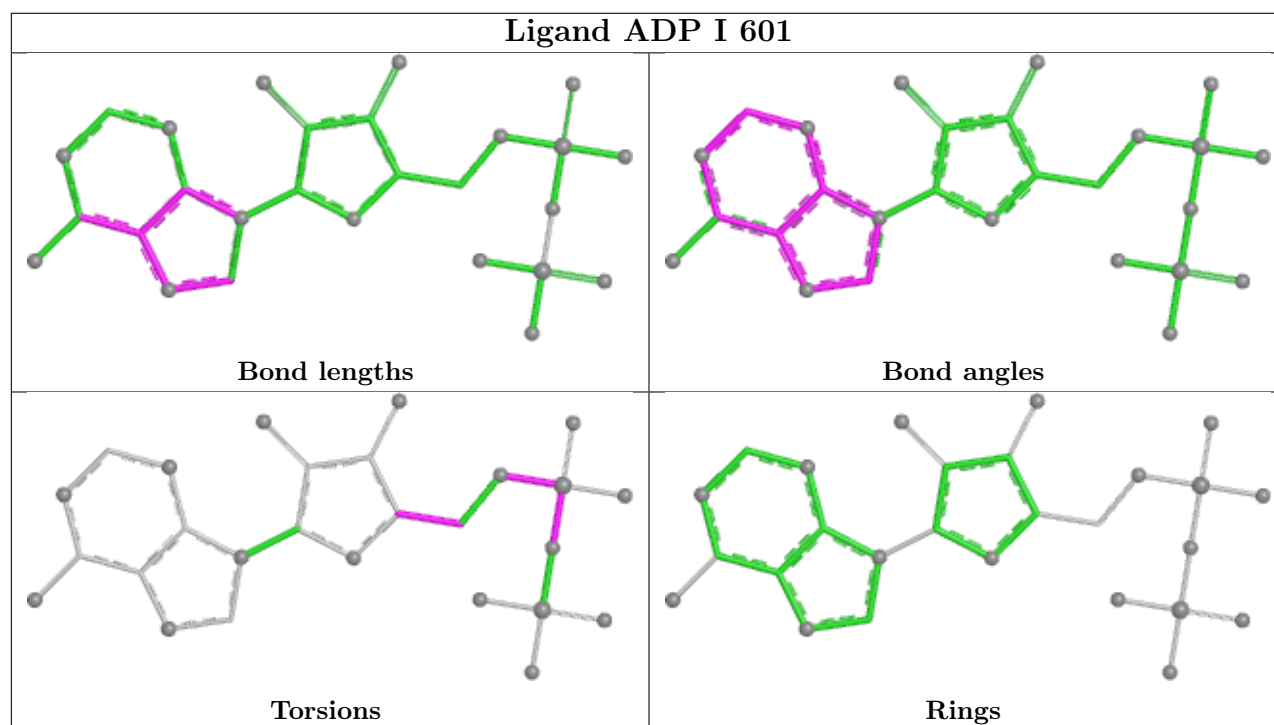
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	601	ADP	3	0
3	J	601	ADP	1	0
4	G	602	BEF	1	0
3	N	601	ADP	5	0
4	F	602	BEF	1	0
3	F	601	ADP	4	0
4	H	602	BEF	4	0
3	B	601	ADP	5	0
4	M	602	BEF	1	0
3	A	601	ADP	1	0
4	E	602	BEF	1	0
3	E	601	ADP	4	0
4	B	602	BEF	3	0
4	L	602	BEF	2	0
4	D	602	BEF	1	0
3	C	601	ADP	4	0
4	C	602	BEF	4	0
4	I	602	BEF	4	0
4	J	602	BEF	2	0
3	M	601	ADP	4	0
4	A	602	BEF	2	0
3	D	601	ADP	4	0
3	K	601	ADP	4	0
3	H	601	ADP	2	0
4	N	602	BEF	3	0
3	G	601	ADP	5	0

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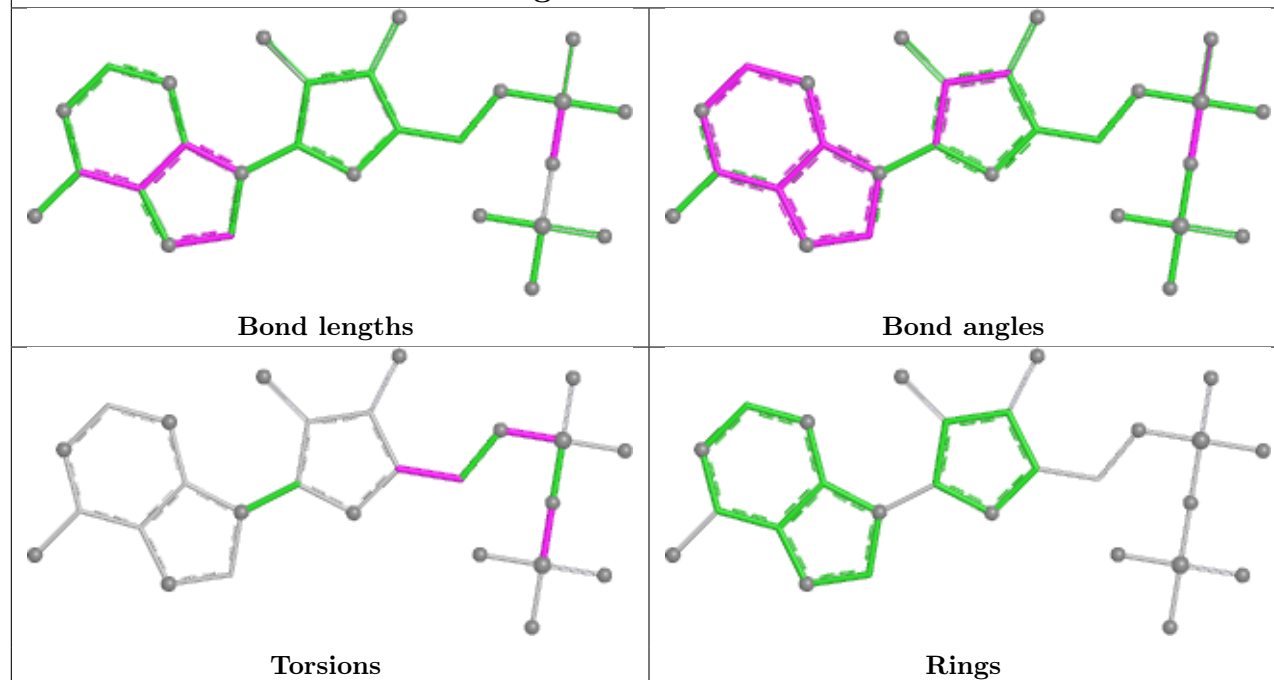
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	601	ADP	2	0
4	K	602	BEF	2	0

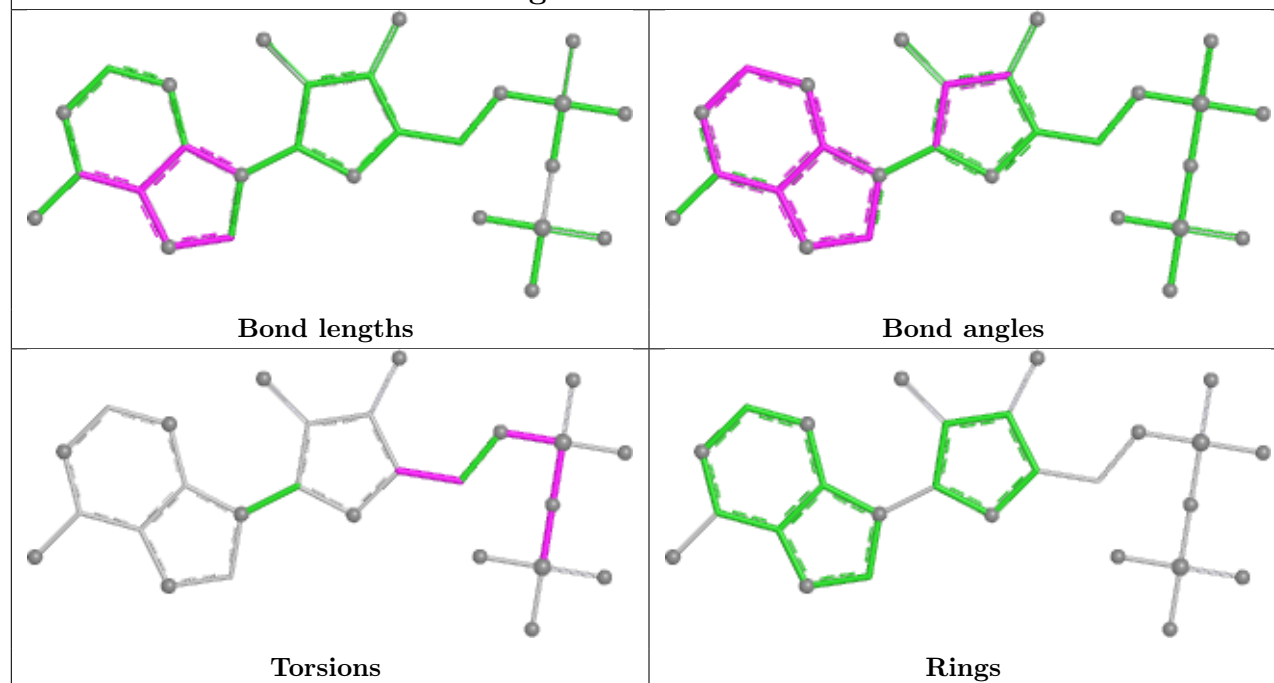
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



