



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:14 AM UTC

PDB ID : 1G3I / pdb_00001g3i
Title : CRYSTAL STRUCTURE OF THE HSLUV PROTEASE-CHAPERONE COMPLEX
Authors : Sousa, M.C.; Trame, C.B.; Tsuruta, H.; Wilbanks, S.M.; Reddy, V.S.; McKay, D.B.
Deposited on : 2000-10-24
Resolution : 3.41 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

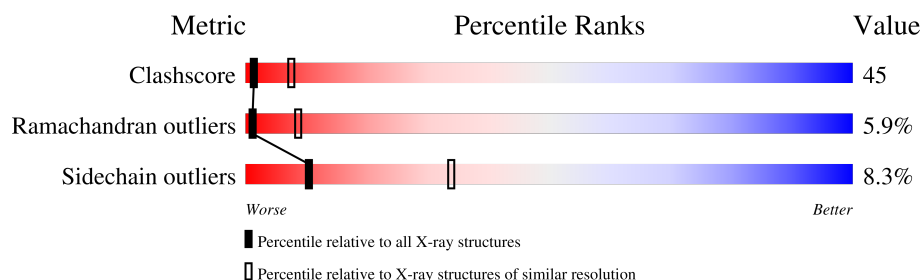
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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))
Clashscore	190562	1234 (3.48-3.36)
Ramachandran outliers	187476	1222 (3.48-3.36)
Sidechain outliers	187428	1222 (3.48-3.36)

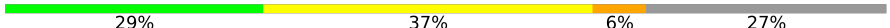
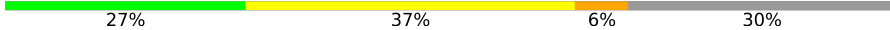
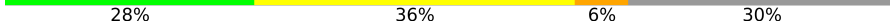
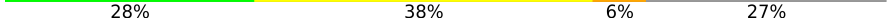
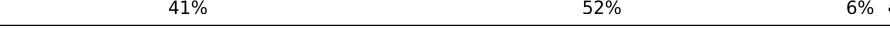
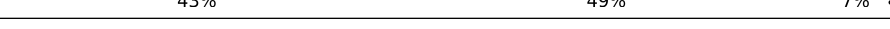
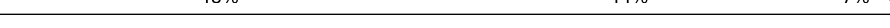
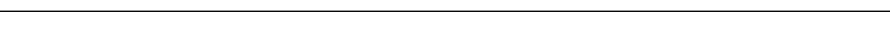
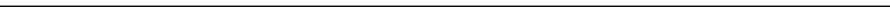
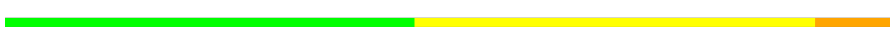
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	444	
1	B	444	
1	C	444	
1	D	444	
1	E	444	
1	F	444	
1	S	444	
1	T	444	

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Mol	Chain	Length	Quality of chain
1	U	444	
1	V	444	
1	W	444	
1	X	444	
2	G	174	
2	H	174	
2	I	174	
2	J	174	
2	K	174	
2	L	174	
2	M	174	
2	N	174	
2	O	174	
2	P	174	
2	Q	174	
2	R	174	

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
3	ATP	E	454	-	-	X	-
3	ATP	S	456	-	-	X	-
3	ATP	U	458	-	-	X	-
3	ATP	X	461	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 45528 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUB-UNIT HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2539	1588	454	487	10			
1	B	326	Total	C	N	O	S	0	0	0
			2539	1588	454	487	10			
1	C	319	Total	C	N	O	S	0	0	0
			2484	1554	446	474	10			
1	D	318	Total	C	N	O	S	0	0	0
			2476	1548	445	473	10			
1	E	317	Total	C	N	O	S	0	0	0
			2462	1540	443	469	10			
1	F	320	Total	C	N	O	S	0	0	0
			2495	1560	450	475	10			
1	S	317	Total	C	N	O	S	0	0	0
			2468	1543	444	471	10			
1	T	331	Total	C	N	O	S	0	0	0
			2570	1602	461	497	10			
1	U	322	Total	C	N	O	S	0	0	0
			2503	1562	449	482	10			
1	V	313	Total	C	N	O	S	0	0	0
			2432	1519	436	467	10			
1	W	312	Total	C	N	O	S	0	0	0
			2428	1516	437	465	10			
1	X	322	Total	C	N	O	S	0	0	0
			2500	1562	446	482	10			

- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

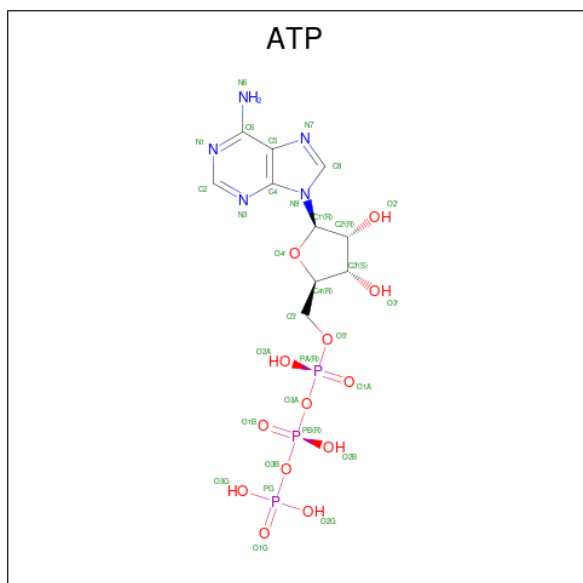
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	173	Total	C	N	O	S	0	0	0
			1280	803	227	246	4			
2	H	173	Total	C	N	O	S	0	0	0
			1280	802	227	247	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	173	Total	C	N	O	S	0	0	0
			1292	810	229	249	4			
2	J	173	Total	C	N	O	S	0	0	0
			1280	802	227	247	4			
2	K	173	Total	C	N	O	S	0	0	0
			1280	802	227	247	4			
2	L	173	Total	C	N	O	S	0	0	0
			1294	810	231	249	4			
2	M	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	N	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	O	173	Total	C	N	O	S	0	0	0
			1257	789	225	240	3			
2	P	173	Total	C	N	O	S	0	0	0
			1257	789	225	240	3			
2	Q	173	Total	C	N	O	S	0	0	0
			1261	791	226	241	3			
2	R	173	Total	C	N	O	S	0	0	0
			1257	789	225	240	3			

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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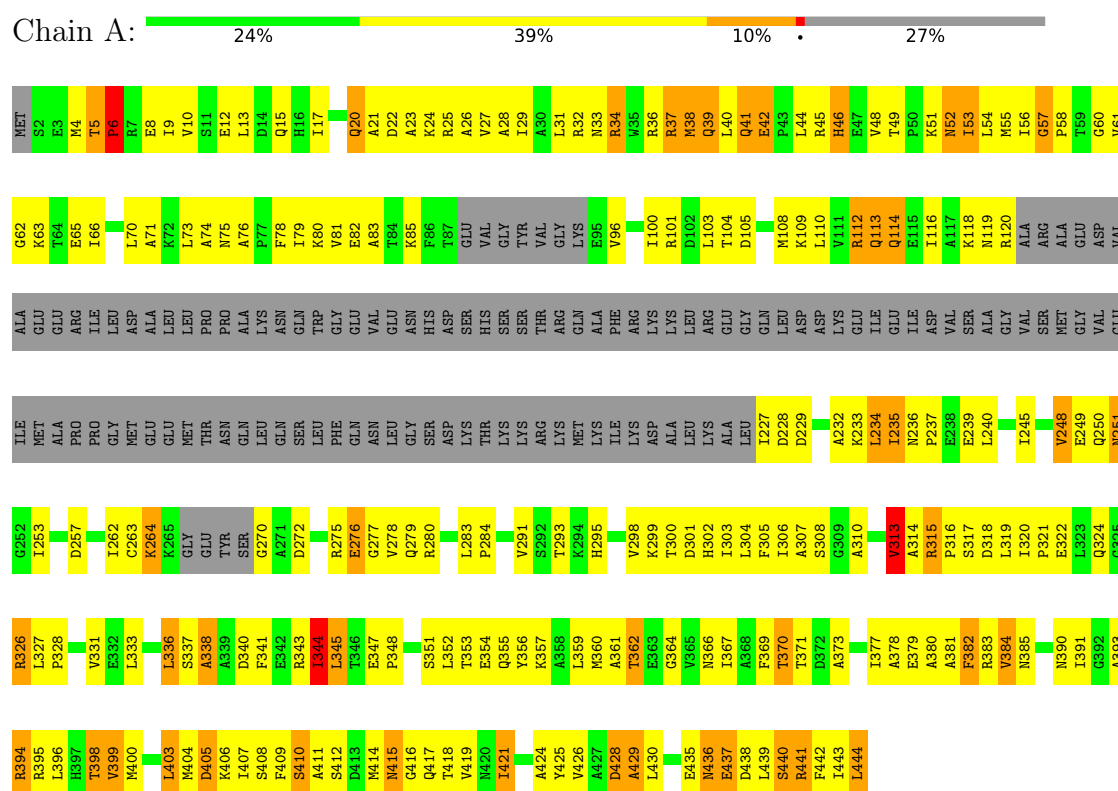
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	S	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	T	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	U	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	V	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	W	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	X	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

3 Residue-property plots

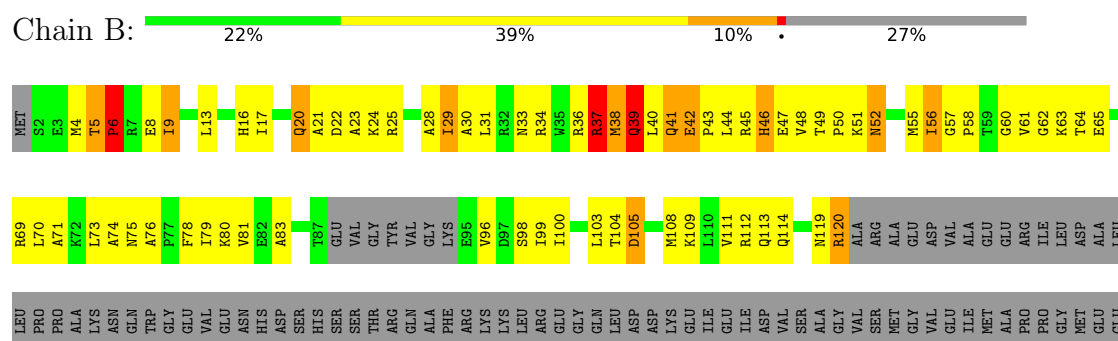
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

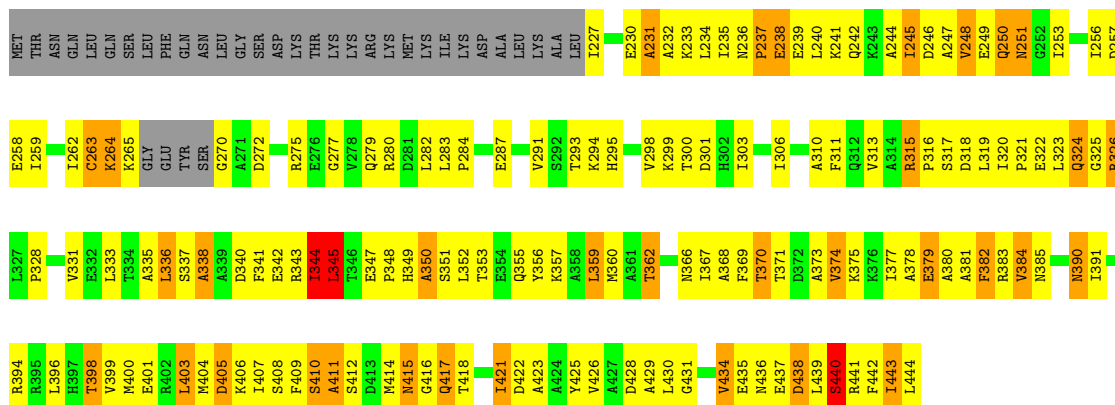
Note EDS was not executed.

• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU



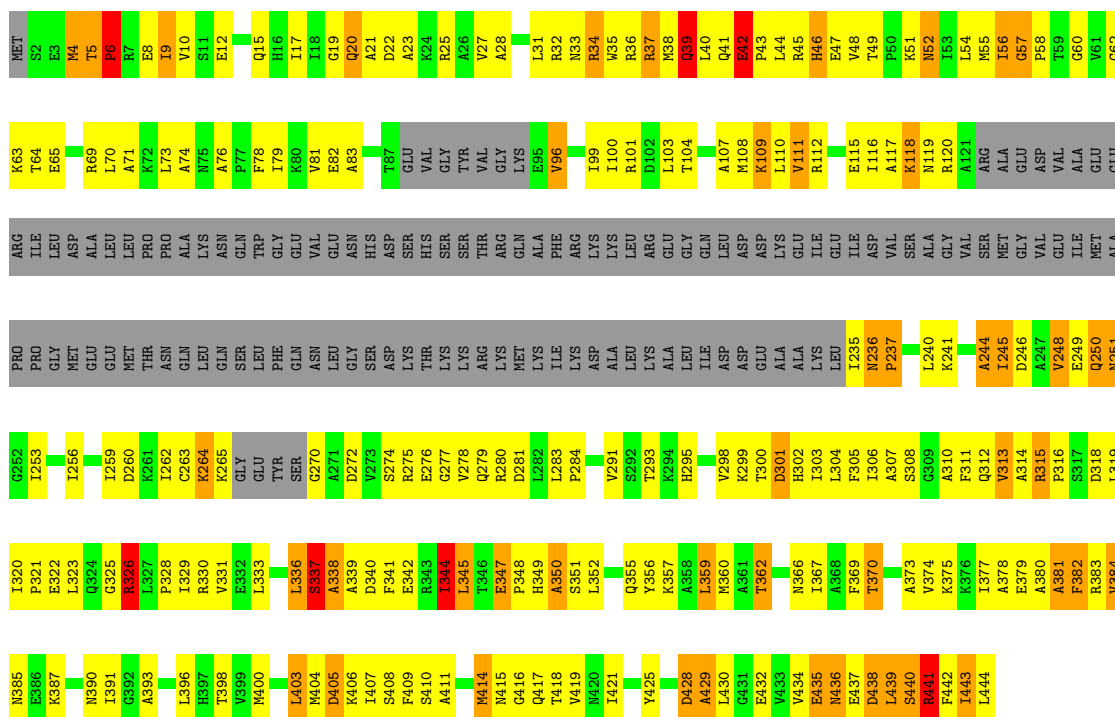
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU





• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

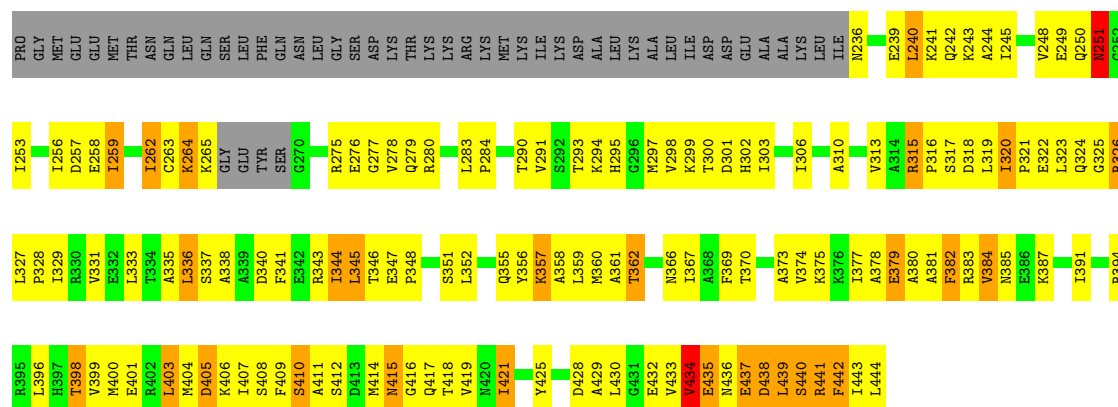
Chain C: 23% 37% 11% 28%



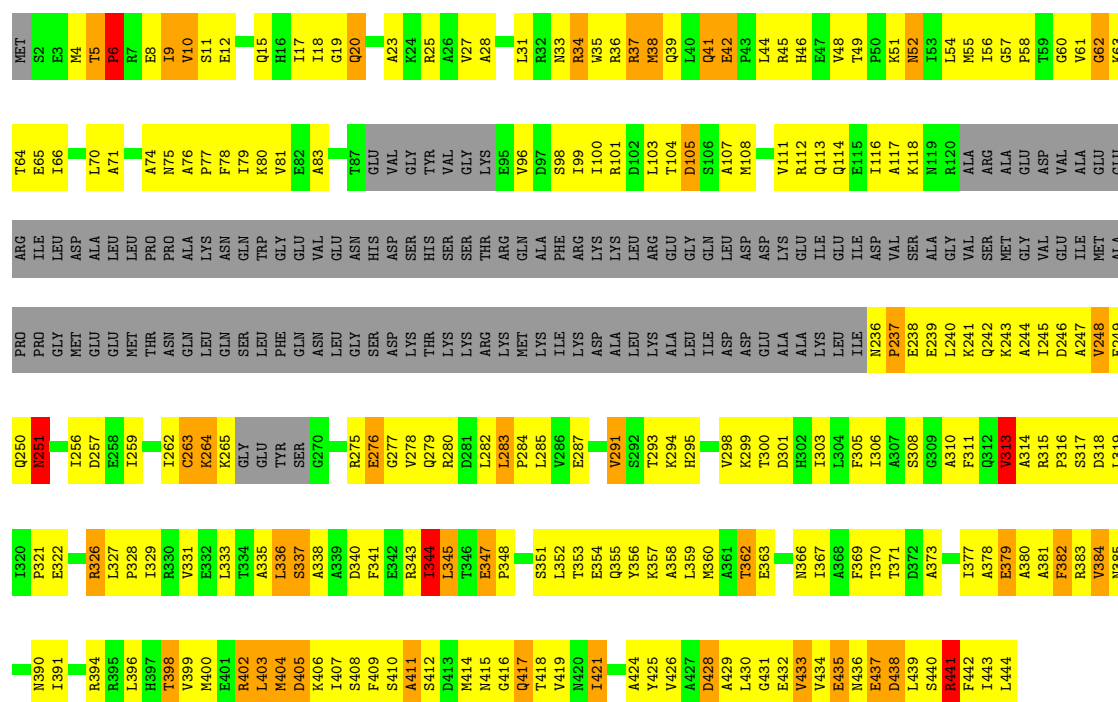
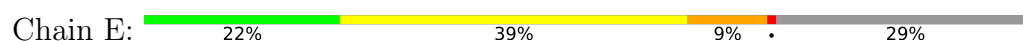
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

Chain D: 22% 40% 9% 28%

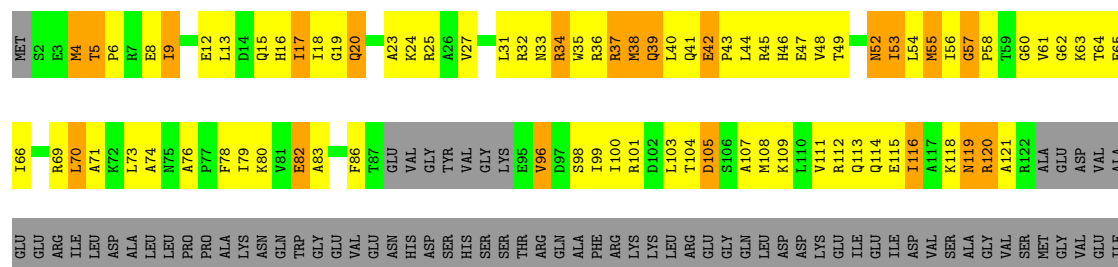
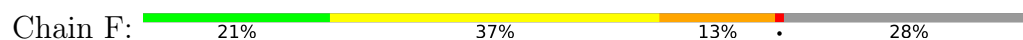


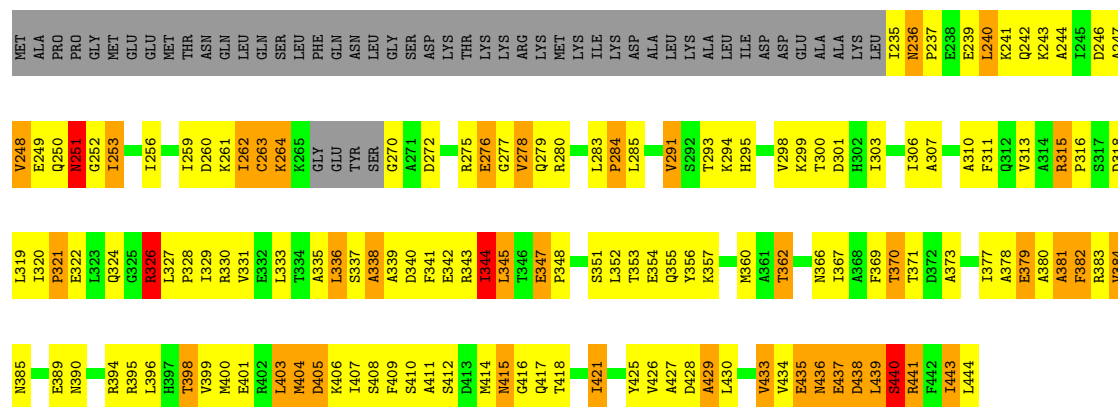


• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

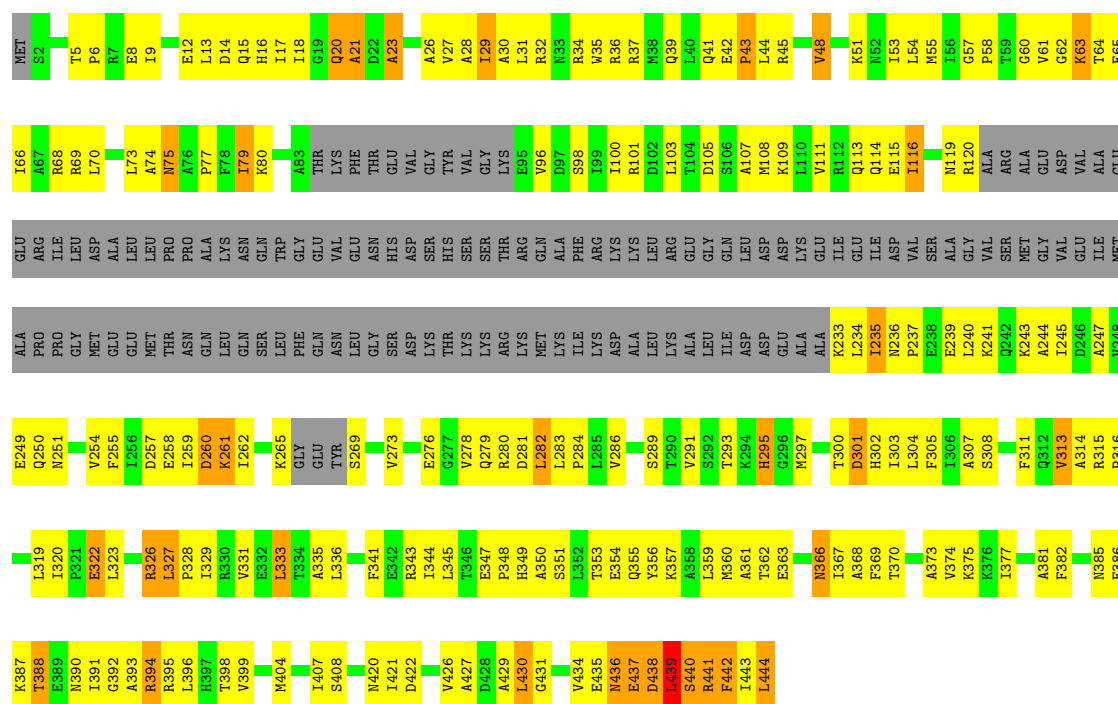
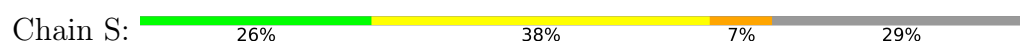


• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

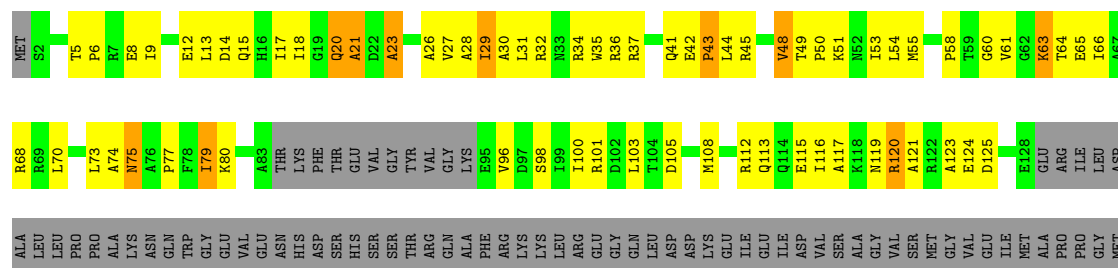


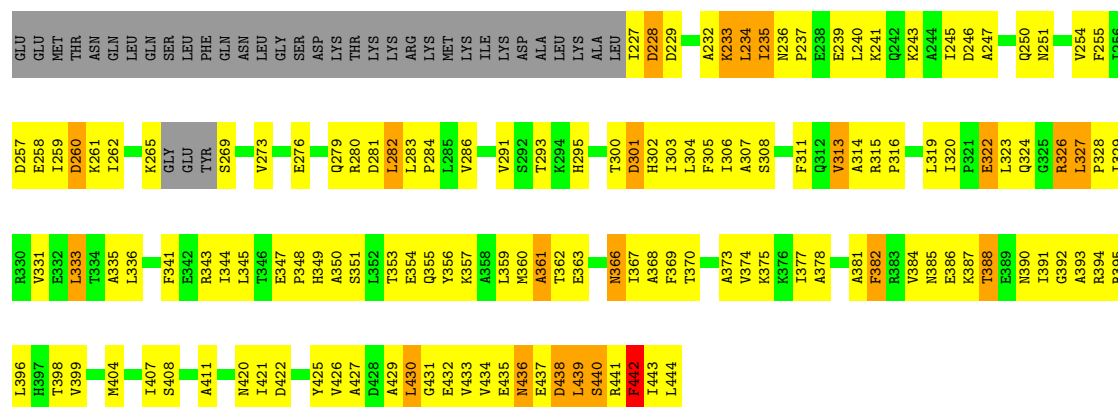


• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU



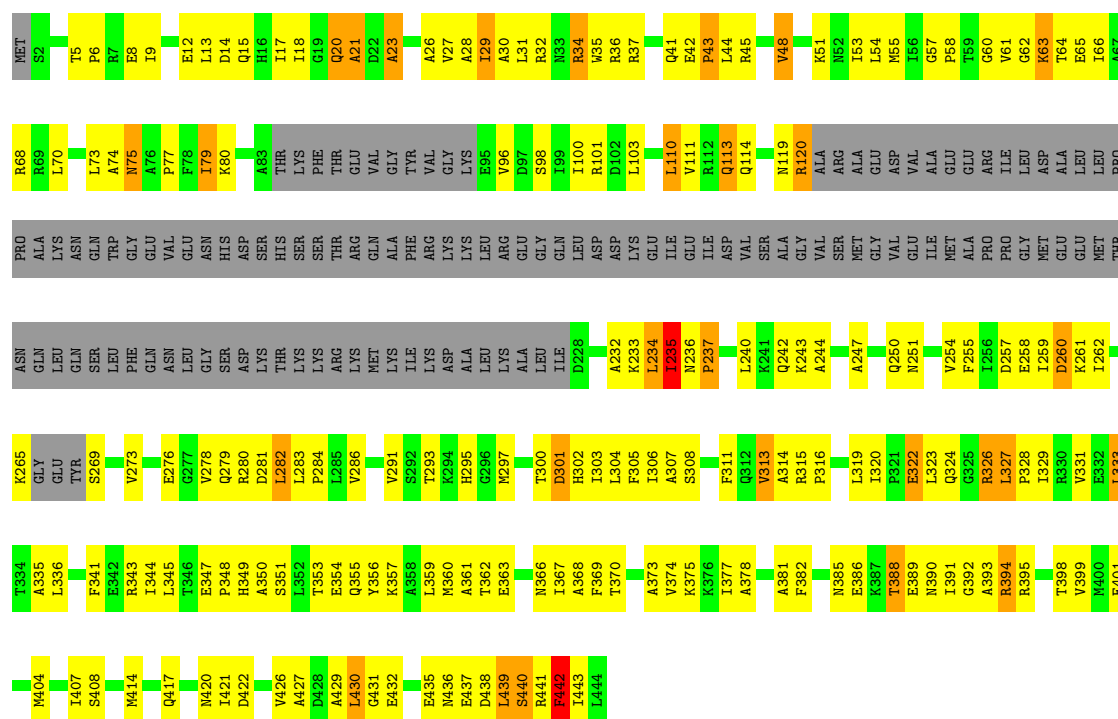
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU





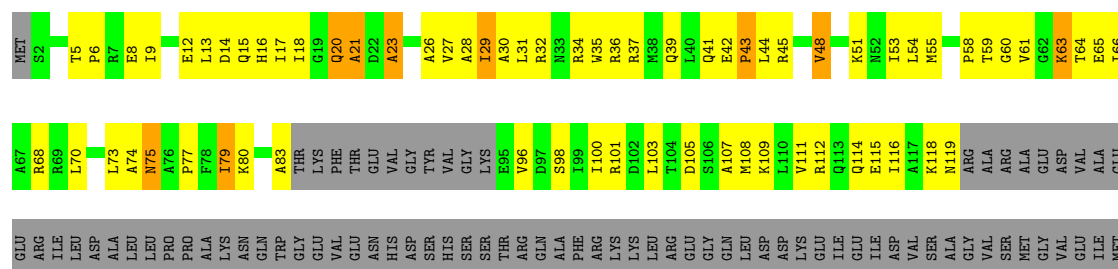
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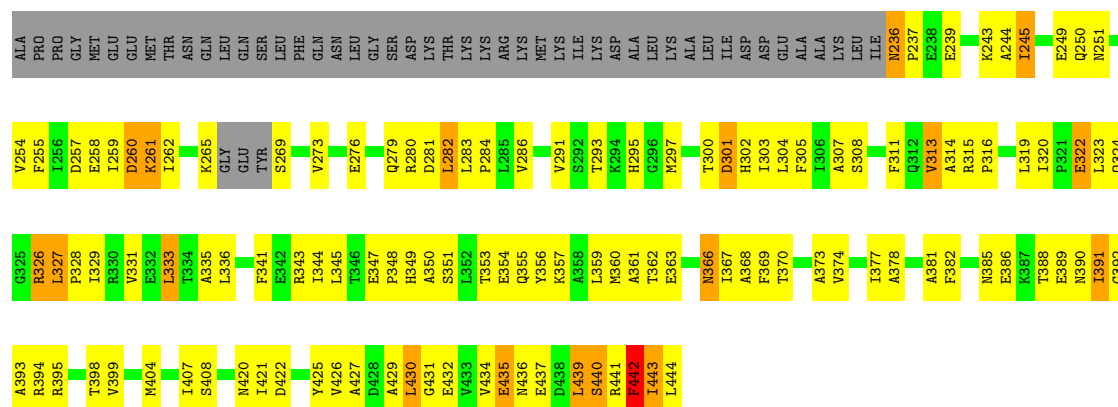
Chain U: 29% 37% 6% 27%



• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

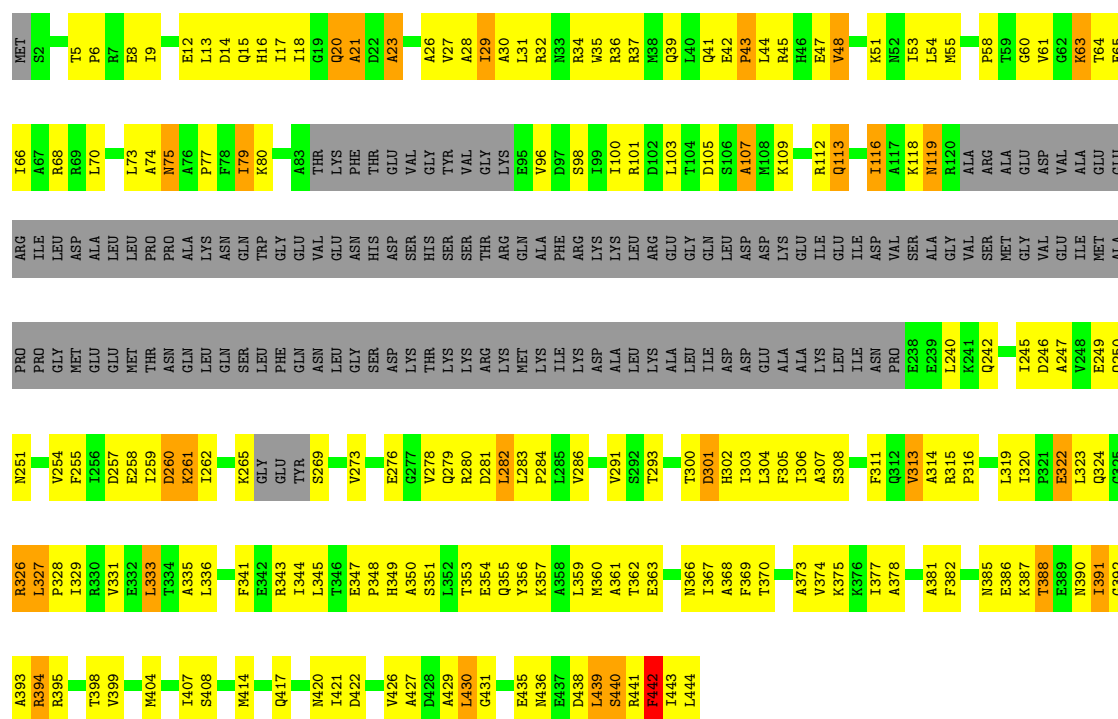
Chain V: 27% 37% 6% 30%





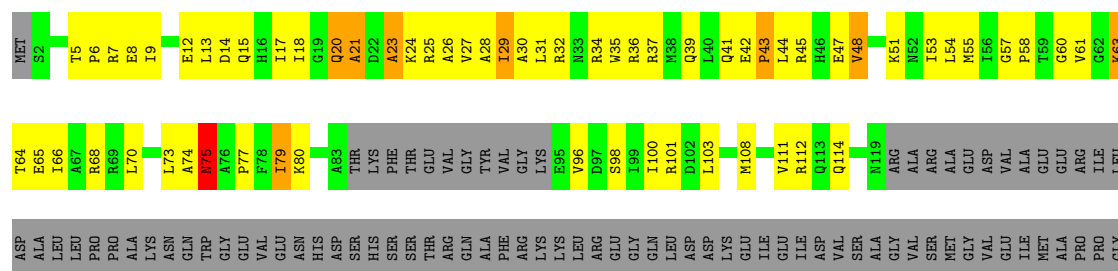
• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

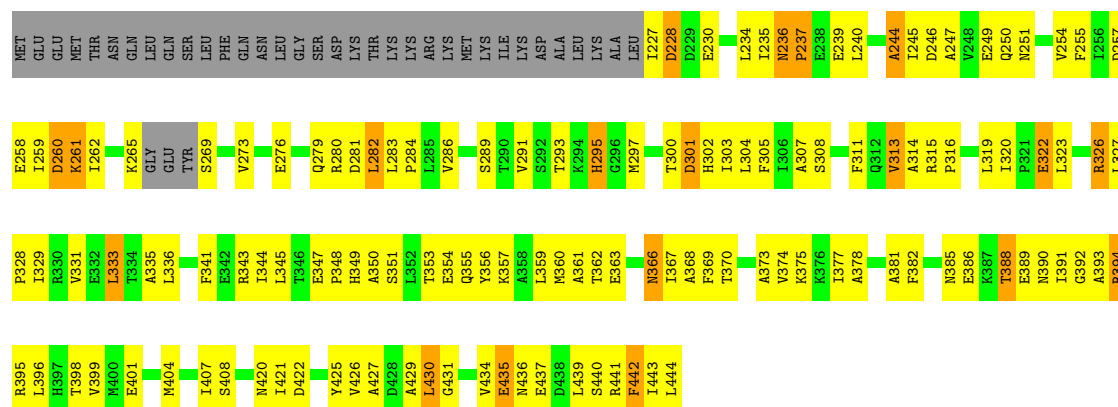
Chain W: 28% 36% 6% 30%



• Molecule 1: ATP-DEPENDENT HSLU PROTEASE ATP-BINDING SUBUNIT HSLU

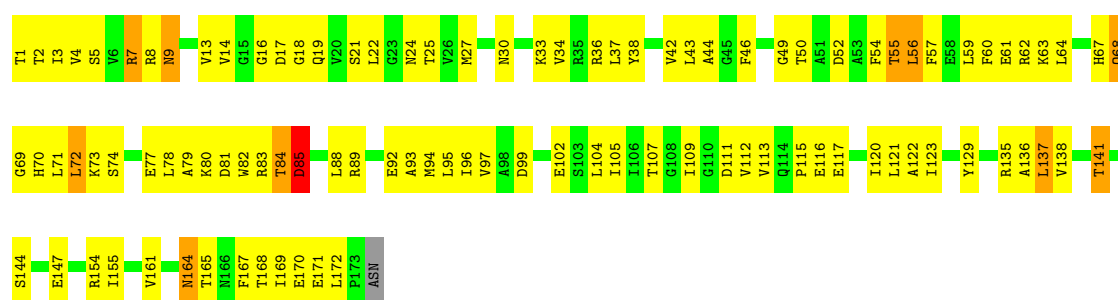
Chain X: 28% 38% 6% 27%





• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain G: 41% 52% 6% ..



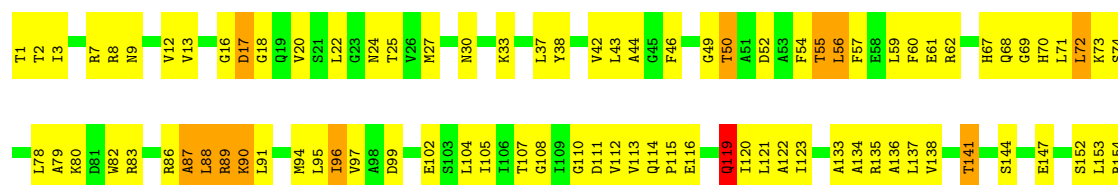
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain H: 41% 48% 9% ..



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

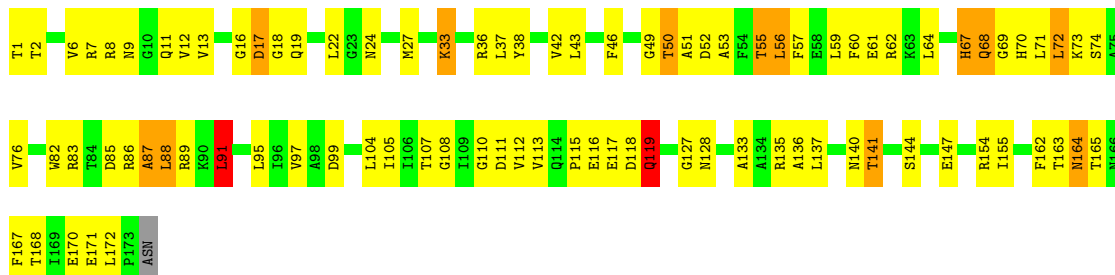
Chain I: 43% 49% 7% ..





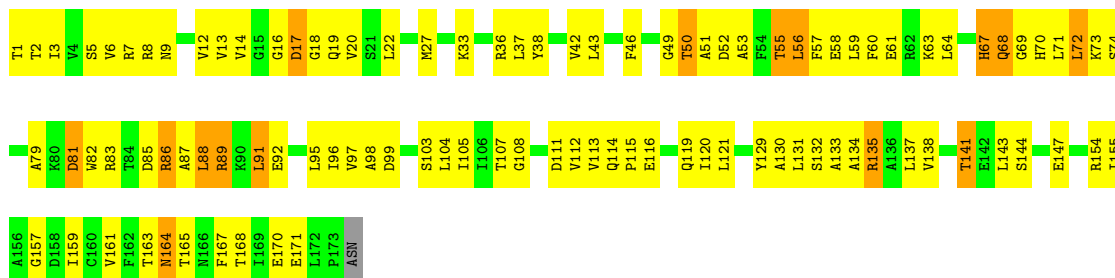
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain J: 48% 44% 7% ..



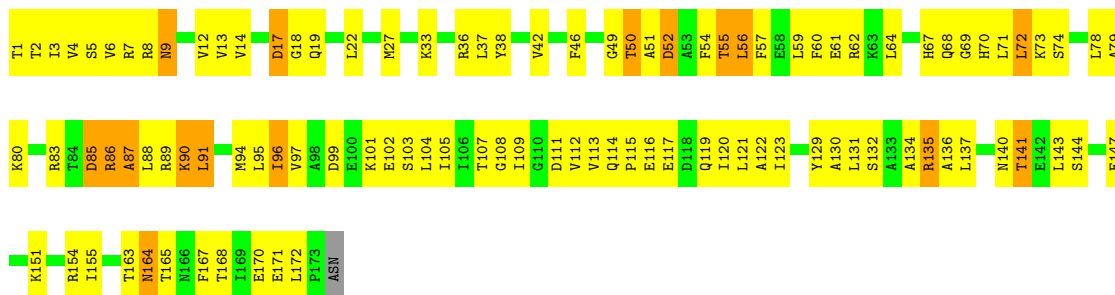
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain K: 41% 50% 9% .



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

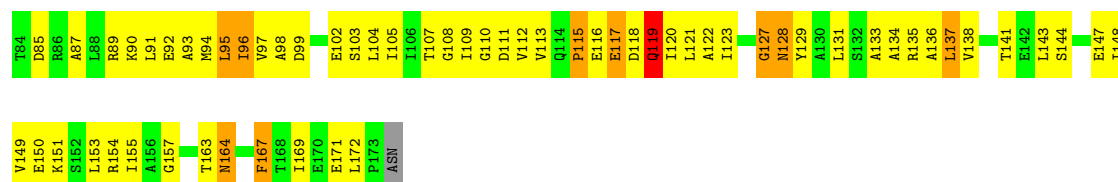
Chain L: 40% 51% 9% .



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

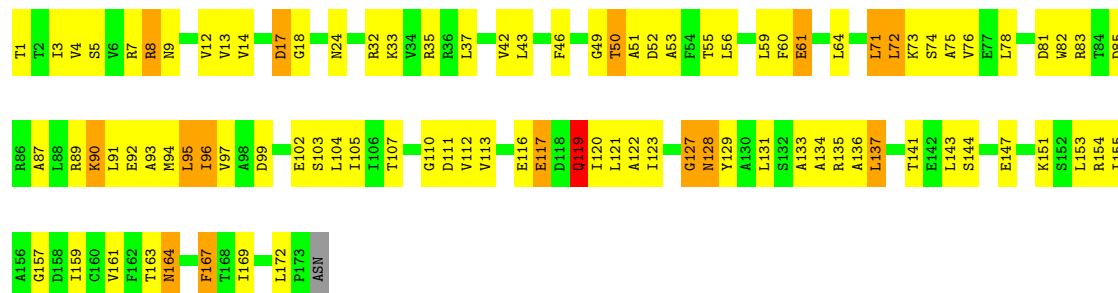
Chain M: 40% 51% 9% ..





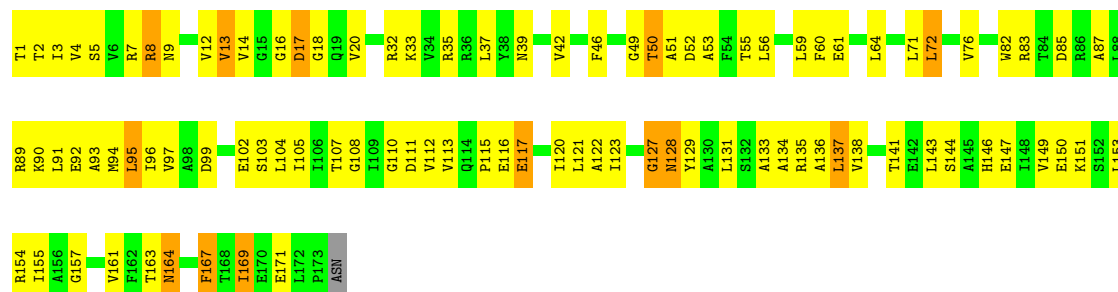
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain N: 45% 45% 9% ..



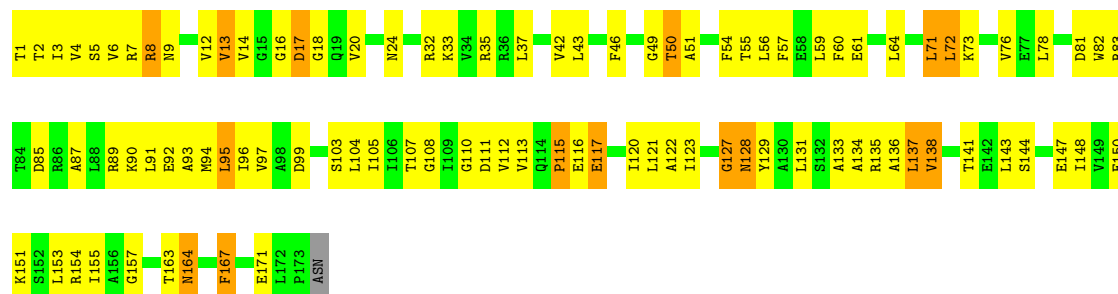
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain O: 45% 47% 7% .



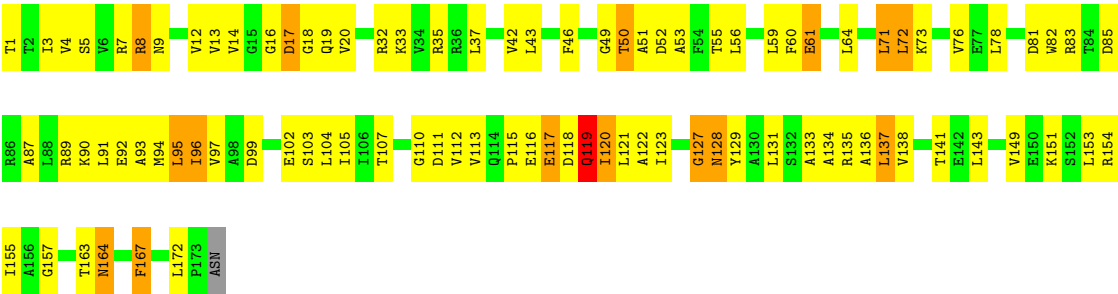
• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain P: 44% 47% 9% .



• Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain Q: 46% 44% 9% ..