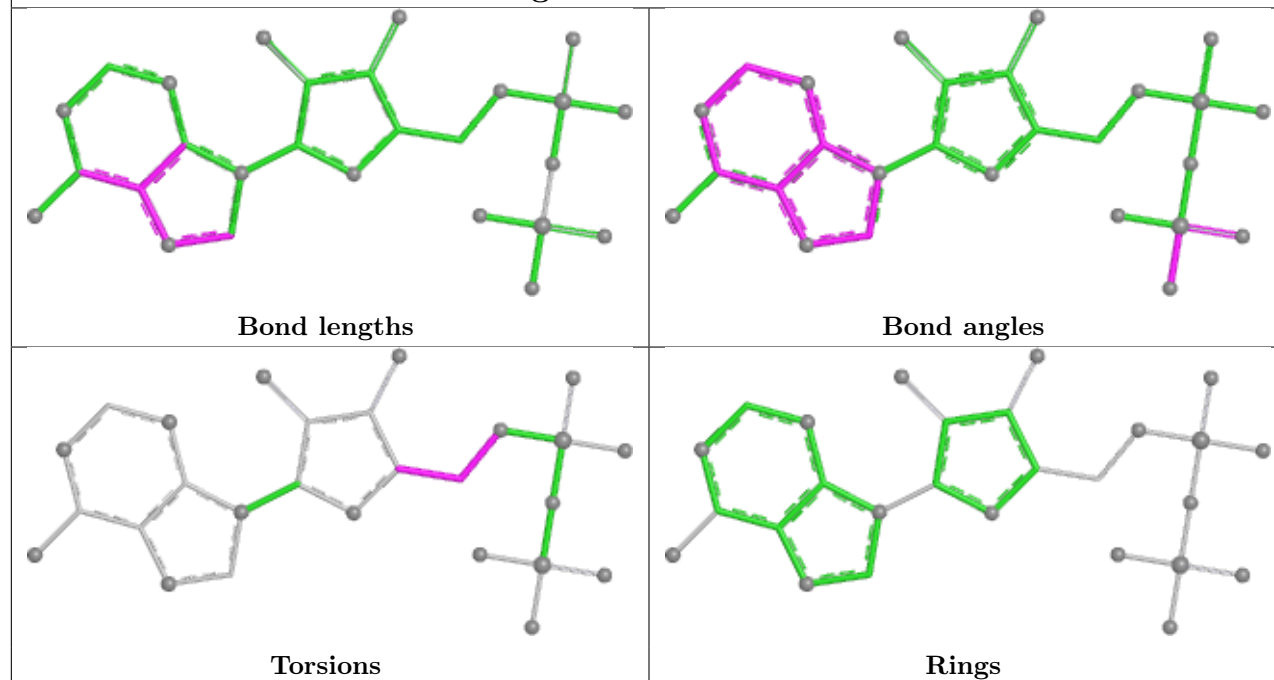
Ligand ADP J 601



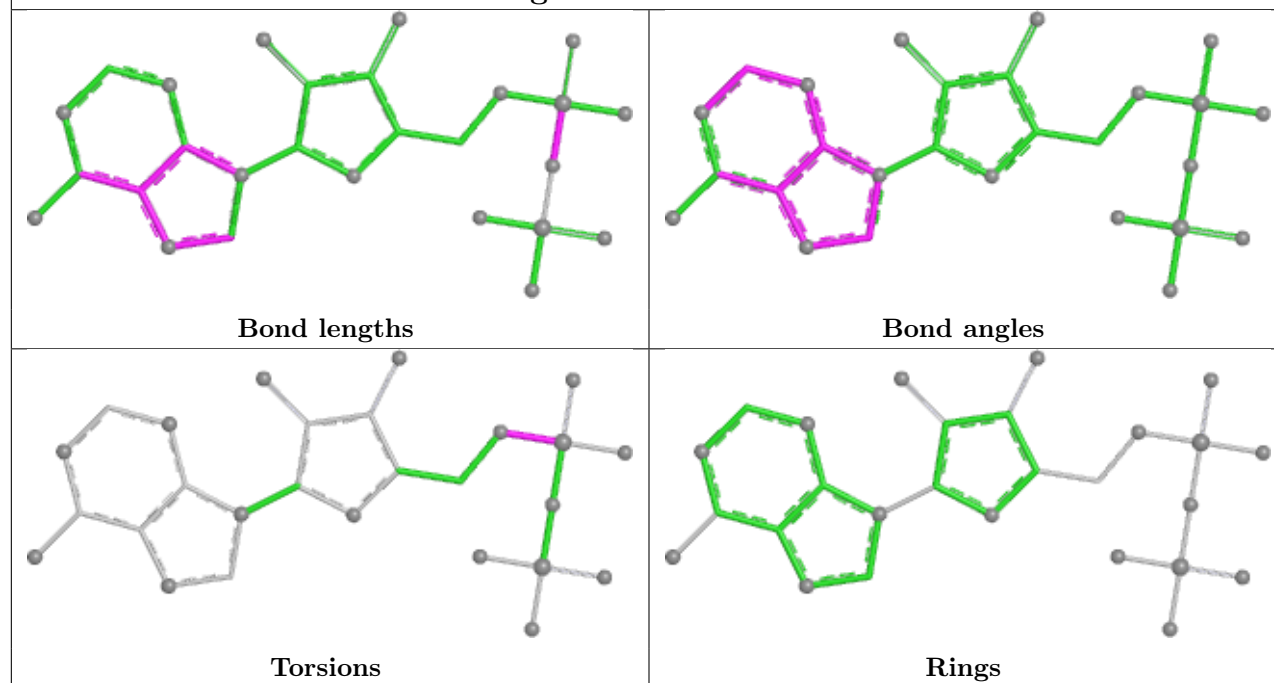
Ligand ADP N 601

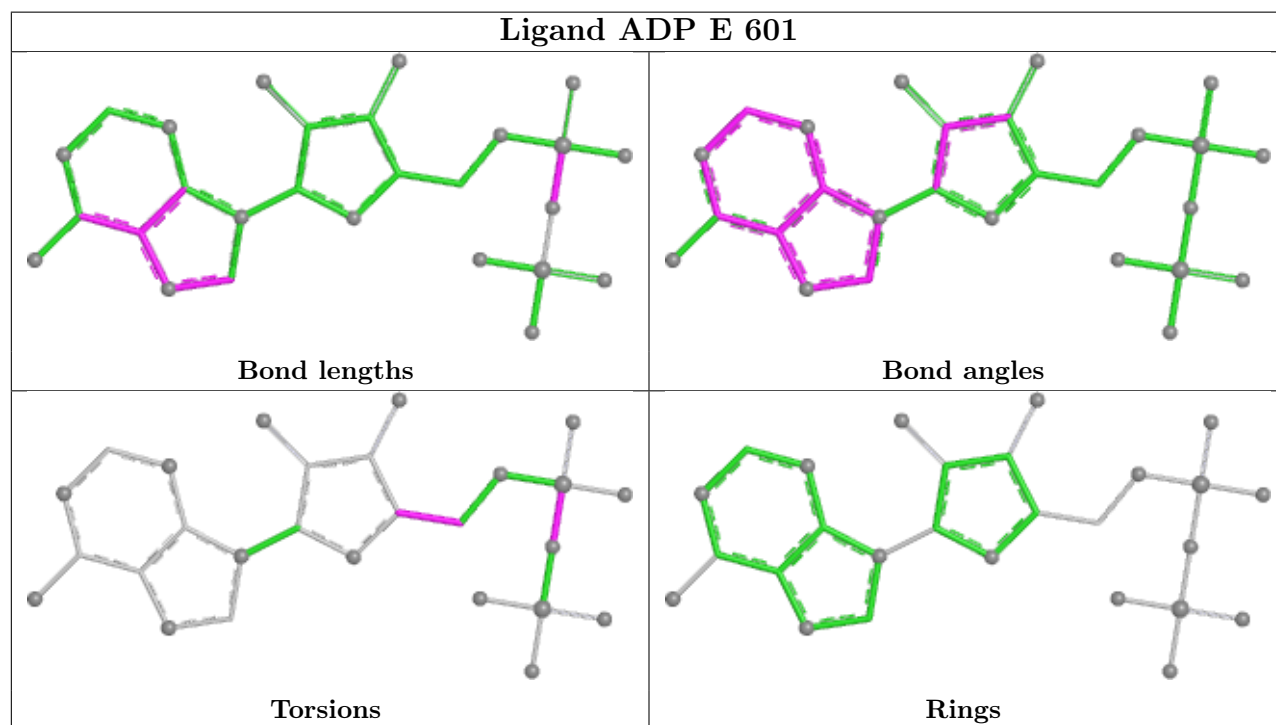
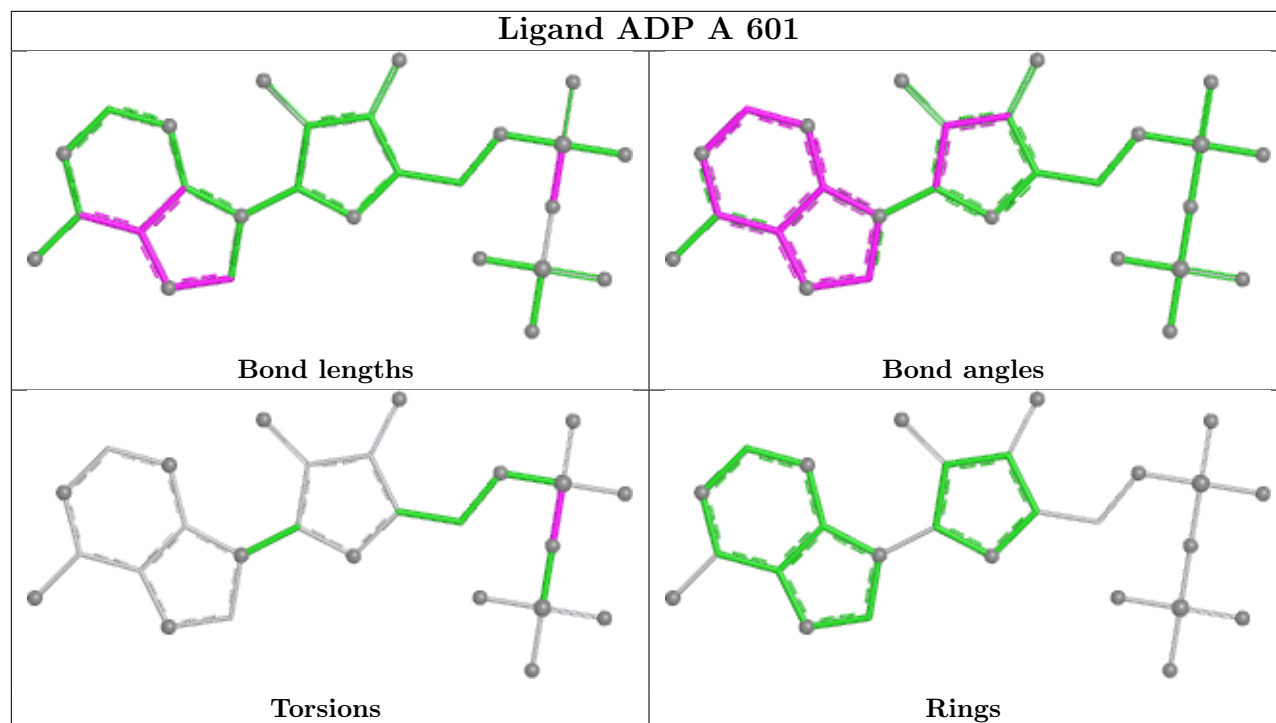