● Molecule 2: ATP-DEPENDENT PROTEASE HSLV



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	209.22Å 220.58Å 241.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.08 – 3.41	Depositor
% Data completeness (in resolution range)	(Not available) (30.08-3.41)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.240 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	45528	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP

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	0.85	2/2566 (0.1%)	1.20	20/3458 (0.6%)
1	B	0.86	0/2566	1.21	24/3458 (0.7%)
1	C	0.77	1/2511 (0.0%)	1.19	31/3384 (0.9%)
1	D	0.85	1/2503 (0.0%)	1.24	26/3373 (0.8%)
1	E	0.89	1/2489 (0.0%)	1.27	28/3354 (0.8%)
1	F	0.86	3/2522 (0.1%)	1.23	29/3398 (0.9%)
1	S	0.38	0/2494	0.95	12/3360 (0.4%)
1	T	0.38	0/2596	0.97	13/3499 (0.4%)
1	U	0.37	0/2529	0.96	16/3408 (0.5%)
1	V	0.38	0/2458	0.96	13/3313 (0.4%)
1	W	0.36	0/2453	0.95	9/3304 (0.3%)
1	X	0.38	0/2526	0.93	10/3405 (0.3%)
2	G	0.73	0/1294	1.07	6/1753 (0.3%)
2	H	0.74	2/1294 (0.2%)	1.12	7/1754 (0.4%)
2	I	0.67	0/1306	1.04	6/1767 (0.3%)
2	J	0.67	0/1294	1.05	5/1754 (0.3%)
2	K	0.69	0/1294	1.06	3/1754 (0.2%)
2	L	0.73	0/1308	1.11	7/1770 (0.4%)
2	M	0.51	0/1275	0.99	6/1732 (0.3%)
2	N	0.48	0/1275	0.97	5/1732 (0.3%)
2	O	0.45	0/1271	0.92	3/1727 (0.2%)
2	P	0.45	0/1271	0.92	2/1727 (0.1%)
2	Q	0.61	3/1275 (0.2%)	0.99	5/1732 (0.3%)
2	R	0.50	0/1271	0.94	2/1727 (0.1%)
All	All	0.64	13/45641 (0.0%)	1.07	288/61643 (0.5%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	120	ILE	N-CA	-7.60	1.37	1.46
2	Q	119	GLN	CA-C	-7.30	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	53	ILE	CA-CB	-7.13	1.45	1.54
1	A	313	VAL	CA-CB	-6.84	1.47	1.55
2	Q	119	GLN	C-N	-6.63	1.24	1.33
1	E	313	VAL	CA-CB	-6.23	1.48	1.55
1	C	414	MET	SD-CE	5.77	1.94	1.79
1	A	399	VAL	CA-CB	-5.65	1.47	1.54
1	D	21	ALA	CA-CB	-5.60	1.44	1.53
2	H	118	ASP	N-CA	5.38	1.53	1.46
1	F	55	MET	CA-C	-5.35	1.46	1.52
2	H	117	GLU	C-N	5.23	1.41	1.34
1	F	307	ALA	CA-CB	-5.13	1.45	1.53

All (288) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ARG	N-CA-C	-10.51	97.16	110.19
1	W	116	ILE	N-CA-C	-10.49	101.99	113.43
2	M	119	GLN	OE1-CD-NE2	-10.24	112.36	122.60
2	Q	119	GLN	OE1-CD-NE2	-10.11	112.49	122.60
1	E	37	ARG	N-CA-C	-9.89	98.25	110.41
2	J	119	GLN	OE1-CD-NE2	-9.82	112.78	122.60
2	I	119	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	37	ARG	N-CA-C	-9.77	98.07	110.19
2	L	119	GLN	OE1-CD-NE2	-9.76	112.84	122.60
2	N	119	GLN	OE1-CD-NE2	-9.76	112.84	122.60
2	K	119	GLN	OE1-CD-NE2	-9.74	112.86	122.60
2	H	119	GLN	OE1-CD-NE2	-9.57	113.03	122.60
1	C	39	GLN	N-CA-C	-8.71	101.40	114.64
1	D	327	LEU	CA-C-N	8.43	130.38	119.84
1	D	327	LEU	C-N-CA	8.43	130.38	119.84
1	S	116	ILE	N-CA-C	-8.41	105.29	113.53
1	B	39	GLN	N-CA-C	-8.39	101.74	114.16
1	D	37	ARG	N-CA-C	-8.32	100.17	110.41
1	U	234	LEU	N-CA-C	-8.23	101.57	111.69
1	T	234	LEU	N-CA-C	-8.17	102.33	111.07
1	C	435	GLU	N-CA-C	8.11	115.43	108.78
1	V	114	GLN	N-CA-C	-8.07	103.57	113.50
1	S	63	LYS	N-CA-C	-8.03	103.95	114.31
1	T	241	LYS	N-CA-C	-7.86	103.75	112.72
1	F	57	GLY	CA-C-N	7.73	129.25	120.98
1	F	57	GLY	C-N-CA	7.73	129.25	120.98
1	V	63	LYS	N-CA-C	-7.73	104.34	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	67	HIS	N-CA-C	7.70	119.68	110.44
1	S	243	LYS	N-CA-C	-7.70	104.49	114.04
1	C	37	ARG	N-CA-C	-7.68	100.42	110.33
1	D	412	SER	N-CA-C	7.68	119.29	111.07
1	W	63	LYS	N-CA-C	-7.68	104.40	114.31
1	D	434	VAL	N-CA-C	7.68	121.25	108.81
1	A	327	LEU	CA-C-N	7.63	129.38	119.84
1	A	327	LEU	C-N-CA	7.63	129.38	119.84
1	F	37	ARG	N-CA-C	-7.62	100.50	110.33
1	U	63	LYS	N-CA-C	-7.53	104.60	114.31
1	T	63	LYS	N-CA-C	-7.48	104.66	114.31
1	X	63	LYS	N-CA-C	-7.38	104.78	114.31
1	T	228	ASP	N-CA-C	-7.35	104.12	113.23
1	E	344	ILE	N-CA-C	-7.28	101.41	111.89
1	W	107	ALA	N-CA-C	-7.22	105.08	114.04
1	C	49	THR	CA-C-N	7.21	128.86	119.84
1	C	49	THR	C-N-CA	7.21	128.86	119.84
1	C	338	ALA	N-CA-C	-7.13	102.32	111.02
2	M	119	GLN	CG-CD-NE2	7.03	126.94	116.40
1	F	327	LEU	CA-C-N	6.92	128.49	119.84
1	F	327	LEU	C-N-CA	6.92	128.49	119.84
2	N	85	ASP	N-CA-C	-6.91	105.13	113.97
1	E	315	ARG	CA-C-N	-6.90	111.87	119.19
1	E	315	ARG	C-N-CA	-6.90	111.87	119.19
1	E	62	GLY	N-CA-C	6.87	122.65	114.48
1	E	49	THR	CA-C-N	6.85	128.40	119.84
1	E	49	THR	C-N-CA	6.85	128.40	119.84
1	F	49	THR	CA-C-N	6.84	126.87	119.89
1	F	49	THR	C-N-CA	6.84	126.87	119.89
2	H	119	GLN	CG-CD-NE2	6.84	126.66	116.40
2	P	85	ASP	N-CA-C	-6.78	105.29	113.97
2	G	85	ASP	N-CA-C	-6.76	103.99	111.36
2	G	117	GLU	N-CA-C	6.75	119.50	111.33
2	M	85	ASP	N-CA-C	-6.73	105.36	113.97
1	B	62	GLY	N-CA-C	6.66	122.41	114.48
1	C	329	ILE	N-CA-C	6.65	117.03	108.12
2	Q	119	GLN	CG-CD-NE2	6.65	126.37	116.40
2	G	67	HIS	N-CA-C	6.65	118.42	110.44
2	I	119	GLN	CG-CD-NE2	6.64	126.37	116.40
2	L	119	GLN	CG-CD-NE2	6.64	126.36	116.40
2	N	119	GLN	CG-CD-NE2	6.64	126.35	116.40
2	J	119	GLN	CG-CD-NE2	6.63	126.35	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	119	GLN	CG-CD-NE2	6.63	126.35	116.40
1	B	335	ALA	N-CA-C	-6.61	101.37	110.35
1	B	344	ILE	N-CA-C	-6.61	102.38	111.89
2	Q	85	ASP	N-CA-C	-6.59	105.53	113.97
2	R	85	ASP	N-CA-C	-6.59	105.54	113.97
2	J	116	GLU	N-CA-C	-6.57	101.06	110.59
2	O	85	ASP	N-CA-C	-6.57	105.56	113.97
2	J	67	HIS	N-CA-C	6.53	118.27	110.44
1	C	57	GLY	CA-C-N	6.51	127.98	119.84
1	C	57	GLY	C-N-CA	6.51	127.98	119.84
1	T	123	ALA	N-CA-C	-6.34	104.00	112.94
1	W	113	GLN	N-CA-C	-6.32	105.33	114.12
1	X	228	ASP	N-CA-C	-6.31	105.23	113.12
1	E	431	GLY	N-CA-C	6.30	128.10	113.18
1	D	251	ASN	N-CA-C	6.28	117.97	110.44
1	D	315	ARG	N-CA-C	-6.26	102.25	110.39
1	F	53	ILE	N-CA-C	6.26	117.61	108.53
1	T	327	LEU	CA-C-N	6.25	125.93	119.56
1	T	327	LEU	C-N-CA	6.25	125.93	119.56
1	C	326	ARG	N-CA-C	-6.20	105.36	113.17
1	D	53	ILE	N-CA-C	6.20	117.41	108.48
1	S	381	ALA	N-CA-C	-6.20	106.04	113.97
1	U	327	LEU	CA-C-N	6.18	125.87	119.56
1	U	327	LEU	C-N-CA	6.18	125.87	119.56
1	D	236	ASN	CA-C-N	6.18	125.59	118.85
1	D	236	ASN	C-N-CA	6.18	125.59	118.85
1	E	10	VAL	N-CA-C	-6.17	104.50	110.42
2	H	67	HIS	N-CA-C	6.12	117.93	109.54
1	A	49	THR	CA-C-N	6.10	127.46	119.84
1	A	49	THR	C-N-CA	6.10	127.46	119.84
1	B	338	ALA	N-CA-C	-6.10	103.58	111.02
1	V	381	ALA	N-CA-C	-6.10	106.17	113.97
1	A	82	GLU	N-CA-C	-6.09	101.91	110.50
1	B	315	ARG	N-CA-C	-6.08	102.21	110.36
1	C	315	ARG	N-CA-C	-6.08	102.22	110.36
1	B	326	ARG	N-CA-C	-6.03	105.57	113.17
1	B	443	ILE	N-CA-C	6.03	118.13	108.85
1	F	263	CYS	N-CA-C	-6.03	101.07	110.17
1	D	436	ASN	N-CA-C	-6.01	101.46	110.06
1	E	246	ASP	N-CA-C	-6.01	104.64	111.07
1	V	243	LYS	N-CA-C	-6.00	105.19	113.18
2	K	67	HIS	N-CA-C	6.00	117.64	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	38	MET	N-CA-C	-6.00	105.91	113.23
1	E	42	GLU	N-CA-C	5.99	123.06	109.81
1	C	244	ALA	N-CA-C	-5.99	104.10	111.40
1	W	381	ALA	N-CA-C	-5.97	106.33	113.97
1	F	42	GLU	N-CA-C	5.96	122.97	109.81
1	D	259	ILE	N-CA-C	-5.95	104.23	112.50
1	V	116	ILE	N-CA-C	-5.94	106.53	112.17
1	B	38	MET	N-CA-C	-5.93	105.63	112.86
1	C	315	ARG	CA-C-N	-5.92	113.58	119.56
1	C	315	ARG	C-N-CA	-5.92	113.58	119.56
1	B	238	GLU	N-CA-C	-5.91	106.40	113.97
1	E	248	VAL	CB-CA-C	-5.91	104.42	111.81
1	E	347	GLU	CA-C-N	5.91	125.93	119.90
1	E	347	GLU	C-N-CA	5.91	125.93	119.90
1	C	302	HIS	N-CA-C	5.90	120.49	112.88
1	E	329	ILE	N-CA-C	5.87	115.99	108.12
1	X	381	ALA	N-CA-C	-5.87	106.45	113.97
1	T	381	ALA	N-CA-C	-5.87	106.46	113.97
1	U	381	ALA	N-CA-C	-5.82	106.52	113.97
1	A	315	ARG	N-CA-C	-5.81	102.78	110.40
1	B	49	THR	CA-C-N	5.80	127.09	119.84
1	B	49	THR	C-N-CA	5.80	127.09	119.84
1	E	118	LYS	N-CA-C	-5.79	104.96	111.28
1	F	326	ARG	N-CA-C	-5.79	105.80	112.92
1	U	110	LEU	N-CA-C	-5.79	108.02	114.62
1	V	236	ASN	CA-C-N	5.77	127.05	119.84
1	V	236	ASN	C-N-CA	5.77	127.05	119.84
2	G	116	GLU	N-CA-C	-5.76	100.94	109.86
1	A	57	GLY	CA-C-N	5.74	127.01	119.84
1	A	57	GLY	C-N-CA	5.74	127.01	119.84
1	D	49	THR	CA-C-N	5.74	127.01	119.84
1	D	49	THR	C-N-CA	5.74	127.01	119.84
1	F	435	GLU	N-CA-C	5.72	117.93	108.49
1	X	382	PHE	N-CA-C	-5.71	104.51	112.45
1	C	443	ILE	N-CA-C	5.68	117.92	109.17
1	U	235	ILE	N-CA-C	5.68	121.15	109.34
1	E	327	LEU	CA-C-N	5.66	126.92	119.84
1	E	327	LEU	C-N-CA	5.66	126.92	119.84
1	T	276	GLU	N-CA-C	-5.66	106.42	113.38
1	C	347	GLU	CA-C-N	5.66	126.92	119.84
1	C	347	GLU	C-N-CA	5.66	126.92	119.84
1	B	9	ILE	CB-CA-C	-5.66	104.41	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	GLU	N-CA-C	-5.62	104.53	111.33
1	E	245	ILE	N-CA-C	5.62	116.26	110.36
1	E	251	ASN	CA-C-N	-5.60	116.93	122.36
1	E	251	ASN	C-N-CA	-5.60	116.93	122.36
1	D	346	THR	N-CA-C	5.59	121.80	114.75
2	H	117	GLU	CA-C-N	5.58	128.79	120.31
2	H	117	GLU	C-N-CA	5.58	128.79	120.31
1	E	242	GLN	N-CA-C	-5.57	104.90	110.97
1	F	443	ILE	N-CA-C	5.56	116.60	108.53
1	C	250	GLN	N-CA-C	5.56	118.18	111.40
2	H	102	GLU	N-CA-C	5.56	117.70	109.69
1	A	42	GLU	N-CA-C	5.55	122.08	109.81
1	E	283	LEU	CA-C-N	5.55	126.78	119.84
1	E	283	LEU	C-N-CA	5.55	126.78	119.84
1	U	243	LYS	N-CA-C	-5.54	106.88	113.97
1	B	345	LEU	N-CA-C	5.53	117.31	111.28
1	D	335	ALA	N-CA-C	-5.52	102.84	110.35
1	U	382	PHE	N-CA-C	-5.52	104.78	112.45
1	F	335	ALA	N-CA-C	-5.51	102.73	110.50
1	A	344	ILE	N-CA-C	-5.49	103.98	111.89
1	A	248	VAL	CB-CA-C	-5.49	104.79	111.87
1	E	9	ILE	CB-CA-C	-5.49	104.89	112.24
2	I	116	GLU	N-CA-C	-5.49	101.36	109.86
1	C	337	SER	N-CA-C	5.48	118.57	110.46
1	E	424	ALA	N-CA-C	-5.48	105.20	111.07
1	S	57	GLY	CA-C-N	5.48	126.69	119.84
1	S	57	GLY	C-N-CA	5.48	126.69	119.84
1	C	344	ILE	N-CA-C	-5.48	104.20	111.05
1	F	70	LEU	N-CA-C	-5.47	104.34	111.02
1	F	315	ARG	N-CA-C	-5.46	103.04	110.36
1	F	329	ILE	N-CA-C	5.46	115.44	108.12
2	I	119	GLN	CA-C-N	-5.46	115.99	123.14
2	I	119	GLN	C-N-CA	-5.46	115.99	123.14
1	T	113	GLN	N-CA-C	-5.46	106.63	113.72
1	F	344	ILE	N-CA-C	-5.44	104.06	111.89
1	U	276	GLU	N-CA-C	-5.44	106.69	113.38
1	F	9	ILE	CB-CA-C	-5.44	104.89	112.02
2	M	150	GLU	N-CA-C	-5.44	105.00	111.03
2	O	150	GLU	N-CA-C	-5.42	105.01	111.03
1	B	374	VAL	N-CA-C	-5.42	105.04	110.30
1	F	120	ARG	N-CA-C	-5.41	106.85	113.50
1	S	276	GLU	N-CA-C	-5.40	106.73	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	329	ILE	N-CA-C	5.40	116.13	107.98
1	X	246	ASP	N-CA-C	-5.39	106.73	113.15
1	B	42	GLU	N-CA-C	5.39	121.72	109.81
2	P	150	GLU	N-CA-C	-5.39	105.05	111.03
1	A	302	HIS	N-CA-C	5.38	120.50	113.30
1	C	329	ILE	CB-CA-C	-5.37	105.50	111.35
1	C	64	THR	N-CA-C	5.37	116.81	111.07
1	E	38	MET	N-CA-C	-5.36	106.33	112.86
2	L	117	GLU	N-CA-C	5.36	118.61	111.75
2	R	61	GLU	N-CA-C	-5.34	105.54	111.36
1	B	29	ILE	N-CA-C	-5.34	105.17	110.62
1	S	107	ALA	N-CA-C	-5.34	107.43	114.31
1	D	302	HIS	N-CA-C	5.32	119.75	112.88
1	V	245	ILE	N-CA-C	-5.32	105.83	113.07
1	W	276	GLU	N-CA-C	-5.32	106.83	113.38
2	L	85	ASP	N-CA-C	-5.30	105.62	111.71
1	D	357	LYS	N-CA-C	-5.29	104.56	111.02
1	F	347	GLU	CA-C-N	5.29	126.45	119.84
1	F	347	GLU	C-N-CA	5.29	126.45	119.84
1	D	320	ILE	CA-C-N	5.29	124.74	119.24
1	D	320	ILE	C-N-CA	5.29	124.74	119.24
1	V	276	GLU	N-CA-C	-5.28	106.88	113.38
2	Q	61	GLU	N-CA-C	-5.27	105.61	111.36
1	A	338	ALA	N-CA-C	-5.27	104.59	111.02
1	F	338	ALA	N-CA-C	-5.27	104.59	111.02
2	Q	53	ALA	N-CA-C	-5.26	105.19	111.03
1	C	439	LEU	CB-CA-C	-5.26	109.53	115.79
1	T	382	PHE	N-CA-C	-5.26	105.14	112.45
1	B	315	ARG	CA-C-N	-5.25	114.25	119.56
1	B	315	ARG	C-N-CA	-5.25	114.25	119.56
1	D	38	MET	N-CA-C	-5.25	106.18	112.58
1	C	9	ILE	CB-CA-C	-5.24	104.99	112.22
1	S	327	LEU	CA-C-N	5.24	126.39	119.84
1	S	327	LEU	C-N-CA	5.24	126.39	119.84
1	A	424	ALA	N-CA-C	-5.24	105.26	110.97
1	C	381	ALA	N-CA-C	-5.23	104.64	111.02
1	D	435	GLU	N-CA-C	5.23	121.93	110.80
2	G	93	ALA	N-CA-C	5.23	116.23	108.60
1	F	248	VAL	CB-CA-C	-5.22	105.01	111.70
1	F	381	ALA	N-CA-C	-5.22	104.65	111.02
2	M	109	ILE	N-CA-C	-5.21	105.39	113.16
1	B	248	VAL	CB-CA-C	-5.21	105.30	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	251	ASN	CA-C-N	-5.21	117.31	122.36
1	F	251	ASN	C-N-CA	-5.21	117.31	122.36
1	E	335	ALA	N-CA-C	-5.20	103.17	110.50
1	C	96	VAL	N-CA-C	5.19	115.96	110.72
1	W	382	PHE	N-CA-C	-5.19	105.24	112.45
1	V	327	LEU	CA-C-N	5.17	126.31	119.84
1	V	327	LEU	C-N-CA	5.17	126.31	119.84
1	C	274	SER	N-CA-C	-5.17	105.82	111.82
1	W	327	LEU	CA-C-N	5.17	126.30	119.84
1	W	327	LEU	C-N-CA	5.17	126.30	119.84
1	X	244	ALA	N-CA-C	-5.17	106.98	113.28
1	C	245	ILE	N-CA-C	-5.17	104.86	110.23
1	V	295	HIS	N-CA-C	-5.16	108.24	114.75
1	X	276	GLU	N-CA-C	-5.16	107.03	113.38
2	L	101	LYS	N-CA-C	5.16	119.62	112.45
1	S	295	HIS	N-CA-C	-5.16	108.25	114.75
1	X	57	GLY	CA-C-N	5.15	126.28	119.84
1	X	57	GLY	C-N-CA	5.15	126.28	119.84
1	U	295	HIS	N-CA-C	-5.15	108.27	114.75
1	U	57	GLY	CA-C-N	5.14	126.27	119.84
1	U	57	GLY	C-N-CA	5.14	126.27	119.84
1	D	118	LYS	N-CA-C	-5.13	105.38	111.69
2	H	169	ILE	N-CA-C	5.13	115.51	108.12
1	U	113	GLN	N-CA-C	-5.13	106.42	113.30
1	C	435	GLU	CB-CA-C	-5.13	109.68	117.07
1	F	116	ILE	N-CA-C	-5.12	107.44	113.42
1	B	245	ILE	N-CA-C	-5.11	105.72	110.53
2	L	96	ILE	N-CA-C	-5.11	100.29	107.75
2	I	96	ILE	N-CA-C	-5.10	100.31	107.75
1	S	382	PHE	N-CA-C	-5.10	105.36	112.45
1	V	382	PHE	N-CA-C	-5.10	105.36	112.45
1	A	53	ILE	N-CA-C	5.09	116.63	108.89
2	J	33	LYS	N-CA-C	5.08	119.20	113.15
1	D	42	GLU	N-CA-C	5.07	121.02	109.81
1	U	34	ARG	N-CA-C	-5.07	106.78	113.17
1	A	39	GLN	N-CA-C	-5.07	100.01	110.80
1	B	434	VAL	N-CA-C	-5.06	102.11	109.29
1	A	38	MET	N-CA-C	-5.05	106.69	112.86
1	X	295	HIS	N-CA-C	-5.05	108.38	114.75
2	O	169	ILE	N-CA-C	5.05	115.24	108.17
1	C	42	GLU	N-CA-C	5.05	120.97	109.81
1	B	250	GLN	N-CA-C	5.04	119.30	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ARG	N-CA-C	-5.03	105.24	111.33
1	U	244	ALA	N-CA-C	-5.03	106.99	113.23
2	N	61	GLU	N-CA-C	-5.02	105.89	111.36
1	D	442	PHE	N-CA-C	5.02	119.38	113.16
2	N	169	ILE	N-CA-C	5.01	115.13	108.11
1	T	361	ALA	N-CA-C	-5.01	106.33	112.90
1	T	411	ALA	N-CA-C	-5.01	107.34	113.50
2	G	169	ILE	N-CA-C	5.01	115.33	108.12
2	M	61	GLU	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

There are no planarity outliers.

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	2539	0	2606	269	0
1	B	2539	0	2606	272	0
1	C	2484	0	2552	261	0
1	D	2476	0	2541	264	0
1	E	2462	0	2521	263	0
1	F	2495	0	2565	279	0
1	S	2468	0	2540	260	0
1	T	2570	0	2628	239	0
1	U	2503	0	2564	242	0
1	V	2432	0	2492	230	0
1	W	2428	0	2492	234	0
1	X	2500	0	2562	256	1
2	G	1280	0	1275	112	0
2	H	1280	0	1270	124	0
2	I	1292	0	1296	116	0
2	J	1280	0	1270	108	0
2	K	1280	0	1270	117	0
2	L	1294	0	1296	114	0
2	M	1261	0	1240	112	0
2	N	1261	0	1240	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	1257	0	1234	102	0
2	P	1257	0	1234	101	0
2	Q	1261	0	1240	101	0
2	R	1257	0	1234	99	0
3	A	31	0	12	2	0
3	B	31	0	12	5	0
3	C	31	0	12	5	0
3	D	31	0	12	4	0
3	E	31	0	12	9	0
3	F	31	0	12	8	0
3	S	31	0	12	14	0
3	T	31	0	12	3	0
3	U	31	0	12	12	0
3	V	31	0	12	3	0
3	W	31	0	12	8	0
3	X	31	0	12	9	0
All	All	45528	0	45912	4131	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (4131) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:LYS:NZ	1:F:279:GLN:HE22	1.38	1.21
2:Q:7:ARG:HD2	2:Q:119:GLN:OE1	1.44	1.17
1:E:264:LYS:NZ	1:E:279:GLN:HE22	1.42	1.15
2:N:7:ARG:HD2	2:N:119:GLN:HE21	1.09	1.15
1:A:264:LYS:NZ	1:A:279:GLN:HE22	1.45	1.12
2:J:91:LEU:H	2:J:91:LEU:HD12	1.06	1.11
2:I:7:ARG:HD2	2:I:119:GLN:OE1	1.50	1.10
1:D:264:LYS:NZ	1:D:279:GLN:HE22	1.50	1.09
1:S:313:VAL:HG23	1:S:314:ALA:H	1.19	1.08
1:T:313:VAL:HG23	1:T:314:ALA:H	1.17	1.08
1:U:313:VAL:HG23	1:U:314:ALA:H	1.18	1.07
2:N:7:ARG:CD	2:N:119:GLN:HE21	1.69	1.05
2:M:7:ARG:HD2	2:M:119:GLN:OE1	1.55	1.05
1:S:279:GLN:HE21	1:S:320:ILE:HG12	1.14	1.04
1:V:279:GLN:HE21	1:V:320:ILE:HG12	1.18	1.04
1:X:313:VAL:HG23	1:X:314:ALA:H	1.19	1.04
1:V:313:VAL:HG23	1:V:314:ALA:H	1.19	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:313:VAL:HG23	1:W:314:ALA:H	1.19	1.03
1:U:279:GLN:HE21	1:U:320:ILE:HG12	1.20	1.03
1:F:406:LYS:H	1:F:406:LYS:HD2	1.24	1.03
1:S:279:GLN:NE2	1:S:320:ILE:H	1.55	1.02
1:X:279:GLN:HE21	1:X:320:ILE:HG12	1.21	1.01
1:V:279:GLN:NE2	1:V:320:ILE:H	1.59	1.00
1:S:279:GLN:HE22	1:S:320:ILE:H	1.10	1.00
1:W:65:GLU:HG2	3:W:460:ATP:H5'2	1.41	1.00
1:T:279:GLN:HE21	1:T:320:ILE:HG12	1.23	1.00
1:U:279:GLN:NE2	1:U:320:ILE:H	1.59	0.99
1:B:406:LYS:H	1:B:406:LYS:HD2	1.25	0.99
1:U:65:GLU:HG2	3:U:458:ATP:H5'2	1.42	0.99
1:C:52:ASN:ND2	1:C:305:PHE:H	1.59	0.99
1:C:264:LYS:NZ	1:C:279:GLN:HE22	1.61	0.99
1:B:264:LYS:NZ	1:B:279:GLN:HE22	1.61	0.99
2:O:20:VAL:HG21	1:V:444:LEU:HD21	1.41	0.99
1:X:279:GLN:NE2	1:X:320:ILE:H	1.61	0.98
1:C:79:ILE:HG22	1:C:103:LEU:HD13	1.44	0.98
1:A:406:LYS:H	1:A:406:LYS:HD2	1.24	0.98
1:D:406:LYS:H	1:D:406:LYS:HD2	1.28	0.98
1:W:279:GLN:NE2	1:W:320:ILE:H	1.61	0.98
1:T:279:GLN:NE2	1:T:320:ILE:H	1.61	0.98
2:M:115:PRO:CB	2:M:119:GLN:HA	1.94	0.97
1:W:279:GLN:HE21	1:W:320:ILE:HG12	1.22	0.97
1:X:357:LYS:HA	1:X:367:ILE:HD11	1.46	0.97
2:I:83:ARG:HG2	2:J:55:THR:HG22	1.46	0.97
1:S:279:GLN:NE2	1:S:320:ILE:HG12	1.80	0.96
2:J:52:ASP:HA	2:J:55:THR:HG23	1.47	0.96
2:R:56:LEU:HB2	2:R:91:LEU:HD23	1.47	0.96
1:T:357:LYS:HA	1:T:367:ILE:HD11	1.48	0.96
1:E:111:VAL:HG21	1:E:244:ALA:HA	1.47	0.96
1:U:357:LYS:HA	1:U:367:ILE:HD11	1.46	0.96
1:S:357:LYS:HA	1:S:367:ILE:HD11	1.45	0.95
1:V:357:LYS:HA	1:V:367:ILE:HD11	1.47	0.95
1:V:279:GLN:NE2	1:V:320:ILE:HG12	1.81	0.95
2:M:56:LEU:HB2	2:M:91:LEU:HD23	1.49	0.95
1:B:264:LYS:HZ1	1:B:279:GLN:HE22	1.14	0.94
1:C:406:LYS:H	1:C:406:LYS:HD2	1.32	0.94
1:W:357:LYS:HA	1:W:367:ILE:HD11	1.47	0.94
1:B:231:ALA:HA	1:B:234:LEU:HD21	1.48	0.94
1:C:60:GLY:HA2	3:C:452:ATP:O3A	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:ASN:ND2	1:E:305:PHE:H	1.65	0.94
1:D:264:LYS:HZ1	1:D:279:GLN:HE22	1.09	0.93
2:O:56:LEU:HB2	2:O:91:LEU:HD23	1.48	0.93
1:S:105:ASP:HB3	1:X:297:MET:HE2	1.51	0.93
1:X:279:GLN:NE2	1:X:320:ILE:HG12	1.83	0.93
1:U:279:GLN:NE2	1:U:320:ILE:HG12	1.82	0.93
2:P:56:LEU:HB2	2:P:91:LEU:HD23	1.48	0.92
1:X:442:PHE:HD1	1:X:442:PHE:H	1.04	0.92
1:B:360:MET:HE1	1:C:36:ARG:NH1	1.84	0.92
1:T:437:GLU:HG3	1:T:438:ASP:H	1.33	0.92
2:Q:56:LEU:HB2	2:Q:91:LEU:HD23	1.50	0.92
1:F:264:LYS:HZ1	1:F:279:GLN:HE22	0.98	0.91
1:S:235:ILE:HG22	1:S:237:PRO:HD3	1.52	0.91
1:F:360:MET:HE2	1:F:360:MET:HA	1.53	0.91
1:T:279:GLN:NE2	1:T:320:ILE:HG12	1.84	0.91
2:K:137:LEU:O	2:K:141:THR:HG23	1.71	0.91
1:V:279:GLN:HE22	1:V:320:ILE:H	1.14	0.91
2:I:52:ASP:HA	2:I:55:THR:HG23	1.51	0.90
2:N:56:LEU:HB2	2:N:91:LEU:HD23	1.52	0.90
1:E:406:LYS:H	1:E:406:LYS:HD2	1.37	0.90
1:A:366:ASN:HB3	1:A:418:THR:HG22	1.53	0.90
1:B:409:PHE:CD1	1:C:6:PRO:HB3	2.07	0.90
1:T:236:ASN:OD1	1:T:239:GLU:HB3	1.72	0.90
1:X:279:GLN:HE22	1:X:320:ILE:H	1.17	0.89
1:W:279:GLN:HE22	1:W:320:ILE:H	1.18	0.89
1:B:360:MET:HE2	1:B:360:MET:HA	1.54	0.89
1:T:64:THR:HB	3:T:457:ATP:O2A	1.73	0.89
1:E:264:LYS:HZ1	1:E:279:GLN:HE22	1.16	0.89
2:Q:7:ARG:CD	2:Q:119:GLN:OE1	2.21	0.88
2:L:52:ASP:HA	2:L:55:THR:HG23	1.53	0.88
1:W:279:GLN:NE2	1:W:320:ILE:HG12	1.88	0.88
1:D:264:LYS:HE3	1:D:264:LYS:N	1.88	0.88
1:E:20:GLN:HE21	1:E:20:GLN:CA	1.86	0.88
2:Q:131:LEU:HD11	2:Q:135:ARG:NE	1.88	0.88
1:A:58:PRO:HD2	1:A:61:VAL:HG21	1.54	0.88
1:E:367:ILE:HD11	1:E:421:ILE:HD11	1.56	0.88
2:J:144:SER:HB3	2:J:147:GLU:HG3	1.55	0.88
1:B:108:MET:HE1	1:B:240:LEU:HD23	1.55	0.88
2:M:112:VAL:HB	1:S:443:ILE:HD12	1.55	0.88
1:U:279:GLN:HE22	1:U:320:ILE:H	1.16	0.88
2:R:76:VAL:HG22	1:X:443:ILE:HD11	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:MET:HE2	1:E:360:MET:HA	1.55	0.87
2:L:137:LEU:O	2:L:141:THR:HG23	1.74	0.87
1:F:23:ALA:HA	1:F:331:VAL:HG21	1.56	0.87
1:T:279:GLN:HE22	1:T:320:ILE:H	1.15	0.87
1:U:300:THR:O	1:U:303:ILE:HG13	1.75	0.87
1:F:264:LYS:NZ	1:F:279:GLN:NE2	2.22	0.87
2:I:7:ARG:CD	2:I:119:GLN:OE1	2.21	0.87
1:A:6:PRO:HB3	1:F:409:PHE:CD1	2.10	0.86
2:J:91:LEU:HD12	2:J:91:LEU:N	1.90	0.86
2:M:17:ASP:HB2	2:M:164:ASN:ND2	1.90	0.86
1:E:20:GLN:HE21	1:E:20:GLN:HA	1.40	0.86
2:K:83:ARG:HG2	2:L:55:THR:HG22	1.57	0.86
2:G:17:ASP:O	2:G:33:LYS:HD2	1.75	0.86
2:J:18:GLY:H	2:J:164:ASN:HD21	1.22	0.86
2:G:56:LEU:HD13	2:G:95:LEU:HG	1.56	0.86
2:N:7:ARG:HD2	2:N:119:GLN:NE2	1.88	0.86
2:H:56:LEU:HD13	2:H:95:LEU:HG	1.58	0.86
2:M:7:ARG:CD	2:M:119:GLN:OE1	2.23	0.86
2:M:115:PRO:HB3	2:M:119:GLN:HA	1.56	0.86
1:D:360:MET:HE2	1:D:360:MET:HA	1.56	0.86
2:Q:17:ASP:HA	2:Q:167:PHE:HB3	1.58	0.86
1:S:369:PHE:HE2	1:S:421:ILE:HD12	1.41	0.85
1:A:409:PHE:CD1	1:B:6:PRO:HB3	2.12	0.85
2:L:56:LEU:HD13	2:L:95:LEU:HG	1.56	0.85
2:N:17:ASP:HB2	2:N:164:ASN:ND2	1.92	0.85
2:J:91:LEU:H	2:J:91:LEU:CD1	1.89	0.85
1:A:435:GLU:HG3	1:A:436:ASN:H	1.40	0.85
1:E:443:ILE:HG23	2:K:112:VAL:HG23	1.59	0.85
1:S:327:LEU:N	1:S:328:PRO:HD3	1.92	0.85
1:D:27:VAL:HB	1:D:70:LEU:HD22	1.57	0.85
1:E:116:ILE:HD12	1:E:117:ALA:N	1.90	0.85
1:T:369:PHE:HE2	1:T:421:ILE:HD12	1.42	0.85
1:D:275:ARG:C	1:D:277:GLY:H	1.82	0.84
2:O:17:ASP:HB2	2:O:164:ASN:ND2	1.92	0.84
1:W:369:PHE:HE2	1:W:421:ILE:HD12	1.42	0.84
2:O:18:GLY:H	2:O:164:ASN:HD21	1.24	0.84
1:E:443:ILE:HD11	2:K:72:LEU:HD11	1.59	0.84
2:H:144:SER:HB3	2:H:147:GLU:HG3	1.59	0.84
1:T:327:LEU:N	1:T:328:PRO:HD3	1.92	0.84
1:C:264:LYS:HZ1	1:C:279:GLN:HE22	1.24	0.84
1:B:111:VAL:HG21	1:B:244:ALA:HA	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:VAL:HG12	1:F:434:VAL:H	1.43	0.84
1:S:393:ALA:HB3	3:S:456:ATP:H1'	1.60	0.84
1:B:20:GLN:HA	1:B:20:GLN:HE21	1.42	0.84
2:Q:17:ASP:HB2	2:Q:164:ASN:ND2	1.91	0.84
1:T:442:PHE:N	1:T:442:PHE:HD1	1.75	0.84
1:A:264:LYS:HZ1	1:A:279:GLN:HE22	1.25	0.84
1:V:63:LYS:HZ2	1:V:308:SER:HB2	1.43	0.84
1:W:439:LEU:HG	1:W:440:SER:H	1.43	0.83
2:N:8:ARG:HB3	2:N:8:ARG:HH11	1.42	0.83
2:R:8:ARG:HB3	2:R:8:ARG:HH11	1.42	0.83
2:R:17:ASP:HA	2:R:167:PHE:HB3	1.60	0.83
1:B:20:GLN:HE21	1:B:20:GLN:CA	1.90	0.83
2:H:137:LEU:O	2:H:141:THR:HG23	1.79	0.83
1:A:360:MET:HE1	1:B:36:ARG:NH1	1.94	0.83
2:M:131:LEU:HD11	2:M:135:ARG:NE	1.93	0.83
2:O:8:ARG:HB3	2:O:8:ARG:HH11	1.42	0.83
2:P:17:ASP:HB2	2:P:164:ASN:ND2	1.94	0.83
2:G:37:LEU:HB2	2:G:42:VAL:HG23	1.60	0.83
2:I:17:ASP:HB2	2:I:164:ASN:ND2	1.94	0.83
2:M:8:ARG:HB3	2:M:8:ARG:HH11	1.41	0.83
2:P:17:ASP:HA	2:P:167:PHE:HB3	1.61	0.83
1:X:369:PHE:HE2	1:X:421:ILE:HD12	1.42	0.83
1:T:442:PHE:HD1	1:T:442:PHE:H	1.27	0.83
2:N:7:ARG:CD	2:N:119:GLN:NE2	2.42	0.83
2:M:17:ASP:HA	2:M:167:PHE:HB3	1.60	0.83
1:U:327:LEU:N	1:U:328:PRO:HD3	1.92	0.82
2:G:137:LEU:O	2:G:141:THR:HG23	1.78	0.82
1:C:337:SER:HB3	1:C:340:ASP:OD2	1.77	0.82
1:F:37:ARG:HD2	1:F:48:VAL:HG13	1.61	0.82
2:N:17:ASP:HA	2:N:167:PHE:HB3	1.61	0.82
1:W:327:LEU:N	1:W:328:PRO:HD3	1.92	0.82
1:D:403:LEU:HD23	1:D:404:MET:N	1.93	0.82
2:M:18:GLY:H	2:M:164:ASN:HD21	1.24	0.82
1:X:300:THR:O	1:X:303:ILE:HG13	1.80	0.82
1:D:108:MET:HE1	1:D:240:LEU:HG	1.61	0.82
1:F:403:LEU:C	1:F:403:LEU:HD23	2.04	0.82
1:E:52:ASN:ND2	1:E:305:PHE:HB2	1.95	0.82
2:H:88:LEU:O	2:H:90:LYS:N	2.12	0.82
2:O:17:ASP:HA	2:O:167:PHE:HB3	1.62	0.82
1:U:369:PHE:HE2	1:U:421:ILE:HD12	1.43	0.82
1:E:403:LEU:HD23	1:E:404:MET:N	1.95	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:403:LEU:HD23	1:F:404:MET:N	1.95	0.82
2:J:83:ARG:HG2	2:K:55:THR:HG22	1.62	0.82
2:Q:8:ARG:HB3	2:Q:8:ARG:HH11	1.44	0.81
1:V:434:VAL:HG12	1:V:435:GLU:H	1.43	0.81
2:G:17:ASP:HB2	2:G:164:ASN:ND2	1.95	0.81
2:R:131:LEU:HD11	2:R:135:ARG:NE	1.94	0.81
1:X:327:LEU:N	1:X:328:PRO:HD3	1.95	0.81
2:M:115:PRO:HB2	2:M:119:GLN:HA	1.58	0.81
2:R:18:GLY:H	2:R:164:ASN:HD21	1.27	0.81
1:S:60:GLY:HA3	1:S:392:GLY:HA3	1.62	0.81
2:P:8:ARG:HB3	2:P:8:ARG:HH11	1.45	0.81
1:B:421:ILE:HG23	1:B:425:TYR:CD1	2.16	0.81
1:E:264:LYS:N	1:E:264:LYS:HE3	1.96	0.81
1:A:55:MET:HE3	1:A:306:ILE:HG21	1.60	0.81
2:H:18:GLY:H	2:H:164:ASN:HD21	1.26	0.81
2:K:79:ALA:HB1	2:K:83:ARG:HH21	1.44	0.81
2:I:83:ARG:HG2	2:J:55:THR:CG2	2.11	0.81
1:V:54:LEU:HD21	1:V:327:LEU:HD13	1.60	0.81
1:B:403:LEU:HD23	1:B:404:MET:N	1.94	0.81
1:F:337:SER:HB3	1:F:340:ASP:OD2	1.81	0.81
1:A:236:ASN:ND2	1:A:239:GLU:HB2	1.96	0.81
2:L:22:LEU:HD22	2:L:27:MET:HE3	1.63	0.81
2:L:88:LEU:HD23	2:L:89:ARG:H	1.43	0.80
1:T:442:PHE:N	1:T:442:PHE:CD1	2.47	0.80
1:C:439:LEU:HA	1:C:443:ILE:HD12	1.62	0.80
2:G:52:ASP:HA	2:G:55:THR:HG23	1.64	0.80
2:H:22:LEU:HD22	2:H:27:MET:HE3	1.63	0.80
2:R:17:ASP:HB2	2:R:164:ASN:ND2	1.95	0.80
1:F:55:MET:HE3	1:F:306:ILE:HG21	1.64	0.80
2:H:82:TRP:HZ2	2:H:91:LEU:HD13	1.45	0.80
2:I:18:GLY:H	2:I:164:ASN:HD21	1.27	0.80
1:S:441:ARG:HB3	1:S:442:PHE:HD1	1.44	0.80
2:L:17:ASP:HB2	2:L:164:ASN:ND2	1.96	0.80
2:N:18:GLY:H	2:N:164:ASN:HD21	1.28	0.80
1:D:79:ILE:HG22	1:D:103:LEU:HD13	1.63	0.80
2:G:18:GLY:H	2:G:164:ASN:HD21	1.28	0.80
1:A:275:ARG:C	1:A:277:GLY:H	1.88	0.80
2:K:18:GLY:H	2:K:164:ASN:HD21	1.26	0.80
1:B:264:LYS:N	1:B:264:LYS:HE3	1.97	0.80
2:J:37:LEU:HB2	2:J:42:VAL:HG23	1.64	0.80
2:I:144:SER:HB3	2:I:147:GLU:HG3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:18:GLY:H	2:Q:164:ASN:HD21	1.27	0.79
1:E:275:ARG:C	1:E:277:GLY:H	1.88	0.79
2:R:5:SER:HB2	2:R:14:VAL:HG22	1.63	0.79
1:T:54:LEU:HD21	1:T:327:LEU:HD13	1.64	0.79
1:X:77:PRO:HD2	1:X:251:ASN:O	1.82	0.79
1:V:77:PRO:HD2	1:V:251:ASN:O	1.81	0.79
2:G:144:SER:HB3	2:G:147:GLU:HG3	1.65	0.79
2:Q:131:LEU:HD11	2:Q:135:ARG:HE	1.47	0.79
1:V:327:LEU:N	1:V:328:PRO:HD3	1.95	0.79
2:P:131:LEU:HD11	2:P:135:ARG:NE	1.96	0.79
1:S:279:GLN:HE22	1:S:320:ILE:N	1.81	0.79
1:X:54:LEU:HD21	1:X:327:LEU:HD13	1.65	0.79
1:T:260:ASP:HB3	1:T:311:PHE:CD2	2.18	0.79
1:U:77:PRO:HD2	1:U:251:ASN:O	1.83	0.79
2:K:144:SER:HB3	2:K:147:GLU:HG3	1.65	0.79
1:B:275:ARG:C	1:B:277:GLY:H	1.90	0.79
2:G:105:ILE:CG2	2:G:113:VAL:HB	2.13	0.79
1:W:260:ASP:HB3	1:W:311:PHE:CD2	2.18	0.79
1:F:57:GLY:O	1:F:310:ALA:HA	1.83	0.78
2:L:38:TYR:CE1	2:L:69:GLY:HA3	2.18	0.78
1:V:369:PHE:HE2	1:V:421:ILE:HD12	1.46	0.78
1:X:64:THR:HB	3:X:461:ATP:O2A	1.83	0.78
2:K:22:LEU:HD22	2:K:27:MET:HE3	1.66	0.78
2:M:131:LEU:HD11	2:M:135:ARG:HE	1.49	0.78
1:E:27:VAL:HB	1:E:70:LEU:HD22	1.64	0.78
1:F:264:LYS:HZ1	1:F:279:GLN:NE2	1.78	0.78
2:M:164:ASN:H	2:M:164:ASN:HD22	1.30	0.78
1:W:54:LEU:HD21	1:W:327:LEU:HD13	1.65	0.78
1:D:440:SER:O	1:D:442:PHE:N	2.16	0.78
1:F:441:ARG:NH2	2:G:37:LEU:HA	1.99	0.78
2:H:52:ASP:HA	2:H:55:THR:HG23	1.65	0.78
2:M:55:THR:HG22	2:N:83:ARG:HG2	1.66	0.78
1:A:403:LEU:HD23	1:A:404:MET:N	1.99	0.78
2:O:5:SER:HB2	2:O:14:VAL:HG22	1.65	0.78
1:F:104:THR:HA	1:F:248:VAL:HG21	1.65	0.78
2:M:42:VAL:HG12	2:M:99:ASP:HB3	1.66	0.78
1:S:260:ASP:HB3	1:S:311:PHE:CD2	2.19	0.78
1:T:96:VAL:HG13	1:T:282:LEU:HD12	1.66	0.78
1:B:337:SER:HB3	1:B:340:ASP:OD2	1.82	0.78
1:C:403:LEU:C	1:C:403:LEU:HD23	2.08	0.78
1:S:77:PRO:HD2	1:S:251:ASN:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:303:ILE:HG22	1:T:304:LEU:H	1.49	0.78
1:C:23:ALA:HA	1:C:331:VAL:HG21	1.66	0.78
1:C:264:LYS:N	1:C:264:LYS:HE3	1.97	0.78
1:E:280:ARG:HH11	1:E:280:ARG:HG3	1.47	0.78
1:S:96:VAL:HG13	1:S:282:LEU:HD12	1.65	0.78
1:C:52:ASN:O	1:C:328:PRO:HD2	1.82	0.78
1:B:60:GLY:HA2	3:B:451:ATP:O3A	1.84	0.78
1:D:37:ARG:HD2	1:D:48:VAL:HG13	1.66	0.78
2:J:118:ASP:O	2:J:119:GLN:O	2.02	0.77
2:K:17:ASP:HB2	2:K:164:ASN:ND2	1.99	0.77
1:U:303:ILE:HG22	1:U:304:LEU:H	1.47	0.77
1:V:300:THR:O	1:V:303:ILE:HG13	1.83	0.77
2:Q:5:SER:HB2	2:Q:14:VAL:HG22	1.66	0.77
1:T:300:THR:O	1:T:303:ILE:HG13	1.83	0.77
1:V:96:VAL:HG13	1:V:282:LEU:HD12	1.66	0.77
1:D:58:PRO:O	1:D:63:LYS:NZ	2.17	0.77
1:E:55:MET:HE3	1:E:306:ILE:HG21	1.66	0.77
2:L:91:LEU:O	2:L:108:GLY:HA3	1.85	0.77
1:C:52:ASN:HD22	1:C:305:PHE:H	1.27	0.77
2:H:7:ARG:HD2	2:H:119:GLN:OE1	1.85	0.77
2:P:5:SER:HB2	2:P:14:VAL:HG22	1.67	0.77
1:V:260:ASP:HB3	1:V:311:PHE:CD2	2.20	0.77
1:A:264:LYS:N	1:A:264:LYS:HE3	2.00	0.77
1:X:108:MET:HE2	1:X:295:HIS:HD2	1.49	0.77
1:X:227:ILE:HG23	1:X:228:ASP:H	1.49	0.77
2:P:18:GLY:H	2:P:164:ASN:HD21	1.31	0.77
1:D:242:GLN:HA	1:D:245:ILE:HD12	1.66	0.77
1:T:77:PRO:HD2	1:T:251:ASN:O	1.84	0.77
1:X:260:ASP:HB3	1:X:311:PHE:CD2	2.19	0.77
1:D:20:GLN:HE21	1:D:20:GLN:H	1.31	0.77
2:M:116:GLU:O	2:M:119:GLN:N	2.11	0.77
2:N:131:LEU:HD11	2:N:135:ARG:NE	2.00	0.77
1:E:79:ILE:HG22	1:E:103:LEU:HD13	1.67	0.77
1:A:37:ARG:HD2	1:A:48:VAL:HG13	1.65	0.77
2:P:42:VAL:HG12	2:P:99:ASP:HB3	1.66	0.77
1:U:313:VAL:HG23	1:U:314:ALA:N	1.99	0.77
1:B:362:THR:CG2	1:C:39:GLN:HG2	2.14	0.76
1:T:439:LEU:O	1:T:441:ARG:N	2.18	0.76
1:W:300:THR:O	1:W:303:ILE:HG13	1.84	0.76
1:A:264:LYS:HZ3	1:A:279:GLN:HE22	1.29	0.76
1:S:439:LEU:H	1:S:439:LEU:HD23	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:443:ILE:HD11	2:I:72:LEU:HD11	1.64	0.76
1:F:275:ARG:C	1:F:277:GLY:H	1.93	0.76
2:H:105:ILE:CG2	2:H:113:VAL:HB	2.16	0.76
1:F:36:ARG:O	1:F:39:GLN:HB3	1.86	0.76
1:S:300:THR:O	1:S:303:ILE:HG13	1.84	0.76
2:J:105:ILE:CG2	2:J:113:VAL:HB	2.14	0.76
2:L:18:GLY:H	2:L:164:ASN:HD21	1.27	0.76
2:R:164:ASN:H	2:R:164:ASN:HD22	1.33	0.76
1:S:65:GLU:HG2	3:S:456:ATP:H5'2	1.66	0.76
1:U:54:LEU:HD21	1:U:327:LEU:HD13	1.67	0.76
1:A:337:SER:HB3	1:A:340:ASP:OD2	1.86	0.76
1:B:23:ALA:HA	1:B:331:VAL:HG21	1.67	0.76
1:D:352:LEU:HD13	1:D:400:MET:HG3	1.67	0.76
2:O:164:ASN:H	2:O:164:ASN:HD22	1.34	0.76
2:Q:164:ASN:HD22	2:Q:164:ASN:H	1.33	0.76
1:F:37:ARG:HH12	1:F:38:MET:HE2	1.50	0.76
2:O:42:VAL:HG12	2:O:99:ASP:HB3	1.68	0.76
1:U:260:ASP:HB3	1:U:311:PHE:CD2	2.21	0.76
2:N:103:SER:O	2:N:104:LEU:HD23	1.86	0.76
1:S:54:LEU:HD21	1:S:327:LEU:HD13	1.67	0.76
2:O:131:LEU:HD11	2:O:135:ARG:NE	2.01	0.76
1:W:313:VAL:HG23	1:W:314:ALA:N	2.00	0.76
1:D:17:ILE:N	1:D:17:ILE:HD12	2.02	0.75
1:W:326:ARG:HB3	1:W:326:ARG:HH11	1.52	0.75
1:A:405:ASP:HB3	1:A:406:LYS:HD2	1.68	0.75
1:X:313:VAL:HG23	1:X:314:ALA:N	2.00	0.75
2:G:57:PHE:HA	2:G:95:LEU:HD11	1.68	0.75
2:L:88:LEU:HD23	2:L:89:ARG:N	2.00	0.75
2:R:42:VAL:HG12	2:R:99:ASP:HB3	1.69	0.75
1:D:403:LEU:HD23	1:D:403:LEU:C	2.11	0.75
1:E:64:THR:HB	3:E:454:ATP:O1A	1.86	0.75
2:L:52:ASP:CA	2:L:55:THR:HG23	2.16	0.75
2:O:76:VAL:HG11	1:U:442:PHE:HD2	1.52	0.75
1:F:108:MET:HE1	1:F:240:LEU:CD2	2.16	0.75
1:U:96:VAL:HG13	1:U:282:LEU:HD12	1.67	0.75
1:W:303:ILE:HG22	1:W:304:LEU:H	1.52	0.75
2:K:52:ASP:HA	2:K:55:THR:HG23	1.69	0.75
2:N:7:ARG:NE	2:N:119:GLN:NE2	2.33	0.75
1:S:393:ALA:CB	3:S:456:ATP:H1'	2.16	0.75
1:B:104:THR:HA	1:B:248:VAL:HG21	1.69	0.75
2:K:105:ILE:CG2	2:K:113:VAL:HB	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:105:ILE:HG23	2:G:113:VAL:HB	1.68	0.75
1:A:233:LYS:HD2	1:A:234:LEU:N	2.02	0.74
1:D:367:ILE:HD11	1:D:421:ILE:HD11	1.69	0.74
1:B:366:ASN:HB3	1:B:418:THR:HG22	1.67	0.74
1:F:17:ILE:N	1:F:17:ILE:HD12	2.03	0.74
1:V:303:ILE:HG22	1:V:304:LEU:H	1.50	0.74
1:C:435:GLU:HG2	1:C:436:ASN:H	1.51	0.74
1:D:407:ILE:O	1:D:411:ALA:HB2	1.87	0.74
1:U:279:GLN:HE22	1:U:320:ILE:N	1.85	0.74
1:W:96:VAL:HG13	1:W:282:LEU:HD12	1.67	0.74
1:B:232:ALA:H	1:B:234:LEU:HD23	1.52	0.74
1:C:104:THR:HA	1:C:248:VAL:HG21	1.68	0.74
1:F:441:ARG:HH22	2:G:37:LEU:HA	1.53	0.74
2:G:13:VAL:HG22	2:G:171:GLU:HB3	1.70	0.74
1:V:326:ARG:HB3	1:V:326:ARG:HH11	1.51	0.74
1:A:403:LEU:HD23	1:A:403:LEU:C	2.13	0.74
1:C:360:MET:HA	1:C:360:MET:HE2	1.69	0.74
1:S:6:PRO:HD3	1:S:32:ARG:HD3	1.70	0.74
1:B:36:ARG:O	1:B:39:GLN:HB3	1.87	0.74
1:D:264:LYS:NZ	1:D:279:GLN:NE2	2.34	0.74
1:F:444:LEU:HD23	1:F:444:LEU:C	2.12	0.74
2:G:13:VAL:HG22	2:G:171:GLU:CB	2.18	0.74
2:I:82:TRP:HZ2	2:I:91:LEU:HD23	1.51	0.74
2:L:37:LEU:HD21	2:L:57:PHE:CZ	2.21	0.74
1:X:279:GLN:HE22	1:X:320:ILE:N	1.86	0.74
1:B:5:THR:H	1:B:8:GLU:HB3	1.53	0.74
1:B:79:ILE:HG22	1:B:103:LEU:HD13	1.70	0.73
1:B:232:ALA:H	1:B:234:LEU:CD2	2.01	0.73
1:D:104:THR:HA	1:D:248:VAL:HG21	1.68	0.73
1:T:442:PHE:O	1:T:443:ILE:HG12	1.88	0.73
1:V:279:GLN:HE22	1:V:320:ILE:N	1.84	0.73
1:X:96:VAL:HG13	1:X:282:LEU:HD12	1.68	0.73
1:B:352:LEU:HD13	1:B:400:MET:HG3	1.68	0.73
1:F:264:LYS:N	1:F:264:LYS:HE3	2.03	0.73
2:P:164:ASN:H	2:P:164:ASN:HD22	1.34	0.73
1:W:6:PRO:HD3	1:W:32:ARG:HD3	1.70	0.73
1:A:83:ALA:HB1	1:A:262:ILE:HD13	1.69	0.73
1:D:36:ARG:O	1:D:39:GLN:HB3	1.88	0.73
2:G:37:LEU:HD21	2:G:57:PHE:CZ	2.23	0.73
1:X:395:ARG:O	1:X:399:VAL:HG23	1.89	0.73
1:E:37:ARG:HD2	1:E:48:VAL:HG13	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:367:ILE:HD11	1:E:421:ILE:CD1	2.19	0.73
2:H:17:ASP:HB2	2:H:164:ASN:ND2	2.03	0.73
1:F:20:GLN:CA	1:F:20:GLN:HE21	2.01	0.73
2:H:91:LEU:CD1	2:H:91:LEU:H	2.02	0.73
1:S:303:ILE:HG22	1:S:304:LEU:H	1.52	0.73
1:U:326:ARG:HB3	1:U:326:ARG:HH11	1.54	0.73
2:O:103:SER:O	2:O:104:LEU:HD23	1.87	0.73
2:Q:42:VAL:HG12	2:Q:99:ASP:HB3	1.70	0.73
1:V:395:ARG:O	1:V:399:VAL:HG23	1.88	0.73
2:L:46:PHE:HB3	2:L:95:LEU:CD2	2.19	0.73
2:R:103:SER:O	2:R:104:LEU:HD23	1.89	0.73
1:W:77:PRO:HD2	1:W:251:ASN:O	1.87	0.73
1:T:6:PRO:HD3	1:T:32:ARG:HD3	1.71	0.73
1:X:303:ILE:HG22	1:X:304:LEU:H	1.53	0.73
1:C:403:LEU:HD23	1:C:404:MET:N	2.03	0.73
1:D:360:MET:HE1	1:E:36:ARG:NH1	2.03	0.73
1:T:326:ARG:HB3	1:T:326:ARG:HH11	1.54	0.73
1:A:367:ILE:HD11	1:A:421:ILE:HD11	1.68	0.72
1:D:116:ILE:HD12	1:D:117:ALA:N	2.04	0.72
1:D:409:PHE:CD1	1:E:6:PRO:HB3	2.24	0.72
1:E:264:LYS:HZ3	1:E:279:GLN:HE22	1.36	0.72
1:F:79:ILE:HG22	1:F:103:LEU:HD13	1.70	0.72
2:I:37:LEU:HB2	2:I:42:VAL:HG23	1.70	0.72
1:X:6:PRO:HD3	1:X:32:ARG:HD3	1.71	0.72
2:Q:103:SER:O	2:Q:104:LEU:HD23	1.89	0.72
1:W:279:GLN:HE22	1:W:320:ILE:N	1.87	0.72
1:A:39:GLN:HG2	1:F:362:THR:CG2	2.18	0.72
1:F:443:ILE:HD11	2:L:72:LEU:HD11	1.72	0.72
2:N:42:VAL:HG12	2:N:99:ASP:HB3	1.70	0.72
1:U:6:PRO:HD3	1:U:32:ARG:HD3	1.69	0.72
1:C:5:THR:H	1:C:8:GLU:HB3	1.55	0.72
2:L:144:SER:HB3	2:L:147:GLU:HG3	1.69	0.72
1:A:362:THR:CG2	1:B:39:GLN:HG2	2.20	0.72
1:B:283:LEU:HB2	1:B:284:PRO:HD3	1.70	0.72
1:C:5:THR:O	1:C:9:ILE:HG13	1.89	0.72
2:R:131:LEU:HD11	2:R:135:ARG:HE	1.53	0.72
1:S:326:ARG:HB3	1:S:326:ARG:HH11	1.55	0.72
1:C:275:ARG:C	1:C:277:GLY:H	1.98	0.72
2:K:83:ARG:HG2	2:L:55:THR:CG2	2.19	0.72
1:D:20:GLN:HE21	1:D:20:GLN:N	1.87	0.72
1:E:108:MET:HG3	1:E:295:HIS:CE1	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:ASN:OD1	1:E:416:GLY:N	2.22	0.72
2:K:56:LEU:HD13	2:K:95:LEU:HG	1.72	0.72
1:V:442:PHE:O	1:V:443:ILE:HG12	1.90	0.72
1:A:52:ASN:O	1:A:328:PRO:HD2	1.90	0.72
1:A:421:ILE:HG23	1:A:425:TYR:CD1	2.25	0.72
1:D:55:MET:HE3	1:D:306:ILE:HG21	1.71	0.72
1:V:313:VAL:HG23	1:V:314:ALA:N	1.99	0.72
1:X:235:ILE:O	1:X:236:ASN:HB2	1.90	0.72
1:E:362:THR:CG2	1:F:39:GLN:HG2	2.20	0.72
1:E:421:ILE:HA	1:E:425:TYR:HD1	1.55	0.72
2:K:37:LEU:HD21	2:K:57:PHE:CZ	2.25	0.72
1:E:366:ASN:HB3	1:E:418:THR:HG22	1.72	0.71
1:F:38:MET:HG3	1:F:45:ARG:NH1	2.05	0.71
1:T:279:GLN:HE22	1:T:320:ILE:N	1.85	0.71
1:W:328:PRO:HB3	1:X:398:THR:HA	1.72	0.71
1:A:360:MET:HE2	1:A:360:MET:HA	1.72	0.71
1:E:264:LYS:NZ	1:E:279:GLN:NE2	2.28	0.71
1:U:395:ARG:O	1:U:399:VAL:HG23	1.89	0.71
1:X:326:ARG:HB3	1:X:326:ARG:HH11	1.54	0.71
1:A:408:SER:O	1:B:36:ARG:NH2	2.22	0.71
1:C:55:MET:HE3	1:C:306:ILE:HG21	1.71	0.71
2:G:37:LEU:HB2	2:G:42:VAL:CG2	2.20	0.71
2:N:5:SER:HB2	2:N:14:VAL:HG22	1.72	0.71
1:A:391:ILE:HG22	1:B:321:PRO:HB3	1.70	0.71
2:I:91:LEU:H	2:I:91:LEU:HD22	1.54	0.71
2:J:37:LEU:HB2	2:J:42:VAL:CG2	2.20	0.71
1:B:63:LYS:HB2	3:B:451:ATP:O2B	1.90	0.71
2:N:164:ASN:HD22	2:N:164:ASN:H	1.38	0.71
1:D:443:ILE:HG12	2:J:112:VAL:HG21	1.72	0.71
2:I:137:LEU:O	2:I:141:THR:HG23	1.90	0.71
2:P:131:LEU:HD11	2:P:135:ARG:HE	1.53	0.71
1:A:104:THR:HA	1:A:248:VAL:HG21	1.72	0.71
1:C:100:ILE:HB	1:C:291:VAL:HG21	1.73	0.71
1:C:256:ILE:HG21	1:C:259:ILE:HD12	1.70	0.71
1:D:20:GLN:OE1	1:D:333:LEU:HB3	1.90	0.71
2:J:137:LEU:CD1	2:P:136:ALA:HB1	2.21	0.71
1:S:261:LYS:HE3	1:X:280:ARG:HH22	1.53	0.71
2:M:5:SER:HB2	2:M:14:VAL:HG22	1.71	0.71
2:L:57:PHE:HA	2:L:95:LEU:HD11	1.70	0.71
1:T:108:MET:O	1:T:112:ARG:HB3	1.90	0.71
1:V:6:PRO:HD3	1:V:32:ARG:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ILE:CG2	1:C:103:LEU:HD13	2.19	0.70
2:I:22:LEU:HD22	2:I:27:MET:HE3	1.73	0.70
2:I:57:PHE:HA	2:I:95:LEU:HD11	1.73	0.70
1:A:100:ILE:HB	1:A:291:VAL:HG21	1.72	0.70
1:B:100:ILE:HB	1:B:291:VAL:HG21	1.73	0.70
1:B:403:LEU:HD23	1:B:403:LEU:C	2.15	0.70
1:C:409:PHE:CD1	1:D:6:PRO:HB3	2.26	0.70
1:S:105:ASP:HB3	1:X:297:MET:CE	2.20	0.70
1:S:313:VAL:HG23	1:S:314:ALA:N	2.00	0.70
2:J:118:ASP:O	2:J:119:GLN:C	2.33	0.70
2:G:82:TRP:CZ2	2:G:88:LEU:HD22	2.25	0.70
1:A:406:LYS:HD2	1:A:406:LYS:N	2.04	0.70
1:C:435:GLU:HG2	1:C:436:ASN:N	2.05	0.70
2:P:103:SER:O	2:P:104:LEU:HD23	1.92	0.70
1:S:37:ARG:HH21	1:S:302:HIS:CE1	2.08	0.70
1:T:313:VAL:HG23	1:T:314:ALA:N	1.98	0.70
1:F:443:ILE:HG12	2:L:112:VAL:HG21	1.73	0.70
2:I:42:VAL:HG12	2:I:99:ASP:HB3	1.72	0.70
2:J:17:ASP:HB2	2:J:164:ASN:ND2	2.07	0.70
2:N:137:LEU:O	2:N:141:THR:HG22	1.91	0.70
2:P:55:THR:HG22	2:Q:83:ARG:HG2	1.73	0.70
1:A:367:ILE:HD11	1:A:421:ILE:CD1	2.22	0.70
1:A:235:ILE:HG22	1:A:237:PRO:HD3	1.72	0.70
1:D:83:ALA:HB1	1:D:262:ILE:HD13	1.73	0.70
2:Q:118:ASP:O	2:Q:119:GLN:HB2	1.92	0.70
1:W:60:GLY:HA3	1:W:392:GLY:HA3	1.72	0.70
1:W:347:GLU:HB2	1:W:348:PRO:HD3	1.74	0.70
1:X:108:MET:HE2	1:X:295:HIS:CD2	2.26	0.70
1:C:421:ILE:HG23	1:C:425:TYR:CD1	2.26	0.70
1:F:366:ASN:HB3	1:F:418:THR:HG22	1.74	0.70
2:G:22:LEU:HD22	2:G:27:MET:HE3	1.74	0.70
1:S:109:LYS:O	1:S:113:GLN:HB3	1.92	0.70
1:S:395:ARG:O	1:S:399:VAL:HG23	1.91	0.70
1:C:52:ASN:ND2	1:C:305:PHE:HB2	2.07	0.70
2:N:105:ILE:HG23	2:N:113:VAL:HB	1.74	0.70
2:O:60:PHE:CE2	2:O:97:VAL:HG11	2.26	0.70
1:U:23:ALA:HA	1:U:331:VAL:HG21	1.74	0.70
1:C:37:ARG:HD2	1:C:48:VAL:HG13	1.74	0.69
1:T:395:ARG:O	1:T:399:VAL:HG23	1.92	0.69
1:X:313:VAL:CG2	1:X:314:ALA:H	2.02	0.69
1:E:52:ASN:HD22	1:E:305:PHE:H	1.36	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:104:THR:HA	1:E:248:VAL:HG21	1.73	0.69
2:Q:137:LEU:O	2:Q:141:THR:HG22	1.91	0.69
1:U:385:ASN:HD21	1:U:395:ARG:HE	1.40	0.69
1:X:42:GLU:HB3	1:X:43:PRO:HD3	1.75	0.69
2:J:52:ASP:CA	2:J:55:THR:HG23	2.21	0.69
1:A:57:GLY:O	1:A:310:ALA:HA	1.92	0.69
1:D:37:ARG:HA	1:D:40:LEU:CD1	2.22	0.69
1:F:405:ASP:HB3	1:F:406:LYS:HD2	1.74	0.69
2:L:37:LEU:HB2	2:L:42:VAL:HG23	1.73	0.69
1:T:235:ILE:HG22	1:T:237:PRO:HD3	1.75	0.69
1:E:5:THR:H	1:E:8:GLU:HB3	1.57	0.69
1:F:100:ILE:HB	1:F:291:VAL:HG21	1.74	0.69
2:I:105:ILE:HG23	2:I:113:VAL:HB	1.74	0.69
1:W:395:ARG:O	1:W:399:VAL:HG23	1.91	0.69
1:F:360:MET:HE2	1:F:360:MET:CA	2.23	0.69
2:G:38:TYR:CE1	2:G:69:GLY:HA3	2.27	0.69
2:G:137:LEU:CD1	2:M:136:ALA:HB1	2.22	0.69
2:I:37:LEU:HD21	2:I:57:PHE:CZ	2.27	0.69
2:I:105:ILE:CG2	2:I:113:VAL:HB	2.23	0.69
1:T:23:ALA:HA	1:T:331:VAL:HG21	1.74	0.69
1:U:347:GLU:HB2	1:U:348:PRO:HD3	1.74	0.69
1:E:57:GLY:O	1:E:310:ALA:HA	1.92	0.69
2:H:37:LEU:HD21	2:H:57:PHE:CZ	2.28	0.69
1:T:347:GLU:HB2	1:T:348:PRO:HD3	1.75	0.69
1:D:64:THR:HB	3:D:453:ATP:O1A	1.92	0.69
2:J:137:LEU:O	2:J:141:THR:HG23	1.93	0.69
2:K:38:TYR:CE1	2:K:69:GLY:HA3	2.28	0.69
1:U:120:ARG:CD	1:U:232:ALA:HA	2.23	0.69
1:V:5:THR:O	1:V:9:ILE:HG13	1.92	0.69
1:V:279:GLN:NE2	1:V:320:ILE:N	2.40	0.69
1:W:37:ARG:HH21	1:W:302:HIS:CE1	2.11	0.69
1:X:63:LYS:HB2	3:X:461:ATP:O2B	1.93	0.69
2:O:20:VAL:CG2	1:V:444:LEU:HD21	2.20	0.69
2:H:91:LEU:H	2:H:91:LEU:HD12	1.57	0.69
1:T:5:THR:O	1:T:9:ILE:HG13	1.93	0.69
1:U:37:ARG:HH21	1:U:302:HIS:CE1	2.11	0.69
1:V:37:ARG:HH21	1:V:302:HIS:CE1	2.11	0.69
1:D:23:ALA:HA	1:D:331:VAL:HG21	1.75	0.68
1:E:264:LYS:HZ1	1:E:279:GLN:NE2	1.90	0.68
2:H:105:ILE:HG23	2:H:113:VAL:HB	1.75	0.68
2:K:37:LEU:HB2	2:K:42:VAL:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:THR:H	1:A:8:GLU:HB3	1.57	0.68
1:B:435:GLU:HG2	1:B:436:ASN:N	2.07	0.68
1:C:36:ARG:O	1:C:39:GLN:HB3	1.93	0.68
1:C:351:SER:O	1:C:355:GLN:HG3	1.94	0.68
1:D:367:ILE:HD11	1:D:421:ILE:CD1	2.24	0.68
1:E:409:PHE:CD1	1:F:6:PRO:HB3	2.28	0.68
1:F:111:VAL:O	1:F:114:GLN:HG2	1.93	0.68
2:I:13:VAL:HG22	2:I:171:GLU:CB	2.22	0.68
1:A:37:ARG:HA	1:A:40:LEU:CD1	2.24	0.68
1:B:37:ARG:HD2	1:B:48:VAL:HG13	1.75	0.68
1:V:23:ALA:HA	1:V:331:VAL:HG21	1.75	0.68
1:C:52:ASN:ND2	1:C:305:PHE:N	2.38	0.68
2:K:120:ILE:HD11	2:K:138:VAL:HG21	1.74	0.68
1:W:5:THR:O	1:W:9:ILE:HG13	1.94	0.68
1:X:23:ALA:HA	1:X:331:VAL:HG21	1.74	0.68
1:D:398:THR:HG22	1:D:399:VAL:N	2.07	0.68
1:W:23:ALA:HA	1:W:331:VAL:HG21	1.74	0.68
1:E:360:MET:HE2	1:E:360:MET:CA	2.23	0.68
2:I:38:TYR:CE1	2:I:69:GLY:HA3	2.27	0.68
2:I:52:ASP:CA	2:I:55:THR:HG23	2.24	0.68
2:J:22:LEU:HD22	2:J:27:MET:HE3	1.75	0.68
2:J:56:LEU:HD13	2:J:95:LEU:HG	1.75	0.68
2:N:131:LEU:HD11	2:N:135:ARG:HE	1.59	0.68
1:A:415:ASN:OD1	1:A:416:GLY:N	2.26	0.68
1:E:337:SER:HB3	1:E:340:ASP:OD2	1.94	0.68
2:I:107:THR:OG1	2:I:111:ASP:OD2	2.10	0.68
1:S:344:ILE:HG23	3:S:456:ATP:C2	2.29	0.68
1:U:439:LEU:HD23	1:U:439:LEU:H	1.59	0.68
1:D:37:ARG:HA	1:D:40:LEU:HD12	1.76	0.68
1:E:344:ILE:CG2	3:E:454:ATP:C2	2.77	0.68
1:E:403:LEU:HD23	1:E:403:LEU:C	2.19	0.68
2:I:79:ALA:HB1	2:I:83:ARG:HH21	1.58	0.68
1:S:23:ALA:HA	1:S:331:VAL:HG21	1.76	0.68
2:N:7:ARG:NE	2:N:119:GLN:HE21	1.91	0.68
1:S:370:THR:HG22	1:S:421:ILE:O	1.94	0.68
1:S:442:PHE:O	1:S:443:ILE:HD13	1.93	0.68
2:K:137:LEU:HD11	2:Q:136:ALA:HB1	1.76	0.68
2:O:131:LEU:HD11	2:O:135:ARG:HE	1.58	0.68
1:V:385:ASN:HD21	1:V:395:ARG:HE	1.42	0.68
1:C:349:HIS:O	1:C:350:ALA:HB3	1.93	0.67
1:E:20:GLN:HA	1:E:20:GLN:NE2	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:88:LEU:O	2:G:88:LEU:HD23	1.94	0.67
1:T:42:GLU:HB3	1:T:43:PRO:HD3	1.76	0.67
1:B:405:ASP:HB3	1:B:406:LYS:HD2	1.76	0.67
1:D:108:MET:HE2	1:D:244:ALA:HB2	1.75	0.67
1:F:406:LYS:HD2	1:F:406:LYS:N	2.05	0.67
2:L:105:ILE:CG2	2:L:113:VAL:HB	2.24	0.67
1:T:227:ILE:HG23	1:T:228:ASP:H	1.59	0.67
1:U:437:GLU:HG3	1:U:440:SER:HB2	1.76	0.67
1:B:360:MET:HE2	1:B:360:MET:CA	2.22	0.67
1:W:42:GLU:HB3	1:W:43:PRO:HD3	1.77	0.67
1:A:79:ILE:HG22	1:A:103:LEU:HD13	1.74	0.67
2:P:60:PHE:CE2	2:P:97:VAL:HG11	2.29	0.67
1:X:37:ARG:HH21	1:X:302:HIS:CE1	2.11	0.67
1:X:344:ILE:HG23	3:X:461:ATP:H2	1.59	0.67
1:F:5:THR:H	1:F:8:GLU:HB3	1.58	0.67
1:F:264:LYS:HZ3	1:F:279:GLN:HE22	1.42	0.67
1:F:367:ILE:HD11	1:F:421:ILE:HD11	1.75	0.67
1:F:439:LEU:O	1:F:440:SER:C	2.36	0.67
2:L:137:LEU:CD1	2:R:136:ALA:HB1	2.24	0.67
2:M:118:ASP:C	2:M:118:ASP:OD1	2.36	0.67
1:S:5:THR:O	1:S:9:ILE:HG13	1.94	0.67
1:D:360:MET:HE2	1:D:360:MET:CA	2.24	0.67
1:E:360:MET:HE1	1:F:36:ARG:NH1	2.09	0.67
1:V:370:THR:HG22	1:V:421:ILE:O	1.95	0.67
1:E:52:ASN:ND2	1:E:305:PHE:N	2.41	0.67
2:G:1:THR:HG23	2:G:33:LYS:NZ	2.09	0.67
2:I:46:PHE:HB3	2:I:95:LEU:CD2	2.25	0.67
1:A:37:ARG:HA	1:A:40:LEU:HD12	1.76	0.67
1:B:57:GLY:O	1:B:310:ALA:HA	1.94	0.67
1:E:23:ALA:HA	1:E:331:VAL:HG21	1.76	0.67
2:K:105:ILE:HG23	2:K:113:VAL:HB	1.76	0.67
1:X:63:LYS:NZ	1:X:308:SER:HB2	2.10	0.67
1:F:250:GLN:HA	1:F:250:GLN:NE2	2.10	0.67
2:L:103:SER:O	2:L:104:LEU:HD12	1.95	0.67
1:T:17:ILE:HD11	1:T:65:GLU:HB3	1.76	0.67
1:A:356:TYR:CD1	1:A:400:MET:HE3	2.31	0.67
1:D:57:GLY:O	1:D:310:ALA:HA	1.94	0.67
1:V:347:GLU:HB2	1:V:348:PRO:HD3	1.76	0.67
2:J:144:SER:HB3	2:J:147:GLU:CG	2.25	0.66
1:W:279:GLN:NE2	1:W:320:ILE:N	2.41	0.66