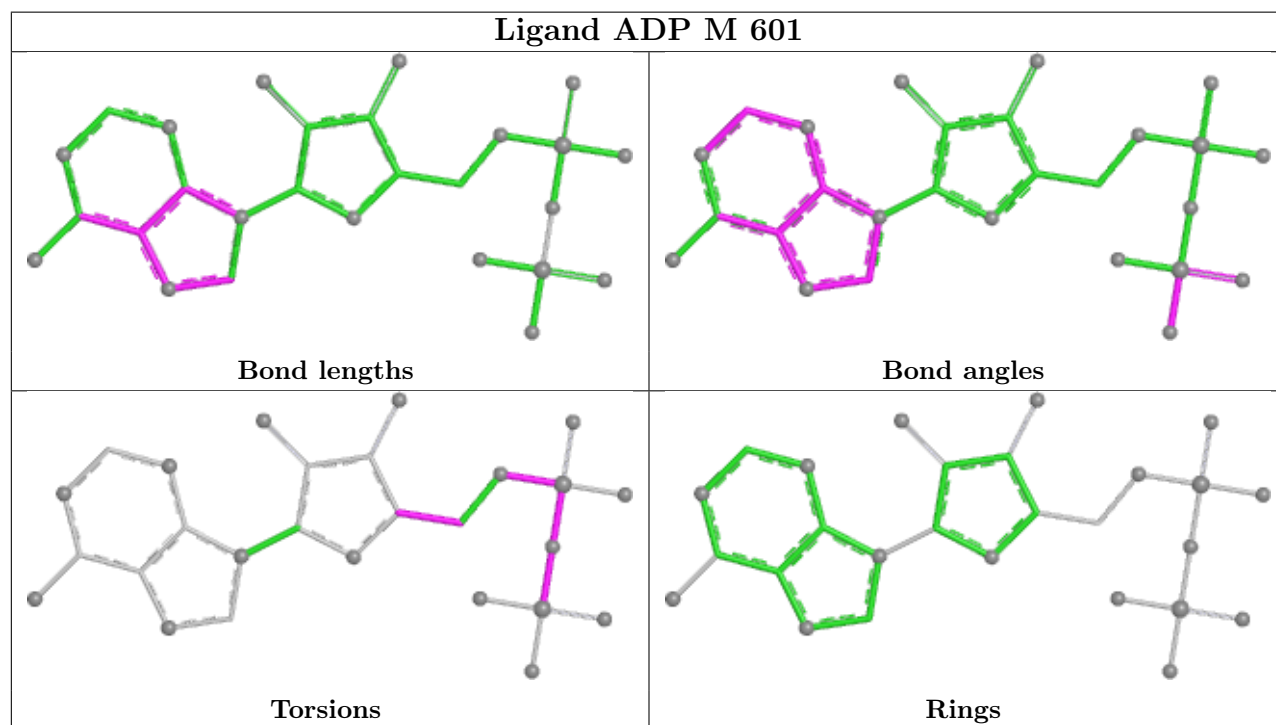
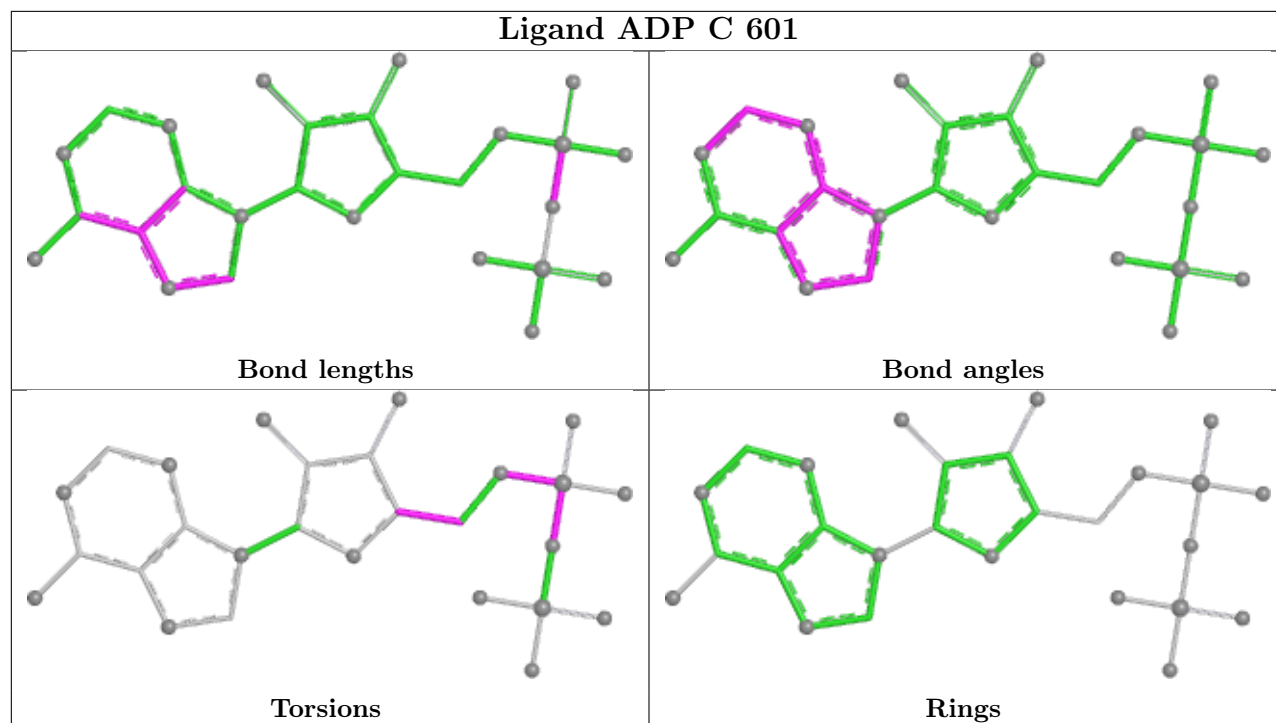
Ligand ADP F 601

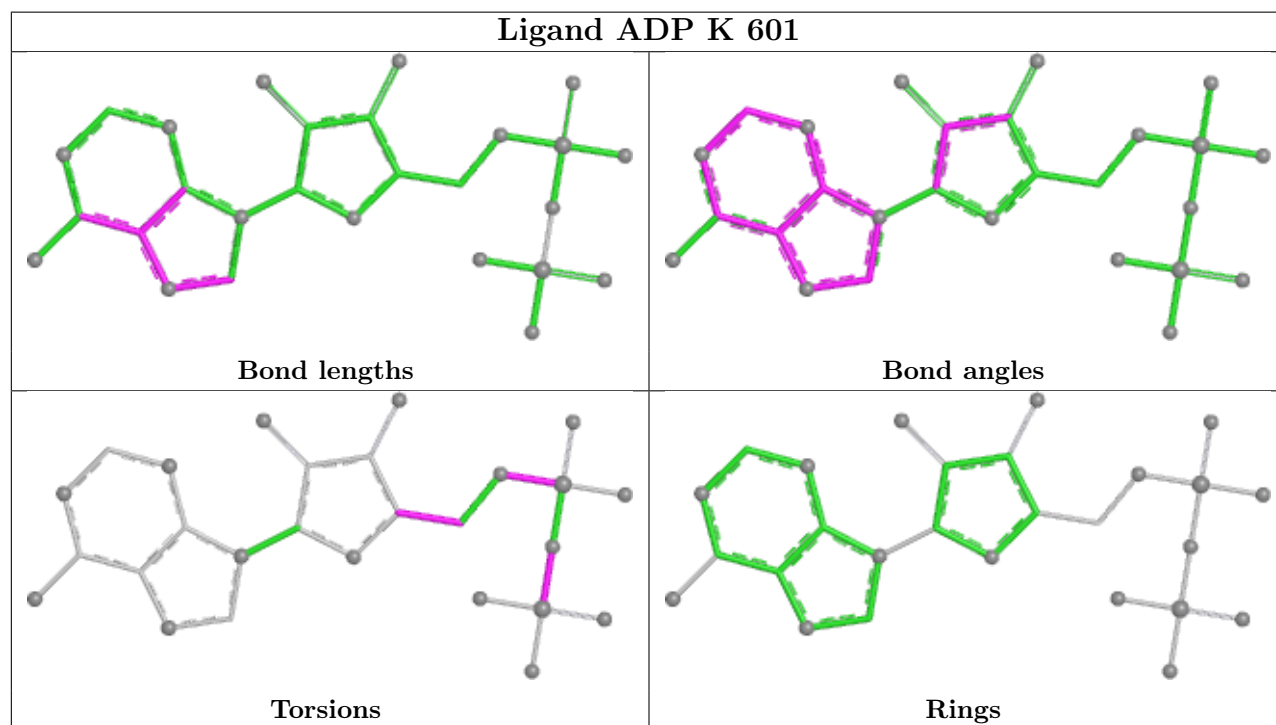
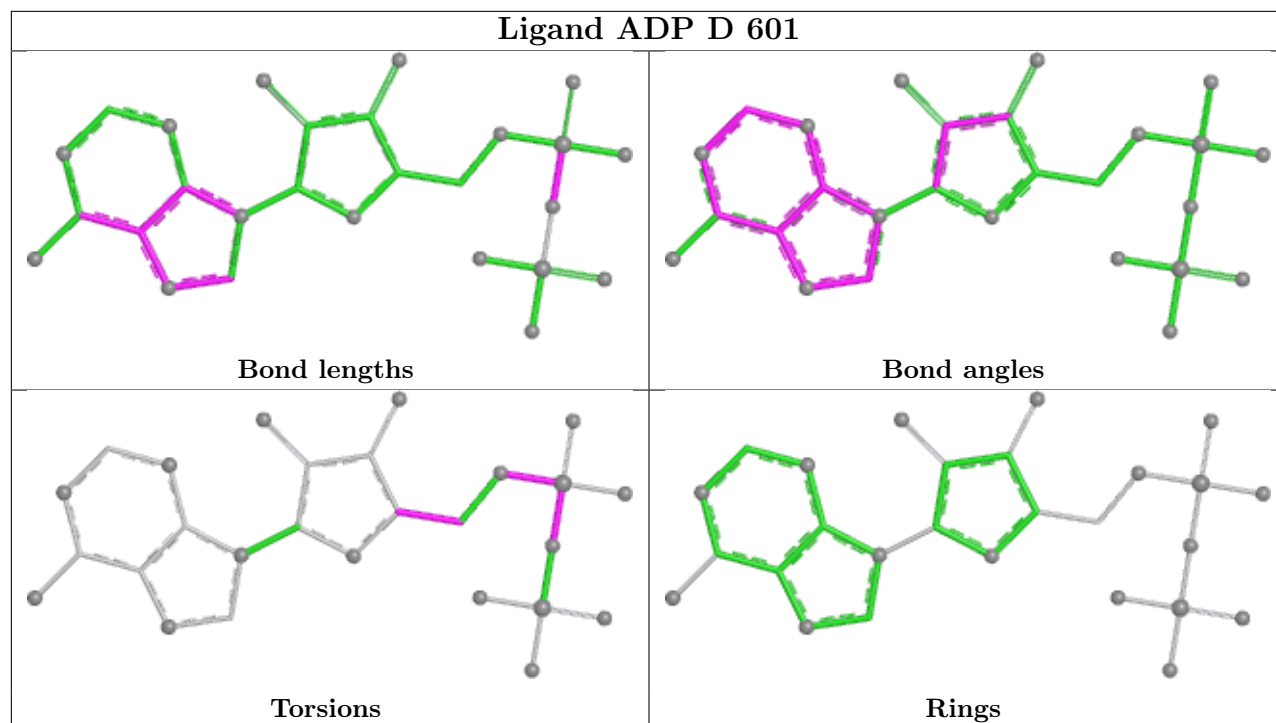


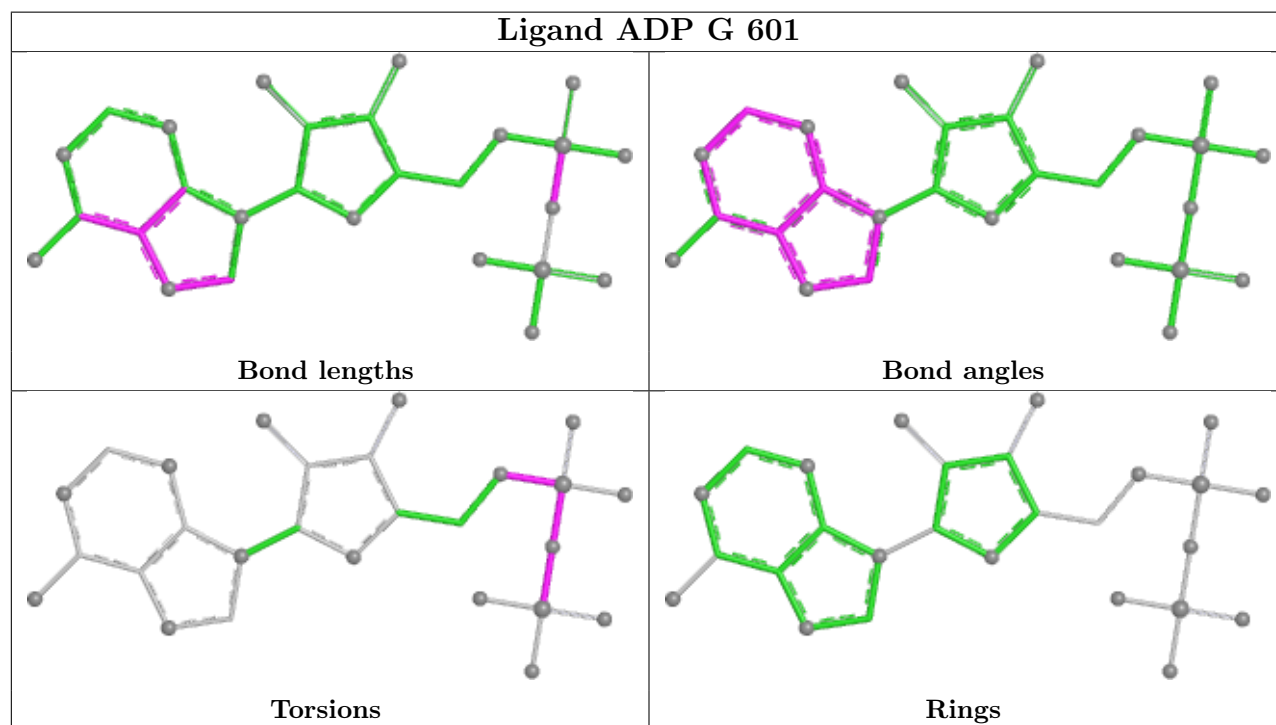
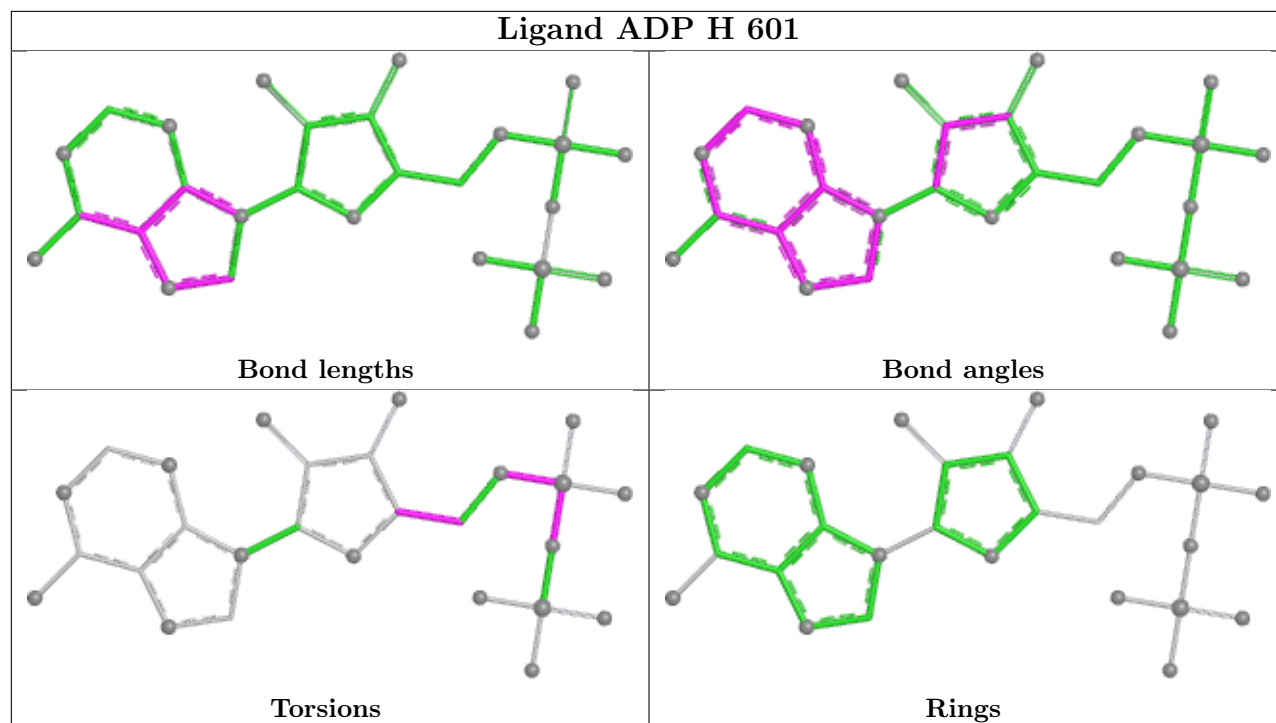
Ligand ADP B 601