1:D:250:GLN:NE2	1:D:250:GLN:HA	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:GLN:HA	1:E:41:GLN:NE2	2.09	0.66
2:G:107:THR:OG1	2:G:111:ASP:OD2	2.10	0.66
2:H:7:ARG:CD	2:H:119:GLN:OE1	2.43	0.66
2:K:91:LEU:O	2:K:108:GLY:HA3	1.95	0.66
2:M:164:ASN:ND2	2:M:164:ASN:H	1.93	0.66
1:A:264:LYS:NZ	1:A:279:GLN:NE2	2.31	0.66
1:D:108:MET:HE3	1:D:241:LYS:HA	1.77	0.66
2:K:55:THR:O	2:K:59:LEU:HD13	1.95	0.66
2:M:137:LEU:O	2:M:141:THR:HG22	1.95	0.66
1:S:279:GLN:NE2	1:S:320:ILE:N	2.36	0.66
1:W:247:ALA:O	1:W:251:ASN:N	2.28	0.66
1:X:347:GLU:HB2	1:X:348:PRO:HD3	1.77	0.66
1:D:421:ILE:HG23	1:D:425:TYR:CD1	2.30	0.66
1:F:63:LYS:HB2	3:F:455:ATP:O2B	1.94	0.66
2:O:105:ILE:HG23	2:O:113:VAL:HB	1.78	0.66
1:X:344:ILE:HG23	3:X:461:ATP:C2	2.30	0.66
2:K:13:VAL:HG22	2:K:171:GLU:HB3	1.78	0.66
1:T:257:ASP:HA	1:T:308:SER:OG	1.95	0.66
1:U:42:GLU:HB3	1:U:43:PRO:HD3	1.75	0.66
1:U:65:GLU:HG2	3:U:458:ATP:C5'	2.22	0.66
1:A:55:MET:HE3	1:A:306:ILE:CG2	2.24	0.66
1:B:256:ILE:HG21	1:B:259:ILE:HD12	1.77	0.66
1:C:414:MET:HG2	1:C:414:MET:O	1.94	0.66
2:P:105:ILE:HG23	2:P:113:VAL:HB	1.77	0.66
2:Q:60:PHE:CE2	2:Q:97:VAL:HG11	2.31	0.66
1:A:377:ILE:O	1:A:380:ALA:HB3	1.95	0.66
1:C:264:LYS:NZ	1:C:279:GLN:NE2	2.40	0.66
1:E:283:LEU:HB2	1:E:284:PRO:HD3	1.77	0.66
1:F:52:ASN:O	1:F:328:PRO:HD2	1.96	0.66
2:G:84:THR:HG22	2:G:85:ASP:H	1.60	0.66
2:I:13:VAL:HG22	2:I:171:GLU:HB3	1.77	0.66
2:L:105:ILE:HG23	2:L:113:VAL:HB	1.78	0.66
1:V:64:THR:HB	3:V:459:ATP:O2A	1.96	0.66
1:B:83:ALA:HB1	1:B:262:ILE:HD13	1.78	0.66
1:C:435:GLU:CG	1:C:436:ASN:H	2.07	0.66
2:M:105:ILE:HG23	2:M:113:VAL:HB	1.77	0.66
2:Q:105:ILE:HG23	2:Q:113:VAL:HB	1.77	0.66
1:A:20:GLN:HE21	1:A:20:GLN:N	1.94	0.66
1:F:415:ASN:OD1	1:F:416:GLY:N	2.29	0.66
2:I:165:THR:HA	2:I:167:PHE:CE2	2.31	0.66
1:S:344:ILE:HG23	3:S:456:ATP:H2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:137:LEU:HD11	2:M:136:ALA:HB1	1.78	0.66
2:K:46:PHE:HB3	2:K:95:LEU:CD2	2.26	0.66
2:K:137:LEU:CD1	2:Q:136:ALA:HB1	2.25	0.66
2:M:83:ARG:CB	2:R:55:THR:HG22	2.25	0.66
2:M:103:SER:O	2:M:104:LEU:HD23	1.95	0.66
1:S:320:ILE:HD11	1:S:323:LEU:HD13	1.77	0.66
1:A:23:ALA:HA	1:A:331:VAL:HG21	1.78	0.65
1:C:366:ASN:HB3	1:C:418:THR:HG22	1.78	0.65
2:R:137:LEU:O	2:R:141:THR:HG22	1.96	0.65
1:S:42:GLU:HB3	1:S:43:PRO:HD3	1.78	0.65
1:V:42:GLU:HB3	1:V:43:PRO:HD3	1.77	0.65
1:B:443:ILE:HD11	2:H:72:LEU:HD11	1.77	0.65
2:I:56:LEU:HD13	2:I:95:LEU:HG	1.78	0.65
2:N:56:LEU:HD23	2:N:95:LEU:HD22	1.78	0.65
2:N:94:MET:HE3	2:N:123:ILE:HB	1.78	0.65
1:A:41:GLN:NE2	1:A:41:GLN:HA	2.09	0.65
1:A:360:MET:HE2	1:A:360:MET:CA	2.26	0.65
1:C:415:ASN:OD1	1:C:416:GLY:N	2.28	0.65
1:F:37:ARG:HA	1:F:40:LEU:HD12	1.78	0.65
1:F:280:ARG:HH11	1:F:280:ARG:HG3	1.61	0.65
2:L:13:VAL:HG22	2:L:171:GLU:HB3	1.79	0.65
2:N:60:PHE:CE2	2:N:97:VAL:HG11	2.32	0.65
2:O:55:THR:HG22	2:P:83:ARG:CB	2.26	0.65
1:T:37:ARG:HH21	1:T:302:HIS:CE1	2.13	0.65
1:U:345:LEU:HD23	1:U:374:VAL:HG13	1.79	0.65
1:E:100:ILE:HB	1:E:291:VAL:HG21	1.76	0.65
2:O:137:LEU:O	2:O:141:THR:HG22	1.96	0.65
1:S:347:GLU:HB2	1:S:348:PRO:HD3	1.76	0.65
1:A:283:LEU:HB2	1:A:284:PRO:HD3	1.78	0.65
1:B:275:ARG:C	1:B:277:GLY:N	2.55	0.65
1:F:27:VAL:HB	1:F:70:LEU:HD22	1.78	0.65
1:F:352:LEU:HD13	1:F:400:MET:HG3	1.78	0.65
1:W:326:ARG:HB3	1:W:326:ARG:NH1	2.11	0.65
1:A:235:ILE:HG22	1:A:237:PRO:CD	2.26	0.65
1:B:37:ARG:HA	1:B:40:LEU:CD1	2.26	0.65
2:I:137:LEU:CD1	2:O:136:ALA:HB1	2.27	0.65
2:R:60:PHE:CE2	2:R:97:VAL:HG11	2.31	0.65
1:V:439:LEU:O	1:V:441:ARG:N	2.30	0.65
1:A:20:GLN:HE21	1:A:20:GLN:H	1.43	0.65
1:C:52:ASN:HD22	1:C:305:PHE:N	1.95	0.65
1:C:352:LEU:HD13	1:C:400:MET:HG3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:63:LYS:NZ	1:T:308:SER:HB2	2.12	0.65
1:V:326:ARG:HB3	1:V:326:ARG:NH1	2.10	0.65
1:W:257:ASP:HA	1:W:308:SER:OG	1.96	0.65
2:J:87:ALA:O	2:J:88:LEU:HB2	1.97	0.65
1:S:18:ILE:HD11	1:S:343:ARG:NH2	2.12	0.65
1:V:36:ARG:HA	1:V:36:ARG:HE	1.62	0.65
1:D:241:LYS:O	1:D:245:ILE:HG13	1.98	0.64
1:S:439:LEU:HG	1:S:440:SER:H	1.61	0.64
1:U:5:THR:O	1:U:9:ILE:HG13	1.97	0.64
1:U:63:LYS:NZ	1:U:308:SER:HB2	2.12	0.64
1:W:63:LYS:HZ2	1:W:308:SER:HB2	1.62	0.64
1:D:367:ILE:CD1	1:D:421:ILE:HD11	2.27	0.64
2:K:107:THR:OG1	2:K:111:ASP:OD2	2.09	0.64
1:V:439:LEU:HG	1:V:440:SER:H	1.62	0.64
1:B:406:LYS:HD2	1:B:406:LYS:N	2.06	0.64
1:F:437:GLU:O	1:F:438:ASP:O	2.14	0.64
2:H:37:LEU:HB2	2:H:42:VAL:HG23	1.80	0.64
2:J:38:TYR:CE1	2:J:69:GLY:HA3	2.32	0.64
2:J:52:ASP:HA	2:J:55:THR:CG2	2.25	0.64
1:S:280:ARG:HH22	1:T:261:LYS:HE3	1.61	0.64
1:T:439:LEU:HG	1:T:440:SER:H	1.60	0.64
1:F:20:GLN:HA	1:F:20:GLN:NE2	2.13	0.64
1:F:377:ILE:O	1:F:380:ALA:HB3	1.97	0.64
2:G:105:ILE:HG22	2:G:113:VAL:O	1.98	0.64
2:Q:55:THR:HG22	2:R:83:ARG:HG2	1.80	0.64
1:S:36:ARG:HA	1:S:36:ARG:HE	1.61	0.64
1:S:385:ASN:HD21	1:S:395:ARG:HE	1.44	0.64
1:W:63:LYS:NZ	1:W:308:SER:HB2	2.13	0.64
1:X:5:THR:O	1:X:9:ILE:HG13	1.97	0.64
1:A:421:ILE:HA	1:A:425:TYR:HD1	1.63	0.64
1:U:279:GLN:NE2	1:U:320:ILE:N	2.40	0.64
1:U:370:THR:HG22	1:U:421:ILE:O	1.97	0.64
1:W:370:THR:HG22	1:W:421:ILE:O	1.97	0.64
1:X:279:GLN:NE2	1:X:320:ILE:N	2.41	0.64
1:C:37:ARG:HH12	1:C:38:MET:HE2	1.63	0.64
1:E:244:ALA:O	1:E:247:ALA:HB3	1.97	0.64
1:S:12:GLU:HG2	1:S:73:LEU:HD23	1.79	0.64
1:T:320:ILE:HD11	1:T:323:LEU:HD13	1.79	0.64
1:U:344:ILE:HG23	3:U:458:ATP:H2	1.62	0.64
1:X:245:ILE:HG22	1:X:249:GLU:HG3	1.80	0.64
1:C:27:VAL:HB	1:C:70:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ARG:HA	1:B:240:LEU:HD21	1.80	0.64
2:H:55:THR:O	2:H:59:LEU:HD13	1.97	0.64
1:S:17:ILE:HD11	1:S:65:GLU:HB3	1.79	0.64
1:V:257:ASP:HA	1:V:308:SER:OG	1.98	0.64
1:A:57:GLY:HA3	1:A:63:LYS:HE3	1.80	0.64
2:J:17:ASP:O	2:J:33:LYS:HD2	1.98	0.64
1:W:36:ARG:HA	1:W:36:ARG:HE	1.62	0.64
1:X:442:PHE:HD1	1:X:442:PHE:N	1.87	0.64
2:L:1:THR:HG22	2:L:2:THR:N	2.11	0.64
1:U:36:ARG:HA	1:U:36:ARG:HE	1.61	0.64
1:U:257:ASP:HA	1:U:308:SER:OG	1.98	0.64
1:A:37:ARG:HH22	1:A:250:GLN:HE22	1.47	0.63
1:B:347:GLU:HB2	1:B:348:PRO:HD3	1.80	0.63
1:B:421:ILE:HG23	1:B:425:TYR:HD1	1.59	0.63
1:C:283:LEU:HB2	1:C:284:PRO:HD3	1.80	0.63
1:D:100:ILE:HB	1:D:291:VAL:HG21	1.79	0.63
1:D:369:PHE:CE2	1:D:421:ILE:HD12	2.33	0.63
2:G:80:LYS:HA	2:G:83:ARG:HD3	1.80	0.63
2:O:76:VAL:HG22	1:U:443:ILE:HD11	1.78	0.63
2:Q:56:LEU:HD23	2:Q:95:LEU:HD22	1.80	0.63
1:S:257:ASP:HA	1:S:308:SER:OG	1.97	0.63
1:W:320:ILE:HD11	1:W:323:LEU:HD13	1.80	0.63
1:X:17:ILE:HD13	1:X:66:ILE:CG1	2.28	0.63
2:R:105:ILE:HG23	2:R:113:VAL:HB	1.80	0.63
1:T:326:ARG:HB3	1:T:326:ARG:NH1	2.13	0.63
1:V:441:ARG:HB3	1:V:442:PHE:CD1	2.33	0.63
1:B:20:GLN:HA	1:B:20:GLN:NE2	2.11	0.63
1:C:391:ILE:HG22	1:D:321:PRO:HB3	1.80	0.63
2:H:91:LEU:HD12	2:H:91:LEU:N	2.13	0.63
2:K:13:VAL:HG22	2:K:171:GLU:CB	2.28	0.63
2:K:86:ARG:HG2	2:K:87:ALA:N	2.13	0.63
1:V:23:ALA:O	1:V:27:VAL:HG23	1.99	0.63
1:B:351:SER:O	1:B:355:GLN:HG3	1.98	0.63
1:S:441:ARG:HB3	1:S:442:PHE:CD1	2.29	0.63
1:T:345:LEU:HD23	1:T:374:VAL:HG13	1.80	0.63
1:T:370:THR:HG22	1:T:421:ILE:O	1.98	0.63
1:U:326:ARG:HB3	1:U:326:ARG:NH1	2.13	0.63
1:A:36:ARG:O	1:A:39:GLN:HB3	1.98	0.63
1:F:56:ILE:HD12	1:F:56:ILE:N	2.13	0.63
2:Q:164:ASN:ND2	2:Q:164:ASN:H	1.95	0.63
1:U:17:ILE:HD11	1:U:65:GLU:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:370:THR:HG22	1:X:421:ILE:O	1.98	0.63
1:E:433:VAL:HG13	1:E:433:VAL:O	1.98	0.63
2:P:56:LEU:HD23	2:P:95:LEU:HD22	1.81	0.63
1:T:385:ASN:HD21	1:T:395:ARG:HE	1.47	0.63
1:X:36:ARG:HE	1:X:36:ARG:HA	1.63	0.63
1:B:104:THR:HA	1:B:248:VAL:CG2	2.28	0.63
1:C:57:GLY:HA3	1:C:63:LYS:HE3	1.81	0.63
2:K:165:THR:HA	2:K:167:PHE:CE2	2.34	0.63
1:S:27:VAL:HG21	1:S:66:ILE:HG21	1.81	0.63
1:A:352:LEU:HD13	1:A:400:MET:HG3	1.80	0.63
1:E:20:GLN:HE21	1:E:20:GLN:N	1.95	0.63
1:E:264:LYS:CE	1:E:279:GLN:HE22	2.11	0.63
2:G:120:ILE:HD11	2:G:138:VAL:HG21	1.80	0.63
1:W:17:ILE:HD11	1:W:65:GLU:HB3	1.79	0.63
1:X:236:ASN:H	1:X:237:PRO:HD3	1.63	0.63
1:E:5:THR:O	1:E:9:ILE:HG13	1.99	0.63
1:E:60:GLY:HA2	3:E:454:ATP:O3A	1.99	0.63
1:F:421:ILE:HG23	1:F:425:TYR:CD1	2.34	0.63
2:I:37:LEU:HB2	2:I:42:VAL:CG2	2.29	0.63
1:X:286:VAL:HA	1:X:305:PHE:CE1	2.34	0.63
1:X:385:ASN:HD21	1:X:395:ARG:HE	1.46	0.63
1:A:367:ILE:CD1	1:A:421:ILE:HD11	2.28	0.62
1:E:36:ARG:O	1:E:39:GLN:HB3	1.99	0.62
1:F:20:GLN:HE21	1:F:20:GLN:HA	1.63	0.62
2:H:17:ASP:O	2:H:33:LYS:HD2	1.98	0.62
2:H:42:VAL:HG12	2:H:99:ASP:HB3	1.80	0.62
2:M:7:ARG:NE	2:M:119:GLN:OE1	2.32	0.62
1:S:439:LEU:O	1:S:441:ARG:N	2.32	0.62
1:U:63:LYS:HZ2	1:U:308:SER:HB2	1.63	0.62
1:W:37:ARG:HG2	1:W:37:ARG:HH11	1.64	0.62
1:X:18:ILE:HD11	1:X:343:ARG:NH2	2.14	0.62
1:C:356:TYR:CD1	1:C:400:MET:HE3	2.34	0.62
2:J:13:VAL:HG22	2:J:171:GLU:HB3	1.79	0.62
1:V:297:MET:HE2	1:W:105:ASP:HB3	1.81	0.62
1:X:326:ARG:HB3	1:X:326:ARG:NH1	2.13	0.62
1:A:112:ARG:O	1:A:114:GLN:N	2.26	0.62
1:C:362:THR:CG2	1:D:39:GLN:HG2	2.28	0.62
1:D:362:THR:CG2	1:E:39:GLN:HG2	2.28	0.62
2:L:37:LEU:HB2	2:L:42:VAL:CG2	2.28	0.62
1:C:20:GLN:CA	1:C:20:GLN:HE21	2.12	0.62
2:Q:105:ILE:CG2	2:Q:113:VAL:HB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:27:VAL:HG21	1:W:66:ILE:HG21	1.81	0.62
1:W:385:ASN:HD21	1:W:395:ARG:HE	1.45	0.62
1:B:58:PRO:O	1:B:63:LYS:NZ	2.32	0.62
1:C:356:TYR:HE1	1:C:400:MET:HB3	1.64	0.62
1:D:337:SER:HB3	1:D:340:ASP:OD2	1.98	0.62
2:K:5:SER:HB2	2:K:14:VAL:HG22	1.81	0.62
2:N:8:ARG:HH11	2:N:8:ARG:CB	2.12	0.62
1:W:326:ARG:HH11	1:W:326:ARG:CB	2.13	0.62
1:A:112:ARG:C	1:A:114:GLN:H	2.07	0.62
1:E:414:MET:O	1:E:414:MET:HG2	1.99	0.62
1:T:12:GLU:HG2	1:T:73:LEU:HD23	1.82	0.62
1:X:320:ILE:HD11	1:X:323:LEU:HD13	1.82	0.62
1:A:233:LYS:NZ	1:A:234:LEU:HB2	2.15	0.62
1:A:316:PRO:C	1:A:318:ASP:H	2.08	0.62
2:N:3:ILE:O	2:N:122:ALA:HA	1.99	0.62
2:P:49:GLY:O	2:P:50:THR:C	2.43	0.62
2:R:94:MET:HE3	2:R:123:ILE:HB	1.80	0.62
1:W:64:THR:HB	3:W:460:ATP:O2A	2.00	0.62
1:C:405:ASP:HB3	1:C:406:LYS:HD2	1.80	0.62
1:D:322:GLU:OE2	1:D:322:GLU:N	2.29	0.62
1:F:55:MET:HE3	1:F:306:ILE:CG2	2.30	0.62
2:J:52:ASP:OD2	2:J:91:LEU:HA	2.00	0.62
2:P:164:ASN:ND2	2:P:164:ASN:H	1.96	0.62
1:S:63:LYS:NZ	1:S:308:SER:HB2	2.15	0.62
1:V:27:VAL:HG21	1:V:66:ILE:HG21	1.82	0.62
1:D:407:ILE:HD11	1:D:419:VAL:HG11	1.82	0.62
1:F:38:MET:HG3	1:F:45:ARG:HH12	1.65	0.62
2:H:137:LEU:CD1	2:N:136:ALA:HB1	2.30	0.62
2:K:1:THR:HG23	2:K:33:LYS:HD3	1.82	0.62
2:N:105:ILE:CG2	2:N:113:VAL:HB	2.30	0.62
1:V:12:GLU:HG2	1:V:73:LEU:HD23	1.81	0.62
1:B:55:MET:HE3	1:B:306:ILE:HG21	1.82	0.62
1:F:264:LYS:HE3	1:F:264:LYS:H	1.64	0.62
2:M:105:ILE:CG2	2:M:113:VAL:HB	2.29	0.62
2:O:56:LEU:HD23	2:O:95:LEU:HD22	1.82	0.62
1:T:36:ARG:HA	1:T:36:ARG:HE	1.63	0.62
1:T:247:ALA:O	1:T:251:ASN:HB2	2.00	0.62
1:T:437:GLU:HG3	1:T:438:ASP:N	2.08	0.62
1:U:17:ILE:HD13	1:U:66:ILE:CG1	2.30	0.62
1:B:293:THR:C	1:B:295:HIS:H	2.08	0.61
1:C:421:ILE:HA	1:C:425:TYR:HD1	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:403:LEU:CD2	1:E:404:MET:SD	2.88	0.61
2:H:46:PHE:HB3	2:H:95:LEU:CD2	2.30	0.61
2:I:52:ASP:HA	2:I:55:THR:CG2	2.29	0.61
2:R:8:ARG:HH11	2:R:8:ARG:CB	2.13	0.61
1:W:345:LEU:HD23	1:W:374:VAL:HG13	1.80	0.61
1:X:112:ARG:HB2	1:X:240:LEU:HD21	1.81	0.61
1:A:60:GLY:HA2	3:A:450:ATP:O3A	2.00	0.61
1:A:232:ALA:HA	1:A:235:ILE:HD12	1.81	0.61
1:B:13:LEU:HD13	1:B:24:LYS:HG2	1.82	0.61
1:C:367:ILE:HD11	1:C:421:ILE:CD1	2.30	0.61
1:D:382:PHE:C	1:D:382:PHE:CD2	2.78	0.61
1:D:391:ILE:HG22	1:E:321:PRO:HB3	1.82	0.61
1:D:405:ASP:HB3	1:D:406:LYS:HD2	1.81	0.61
1:F:381:ALA:O	1:F:384:VAL:HG13	2.00	0.61
2:M:7:ARG:HH21	2:M:103:SER:HB3	1.64	0.61
2:M:55:THR:HG22	2:N:83:ARG:CG	2.28	0.61
2:Q:94:MET:HE3	2:Q:123:ILE:HB	1.81	0.61
2:R:164:ASN:ND2	2:R:164:ASN:H	1.98	0.61
1:S:326:ARG:HB3	1:S:326:ARG:NH1	2.14	0.61
1:V:63:LYS:NZ	1:V:308:SER:HB2	2.13	0.61
1:F:20:GLN:HE21	1:F:20:GLN:N	1.98	0.61
2:M:17:ASP:HB2	2:M:164:ASN:HD22	1.66	0.61
2:Q:17:ASP:HB2	2:Q:164:ASN:HD21	1.64	0.61
1:S:398:THR:HA	1:X:328:PRO:HB3	1.81	0.61
1:T:120:ARG:NH2	1:T:121:ALA:HB2	2.16	0.61
1:W:280:ARG:HH22	1:X:261:LYS:HE3	1.64	0.61
1:C:370:THR:HG23	1:C:421:ILE:O	1.99	0.61
1:D:79:ILE:CG2	1:D:103:LEU:HD13	2.31	0.61
1:D:283:LEU:HB2	1:D:284:PRO:HD3	1.82	0.61
2:G:17:ASP:OD2	2:G:33:LYS:HE3	2.00	0.61
2:O:8:ARG:HH11	2:O:8:ARG:CB	2.12	0.61
2:Q:7:ARG:HH21	2:Q:103:SER:HB3	1.65	0.61
2:Q:72:LEU:O	2:Q:76:VAL:HG23	2.01	0.61
2:R:3:ILE:O	2:R:122:ALA:HA	2.01	0.61
1:S:233:LYS:C	1:S:235:ILE:H	2.08	0.61
1:V:51:LYS:HE2	1:W:356:TYR:OH	2.00	0.61
2:I:83:ARG:HG2	2:J:55:THR:CB	2.29	0.61
2:J:105:ILE:HG23	2:J:113:VAL:HB	1.80	0.61
2:P:105:ILE:CG2	2:P:113:VAL:HB	2.29	0.61
2:P:137:LEU:O	2:P:141:THR:HG22	2.00	0.61
1:V:326:ARG:HH11	1:V:326:ARG:CB	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASN:O	1:B:328:PRO:HD2	2.00	0.61
1:C:237:PRO:HB3	1:C:241:LYS:HZ1	1.66	0.61
1:D:264:LYS:HE3	1:D:264:LYS:H	1.63	0.61
1:E:367:ILE:CD1	1:E:421:ILE:HD11	2.29	0.61
1:E:440:SER:O	1:E:442:PHE:N	2.34	0.61
2:G:71:LEU:HD13	2:G:71:LEU:C	2.26	0.61
2:J:42:VAL:HG12	2:J:99:ASP:HB3	1.82	0.61
2:K:71:LEU:C	2:K:71:LEU:HD13	2.26	0.61
2:M:8:ARG:HH11	2:M:8:ARG:CB	2.10	0.61
2:P:94:MET:HE3	2:P:123:ILE:HB	1.83	0.61
1:S:64:THR:HB	3:S:456:ATP:O2A	2.00	0.61
1:T:63:LYS:HZ2	1:T:308:SER:HB2	1.65	0.61
1:T:283:LEU:HD13	1:T:323:LEU:HD12	1.83	0.61
1:A:435:GLU:C	1:A:437:GLU:H	2.08	0.61
1:B:227:ILE:O	1:B:227:ILE:HG12	1.99	0.61
1:F:57:GLY:HA3	1:F:63:LYS:HE3	1.83	0.61
2:H:144:SER:HB3	2:H:147:GLU:CG	2.31	0.61
2:K:49:GLY:O	2:K:50:THR:C	2.42	0.61
2:K:57:PHE:HA	2:K:95:LEU:HD11	1.82	0.61
2:Q:3:ILE:O	2:Q:122:ALA:HA	2.00	0.61
1:U:12:GLU:HG2	1:U:73:LEU:HD23	1.83	0.61
1:C:443:ILE:HG12	2:I:112:VAL:HG21	1.82	0.61
1:F:37:ARG:HH22	1:F:250:GLN:HE22	1.48	0.61
1:F:351:SER:O	1:F:355:GLN:HG3	2.00	0.61
1:S:15:GLN:O	1:S:349:HIS:N	2.31	0.61
1:V:80:LYS:HG3	1:V:255:PHE:HD2	1.66	0.61
1:X:12:GLU:HG2	1:X:73:LEU:HD23	1.83	0.61
1:X:345:LEU:HD23	1:X:374:VAL:HG13	1.82	0.61
1:B:362:THR:HG21	1:C:39:GLN:HG2	1.82	0.61
1:B:370:THR:HG23	1:B:421:ILE:O	2.00	0.61
2:K:105:ILE:HG22	2:K:113:VAL:O	2.01	0.61
1:V:5:THR:OG1	1:V:6:PRO:HD2	2.01	0.61
1:X:326:ARG:HH11	1:X:326:ARG:CB	2.14	0.61
1:B:264:LYS:HE3	1:B:264:LYS:H	1.64	0.61
1:C:37:ARG:HG2	1:C:38:MET:N	2.15	0.61
1:C:235:ILE:HG22	1:C:236:ASN:N	2.14	0.61
1:F:34:ARG:CZ	1:F:251:ASN:HA	2.31	0.61
1:S:442:PHE:CD1	1:S:442:PHE:N	2.69	0.61
1:V:37:ARG:HG2	1:V:37:ARG:HH11	1.66	0.61
1:W:283:LEU:HD13	1:W:323:LEU:HD12	1.83	0.61
1:A:407:ILE:HD11	1:A:419:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:THR:HA	1:D:248:VAL:CG2	2.31	0.60
1:F:37:ARG:HB2	1:F:48:VAL:HG11	1.83	0.60
2:H:13:VAL:HG22	2:H:171:GLU:HB3	1.82	0.60
2:J:37:LEU:HD21	2:J:57:PHE:CZ	2.36	0.60
1:V:60:GLY:HA3	1:V:392:GLY:HA3	1.82	0.60
1:A:435:GLU:O	1:A:437:GLU:N	2.28	0.60
1:B:316:PRO:C	1:B:318:ASP:H	2.08	0.60
1:F:438:ASP:O	1:F:439:LEU:C	2.43	0.60
2:I:17:ASP:HB2	2:I:164:ASN:HD22	1.63	0.60
2:M:60:PHE:CE2	2:M:97:VAL:HG11	2.37	0.60
2:O:55:THR:HG22	2:P:83:ARG:HG2	1.83	0.60
1:S:362:THR:HG21	1:X:39:GLN:HB2	1.83	0.60
1:A:443:ILE:HD11	2:G:72:LEU:HD11	1.83	0.60
1:D:12:GLU:O	1:D:15:GLN:HB2	2.01	0.60
1:D:250:GLN:HA	1:D:250:GLN:HE21	1.65	0.60
1:D:437:GLU:O	1:D:438:ASP:C	2.44	0.60
1:E:25:ARG:O	1:E:28:ALA:HB3	2.02	0.60
1:S:37:ARG:HH11	1:S:37:ARG:HG2	1.66	0.60
1:S:108:MET:HE1	1:S:244:ALA:CB	2.30	0.60
1:V:20:GLN:O	1:V:21:ALA:HB2	2.01	0.60
1:A:443:ILE:HG12	2:G:112:VAL:HG21	1.83	0.60
1:C:370:THR:O	1:C:373:ALA:HB3	2.01	0.60
1:D:275:ARG:C	1:D:277:GLY:N	2.48	0.60
1:F:5:THR:O	1:F:9:ILE:HG13	2.02	0.60
2:J:137:LEU:HD11	2:P:136:ALA:HB1	1.82	0.60
2:O:164:ASN:ND2	2:O:164:ASN:H	1.98	0.60
1:S:286:VAL:HA	1:S:305:PHE:CE1	2.37	0.60
1:U:303:ILE:HG22	1:U:304:LEU:N	2.16	0.60
1:W:20:GLN:O	1:W:21:ALA:HB2	2.02	0.60
1:W:386:GLU:O	1:W:386:GLU:HG2	2.00	0.60
1:B:437:GLU:O	1:B:438:ASP:O	2.18	0.60
1:C:20:GLN:HE21	1:C:20:GLN:N	1.99	0.60
1:C:300:THR:HA	1:C:303:ILE:HG12	1.83	0.60
2:G:17:ASP:HB2	2:G:164:ASN:HD22	1.66	0.60
1:V:434:VAL:HG12	1:V:435:GLU:N	2.15	0.60
1:A:118:LYS:C	1:A:120:ARG:H	2.10	0.60
1:B:415:ASN:OD1	1:B:416:GLY:N	2.34	0.60
1:C:55:MET:HE3	1:C:306:ILE:CG2	2.31	0.60
1:C:57:GLY:O	1:C:310:ALA:HA	2.01	0.60
1:F:109:LYS:O	1:F:113:GLN:HB2	2.01	0.60
2:G:60:PHE:CE2	2:G:97:VAL:HG11	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:42:VAL:HG12	2:L:99:ASP:HB3	1.82	0.60
2:R:105:ILE:CG2	2:R:113:VAL:HB	2.32	0.60
1:U:326:ARG:HH11	1:U:326:ARG:CB	2.15	0.60
1:W:387:LYS:HZ1	1:W:435:GLU:HG3	1.67	0.60
1:X:257:ASP:HA	1:X:308:SER:OG	2.02	0.60
1:A:440:SER:O	1:A:443:ILE:N	2.34	0.60
2:Q:8:ARG:HH11	2:Q:8:ARG:CB	2.14	0.60
1:V:17:ILE:HD11	1:V:65:GLU:HB3	1.83	0.60
1:X:17:ILE:HD11	1:X:65:GLU:HB3	1.82	0.60
1:A:36:ARG:NH1	1:F:360:MET:HE1	2.17	0.60
1:A:41:GLN:HA	1:A:41:GLN:HE21	1.65	0.60
1:A:275:ARG:C	1:A:277:GLY:N	2.56	0.60
1:B:338:ALA:N	1:B:382:PHE:HD1	2.00	0.60
1:E:31:LEU:HD21	1:E:74:ALA:HB2	1.82	0.60
2:M:72:LEU:O	2:M:76:VAL:HG23	2.02	0.60
1:X:17:ILE:HD13	1:X:66:ILE:HG12	1.83	0.60
1:X:442:PHE:N	1:X:442:PHE:CD1	2.59	0.60
1:C:56:ILE:HD12	1:C:56:ILE:N	2.16	0.60
2:G:1:THR:HG22	2:G:2:THR:N	2.17	0.60
2:L:52:ASP:HA	2:L:55:THR:CG2	2.27	0.60
1:C:360:MET:HE2	1:C:360:MET:CA	2.30	0.60
1:D:316:PRO:C	1:D:318:ASP:H	2.09	0.60
1:F:108:MET:HG3	1:F:295:HIS:CE1	2.37	0.60
1:T:23:ALA:O	1:T:27:VAL:HG23	2.02	0.60
1:T:439:LEU:HD23	1:T:439:LEU:H	1.67	0.60
1:U:27:VAL:HG21	1:U:66:ILE:HG21	1.84	0.60
1:A:347:GLU:HB2	1:A:348:PRO:HD3	1.84	0.59
1:B:377:ILE:O	1:B:380:ALA:HB3	2.02	0.59
1:D:52:ASN:O	1:D:328:PRO:HD2	2.01	0.59
1:E:409:PHE:CD2	1:F:25:ARG:CZ	2.84	0.59
1:E:443:ILE:HG12	2:K:112:VAL:HG21	1.84	0.59
1:F:441:ARG:NH2	2:G:36:ARG:O	2.34	0.59
2:N:112:VAL:HB	1:T:443:ILE:HD13	1.85	0.59
1:S:20:GLN:O	1:S:21:ALA:HB2	2.01	0.59
1:V:300:THR:HG22	1:V:303:ILE:HD11	1.84	0.59
1:W:12:GLU:HG2	1:W:73:LEU:HD23	1.83	0.59
2:G:8:ARG:O	2:G:9:ASN:HB2	2.02	0.59
2:N:55:THR:HG22	2:O:83:ARG:HG2	1.83	0.59
1:U:283:LEU:HD13	1:U:323:LEU:HD12	1.82	0.59
1:U:300:THR:HG22	1:U:303:ILE:HD11	1.84	0.59
1:W:48:VAL:HA	1:X:355:GLN:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ARG:HG3	1:C:330:ARG:HH11	1.68	0.59
1:D:437:GLU:HG2	1:D:438:ASP:N	2.17	0.59
2:H:79:ALA:HB1	2:H:83:ARG:HH21	1.66	0.59
2:O:94:MET:HE3	2:O:123:ILE:HB	1.83	0.59
2:P:7:ARG:HH21	2:P:103:SER:HB3	1.67	0.59
1:S:27:VAL:HG21	1:S:66:ILE:CG2	2.32	0.59
1:T:17:ILE:HD13	1:T:66:ILE:CG1	2.32	0.59
1:X:300:THR:HG22	1:X:303:ILE:HD11	1.82	0.59
1:F:264:LYS:CE	1:F:279:GLN:HE22	2.14	0.59
2:G:52:ASP:CA	2:G:55:THR:HG23	2.33	0.59
2:H:13:VAL:HG22	2:H:171:GLU:CB	2.33	0.59
2:P:89:ARG:HH11	2:Q:87:ALA:HB2	1.67	0.59
1:S:326:ARG:HH11	1:S:326:ARG:CB	2.15	0.59
1:T:326:ARG:HH11	1:T:326:ARG:CB	2.14	0.59
1:B:234:LEU:HD23	1:B:234:LEU:H	1.68	0.59
2:J:13:VAL:HG22	2:J:171:GLU:CB	2.33	0.59
2:N:89:ARG:HH11	2:O:87:ALA:HB2	1.67	0.59
2:P:3:ILE:O	2:P:122:ALA:HA	2.01	0.59
1:S:23:ALA:O	1:S:27:VAL:HG23	2.03	0.59
1:T:23:ALA:HA	1:T:331:VAL:CG2	2.33	0.59
1:U:20:GLN:O	1:U:21:ALA:HB2	2.02	0.59
1:X:283:LEU:HD13	1:X:323:LEU:HD12	1.84	0.59
1:B:20:GLN:HE21	1:B:20:GLN:N	2.00	0.59
1:E:353:THR:O	1:E:354:GLU:C	2.42	0.59
1:F:250:GLN:HA	1:F:250:GLN:HE21	1.67	0.59
2:I:83:ARG:CG	2:J:55:THR:HG22	2.26	0.59
2:L:83:ARG:HH21	2:L:111:ASP:HA	1.68	0.59
1:S:283:LEU:HD13	1:S:323:LEU:HD12	1.82	0.59
1:V:320:ILE:HD11	1:V:323:LEU:HD13	1.85	0.59
1:W:23:ALA:O	1:W:27:VAL:HG23	2.01	0.59
1:W:39:GLN:HB2	1:X:362:THR:HG21	1.84	0.59
1:W:442:PHE:N	1:W:442:PHE:HD1	2.01	0.59
1:C:58:PRO:O	1:C:63:LYS:NZ	2.30	0.59
1:C:439:LEU:O	1:C:440:SER:C	2.45	0.59
1:E:236:ASN:ND2	1:E:239:GLU:HB2	2.18	0.59
1:F:403:LEU:C	1:F:405:ASP:H	2.10	0.59
2:H:78:LEU:HD11	2:H:82:TRP:CZ3	2.38	0.59
2:N:7:ARG:HH21	2:N:103:SER:HB3	1.66	0.59
2:O:76:VAL:CG1	1:U:442:PHE:HD2	2.14	0.59
2:Q:112:VAL:HB	1:W:443:ILE:HD13	1.83	0.59
1:S:15:GLN:O	1:S:348:PRO:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:79:ILE:HG22	1:T:103:LEU:HD13	1.84	0.59
1:T:279:GLN:NE2	1:T:320:ILE:N	2.41	0.59
1:U:286:VAL:HA	1:U:305:PHE:CE1	2.36	0.59
1:A:406:LYS:H	1:A:406:LYS:CD	2.04	0.59
1:C:37:ARG:HH22	1:C:250:GLN:HE22	1.51	0.59
1:D:275:ARG:O	1:D:277:GLY:N	2.35	0.59
1:E:391:ILE:HG22	1:F:321:PRO:HB3	1.83	0.59
2:I:120:ILE:HD11	2:I:138:VAL:HG21	1.84	0.59
2:O:7:ARG:HH21	2:O:103:SER:HB3	1.68	0.59
2:R:49:GLY:O	2:R:50:THR:C	2.46	0.59
1:S:345:LEU:HD23	1:S:374:VAL:HG13	1.84	0.59
1:T:60:GLY:HA3	1:T:392:GLY:HA3	1.84	0.59
1:T:386:GLU:O	1:T:386:GLU:HG2	2.02	0.59
1:U:259:ILE:O	1:U:262:ILE:HG12	2.03	0.59
1:X:23:ALA:O	1:X:27:VAL:HG23	2.03	0.59
1:B:56:ILE:N	1:B:56:ILE:HD12	2.18	0.59
1:C:245:ILE:O	1:C:246:ASP:C	2.46	0.59
1:E:378:ALA:O	1:E:379:GLU:C	2.46	0.59
1:E:384:VAL:O	1:E:385:ASN:C	2.46	0.59
1:F:4:MET:HE2	1:F:9:ILE:HA	1.84	0.59
2:H:17:ASP:OD2	2:H:33:LYS:HE3	2.03	0.59
2:M:49:GLY:O	2:M:50:THR:C	2.44	0.59
2:N:164:ASN:ND2	2:N:164:ASN:H	2.01	0.59
2:O:89:ARG:HH11	2:P:87:ALA:HB2	1.68	0.59
2:O:105:ILE:CG2	2:O:113:VAL:HB	2.32	0.59
2:R:37:LEU:HD23	1:S:441:ARG:HH22	1.68	0.59
1:U:439:LEU:O	1:U:441:ARG:N	2.36	0.59
1:V:245:ILE:O	1:V:249:GLU:HG3	2.03	0.59
1:B:230:GLU:O	1:B:231:ALA:CB	2.51	0.59
1:D:351:SER:O	1:D:355:GLN:HG3	2.03	0.59
2:G:1:THR:HG23	2:G:33:LYS:HZ1	1.67	0.59
2:G:61:GLU:O	2:G:62:ARG:C	2.46	0.59
2:I:24:ASN:O	2:N:161:VAL:HG13	2.03	0.59
2:N:56:LEU:CD2	2:N:95:LEU:HD22	2.33	0.59
1:D:264:LYS:NZ	1:D:319:LEU:HA	2.18	0.58
1:D:377:ILE:O	1:D:380:ALA:HB3	2.03	0.58
1:F:316:PRO:C	1:F:318:ASP:H	2.11	0.58
2:G:46:PHE:HB3	2:G:95:LEU:CD2	2.33	0.58
2:J:1:THR:CG2	2:J:33:LYS:HD3	2.33	0.58
1:X:20:GLN:O	1:X:21:ALA:HB2	2.02	0.58
1:D:280:ARG:HH11	1:D:280:ARG:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:82:TRP:CE2	2:I:88:LEU:HD13	2.38	0.58
1:U:235:ILE:HG22	1:U:236:ASN:N	2.18	0.58
1:U:283:LEU:HD11	1:U:322:GLU:HB3	1.85	0.58
1:V:286:VAL:HA	1:V:305:PHE:CE1	2.37	0.58
1:B:17:ILE:HD12	1:B:17:ILE:N	2.18	0.58
1:B:41:GLN:HA	1:B:41:GLN:NE2	2.18	0.58
1:D:16:HIS:C	1:D:17:ILE:HD12	2.28	0.58
1:F:4:MET:CE	1:F:9:ILE:HA	2.34	0.58
2:H:55:THR:HG21	2:H:89:ARG:NH2	2.18	0.58
2:H:107:THR:OG1	2:H:111:ASP:OD2	2.11	0.58
2:J:17:ASP:CG	2:J:163:THR:HG23	2.28	0.58
2:K:134:ALA:O	2:K:138:VAL:HG23	2.04	0.58
2:L:8:ARG:O	2:L:9:ASN:HB2	2.03	0.58
2:Q:17:ASP:HB2	2:Q:164:ASN:HD22	1.68	0.58
1:T:327:LEU:N	1:T:328:PRO:CD	2.64	0.58
1:U:386:GLU:O	1:U:386:GLU:HG2	2.03	0.58
1:A:360:MET:HE2	1:A:360:MET:N	2.18	0.58
1:B:283:LEU:CB	1:B:284:PRO:HD3	2.32	0.58
1:C:275:ARG:C	1:C:277:GLY:N	2.59	0.58
1:F:275:ARG:C	1:F:277:GLY:N	2.58	0.58
1:W:51:LYS:HE2	1:X:356:TYR:OH	2.03	0.58
1:W:300:THR:HG22	1:W:303:ILE:HD11	1.84	0.58
1:A:322:GLU:OE2	1:A:322:GLU:N	2.35	0.58
1:C:264:LYS:HE3	1:C:264:LYS:H	1.68	0.58
2:L:13:VAL:HG22	2:L:171:GLU:CB	2.33	0.58
1:U:23:ALA:HA	1:U:331:VAL:CG2	2.32	0.58
1:U:113:GLN:HG3	1:U:113:GLN:O	2.04	0.58
1:A:382:PHE:HD2	1:A:382:PHE:C	2.11	0.58
1:B:264:LYS:NZ	1:B:279:GLN:NE2	2.44	0.58
1:C:235:ILE:O	1:C:236:ASN:HB3	2.02	0.58
1:C:407:ILE:HD11	1:C:419:VAL:HG11	1.85	0.58
1:D:5:THR:H	1:D:8:GLU:HB3	1.69	0.58
1:F:37:ARG:NH1	1:F:38:MET:HE2	2.16	0.58
2:N:72:LEU:O	2:N:76:VAL:HG23	2.03	0.58
2:O:17:ASP:HB2	2:O:164:ASN:HD22	1.67	0.58
2:O:72:LEU:O	2:O:76:VAL:HG23	2.02	0.58
2:Q:164:ASN:HD22	2:Q:164:ASN:N	1.96	0.58
1:S:373:ALA:HB2	1:S:422:ASP:HA	1.85	0.58
1:U:37:ARG:HG2	1:U:37:ARG:HH11	1.69	0.58
1:V:313:VAL:CG2	1:V:314:ALA:H	2.02	0.58
1:V:386:GLU:HG2	1:V:386:GLU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:23:ALA:HA	1:W:331:VAL:CG2	2.34	0.58
1:W:283:LEU:HD11	1:W:322:GLU:HB3	1.85	0.58
1:A:403:LEU:CD2	1:A:404:MET:SD	2.92	0.58
1:B:250:GLN:NE2	1:B:250:GLN:HA	2.18	0.58
1:C:264:LYS:CE	1:C:279:GLN:HE22	2.16	0.58
1:C:316:PRO:C	1:C:318:ASP:H	2.12	0.58
1:C:356:TYR:HD1	1:C:400:MET:HE3	1.69	0.58
1:D:443:ILE:HG12	2:J:112:VAL:CG2	2.32	0.58
1:E:405:ASP:HB3	1:E:406:LYS:HD2	1.85	0.58
2:L:137:LEU:HD11	2:R:136:ALA:HB1	1.85	0.58
1:S:355:GLN:OE1	1:X:48:VAL:HA	2.04	0.58
1:S:386:GLU:HG2	1:S:386:GLU:O	2.04	0.58
1:T:37:ARG:HG2	1:T:37:ARG:HH11	1.69	0.58
1:T:120:ARG:O	1:T:124:GLU:HB3	2.04	0.58
1:T:286:VAL:HA	1:T:305:PHE:CE1	2.38	0.58
1:U:320:ILE:HD11	1:U:323:LEU:HD13	1.85	0.58
1:U:327:LEU:N	1:U:328:PRO:CD	2.64	0.58
1:V:345:LEU:HD23	1:V:374:VAL:HG13	1.85	0.58
1:W:63:LYS:HB2	3:W:460:ATP:O2B	2.03	0.58
1:X:23:ALA:HA	1:X:331:VAL:CG2	2.34	0.58
1:B:406:LYS:H	1:B:406:LYS:CD	2.09	0.58
2:J:1:THR:HG22	2:J:2:THR:N	2.19	0.58
2:K:86:ARG:HG2	2:K:87:ALA:H	1.67	0.58
1:W:259:ILE:O	1:W:262:ILE:HG12	2.04	0.58
1:W:327:LEU:N	1:W:328:PRO:CD	2.64	0.58
1:C:443:ILE:HG21	2:I:114:GLN:HG3	1.85	0.58
1:E:316:PRO:C	1:E:318:ASP:H	2.12	0.58
2:K:37:LEU:HB2	2:K:42:VAL:CG2	2.33	0.58
1:T:20:GLN:O	1:T:21:ALA:HB2	2.03	0.58
1:U:5:THR:OG1	1:U:6:PRO:HD2	2.04	0.58
1:U:313:VAL:CG2	1:U:314:ALA:H	2.02	0.58
1:V:18:ILE:HG22	1:V:344:ILE:HG12	1.86	0.58
1:W:27:VAL:HG21	1:W:66:ILE:CG2	2.33	0.58
1:A:34:ARG:CZ	1:A:251:ASN:HA	2.34	0.58
1:C:403:LEU:CD2	1:C:404:MET:SD	2.92	0.58
1:E:313:VAL:HG23	1:E:314:ALA:H	1.69	0.58
1:E:403:LEU:HD22	1:E:404:MET:HG2	1.85	0.58
1:F:435:GLU:O	1:F:436:ASN:HB3	2.03	0.58
2:G:55:THR:O	2:G:59:LEU:HD13	2.04	0.58
2:J:55:THR:O	2:J:59:LEU:HD13	2.04	0.58
2:R:56:LEU:HD23	2:R:95:LEU:HD22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:108:MET:HE3	1:S:295:HIS:CD2	2.38	0.58
1:T:80:LYS:HG3	1:T:255:PHE:HD2	1.66	0.58
1:W:442:PHE:N	1:W:442:PHE:CD1	2.72	0.58
1:X:61:VAL:HA	1:X:336:LEU:HD21	1.85	0.58
1:X:386:GLU:HG2	1:X:386:GLU:O	2.04	0.58
1:C:108:MET:O	1:C:109:LYS:C	2.46	0.57
1:E:34:ARG:CZ	1:E:251:ASN:HA	2.34	0.57
1:F:406:LYS:H	1:F:406:LYS:CD	2.06	0.57
2:K:82:TRP:CD1	2:K:88:LEU:HB3	2.39	0.57
2:N:17:ASP:HB2	2:N:164:ASN:HD22	1.68	0.57
2:P:17:ASP:HB2	2:P:164:ASN:HD21	1.67	0.57
2:P:72:LEU:O	2:P:76:VAL:HG23	2.04	0.57
2:R:7:ARG:HH21	2:R:103:SER:HB3	1.69	0.57
1:U:111:VAL:HG12	1:U:240:LEU:HD11	1.85	0.57
1:V:373:ALA:HB2	1:V:422:ASP:HA	1.86	0.57
1:X:27:VAL:HG21	1:X:66:ILE:HG21	1.86	0.57
1:B:407:ILE:O	1:B:411:ALA:HB2	2.04	0.57
1:C:237:PRO:CB	1:C:241:LYS:HZ1	2.17	0.57
1:E:54:LEU:HG	1:E:56:ILE:HD11	1.86	0.57
2:G:144:SER:HB3	2:G:147:GLU:CG	2.32	0.57
2:R:72:LEU:O	2:R:76:VAL:HG23	2.03	0.57
1:S:80:LYS:HG3	1:S:255:PHE:HD2	1.69	0.57
1:S:120:ARG:HD2	1:S:120:ARG:C	2.29	0.57
1:S:259:ILE:O	1:S:262:ILE:HG12	2.04	0.57
1:T:27:VAL:HG21	1:T:66:ILE:HG21	1.85	0.57
1:T:227:ILE:HG23	1:T:228:ASP:N	2.18	0.57
1:T:240:LEU:HD12	1:T:243:LYS:HB3	1.86	0.57
1:V:23:ALA:HA	1:V:331:VAL:CG2	2.34	0.57
1:V:333:LEU:N	1:V:333:LEU:HD23	2.18	0.57
1:W:37:ARG:HG2	1:W:37:ARG:NH1	2.18	0.57
1:W:80:LYS:HG3	1:W:255:PHE:HD2	1.68	0.57
1:A:275:ARG:O	1:A:277:GLY:N	2.37	0.57
2:I:17:ASP:O	2:I:33:LYS:HD2	2.03	0.57
2:M:120:ILE:O	2:M:121:LEU:HD23	2.03	0.57
1:S:79:ILE:HG22	1:S:103:LEU:HD13	1.86	0.57
1:V:55:MET:HE1	1:V:63:LYS:O	2.03	0.57
1:X:63:LYS:HZ2	1:X:308:SER:HB2	1.68	0.57
1:X:259:ILE:O	1:X:262:ILE:HG12	2.03	0.57
1:A:41:GLN:HE21	1:A:41:GLN:CA	2.16	0.57
1:A:315:ARG:O	1:A:318:ASP:HB2	2.04	0.57
1:C:54:LEU:HG	1:C:56:ILE:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:GLY:HA2	3:F:455:ATP:O1B	2.04	0.57
2:H:137:LEU:HD11	2:N:136:ALA:HB1	1.85	0.57
2:K:52:ASP:CA	2:K:55:THR:HG23	2.34	0.57
2:O:37:LEU:HB2	2:O:42:VAL:HG23	1.86	0.57
1:S:333:LEU:N	1:S:333:LEU:HD23	2.19	0.57
1:U:23:ALA:O	1:U:27:VAL:HG23	2.04	0.57
1:V:27:VAL:HG21	1:V:66:ILE:CG2	2.34	0.57
1:X:20:GLN:OE1	1:X:333:LEU:HB3	2.04	0.57
1:X:327:LEU:N	1:X:328:PRO:CD	2.67	0.57
1:A:27:VAL:HB	1:A:70:LEU:HD22	1.86	0.57
1:A:435:GLU:HG3	1:A:436:ASN:N	2.16	0.57
1:C:104:THR:HA	1:C:248:VAL:CG2	2.32	0.57
1:C:366:ASN:O	1:C:418:THR:HA	2.03	0.57
1:E:58:PRO:O	1:E:63:LYS:NZ	2.28	0.57
1:E:293:THR:C	1:E:295:HIS:H	2.11	0.57
2:I:86:ARG:O	2:I:87:ALA:HB2	2.04	0.57
2:I:88:LEU:O	2:I:89:ARG:C	2.47	0.57
2:M:17:ASP:HB2	2:M:164:ASN:HD21	1.66	0.57
1:S:55:MET:HE1	1:S:63:LYS:O	2.05	0.57
1:T:328:PRO:HB3	1:U:398:THR:HA	1.85	0.57
1:U:328:PRO:HB3	1:V:398:THR:HA	1.85	0.57
1:V:370:THR:CG2	1:V:422:ASP:HA	2.35	0.57
1:B:235:ILE:O	1:B:236:ASN:HB3	2.05	0.57
1:B:378:ALA:O	1:B:379:GLU:C	2.44	0.57
1:C:54:LEU:HD12	1:C:307:ALA:O	2.04	0.57
1:C:62:GLY:O	1:C:63:LYS:C	2.46	0.57
1:C:264:LYS:O	1:C:265:LYS:HB3	2.03	0.57
1:D:55:MET:HE3	1:D:306:ILE:CG2	2.34	0.57
1:E:41:GLN:HA	1:E:41:GLN:HE21	1.68	0.57
1:E:52:ASN:O	1:E:328:PRO:HD2	2.05	0.57
2:J:17:ASP:HB2	2:J:164:ASN:HD22	1.69	0.57
2:K:1:THR:HG23	2:K:33:LYS:NZ	2.19	0.57
1:V:341:PHE:O	1:V:345:LEU:HB2	2.05	0.57
1:X:79:ILE:HG22	1:X:103:LEU:HD13	1.86	0.57
1:D:333:LEU:N	1:D:333:LEU:HD12	2.19	0.57
1:E:264:LYS:O	1:E:265:LYS:HB3	2.05	0.57
1:E:280:ARG:HG3	1:E:280:ARG:NH1	2.16	0.57
2:K:17:ASP:HB2	2:K:164:ASN:HD22	1.67	0.57
2:M:1:THR:HG23	2:M:33:LYS:HD3	1.86	0.57
2:N:37:LEU:HB2	2:N:42:VAL:HG23	1.87	0.57
1:V:327:LEU:N	1:V:328:PRO:CD	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:PRO:HD3	1:D:32:ARG:HG2	1.87	0.57
1:E:41:GLN:HE21	1:E:41:GLN:CA	2.18	0.57