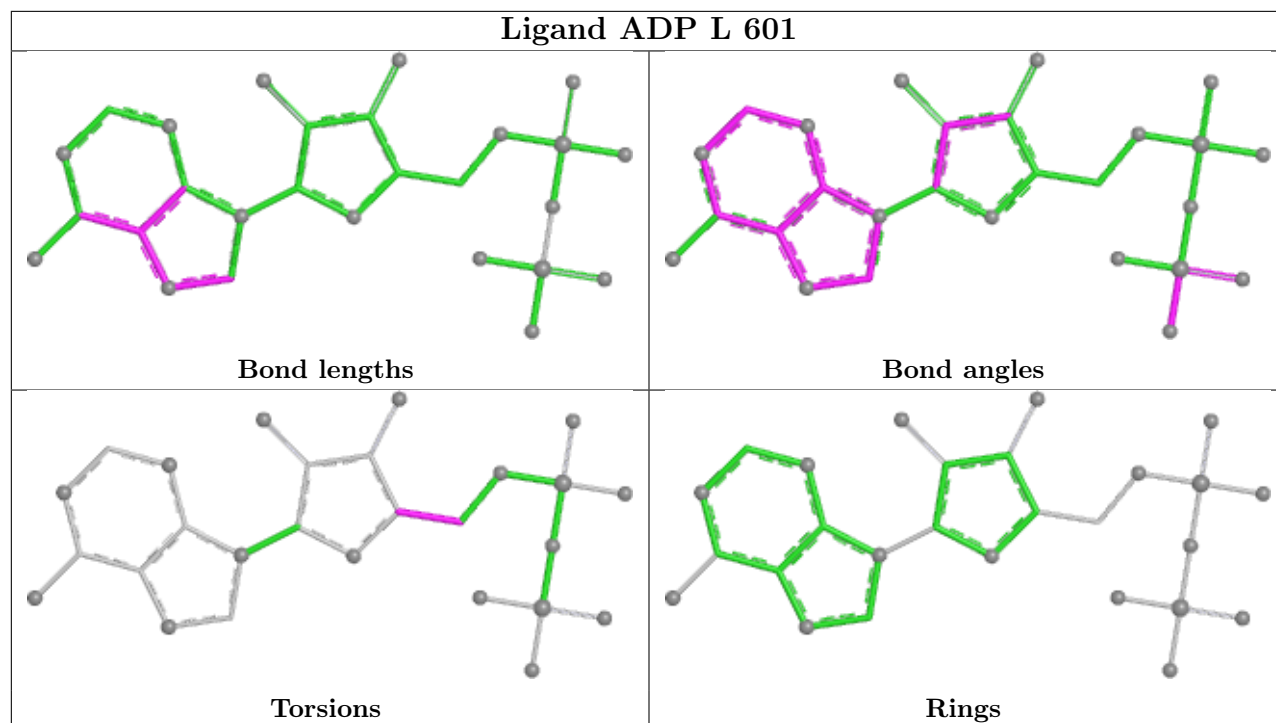












5.7 Other polymers [i](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	524/548 (95%)	-0.38	1 (0%) 91 82	54, 121, 305, 467	0
1	B	524/548 (95%)	-0.41	1 (0%) 91 82	57, 135, 293, 355	0
1	C	524/548 (95%)	-0.43	1 (0%) 91 82	54, 126, 274, 415	0
1	D	524/548 (95%)	-0.41	1 (0%) 91 82	53, 113, 212, 321	0
1	E	524/548 (95%)	-0.38	1 (0%) 91 82	62, 139, 293, 376	0
1	F	524/548 (95%)	-0.31	4 (0%) 82 63	51, 122, 288, 363	0
1	G	524/548 (95%)	-0.35	3 (0%) 85 68	43, 111, 278, 398	0
1	H	524/548 (95%)	-0.43	1 (0%) 91 82	61, 150, 325, 459	0
1	I	524/548 (95%)	-0.40	0 100 100	49, 117, 213, 354	0
1	J	524/548 (95%)	-0.43	0 100 100	63, 139, 287, 398	0
1	K	524/548 (95%)	-0.36	3 (0%) 85 68	59, 141, 293, 379	0
1	L	524/548 (95%)	-0.37	2 (0%) 88 74	53, 130, 298, 397	0
1	M	524/548 (95%)	-0.37	1 (0%) 91 82	71, 146, 330, 456	0
1	N	524/548 (95%)	-0.41	1 (0%) 91 82	70, 159, 306, 375	0
2	1	97/97 (100%)	-0.20	1 (1%) 79 58	93, 149, 321, 352	0
2	2	97/97 (100%)	-0.10	1 (1%) 79 58	98, 162, 314, 350	0
2	O	95/97 (97%)	-0.21	0 100 100	88, 136, 315, 390	0
2	P	97/97 (100%)	-0.17	1 (1%) 79 58	74, 152, 323, 361	0
2	Q	96/97 (98%)	-0.22	0 100 100	113, 182, 322, 375	0
2	R	97/97 (100%)	-0.06	0 100 100	112, 168, 267, 319	0
2	S	96/97 (98%)	0.10	1 (1%) 79 58	106, 165, 341, 367	0
2	T	97/97 (100%)	-0.13	1 (1%) 79 58	116, 178, 338, 434	0
2	U	97/97 (100%)	-0.14	0 100 100	88, 156, 354, 422	0
2	V	97/97 (100%)	-0.21	0 100 100	119, 183, 325, 378	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	W	97/97 (100%)	-0.04	1 (1%) 79 58	106, 161, 248, 306	0
2	X	97/97 (100%)	0.10	6 (6%) 26 22	101, 153, 297, 380	0
2	Y	96/97 (98%)	-0.20	0 100 100	104, 155, 304, 366	0
2	Z	95/97 (97%)	-0.18	0 100 100	108, 160, 312, 358	0
All	All	8687/9030 (96%)	-0.35	32 (0%) 88 74	43, 139, 302, 467	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	227	ILE	5.4
2	S	59	VAL	3.6
1	K	249	ILE	3.5
1	M	273	VAL	3.4
2	X	59	VAL	3.4
1	L	233	MET	3.2
1	G	233	MET	3.1
2	X	10	VAL	3.0
1	K	223	ALA	2.8
1	E	248	LEU	2.7
1	F	275	ALA	2.5
1	G	223	ALA	2.5
2	X	5	PRO	2.5
2	X	42	ALA	2.4
1	N	248	LEU	2.3
2	X	43	VAL	2.3
1	D	519	CYS	2.3
1	H	512	GLY	2.3
1	F	233	MET	2.3
2	1	97	ALA	2.3
1	C	495	ASP	2.2
1	F	227	ILE	2.2
2	W	10	VAL	2.2
1	B	249	ILE	2.2
1	L	249	ILE	2.2
2	X	85	ILE	2.1
1	A	250	ILE	2.1
1	G	499	VAL	2.1
2	T	65	VAL	2.1
2	2	86	MET	2.0
1	F	250	ILE	2.0
2	P	10	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BEF	F	602	4/4	0.84	0.21	53,80,165,206	0
4	BEF	A	602	4/4	0.88	0.12	62,131,196,204	0
4	BEF	K	602	4/4	0.90	0.14	54,86,101,160	0
4	BEF	N	602	4/4	0.91	0.10	98,99,105,118	0
4	BEF	B	602	4/4	0.92	0.16	45,60,96,100	0
4	BEF	J	602	4/4	0.93	0.09	40,132,142,204	0
5	MG	B	603	1/1	0.93	0.14	66,66,66,66	0
4	BEF	D	602	4/4	0.94	0.09	31,64,104,109	0
3	ADP	H	601	27/27	0.94	0.10	72,93,142,191	0
3	ADP	K	601	27/27	0.94	0.11	80,97,118,125	0
5	MG	L	603	1/1	0.94	0.11	66,66,66,66	0
4	BEF	M	602	4/4	0.95	0.12	119,139,180,221	0
3	ADP	J	601	27/27	0.95	0.11	35,90,137,139	0
3	ADP	C	601	27/27	0.95	0.08	66,83,148,156	0
5	MG	I	603	1/1	0.95	0.17	81,81,81,81	0
3	ADP	M	601	27/27	0.95	0.10	25,77,196,198	0
6	K	J	604	1/1	0.95	0.11	122,122,122,122	0
3	ADP	I	601	27/27	0.96	0.09	47,72,117,158	0
4	BEF	I	602	4/4	0.96	0.09	59,65,81,85	0
5	MG	G	603	1/1	0.96	0.17	48,48,48,48	0
3	ADP	F	601	27/27	0.96	0.10	44,79,128,140	0
3	ADP	A	601	27/27	0.96	0.10	34,80,131,147	0
6	K	C	604	1/1	0.96	0.05	126,126,126,126	0
6	K	F	604	1/1	0.96	0.07	103,103,103,103	0
3	ADP	L	601	27/27	0.96	0.09	69,83,118,128	0
6	K	K	604	1/1	0.96	0.05	110,110,110,110	0
3	ADP	G	601	27/27	0.97	0.08	3,59,88,94	0