1:E:409:PHE:CZ	1:F:25:ARG:HG3	2.40	0.57
2:I:115:PRO:HB2	2:I:119:GLN:HA	1.87	0.57
2:L:86:ARG:O	2:L:87:ALA:CB	2.53	0.57
1:D:406:LYS:HD2	1:D:406:LYS:N	2.10	0.57
2:I:164:ASN:HD22	2:I:164:ASN:C	2.11	0.57
2:M:3:ILE:O	2:M:122:ALA:HA	2.04	0.57
2:R:37:LEU:HB2	2:R:42:VAL:HG23	1.87	0.57
1:T:20:GLN:OE1	1:T:333:LEU:HB3	2.05	0.57
1:E:38:MET:HG3	1:E:45:ARG:NH1	2.20	0.57
2:M:56:LEU:HD23	2:M:95:LEU:HD22	1.86	0.57
2:N:49:GLY:O	2:N:50:THR:C	2.47	0.57
2:Q:120:ILE:O	2:Q:121:LEU:HD23	2.05	0.57
2:R:17:ASP:HB2	2:R:164:ASN:HD22	1.70	0.57
1:A:25:ARG:O	1:A:28:ALA:N	2.38	0.56
1:A:370:THR:HG23	1:A:421:ILE:O	2.04	0.56
1:B:245:ILE:HG23	1:B:298:VAL:HG12	1.87	0.56
1:B:382:PHE:C	1:B:382:PHE:CD2	2.83	0.56
1:C:4:MET:HE3	1:C:8:GLU:HG2	1.86	0.56
2:G:38:TYR:CD1	2:G:69:GLY:HA3	2.39	0.56
1:S:327:LEU:N	1:S:328:PRO:CD	2.64	0.56
1:S:359:LEU:O	1:S:360:MET:HE2	2.05	0.56
1:V:17:ILE:HD13	1:V:66:ILE:CG1	2.35	0.56
1:V:303:ILE:HG22	1:V:304:LEU:N	2.20	0.56
1:X:37:ARG:HG2	1:X:37:ARG:HH11	1.69	0.56
1:A:264:LYS:HD3	1:A:276:GLU:CD	2.30	0.56
1:D:256:ILE:HG21	1:D:259:ILE:HD12	1.85	0.56
1:E:382:PHE:C	1:E:382:PHE:CD2	2.83	0.56
1:F:341:PHE:O	1:F:345:LEU:HB2	2.04	0.56
2:J:8:ARG:O	2:J:9:ASN:HB2	2.05	0.56
2:L:36:ARG:NH1	2:L:170:GLU:OE2	2.39	0.56
2:O:56:LEU:HD21	2:O:95:LEU:HB2	1.87	0.56
2:O:120:ILE:O	2:O:121:LEU:HD23	2.05	0.56
2:P:37:LEU:HB2	2:P:42:VAL:HG23	1.87	0.56
1:S:283:LEU:HD11	1:S:322:GLU:HB3	1.88	0.56
1:U:79:ILE:HG22	1:U:103:LEU:HD13	1.86	0.56
1:V:59:THR:HG23	3:V:459:ATP:O1G	2.06	0.56
1:V:79:ILE:HG22	1:V:103:LEU:HD13	1.86	0.56
1:W:324:GLN:HE22	1:X:389:GLU:HG2	1.70	0.56
1:A:104:THR:HA	1:A:248:VAL:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ARG:HH22	1:B:250:GLN:HE22	1.52	0.56
1:E:370:THR:O	1:E:373:ALA:HB3	2.06	0.56
1:F:373:ALA:O	1:F:377:ILE:HG13	2.06	0.56
2:H:17:ASP:HB2	2:H:164:ASN:HD22	1.68	0.56
2:H:105:ILE:HG22	2:H:113:VAL:O	2.05	0.56
2:K:8:ARG:O	2:K:9:ASN:HB2	2.04	0.56
2:M:89:ARG:HH11	2:N:87:ALA:HB2	1.70	0.56
1:S:68:ARG:HG3	1:S:68:ARG:HH11	1.70	0.56
1:S:300:THR:HG22	1:S:303:ILE:HD11	1.86	0.56
1:S:303:ILE:HG22	1:S:304:LEU:N	2.21	0.56
1:T:115:GLU:C	1:T:117:ALA:H	2.12	0.56
1:U:315:ARG:HB3	1:U:316:PRO:HD2	1.87	0.56
1:V:39:GLN:HB2	1:W:362:THR:HG21	1.86	0.56
1:W:112:ARG:O	1:W:116:ILE:HB	2.06	0.56
1:X:283:LEU:HB3	1:X:284:PRO:HD3	1.88	0.56
1:A:382:PHE:C	1:A:382:PHE:CD2	2.81	0.56
1:C:65:GLU:HG3	3:C:452:ATP:H2'	1.88	0.56
1:D:403:LEU:CD2	1:D:404:MET:SD	2.93	0.56
1:E:55:MET:HE3	1:E:306:ILE:CG2	2.36	0.56
1:E:275:ARG:C	1:E:277:GLY:N	2.54	0.56
1:E:352:LEU:HD13	1:E:400:MET:HG3	1.87	0.56
2:G:83:ARG:HB3	2:H:55:THR:HB	1.88	0.56
2:J:86:ARG:O	2:J:87:ALA:CB	2.53	0.56
2:L:71:LEU:HD13	2:L:71:LEU:C	2.30	0.56
2:O:8:ARG:O	2:O:9:ASN:HB2	2.05	0.56
2:R:8:ARG:O	2:R:9:ASN:HB2	2.04	0.56
1:S:18:ILE:HG22	1:S:344:ILE:HG12	1.86	0.56
1:S:20:GLN:OE1	1:S:333:LEU:HB3	2.05	0.56
1:T:283:LEU:HD11	1:T:322:GLU:HB3	1.88	0.56
1:V:65:GLU:HG2	3:V:459:ATP:H5'2	1.88	0.56
1:W:369:PHE:CE2	1:W:421:ILE:HD12	2.33	0.56
1:X:227:ILE:HG23	1:X:228:ASP:N	2.20	0.56
1:A:366:ASN:O	1:A:418:THR:HA	2.05	0.56
1:B:341:PHE:HA	1:B:344:ILE:HG12	1.87	0.56
1:C:52:ASN:HD21	1:C:305:PHE:H	1.49	0.56
1:D:315:ARG:O	1:D:318:ASP:HB2	2.05	0.56
1:D:382:PHE:C	1:D:382:PHE:HD2	2.13	0.56
1:E:264:LYS:NZ	1:E:319:LEU:HA	2.21	0.56
2:I:7:ARG:NE	2:I:119:GLN:OE1	2.38	0.56
2:J:46:PHE:HB3	2:J:95:LEU:CD2	2.35	0.56
2:N:56:LEU:HD21	2:N:95:LEU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:17:ASP:HB2	2:O:164:ASN:HD21	1.68	0.56
1:S:23:ALA:HA	1:S:331:VAL:CG2	2.35	0.56
1:T:55:MET:HE1	1:T:63:LYS:O	2.05	0.56
1:T:300:THR:HG22	1:T:303:ILE:HD11	1.88	0.56
1:U:247:ALA:O	1:U:251:ASN:HB2	2.06	0.56
1:V:37:ARG:HG2	1:V:37:ARG:NH1	2.19	0.56
1:V:328:PRO:HB3	1:W:398:THR:HA	1.86	0.56
1:W:359:LEU:O	1:W:360:MET:HE2	2.06	0.56
1:B:236:ASN:O	1:B:238:GLU:N	2.38	0.56
1:C:20:GLN:HE21	1:C:20:GLN:H	1.54	0.56
1:D:373:ALA:O	1:D:377:ILE:HG13	2.05	0.56
1:F:65:GLU:O	1:F:66:ILE:C	2.48	0.56
1:F:369:PHE:CE2	1:F:421:ILE:HD12	2.40	0.56
2:K:17:ASP:OD2	2:K:33:LYS:HE3	2.05	0.56
2:M:83:ARG:HG2	2:R:55:THR:HG22	1.87	0.56
2:N:7:ARG:HE	2:N:119:GLN:NE2	2.04	0.56
2:O:3:ILE:O	2:O:122:ALA:HA	2.05	0.56
2:P:56:LEU:CD2	2:P:95:LEU:HD22	2.35	0.56
1:S:349:HIS:O	1:S:350:ALA:HB3	2.06	0.56
1:T:359:LEU:O	1:T:360:MET:HE2	2.06	0.56
1:X:373:ALA:HB2	1:X:422:ASP:HA	1.87	0.56
1:A:264:LYS:HZ1	1:A:279:GLN:NE2	2.00	0.56
1:E:52:ASN:HD22	1:E:305:PHE:N	2.01	0.56
1:F:283:LEU:HB2	1:F:284:PRO:HD3	1.88	0.56
1:F:293:THR:C	1:F:295:HIS:H	2.14	0.56
1:F:384:VAL:O	1:F:385:ASN:C	2.48	0.56
2:M:95:LEU:O	2:M:105:ILE:HA	2.06	0.56
2:M:164:ASN:HD22	2:M:164:ASN:N	1.95	0.56
2:R:5:SER:CB	2:R:14:VAL:HG22	2.35	0.56
1:T:27:VAL:HG21	1:T:66:ILE:CG2	2.36	0.56
1:T:353:THR:HG22	1:T:369:PHE:CD1	2.40	0.56
1:T:430:LEU:HG	1:T:431:GLY:H	1.70	0.56
1:U:17:ILE:HD13	1:U:66:ILE:HG12	1.87	0.56
1:U:54:LEU:HD21	1:U:327:LEU:HD22	1.87	0.56
1:U:373:ALA:HB2	1:U:422:ASP:HA	1.88	0.56
1:V:17:ILE:HD13	1:V:66:ILE:HG12	1.88	0.56
1:C:443:ILE:HG12	2:I:112:VAL:CG2	2.35	0.56
1:F:41:GLN:NE2	1:F:41:GLN:HA	2.21	0.56
2:H:8:ARG:O	2:H:9:ASN:HB2	2.05	0.56
2:K:144:SER:HB3	2:K:147:GLU:CG	2.35	0.56
2:M:115:PRO:HB3	2:M:119:GLN:CA	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:48:VAL:HG21	1:W:359:LEU:HD11	1.88	0.56
1:V:111:VAL:O	1:V:115:GLU:HB2	2.05	0.56
1:C:382:PHE:C	1:C:382:PHE:CD2	2.84	0.56
1:D:111:VAL:HG21	1:D:244:ALA:HA	1.88	0.56
1:D:370:THR:O	1:D:373:ALA:HB3	2.06	0.56
1:E:58:PRO:HD2	1:E:61:VAL:HG21	1.88	0.56
1:F:240:LEU:O	1:F:243:LYS:N	2.31	0.56
1:F:370:THR:HG23	1:F:421:ILE:O	2.06	0.56
2:N:17:ASP:HB2	2:N:164:ASN:HD21	1.66	0.56
2:R:56:LEU:CD2	2:R:95:LEU:HD13	2.36	0.56
1:V:283:LEU:HB3	1:V:284:PRO:HD3	1.87	0.56
1:X:54:LEU:HD21	1:X:327:LEU:HD22	1.86	0.56
1:A:20:GLN:OE1	1:A:333:LEU:HB3	2.06	0.56
1:B:37:ARG:HA	1:B:40:LEU:HD12	1.88	0.56
1:B:349:HIS:O	1:B:350:ALA:HB3	2.06	0.56
1:D:41:GLN:NE2	1:D:41:GLN:HA	2.21	0.56
2:H:38:TYR:CE1	2:H:69:GLY:HA3	2.41	0.56
2:J:43:LEU:O	2:J:97:VAL:HA	2.05	0.56
2:J:115:PRO:HB2	2:J:119:GLN:HA	1.88	0.56
2:L:86:ARG:O	2:L:87:ALA:HB2	2.05	0.56
2:Q:8:ARG:O	2:Q:9:ASN:HB2	2.05	0.56
2:Q:56:LEU:CD2	2:Q:95:LEU:HD22	2.36	0.56
2:R:128:ASN:HA	2:R:131:LEU:HB3	1.88	0.56
1:S:37:ARG:HG2	1:S:37:ARG:NH1	2.20	0.56
1:S:439:LEU:HD23	1:S:439:LEU:N	2.19	0.56
1:T:435:GLU:O	1:T:436:ASN:O	2.22	0.56
1:B:391:ILE:HG22	1:C:321:PRO:HB3	1.88	0.55
1:C:341:PHE:HA	1:C:344:ILE:HG12	1.89	0.55
1:E:437:GLU:O	1:E:438:ASP:O	2.23	0.55
2:Q:37:LEU:HB2	2:Q:42:VAL:HG23	1.88	0.55
2:Q:56:LEU:HD21	2:Q:95:LEU:HB2	1.88	0.55
1:S:17:ILE:HG23	3:S:456:ATP:N6	2.21	0.55
1:S:233:LYS:C	1:S:235:ILE:N	2.59	0.55
1:S:370:THR:CG2	1:S:422:ASP:HA	2.36	0.55
1:V:283:LEU:HD13	1:V:323:LEU:HD12	1.88	0.55
1:B:113:GLN:O	1:B:113:GLN:HG2	2.05	0.55
1:B:352:LEU:HD13	1:B:400:MET:CG	2.35	0.55
2:G:5:SER:HB2	2:G:14:VAL:HG22	1.87	0.55
2:J:61:GLU:O	2:J:62:ARG:C	2.46	0.55
1:S:5:THR:OG1	1:S:6:PRO:HD2	2.06	0.55
1:U:27:VAL:HG21	1:U:66:ILE:CG2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:120:ARG:HG3	1:U:232:ALA:CB	2.36	0.55
1:U:297:MET:HE2	1:V:105:ASP:HB3	1.88	0.55
1:A:37:ARG:CG	1:A:38:MET:N	2.69	0.55
1:A:414:MET:HG2	1:A:414:MET:O	2.06	0.55
1:C:338:ALA:N	1:C:382:PHE:HD1	2.03	0.55
1:F:31:LEU:HD21	1:F:74:ALA:HB2	1.88	0.55
1:F:250:GLN:HE21	1:F:250:GLN:CA	2.19	0.55
2:H:115:PRO:HG3	2:H:121:LEU:HD11	1.88	0.55
1:T:283:LEU:HB3	1:T:284:PRO:HD3	1.88	0.55
1:T:373:ALA:HB2	1:T:422:ASP:HA	1.88	0.55
1:V:359:LEU:O	1:V:360:MET:HE2	2.07	0.55
1:A:53:ILE:HG22	1:A:54:LEU:N	2.21	0.55
1:A:233:LYS:HD2	1:A:233:LYS:C	2.32	0.55
2:I:55:THR:O	2:I:59:LEU:HD13	2.06	0.55
2:J:105:ILE:HG22	2:J:113:VAL:O	2.07	0.55
2:K:43:LEU:O	2:K:97:VAL:HA	2.07	0.55
2:M:94:MET:HE3	2:M:123:ILE:HB	1.89	0.55
2:P:56:LEU:HD21	2:P:95:LEU:HB2	1.89	0.55
1:S:55:MET:HA	1:S:331:VAL:HG13	1.88	0.55
1:T:341:PHE:O	1:T:345:LEU:HB2	2.07	0.55
1:W:68:ARG:HH11	1:W:68:ARG:HG3	1.71	0.55
1:W:341:PHE:O	1:W:345:LEU:HB2	2.07	0.55
1:C:322:GLU:OE2	1:C:322:GLU:N	2.39	0.55
1:D:358:ALA:O	1:D:361:ALA:HB3	2.07	0.55
1:F:17:ILE:HG12	1:F:66:ILE:HG13	1.89	0.55
1:F:69:ARG:O	1:F:70:LEU:C	2.50	0.55
2:M:87:ALA:HB2	2:R:89:ARG:HH11	1.72	0.55
1:U:280:ARG:HH22	1:V:261:LYS:HE3	1.72	0.55
1:W:303:ILE:HG22	1:W:304:LEU:N	2.20	0.55
1:X:60:GLY:HA3	1:X:392:GLY:HA3	1.88	0.55
1:A:245:ILE:HG23	1:A:298:VAL:HG12	1.88	0.55
1:A:404:MET:O	1:A:408:SER:HB2	2.07	0.55
1:C:54:LEU:HG	1:C:56:ILE:HD11	1.89	0.55
1:C:250:GLN:HA	1:C:250:GLN:NE2	2.20	0.55
1:D:421:ILE:HA	1:D:425:TYR:HD1	1.70	0.55
1:F:65:GLU:HG3	3:F:455:ATP:H2'	1.88	0.55
1:F:275:ARG:O	1:F:277:GLY:N	2.40	0.55
1:F:367:ILE:HD11	1:F:421:ILE:CD1	2.35	0.55
1:F:443:ILE:HG12	2:L:112:VAL:CG2	2.35	0.55
2:M:37:LEU:HB2	2:M:42:VAL:HG23	1.88	0.55
2:M:105:ILE:HG22	2:M:113:VAL:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:49:GLY:O	2:O:50:THR:C	2.49	0.55
2:O:128:ASN:HA	2:O:131:LEU:HB3	1.88	0.55
1:T:313:VAL:CG2	1:T:314:ALA:H	2.00	0.55
1:T:349:HIS:O	1:T:350:ALA:HB3	2.07	0.55
1:W:48:VAL:HG23	1:X:355:GLN:OE1	2.06	0.55
1:W:442:PHE:HD1	1:W:442:PHE:H	1.53	0.55
1:X:55:MET:HE1	1:X:63:LYS:O	2.06	0.55
1:B:315:ARG:O	1:B:318:ASP:HB2	2.07	0.55
1:D:20:GLN:CA	1:D:20:GLN:NE2	2.69	0.55
1:E:357:LYS:HE3	1:E:367:ILE:O	2.06	0.55
2:G:55:THR:HG22	2:L:83:ARG:HG2	1.89	0.55
2:I:8:ARG:O	2:I:9:ASN:HB2	2.06	0.55
2:M:128:ASN:HA	2:M:131:LEU:HB3	1.89	0.55
2:P:55:THR:HG22	2:Q:83:ARG:CG	2.36	0.55
1:T:98:SER:HA	1:T:101:ARG:NH1	2.22	0.55
1:U:359:LEU:O	1:U:360:MET:HE2	2.06	0.55
1:V:362:THR:O	1:V:362:THR:HG22	2.07	0.55
1:B:374:VAL:O	1:B:375:LYS:C	2.50	0.55
1:C:73:LEU:C	1:C:73:LEU:HD12	2.32	0.55
1:C:406:LYS:H	1:C:406:LYS:CD	2.13	0.55
1:D:250:GLN:HE21	1:D:250:GLN:CA	2.18	0.55
1:E:104:THR:HA	1:E:248:VAL:CG2	2.36	0.55
2:J:57:PHE:HA	2:J:95:LEU:HD11	1.88	0.55
2:L:17:ASP:O	2:L:33:LYS:HD2	2.06	0.55
2:O:56:LEU:CD2	2:O:95:LEU:HD22	2.37	0.55
2:R:56:LEU:HD21	2:R:95:LEU:HB2	1.87	0.55
1:S:353:THR:HG22	1:S:369:PHE:CD1	2.42	0.55
1:T:259:ILE:O	1:T:262:ILE:HG12	2.05	0.55
1:T:315:ARG:HB3	1:T:316:PRO:HD2	1.89	0.55
1:V:283:LEU:HD11	1:V:322:GLU:HB3	1.88	0.55
1:A:439:LEU:HD23	1:A:443:ILE:HD12	1.89	0.55
1:D:41:GLN:HA	1:D:41:GLN:HE21	1.71	0.55
1:D:366:ASN:HB3	1:D:418:THR:HG22	1.88	0.55
1:D:428:ASP:O	1:D:430:LEU:N	2.40	0.55
1:E:355:GLN:O	1:E:359:LEU:HD23	2.07	0.55
1:F:104:THR:HA	1:F:248:VAL:CG2	2.36	0.55
2:R:1:THR:HG23	2:R:33:LYS:HD3	1.87	0.55
1:S:17:ILE:HD13	1:S:66:ILE:CG1	2.37	0.55
1:T:61:VAL:HA	1:T:336:LEU:HD21	1.89	0.55
1:U:98:SER:HA	1:U:101:ARG:NH1	2.22	0.55
1:V:55:MET:HA	1:V:331:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:68:ARG:HH11	1:V:68:ARG:HG3	1.72	0.55
2:H:37:LEU:HB2	2:H:42:VAL:CG2	2.37	0.55
2:I:1:THR:HG23	2:I:33:LYS:NZ	2.22	0.55
2:N:8:ARG:O	2:N:9:ASN:HB2	2.07	0.55
2:O:56:LEU:CD2	2:O:95:LEU:HD13	2.37	0.55
2:P:4:VAL:HG12	2:P:153:LEU:HD21	1.89	0.55
2:P:20:VAL:HG21	1:W:444:LEU:HD21	1.87	0.55
2:Q:128:ASN:HA	2:Q:131:LEU:HB3	1.89	0.55
1:S:393:ALA:HB3	3:S:456:ATP:C1'	2.35	0.55
1:T:280:ARG:HH22	1:U:261:LYS:HE3	1.71	0.55
1:W:17:ILE:HD13	1:W:66:ILE:CG1	2.36	0.55
1:W:373:ALA:HB2	1:W:422:ASP:HA	1.87	0.55
1:X:27:VAL:HG21	1:X:66:ILE:CG2	2.37	0.55
1:C:38:MET:HG3	1:C:45:ARG:NH1	2.21	0.54
1:C:76:ALA:HB1	1:C:251:ASN:O	2.07	0.54
1:D:249:GLU:OE1	1:D:299:LYS:HG3	2.07	0.54
2:G:78:LEU:O	2:G:81:ASP:HB2	2.06	0.54
2:N:55:THR:HG22	2:O:83:ARG:CB	2.37	0.54
2:N:105:ILE:HG22	2:N:113:VAL:O	2.06	0.54
2:Q:49:GLY:O	2:Q:50:THR:C	2.50	0.54
1:U:37:ARG:HG2	1:U:37:ARG:NH1	2.22	0.54
1:U:341:PHE:O	1:U:345:LEU:HB2	2.07	0.54
1:W:79:ILE:HG22	1:W:103:LEU:HD13	1.88	0.54
1:X:55:MET:HA	1:X:331:VAL:HG13	1.89	0.54
1:D:264:LYS:HZ1	1:D:279:GLN:NE2	1.92	0.54
2:H:105:ILE:HG23	2:H:105:ILE:O	2.06	0.54
2:L:38:TYR:CD1	2:L:69:GLY:HA3	2.42	0.54
2:L:56:LEU:CD2	2:L:56:LEU:C	2.80	0.54
2:P:17:ASP:HB2	2:P:164:ASN:HD22	1.70	0.54
1:S:18:ILE:CG2	1:S:344:ILE:HG13	2.36	0.54
1:S:96:VAL:CG1	1:S:282:LEU:HD12	2.37	0.54
1:S:362:THR:O	1:S:362:THR:HG22	2.06	0.54
1:S:430:LEU:HG	1:S:431:GLY:H	1.72	0.54
1:X:63:LYS:HB2	1:X:63:LYS:HZ2	1.71	0.54
1:A:61:VAL:HA	1:A:336:LEU:HD22	1.90	0.54
1:A:264:LYS:CE	1:A:279:GLN:HE22	2.17	0.54
1:A:362:THR:HG21	1:B:39:GLN:HG2	1.90	0.54
1:A:407:ILE:O	1:A:411:ALA:HB2	2.08	0.54
1:D:370:THR:HG23	1:D:421:ILE:O	2.07	0.54
1:F:73:LEU:C	1:F:73:LEU:HD12	2.33	0.54
2:H:1:THR:HG23	2:H:33:LYS:NZ	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:105:ILE:HG22	2:P:113:VAL:O	2.07	0.54
1:T:55:MET:HA	1:T:331:VAL:HG13	1.89	0.54
1:T:303:ILE:HG22	1:T:304:LEU:N	2.18	0.54
1:T:369:PHE:CE2	1:T:421:ILE:HD12	2.33	0.54
1:W:18:ILE:HG22	1:W:344:ILE:HG12	1.89	0.54
1:W:362:THR:HG22	1:W:362:THR:O	2.07	0.54
1:B:352:LEU:O	1:B:355:GLN:HB2	2.07	0.54
1:B:356:TYR:O	1:B:357:LYS:C	2.50	0.54
1:B:378:ALA:C	1:B:380:ALA:N	2.63	0.54
1:C:41:GLN:HA	1:C:41:GLN:NE2	2.21	0.54
2:G:46:PHE:HB3	2:G:95:LEU:HD21	1.89	0.54
2:L:89:ARG:O	2:L:90:LYS:CB	2.55	0.54
2:P:8:ARG:O	2:P:9:ASN:HB2	2.06	0.54
1:T:5:THR:OG1	1:T:6:PRO:HD2	2.06	0.54
1:T:37:ARG:HG2	1:T:37:ARG:NH1	2.22	0.54
1:U:55:MET:HA	1:U:331:VAL:HG13	1.89	0.54
1:W:349:HIS:O	1:W:350:ALA:HB3	2.07	0.54
1:X:68:ARG:HG3	1:X:68:ARG:HH11	1.72	0.54
1:X:344:ILE:CG2	3:X:461:ATP:C2	2.90	0.54
1:B:34:ARG:CZ	1:B:251:ASN:HA	2.38	0.54
1:C:6:PRO:HD3	1:C:32:ARG:HG2	1.90	0.54
1:D:280:ARG:HA	1:D:283:LEU:HD12	1.89	0.54
2:K:1:THR:CG2	2:K:33:LYS:HD3	2.37	0.54
2:L:164:ASN:HD22	2:L:164:ASN:C	2.16	0.54
1:U:283:LEU:HB3	1:U:284:PRO:HD3	1.89	0.54
1:U:349:HIS:O	1:U:350:ALA:HB3	2.08	0.54
1:X:245:ILE:CG2	1:X:249:GLU:HG3	2.37	0.54
1:B:241:LYS:HG2	1:B:295:HIS:ND1	2.22	0.54
1:B:250:GLN:HA	1:B:250:GLN:HE21	1.72	0.54
1:B:370:THR:O	1:B:373:ALA:HB3	2.08	0.54
1:D:9:ILE:HD13	1:D:31:LEU:HD23	1.88	0.54
1:E:37:ARG:HH12	1:E:38:MET:HE2	1.72	0.54
1:E:398:THR:HG22	1:E:399:VAL:N	2.22	0.54
1:F:13:LEU:HD13	1:F:24:LYS:HG2	1.90	0.54
2:K:38:TYR:CD1	2:K:69:GLY:HA3	2.42	0.54
2:N:104:LEU:HD13	2:N:112:VAL:CG1	2.38	0.54
1:T:63:LYS:N	3:T:457:ATP:O2B	2.35	0.54
1:T:235:ILE:HG22	1:T:236:ASN:N	2.23	0.54
1:T:333:LEU:HD23	1:T:333:LEU:N	2.23	0.54
1:U:96:VAL:HG11	1:U:281:ASP:O	2.08	0.54
1:U:100:ILE:HG13	1:U:291:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:120:ARG:HG3	1:U:232:ALA:HB2	1.89	0.54
1:W:5:THR:OG1	1:W:6:PRO:HD2	2.08	0.54
1:W:98:SER:HA	1:W:101:ARG:NH1	2.23	0.54
1:X:236:ASN:N	1:X:237:PRO:HD3	2.21	0.54
1:X:333:LEU:N	1:X:333:LEU:HD23	2.23	0.54
1:A:443:ILE:HG12	2:G:112:VAL:CG2	2.38	0.54
1:B:409:PHE:CE1	1:C:6:PRO:HB3	2.41	0.54
1:C:347:GLU:HB2	1:C:348:PRO:HD3	1.89	0.54
1:E:17:ILE:HD12	1:E:17:ILE:N	2.22	0.54
2:H:4:VAL:HG22	2:H:5:SER:N	2.22	0.54
2:N:128:ASN:HA	2:N:131:LEU:HB3	1.90	0.54
2:Q:105:ILE:HG22	2:Q:113:VAL:O	2.07	0.54
1:T:68:ARG:HH11	1:T:68:ARG:HG3	1.73	0.54
1:U:20:GLN:OE1	1:U:333:LEU:HB3	2.08	0.54
1:U:120:ARG:HH12	1:U:234:LEU:HB3	1.72	0.54
1:W:315:ARG:HB3	1:W:316:PRO:HD2	1.90	0.54
1:X:80:LYS:HG3	1:X:255:PHE:HD2	1.72	0.54
1:A:235:ILE:HG22	1:A:236:ASN:N	2.23	0.54
1:B:283:LEU:O	1:B:287:GLU:HB2	2.06	0.54
2:H:52:ASP:CA	2:H:55:THR:HG23	2.35	0.54
1:S:341:PHE:O	1:S:345:LEU:HB2	2.08	0.54
1:U:437:GLU:OE2	1:U:439:LEU:HG	2.08	0.54
1:W:112:ARG:O	1:W:112:ARG:HG2	2.08	0.54
1:A:6:PRO:HB3	1:F:409:PHE:HD1	1.69	0.54
1:B:37:ARG:CG	1:B:38:MET:N	2.71	0.54
1:C:55:MET:C	1:C:56:ILE:HD12	2.32	0.54
1:C:382:PHE:C	1:C:382:PHE:HD2	2.16	0.54
1:E:283:LEU:CB	1:E:284:PRO:HD3	2.37	0.54
1:F:20:GLN:HE21	1:F:20:GLN:H	1.55	0.54
1:F:382:PHE:O	1:F:383:ARG:C	2.50	0.54
2:H:98:ALA:HB2	2:H:103:SER:HA	1.90	0.54
2:O:55:THR:HG22	2:P:83:ARG:CG	2.37	0.54
1:T:54:LEU:HD21	1:T:327:LEU:HD22	1.90	0.54
1:T:441:ARG:HH11	1:T:441:ARG:HG3	1.72	0.54
1:W:28:ALA:C	1:W:30:ALA:H	2.16	0.54
1:A:227:ILE:HG23	1:A:228:ASP:H	1.72	0.54
1:B:61:VAL:HA	1:B:336:LEU:HD22	1.89	0.54
1:B:300:THR:HA	1:B:303:ILE:HG12	1.90	0.54
1:D:113:GLN:HG2	1:D:113:GLN:O	2.08	0.54
1:E:356:TYR:CD1	1:E:400:MET:HE3	2.43	0.54
1:F:433:VAL:HG12	1:F:434:VAL:N	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:42:VAL:HG12	2:G:99:ASP:HB3	1.89	0.54
2:P:1:THR:HG23	2:P:33:LYS:HD3	1.90	0.54
1:S:370:THR:HG23	1:S:373:ALA:HB3	1.90	0.54
1:U:311:PHE:HE1	1:U:316:PRO:HA	1.73	0.54
1:X:37:ARG:HG2	1:X:37:ARG:NH1	2.22	0.54
1:X:98:SER:HA	1:X:101:ARG:NH1	2.23	0.54
1:A:38:MET:HG3	1:A:45:ARG:NH1	2.23	0.53
1:A:250:GLN:NE2	1:A:250:GLN:HA	2.23	0.53
1:B:13:LEU:CD1	1:B:24:LYS:HG2	2.38	0.53
1:B:236:ASN:C	1:B:238:GLU:H	2.16	0.53
1:B:343:ARG:C	1:B:345:LEU:N	2.62	0.53
1:C:34:ARG:CZ	1:C:251:ASN:HA	2.39	0.53
1:C:56:ILE:N	1:C:56:ILE:CD1	2.71	0.53
1:C:341:PHE:O	1:C:345:LEU:HB2	2.08	0.53
1:C:367:ILE:HD11	1:C:421:ILE:HD11	1.89	0.53
1:C:440:SER:O	1:C:442:PHE:N	2.41	0.53
1:D:262:ILE:HG13	1:D:262:ILE:O	2.07	0.53
1:T:362:THR:HG22	1:T:362:THR:O	2.08	0.53
1:T:426:VAL:O	1:T:429:ALA:HB3	2.07	0.53
1:U:55:MET:HE1	1:U:63:LYS:O	2.07	0.53
1:V:370:THR:HG23	1:V:373:ALA:HB3	1.89	0.53
1:V:444:LEU:HD23	1:V:444:LEU:C	2.32	0.53
1:W:63:LYS:NZ	3:W:460:ATP:O2G	2.41	0.53
1:W:283:LEU:HB3	1:W:284:PRO:HD3	1.90	0.53
1:W:313:VAL:CG2	1:W:314:ALA:H	2.02	0.53
1:A:37:ARG:HH12	1:A:38:MET:HE2	1.72	0.53
1:D:41:GLN:HE21	1:D:41:GLN:CA	2.21	0.53
1:E:71:ALA:HB1	1:E:78:PHE:HB2	1.89	0.53
1:E:275:ARG:O	1:E:277:GLY:N	2.41	0.53
1:E:326:ARG:O	1:E:328:PRO:HD3	2.09	0.53
1:E:377:ILE:O	1:E:380:ALA:HB3	2.09	0.53
2:G:137:LEU:CD1	2:G:137:LEU:N	2.71	0.53
2:G:164:ASN:HD22	2:G:164:ASN:C	2.13	0.53
2:K:42:VAL:HG12	2:K:99:ASP:HB3	1.90	0.53
2:L:17:ASP:HB2	2:L:164:ASN:HD22	1.68	0.53
2:N:107:THR:OG1	2:N:111:ASP:OD2	2.21	0.53
1:S:260:ASP:HB3	1:S:311:PHE:CE2	2.43	0.53
1:C:20:GLN:CA	1:C:20:GLN:NE2	2.71	0.53
1:E:77:PRO:HD2	1:E:251:ASN:O	2.09	0.53
2:J:165:THR:HA	2:J:167:PHE:CE2	2.44	0.53
2:N:56:LEU:CD2	2:N:95:LEU:HD13	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:55:THR:O	2:Q:59:LEU:HB2	2.08	0.53
1:S:63:LYS:HB2	1:S:63:LYS:HZ2	1.72	0.53
1:S:63:LYS:HZ2	1:S:308:SER:HB2	1.72	0.53
1:V:236:ASN:HD21	1:V:239:GLU:HB3	1.73	0.53
1:A:409:PHE:O	1:B:6:PRO:HG2	2.09	0.53
1:D:3:GLU:HG3	1:D:4:MET:N	2.22	0.53
1:D:37:ARG:HG2	1:D:38:MET:N	2.23	0.53
1:D:384:VAL:O	1:D:385:ASN:C	2.50	0.53
1:F:5:THR:OG1	1:F:8:GLU:HB2	2.08	0.53
1:F:12:GLU:O	1:F:15:GLN:HB2	2.09	0.53
1:F:341:PHE:HA	1:F:344:ILE:CG1	2.38	0.53
2:H:88:LEU:C	2:H:90:LYS:N	2.64	0.53
2:R:17:ASP:HB2	2:R:164:ASN:HD21	1.72	0.53
1:S:311:PHE:HE1	1:S:316:PRO:HA	1.73	0.53
1:S:437:GLU:HG3	1:S:440:SER:HB2	1.89	0.53
1:T:17:ILE:HD13	1:T:66:ILE:HG12	1.91	0.53
1:T:96:VAL:CG1	1:T:282:LEU:HD12	2.37	0.53
1:X:341:PHE:O	1:X:345:LEU:HB2	2.08	0.53
1:B:5:THR:O	1:B:9:ILE:HG13	2.08	0.53
1:D:17:ILE:N	1:D:17:ILE:CD1	2.69	0.53
2:I:144:SER:HB3	2:I:147:GLU:CG	2.35	0.53
1:S:28:ALA:C	1:S:30:ALA:H	2.17	0.53
1:S:98:SER:HA	1:S:101:ARG:NH1	2.24	0.53
1:U:370:THR:CG2	1:U:422:ASP:HA	2.38	0.53
1:U:442:PHE:O	1:U:443:ILE:HD13	2.08	0.53
1:V:20:GLN:OE1	1:V:333:LEU:HB3	2.08	0.53
1:X:349:HIS:O	1:X:350:ALA:HB3	2.07	0.53
1:X:359:LEU:O	1:X:360:MET:HE2	2.08	0.53
1:A:76:ALA:HB1	1:A:251:ASN:O	2.08	0.53
1:C:20:GLN:NE2	1:C:20:GLN:HA	2.24	0.53
1:D:37:ARG:HH22	1:D:250:GLN:HE22	1.55	0.53
1:E:380:ALA:O	1:E:383:ARG:HB3	2.09	0.53
1:F:37:ARG:HG2	1:F:38:MET:N	2.22	0.53
2:G:85:ASP:OD2	2:G:85:ASP:N	2.39	0.53
2:H:82:TRP:CZ2	2:H:91:LEU:HD13	2.35	0.53
2:H:165:THR:HA	2:H:167:PHE:CE2	2.44	0.53
2:I:67:HIS:CD2	2:I:73:LYS:HD3	2.44	0.53
2:L:17:ASP:CG	2:L:163:THR:HG23	2.33	0.53
1:S:21:ALA:C	1:S:23:ALA:N	2.64	0.53
1:U:60:GLY:HA3	1:U:392:GLY:HA3	1.90	0.53
1:U:68:ARG:HH11	1:U:68:ARG:HG3	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:315:ARG:HB3	1:V:316:PRO:HD2	1.91	0.53
1:W:55:MET:HA	1:W:331:VAL:HG13	1.90	0.53
1:X:353:THR:HG22	1:X:369:PHE:CD1	2.43	0.53
1:C:104:THR:O	1:C:107:ALA:HB3	2.07	0.53
1:C:341:PHE:HA	1:C:344:ILE:CG1	2.38	0.53
1:E:322:GLU:OE2	1:E:322:GLU:N	2.37	0.53
1:F:105:ASP:OD1	1:F:294:LYS:HE2	2.09	0.53
2:H:83:ARG:HG3	2:I:55:THR:HG22	1.90	0.53
2:K:131:LEU:O	2:K:132:SER:C	2.51	0.53
2:K:161:VAL:HG22	2:P:24:ASN:O	2.09	0.53
2:L:1:THR:CG2	2:L:33:LYS:HD3	2.39	0.53
2:M:55:THR:HG22	2:N:83:ARG:CB	2.38	0.53
2:M:83:ARG:HB3	2:R:55:THR:HG22	1.91	0.53
2:R:164:ASN:HD22	2:R:164:ASN:N	1.97	0.53
1:S:18:ILE:HG22	1:S:344:ILE:CG1	2.39	0.53
1:U:120:ARG:NE	1:U:232:ALA:HA	2.23	0.53
1:U:439:LEU:C	1:U:441:ARG:N	2.66	0.53
1:V:259:ILE:O	1:V:262:ILE:HG12	2.08	0.53
1:V:437:GLU:O	1:V:437:GLU:HG2	2.09	0.53
1:W:17:ILE:HD13	1:W:66:ILE:HG12	1.89	0.53
1:X:5:THR:OG1	1:X:6:PRO:HD2	2.07	0.53
1:X:283:LEU:HD11	1:X:322:GLU:HB3	1.90	0.53
1:A:104:THR:OG1	1:A:293:THR:HG21	2.08	0.53
1:B:382:PHE:C	1:B:382:PHE:HD2	2.16	0.53
1:C:384:VAL:O	1:C:385:ASN:C	2.49	0.53
1:F:54:LEU:HG	1:F:56:ILE:HD11	1.91	0.53
2:N:4:VAL:HG12	2:N:153:LEU:HD21	1.91	0.53
2:P:55:THR:HG22	2:Q:83:ARG:CB	2.38	0.53
1:S:369:PHE:CE2	1:S:421:ILE:HD12	2.32	0.53
1:T:65:GLU:HG2	3:T:457:ATP:H5'2	1.90	0.53
1:T:370:THR:CG2	1:T:422:ASP:HA	2.39	0.53
1:U:21:ALA:C	1:U:23:ALA:N	2.65	0.53
1:U:48:VAL:HG23	1:V:355:GLN:OE1	2.08	0.53
1:U:369:PHE:CE2	1:U:421:ILE:HD12	2.34	0.53
1:A:57:GLY:CA	1:A:63:LYS:HE3	2.38	0.53
1:B:436:ASN:O	1:B:437:GLU:C	2.52	0.53
1:C:37:ARG:CG	1:C:38:MET:N	2.72	0.53
1:D:240:LEU:O	1:D:241:LYS:C	2.52	0.53
1:E:56:ILE:N	1:E:56:ILE:HD12	2.24	0.53
1:F:37:ARG:HA	1:F:40:LEU:CD1	2.38	0.53
2:G:1:THR:HG22	2:G:2:THR:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:137:LEU:HD11	2:O:136:ALA:HB1	1.91	0.53
2:L:154:ARG:O	2:L:155:ILE:C	2.50	0.53
2:L:165:THR:HA	2:L:167:PHE:CE2	2.43	0.53
2:O:95:LEU:O	2:O:105:ILE:HA	2.09	0.53
2:P:8:ARG:HH11	2:P:8:ARG:CB	2.16	0.53
2:P:127:GLY:O	2:P:129:TYR:N	2.41	0.53
1:S:444:LEU:HD13	1:S:444:LEU:H	1.73	0.53
1:U:235:ILE:CG2	1:U:236:ASN:N	2.72	0.53
1:V:441:ARG:HG3	1:V:441:ARG:HH11	1.73	0.53
1:A:249:GLU:HG2	1:A:299:LYS:H	1.74	0.53
1:B:264:LYS:O	1:B:265:LYS:HB3	2.09	0.53
1:E:262:ILE:HD12	1:E:278:VAL:HB	1.91	0.53
1:F:441:ARG:NH2	2:G:37:LEU:HD23	2.24	0.53
1:F:443:ILE:HG21	2:L:114:GLN:HG3	1.90	0.53
2:I:7:ARG:HD2	2:I:119:GLN:CD	2.32	0.53
2:O:104:LEU:HD13	2:O:112:VAL:CG1	2.39	0.53
1:S:26:ALA:HA	1:S:29:ILE:HG12	1.91	0.53
1:S:283:LEU:HB3	1:S:284:PRO:HD3	1.90	0.53
1:S:356:TYR:OH	1:X:51:LYS:HE2	2.08	0.53
1:S:426:VAL:O	1:S:429:ALA:HB3	2.09	0.53
1:B:366:ASN:O	1:B:418:THR:HA	2.09	0.52
1:D:347:GLU:N	1:D:348:PRO:CD	2.71	0.52
2:K:129:TYR:O	2:K:130:ALA:C	2.53	0.52
2:R:56:LEU:CD2	2:R:95:LEU:HD22	2.38	0.52
1:U:333:LEU:N	1:U:333:LEU:HD23	2.24	0.52
1:W:286:VAL:HA	1:W:305:PHE:CE1	2.43	0.52
1:W:370:THR:CG2	1:W:422:ASP:HA	2.38	0.52
1:A:398:THR:HG22	1:A:399:VAL:N	2.22	0.52
1:B:280:ARG:HG3	1:B:280:ARG:HH11	1.74	0.52
1:B:403:LEU:CD1	1:B:426:VAL:HG22	2.39	0.52
1:B:404:MET:O	1:B:408:SER:HB2	2.10	0.52
1:B:444:LEU:C	1:B:444:LEU:HD23	2.34	0.52
2:H:1:THR:HG23	2:H:33:LYS:HD3	1.91	0.52
2:H:1:THR:HG22	2:H:2:THR:N	2.24	0.52
2:I:105:ILE:HG22	2:I:113:VAL:O	2.09	0.52
1:S:61:VAL:HA	1:S:336:LEU:HD21	1.92	0.52
1:S:315:ARG:HB3	1:S:316:PRO:HD2	1.90	0.52
1:U:111:VAL:CG1	1:U:240:LEU:HD11	2.39	0.52
1:U:353:THR:HG22	1:U:369:PHE:CD1	2.44	0.52
1:V:356:TYR:HB3	1:V:404:MET:HE2	1.90	0.52
1:W:260:ASP:HB3	1:W:311:PHE:CE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:369:PHE:CE2	1:X:421:ILE:HD12	2.33	0.52
1:A:119:ASN:HB3	1:A:234:LEU:CD1	2.39	0.52
1:B:357:LYS:HA	1:B:367:ILE:CG2	2.40	0.52
1:B:370:THR:O	1:B:373:ALA:N	2.40	0.52
1:C:381:ALA:HB2	1:C:396:LEU:HD23	1.91	0.52
1:E:54:LEU:HG	1:E:56:ILE:CD1	2.39	0.52
2:M:4:VAL:HG12	2:M:153:LEU:HD21	1.91	0.52
1:S:436:ASN:HD22	1:S:436:ASN:C	2.17	0.52
1:T:18:ILE:HG22	1:T:344:ILE:HG12	1.90	0.52
1:W:430:LEU:HG	1:W:431:GLY:H	1.73	0.52
1:X:245:ILE:C	1:X:247:ALA:H	2.15	0.52
1:X:315:ARG:HB3	1:X:316:PRO:HD2	1.91	0.52
1:B:51:LYS:O	1:B:52:ASN:O	2.27	0.52
1:E:249:GLU:HG2	1:E:299:LYS:H	1.75	0.52
2:G:73:LYS:O	2:G:74:SER:C	2.53	0.52
2:H:43:LEU:O	2:H:97:VAL:HA	2.09	0.52
2:H:46:PHE:HB3	2:H:95:LEU:HD21	1.91	0.52
2:H:70:HIS:O	2:H:71:LEU:C	2.51	0.52
2:I:91:LEU:O	2:I:108:GLY:HA3	2.10	0.52
2:K:18:GLY:N	2:K:164:ASN:HD21	2.03	0.52
2:M:56:LEU:HD21	2:M:95:LEU:HB2	1.90	0.52
1:S:355:GLN:OE1	1:X:48:VAL:HG23	2.10	0.52
1:S:427:ALA:C	1:S:429:ALA:H	2.18	0.52
1:U:362:THR:O	1:U:362:THR:HG22	2.09	0.52
1:V:349:HIS:O	1:V:350:ALA:HB3	2.08	0.52
1:W:55:MET:HE1	1:W:63:LYS:O	2.08	0.52
1:X:439:LEU:O	1:X:441:ARG:N	2.43	0.52
1:A:101:ARG:HA	1:A:293:THR:HG22	1.90	0.52
1:D:38:MET:HG3	1:D:45:ARG:NH1	2.24	0.52
1:E:360:MET:HA	1:E:360:MET:CE	2.36	0.52
1:E:403:LEU:C	1:E:405:ASP:H	2.17	0.52
1:F:403:LEU:CD2	1:F:404:MET:SD	2.97	0.52
2:G:77:GLU:O	2:G:80:LYS:HG2	2.09	0.52
2:H:88:LEU:C	2:H:90:LYS:H	2.18	0.52
2:H:128:ASN:O	2:H:131:LEU:HB3	2.10	0.52
2:Q:89:ARG:HH11	2:R:87:ALA:HB2	1.73	0.52
2:Q:127:GLY:O	2:Q:129:TYR:N	2.42	0.52
2:R:7:ARG:NH1	2:R:12:VAL:CG2	2.73	0.52
2:R:157:GLY:HA2	2:R:163:THR:HG22	1.92	0.52
1:S:404:MET:HA	1:S:407:ILE:HG22	1.92	0.52
1:S:422:ASP:O	1:S:426:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:260:ASP:HB3	1:T:311:PHE:CE2	2.44	0.52
1:V:96:VAL:CG1	1:V:282:LEU:HD12	2.38	0.52
1:V:353:THR:HG22	1:V:369:PHE:CD1	2.43	0.52
1:X:20:GLN:HB3	1:X:23:ALA:HB3	1.91	0.52
1:X:260:ASP:HB3	1:X:311:PHE:CE2	2.43	0.52
1:A:233:LYS:HD2	1:A:234:LEU:HB2	1.91	0.52
1:C:55:MET:CE	1:C:306:ILE:HG21	2.39	0.52
1:F:283:LEU:O	1:F:284:PRO:C	2.53	0.52
2:P:157:GLY:HA2	2:P:163:THR:HG22	1.91	0.52
1:S:16:HIS:HA	1:S:348:PRO:HB3	1.92	0.52
1:S:313:VAL:CG2	1:S:314:ALA:H	2.02	0.52
1:S:359:LEU:HD11	1:X:48:VAL:HG21	1.90	0.52
1:V:34:ARG:HG2	1:V:250:GLN:HE21	1.75	0.52
1:V:96:VAL:HG11	1:V:281:ASP:O	2.09	0.52
1:X:370:THR:CG2	1:X:422:ASP:HA	2.38	0.52
1:A:370:THR:O	1:A:373:ALA:HB3	2.09	0.52
1:F:370:THR:O	1:F:371:THR:C	2.52	0.52
2:K:3:ILE:HG22	2:K:96:ILE:HD12	1.90	0.52
2:M:8:ARG:O	2:M:9:ASN:HB2	2.08	0.52
2:P:95:LEU:O	2:P:105:ILE:HA	2.10	0.52
2:P:128:ASN:HA	2:P:131:LEU:HB3	1.92	0.52
2:R:55:THR:O	2:R:59:LEU:HB2	2.09	0.52
2:R:95:LEU:O	2:R:105:ILE:HA	2.10	0.52
1:S:247:ALA:O	1:S:251:ASN:N	2.37	0.52
1:T:26:ALA:HA	1:T:29:ILE:HG12	1.91	0.52
1:V:54:LEU:HD21	1:V:327:LEU:HD22	1.91	0.52
1:X:100:ILE:HG13	1:X:291:VAL:HG21	1.92	0.52
1:D:347:GLU:HB2	1:D:348:PRO:HD3	1.91	0.52
1:E:326:ARG:C	1:E:328:PRO:HD3	2.34	0.52
1:F:403:LEU:HD22	1:F:404:MET:HG2	1.92	0.52
2:M:56:LEU:CD2	2:M:95:LEU:HD22	2.40	0.52
2:M:118:ASP:O	2:M:120:ILE:N	2.43	0.52
1:X:96:VAL:CG1	1:X:282:LEU:HD12	2.39	0.52
1:A:439:LEU:HA	1:A:443:ILE:HD12	1.91	0.52
1:B:73:LEU:C	1:B:73:LEU:HD12	2.35	0.52
1:E:337:SER:OG	1:E:338:ALA:N	2.42	0.52
1:F:108:MET:HE1	1:F:240:LEU:HD21	1.92	0.52
2:N:49:GLY:O	2:N:51:ALA:N	2.43	0.52
1:S:17:ILE:HD13	1:S:66:ILE:HG12	1.92	0.52
1:S:344:ILE:CG2	3:S:456:ATP:C2	2.93	0.52
1:T:21:ALA:C	1:T:23:ALA:N	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:421:ILE:O	1:T:421:ILE:HG22	2.09	0.52
1:U:422:ASP:O	1:U:426:VAL:HG23	2.10	0.52
1:W:322:GLU:HG3	1:X:394:ARG:HH12	1.74	0.52
1:W:333:LEU:N	1:W:333:LEU:HD23	2.25	0.52
1:A:54:LEU:HG	1:A:56:ILE:CD1	2.40	0.52
1:B:360:MET:HE1	1:C:36:ARG:HH11	1.71	0.52
1:C:101:ARG:HA	1:C:293:THR:HG22	1.91	0.52
1:F:6:PRO:HD3	1:F:32:ARG:HG2	1.92	0.52
2:L:7:ARG:CZ	2:L:12:VAL:HG22	2.39	0.52
1:S:63:LYS:HB2	3:S:456:ATP:O2B	2.10	0.52
1:T:437:GLU:O	1:T:439:LEU:HD23	2.09	0.52
1:V:98:SER:HA	1:V:101:ARG:NH1	2.24	0.52
1:W:26:ALA:HA	1:W:29:ILE:HG12	1.92	0.52
1:W:34:ARG:HG2	1:W:250:GLN:HE21	1.74	0.52
1:A:276:GLU:HG2	1:A:276:GLU:O	2.11	0.51
1:D:415:ASN:OD1	1:D:416:GLY:N	2.42	0.51
1:E:79:ILE:CG2	1:E:103:LEU:HD13	2.37	0.51
1:E:83:ALA:HB1	1:E:262:ILE:HD13	1.92	0.51
2:M:7:ARG:NH1	2:M:12:VAL:CG2	2.73	0.51
1:V:370:THR:HG23	1:V:373:ALA:CB	2.40	0.51
1:W:20:GLN:OE1	1:W:333:LEU:HB3	2.10	0.51
1:A:403:LEU:C	1:A:405:ASP:H	2.18	0.51
1:B:57:GLY:HA3	1:B:63:LYS:HE3	1.91	0.51
1:C:406:LYS:HD2	1:C:406:LYS:N	2.13	0.51
1:E:250:GLN:HA	1:E:250:GLN:NE2	2.25	0.51
1:E:381:ALA:HB2	1:E:396:LEU:HD23	1.92	0.51
1:F:280:ARG:HG3	1:F:280:ARG:NH1	2.25	0.51
1:F:356:TYR:CD1	1:F:400:MET:HE3	2.46	0.51
2:I:115:PRO:CB	2:I:119:GLN:HA	2.41	0.51
2:J:140:ASN:C	2:J:141:THR:HG22	2.36	0.51
2:N:55:THR:O	2:N:59:LEU:HB2	2.09	0.51
2:R:120:ILE:O	2:R:121:LEU:HD23	2.11	0.51
1:S:96:VAL:HG11	1:S:281:ASP:O	2.09	0.51
1:V:21:ALA:C	1:V:23:ALA:N	2.65	0.51
1:V:108:MET:SD	1:V:244:ALA:CB	2.97	0.51
1:F:338:ALA:N	1:F:382:PHE:HD1	2.08	0.51
2:I:1:THR:HG22	2:I:2:THR:N	2.25	0.51
2:M:83:ARG:CG	2:R:55:THR:HG22	2.39	0.51
2:N:120:ILE:O	2:N:121:LEU:HD23	2.10	0.51
2:Q:5:SER:CB	2:Q:14:VAL:HG22	2.38	0.51
1:T:48:VAL:HG23	1:U:355:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:21:ALA:C	1:X:23:ALA:N	2.64	0.51
1:A:304:LEU:HD12	1:A:305:PHE:N	2.26	0.51
1:C:360:MET:HE1	1:D:36:ARG:NH1	2.25	0.51
1:F:33:ASN:HA	1:F:36:ARG:HD2	1.91	0.51
2:H:71:LEU:C	2:H:71:LEU:HD13	2.35	0.51
2:K:82:TRP:CE2	2:K:88:LEU:HD13	2.45	0.51
2:L:115:PRO:HG3	2:L:121:LEU:HD11	1.92	0.51
2:M:55:THR:O	2:M:59:LEU:HB2	2.11	0.51
2:R:105:ILE:HG22	2:R:113:VAL:O	2.11	0.51