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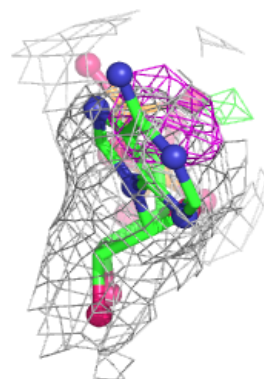
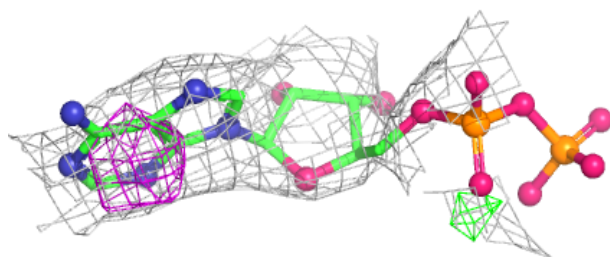
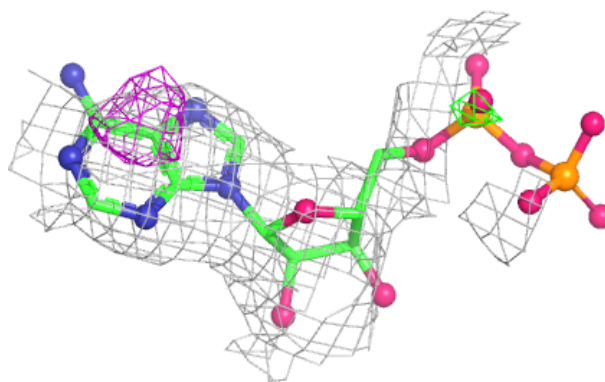
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BEF	L	602	4/4	0.97	0.06	43,102,141,206	0
5	MG	M	603	1/1	0.97	0.09	73,73,73,73	0
4	BEF	E	602	4/4	0.97	0.06	55,87,89,89	0
3	ADP	N	601	27/27	0.97	0.07	66,106,128,133	0
3	ADP	D	601	27/27	0.97	0.07	25,73,84,87	0
3	ADP	B	601	27/27	0.97	0.08	16,86,98,110	0
6	K	N	604	1/1	0.97	0.04	107,107,107,107	0
4	BEF	C	602	4/4	0.98	0.09	2,4,92,93	0
5	MG	K	603	1/1	0.98	0.11	50,50,50,50	0
3	ADP	E	601	27/27	0.98	0.07	36,84,99,115	0
5	MG	A	603	1/1	0.98	0.08	78,78,78,78	0
6	K	A	604	1/1	0.98	0.07	84,84,84,84	0
6	K	B	604	1/1	0.98	0.03	79,79,79,79	0
4	BEF	G	602	4/4	0.98	0.07	36,46,68,99	0
6	K	D	604	1/1	0.98	0.04	82,82,82,82	0
6	K	E	604	1/1	0.98	0.07	89,89,89,89	0
5	MG	D	603	1/1	0.98	0.08	44,44,44,44	0
6	K	H	604	1/1	0.98	0.03	110,110,110,110	0
5	MG	F	603	1/1	0.98	0.12	51,51,51,51	0
4	BEF	H	602	4/4	0.98	0.05	13,85,125,156	0
5	MG	H	603	1/1	0.98	0.07	103,103,103,103	0
6	K	G	604	1/1	0.99	0.04	67,67,67,67	0
5	MG	J	603	1/1	0.99	0.08	56,56,56,56	0
6	K	I	604	1/1	0.99	0.06	75,75,75,75	0
5	MG	N	603	1/1	0.99	0.04	71,71,71,71	0
5	MG	C	603	1/1	0.99	0.07	57,57,57,57	0
6	K	L	604	1/1	0.99	0.04	87,87,87,87	0
6	K	M	604	1/1	0.99	0.05	94,94,94,94	0
5	MG	E	603	1/1	0.99	0.07	45,45,45,45	0

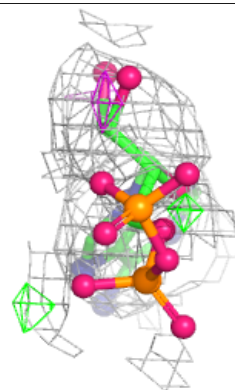
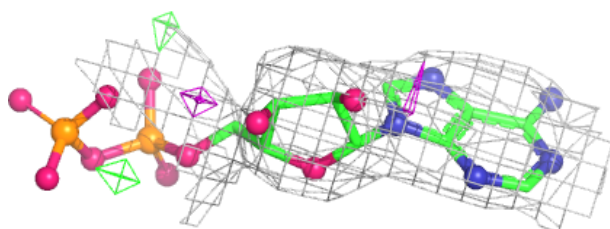
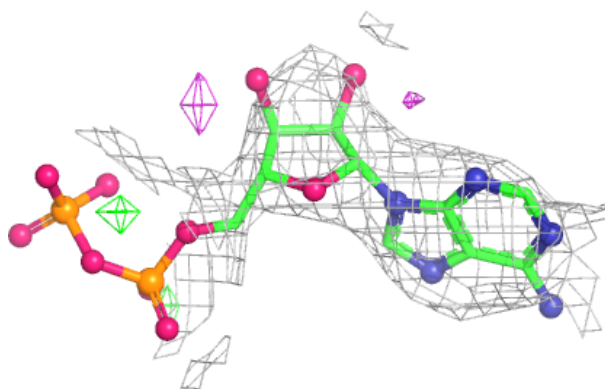
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP H 601:

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

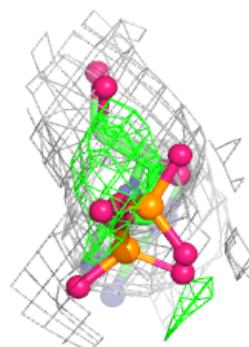
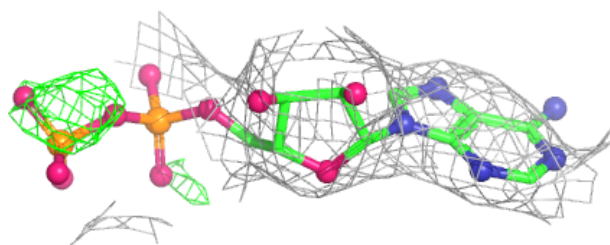
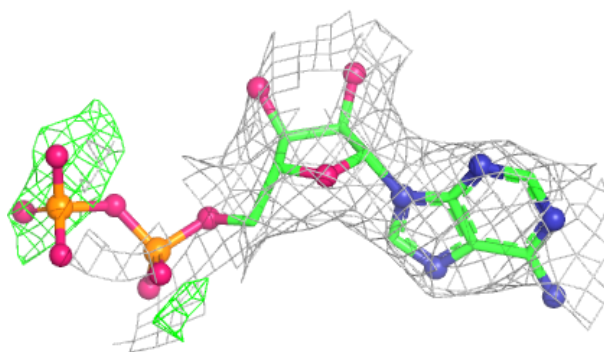
**Electron density around ADP K 601:**

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

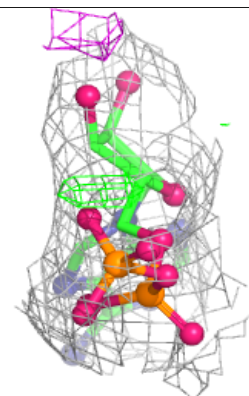
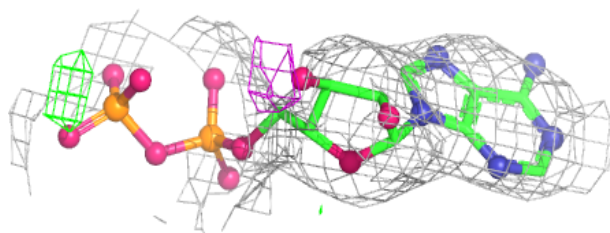
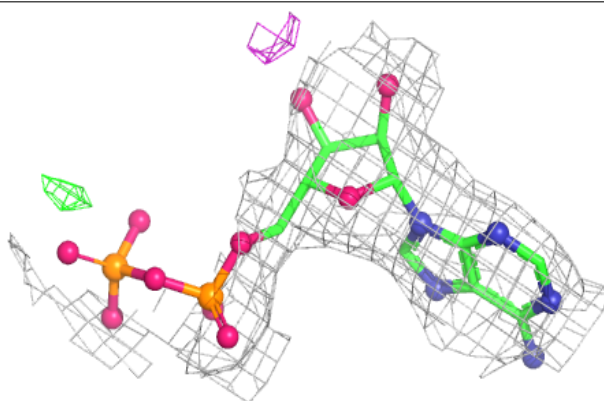


Electron density around ADP J 601:

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

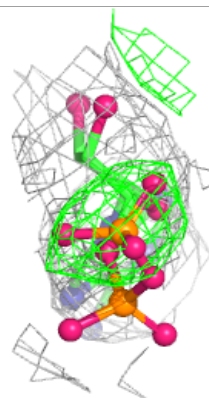
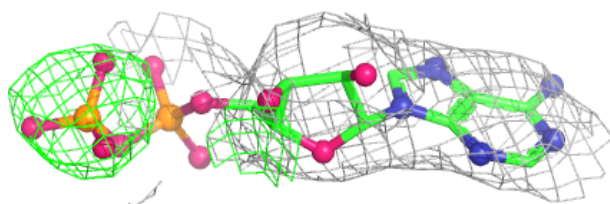
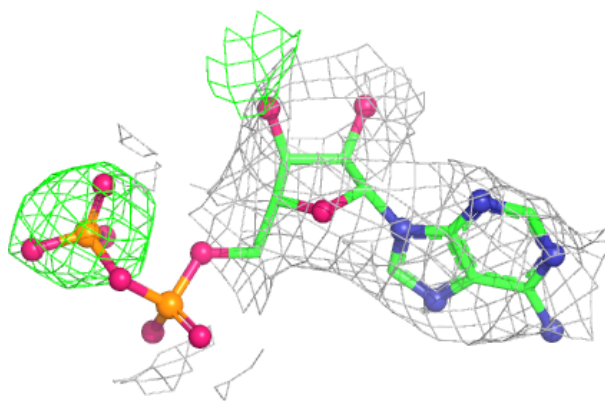
**Electron density around ADP C 601:**

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

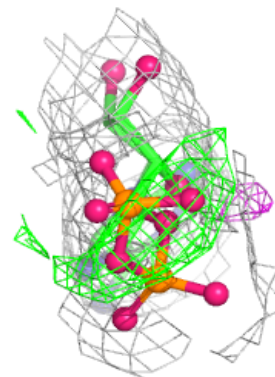
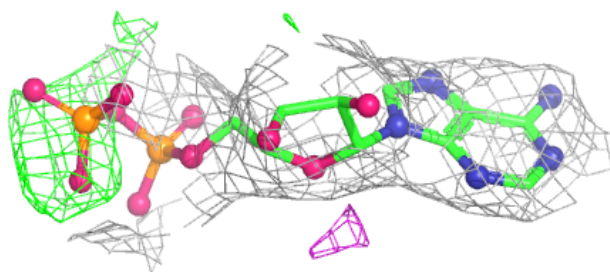
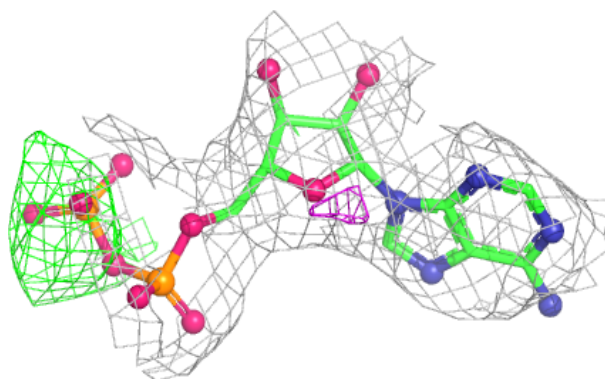


Electron density around ADP M 601:

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

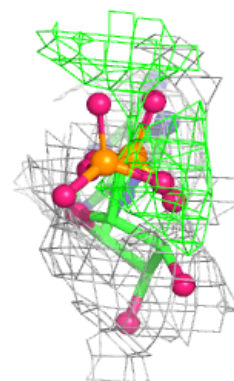
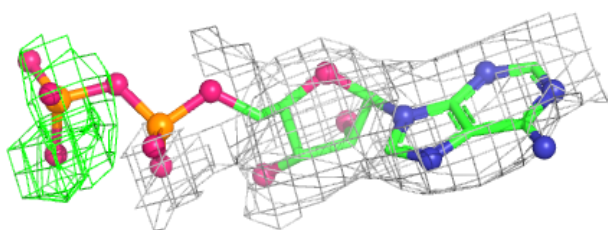
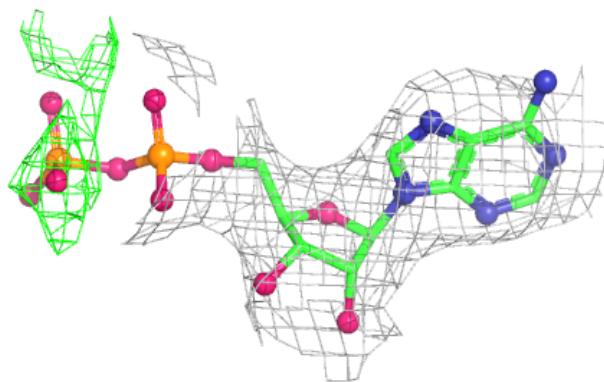
**Electron density around ADP I 601:**

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

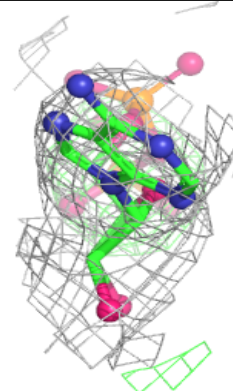
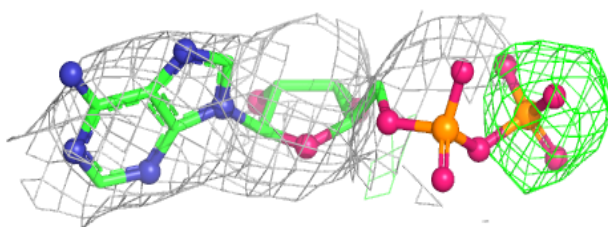
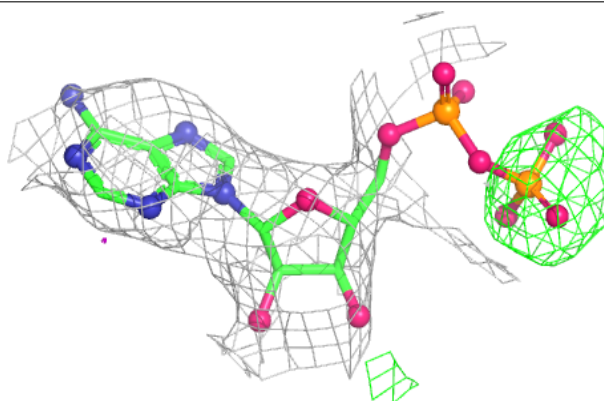


Electron density around ADP F 601:

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

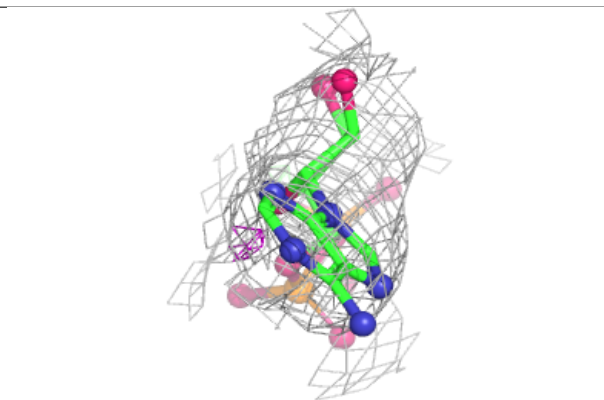
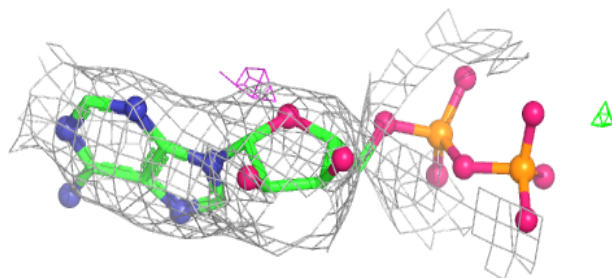
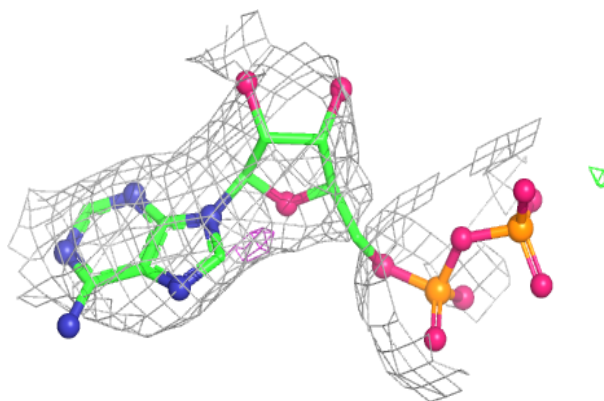
**Electron density around ADP A 601:**