2:R:133:ALA:O	2:R:136:ALA:HB3	2.10	0.51
1:U:80:LYS:HG3	1:U:255:PHE:HD2	1.73	0.51
1:U:120:ARG:HG3	1:U:232:ALA:HA	1.93	0.51
1:W:28:ALA:C	1:W:30:ALA:N	2.68	0.51
1:W:370:THR:HG23	1:W:373:ALA:HB3	1.92	0.51
1:X:9:ILE:HD13	1:X:31:LEU:HD23	1.92	0.51
1:X:422:ASP:O	1:X:426:VAL:HG23	2.10	0.51
1:A:338:ALA:N	1:A:382:PHE:HD1	2.08	0.51
1:B:41:GLN:HA	1:B:41:GLN:HE21	1.75	0.51
1:B:403:LEU:C	1:B:405:ASP:H	2.19	0.51
2:J:82:TRP:CE3	2:J:110:GLY:HA2	2.45	0.51
2:K:1:THR:HG23	2:K:33:LYS:CE	2.41	0.51
2:L:6:VAL:HG22	2:L:120:ILE:HG23	1.93	0.51
2:O:55:THR:O	2:O:59:LEU:HB2	2.11	0.51
2:O:105:ILE:HG22	2:O:113:VAL:O	2.10	0.51
1:T:96:VAL:HG11	1:T:281:ASP:O	2.10	0.51
1:U:315:ARG:HB3	1:U:316:PRO:CD	2.41	0.51
1:U:430:LEU:HG	1:U:431:GLY:H	1.76	0.51
1:B:250:GLN:HE21	1:B:250:GLN:CA	2.21	0.51
1:C:377:ILE:O	1:C:380:ALA:HB3	2.11	0.51
1:E:101:ARG:HA	1:E:293:THR:HG22	1.93	0.51
1:E:107:ALA:O	1:E:111:VAL:HG23	2.11	0.51
2:H:161:VAL:HG22	2:M:24:ASN:O	2.10	0.51
2:J:70:HIS:O	2:J:71:LEU:C	2.53	0.51
2:O:164:ASN:HD22	2:O:164:ASN:N	1.98	0.51
1:S:54:LEU:HD21	1:S:327:LEU:HD22	1.93	0.51
1:T:427:ALA:C	1:T:429:ALA:H	2.19	0.51
1:C:347:GLU:N	1:C:348:PRO:CD	2.74	0.51
1:D:34:ARG:NH2	1:D:253:ILE:HD13	2.25	0.51
1:E:403:LEU:CD2	1:E:404:MET:N	2.72	0.51
2:K:83:ARG:HG2	2:L:55:THR:CB	2.41	0.51
2:R:56:LEU:HD23	2:R:95:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:244:ALA:O	1:S:247:ALA:HB3	2.10	0.51
1:T:324:GLN:HE22	1:U:389:GLU:HG2	1.75	0.51
1:W:369:PHE:HE2	1:W:421:ILE:CD1	2.20	0.51
1:X:108:MET:HE1	1:X:240:LEU:O	2.11	0.51
1:A:234:LEU:O	1:A:235:ILE:C	2.54	0.51
1:A:337:SER:OG	1:A:338:ALA:N	2.43	0.51
1:C:337:SER:OG	1:C:338:ALA:N	2.43	0.51
1:C:403:LEU:C	1:C:403:LEU:CD2	2.80	0.51
1:F:37:ARG:CG	1:F:38:MET:N	2.74	0.51
2:H:116:GLU:HG2	2:I:30:ASN:ND2	2.26	0.51
2:I:7:ARG:NH2	2:I:102:GLU:O	2.44	0.51
2:Q:1:THR:HG23	2:Q:33:LYS:HD3	1.92	0.51
2:R:37:LEU:HD22	2:R:61:GLU:HG3	1.93	0.51
1:V:311:PHE:HE1	1:V:316:PRO:HA	1.75	0.51
1:X:356:TYR:HB3	1:X:404:MET:HE2	1.93	0.51
1:A:74:ALA:O	1:A:75:ASN:C	2.53	0.51
1:B:381:ALA:O	1:B:384:VAL:HG13	2.11	0.51
1:D:34:ARG:CZ	1:D:251:ASN:HA	2.41	0.51
1:D:78:PHE:CG	1:D:79:ILE:N	2.78	0.51
1:E:356:TYR:HE1	1:E:400:MET:HB3	1.75	0.51
2:I:46:PHE:HB3	2:I:95:LEU:HD23	1.92	0.51
2:J:164:ASN:HD22	2:J:164:ASN:C	2.18	0.51
2:M:56:LEU:CD2	2:M:95:LEU:HD13	2.41	0.51
2:N:90:LYS:O	2:N:91:LEU:HD12	2.11	0.51
1:T:34:ARG:HG2	1:T:250:GLN:HE21	1.76	0.51
1:T:112:ARG:O	1:T:116:ILE:HB	2.10	0.51
1:U:427:ALA:C	1:U:429:ALA:H	2.19	0.51
1:V:20:GLN:HB3	1:V:23:ALA:HB3	1.92	0.51
1:X:303:ILE:HG22	1:X:304:LEU:N	2.23	0.51
1:X:434:VAL:O	1:X:435:GLU:O	2.29	0.51
1:B:378:ALA:O	1:B:380:ALA:N	2.44	0.51
1:D:44:LEU:HA	1:D:47:GLU:HB2	1.93	0.51
1:D:111:VAL:HG21	1:D:244:ALA:CA	2.41	0.51
1:D:112:ARG:C	1:D:114:GLN:H	2.19	0.51
1:D:116:ILE:CD1	1:D:117:ALA:N	2.74	0.51
1:F:58:PRO:O	1:F:63:LYS:NZ	2.41	0.51
1:F:407:ILE:O	1:F:411:ALA:HB2	2.11	0.51
2:N:33:LYS:HA	2:N:46:PHE:CZ	2.46	0.51
1:S:28:ALA:C	1:S:30:ALA:N	2.68	0.51
1:S:357:LYS:CA	1:S:367:ILE:HD11	2.32	0.51
1:S:439:LEU:H	1:S:439:LEU:CD2	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:370:THR:HG23	1:T:373:ALA:HB3	1.93	0.51
1:V:28:ALA:C	1:V:30:ALA:H	2.18	0.51
1:V:441:ARG:O	1:V:443:ILE:N	2.44	0.51
1:W:65:GLU:HG2	3:W:460:ATP:C5'	2.29	0.51
1:A:283:LEU:CB	1:A:284:PRO:HD3	2.42	0.50
1:C:439:LEU:HD23	1:C:443:ILE:HD12	1.93	0.50
1:D:439:LEU:HD23	2:J:72:LEU:HG	1.91	0.50
1:E:52:ASN:ND2	1:E:305:PHE:CB	2.72	0.50
1:E:382:PHE:C	1:E:382:PHE:HD2	2.19	0.50
1:F:54:LEU:HG	1:F:56:ILE:CD1	2.41	0.50
2:M:37:LEU:HD22	2:M:61:GLU:HG3	1.94	0.50
1:S:96:VAL:HG21	1:S:281:ASP:HB3	1.93	0.50
1:T:28:ALA:C	1:T:30:ALA:H	2.18	0.50
1:T:439:LEU:O	1:T:440:SER:C	2.53	0.50
1:U:45:ARG:O	1:U:48:VAL:HG12	2.11	0.50
1:W:353:THR:HG22	1:W:369:PHE:CD1	2.46	0.50
1:X:48:VAL:HG13	1:X:48:VAL:O	2.10	0.50
1:B:71:ALA:HB1	1:B:78:PHE:HB2	1.92	0.50
1:C:12:GLU:O	1:C:15:GLN:HB2	2.11	0.50
1:F:31:LEU:CD2	1:F:74:ALA:HB2	2.41	0.50
1:F:119:ASN:ND2	1:F:235:ILE:N	2.58	0.50
1:F:403:LEU:CD2	1:F:404:MET:N	2.71	0.50
2:G:54:PHE:O	2:G:55:THR:C	2.54	0.50
2:K:70:HIS:O	2:K:71:LEU:C	2.54	0.50
2:L:61:GLU:O	2:L:62:ARG:C	2.54	0.50
2:P:92:GLU:O	2:P:93:ALA:HB2	2.12	0.50
2:P:112:VAL:HB	1:V:443:ILE:CD1	2.42	0.50
1:T:63:LYS:HZ2	1:T:63:LYS:HB2	1.76	0.50
1:T:336:LEU:HB2	1:T:341:PHE:HE1	1.75	0.50
1:U:356:TYR:HB3	1:U:404:MET:HE2	1.93	0.50
1:V:96:VAL:HG21	1:V:281:ASP:HB3	1.94	0.50
1:X:427:ALA:C	1:X:429:ALA:H	2.19	0.50
1:A:9:ILE:O	1:A:10:VAL:C	2.54	0.50
1:B:403:LEU:HD12	1:B:426:VAL:HG22	1.94	0.50
1:D:443:ILE:HD11	2:J:72:LEU:HD11	1.92	0.50
1:E:33:ASN:HA	1:E:36:ARG:HD2	1.91	0.50
1:F:239:GLU:O	1:F:240:LEU:C	2.54	0.50
1:F:341:PHE:HA	1:F:344:ILE:HG12	1.94	0.50
1:F:366:ASN:O	1:F:418:THR:HA	2.10	0.50
1:F:378:ALA:O	1:F:379:GLU:C	2.52	0.50
2:H:55:THR:HG21	2:H:89:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:57:PHE:HA	2:H:95:LEU:HD11	1.92	0.50
2:M:90:LYS:C	2:M:91:LEU:HD12	2.36	0.50
1:S:34:ARG:HG2	1:S:250:GLN:HE21	1.75	0.50
1:U:26:ALA:HA	1:U:29:ILE:HG12	1.92	0.50
1:U:34:ARG:HG2	1:U:250:GLN:HE21	1.76	0.50
1:U:370:THR:HG23	1:U:373:ALA:HB3	1.92	0.50
1:V:280:ARG:HH22	1:W:261:LYS:HE3	1.75	0.50
1:V:427:ALA:C	1:V:429:ALA:H	2.18	0.50
1:W:54:LEU:HD21	1:W:327:LEU:HD22	1.93	0.50
1:X:96:VAL:HG11	1:X:281:ASP:O	2.12	0.50
1:X:336:LEU:HB2	1:X:341:PHE:HE1	1.76	0.50
1:X:439:LEU:C	1:X:441:ARG:N	2.67	0.50
1:B:337:SER:OG	1:B:338:ALA:N	2.43	0.50
1:D:262:ILE:HD12	1:D:278:VAL:HB	1.94	0.50
1:E:79:ILE:HD12	1:E:80:LYS:H	1.75	0.50
1:E:264:LYS:HE3	1:E:264:LYS:H	1.73	0.50
1:F:107:ALA:HB2	1:F:248:VAL:HG23	1.94	0.50
2:L:1:THR:HG23	2:L:33:LYS:HD3	1.94	0.50
2:N:90:LYS:C	2:N:91:LEU:HD12	2.36	0.50
2:N:95:LEU:O	2:N:105:ILE:HA	2.12	0.50
2:O:1:THR:HG23	2:O:33:LYS:HD3	1.93	0.50
2:Q:76:VAL:HG22	1:W:443:ILE:HD11	1.93	0.50
2:R:83:ARG:HH12	1:X:442:PHE:HB2	1.76	0.50
2:R:134:ALA:O	2:R:137:LEU:N	2.45	0.50
1:S:100:ILE:HG13	1:S:291:VAL:HG21	1.93	0.50
1:S:370:THR:HG23	1:S:373:ALA:CB	2.41	0.50
1:T:45:ARG:O	1:T:48:VAL:HG12	2.11	0.50
1:V:107:ALA:O	1:V:111:VAL:HG23	2.12	0.50
1:V:236:ASN:ND2	1:V:239:GLU:HB3	2.27	0.50
1:W:245:ILE:HG22	1:W:249:GLU:HG3	1.94	0.50
1:W:315:ARG:HB3	1:W:316:PRO:CD	2.41	0.50
1:W:404:MET:HA	1:W:407:ILE:HG22	1.93	0.50
1:X:34:ARG:HG2	1:X:250:GLN:HE21	1.76	0.50
1:X:361:ALA:C	1:X:363:GLU:H	2.19	0.50
1:B:5:THR:O	1:B:6:PRO:C	2.54	0.50
1:B:41:GLN:HE21	1:B:41:GLN:CA	2.24	0.50
1:C:403:LEU:HD22	1:C:404:MET:HG2	1.94	0.50
1:D:337:SER:OG	1:D:338:ALA:N	2.44	0.50
1:F:119:ASN:HD21	1:F:235:ILE:N	2.09	0.50
2:L:17:ASP:OD2	2:L:33:LYS:HE3	2.11	0.50
2:N:55:THR:HG22	2:O:83:ARG:CG	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:37:LEU:HD22	2:O:61:GLU:HG3	1.93	0.50
2:Q:7:ARG:NH1	2:Q:12:VAL:CG2	2.75	0.50
2:Q:95:LEU:O	2:Q:105:ILE:HA	2.11	0.50
1:S:20:GLN:HB3	1:S:23:ALA:HB3	1.93	0.50
1:U:260:ASP:HB3	1:U:311:PHE:CE2	2.46	0.50
1:U:279:GLN:O	1:U:320:ILE:HD11	2.11	0.50
1:V:119:ASN:C	1:V:119:ASN:HD22	2.18	0.50
1:W:96:VAL:HG11	1:W:281:ASP:O	2.10	0.50
1:A:236:ASN:ND2	1:A:239:GLU:CB	2.73	0.50
1:B:5:THR:HG23	1:B:8:GLU:CD	2.36	0.50
1:B:38:MET:HG3	1:B:45:ARG:NH1	2.26	0.50
1:C:439:LEU:HA	1:C:443:ILE:CD1	2.38	0.50
1:D:20:GLN:HE21	1:D:20:GLN:CA	2.24	0.50
1:E:356:TYR:HD1	1:E:400:MET:HE3	1.76	0.50
1:F:249:GLU:HG2	1:F:299:LYS:H	1.77	0.50
2:G:17:ASP:C	2:G:33:LYS:HD2	2.36	0.50
2:P:133:ALA:O	2:P:136:ALA:HB3	2.11	0.50
2:Q:107:THR:OG1	2:Q:111:ASP:OD2	2.24	0.50
1:S:236:ASN:HB3	1:S:239:GLU:CB	2.41	0.50
1:S:363:GLU:OE1	1:X:32:ARG:NH2	2.40	0.50
1:V:404:MET:HA	1:V:407:ILE:HG22	1.94	0.50
1:V:426:VAL:O	1:V:429:ALA:HB3	2.12	0.50
1:W:63:LYS:HZ2	1:W:63:LYS:HB2	1.77	0.50
1:W:96:VAL:HG21	1:W:281:ASP:HB3	1.94	0.50
1:W:357:LYS:HA	1:W:367:ILE:CD1	2.32	0.50
1:W:421:ILE:O	1:W:421:ILE:HG22	2.11	0.50
1:X:18:ILE:HG22	1:X:344:ILE:HG12	1.94	0.50
1:X:370:THR:HG23	1:X:373:ALA:HB3	1.93	0.50
1:A:44:LEU:O	1:A:48:VAL:HG12	2.12	0.50
1:E:37:ARG:HH22	1:E:250:GLN:HE22	1.59	0.50
2:N:151:LYS:O	2:N:155:ILE:HD13	2.12	0.50
2:O:5:SER:CB	2:O:14:VAL:HG22	2.40	0.50
2:P:7:ARG:NH1	2:P:12:VAL:CG2	2.75	0.50
2:Q:37:LEU:HD22	2:Q:61:GLU:HG3	1.93	0.50
2:R:37:LEU:HD23	1:S:441:ARG:NH2	2.26	0.50
1:T:315:ARG:HB3	1:T:316:PRO:CD	2.41	0.50
1:U:344:ILE:HG23	3:U:458:ATP:C2	2.44	0.50
1:V:422:ASP:O	1:V:426:VAL:HG23	2.12	0.50
1:X:28:ALA:C	1:X:30:ALA:H	2.20	0.50
1:X:311:PHE:HE1	1:X:316:PRO:HA	1.77	0.50
1:B:44:LEU:HA	1:B:47:GLU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:MET:O	1:B:109:LYS:C	2.54	0.50
1:B:384:VAL:O	1:B:385:ASN:C	2.55	0.50
1:C:262:ILE:HD12	1:C:278:VAL:HB	1.93	0.50
1:D:410:SER:O	1:D:411:ALA:C	2.53	0.50
1:E:20:GLN:HE21	1:E:20:GLN:H	1.60	0.50
1:E:65:GLU:HG3	3:E:454:ATP:H2'	1.92	0.50
1:F:356:TYR:O	1:F:357:LYS:C	2.55	0.50
2:H:6:VAL:HG12	2:H:7:ARG:N	2.26	0.50
2:H:78:LEU:HD11	2:H:82:TRP:HZ3	1.76	0.50
2:J:137:LEU:HD13	2:P:136:ALA:HB1	1.92	0.50
2:K:73:LYS:O	2:K:74:SER:C	2.54	0.50
2:O:7:ARG:NH1	2:O:12:VAL:CG2	2.75	0.50
2:P:37:LEU:HD22	2:P:61:GLU:HG3	1.94	0.50
1:T:422:ASP:O	1:T:426:VAL:HG23	2.11	0.50
1:W:48:VAL:O	1:W:48:VAL:HG13	2.12	0.50
1:W:422:ASP:O	1:W:426:VAL:HG23	2.11	0.50
1:A:62:GLY:O	1:A:63:LYS:C	2.54	0.50
1:C:357:LYS:HG2	1:C:367:ILE:HG23	1.94	0.50
1:D:355:GLN:O	1:D:359:LEU:HD23	2.12	0.50
1:E:356:TYR:O	1:E:357:LYS:C	2.55	0.50
2:N:7:ARG:NH1	2:N:12:VAL:CG2	2.75	0.50
1:T:311:PHE:HE1	1:T:316:PRO:HA	1.77	0.50
1:W:370:THR:HG23	1:W:373:ALA:CB	2.42	0.50
1:X:393:ALA:HB3	3:X:461:ATP:H1'	1.93	0.50
1:A:326:ARG:C	1:A:328:PRO:HD3	2.37	0.49
1:B:344:ILE:CG2	3:B:451:ATP:C2	2.95	0.49
1:C:330:ARG:HG3	1:C:330:ARG:NH1	2.27	0.49
1:C:403:LEU:CD2	1:C:404:MET:N	2.75	0.49
1:D:5:THR:O	1:D:6:PRO:C	2.56	0.49
1:D:290:THR:CG2	1:D:297:MET:HE3	2.41	0.49
1:E:347:GLU:HB2	1:E:348:PRO:HD3	1.94	0.49
2:G:25:THR:HA	2:R:159:ILE:O	2.11	0.49
2:H:164:ASN:HD22	2:H:164:ASN:H	1.60	0.49
2:I:94:MET:HE3	2:I:123:ILE:HB	1.93	0.49
2:J:105:ILE:HG23	2:J:105:ILE:O	2.11	0.49
1:S:54:LEU:CD2	1:S:307:ALA:HB3	2.42	0.49
1:S:336:LEU:HB2	1:S:341:PHE:HE1	1.77	0.49
1:T:48:VAL:O	1:T:48:VAL:HG13	2.12	0.49
1:T:100:ILE:HG13	1:T:291:VAL:HG21	1.93	0.49
1:U:28:ALA:C	1:U:30:ALA:H	2.20	0.49
1:W:45:ARG:O	1:W:48:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:VAL:O	1:C:375:LYS:C	2.55	0.49
2:I:43:LEU:O	2:I:97:VAL:HA	2.11	0.49
2:J:1:THR:HG23	2:J:33:LYS:CE	2.41	0.49
2:L:17:ASP:HB2	2:L:164:ASN:HD21	1.75	0.49
1:T:229:ASP:O	1:T:233:LYS:HG3	2.11	0.49
1:T:431:GLY:O	1:T:432:GLU:HG3	2.12	0.49
1:V:260:ASP:HB3	1:V:311:PHE:CE2	2.46	0.49
1:C:387:LYS:HD2	1:C:435:GLU:OE1	2.13	0.49
1:D:57:GLY:HA3	1:D:63:LYS:HE3	1.94	0.49
1:D:264:LYS:HZ3	1:D:279:GLN:HE22	1.49	0.49
1:F:235:ILE:HG22	1:F:237:PRO:HD3	1.95	0.49
2:I:1:THR:HG23	2:I:33:LYS:CE	2.43	0.49
2:K:82:TRP:NE1	2:K:88:LEU:HB3	2.27	0.49
2:K:86:ARG:CG	2:K:87:ALA:H	2.22	0.49
2:K:137:LEU:O	2:K:141:THR:CG2	2.52	0.49
1:S:369:PHE:HE2	1:S:421:ILE:CD1	2.21	0.49
1:U:426:VAL:O	1:U:429:ALA:HB3	2.12	0.49
1:W:260:ASP:HB3	1:W:311:PHE:HD2	1.73	0.49
1:B:310:ALA:O	1:B:311:PHE:HB2	2.10	0.49
1:E:257:ASP:OD1	1:E:308:SER:OG	2.31	0.49
1:F:57:GLY:CA	1:F:63:LYS:HE3	2.41	0.49
1:F:337:SER:OG	1:F:338:ALA:N	2.43	0.49
1:F:356:TYR:HE1	1:F:400:MET:HB3	1.76	0.49
2:G:164:ASN:ND2	2:G:164:ASN:C	2.70	0.49
2:K:17:ASP:O	2:K:33:LYS:HD2	2.11	0.49
2:O:133:ALA:O	2:O:136:ALA:HB3	2.12	0.49
1:T:404:MET:HA	1:T:407:ILE:HG22	1.94	0.49
1:U:63:LYS:HZ2	1:U:63:LYS:HB2	1.77	0.49
1:U:96:VAL:CG1	1:U:282:LEU:HD12	2.39	0.49
1:V:26:ALA:HA	1:V:29:ILE:HG12	1.94	0.49
1:W:356:TYR:HB3	1:W:404:MET:HE2	1.94	0.49
1:X:65:GLU:HG2	3:X:461:ATP:H5'2	1.94	0.49
1:A:382:PHE:O	1:A:383:ARG:C	2.55	0.49
1:A:440:SER:O	1:A:442:PHE:N	2.45	0.49
1:E:403:LEU:HD12	1:E:426:VAL:HG13	1.94	0.49
1:E:407:ILE:HD11	1:E:425:TYR:OH	2.12	0.49
1:F:256:ILE:HG21	1:F:259:ILE:HD12	1.93	0.49
2:L:151:LYS:O	2:L:155:ILE:HG13	2.13	0.49
2:N:4:VAL:HA	2:N:121:LEU:O	2.13	0.49
2:P:120:ILE:O	2:P:121:LEU:HD23	2.12	0.49
1:T:245:ILE:HD11	1:T:295:HIS:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:369:PHE:HE2	1:T:421:ILE:CD1	2.21	0.49
1:U:297:MET:HB2	1:V:109:LYS:NZ	2.28	0.49
1:U:441:ARG:O	1:U:443:ILE:N	2.44	0.49
1:V:315:ARG:HB3	1:V:316:PRO:CD	2.42	0.49
1:W:9:ILE:HD13	1:W:31:LEU:HD23	1.94	0.49
1:B:438:ASP:CG	1:B:439:LEU:H	2.19	0.49
1:D:34:ARG:HH22	1:D:253:ILE:HD13	1.78	0.49
1:E:402:ARG:O	1:E:405:ASP:HB2	2.13	0.49
1:F:410:SER:O	1:F:411:ALA:C	2.56	0.49
2:J:71:LEU:C	2:J:71:LEU:HD13	2.38	0.49
2:J:117:GLU:C	2:J:119:GLN:H	2.21	0.49
1:U:120:ARG:NH1	1:U:234:LEU:HB3	2.28	0.49
1:W:21:ALA:C	1:W:23:ALA:N	2.67	0.49
1:W:427:ALA:C	1:W:429:ALA:H	2.20	0.49
1:W:439:LEU:HG	1:W:440:SER:N	2.20	0.49
1:B:108:MET:HG3	1:B:295:HIS:CE1	2.48	0.49
1:D:341:PHE:HA	1:D:344:ILE:CG1	2.42	0.49
1:D:360:MET:HA	1:D:360:MET:CE	2.33	0.49
1:E:382:PHE:O	1:E:383:ARG:C	2.56	0.49
1:F:41:GLN:CA	1:F:41:GLN:HE21	2.26	0.49
1:F:242:GLN:OE1	1:F:242:GLN:HA	2.12	0.49
1:F:315:ARG:O	1:F:318:ASP:HB2	2.13	0.49
2:J:83:ARG:HG2	2:K:55:THR:CG2	2.39	0.49
2:J:107:THR:OG1	2:J:111:ASP:OD2	2.26	0.49
2:Q:118:ASP:OD1	2:Q:119:GLN:N	2.43	0.49
1:U:9:ILE:HD13	1:U:31:LEU:HD23	1.94	0.49
1:U:20:GLN:HB3	1:U:23:ALA:HB3	1.94	0.49
1:X:421:ILE:O	1:X:421:ILE:HG22	2.11	0.49
1:A:113:GLN:OE1	1:A:113:GLN:HA	2.13	0.49
1:C:81:VAL:HG11	1:C:99:ILE:HG12	1.93	0.49
1:E:5:THR:OG1	1:E:8:GLU:HB2	2.12	0.49
1:E:404:MET:O	1:E:408:SER:HB2	2.12	0.49
2:G:36:ARG:NH1	2:G:170:GLU:OE2	2.46	0.49
1:T:28:ALA:C	1:T:30:ALA:N	2.69	0.49
1:T:436:ASN:O	1:T:437:GLU:C	2.56	0.49
1:U:404:MET:HA	1:U:407:ILE:HG22	1.95	0.49
1:A:341:PHE:O	1:A:345:LEU:HB2	2.12	0.49
1:C:51:LYS:O	1:C:52:ASN:O	2.30	0.49
1:D:20:GLN:NE2	1:D:20:GLN:HA	2.27	0.49
1:D:437:GLU:O	1:D:439:LEU:N	2.46	0.49
1:E:381:ALA:CB	1:E:396:LEU:HD23	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:454:ATP:C8	3:E:454:ATP:H5'1	2.48	0.49
1:F:83:ALA:HB1	1:F:262:ILE:HD13	1.95	0.49
2:G:137:LEU:O	2:G:141:THR:CG2	2.56	0.49
2:O:55:THR:HG22	2:P:83:ARG:HB3	1.95	0.49
2:P:5:SER:CB	2:P:14:VAL:HG22	2.40	0.49
1:S:328:PRO:HB3	1:T:398:THR:HA	1.94	0.49
1:U:48:VAL:HG13	1:U:48:VAL:O	2.12	0.49
1:V:45:ARG:O	1:V:48:VAL:HG12	2.12	0.49
1:V:436:ASN:O	1:V:437:GLU:C	2.56	0.49
1:W:65:GLU:CG	3:W:460:ATP:H5'2	2.26	0.49
1:A:264:LYS:HZ3	1:A:279:GLN:NE2	2.03	0.49
1:C:83:ALA:HB1	1:C:262:ILE:HD13	1.93	0.49
1:C:349:HIS:O	1:C:350:ALA:CB	2.59	0.49
1:F:41:GLN:HA	1:F:41:GLN:HE21	1.77	0.49
2:G:49:GLY:O	2:G:50:THR:C	2.55	0.49
2:H:120:ILE:HD11	2:H:138:VAL:HG21	1.95	0.49
2:I:17:ASP:CG	2:I:163:THR:HG23	2.38	0.49
1:S:15:GLN:O	1:S:348:PRO:CA	2.61	0.49
1:U:370:THR:HG23	1:U:373:ALA:CB	2.43	0.49
1:W:61:VAL:HA	1:W:336:LEU:HD21	1.94	0.49
1:A:293:THR:C	1:A:295:HIS:H	2.21	0.48
1:B:38:MET:HA	1:B:45:ARG:HH11	1.78	0.48
1:C:367:ILE:HD11	1:C:421:ILE:HD12	1.93	0.48
1:D:444:LEU:HD21	2:K:20:VAL:HG21	1.94	0.48
1:E:343:ARG:C	1:E:345:LEU:N	2.66	0.48
1:E:443:ILE:HG21	2:K:114:GLN:HG3	1.94	0.48
2:H:88:LEU:O	2:H:89:ARG:C	2.55	0.48
2:I:79:ALA:CB	2:I:83:ARG:HH21	2.25	0.48
2:K:81:ASP:HB3	2:K:88:LEU:HD12	1.94	0.48
2:L:78:LEU:HD12	2:L:78:LEU:O	2.13	0.48
2:Q:49:GLY:O	2:Q:51:ALA:N	2.45	0.48
2:Q:104:LEU:HD13	2:Q:112:VAL:CG1	2.44	0.48
2:R:116:GLU:O	2:R:117:GLU:C	2.56	0.48
1:S:315:ARG:HB3	1:S:316:PRO:CD	2.42	0.48
1:T:20:GLN:HB3	1:T:23:ALA:HB3	1.94	0.48
1:V:322:GLU:HG3	1:W:394:ARG:HH12	1.78	0.48
1:X:45:ARG:O	1:X:48:VAL:HG12	2.13	0.48
1:A:380:ALA:O	1:A:383:ARG:HB3	2.13	0.48
1:B:119:ASN:O	1:B:120:ARG:C	2.55	0.48
1:C:41:GLN:CA	1:C:41:GLN:HE21	2.25	0.48
1:C:444:LEU:HB3	2:I:113:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:MET:HE2	1:D:244:ALA:CB	2.43	0.48
2:G:7:ARG:NH2	2:G:102:GLU:O	2.46	0.48
2:L:137:LEU:O	2:L:141:THR:CG2	2.56	0.48
1:V:361:ALA:C	1:V:363:GLU:H	2.21	0.48
1:W:28:ALA:O	1:W:30:ALA:N	2.46	0.48
1:X:430:LEU:HG	1:X:431:GLY:H	1.78	0.48
1:A:38:MET:HG3	1:A:45:ARG:HH12	1.77	0.48
1:C:32:ARG:CZ	1:C:35:TRP:CE3	2.96	0.48
1:D:37:ARG:CG	1:D:38:MET:N	2.76	0.48
1:D:240:LEU:O	1:D:243:LYS:N	2.45	0.48
1:D:340:ASP:O	1:D:344:ILE:CD1	2.62	0.48
1:F:367:ILE:CD1	1:F:421:ILE:HD11	2.43	0.48
2:G:43:LEU:O	2:G:97:VAL:HA	2.14	0.48
2:I:154:ARG:O	2:I:155:ILE:C	2.55	0.48
1:S:48:VAL:HG13	1:S:48:VAL:O	2.13	0.48
1:T:120:ARG:O	1:T:120:ARG:HD2	2.13	0.48
1:U:361:ALA:C	1:U:363:GLU:H	2.20	0.48
1:U:430:LEU:HD23	1:U:430:LEU:H	1.78	0.48
1:V:61:VAL:HA	1:V:336:LEU:HD21	1.95	0.48
1:W:20:GLN:HB3	1:W:23:ALA:HB3	1.93	0.48
1:X:112:ARG:CB	1:X:240:LEU:HD21	2.43	0.48
1:X:235:ILE:O	1:X:236:ASN:CB	2.60	0.48
1:X:430:LEU:HD23	1:X:430:LEU:H	1.78	0.48
1:A:85:LYS:HG2	1:A:85:LYS:O	2.12	0.48
1:A:403:LEU:CD2	1:A:404:MET:N	2.75	0.48
1:B:410:SER:O	1:B:412:SER:N	2.46	0.48
1:C:250:GLN:HA	1:C:250:GLN:HE21	1.79	0.48
1:C:409:PHE:CE1	1:D:6:PRO:HB3	2.49	0.48
1:C:437:GLU:O	1:C:438:ASP:O	2.32	0.48
1:D:26:ALA:O	1:D:29:ILE:HG12	2.13	0.48
1:D:374:VAL:O	1:D:375:LYS:C	2.57	0.48
1:D:403:LEU:C	1:D:403:LEU:CD2	2.85	0.48
1:F:275:ARG:O	1:F:278:VAL:HG23	2.14	0.48
2:H:134:ALA:O	2:H:138:VAL:HG23	2.12	0.48
2:I:38:TYR:CD1	2:I:69:GLY:HA3	2.48	0.48
2:I:67:HIS:HD2	2:I:73:LYS:HD3	1.78	0.48
2:O:90:LYS:O	2:O:91:LEU:HD12	2.14	0.48
1:S:437:GLU:O	1:S:438:ASP:C	2.57	0.48
1:T:115:GLU:O	1:T:119:ASN:HB3	2.13	0.48
1:T:356:TYR:HB3	1:T:404:MET:HE2	1.94	0.48
1:U:385:ASN:ND2	1:U:395:ARG:HE	2.08	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:HG23	1:A:228:ASP:N	2.28	0.48
1:B:381:ALA:HB2	1:B:396:LEU:HD23	1.96	0.48
1:B:436:ASN:HB3	1:B:439:LEU:CD1	2.44	0.48
1:C:17:ILE:N	1:C:17:ILE:HD12	2.29	0.48
1:C:373:ALA:O	1:C:377:ILE:HG13	2.12	0.48
2:H:1:THR:HG23	2:H:33:LYS:HZ2	1.79	0.48
2:H:83:ARG:HG2	2:I:55:THR:CB	2.42	0.48
2:H:91:LEU:CD1	2:H:91:LEU:N	2.71	0.48
1:U:322:GLU:OE1	1:U:322:GLU:N	2.46	0.48
1:V:61:VAL:HG11	1:V:335:ALA:HA	1.94	0.48
1:W:15:GLN:O	1:W:349:HIS:N	2.41	0.48
1:W:311:PHE:HE1	1:W:316:PRO:HA	1.78	0.48
1:W:361:ALA:C	1:W:363:GLU:H	2.22	0.48
1:A:6:PRO:HB3	1:F:409:PHE:CE1	2.45	0.48
1:D:293:THR:C	1:D:295:HIS:H	2.20	0.48
1:D:357:LYS:HE3	1:D:367:ILE:O	2.13	0.48
1:F:16:HIS:C	1:F:17:ILE:HD12	2.39	0.48
1:F:381:ALA:HB2	1:F:396:LEU:HD23	1.95	0.48
2:I:91:LEU:HD22	2:I:91:LEU:N	2.27	0.48
2:P:56:LEU:CD2	2:P:95:LEU:HD13	2.43	0.48
2:P:112:VAL:HB	1:V:443:ILE:HD13	1.96	0.48
2:Q:7:ARG:NE	2:Q:119:GLN:OE1	2.47	0.48
2:Q:20:VAL:HG21	1:X:444:LEU:HD21	1.95	0.48
1:S:357:LYS:HA	1:S:367:ILE:CD1	2.31	0.48
1:T:322:GLU:OE1	1:T:322:GLU:N	2.47	0.48
1:U:439:LEU:C	1:U:441:ARG:H	2.21	0.48
1:W:322:GLU:OE1	1:W:322:GLU:N	2.46	0.48
1:A:54:LEU:HD12	1:A:307:ALA:O	2.13	0.48
1:B:263:CYS:SG	1:B:319:LEU:HD23	2.53	0.48
1:C:362:THR:HG23	1:D:39:GLN:HG2	1.95	0.48
1:C:381:ALA:O	1:C:384:VAL:HG13	2.14	0.48
1:F:23:ALA:CA	1:F:331:VAL:HG21	2.34	0.48
1:F:264:LYS:HD3	1:F:276:GLU:CD	2.38	0.48
2:H:164:ASN:ND2	2:H:164:ASN:H	2.12	0.48
2:J:1:THR:HG23	2:J:33:LYS:HD3	1.94	0.48
2:L:5:SER:HB2	2:L:14:VAL:HG22	1.95	0.48
2:M:4:VAL:HG12	2:M:153:LEU:CD2	2.44	0.48
2:P:4:VAL:HG12	2:P:153:LEU:CD2	2.44	0.48
1:S:353:THR:HG22	1:S:369:PHE:HD1	1.79	0.48
1:S:385:ASN:ND2	1:S:395:ARG:HE	2.12	0.48
1:U:101:ARG:HA	1:U:293:THR:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:439:LEU:HD23	1:V:439:LEU:H	1.77	0.48
1:X:26:ALA:HA	1:X:29:ILE:HG12	1.95	0.48
1:B:56:ILE:N	1:B:56:ILE:CD1	2.76	0.48
1:B:440:SER:O	1:B:442:PHE:N	2.47	0.48
1:D:433:VAL:HG22	1:D:434:VAL:N	2.29	0.48
1:E:12:GLU:O	1:E:15:GLN:HB2	2.14	0.48
2:I:46:PHE:HB3	2:I:95:LEU:HD21	1.95	0.48
2:J:1:THR:HG23	2:J:33:LYS:NZ	2.28	0.48
2:K:141:THR:HG21	2:K:143:LEU:HD12	1.95	0.48
2:K:154:ARG:O	2:K:155:ILE:C	2.57	0.48
2:L:107:THR:OG1	2:L:111:ASP:OD2	2.24	0.48
2:R:4:VAL:HG12	2:R:153:LEU:HD21	1.96	0.48
1:U:336:LEU:HB2	1:U:341:PHE:HE1	1.79	0.48
1:V:118:LYS:HG3	1:V:118:LYS:O	2.14	0.48
1:V:441:ARG:HG3	1:V:441:ARG:NH1	2.29	0.48
1:W:96:VAL:CG1	1:W:282:LEU:HD12	2.39	0.48
1:X:315:ARG:HB3	1:X:316:PRO:CD	2.44	0.48
1:X:362:THR:O	1:X:362:THR:HG22	2.13	0.48
1:A:262:ILE:HD12	1:A:278:VAL:HB	1.96	0.48
1:A:352:LEU:HD13	1:A:400:MET:CG	2.43	0.48
1:B:435:GLU:HG2	1:B:436:ASN:H	1.79	0.48
1:C:34:ARG:HH22	1:C:253:ILE:HD13	1.79	0.48
1:D:360:MET:O	1:D:361:ALA:C	2.57	0.48
1:D:403:LEU:C	1:D:405:ASP:H	2.20	0.48
1:F:55:MET:C	1:F:56:ILE:HD12	2.38	0.48
2:L:49:GLY:O	2:L:50:THR:C	2.57	0.48
2:M:7:ARG:NH1	2:M:12:VAL:HG21	2.29	0.48
2:N:154:ARG:O	2:N:155:ILE:C	2.57	0.48
2:P:49:GLY:O	2:P:51:ALA:N	2.47	0.48
1:U:283:LEU:CD1	1:U:323:LEU:HD12	2.44	0.48
1:V:421:ILE:O	1:V:421:ILE:HG22	2.14	0.48
1:X:234:LEU:HD13	1:X:234:LEU:C	2.39	0.48
1:X:404:MET:HA	1:X:407:ILE:HG22	1.95	0.48
1:A:403:LEU:HD22	1:A:404:MET:HG2	1.96	0.48
1:C:111:VAL:HG12	1:C:112:ARG:N	2.29	0.48
1:F:260:ASP:HB3	1:F:311:PHE:CE2	2.49	0.48
2:G:105:ILE:HG23	2:G:105:ILE:O	2.14	0.48
2:H:83:ARG:CG	2:I:55:THR:HG22	2.44	0.48
2:L:46:PHE:HB3	2:L:95:LEU:HD23	1.92	0.48
2:P:151:LYS:O	2:P:155:ILE:HD13	2.13	0.48
1:S:28:ALA:O	1:S:30:ALA:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:100:ILE:HG13	1:W:291:VAL:HG21	1.95	0.48
1:A:20:GLN:CA	1:A:20:GLN:NE2	2.77	0.47
1:A:439:LEU:O	1:A:440:SER:C	2.58	0.47
1:B:73:LEU:HD12	1:B:73:LEU:O	2.14	0.47
1:B:439:LEU:CD2	2:H:72:LEU:HG	2.44	0.47
1:C:44:LEU:HA	1:C:47:GLU:HB2	1.96	0.47
1:C:278:VAL:O	1:C:281:ASP:HB2	2.14	0.47
1:D:326:ARG:C	1:D:328:PRO:HD3	2.39	0.47
1:E:19:GLY:O	1:E:20:GLN:C	2.55	0.47
1:F:17:ILE:N	1:F:17:ILE:CD1	2.72	0.47
1:F:382:PHE:C	1:F:382:PHE:CD2	2.91	0.47
2:J:18:GLY:H	2:J:164:ASN:ND2	2.01	0.47
2:K:6:VAL:HG12	2:K:7:ARG:N	2.29	0.47
2:P:104:LEU:HD13	2:P:112:VAL:CG1	2.44	0.47
2:Q:151:LYS:O	2:Q:155:ILE:HD13	2.14	0.47
1:T:353:THR:HG22	1:T:369:PHE:HD1	1.78	0.47
1:T:370:THR:HG23	1:T:373:ALA:CB	2.43	0.47
1:V:336:LEU:HB2	1:V:341:PHE:HE1	1.78	0.47
1:W:426:VAL:O	1:W:429:ALA:HB3	2.13	0.47
1:X:61:VAL:HG11	1:X:335:ALA:HA	1.94	0.47
1:X:336:LEU:HB2	1:X:341:PHE:CE1	2.49	0.47
1:X:370:THR:HG23	1:X:373:ALA:CB	2.43	0.47
1:A:17:ILE:N	1:A:17:ILE:HD12	2.29	0.47
1:B:20:GLN:HE21	1:B:20:GLN:H	1.62	0.47
1:B:33:ASN:HA	1:B:36:ARG:HD2	1.96	0.47
1:B:241:LYS:O	1:B:242:GLN:C	2.56	0.47
1:C:38:MET:HG3	1:C:45:ARG:HH12	1.79	0.47
1:E:112:ARG:O	1:E:114:GLN:N	2.47	0.47
1:E:358:ALA:HB1	1:F:40:LEU:HD22	1.97	0.47
2:I:61:GLU:O	2:I:62:ARG:C	2.55	0.47
2:J:82:TRP:HZ2	2:J:91:LEU:HD13	1.79	0.47
2:Q:153:LEU:HB3	2:Q:167:PHE:CE2	2.49	0.47
1:S:362:THR:O	1:X:36:ARG:NH1	2.47	0.47
1:S:363:GLU:HG2	1:X:36:ARG:HH11	1.78	0.47
1:T:96:VAL:HG21	1:T:281:ASP:HB3	1.95	0.47
1:T:260:ASP:HB3	1:T:311:PHE:HD2	1.73	0.47
1:U:60:GLY:N	3:U:458:ATP:O1B	2.47	0.47
1:U:62:GLY:HA3	3:U:458:ATP:N7	2.29	0.47
1:U:120:ARG:HH21	1:U:235:ILE:HD13	1.79	0.47
1:U:421:ILE:O	1:U:421:ILE:HG22	2.13	0.47
1:V:331:VAL:HG13	1:V:331:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:35:TRP:C	1:X:37:ARG:N	2.72	0.47
1:A:65:GLU:HG3	3:A:450:ATP:H2'	1.95	0.47
1:B:41:GLN:O	1:B:43:PRO:HD2	2.14	0.47
1:C:262:ILE:O	1:C:262:ILE:HG13	2.13	0.47
1:D:84:THR:C	1:D:86:PHE:N	2.69	0.47
1:E:37:ARG:CG	1:E:38:MET:N	2.76	0.47
1:E:237:PRO:O	1:E:238:GLU:C	2.57	0.47
1:S:351:SER:OG	1:S:354:GLU:HG2	2.14	0.47
1:S:361:ALA:C	1:S:363:GLU:H	2.22	0.47
1:S:434:VAL:HG12	1:S:435:GLU:N	2.28	0.47
1:T:357:LYS:HA	1:T:367:ILE:CD1	2.33	0.47
1:T:361:ALA:C	1:T:363:GLU:H	2.21	0.47
1:U:17:ILE:HD13	1:U:66:ILE:HG13	1.96	0.47
1:U:254:VAL:HB	1:U:305:PHE:CD2	2.48	0.47
1:V:48:VAL:HG13	1:V:48:VAL:O	2.13	0.47
1:A:13:LEU:HD13	1:A:24:LYS:HG2	1.96	0.47
1:A:283:LEU:HD11	1:A:320:ILE:HD12	1.95	0.47
1:A:410:SER:O	1:A:411:ALA:C	2.53	0.47
1:A:428:ASP:OD1	1:A:429:ALA:N	2.47	0.47
1:B:275:ARG:O	1:B:277:GLY:N	2.47	0.47
1:D:326:ARG:O	1:D:328:PRO:HD3	2.14	0.47
1:D:352:LEU:HD13	1:D:400:MET:CG	2.40	0.47
1:D:441:ARG:NH2	2:K:61:GLU:OE2	2.48	0.47
1:E:409:PHE:CD2	1:F:25:ARG:NH2	2.83	0.47
1:F:64:THR:HB	3:F:455:ATP:O1A	2.14	0.47
1:F:79:ILE:CG2	1:F:103:LEU:HD13	2.42	0.47
2:H:38:TYR:CD1	2:H:69:GLY:HA3	2.49	0.47
2:K:137:LEU:CD1	2:K:137:LEU:N	2.77	0.47
2:L:6:VAL:HG12	2:L:7:ARG:N	2.28	0.47
2:Q:90:LYS:C	2:Q:91:LEU:HD12	2.39	0.47
1:S:254:VAL:HB	1:S:305:PHE:CD2	2.49	0.47
1:S:421:ILE:O	1:S:421:ILE:HG22	2.13	0.47
1:S:444:LEU:H	1:S:444:LEU:CD1	2.28	0.47
1:T:336:LEU:HB2	1:T:341:PHE:CE1	2.50	0.47
1:V:28:ALA:C	1:V:30:ALA:N	2.69	0.47
1:W:54:LEU:CD2	1:W:307:ALA:HB3	2.44	0.47
1:X:54:LEU:CD2	1:X:307:ALA:HB3	2.44	0.47
1:X:254:VAL:HB	1:X:305:PHE:CD2	2.49	0.47
1:X:426:VAL:O	1:X:429:ALA:HB3	2.14	0.47
1:B:264:LYS:NZ	1:B:318:ASP:O	2.45	0.47
1:B:356:TYR:HE1	1:B:400:MET:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:MET:HA	1:B:360:MET:CE	2.32	0.47
1:D:118:LYS:O	1:D:118:LYS:HD2	2.14	0.47
1:E:63:LYS:HB2	3:E:454:ATP:O2B	2.13	0.47
1:E:362:THR:HG23	1:F:39:GLN:HG2	1.97	0.47
2:G:88:LEU:O	2:G:89:ARG:HB2	2.13	0.47
2:H:98:ALA:CB	2:H:103:SER:HA	2.45	0.47
2:J:18:GLY:N	2:J:164:ASN:HD21	2.02	0.47
2:Q:4:VAL:HA	2:Q:121:LEU:O	2.13	0.47
2:Q:116:GLU:O	2:Q:117:GLU:C	2.57	0.47
2:R:8:ARG:HH22	2:R:143:LEU:H	1.62	0.47
1:S:62:GLY:HA3	3:S:456:ATP:N7	2.28	0.47
1:S:236:ASN:HB3	1:S:239:GLU:HB3	1.95	0.47
1:U:54:LEU:CD2	1:U:307:ALA:HB3	2.44	0.47
1:W:254:VAL:HB	1:W:305:PHE:CD2	2.50	0.47
1:A:264:LYS:NZ	1:A:319:LEU:HA	2.30	0.47
1:F:330:ARG:HG3	1:F:330:ARG:HH11	1.79	0.47
2:L:51:ALA:O	2:L:54:PHE:N	2.47	0.47
2:O:56:LEU:HD23	2:O:95:LEU:HD13	1.96	0.47
2:R:127:GLY:O	2:R:129:TYR:N	2.48	0.47
1:U:297:MET:HB2	1:V:109:LYS:CE	2.45	0.47
1:V:9:ILE:HD13	1:V:31:LEU:HD23	1.96	0.47
1:V:17:ILE:O	1:V:17:ILE:HG22	2.14	0.47
1:V:260:ASP:HB3	1:V:311:PHE:HD2	1.73	0.47
1:V:273:VAL:O	1:V:273:VAL:HG12	2.15	0.47
1:A:20:GLN:HE21	1:A:20:GLN:CA	2.28	0.47
1:A:38:MET:HA	1:A:45:ARG:HH11	1.80	0.47
1:A:39:GLN:HG2	1:F:362:THR:HG21	1.93	0.47
1:B:236:ASN:N	1:B:237:PRO:HD3	2.30	0.47
1:C:37:ARG:NH1	1:C:38:MET:HE2	2.28	0.47
1:C:280:ARG:HH11	1:C:280:ARG:HG3	1.79	0.47
1:C:283:LEU:HA	1:C:283:LEU:HD23	1.54	0.47
1:D:5:THR:O	1:D:9:ILE:HG13	2.15	0.47
1:D:6:PRO:HD3	1:D:32:ARG:CG	2.45	0.47
1:D:32:ARG:CZ	1:D:35:TRP:CE3	2.98	0.47
1:D:406:LYS:H	1:D:406:LYS:CD	2.11	0.47
1:E:352:LEU:O	1:E:355:GLN:N	2.48	0.47
1:E:406:LYS:O	1:E:407:ILE:C	2.58	0.47
1:F:321:PRO:O	1:F:322:GLU:C	2.57	0.47
2:H:60:PHE:CE2	2:H:97:VAL:HG11	2.49	0.47
2:I:7:ARG:CZ	2:I:12:VAL:HG22	2.44	0.47
2:I:105:ILE:HG23	2:I:105:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:7:ARG:CZ	2:J:12:VAL:HG22	2.44	0.47
2:J:73:LYS:O	2:J:74:SER:C	2.58	0.47
2:K:49:GLY:O	2:K:51:ALA:N	2.47	0.47
2:O:4:VAL:HG12	2:O:153:LEU:HD21	1.97	0.47
2:O:32:ARG:HB2	2:O:35:ARG:HE	1.80	0.47
2:P:153:LEU:HB3	2:P:167:PHE:CE2	2.50	0.47
2:Q:133:ALA:O	2:Q:136:ALA:HB3	2.14	0.47
2:Q:154:ARG:O	2:Q:155:ILE:C	2.57	0.47
2:R:49:GLY:O	2:R:51:ALA:N	2.48	0.47
2:R:112:VAL:HB	1:X:443:ILE:HD12	1.96	0.47
1:T:61:VAL:HG11	1:T:335:ALA:HA	1.96	0.47
1:U:96:VAL:HG21	1:U:281:ASP:HB3	1.96	0.47
1:V:254:VAL:HB	1:V:305:PHE:CD2	2.50	0.47
1:V:322:GLU:N	1:V:322:GLU:OE1	2.48	0.47
1:W:63:LYS:CB	3:W:460:ATP:O2B	2.63	0.47
1:B:443:ILE:HG23	2:H:112:VAL:HG23	1.96	0.47
1:F:264:LYS:HZ3	1:F:279:GLN:NE2	2.06	0.47
2:K:133:ALA:HB1	2:K:155:ILE:HD12	1.97	0.47
1:T:17:ILE:HD13	1:T:66:ILE:HG13	1.96	0.47
1:V:100:ILE:HG13	1:V:291:VAL:HG21	1.95	0.47
1:V:297:MET:CE	1:W:105:ASP:HB3	2.44	0.47
1:W:273:VAL:HG12	1:W:273:VAL:O	2.15	0.47
1:X:439:LEU:C	1:X:441:ARG:H	2.22	0.47
1:A:5:THR:O	1:A:6:PRO:C	2.58	0.47
1:B:338:ALA:N	1:B:382:PHE:CD1	2.80	0.47
1:C:275:ARG:O	1:C:277:GLY:N	2.48	0.47
1:C:410:SER:O	1:C:411:ALA:C	2.58	0.47
1:D:85:LYS:O	1:D:85:LYS:HG2	2.14	0.47
2:G:3:ILE:O	2:G:122:ALA:HA	2.15	0.47
2:I:137:LEU:HD13	2:O:136:ALA:HB1	1.95	0.47
2:J:2:THR:O	2:J:16:GLY:HA2	2.15	0.47
2:J:137:LEU:CD1	2:J:137:LEU:N	2.77	0.47
2:K:88:LEU:O	2:K:89:ARG:HB2	2.13	0.47
2:L:1:THR:HG22	2:L:2:THR:H	1.78	0.47
2:N:1:THR:HG23	2:N:33:LYS:HD3	1.95	0.47
1:S:13:LEU:C	1:S:15:GLN:H	2.23	0.47
1:S:48:VAL:HG23	1:T:355:GLN:OE1	2.15	0.47
1:S:439:LEU:C	1:S:441:ARG:H	2.21	0.47
1:U:17:ILE:HG22	1:U:17:ILE:O	2.14	0.47
1:V:341:PHE:CB	1:V:378:ALA:HB1	2.45	0.47
1:X:68:ARG:C	1:X:70:LEU:H	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:C	1:A:114:GLN:N	2.70	0.47
1:A:410:SER:C	1:A:412:SER:N	2.72	0.47
1:C:37:ARG:HA	1:C:40:LEU:HD12	1.95	0.47
1:D:290:THR:HG21	1:D:297:MET:HE3	1.97	0.47
1:D:356:TYR:O	1:D:357:LYS:C	2.56	0.47
1:D:381:ALA:HB2	1:D:396:LEU:HD23	1.96	0.47
1:E:38:MET:HG3	1:E:45:ARG:HH12	1.79	0.47
2:H:131:LEU:O	2:H:132:SER:C	2.58	0.47
2:L:3:ILE:O	2:L:122:ALA:HA	2.15	0.47
2:M:144:SER:OG	2:M:147:GLU:HB2	2.15	0.47
2:P:107:THR:OG1	2:P:111:ASP:OD2	2.23	0.47
1:T:112:ARG:O	1:T:112:ARG:HG2	2.14	0.47
1:T:357:LYS:CA	1:T:367:ILE:HD11	2.34	0.47
1:U:61:VAL:HA	1:U:336:LEU:HD21	1.96	0.47
1:U:326:ARG:C	1:U:328:PRO:HD3	2.40	0.47
1:W:107:ALA:C	1:W:109:LYS:H	2.22	0.47
1:A:37:ARG:HB2	1:A:48:VAL:HG11	1.96	0.46
1:A:356:TYR:HD1	1:A:400:MET:HE3	1.76	0.46
1:B:244:ALA:O	1:B:247:ALA:HB3	2.15	0.46
1:C:236:ASN:O	1:C:240:LEU:HD13	2.15	0.46
1:D:110:LEU:O	1:D:114:GLN:HB2	2.15	0.46