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

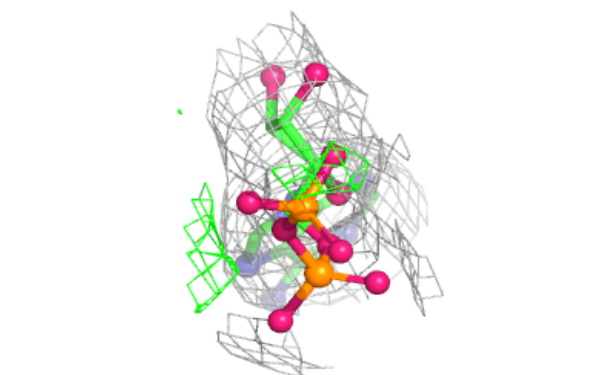
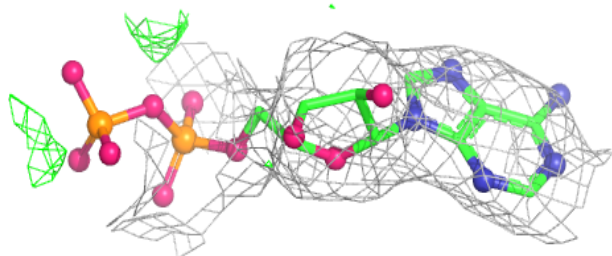
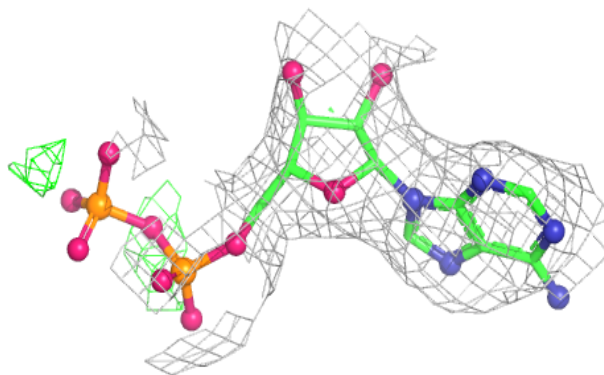


Electron density around ADP L 601:

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

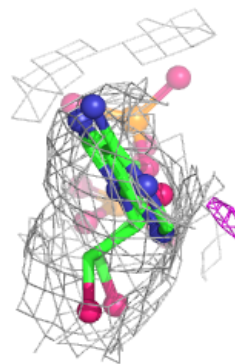
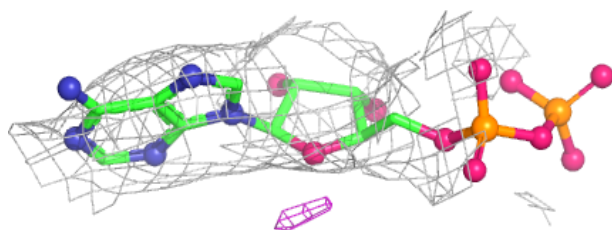
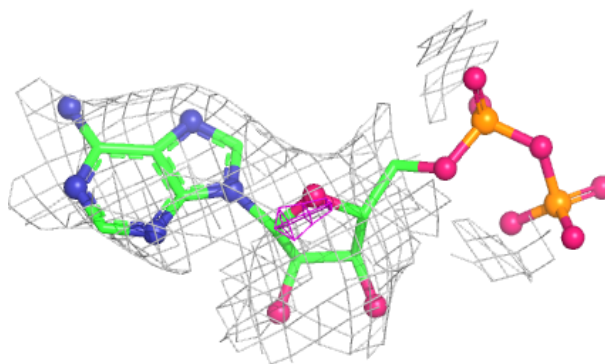
**Electron density around ADP G 601:**

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

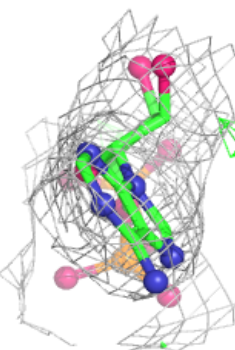
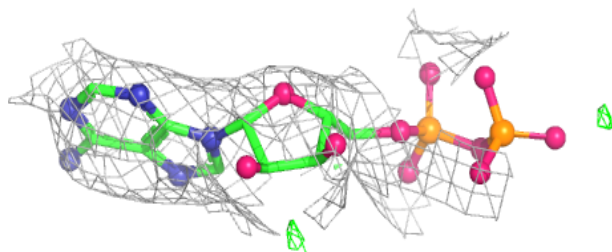
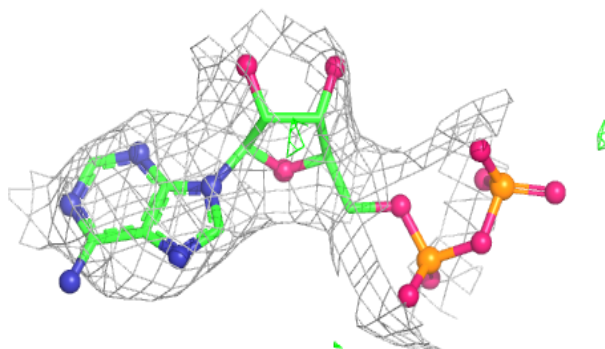


Electron density around ADP N 601:

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

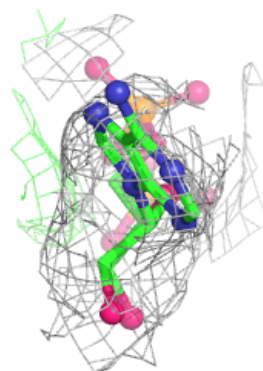
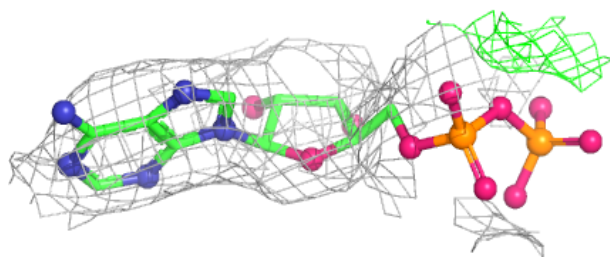
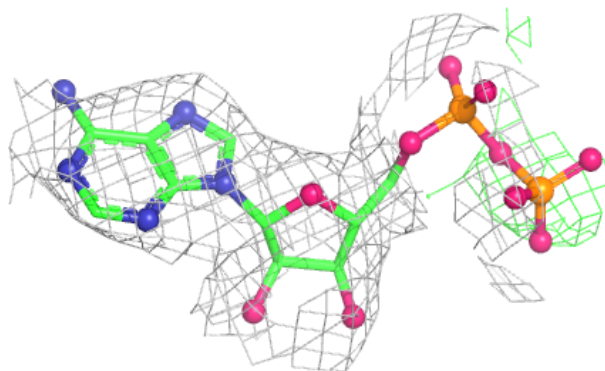
**Electron density around ADP D 601:**

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

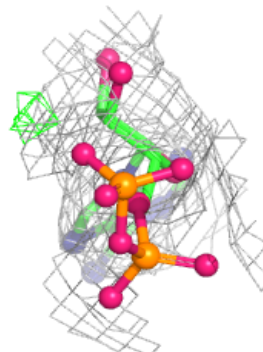
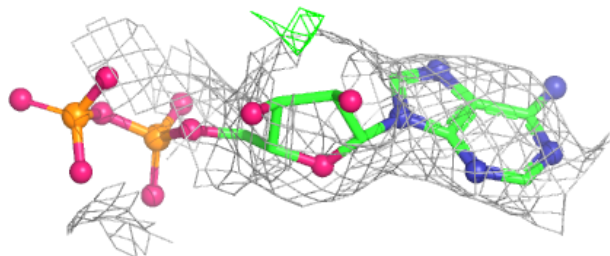
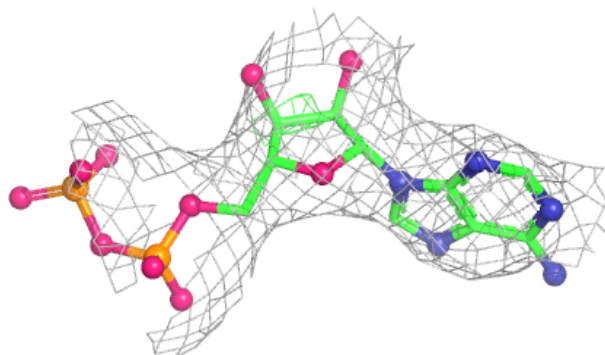


Electron density around ADP B 601:

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

**Electron density around ADP E 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.