1:D:401:GLU:OE1	1:E:51:LYS:HG3	2.16	0.46
1:E:240:LEU:O	1:E:241:LYS:C	2.59	0.46
1:F:38:MET:HA	1:F:45:ARG:HH11	1.79	0.46
1:F:115:GLU:OE2	1:F:118:LYS:HD3	2.15	0.46
1:F:382:PHE:C	1:F:382:PHE:HD2	2.24	0.46
2:G:82:TRP:CE2	2:G:88:LEU:HD22	2.50	0.46
2:G:161:VAL:HG22	2:R:24:ASN:O	2.15	0.46
2:H:7:ARG:NH2	2:H:102:GLU:O	2.48	0.46
2:I:78:LEU:HG	2:I:82:TRP:HZ3	1.80	0.46
2:P:8:ARG:HH22	2:P:143:LEU:H	1.63	0.46
2:P:71:LEU:O	2:P:73:LYS:N	2.48	0.46
2:Q:55:THR:HG22	2:R:83:ARG:CG	2.44	0.46
1:S:9:ILE:HD13	1:S:31:LEU:HD23	1.97	0.46
1:S:45:ARG:O	1:S:48:VAL:HG12	2.15	0.46
1:S:68:ARG:HG3	1:S:68:ARG:NH1	2.30	0.46
1:S:68:ARG:C	1:S:70:LEU:H	2.23	0.46
1:S:279:GLN:O	1:S:320:ILE:HD11	2.15	0.46
1:U:28:ALA:C	1:U:30:ALA:N	2.72	0.46
1:U:35:TRP:C	1:U:37:ARG:N	2.73	0.46
1:W:68:ARG:C	1:W:70:LEU:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:435:GLU:HB3	1:X:436:ASN:H	1.51	0.46
1:A:250:GLN:HA	1:A:250:GLN:HE21	1.80	0.46
1:B:81:VAL:HG11	1:B:99:ILE:HG12	1.97	0.46
1:B:311:PHE:CE1	1:B:316:PRO:HA	2.51	0.46
1:B:367:ILE:HD11	1:B:421:ILE:HD11	1.96	0.46
1:B:382:PHE:O	1:B:383:ARG:C	2.57	0.46
1:C:17:ILE:HA	3:C:452:ATP:C2	2.50	0.46
1:C:41:GLN:HA	1:C:41:GLN:HE21	1.79	0.46
1:E:240:LEU:O	1:E:243:LYS:N	2.48	0.46
1:E:394:ARG:HD3	1:E:394:ARG:HA	1.78	0.46
1:F:32:ARG:CZ	1:F:35:TRP:CE3	2.98	0.46
1:F:403:LEU:C	1:F:403:LEU:CD2	2.79	0.46
1:F:435:GLU:O	1:F:436:ASN:CB	2.62	0.46
2:H:154:ARG:O	2:H:155:ILE:C	2.58	0.46
2:I:133:ALA:HB1	2:I:155:ILE:HD12	1.97	0.46
2:N:4:VAL:HG12	2:N:153:LEU:CD2	2.45	0.46
2:Q:90:LYS:O	2:Q:91:LEU:HD12	2.15	0.46
1:V:48:VAL:CG2	1:W:359:LEU:HD11	2.44	0.46
1:V:54:LEU:CD2	1:V:307:ALA:HB3	2.45	0.46
1:W:48:VAL:HG21	1:X:359:LEU:HD11	1.96	0.46
1:W:101:ARG:HA	1:W:293:THR:HG22	1.96	0.46
1:X:436:ASN:O	1:X:437:GLU:C	2.58	0.46
1:A:439:LEU:HD23	2:G:72:LEU:HD11	1.98	0.46
1:B:414:MET:O	1:B:414:MET:HG2	2.14	0.46
1:C:4:MET:HE2	1:C:9:ILE:HA	1.96	0.46
1:C:51:LYS:O	1:C:52:ASN:C	2.58	0.46
1:E:366:ASN:O	1:E:418:THR:HA	2.15	0.46
1:F:370:THR:O	1:F:373:ALA:N	2.45	0.46
2:J:60:PHE:CE2	2:J:97:VAL:HG11	2.50	0.46
2:J:91:LEU:O	2:J:108:GLY:HA3	2.15	0.46
2:K:98:ALA:HB2	2:K:103:SER:HA	1.98	0.46
2:L:3:ILE:HG22	2:L:96:ILE:HD12	1.96	0.46
2:O:90:LYS:C	2:O:91:LEU:HD12	2.39	0.46
2:R:151:LYS:O	2:R:155:ILE:HD13	2.15	0.46
1:S:350:ALA:HB2	1:X:47:GLU:OE1	2.16	0.46
1:T:9:ILE:HD13	1:T:31:LEU:HD23	1.97	0.46
1:U:120:ARG:CG	1:U:232:ALA:HA	2.45	0.46
1:U:235:ILE:C	1:U:237:PRO:HD3	2.40	0.46
1:U:260:ASP:HB3	1:U:311:PHE:HD2	1.77	0.46
1:U:430:LEU:HD23	1:U:430:LEU:N	2.31	0.46
1:W:68:ARG:HG3	1:W:68:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:9:ILE:O	1:X:13:LEU:HG	2.15	0.46
1:A:280:ARG:HD3	1:F:82:GLU:OE2	2.16	0.46
1:A:353:THR:O	1:A:354:GLU:C	2.58	0.46
1:A:403:LEU:CD1	1:A:426:VAL:HG22	2.46	0.46
1:B:9:ILE:HD13	1:B:31:LEU:HD23	1.98	0.46
1:B:65:GLU:HG3	3:B:451:ATP:H2'	1.97	0.46
1:C:116:ILE:O	1:C:120:ARG:HB2	2.16	0.46
1:D:63:LYS:HB2	3:D:453:ATP:O2B	2.15	0.46
1:F:76:ALA:HB1	1:F:251:ASN:O	2.14	0.46
1:F:262:ILE:O	1:F:262:ILE:HG13	2.15	0.46
2:G:57:PHE:CA	2:G:95:LEU:HD11	2.41	0.46
2:G:94:MET:HE3	2:G:123:ILE:HB	1.97	0.46
2:G:99:ASP:HA	2:G:172:LEU:CD1	2.46	0.46
2:G:144:SER:CB	2:G:147:GLU:HG3	2.42	0.46
2:H:137:LEU:CD1	2:H:137:LEU:N	2.78	0.46
2:M:33:LYS:HA	2:M:46:PHE:CZ	2.51	0.46
2:N:8:ARG:HH22	2:N:143:LEU:H	1.63	0.46
2:O:7:ARG:NH1	2:O:12:VAL:HG21	2.30	0.46
2:P:90:LYS:C	2:P:91:LEU:HD12	2.40	0.46
2:Q:8:ARG:HH22	2:Q:143:LEU:H	1.63	0.46
1:S:336:LEU:HB2	1:S:341:PHE:CE1	2.51	0.46
1:T:13:LEU:C	1:T:15:GLN:H	2.24	0.46
1:W:35:TRP:C	1:W:37:ARG:N	2.73	0.46
1:B:245:ILE:O	1:B:246:ASP:C	2.57	0.46
1:E:338:ALA:N	1:E:382:PHE:HD1	2.13	0.46
1:F:240:LEU:O	1:F:241:LYS:C	2.58	0.46
2:H:159:ILE:O	2:M:25:THR:HA	2.16	0.46
2:J:38:TYR:CD1	2:J:69:GLY:HA3	2.50	0.46
2:K:7:ARG:CZ	2:K:12:VAL:HG22	2.45	0.46
2:N:35:ARG:HG3	2:N:35:ARG:HH11	1.80	0.46
2:N:37:LEU:HD22	2:N:61:GLU:HG3	1.96	0.46
2:O:151:LYS:O	2:O:155:ILE:HD13	2.16	0.46
1:U:390:ASN:HD22	1:U:390:ASN:C	2.24	0.46
1:U:442:PHE:CD1	1:U:442:PHE:N	2.83	0.46
1:V:28:ALA:O	1:V:30:ALA:N	2.49	0.46
1:V:385:ASN:ND2	1:V:395:ARG:HE	2.10	0.46
1:A:21:ALA:O	1:A:22:ASP:C	2.57	0.46
1:A:233:LYS:HZ2	1:A:234:LEU:HB2	1.81	0.46
1:A:428:ASP:O	1:A:430:LEU:N	2.49	0.46
1:C:356:TYR:CE1	1:C:400:MET:HB3	2.48	0.46
1:D:280:ARG:HG3	1:D:280:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:VAL:HG22	1:D:385:ASN:N	2.31	0.46
2:G:107:THR:OG1	2:G:109:ILE:HG12	2.16	0.46
2:H:52:ASP:OD2	2:H:91:LEU:HA	2.16	0.46
2:H:85:ASP:O	2:H:87:ALA:N	2.49	0.46
2:L:55:THR:O	2:L:59:LEU:HD13	2.16	0.46
2:M:127:GLY:O	2:M:129:TYR:N	2.48	0.46
2:Q:56:LEU:CD2	2:Q:95:LEU:HD13	2.46	0.46
2:R:4:VAL:HA	2:R:121:LEU:O	2.16	0.46
2:R:7:ARG:NH1	2:R:12:VAL:HG21	2.30	0.46
1:T:28:ALA:O	1:T:30:ALA:N	2.49	0.46
1:X:351:SER:O	1:X:355:GLN:HG3	2.16	0.46
1:A:54:LEU:HG	1:A:56:ILE:HD11	1.98	0.46
1:B:69:ARG:O	1:B:70:LEU:C	2.58	0.46
1:B:428:ASP:O	1:B:430:LEU:N	2.49	0.46
1:C:249:GLU:HG2	1:C:299:LYS:H	1.80	0.46
1:D:112:ARG:C	1:D:114:GLN:N	2.74	0.46
3:D:453:ATP:C8	3:D:453:ATP:H5'1	2.51	0.46
1:F:112:ARG:HB2	1:F:240:LEU:HD21	1.96	0.46
2:I:2:THR:O	2:I:16:GLY:HA2	2.15	0.46
2:L:134:ALA:O	2:L:135:ARG:C	2.59	0.46
2:M:151:LYS:O	2:M:155:ILE:HD13	2.16	0.46
2:N:56:LEU:HD23	2:N:95:LEU:HD13	1.98	0.46
2:N:164:ASN:ND2	2:N:164:ASN:N	2.62	0.46
2:R:104:LEU:HD13	2:R:112:VAL:CG1	2.46	0.46
2:R:134:ALA:O	2:R:135:ARG:C	2.59	0.46
1:S:61:VAL:HG11	1:S:335:ALA:HA	1.96	0.46
1:S:240:LEU:N	1:S:240:LEU:HD12	2.30	0.46
1:U:120:ARG:HG3	1:U:232:ALA:CA	2.46	0.46
1:W:430:LEU:HD23	1:W:430:LEU:H	1.81	0.46
1:A:25:ARG:O	1:A:28:ALA:HB3	2.15	0.46
1:A:41:GLN:NE2	1:A:41:GLN:CA	2.74	0.46
1:A:360:MET:HA	1:A:360:MET:CE	2.40	0.46
1:A:390:ASN:OD1	1:A:390:ASN:C	2.59	0.46
1:B:409:PHE:O	1:C:6:PRO:HG2	2.16	0.46
1:D:321:PRO:O	1:D:322:GLU:C	2.59	0.46
1:E:369:PHE:CE2	1:E:421:ILE:HD12	2.51	0.46
2:K:164:ASN:HD22	2:K:164:ASN:C	2.24	0.46
2:M:4:VAL:HA	2:M:121:LEU:O	2.16	0.46
2:M:42:VAL:HG21	2:M:64:LEU:CD1	2.46	0.46
2:N:56:LEU:HB2	2:N:91:LEU:CD2	2.36	0.46
1:S:119:ASN:O	1:S:234:LEU:HD22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:430:LEU:HD23	1:S:430:LEU:H	1.79	0.46
1:T:265:LYS:H	1:T:269:SER:HB3	1.81	0.46
1:T:283:LEU:CD1	1:T:323:LEU:HD12	2.45	0.46
1:T:300:THR:O	1:T:301:ASP:C	2.59	0.46
1:W:17:ILE:HG22	1:W:17:ILE:O	2.14	0.46
1:W:47:GLU:OE1	1:X:350:ALA:HB2	2.16	0.46
1:X:28:ALA:C	1:X:30:ALA:N	2.72	0.46
1:X:322:GLU:OE1	1:X:322:GLU:N	2.48	0.46
1:A:381:ALA:HB2	1:A:396:LEU:HD23	1.97	0.46
1:B:76:ALA:HB1	1:B:251:ASN:O	2.16	0.46
1:D:4:MET:HE2	1:D:4:MET:HB3	1.84	0.46
1:E:408:SER:O	1:F:36:ARG:NH2	2.37	0.46
1:E:439:LEU:HA	1:E:443:ILE:CD1	2.46	0.46
1:F:316:PRO:C	1:F:318:ASP:N	2.74	0.46
1:F:353:THR:O	1:F:354:GLU:C	2.57	0.46
1:F:421:ILE:HG23	1:F:425:TYR:HD1	1.80	0.46
2:H:83:ARG:HG2	2:I:55:THR:HB	1.97	0.46
2:M:90:LYS:O	2:M:91:LEU:HD12	2.16	0.46
2:O:131:LEU:HD12	2:O:135:ARG:HG3	1.98	0.46
2:O:154:ARG:O	2:O:155:ILE:C	2.59	0.46
2:P:55:THR:O	2:P:59:LEU:HB2	2.16	0.46
1:S:300:THR:O	1:S:301:ASP:C	2.59	0.46
1:V:101:ARG:HA	1:V:293:THR:HG22	1.97	0.46
1:V:430:LEU:HD23	1:V:430:LEU:H	1.80	0.46
1:W:34:ARG:HG2	1:W:250:GLN:NE2	2.31	0.46
1:X:65:GLU:OE1	1:X:65:GLU:HA	2.16	0.46
1:A:313:VAL:HG23	1:A:314:ALA:H	1.80	0.46
1:B:37:ARG:HG3	1:B:38:MET:N	2.31	0.46
1:C:33:ASN:HA	1:C:36:ARG:HD2	1.98	0.46
1:D:404:MET:O	1:D:408:SER:HB2	2.16	0.46
1:E:341:PHE:O	1:E:345:LEU:HB2	2.16	0.46
2:G:115:PRO:HG3	2:G:121:LEU:HD11	1.98	0.46
2:H:72:LEU:CD1	2:H:72:LEU:C	2.88	0.46
2:K:86:ARG:CG	2:K:87:ALA:N	2.77	0.46
2:L:13:VAL:HG12	2:L:14:VAL:N	2.30	0.46
2:M:133:ALA:O	2:M:136:ALA:HB3	2.16	0.46
2:P:154:ARG:O	2:P:155:ILE:C	2.58	0.46
1:S:35:TRP:C	1:S:37:ARG:N	2.72	0.46
1:T:390:ASN:C	1:T:390:ASN:HD22	2.24	0.46
1:U:51:LYS:HE2	1:V:356:TYR:OH	2.15	0.46
1:U:273:VAL:O	1:U:273:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:265:LYS:H	1:W:269:SER:HB3	1.79	0.46
1:X:6:PRO:C	1:X:8:GLU:N	2.74	0.46
1:X:18:ILE:CG2	1:X:344:ILE:HG13	2.46	0.46
1:X:369:PHE:HE2	1:X:421:ILE:CD1	2.21	0.46
1:A:343:ARG:O	1:A:348:PRO:HD3	2.16	0.45
1:B:58:PRO:HD2	1:B:61:VAL:HG21	1.97	0.45
1:B:347:GLU:N	1:B:348:PRO:CD	2.79	0.45
1:B:438:ASP:CG	1:B:439:LEU:N	2.75	0.45
1:C:71:ALA:HB1	1:C:78:PHE:HB2	1.98	0.45
1:C:421:ILE:HG12	1:C:425:TYR:CE1	2.51	0.45
1:D:51:LYS:O	1:D:52:ASN:O	2.33	0.45
1:D:53:ILE:HG22	1:D:54:LEU:N	2.30	0.45
1:E:98:SER:O	1:E:99:ILE:C	2.59	0.45
1:E:249:GLU:OE1	1:E:299:LYS:HG3	2.16	0.45
1:F:44:LEU:HA	1:F:47:GLU:HB2	1.98	0.45
1:F:403:LEU:HD23	1:F:404:MET:CA	2.45	0.45
2:I:86:ARG:O	2:I:87:ALA:CB	2.64	0.45
2:K:79:ALA:HB1	2:K:83:ARG:NH2	2.24	0.45
2:M:153:LEU:HB3	2:M:167:PHE:CE2	2.51	0.45
2:N:7:ARG:NH1	2:N:12:VAL:HG21	2.32	0.45
2:P:134:ALA:O	2:P:137:LEU:N	2.49	0.45
2:Q:33:LYS:HA	2:Q:46:PHE:CZ	2.51	0.45
1:S:430:LEU:HD23	1:S:430:LEU:N	2.31	0.45
1:W:17:ILE:CD1	1:W:65:GLU:HB3	2.46	0.45
1:W:61:VAL:HG11	1:W:335:ALA:HA	1.97	0.45
1:W:439:LEU:O	1:W:441:ARG:N	2.49	0.45
1:W:441:ARG:O	1:W:443:ILE:N	2.49	0.45
1:X:17:ILE:HD13	1:X:66:ILE:HG13	1.97	0.45
1:X:351:SER:OG	1:X:354:GLU:HG2	2.16	0.45
1:A:263:CYS:C	1:A:264:LYS:HE3	2.40	0.45
1:B:283:LEU:HD23	1:B:283:LEU:HA	1.60	0.45
1:E:300:THR:HA	1:E:303:ILE:HG12	1.97	0.45
1:E:357:LYS:HG2	1:E:367:ILE:HG23	1.99	0.45
1:F:39:GLN:HE21	1:F:39:GLN:HB2	1.50	0.45
2:K:1:THR:CG2	2:K:33:LYS:NZ	2.79	0.45
2:K:51:ALA:O	2:K:52:ASP:C	2.58	0.45
2:N:113:VAL:HG22	1:T:444:LEU:HD21	1.99	0.45
2:O:144:SER:OG	2:O:147:GLU:HB2	2.15	0.45
2:Q:42:VAL:HG21	2:Q:64:LEU:CD1	2.46	0.45
1:T:17:ILE:O	1:T:17:ILE:HG22	2.15	0.45
1:T:273:VAL:O	1:T:273:VAL:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:322:GLU:HA	1:X:394:ARG:NH1	2.31	0.45
1:X:68:ARG:HG3	1:X:68:ARG:NH1	2.32	0.45
1:X:101:ARG:HA	1:X:293:THR:HG22	1.97	0.45
1:B:38:MET:HG3	1:B:45:ARG:HH12	1.82	0.45
1:B:249:GLU:HG2	1:B:299:LYS:H	1.81	0.45
1:C:34:ARG:NH2	1:C:253:ILE:HD13	2.30	0.45
1:F:426:VAL:O	1:F:427:ALA:C	2.59	0.45
2:I:49:GLY:O	2:I:50:THR:C	2.60	0.45
2:I:70:HIS:O	2:I:71:LEU:C	2.60	0.45
2:K:155:ILE:O	2:K:159:ILE:HG13	2.16	0.45
2:L:73:LYS:O	2:L:74:SER:C	2.57	0.45
2:P:32:ARG:HB2	2:P:35:ARG:HE	1.81	0.45
2:P:134:ALA:O	2:P:135:ARG:C	2.59	0.45
2:P:164:ASN:HD22	2:P:164:ASN:N	1.97	0.45
2:Q:43:LEU:HD11	2:Q:172:LEU:HG	1.98	0.45
1:U:344:ILE:CG2	3:U:458:ATP:C2	2.99	0.45
1:X:357:LYS:HA	1:X:367:ILE:CD1	2.32	0.45
1:X:430:LEU:HD23	1:X:430:LEU:N	2.31	0.45
1:B:233:LYS:O	1:B:233:LYS:HG2	2.17	0.45
1:B:321:PRO:HA	1:B:324:GLN:HB3	1.97	0.45
1:C:25:ARG:O	1:C:28:ALA:HB3	2.16	0.45
1:D:283:LEU:CB	1:D:284:PRO:HD3	2.43	0.45
1:F:381:ALA:O	1:F:382:PHE:C	2.60	0.45
2:I:1:THR:CG2	2:I:33:LYS:HD3	2.46	0.45
2:J:49:GLY:O	2:J:50:THR:C	2.59	0.45
2:P:17:ASP:C	2:P:33:LYS:HD2	2.42	0.45
1:S:18:ILE:HD11	1:S:343:ARG:HH21	1.81	0.45
1:T:433:VAL:HG12	1:T:434:VAL:N	2.32	0.45
1:V:430:LEU:HG	1:V:431:GLY:H	1.81	0.45
1:W:439:LEU:O	1:W:440:SER:C	2.59	0.45
1:X:63:LYS:H	3:X:461:ATP:PB	2.40	0.45
1:A:31:LEU:HD21	1:A:74:ALA:HB2	1.98	0.45
1:B:444:LEU:HD21	2:I:20:VAL:HG21	1.98	0.45
1:C:357:LYS:HE3	1:C:367:ILE:O	2.17	0.45
1:D:25:ARG:O	1:D:28:ALA:HB3	2.16	0.45
1:E:10:VAL:O	1:E:11:SER:C	2.60	0.45
1:F:19:GLY:O	1:F:20:GLN:C	2.58	0.45
1:F:347:GLU:N	1:F:348:PRO:CD	2.79	0.45
2:G:13:VAL:CG2	2:G:171:GLU:HB3	2.45	0.45
2:G:71:LEU:C	2:G:71:LEU:CD1	2.89	0.45
2:H:172:LEU:HD23	2:H:172:LEU:HA	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:136:ALA:HB1	2:P:137:LEU:HD13	1.99	0.45
2:R:42:VAL:HG21	2:R:64:LEU:CD1	2.47	0.45
1:S:6:PRO:C	1:S:8:GLU:N	2.73	0.45
1:S:39:GLN:HB2	1:T:362:THR:HG21	1.99	0.45
1:S:356:TYR:HB3	1:S:404:MET:HE2	1.97	0.45
1:T:68:ARG:C	1:T:70:LEU:H	2.24	0.45
1:T:254:VAL:HB	1:T:305:PHE:CD2	2.52	0.45
1:T:387:LYS:HZ3	1:T:435:GLU:CD	2.25	0.45
1:V:65:GLU:OE1	1:V:65:GLU:HA	2.17	0.45
1:W:13:LEU:C	1:W:15:GLN:H	2.24	0.45
1:B:283:LEU:CB	1:B:284:PRO:CD	2.95	0.45
1:B:403:LEU:CD2	1:B:404:MET:N	2.74	0.45
1:D:263:CYS:C	1:D:264:LYS:HE3	2.41	0.45
1:E:4:MET:CE	1:E:9:ILE:HA	2.47	0.45
1:F:34:ARG:NH2	1:F:253:ILE:HD13	2.32	0.45
1:F:339:ALA:O	1:F:342:GLU:HB2	2.17	0.45
1:F:441:ARG:NH1	2:G:36:ARG:O	2.50	0.45
2:G:165:THR:HA	2:G:167:PHE:CE2	2.51	0.45
2:L:1:THR:CG2	2:L:2:THR:N	2.79	0.45
2:P:116:GLU:O	2:P:117:GLU:C	2.59	0.45
2:Q:7:ARG:NH1	2:Q:12:VAL:HG21	2.31	0.45
1:S:283:LEU:CD1	1:S:323:LEU:HD12	2.46	0.45
1:U:265:LYS:H	1:U:269:SER:HB3	1.81	0.45
1:W:300:THR:O	1:W:301:ASP:C	2.60	0.45
1:W:387:LYS:NZ	1:W:435:GLU:HG3	2.31	0.45
1:X:18:ILE:HD11	1:X:343:ARG:HH21	1.81	0.45
1:X:96:VAL:HG21	1:X:281:ASP:HB3	1.98	0.45
1:X:227:ILE:N	1:X:230:GLU:HB2	2.32	0.45
1:X:265:LYS:H	1:X:269:SER:HB3	1.79	0.45
1:X:357:LYS:CA	1:X:367:ILE:HD11	2.33	0.45
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.79	0.45
1:B:293:THR:C	1:B:295:HIS:N	2.71	0.45
1:B:356:TYR:HB3	1:B:404:MET:HE2	1.98	0.45
1:C:108:MET:O	1:C:110:LEU:N	2.50	0.45
1:C:249:GLU:OE1	1:C:299:LYS:HG3	2.17	0.45
1:D:38:MET:HA	1:D:45:ARG:HH11	1.82	0.45
1:D:84:THR:C	1:D:86:PHE:H	2.24	0.45
1:E:55:MET:C	1:E:56:ILE:HD12	2.41	0.45
1:F:443:ILE:CD1	2:L:72:LEU:HD11	2.44	0.45
2:K:19:GLN:HB2	2:K:164:ASN:CG	2.41	0.45
2:K:42:VAL:HG21	2:K:64:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:72:LEU:C	2:K:72:LEU:HD13	2.41	0.45
2:L:86:ARG:HB3	2:L:87:ALA:H	1.48	0.45
2:M:92:GLU:O	2:M:93:ALA:HB2	2.16	0.45
2:M:157:GLY:HA2	2:M:163:THR:HG22	1.99	0.45
1:S:344:ILE:O	1:S:344:ILE:HG22	2.16	0.45
1:U:55:MET:HE2	1:U:306:ILE:HG21	1.97	0.45
1:U:61:VAL:HG11	1:U:335:ALA:HA	1.98	0.45
1:X:17:ILE:O	1:X:17:ILE:HG22	2.15	0.45
1:X:273:VAL:O	1:X:273:VAL:HG12	2.16	0.45
1:X:279:GLN:O	1:X:320:ILE:HD11	2.17	0.45
1:B:377:ILE:HD13	1:B:400:MET:SD	2.57	0.45
1:C:60:GLY:HA2	3:C:452:ATP:PB	2.56	0.45
1:C:250:GLN:HE21	1:C:250:GLN:CA	2.27	0.45
1:C:378:ALA:C	1:C:380:ALA:N	2.71	0.45
1:D:17:ILE:HG22	1:D:18:ILE:N	2.31	0.45
1:D:37:ARG:HH12	1:D:38:MET:HE2	1.82	0.45
1:E:439:LEU:HA	1:E:443:ILE:HG13	1.97	0.45
1:F:421:ILE:HA	1:F:425:TYR:HD1	1.81	0.45
1:F:428:ASP:O	1:F:430:LEU:N	2.50	0.45
2:J:36:ARG:NH1	2:J:170:GLU:OE2	2.50	0.45
2:N:116:GLU:O	2:N:117:GLU:C	2.60	0.45
2:P:35:ARG:HH11	2:P:35:ARG:HG3	1.80	0.45
1:S:17:ILE:CD1	1:S:65:GLU:HB3	2.46	0.45
1:S:260:ASP:HB3	1:S:311:PHE:HD2	1.74	0.45
1:T:232:ALA:C	1:T:234:LEU:H	2.24	0.45
1:T:331:VAL:HG13	1:T:331:VAL:O	2.17	0.45
1:U:18:ILE:HG22	1:U:344:ILE:HG12	1.99	0.45
1:W:6:PRO:C	1:W:8:GLU:N	2.74	0.45
1:W:119:ASN:O	1:W:119:ASN:ND2	2.50	0.45
1:B:64:THR:N	3:B:451:ATP:O2B	2.42	0.45
1:B:74:ALA:O	1:B:75:ASN:C	2.60	0.45
1:C:338:ALA:N	1:C:382:PHE:CD1	2.85	0.45
1:D:381:ALA:CB	1:D:396:LEU:HD23	2.47	0.45
2:G:137:LEU:HD13	2:M:136:ALA:HB1	1.93	0.45
2:H:7:ARG:CZ	2:H:12:VAL:HG22	2.45	0.45
2:H:164:ASN:HD22	2:H:164:ASN:N	2.13	0.45
2:K:115:PRO:HG3	2:K:121:LEU:HD11	1.99	0.45
2:P:90:LYS:O	2:P:91:LEU:HD12	2.17	0.45
2:Q:92:GLU:O	2:Q:93:ALA:HB2	2.17	0.45
2:R:154:ARG:O	2:R:155:ILE:C	2.60	0.45
1:S:101:ARG:HA	1:S:293:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:236:ASN:O	1:S:239:GLU:HB3	2.17	0.45
1:U:357:LYS:CA	1:U:367:ILE:HD11	2.32	0.45
1:W:36:ARG:HH11	1:X:363:GLU:HG2	1.82	0.45
1:W:329:ILE:HG12	1:X:401:GLU:HG2	1.99	0.45
1:W:390:ASN:C	1:W:390:ASN:HD22	2.24	0.45
1:A:108:MET:HG3	1:A:295:HIS:CE1	2.51	0.45
1:A:316:PRO:C	1:A:318:ASP:N	2.74	0.45
1:C:107:ALA:CB	1:C:248:VAL:HG23	2.47	0.45
1:D:33:ASN:HA	1:D:36:ARG:HD2	1.98	0.45
1:F:367:ILE:CD1	1:F:404:MET:HE1	2.46	0.45
2:G:154:ARG:O	2:G:155:ILE:C	2.60	0.45
2:M:82:TRP:CE3	2:M:110:GLY:HA2	2.52	0.45
1:S:326:ARG:C	1:S:328:PRO:HD3	2.42	0.45
1:V:20:GLN:O	1:V:21:ALA:CB	2.65	0.45
1:W:344:ILE:O	1:W:344:ILE:HG22	2.17	0.45
1:X:75:ASN:HD22	1:X:75:ASN:HA	1.53	0.45
1:A:34:ARG:NH2	1:A:253:ILE:HD13	2.32	0.44
1:A:73:LEU:C	1:A:73:LEU:HD12	2.42	0.44
1:A:79:ILE:CG2	1:A:103:LEU:HD13	2.44	0.44
1:A:403:LEU:HD11	1:A:426:VAL:HG22	2.00	0.44
1:B:227:ILE:O	1:B:227:ILE:CG1	2.64	0.44
1:C:118:LYS:HD2	1:C:118:LYS:C	2.42	0.44
1:C:283:LEU:CB	1:C:284:PRO:HD3	2.45	0.44
1:E:37:ARG:HG2	1:E:38:MET:N	2.32	0.44
1:F:108:MET:HE1	1:F:240:LEU:HD23	1.98	0.44
1:F:340:ASP:O	1:F:344:ILE:CD1	2.65	0.44
2:I:52:ASP:OD2	2:I:91:LEU:HA	2.17	0.44
2:L:60:PHE:CE2	2:L:97:VAL:HG11	2.52	0.44
2:L:72:LEU:C	2:L:72:LEU:HD13	2.41	0.44
2:L:141:THR:HG21	2:L:143:LEU:HD12	1.99	0.44
2:L:164:ASN:ND2	2:L:164:ASN:C	2.75	0.44
2:Q:5:SER:N	2:Q:121:LEU:O	2.45	0.44
2:R:2:THR:O	2:R:16:GLY:HA2	2.17	0.44
2:R:71:LEU:O	2:R:73:LYS:N	2.50	0.44
1:V:430:LEU:HD23	1:V:430:LEU:N	2.32	0.44
1:W:109:LYS:O	1:W:113:GLN:HB2	2.17	0.44
1:W:118:LYS:HG2	1:W:119:ASN:N	2.32	0.44
1:A:12:GLU:O	1:A:15:GLN:HB2	2.17	0.44
1:A:227:ILE:C	1:A:229:ASP:H	2.25	0.44
1:B:231:ALA:CA	1:B:234:LEU:HD21	2.34	0.44
1:B:264:LYS:NZ	1:B:319:LEU:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ILE:HG22	1:C:298:VAL:HG21	1.97	0.44
1:D:76:ALA:HB1	1:D:251:ASN:O	2.17	0.44
1:D:108:MET:CE	1:D:241:LYS:HA	2.46	0.44
1:D:116:ILE:CG1	1:D:117:ALA:N	2.80	0.44
1:E:280:ARG:HA	1:E:283:LEU:HD12	1.99	0.44
1:E:403:LEU:CD2	1:E:404:MET:HG2	2.45	0.44
1:F:41:GLN:O	1:F:43:PRO:HD2	2.17	0.44
1:F:270:GLY:C	1:F:272:ASP:H	2.24	0.44
2:G:77:GLU:HA	2:G:80:LYS:HG2	1.97	0.44
2:H:36:ARG:NH1	2:H:170:GLU:OE2	2.50	0.44
2:K:2:THR:O	2:K:16:GLY:HA2	2.17	0.44
2:K:17:ASP:HB2	2:K:164:ASN:HD21	1.81	0.44
2:K:52:ASP:O	2:K:53:ALA:C	2.59	0.44
2:M:35:ARG:HH11	2:M:35:ARG:HG3	1.81	0.44
2:M:104:LEU:HD13	2:M:112:VAL:CG1	2.48	0.44
2:P:82:TRP:CE3	2:P:110:GLY:HA2	2.52	0.44
1:S:65:GLU:OE1	1:S:65:GLU:HA	2.17	0.44
1:T:326:ARG:C	1:T:328:PRO:HD3	2.41	0.44
1:T:343:ARG:C	1:T:345:LEU:H	2.25	0.44
1:T:344:ILE:HG22	1:T:344:ILE:O	2.16	0.44
1:U:68:ARG:C	1:U:70:LEU:H	2.24	0.44
1:V:283:LEU:CD1	1:V:323:LEU:HD12	2.48	0.44
1:V:326:ARG:C	1:V:328:PRO:HD3	2.42	0.44
1:W:36:ARG:HE	1:W:36:ARG:CA	2.29	0.44
1:W:336:LEU:HB2	1:W:341:PHE:HE1	1.81	0.44
1:X:344:ILE:O	1:X:344:ILE:HG22	2.17	0.44
1:A:394:ARG:HD3	1:A:394:ARG:HA	1.74	0.44
1:B:29:ILE:HG13	1:B:30:ALA:N	2.32	0.44
1:C:356:TYR:HB3	1:C:404:MET:HE2	1.98	0.44
1:D:116:ILE:HD12	1:D:116:ILE:C	2.43	0.44
1:D:404:MET:HE3	1:D:404:MET:HB3	1.78	0.44
1:E:52:ASN:HB2	1:E:326:ARG:O	2.17	0.44
1:E:404:MET:HE3	1:E:404:MET:HB3	1.79	0.44
1:F:71:ALA:HB1	1:F:78:PHE:HB2	2.00	0.44
2:G:70:HIS:O	2:G:71:LEU:C	2.60	0.44
2:I:82:TRP:CE2	2:I:108:GLY:O	2.70	0.44
2:M:8:ARG:HH22	2:M:143:LEU:H	1.66	0.44
2:M:154:ARG:O	2:M:155:ILE:C	2.60	0.44
2:O:107:THR:OG1	2:O:111:ASP:OD2	2.25	0.44
2:Q:127:GLY:O	2:Q:128:ASN:C	2.60	0.44
2:R:52:ASP:HA	2:R:55:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:17:ILE:O	1:S:17:ILE:HG22	2.16	0.44
1:T:6:PRO:C	1:T:8:GLU:N	2.74	0.44
1:T:101:ARG:HA	1:T:293:THR:HG22	1.98	0.44
1:T:368:ALA:HB3	1:T:420:ASN:HA	1.99	0.44
1:U:336:LEU:HB2	1:U:341:PHE:CE1	2.52	0.44
1:U:435:GLU:CG	1:U:436:ASN:N	2.80	0.44
1:V:112:ARG:O	1:V:112:ARG:HG2	2.17	0.44
1:V:341:PHE:HB2	1:V:378:ALA:HB1	1.99	0.44
1:W:283:LEU:CD1	1:W:323:LEU:HD12	2.46	0.44
1:C:36:ARG:C	1:C:37:ARG:O	2.55	0.44
1:C:421:ILE:HG12	1:C:425:TYR:CD1	2.51	0.44
1:D:407:ILE:O	1:D:411:ALA:CB	2.63	0.44
1:E:81:VAL:HG11	1:E:99:ILE:HG12	2.00	0.44
1:F:56:ILE:N	1:F:56:ILE:CD1	2.79	0.44
1:F:60:GLY:CA	3:F:455:ATP:O1B	2.65	0.44
1:F:293:THR:C	1:F:295:HIS:N	2.75	0.44
2:I:1:THR:CG2	2:I:33:LYS:NZ	2.81	0.44
2:I:82:TRP:CE3	2:I:110:GLY:HA2	2.52	0.44
2:I:89:ARG:O	2:I:90:LYS:CB	2.65	0.44
2:L:172:LEU:HA	2:L:172:LEU:HD23	1.64	0.44
2:M:43:LEU:HD11	2:M:172:LEU:HG	1.99	0.44
2:N:164:ASN:HD22	2:N:164:ASN:N	2.01	0.44
2:O:157:GLY:HA2	2:O:163:THR:HG22	1.99	0.44
2:P:7:ARG:NH1	2:P:12:VAL:HG21	2.32	0.44
2:P:13:VAL:HG13	2:P:171:GLU:HB3	2.00	0.44
2:R:33:LYS:HA	2:R:46:PHE:CZ	2.52	0.44
2:R:75:ALA:O	2:R:78:LEU:HB3	2.17	0.44
2:R:144:SER:OG	2:R:147:GLU:HB2	2.17	0.44
1:S:36:ARG:HA	1:S:36:ARG:NE	2.31	0.44
1:U:233:LYS:HA	1:U:235:ILE:HG12	2.00	0.44
1:U:351:SER:OG	1:U:354:GLU:HG2	2.18	0.44
1:V:6:PRO:C	1:V:8:GLU:N	2.74	0.44
1:V:345:LEU:HD21	1:V:377:ILE:HG22	1.99	0.44
1:V:369:PHE:HE2	1:V:421:ILE:CD1	2.24	0.44
1:W:279:GLN:HE22	1:W:319:LEU:CA	2.30	0.44
1:X:61:VAL:HG12	1:X:336:LEU:HG	1.99	0.44
1:A:321:PRO:HA	1:A:324:GLN:HB3	2.00	0.44
1:A:381:ALA:O	1:A:384:VAL:HG13	2.18	0.44
1:B:79:ILE:HD12	1:B:80:LYS:H	1.83	0.44
1:D:323:LEU:C	1:D:325:GLY:N	2.75	0.44
1:D:442:PHE:CD2	2:J:76:VAL:HG11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:LYS:O	1:E:52:ASN:O	2.35	0.44
1:E:313:VAL:HG23	1:E:314:ALA:N	2.31	0.44
1:E:352:LEU:O	1:E:355:GLN:HB2	2.17	0.44
1:E:414:MET:O	1:E:417:GLN:HG3	2.17	0.44
1:F:410:SER:C	1:F:412:SER:N	2.74	0.44
2:G:17:ASP:HB2	2:G:164:ASN:HD21	1.75	0.44
2:H:91:LEU:O	2:H:108:GLY:HA3	2.18	0.44
2:I:73:LYS:O	2:I:74:SER:C	2.60	0.44
2:I:83:ARG:HG2	2:J:55:THR:HB	1.97	0.44
2:I:155:ILE:O	2:I:159:ILE:HG13	2.18	0.44
2:J:67:HIS:CD2	2:J:73:LYS:HD3	2.52	0.44
2:K:1:THR:HG23	2:K:33:LYS:CD	2.46	0.44
2:K:61:GLU:C	2:K:63:LYS:N	2.74	0.44
2:M:116:GLU:O	2:M:117:GLU:C	2.60	0.44
2:Q:7:ARG:NH2	2:Q:102:GLU:O	2.50	0.44
1:S:20:GLN:O	1:S:21:ALA:CB	2.66	0.44
1:T:54:LEU:CD2	1:T:307:ALA:HB3	2.47	0.44
1:V:35:TRP:C	1:V:37:ARG:N	2.74	0.44
1:W:385:ASN:ND2	1:W:395:ARG:HE	2.14	0.44
1:X:235:ILE:HG22	1:X:236:ASN:N	2.32	0.44
1:B:20:GLN:HG3	1:B:333:LEU:HD23	1.99	0.44
1:B:21:ALA:O	1:B:22:ASP:C	2.61	0.44
1:B:227:ILE:O	1:B:230:GLU:HB3	2.17	0.44
1:B:239:GLU:O	1:B:240:LEU:C	2.59	0.44
1:B:257:ASP:O	1:B:258:GLU:C	2.61	0.44
1:B:322:GLU:OE2	1:B:322:GLU:N	2.44	0.44
1:C:404:MET:O	1:C:408:SER:HB2	2.17	0.44
1:D:264:LYS:CE	1:D:279:GLN:HE22	2.27	0.44
1:F:13:LEU:CD1	1:F:24:LYS:HG2	2.47	0.44
1:F:283:LEU:O	1:F:285:LEU:N	2.51	0.44
1:F:326:ARG:C	1:F:328:PRO:HD3	2.42	0.44
2:I:136:ALA:HB1	2:O:137:LEU:HD13	1.99	0.44
2:N:144:SER:OG	2:N:147:GLU:HB2	2.17	0.44
1:S:36:ARG:HE	1:S:36:ARG:CA	2.29	0.44
1:S:344:ILE:CG2	1:S:344:ILE:O	2.65	0.44
1:T:18:ILE:HD11	1:T:343:ARG:NH2	2.32	0.44
1:T:68:ARG:HG3	1:T:68:ARG:NH1	2.32	0.44
1:T:351:SER:OG	1:T:354:GLU:HG2	2.17	0.44
1:V:68:ARG:HG3	1:V:68:ARG:NH1	2.32	0.44
1:V:68:ARG:C	1:V:70:LEU:H	2.25	0.44
1:W:32:ARG:NH2	1:X:363:GLU:OE1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:265:LYS:H	1:X:269:SER:CB	2.31	0.44
1:A:300:THR:HA	1:A:303:ILE:HG12	1.99	0.44
1:A:361:ALA:O	1:A:364:GLY:N	2.41	0.44
1:B:36:ARG:C	1:B:37:ARG:O	2.58	0.44
1:B:55:MET:HE3	1:B:306:ILE:CG2	2.46	0.44
1:B:262:ILE:O	1:B:262:ILE:HG13	2.18	0.44
1:C:115:GLU:C	1:C:117:ALA:H	2.23	0.44
1:E:44:LEU:O	1:E:45:ARG:C	2.60	0.44
1:E:264:LYS:HD3	1:E:276:GLU:CD	2.41	0.44
1:E:338:ALA:O	1:E:341:PHE:HB2	2.17	0.44
2:H:72:LEU:C	2:H:72:LEU:HD13	2.43	0.44
2:O:92:GLU:O	2:O:93:ALA:HB2	2.18	0.44
1:T:235:ILE:CG2	1:T:236:ASN:N	2.80	0.44
1:T:300:THR:O	1:T:302:HIS:N	2.50	0.44
1:T:430:LEU:N	1:T:430:LEU:HD23	2.33	0.44
1:T:430:LEU:HD23	1:T:430:LEU:H	1.81	0.44
1:U:36:ARG:HE	1:U:36:ARG:CA	2.30	0.44
1:U:53:ILE:HG12	1:U:329:ILE:HB	1.99	0.44
1:V:36:ARG:HE	1:V:36:ARG:CA	2.30	0.44
1:V:368:ALA:HB3	1:V:420:ASN:HA	2.00	0.44
1:X:368:ALA:HB3	1:X:420:ASN:HA	1.99	0.44
1:X:442:PHE:O	1:X:443:ILE:HD13	2.18	0.44
1:A:403:LEU:HD23	1:A:404:MET:CA	2.48	0.44
1:D:3:GLU:CG	1:D:4:MET:N	2.81	0.44
1:D:357:LYS:HA	1:D:367:ILE:CG2	2.47	0.44
1:E:293:THR:C	1:E:295:HIS:N	2.73	0.44
1:F:5:THR:O	1:F:6:PRO:C	2.60	0.44
1:F:425:TYR:O	1:F:428:ASP:HB3	2.18	0.44
3:F:455:ATP:C8	3:F:455:ATP:H5'1	2.53	0.44
2:H:42:VAL:HG21	2:H:64:LEU:HD13	2.00	0.44
2:H:141:THR:HG21	2:H:143:LEU:HD12	2.00	0.44
2:J:49:GLY:O	2:J:51:ALA:N	2.51	0.44
2:L:71:LEU:C	2:L:71:LEU:CD1	2.90	0.44
2:M:107:THR:OG1	2:M:111:ASP:OD2	2.22	0.44
2:N:32:ARG:HH11	2:N:32:ARG:HG3	1.83	0.44
2:N:127:GLY:O	2:N:129:TYR:N	2.51	0.44
2:N:134:ALA:O	2:N:135:ARG:C	2.61	0.44
2:O:35:ARG:HH11	2:O:35:ARG:HG3	1.83	0.44
1:T:17:ILE:CD1	1:T:65:GLU:HB3	2.45	0.44
1:T:115:GLU:C	1:T:117:ALA:N	2.75	0.44
1:T:441:ARG:HG3	1:T:441:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:344:ILE:CG2	3:U:458:ATP:H2	2.29	0.44
1:X:343:ARG:C	1:X:345:LEU:H	2.26	0.44
1:A:53:ILE:CG2	1:A:54:LEU:N	2.81	0.44
1:A:58:PRO:O	1:A:63:LYS:NZ	2.37	0.44
1:B:436:ASN:HB3	1:B:439:LEU:HD11	2.00	0.44
1:C:100:ILE:HG13	1:C:300:THR:CG2	2.48	0.44
1:C:315:ARG:O	1:C:318:ASP:HB2	2.18	0.44
1:D:108:MET:HG3	1:D:295:HIS:CE1	2.52	0.44
1:E:100:ILE:CG2	1:E:298:VAL:HG21	2.48	0.44
1:E:321:PRO:O	1:E:322:GLU:C	2.60	0.44
1:F:116:ILE:C	1:F:116:ILE:HD12	2.43	0.44
2:H:17:ASP:C	2:H:33:LYS:HD2	2.43	0.44
2:H:78:LEU:HD12	2:H:78:LEU:C	2.43	0.44
2:I:25:THR:HA	2:N:159:ILE:O	2.17	0.44
2:M:32:ARG:HB2	2:M:35:ARG:HE	1.83	0.44
2:Q:134:ALA:O	2:Q:135:ARG:C	2.60	0.44
1:S:64:THR:OG1	1:S:255:PHE:HE2	2.01	0.44
1:S:111:VAL:O	1:S:115:GLU:HB2	2.18	0.44
1:T:65:GLU:OE1	1:T:65:GLU:HA	2.17	0.44
1:V:265:LYS:H	1:V:269:SER:HB3	1.82	0.44
1:V:344:ILE:O	1:V:344:ILE:HG22	2.17	0.44
1:X:300:THR:O	1:X:301:ASP:C	2.60	0.44
1:A:28:ALA:O	1:A:29:ILE:C	2.61	0.43
1:A:337:SER:O	1:A:340:ASP:HB2	2.17	0.43
1:A:384:VAL:O	1:A:385:ASN:C	2.58	0.43
1:B:357:LYS:HE3	1:B:367:ILE:O	2.17	0.43
1:C:23:ALA:CA	1:C:331:VAL:HG21	2.43	0.43
1:D:438:ASP:O	1:D:439:LEU:C	2.61	0.43
1:E:111:VAL:O	1:E:111:VAL:HG12	2.18	0.43
1:F:98:SER:O	1:F:99:ILE:C	2.61	0.43
1:F:356:TYR:HB3	1:F:404:MET:HE2	2.00	0.43
2:K:13:VAL:HG12	2:K:14:VAL:N	2.32	0.43
2:L:105:ILE:HG23	2:L:105:ILE:O	2.17	0.43
2:M:49:GLY:O	2:M:51:ALA:N	2.51	0.43
2:Q:157:GLY:HA2	2:Q:163:THR:HG22	1.99	0.43
2:R:5:SER:N	2:R:121:LEU:O	2.45	0.43
1:U:65:GLU:CG	3:U:458:ATP:H5'2	2.30	0.43
1:A:360:MET:HE1	1:B:36:ARG:HH11	1.81	0.43
1:B:240:LEU:O	1:B:241:LYS:C	2.61	0.43
1:B:293:THR:O	1:B:295:HIS:N	2.51	0.43
1:B:323:LEU:C	1:B:325:GLY:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ASP:O	1:B:423:ALA:C	2.61	0.43
1:D:29:ILE:HG13	1:D:30:ALA:N	2.33	0.43
1:D:60:GLY:HA2	3:D:453:ATP:O1B	2.18	0.43
1:D:336:LEU:HD12	1:D:336:LEU:HA	1.65	0.43
1:F:79:ILE:HD12	1:F:80:LYS:H	1.83	0.43
1:F:107:ALA:CB	1:F:248:VAL:HG23	2.48	0.43
1:F:428:ASP:OD1	1:F:429:ALA:N	2.51	0.43
2:K:71:LEU:C	2:K:71:LEU:CD1	2.90	0.43
2:K:83:ARG:CG	2:L:55:THR:HG22	2.38	0.43
2:L:70:HIS:O	2:L:71:LEU:C	2.61	0.43
2:O:55:THR:HG22	2:P:83:ARG:HA	2.00	0.43
2:Q:82:TRP:CE3	2:Q:110:GLY:HA2	2.53	0.43
1:S:390:ASN:HD22	1:S:390:ASN:C	2.25	0.43
1:U:66:ILE:O	1:U:66:ILE:HG22	2.18	0.43
1:V:9:ILE:O	1:V:13:LEU:HG	2.19	0.43
1:V:34:ARG:HG2	1:V:250:GLN:NE2	2.32	0.43
1:V:279:GLN:O	1:V:320:ILE:HD11	2.17	0.43
1:W:351:SER:OG	1:W:354:GLU:HG2	2.18	0.43
1:X:111:VAL:HG11	1:X:244:ALA:HA	2.00	0.43
1:X:343:ARG:C	1:X:345:LEU:N	2.77	0.43
1:X:353:THR:HG22	1:X:369:PHE:HD1	1.82	0.43
1:A:39:GLN:HG2	1:F:362:THR:HG23	1.97	0.43
1:A:114:GLN:HE21	1:A:114:GLN:HB3	1.57	0.43
1:C:107:ALA:HB2	1:C:248:VAL:CG2	2.48	0.43
1:C:260:ASP:HB3	1:C:311:PHE:CE2	2.52	0.43
1:E:6:PRO:O	1:E:10:VAL:HG23	2.19	0.43
1:E:283:LEU:O	1:E:287:GLU:HB2	2.18	0.43
1:E:347:GLU:N	1:E:348:PRO:CD	2.81	0.43
1:E:360:MET:CA	1:E:360:MET:CE	2.94	0.43
1:E:370:THR:O	1:E:371:THR:C	2.60	0.43
1:E:381:ALA:O	1:E:384:VAL:HG13	2.17	0.43
2:G:3:ILE:HG22	2:G:96:ILE:HD12	2.00	0.43
2:I:157:GLY:HA2	2:I:163:THR:HB	2.01	0.43
2:L:94:MET:HE3	2:L:123:ILE:HB	2.01	0.43
2:M:13:VAL:HG13	2:M:171:GLU:HB3	2.00	0.43
2:M:56:LEU:HD23	2:M:95:LEU:HD13	1.99	0.43
2:N:42:VAL:HG21	2:N:64:LEU:CD1	2.49	0.43
2:N:113:VAL:HG22	1:T:444:LEU:CD2	2.48	0.43
2:N:157:GLY:HA2	2:N:163:THR:HG22	2.00	0.43
1:S:34:ARG:HG2	1:S:250:GLN:NE2	2.32	0.43
1:T:344:ILE:O	1:T:344:ILE:CG2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:441:ARG:O	1:T:443:ILE:N	2.50	0.43
1:V:54:LEU:HD21	1:V:327:LEU:CD1	2.41	0.43
1:V:351:SER:OG	1:V:354:GLU:HG2	2.17	0.43
1:W:265:LYS:H	1:W:269:SER:CB	2.31	0.43
1:W:430:LEU:HD23	1:W:430:LEU:N	2.33	0.43
1:W:439:LEU:N	1:W:439:LEU:HD23	2.33	0.43
1:X:279:GLN:HE22	1:X:319:LEU:CA	2.31	0.43
1:A:257:ASP:OD1	1:A:308:SER:OG	2.37	0.43
1:B:44:LEU:O	1:B:45:ARG:C	2.60	0.43
1:D:101:ARG:HA	1:D:293:THR:HG22	2.00	0.43
1:D:264:LYS:O	1:D:265:LYS:HB3	2.18	0.43
1:D:341:PHE:O	1:D:345:LEU:HB2	2.18	0.43
1:D:403:LEU:CD2	1:D:404:MET:N	2.74	0.43
1:D:409:PHE:CE1	1:E:6:PRO:HB3	2.53	0.43
1:E:108:MET:HG3	1:E:295:HIS:NE2	2.33	0.43
1:F:390:ASN:C	1:F:390:ASN:OD1	2.61	0.43
2:H:105:ILE:HD11	2:H:123:ILE:HG22	1.99	0.43
2:N:82:TRP:CE3	2:N:110:GLY:HA2	2.53	0.43
2:O:112:VAL:HB	1:U:443:ILE:HD12	2.01	0.43
2:P:127:GLY:O	2:P:128:ASN:C	2.61	0.43
2:Q:35:ARG:HH11	2:Q:35:ARG:HG3	1.83	0.43
2:R:90:LYS:C	2:R:91:LEU:HD12	2.44	0.43
1:T:439:LEU:C	1:T:441:ARG:N	2.76	0.43
1:W:18:ILE:HD11	1:W:343:ARG:NH2	2.33	0.43
1:X:283:LEU:CD1	1:X:323:LEU:HD12	2.47	0.43
1:B:357:LYS:NZ	1:B:368:ALA:HA	2.34	0.43
1:D:109:LYS:O	1:D:110:LEU:C	2.60	0.43
1:F:100:ILE:HG22	1:F:298:VAL:HG21	2.00	0.43
1:F:261:LYS:C	1:F:263:CYS:H	2.27	0.43
1:F:336:LEU:HD12	1:F:336:LEU:HA	1.74	0.43
1:F:439:LEU:CD2	2:L:72:LEU:HG	2.49	0.43
2:H:52:ASP:HA	2:H:55:THR:CG2	2.43	0.43
2:J:83:ARG:NH1	2:K:58:GLU:OE2	2.51	0.43
2:J:86:ARG:O	2:J:87:ALA:HB2	2.17	0.43
2:K:67:HIS:O	2:K:68:GLN:C	2.61	0.43
2:L:107:THR:OG1	2:L:109:ILE:HG12	2.19	0.43
2:O:116:GLU:O	2:O:117:GLU:C	2.61	0.43
2:Q:120:ILE:HD11	2:Q:138:VAL:HG21	2.01	0.43
1:S:18:ILE:CG2	1:S:344:ILE:CG1	2.97	0.43
1:S:51:LYS:HE2	1:T:356:TYR:OH	2.18	0.43
1:U:110:LEU:O	1:U:114:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:375:LYS:C	1:U:377:ILE:H	2.27	0.43
1:V:300:THR:O	1:V:301:ASP:C	2.62	0.43
1:V:336:LEU:HB2	1:V:341:PHE:CE1	2.53	0.43
1:V:390:ASN:C	1:V:390:ASN:HD22	2.25	0.43
1:W:20:GLN:O	1:W:21:ALA:CB	2.66	0.43
1:W:343:ARG:C	1:W:345:LEU:H	2.27	0.43
1:X:390:ASN:HD22	1:X:390:ASN:C	2.26	0.43
1:A:25:ARG:O	1:A:26:ALA:C	2.61	0.43
1:A:336:LEU:HD12	1:A:336:LEU:HA	1.70	0.43
1:A:378:ALA:C	1:A:380:ALA:N	2.74	0.43
1:B:390:ASN:C	1:B:390:ASN:OD1	2.61	0.43
1:C:237:PRO:HB3	1:C:241:LYS:NZ	2.33	0.43
1:C:336:LEU:HD12	1:C:336:LEU:HA	1.81	0.43
1:C:428:ASP:O	1:C:430:LEU:N	2.51	0.43
1:E:57:GLY:HA3	1:E:63:LYS:HE3	2.00	0.43
1:E:100:ILE:HG22	1:E:298:VAL:HG21	2.01	0.43
1:F:36:ARG:O	1:F:39:GLN:CB	2.63	0.43
2:H:73:LYS:O	2:H:74:SER:C	2.61	0.43
2:J:19:GLN:OE1	2:J:162:PHE:HA	2.18	0.43
2:K:46:PHE:HB3	2:K:95:LEU:HD21	1.99	0.43
2:K:85:ASP:OD1	2:K:85:ASP:N	2.51	0.43
2:L:164:ASN:ND2	2:L:164:ASN:H	2.16	0.43
2:M:6:VAL:HG21	2:M:148:ILE:CG2	2.49	0.43
2:N:134:ALA:O	2:N:137:LEU:N	2.51	0.43
1:S:262:ILE:HD12	1:S:279:GLN:HB2	2.01	0.43
1:S:273:VAL:O	1:S:273:VAL:HG12	2.18	0.43
1:S:322:GLU:N	1:S:322:GLU:OE1	2.51	0.43
1:U:36:ARG:HA	1:U:36:ARG:NE	2.31	0.43
1:V:13:LEU:C	1:V:15:GLN:H	2.26	0.43
1:W:9:ILE:O	1:W:13:LEU:HG	2.18	0.43
1:A:347:GLU:N	1:A:348:PRO:CD	2.82	0.43
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.80	0.43
1:B:4:MET:HE3	1:B:8:GLU:HG2	2.00	0.43
1:B:57:GLY:CA	1:B:63:LYS:HE3	2.48	0.43
1:B:241:LYS:O	1:B:244:ALA:N	2.51	0.43
1:E:239:GLU:O	1:E:243:LYS:HB2	2.19	0.43
1:E:403:LEU:HD23	1:E:404:MET:CA	2.49	0.43
1:F:20:GLN:OE1	1:F:333:LEU:HB3	2.17	0.43
2:H:49:GLY:O	2:H:50:THR:C	2.61	0.43
2:I:164:ASN:ND2	2:I:164:ASN:C	2.71	0.43
2:K:36:ARG:NH1	2:K:170:GLU:OE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:VAL:CG1	2:L:7:ARG:N	2.81	0.43
2:L:42:VAL:HG21	2:L:64:LEU:HD13	1.99	0.43
2:O:49:GLY:O	2:O:51:ALA:N	2.52	0.43
2:P:2:THR:O	2:P:16:GLY:HA2	2.18	0.43
2:Q:120:ILE:HD13	2:Q:134:ALA:HB1	2.01	0.43
2:R:35:ARG:HH11	2:R:35:ARG:HG3	1.82	0.43
1:S:53:ILE:HG12	1:S:329:ILE:HB	2.00	0.43
1:W:63:LYS:N	3:W:460:ATP:O2B	2.52	0.43
1:W:279:GLN:O	1:W:320:ILE:HD11	2.19	0.43
1:W:375:LYS:C	1:W:377:ILE:H	2.27	0.43
1:C:357:LYS:HA	1:C:367:ILE:CG2	2.48	0.43
1:D:283:LEU:HD23	1:D:283:LEU:HA	1.87	0.43
1:D:352:LEU:O	1:D:355:GLN:HB2	2.19	0.43
1:E:344:ILE:HG22	3:E:454:ATP:C2	2.52	0.43
1:E:363:GLU:HB3	1:E:411:ALA:O	2.18	0.43
2:G:60:PHE:HA	2:G:78:LEU:HD22	2.00	0.43
2:J:1:THR:CG2	2:J:33:LYS:NZ	2.82	0.43
2:J:91:LEU:N	2:J:91:LEU:CD1	2.64	0.43
2:K:46:PHE:HB3	2:K:95:LEU:HD23	2.01	0.43
2:L:46:PHE:HB3	2:L:95:LEU:HD21	1.97	0.43
2:O:2:THR:O	2:O:16:GLY:HA2	2.18	0.43
1:S:79:ILE:HG23	1:S:79:ILE:O	2.19	0.43
1:T:343:ARG:C	1:T:345:LEU:N	2.76	0.43
1:U:68:ARG:HG3	1:U:68:ARG:NH1	2.33	0.43
1:U:279:GLN:HE22	1:U:319:LEU:CA	2.31	0.43
1:U:300:THR:O	1:U:301:ASP:C	2.61	0.43
1:W:259:ILE:HG23	1:W:260:ASP:N	2.34	0.43
1:W:353:THR:HG22	1:W:369:PHE:HD1	1.84	0.43
1:X:28:ALA:O	1:X:30:ALA:N	2.51	0.43
1:A:37:ARG:HG2	1:A:38:MET:N	2.34	0.43
1:A:108:MET:O	1:A:109:LYS:C	2.59	0.43
1:A:351:SER:O	1:A:355:GLN:HG3	2.18	0.43
1:B:381:ALA:CB	1:B:396:LEU:HD23	2.48	0.43
1:C:6:PRO:O	1:C:10:VAL:HG23	2.18	0.43
1:C:37:ARG:HA	1:C:40:LEU:CD1	2.49	0.43
1:C:403:LEU:C	1:C:405:ASP:H	2.26	0.43
1:D:37:ARG:HB2	1:D:48:VAL:HG11	2.01	0.43
1:D:58:PRO:HD2	1:D:61:VAL:HG21	1.99	0.43
1:E:78:PHE:CD2	1:E:78:PHE:C	2.97	0.43
1:E:357:LYS:HA	1:E:367:ILE:CG2	2.48	0.43
1:F:378:ALA:C	1:F:380:ALA:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:433:VAL:CG1	1:F:434:VAL:H	2.23	0.43
2:I:18:GLY:N	2:I:164:ASN:HD21	2.06	0.43
2:K:60:PHE:HZ	2:K:71:LEU:HD22	1.83	0.43
2:O:33:LYS:HA	2:O:46:PHE:CZ	2.54	0.43
2:P:138:VAL:HG23	2:P:148:ILE:HD13	2.00	0.43
2:R:13:VAL:HG21	2:R:146:HIS:HA	2.00	0.43
2:R:17:ASP:OD2	2:R:33:LYS:HE3	2.18	0.43
1:S:437:GLU:O	1:S:439:LEU:N	2.52	0.43
1:T:279:GLN:HE22	1:T:319:LEU:CA	2.32	0.43
1:T:329:ILE:HG12	1:U:401:GLU:HG2	2.00	0.43
1:T:375:LYS:C	1:T:377:ILE:H	2.27	0.43
1:U:300:THR:O	1:U:302:HIS:N	2.52	0.43
1:U:439:LEU:HA	1:U:443:ILE:HB	2.01	0.43
1:X:21:ALA:C	1:X:23:ALA:H	2.25	0.43
1:X:331:VAL:HG13	1:X:331:VAL:O	2.19	0.43
1:X:356:TYR:CD1	1:X:404:MET:HG3	2.54	0.43
1:X:366:ASN:HD22	1:X:366:ASN:HA	1.63	0.43
1:A:270:GLY:C	1:A:272:ASP:H	2.25	0.43
1:A:390:ASN:HB2	2:G:68:GLN:OE1	2.18	0.43
1:B:37:ARG:O	1:B:38:MET:HB3	2.19	0.43
1:B:79:ILE:HD12	1:B:80:LYS:N	2.34	0.43
1:D:283:LEU:HD11	1:D:320:ILE:HD12	2.01	0.43
1:E:264:LYS:HZ1	1:E:319:LEU:HA	1.84	0.43
1:F:58:PRO:HD2	1:F:61:VAL:HG21	2.00	0.43
1:F:60:GLY:HA2	3:F:455:ATP:PB	2.59	0.43
2:G:61:GLU:O	2:G:64:LEU:N	2.52	0.43
2:H:7:ARG:HA	2:H:11:GLN:O	2.19	0.43
2:H:115:PRO:HG3	2:H:121:LEU:HD21	2.01	0.43
2:K:86:ARG:O	2:L:89:ARG:HD3	2.18	0.43
2:K:157:GLY:HA2	2:K:163:THR:HB	2.00	0.43
2:P:17:ASP:OD2	2:P:33:LYS:HE3	2.18	0.43
2:Q:76:VAL:HG21	1:W:438:ASP:CG	2.44	0.43
2:R:83:ARG:NH1	1:X:442:PHE:HB2	2.34	0.43
1:T:35:TRP:C	1:T:37:ARG:N	2.73	0.43
1:U:6:PRO:C	1:U:8:GLU:N	2.75	0.43
1:U:21:ALA:C	1:U:23:ALA:H	2.27	0.43
1:U:35:TRP:C	1:U:37:ARG:H	2.27	0.43
1:W:79:ILE:HG23	1:W:79:ILE:O	2.18	0.43
1:W:283:LEU:N	1:W:284:PRO:CD	2.82	0.43
1:W:441:ARG:HA	1:W:441:ARG:HD3	1.78	0.43
1:A:239:GLU:O	1:A:240:LEU:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLN:HE21	1:A:250:GLN:CA	2.32	0.42
1:A:343:ARG:C	1:A:345:LEU:N	2.75	0.42
1:B:401:GLU:OE1	1:C:51:LYS:HG3	2.19	0.42
1:B:410:SER:C	1:B:412:SER:N	2.74	0.42
1:C:110:LEU:HD12	1:C:110:LEU:HA	1.86	0.42
1:D:340:ASP:C	1:D:344:ILE:HD11	2.43	0.42
1:D:360:MET:CA	1:D:360:MET:CE	2.94	0.42
1:D:443:ILE:HG22	1:D:444:LEU:N	2.34	0.42
1:E:35:TRP:O	1:E:39:GLN:HB2	2.18	0.42
1:E:111:VAL:HG12	1:E:240:LEU:CD1	2.48	0.42
1:E:264:LYS:CE	1:E:279:GLN:NE2	2.80	0.42
1:F:398:THR:HG22	1:F:399:VAL:N	2.32	0.42
2:I:18:GLY:H	2:I:164:ASN:ND2	2.06	0.42
2:O:134:ALA:O	2:O:137:LEU:N	2.52	0.42
2:P:6:VAL:HG21	2:P:148:ILE:CG2	2.49	0.42
2:Q:4:VAL:HG12	2:Q:153:LEU:HD21	2.01	0.42
2:Q:137:LEU:C	2:Q:141:THR:HG22	2.44	0.42
1:S:345:LEU:HD13	1:S:396:LEU:HD22	2.01	0.42
1:S:439:LEU:C	1:S:441:ARG:N	2.76	0.42
1:T:34:ARG:HG2	1:T:250:GLN:NE2	2.34	0.42
1:U:34:ARG:HG2	1:U:250:GLN:NE2	2.34	0.42
1:U:324:GLN:HE22	1:V:389:GLU:HG2	1.84	0.42
1:U:345:LEU:HD21	1:U:377:ILE:HG22	2.01	0.42
1:V:366:ASN:HD22	1:V:366:ASN:HA	1.65	0.42
1:W:259:ILE:O	1:W:260:ASP:C	2.61	0.42
1:W:319:LEU:O	1:W:324:GLN:NE2	2.52	0.42
1:W:344:ILE:O	1:W:344:ILE:CG2	2.67	0.42
1:X:245:ILE:C	1:X:247:ALA:N	2.78	0.42
1:A:410:SER:O	1:A:412:SER:N	2.52	0.42
1:C:283:LEU:HD11	1:C:320:ILE:CD1	2.49	0.42
1:C:340:ASP:O	1:C:344:ILE:CD1	2.67	0.42
1:D:34:ARG:NH2	1:D:253:ILE:CD1	2.82	0.42
1:D:241:LYS:O	1:D:242:GLN:C	2.61	0.42
1:E:65:GLU:O	1:E:66:ILE:C	2.60	0.42
1:F:18:ILE:N	3:F:455:ATP:N1	2.52	0.42
1:F:243:LYS:O	1:F:246:ASP:N	2.53	0.42
1:F:404:MET:O	1:F:408:SER:HB2	2.18	0.42
2:H:19:GLN:HB2	2:H:164:ASN:CG	2.44	0.42
2:K:5:SER:CB	2:K:14:VAL:HG22	2.48	0.42
2:L:18:GLY:N	2:L:164:ASN:HD21	2.06	0.42
2:L:103:SER:O	2:L:104:LEU:CD1	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:32:ARG:HG3	2:M:32:ARG:HH11	1.83	0.42
2:M:91:LEU:HB2	2:M:108:GLY:HA3	2.02	0.42
2:N:32:ARG:HB2	2:N:35:ARG:HE	1.83	0.42
1:S:63:LYS:H	3:S:456:ATP:PB	2.42	0.42
1:S:265:LYS:H	1:S:269:SER:HB3	1.83	0.42
1:S:300:THR:O	1:S:302:HIS:N	2.51	0.42
1:S:368:ALA:HB3	1:S:420:ASN:HA	2.01	0.42
1:T:36:ARG:HE	1:T:36:ARG:CA	2.30	0.42
1:T:283:LEU:CD1	1:T:322:GLU:HB3	2.50	0.42
1:T:393:ALA:C	1:T:395:ARG:N	2.77	0.42
1:U:65:GLU:OE1	1:U:65:GLU:HA	2.18	0.42
1:V:421:ILE:HG12	1:V:425:TYR:CD1	2.54	0.42
1:X:344:ILE:CG2	1:X:344:ILE:O	2.66	0.42
1:X:407:ILE:HG23	1:X:408:SER:N	2.34	0.42
1:A:17:ILE:HB	1:A:24:LYS:HE3	2.01	0.42
1:A:341:PHE:HA	1:A:344:ILE:CG1	2.49	0.42
1:A:393:ALA:O	1:A:394:ARG:C	2.61	0.42
1:C:359:LEU:HD12	1:D:36:ARG:HB3	2.02	0.42
1:E:74:ALA:O	1:E:75:ASN:C	2.59	0.42
1:E:415:ASN:OD1	1:E:415:ASN:C	2.62	0.42
1:F:101:ARG:HA	1:F:293:THR:HG22	2.02	0.42
2:G:83:ARG:HG2	2:G:83:ARG:HH11	1.84	0.42
2:H:75:ALA:O	2:H:78:LEU:HB3	2.19	0.42
2:H:84:THR:HB	2:H:85:ASP:H	1.65	0.42
2:I:17:ASP:HB2	2:I:164:ASN:HD21	1.76	0.42
2:P:42:VAL:HG21	2:P:64:LEU:CD1	2.49	0.42
2:R:4:VAL:HG12	2:R:153:LEU:CD2	2.49	0.42
1:S:394:ARG:HH12	1:X:322:GLU:HG3	1.84	0.42
1:S:436:ASN:C	1:S:436:ASN:ND2	2.76	0.42
1:U:13:LEU:C	1:U:15:GLN:H	2.27	0.42
1:W:53:ILE:HG12	1:W:329:ILE:HB	2.01	0.42
1:W:65:GLU:HA	1:W:65:GLU:OE1	2.18	0.42
1:X:34:ARG:HG2	1:X:250:GLN:NE2	2.34	0.42
1:X:79:ILE:O	1:X:79:ILE:HG23	2.19	0.42
1:A:20:GLN:NE2	1:A:20:GLN:HA	2.35	0.42
1:A:32:ARG:O	1:A:33:ASN:C	2.61	0.42
1:A:367:ILE:HD11	1:A:421:ILE:HD12	2.00	0.42
1:B:98:SER:O	1:B:99:ILE:C	2.63	0.42
1:C:4:MET:CE	1:C:9:ILE:HA	2.49	0.42
1:C:311:PHE:CE1	1:C:316:PRO:HA	2.53	0.42
1:E:256:ILE:HG21	1:E:259:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:SER:O	1:E:412:SER:N	2.53	0.42
1:E:440:SER:O	1:E:441:ARG:C	2.61	0.42
2:G:4:VAL:HG23	2:G:122:ALA:HB2	2.00	0.42
2:J:164:ASN:ND2	2:J:164:ASN:C	2.77	0.42
2:L:131:LEU:O	2:L:132:SER:C	2.62	0.42
2:N:17:ASP:C	2:N:33:LYS:HD2	2.44	0.42
2:P:4:VAL:HA	2:P:121:LEU:O	2.18	0.42
2:P:43:LEU:O	2:P:97:VAL:HA	2.20	0.42
2:Q:52:ASP:HA	2:Q:55:THR:OG1	2.19	0.42
1:S:35:TRP:C	1:S:37:ARG:H	2.27	0.42
1:S:283:LEU:N	1:S:284:PRO:CD	2.83	0.42
1:S:343:ARG:C	1:S:345:LEU:H	2.28	0.42
1:T:20:GLN:O	1:T:21:ALA:CB	2.67	0.42
1:T:79:ILE:HG23	1:T:79:ILE:O	2.20	0.42
1:T:393:ALA:O	1:T:396:LEU:N	2.50	0.42
1:U:344:ILE:HD13	3:U:458:ATP:N1	2.34	0.42
1:W:341:PHE:CB	1:W:378:ALA:HB1	2.50	0.42
1:W:387:LYS:NZ	1:W:435:GLU:CG	2.83	0.42
1:X:36:ARG:HA	1:X:36:ARG:NE	2.33	0.42
1:X:326:ARG:C	1:X:328:PRO:HD3	2.42	0.42
1:A:51:LYS:HG3	1:F:401:GLU:OE1	2.19	0.42
1:A:110:LEU:O	1:A:114:GLN:HB2	2.19	0.42
1:A:359:LEU:C	1:A:360:MET:HE2	2.44	0.42
1:A:369:PHE:CE2	1:A:421:ILE:HD12	2.55	0.42
1:A:435:GLU:C	1:A:437:GLU:N	2.74	0.42
1:B:79:ILE:CG2	1:B:103:LEU:HD13	2.46	0.42
1:B:236:ASN:H	1:B:237:PRO:HD3	1.85	0.42
1:B:357:LYS:HA	1:B:367:ILE:HG23	2.01	0.42
1:B:398:THR:HG22	1:B:399:VAL:N	2.33	0.42
1:C:44:LEU:C	1:C:46:HIS:N	2.76	0.42
1:C:244:ALA:O	1:C:245:ILE:C	2.59	0.42
1:C:323:LEU:C	1:C:325:GLY:N	2.75	0.42
1:C:443:ILE:CG2	1:C:444:LEU:N	2.82	0.42
1:F:235:ILE:O	1:F:236:ASN:CB	2.67	0.42
2:G:19:GLN:OE1	2:G:21:SER:OG	2.38	0.42
2:G:172:LEU:HD23	2:G:172:LEU:HA	1.70	0.42
2:H:1:THR:CG2	2:H:33:LYS:HD3	2.49	0.42
2:I:60:PHE:CE2	2:I:97:VAL:HG11	2.54	0.42
2:L:72:LEU:HD22	2:L:104:LEU:HD21	2.00	0.42
2:O:52:ASP:HA	2:O:55:THR:OG1	2.20	0.42
2:P:144:SER:OG	2:P:147:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:99:ASP:C	2:R:99:ASP:OD2	2.63	0.42
1:S:21:ALA:C	1:S:23:ALA:H	2.26	0.42
1:S:289:SER:H	1:S:300:THR:HG1	1.66	0.42
1:S:366:ASN:HD22	1:S:366:ASN:HA	1.63	0.42
1:T:235:ILE:HG22	1:T:237:PRO:CD	2.48	0.42
1:U:17:ILE:CD1	1:U:65:GLU:HB3	2.47	0.42
1:U:344:ILE:O	1:U:344:ILE:HG22	2.19	0.42
1:W:16:HIS:C	1:W:17:ILE:HG13	2.45	0.42
1:W:240:LEU:HD12	1:W:240:LEU:N	2.34	0.42
1:W:326:ARG:C	1:W:328:PRO:HD3	2.41	0.42
1:X:37:ARG:HG3	1:X:48:VAL:HG11	2.01	0.42
1:X:421:ILE:HG12	1:X:425:TYR:CD1	2.55	0.42
1:B:356:TYR:CE1	1:B:400:MET:HB3	2.54	0.42
1:C:34:ARG:NH2	1:C:253:ILE:CD1	2.82	0.42
1:C:42:GLU:HB3	1:C:43:PRO:HD3	2.00	0.42
1:C:52:ASN:ND2	1:C:305:PHE:CB	2.81	0.42
1:D:37:ARG:O	1:D:38:MET:HB3	2.19	0.42
1:E:263:CYS:C	1:E:264:LYS:HE3	2.44	0.42
1:E:384:VAL:H	1:E:384:VAL:HG12	1.64	0.42
2:L:72:LEU:C	2:L:72:LEU:CD1	2.91	0.42
2:M:5:SER:CB	2:M:14:VAL:HG22	2.44	0.42
2:N:78:LEU:O	2:N:81:ASP:HB2	2.19	0.42
2:Q:153:LEU:HB3	2:Q:167:PHE:CD2	2.54	0.42
2:R:127:GLY:O	2:R:128:ASN:C	2.63	0.42
1:S:245:ILE:CG2	1:S:249:GLU:HG3	2.49	0.42
1:U:247:ALA:O	1:U:251:ASN:O	2.38	0.42
1:U:437:GLU:HG3	1:U:437:GLU:O	2.20	0.42
1:V:15:GLN:O	1:V:349:HIS:N	2.50	0.42
1:V:35:TRP:C	1:V:37:ARG:H	2.28	0.42
1:V:79:ILE:HG23	1:V:79:ILE:O	2.19	0.42
1:V:118:LYS:O	1:V:119:ASN:HB2	2.18	0.42
1:V:262:ILE:HD12	1:V:279:GLN:HB2	2.02	0.42
1:V:279:GLN:HE22	1:V:319:LEU:CA	2.32	0.42
1:V:344:ILE:O	1:V:344:ILE:CG2	2.67	0.42
1:W:393:ALA:C	1:W:395:ARG:N	2.78	0.42
1:A:32:ARG:C	1:A:34:ARG:N	2.76	0.42
1:B:16:HIS:C	1:B:17:ILE:HD12	2.45	0.42
1:B:394:ARG:HD3	1:B:394:ARG:HA	1.83	0.42
1:B:403:LEU:HD23	1:B:404:MET:CA	2.49	0.42
1:B:443:ILE:HG22	1:B:444:LEU:N	2.34	0.42
1:C:12:GLU:HG2	1:C:73:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:THR:C	1:C:295:HIS:H	2.26	0.42
1:D:25:ARG:O	1:D:26:ALA:C	2.63	0.42
1:D:27:VAL:HB	1:D:70:LEU:CD2	2.41	0.42
1:F:62:GLY:O	1:F:63:LYS:C	2.61	0.42
1:F:252:GLY:C	1:F:253:ILE:HD13	2.44	0.42
2:G:1:THR:CG2	2:G:33:LYS:NZ	2.82	0.42
2:H:60:PHE:HZ	2:H:71:LEU:HD22	1.84	0.42
2:L:78:LEU:HD12	2:L:78:LEU:C	2.44	0.42
2:L:79:ALA:O	2:L:80:LYS:C	2.63	0.42
2:M:7:ARG:NH2	2:M:102:GLU:O	2.53	0.42
2:M:164:ASN:ND2	2:M:164:ASN:N	2.56	0.42
2:R:92:GLU:O	2:R:93:ALA:HB2	2.20	0.42
1:T:36:ARG:HA	1:T:36:ARG:NE	2.33	0.42
1:V:21:ALA:C	1:V:23:ALA:H	2.27	0.42
1:V:66:ILE:O	1:V:66:ILE:HG22	2.20	0.42
1:V:300:THR:O	1:V:302:HIS:N	2.52	0.42
1:X:262:ILE:HD12	1:X:279:GLN:HB2	2.02	0.42
1:X:341:PHE:CB	1:X:378:ALA:HB1	2.49	0.42
1:X:345:LEU:HD13	1:X:396:LEU:HD22	2.01	0.42
1:X:375:LYS:C	1:X:377:ILE:H	2.27	0.42
1:A:337:SER:O	1:A:338:ALA:C	2.63	0.42
1:B:321:PRO:O	1:B:322:GLU:C	2.61	0.42
1:B:434:VAL:O	1:B:435:GLU:HB2	2.19	0.42
1:C:9:ILE:HD13	1:C:31:LEU:HD23	2.01	0.42
1:D:38:MET:HG3	1:D:45:ARG:HH12	1.83	0.42
1:E:62:GLY:O	1:E:63:LYS:C	2.62	0.42
1:E:283:LEU:CB	1:E:284:PRO:CD	2.98	0.42
1:E:440:SER:C	1:E:442:PHE:N	2.78	0.42
2:J:144:SER:CB	2:J:147:GLU:HG3	2.38	0.42
2:K:72:LEU:C	2:K:72:LEU:CD1	2.93	0.42
2:L:105:ILE:HG22	2:L:113:VAL:O	2.19	0.42
2:L:129:TYR:O	2:L:130:ALA:C	2.62	0.42
2:M:149:VAL:O	2:M:153:LEU:HG	2.19	0.42
2:O:4:VAL:HG12	2:O:153:LEU:CD2	2.50	0.42
2:Q:71:LEU:O	2:Q:73:LYS:N	2.52	0.42
1:U:28:ALA:O	1:U:30:ALA:N	2.52	0.42
1:U:48:VAL:O	1:U:48:VAL:HG22	2.20	0.42
1:W:368:ALA:HB3	1:W:420:ASN:HA	2.02	0.42
1:W:441:ARG:HB3	1:W:442:PHE:HD1	1.85	0.42
1:X:434:VAL:HG12	1:X:435:GLU:N	2.35	0.42
1:A:65:GLU:O	1:A:66:ILE:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:LEU:C	1:B:325:GLY:N	2.78	0.42
1:B:360:MET:CA	1:B:360:MET:CE	2.94	0.42
1:B:369:PHE:CE2	1:B:421:ILE:HD12	2.53	0.42
1:C:52:ASN:HB2	1:C:326:ARG:O	2.20	0.42
1:D:110:LEU:O	1:D:111:VAL:C	2.63	0.42
1:D:396:LEU:HD23	1:D:396:LEU:HA	1.83	0.42
1:E:37:ARG:NH1	1:E:38:MET:HE2	2.34	0.42
1:E:378:ALA:C	1:E:380:ALA:N	2.76	0.42
1:F:86:PHE:HB2	1:F:278:VAL:HG13	2.01	0.42
1:F:343:ARG:O	1:F:348:PRO:HD3	2.20	0.42
2:H:72:LEU:HD13	2:H:72:LEU:O	2.19	0.42
2:H:82:TRP:CD1	2:H:88:LEU:HB2	2.55	0.42
2:H:164:ASN:HD22	2:H:164:ASN:C	2.28	0.42
2:K:6:VAL:CG1	2:K:7:ARG:N	2.83	0.42
2:N:43:LEU:HD11	2:N:172:LEU:HG	2.01	0.42
2:O:13:VAL:HG12	2:O:169:ILE:HG22	2.02	0.42
2:O:42:VAL:HG21	2:O:64:LEU:CD1	2.50	0.42
2:P:127:GLY:C	2:P:129:TYR:N	2.78	0.42
2:P:153:LEU:HB3	2:P:167:PHE:CD2	2.55	0.42
1:S:359:LEU:HD11	1:X:48:VAL:CG2	2.49	0.42
1:T:51:LYS:HE2	1:U:356:TYR:OH	2.20	0.42
1:T:61:VAL:HG12	1:T:336:LEU:HG	2.02	0.42
1:T:64:THR:OG1	1:T:255:PHE:HE2	2.03	0.42
1:T:351:SER:O	1:T:355:GLN:HG3	2.20	0.42
1:U:120:ARG:NH2	1:U:235:ILE:H	2.18	0.42
1:U:341:PHE:CB	1:U:378:ALA:HB1	2.49	0.42
1:U:357:LYS:HA	1:U:367:ILE:CD1	2.31	0.42
1:V:17:ILE:CD1	1:V:65:GLU:HB3	2.49	0.42
1:A:71:ALA:HB1	1:A:78:PHE:HB2	2.00	0.42
1:B:343:ARG:C	1:B:345:LEU:H	2.28	0.42
1:B:370:THR:O	1:B:371:THR:C	2.63	0.42
1:B:435:GLU:CG	1:B:436:ASN:N	2.80	0.42
1:C:264:LYS:NZ	1:C:319:LEU:HA	2.35	0.42
1:C:383:ARG:O	1:C:387:LYS:HG2	2.20	0.42
1:D:249:GLU:HG2	1:D:299:LYS:H	1.85	0.42
1:D:257:ASP:O	1:D:258:GLU:C	2.63	0.42
1:D:323:LEU:O	1:D:325:GLY:N	2.53	0.42
1:D:357:LYS:HA	1:D:367:ILE:HG23	2.02	0.42
1:D:414:MET:HG2	1:D:414:MET:O	2.20	0.42
1:E:111:VAL:HG12	1:E:240:LEU:HD11	2.02	0.42
1:E:250:GLN:CA	1:E:250:GLN:HE21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ARG:NH2	1:F:251:ASN:HA	2.35	0.42
1:F:380:ALA:O	1:F:384:VAL:HG12	2.20	0.42
1:F:394:ARG:HD3	1:F:394:ARG:HA	1.86	0.42
2:H:96:ILE:HD11	2:H:123:ILE:HG23	2.01	0.42
2:H:137:LEU:O	2:H:141:THR:CG2	2.58	0.42
2:I:3:ILE:O	2:I:122:ALA:HA	2.20	0.42
2:M:153:LEU:HB3	2:M:167:PHE:CD2	2.55	0.42
2:N:5:SER:CB	2:N:14:VAL:HG22	2.45	0.42
2:N:75:ALA:O	2:N:78:LEU:HB3	2.19	0.42
2:N:83:ARG:HH21	2:N:111:ASP:HA	1.85	0.42
2:N:133:ALA:O	2:N:136:ALA:HB3	2.19	0.42
1:S:375:LYS:C	1:S:377:ILE:H	2.28	0.42
1:T:341:PHE:CB	1:T:378:ALA:HB1	2.50	0.42
1:T:407:ILE:HG23	1:T:408:SER:N	2.35	0.42
1:U:63:LYS:HB2	3:U:458:ATP:O2B	2.20	0.42
1:U:368:ALA:HB3	1:U:420:ASN:HA	2.01	0.42
1:V:53:ILE:HG12	1:V:329:ILE:HB	2.01	0.42
1:W:35:TRP:C	1:W:37:ARG:H	2.28	0.42
1:W:55:MET:HE2	1:W:306:ILE:HG21	2.01	0.42
1:A:80:LYS:C	1:A:81:VAL:HG13	2.43	0.41
1:B:341:PHE:O	1:B:342:GLU:C	2.63	0.41
1:B:359:LEU:HD12	1:C:36:ARG:CB	2.50	0.41
1:C:112:ARG:HG2	1:C:112:ARG:HH11	1.84	0.41
1:C:438:ASP:O	1:C:439:LEU:C	2.60	0.41
1:D:428:ASP:C	1:D:430:LEU:N	2.77	0.41
1:E:79:ILE:HD12	1:E:80:LYS:N	2.34	0.41
1:E:333:LEU:N	1:E:333:LEU:HD12	2.35	0.41
1:F:330:ARG:HG3	1:F:330:ARG:NH1	2.35	0.41
2:G:1:THR:CG2	2:G:33:LYS:HD3	2.49	0.41
2:G:30:ASN:ND2	2:L:116:GLU:HG2	2.35	0.41
2:G:136:ALA:HB1	2:M:137:LEU:HD13	2.01	0.41
2:I:71:LEU:C	2:I:71:LEU:HD13	2.45	0.41
2:I:91:LEU:H	2:I:91:LEU:CD2	2.30	0.41
2:J:133:ALA:HB1	2:J:155:ILE:HD12	2.01	0.41
2:L:7:ARG:CZ	2:L:12:VAL:CG2	2.98	0.41
2:L:144:SER:HB3	2:L:147:GLU:CG	2.43	0.41
2:O:13:VAL:HG21	2:O:146:HIS:HA	2.02	0.41
2:Q:96:ILE:O	2:Q:96:ILE:HG22	2.20	0.41
2:Q:127:GLY:C	2:Q:129:TYR:N	2.78	0.41
1:T:17:ILE:HD11	1:T:65:GLU:C	2.45	0.41
1:U:283:LEU:CD1	1:U:322:GLU:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:341:PHE:HB2	1:U:378:ALA:HB1	2.02	0.41
1:U:353:THR:HG22	1:U:369:PHE:HD1	1.84	0.41
1:V:356:TYR:CD1	1:V:404:MET:HG3	2.55	0.41
1:W:391:ILE:H	1:W:391:ILE:HG12	1.58	0.41
1:X:53:ILE:HG12	1:X:329:ILE:HB	2.01	0.41
1:X:300:THR:O	1:X:302:HIS:N	2.52	0.41
1:A:233:LYS:C	1:A:233:LYS:CD	2.93	0.41
1:A:395:ARG:HD3	1:A:395:ARG:HA	1.89	0.41
1:B:341:PHE:HA	1:B:344:ILE:CG1	2.50	0.41
1:C:21:ALA:O	1:C:22:ASP:C	2.63	0.41
1:C:69:ARG:O	1:C:70:LEU:C	2.63	0.41
1:C:421:ILE:HA	1:C:425:TYR:CD1	2.49	0.41
1:D:42:GLU:HB3	1:D:43:PRO:HD3	2.02	0.41
1:D:112:ARG:O	1:D:114:GLN:N	2.53	0.41
1:D:239:GLU:O	1:D:240:LEU:C	2.63	0.41
1:F:53:ILE:O	1:F:306:ILE:HA	2.20	0.41
2:G:83:ARG:HG2	2:G:83:ARG:NH1	2.35	0.41
2:L:19:GLN:HB2	2:L:164:ASN:CG	2.45	0.41
2:L:136:ALA:HB1	2:R:137:LEU:HD13	2.02	0.41
2:M:19:GLN:HB2	2:M:164:ASN:CG	2.45	0.41
2:N:7:ARG:NH2	2:N:102:GLU:O	2.52	0.41
2:O:13:VAL:HG13	2:O:171:GLU:HB3	2.02	0.41
2:Q:16:GLY:O	2:Q:167:PHE:CB	2.68	0.41
2:R:7:ARG:NH2	2:R:102:GLU:O	2.53	0.41
1:T:283:LEU:N	1:T:284:PRO:CD	2.83	0.41
1:T:368:ALA:O	1:T:421:ILE:HB	2.20	0.41
1:U:259:ILE:HG23	1:U:260:ASP:N	2.34	0.41
1:V:319:LEU:O	1:V:324:GLN:NE2	2.53	0.41
1:W:300:THR:O	1:W:302:HIS:N	2.53	0.41
1:W:336:LEU:HB2	1:W:341:PHE:CE1	2.55	0.41
1:B:232:ALA:H	1:B:234:LEU:HD21	1.83	0.41
1:B:270:GLY:C	1:B:272:ASP:H	2.28	0.41
1:B:428:ASP:O	1:B:431:GLY:N	2.51	0.41
1:C:36:ARG:O	1:C:39:GLN:CB	2.64	0.41
1:C:393:ALA:HB3	3:C:452:ATP:C8	2.55	0.41
1:D:256:ILE:O	1:D:256:ILE:HG22	2.20	0.41
1:D:264:LYS:HZ1	1:D:319:LEU:HA	1.85	0.41
1:E:76:ALA:HB1	1:E:251:ASN:O	2.20	0.41
1:E:311:PHE:CE1	1:E:316:PRO:HA	2.55	0.41
1:F:120:ARG:O	1:F:121:ALA:C	2.62	0.41
1:F:244:ALA:O	1:F:247:ALA:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:77:GLU:OE2	2:G:80:LYS:HD2	2.19	0.41
2:G:78:LEU:HG	2:G:82:TRP:HZ3	1.85	0.41
2:G:129:TYR:N	2:G:129:TYR:CD2	2.88	0.41
2:H:172:LEU:HA	2:H:173:PRO:HD2	1.98	0.41
2:K:83:ARG:HG2	2:L:55:THR:HB	2.02	0.41
2:L:140:ASN:C	2:L:141:THR:HG22	2.45	0.41
2:M:96:ILE:O	2:M:96:ILE:HG22	2.20	0.41
2:N:71:LEU:O	2:N:73:LYS:N	2.53	0.41
2:N:153:LEU:HB3	2:N:167:PHE:CE2	2.54	0.41
1:S:297:MET:HE2	1:T:105:ASP:HB3	2.02	0.41
1:T:117:ALA:O	1:T:121:ALA:N	2.53	0.41
1:V:64:THR:OG1	1:V:255:PHE:HE2	2.04	0.41
1:X:35:TRP:C	1:X:37:ARG:H	2.27	0.41
1:X:48:VAL:O	1:X:48:VAL:HG22	2.19	0.41
1:C:428:ASP:O	1:C:429:ALA:C	2.63	0.41
1:D:71:ALA:HB1	1:D:78:PHE:HB2	2.02	0.41
1:E:61:VAL:HA	1:E:336:LEU:HD22	2.02	0.41
1:E:351:SER:O	1:E:355:GLN:HG3	2.21	0.41
1:E:381:ALA:O	1:E:382:PHE:C	2.62	0.41
1:E:421:ILE:HA	1:E:425:TYR:CD1	2.45	0.41
1:E:428:ASP:O	1:E:430:LEU:N	2.54	0.41
1:F:414:MET:HG2	1:F:414:MET:O	2.20	0.41
2:I:172:LEU:HD23	2:I:172:LEU:HA	1.74	0.41
2:J:46:PHE:HB3	2:J:95:LEU:HD21	2.03	0.41
2:L:7:ARG:NH2	2:L:12:VAL:HG21	2.35	0.41
2:O:4:VAL:HA	2:O:121:LEU:O	2.20	0.41
2:Q:32:ARG:HH11	2:Q:32:ARG:HG3	1.86	0.41
2:Q:134:ALA:O	2:Q:137:LEU:N	2.54	0.41
1:S:9:ILE:O	1:S:13:LEU:HG	2.21	0.41
1:S:435:GLU:O	1:S:436:ASN:C	2.64	0.41
1:T:387:LYS:NZ	1:T:435:GLU:CD	2.78	0.41
1:U:79:ILE:O	1:U:79:ILE:HG23	2.20	0.41
1:X:393:ALA:CB	3:X:461:ATP:H1'	2.51	0.41
1:X:441:ARG:HB3	1:X:442:PHE:H	1.70	0.41
1:A:444:LEU:HD23	1:A:444:LEU:C	2.45	0.41
1:B:256:ILE:HD13	1:B:282:LEU:HD13	2.02	0.41
1:C:38:MET:HA	1:C:45:ARG:HH11	1.86	0.41
1:C:367:ILE:CD1	1:C:421:ILE:HD11	2.51	0.41
1:D:55:MET:CE	1:D:306:ILE:HG21	2.45	0.41
1:D:73:LEU:C	1:D:73:LEU:HD12	2.46	0.41
1:D:300:THR:HA	1:D:303:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:LEU:HD23	1:D:404:MET:CA	2.51	0.41
1:E:71:ALA:CB	1:E:78:PHE:HB2	2.51	0.41
1:E:344:ILE:HG23	3:E:454:ATP:C2	2.55	0.41
2:K:105:ILE:HG23	2:K:105:ILE:O	2.21	0.41
2:O:82:TRP:CE3	2:O:110:GLY:HA2	2.55	0.41
2:O:127:GLY:O	2:O:129:TYR:N	2.53	0.41
2:O:149:VAL:O	2:O:153:LEU:HG	2.21	0.41
2:Q:64:LEU:HD23	2:Q:64:LEU:HA	1.96	0.41
2:R:137:LEU:C	2:R:141:THR:HG22	2.45	0.41
2:R:157:GLY:HA2	2:R:163:THR:CG2	2.50	0.41
1:S:61:VAL:HG12	1:S:336:LEU:HG	2.02	0.41
1:S:108:MET:CE	1:S:244:ALA:HB1	2.51	0.41
1:S:279:GLN:HE22	1:S:319:LEU:CA	2.33	0.41
1:S:393:ALA:C	1:S:395:ARG:N	2.77	0.41
1:T:356:TYR:CD1	1:T:404:MET:HG3	2.56	0.41
1:U:54:LEU:HD11	1:U:327:LEU:HB3	2.02	0.41
1:U:343:ARG:C	1:U:345:LEU:H	2.29	0.41
1:W:66:ILE:O	1:W:66:ILE:HG22	2.20	0.41
1:W:407:ILE:HG23	1:W:408:SER:N	2.36	0.41
1:A:4:MET:HE2	1:A:4:MET:HB3	1.82	0.41
1:A:100:ILE:HG22	1:A:298:VAL:HG21	2.01	0.41
1:B:4:MET:CE	1:B:9:ILE:HA	2.51	0.41
1:B:44:LEU:C	1:B:46:HIS:N	2.76	0.41
1:C:406:LYS:O	1:C:407:ILE:C	2.63	0.41
1:E:105:ASP:O	1:E:108:MET:HB2	2.21	0.41
1:F:31:LEU:HD12	1:F:31:LEU:O	2.21	0.41
1:F:260:ASP:HB3	1:F:311:PHE:CD2	2.55	0.41
1:F:300:THR:HA	1:F:303:ILE:HG12	2.03	0.41
1:F:403:LEU:HB2	1:F:430:LEU:HD21	2.01	0.41
2:H:78:LEU:HD12	2:H:78:LEU:O	2.20	0.41
2:H:83:ARG:HD3	2:I:54:PHE:CB	2.49	0.41
2:I:44:ALA:HA	2:I:96:ILE:O	2.20	0.41
2:J:127:GLY:O	2:J:128:ASN:C	2.63	0.41
2:J:154:ARG:O	2:J:155:ILE:C	2.62	0.41
2:N:17:ASP:OD2	2:N:33:LYS:HE3	2.20	0.41
2:N:104:LEU:HD13	2:N:112:VAL:HG11	2.00	0.41
2:O:7:ARG:NH2	2:O:102:GLU:O	2.53	0.41
2:O:91:LEU:HB2	2:O:108:GLY:HA3	2.03	0.41
2:O:104:LEU:HD13	2:O:112:VAL:HG11	2.02	0.41
1:S:16:HIS:C	1:S:17:ILE:HG13	2.45	0.41
1:S:278:VAL:C	1:S:280:ARG:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:345:LEU:HD21	1:S:377:ILE:HG22	2.03	0.41
1:T:49:THR:HA	1:T:50:PRO:HD3	1.95	0.41
1:T:385:ASN:ND2	1:T:395:ARG:HE	2.14	0.41
1:U:369:PHE:HE2	1:U:421:ILE:CD1	2.22	0.41
1:W:414:MET:HE2	1:W:417:GLN:HE22	1.85	0.41
1:X:393:ALA:C	1:X:395:ARG:N	2.78	0.41
1:A:37:ARG:NH1	1:A:38:MET:HE2	2.35	0.41
1:A:73:LEU:HD12	1:A:73:LEU:O	2.20	0.41
1:A:331:VAL:O	1:A:331:VAL:HG13	2.21	0.41
1:A:356:TYR:O	1:A:357:LYS:C	2.63	0.41
1:A:407:ILE:O	1:A:411:ALA:CB	2.69	0.41
1:B:367:ILE:HD11	1:B:421:ILE:CD1	2.49	0.41
1:C:20:GLN:OE1	1:C:333:LEU:HB3	2.21	0.41
1:C:57:GLY:CA	1:C:63:LYS:HE3	2.47	0.41
1:C:253:ILE:HG23	1:C:304:LEU:HD23	2.01	0.41
1:D:32:ARG:NH1	1:D:35:TRP:CE3	2.89	0.41
1:D:98:SER:O	1:D:99:ILE:C	2.63	0.41
1:D:116:ILE:HD12	1:D:117:ALA:CA	2.50	0.41
1:D:408:SER:O	1:E:36:ARG:NH2	2.46	0.41
1:E:103:LEU:HD23	1:E:248:VAL:HG13	2.03	0.41
1:E:316:PRO:C	1:E:318:ASP:N	2.78	0.41
1:E:341:PHE:HA	1:E:344:ILE:CG1	2.51	0.41
1:F:32:ARG:C	1:F:34:ARG:N	2.77	0.41
2:G:2:THR:O	2:G:16:GLY:HA2	2.21	0.41
2:I:152:SER:O	2:I:153:LEU:C	2.63	0.41
2:K:72:LEU:HD13	2:K:72:LEU:O	2.19	0.41
2:L:7:ARG:NH2	2:L:102:GLU:O	2.53	0.41
2:M:13:VAL:HG12	2:M:169:ILE:HG22	2.02	0.41
2:M:78:LEU:O	2:M:81:ASP:HB2	2.21	0.41
2:N:51:ALA:C	2:N:53:ALA:N	2.78	0.41
2:N:52:ASP:HA	2:N:55:THR:OG1	2.21	0.41
2:O:8:ARG:HH22	2:O:143:LEU:H	1.67	0.41
1:U:331:VAL:HG13	1:U:331:VAL:O	2.21	0.41
1:U:356:TYR:CD1	1:U:404:MET:HG3	2.56	0.41
1:V:48:VAL:O	1:V:48:VAL:HG22	2.20	0.41
1:V:421:ILE:HG12	1:V:425:TYR:CE1	2.56	0.41
1:W:283:LEU:CD1	1:W:322:GLU:HB3	2.48	0.41
1:W:439:LEU:C	1:W:441:ARG:N	2.78	0.41
1:A:5:THR:HG23	1:A:8:GLU:CD	2.46	0.41
1:A:54:LEU:HG	1:A:56:ILE:HD12	2.02	0.41
1:A:100:ILE:CG2	1:A:298:VAL:HG21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ILE:HG22	1:A:237:PRO:N	2.36	0.41
1:A:326:ARG:HD2	1:F:394:ARG:NH2	2.35	0.41
1:A:360:MET:CA	1:A:360:MET:CE	2.94	0.41
1:A:410:SER:HB2	1:A:414:MET:HE3	2.02	0.41
1:B:25:ARG:O	1:B:28:ALA:HB3	2.21	0.41
1:B:34:ARG:NH2	1:B:253:ILE:HD13	2.36	0.41
1:B:357:LYS:HG2	1:B:367:ILE:HG23	2.02	0.41
1:B:407:ILE:O	1:B:411:ALA:CB	2.68	0.41
1:D:57:GLY:CA	1:D:63:LYS:HE3	2.50	0.41
1:D:384:VAL:O	1:D:387:LYS:N	2.53	0.41
1:E:52:ASN:HD22	1:E:305:PHE:HB2	1.80	0.41
1:F:17:ILE:HG12	1:F:66:ILE:CG1	2.51	0.41
2:H:44:ALA:HA	2:H:96:ILE:O	2.20	0.41
2:K:46:PHE:CD2	2:K:46:PHE:O	2.73	0.41
2:L:1:THR:HG23	2:L:33:LYS:CE	2.51	0.41
2:M:76:VAL:CG1	1:S:442:PHE:CE2	3.04	0.41
2:M:134:ALA:O	2:M:135:ARG:C	2.62	0.41
2:O:134:ALA:O	2:O:135:ARG:C	2.63	0.41
2:O:164:ASN:ND2	2:O:164:ASN:N	2.59	0.41
2:P:33:LYS:HA	2:P:46:PHE:CZ	2.55	0.41
1:T:437:GLU:CG	1:T:438:ASP:H	2.17	0.41
1:U:278:VAL:C	1:U:280:ARG:N	2.79	0.41
1:U:368:ALA:O	1:U:421:ILE:HB	2.21	0.41
1:V:18:ILE:CG2	1:V:344:ILE:HG13	2.50	0.41
1:V:265:LYS:H	1:V:269:SER:CB	2.34	0.41
1:V:353:THR:HG22	1:V:369:PHE:HD1	1.82	0.41
1:V:357:LYS:CA	1:V:367:ILE:HD11	2.34	0.41
1:W:368:ALA:O	1:W:421:ILE:HB	2.21	0.41
1:X:341:PHE:HB2	1:X:378:ALA:HB1	2.03	0.41
1:X:345:LEU:HD21	1:X:377:ILE:HG22	2.03	0.41
1:A:34:ARG:HH22	1:A:253:ILE:HD13	1.85	0.41
1:A:44:LEU:C	1:A:46:HIS:N	2.76	0.41
1:A:341:PHE:HA	1:A:344:ILE:HG12	2.02	0.41
1:A:360:MET:O	1:A:361:ALA:C	2.63	0.41
1:B:100:ILE:HG22	1:B:298:VAL:HG21	2.02	0.41
1:B:336:LEU:HA	1:B:336:LEU:HD12	1.65	0.41
1:B:337:SER:O	1:B:338:ALA:C	2.64	0.41
1:B:380:ALA:O	1:B:383:ARG:HB3	2.21	0.41
1:C:313:VAL:HG23	1:C:314:ALA:H	1.85	0.41
1:C:369:PHE:CE2	1:C:421:ILE:HD12	2.55	0.41
1:D:19:GLY:O	1:D:20:GLN:C	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:PHE:HD1	1:D:253:ILE:HB	1.85	0.41
1:D:100:ILE:HG13	1:D:300:THR:CG2	2.51	0.41
1:D:245:ILE:HG23	1:D:298:VAL:HG12	2.02	0.41
1:D:341:PHE:HA	1:D:344:ILE:HG12	2.02	0.41
1:D:343:ARG:C	1:D:345:LEU:N	2.73	0.41
1:E:104:THR:OG1	1:E:293:THR:HG21	2.20	0.41
1:E:282:LEU:O	1:E:285:LEU:HB2	2.21	0.41
1:E:336:LEU:HA	1:E:336:LEU:HD12	1.77	0.41
1:E:344:ILE:H	1:E:344:ILE:HG12	1.58	0.41
1:F:17:ILE:HB	1:F:24:LYS:HE3	2.02	0.41
1:F:235:ILE:O	1:F:236:ASN:HB3	2.21	0.41
2:G:164:ASN:HD22	2:G:164:ASN:H	1.69	0.41
2:I:161:VAL:HG13	2:N:24:ASN:O	2.21	0.41
2:J:7:ARG:HA	2:J:11:GLN:O	2.20	0.41
2:J:24:ASN:O	2:O:161:VAL:HG13	2.21	0.41
2:J:115:PRO:CB	2:J:119:GLN:HA	2.51	0.41
2:K:88:LEU:O	2:K:89:ARG:O	2.37	0.41
2:K:91:LEU:HD12	2:K:91:LEU:HA	1.82	0.41
2:K:98:ALA:CB	2:K:103:SER:HA	2.50	0.41
2:K:131:LEU:HD21	2:K:135:ARG:NH2	2.36	0.41
2:N:73:LYS:O	2:N:74:SER:C	2.63	0.41
2:N:92:GLU:O	2:N:93:ALA:HB2	2.20	0.41
2:N:96:ILE:O	2:N:96:ILE:HG22	2.20	0.41
2:N:137:LEU:C	2:N:141:THR:HG22	2.45	0.41
2:N:153:LEU:HB3	2:N:167:PHE:CD2	2.56	0.41
2:O:32:ARG:HH11	2:O:32:ARG:HG3	1.86	0.41
2:P:131:LEU:HD12	2:P:135:ARG:HG3	2.03	0.41
2:R:82:TRP:CE3	2:R:110:GLY:HA2	2.56	0.41
1:S:54:LEU:HD23	1:S:307:ALA:HB3	2.01	0.41
1:S:326:ARG:HA	1:S:326:ARG:HD2	1.96	0.41
1:S:387:LYS:NZ	1:S:435:GLU:CG	2.84	0.41
1:T:382:PHE:C	1:T:384:VAL:N	2.79	0.41
1:U:65:GLU:HG3	3:U:458:ATP:H2'	2.03	0.41
1:V:16:HIS:C	1:V:17:ILE:HG13	2.46	0.41
1:V:48:VAL:HA	1:W:355:GLN:OE1	2.21	0.41
1:V:54:LEU:HD23	1:V:307:ALA:HB3	2.03	0.41
1:V:259:ILE:HG23	1:V:260:ASP:N	2.36	0.41
1:V:343:ARG:C	1:V:345:LEU:N	2.78	0.41
1:V:343:ARG:C	1:V:345:LEU:H	2.28	0.41
1:V:373:ALA:CB	1:V:422:ASP:HA	2.50	0.41
1:V:407:ILE:HG23	1:V:408:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:331:VAL:HG13	1:W:331:VAL:O	2.20	0.41
1:X:15:GLN:O	1:X:348:PRO:HA	2.20	0.41
1:X:24:LYS:O	1:X:25:ARG:C	2.63	0.41
1:X:73:LEU:HD12	1:X:73:LEU:N	2.36	0.41
1:X:259:ILE:O	1:X:260:ASP:C	2.63	0.41
1:A:4:MET:CE	1:A:9:ILE:HA	2.51	0.41
1:B:37:ARG:C	1:B:39:GLN:N	2.77	0.41
1:B:105:ASP:O	1:B:108:MET:HB2	2.21	0.41
1:C:19:GLY:O	1:C:20:GLN:C	2.62	0.41
1:C:31:LEU:HD21	1:C:74:ALA:HB2	2.03	0.41
1:D:37:ARG:O	1:D:38:MET:CB	2.67	0.41
1:E:250:GLN:HA	1:E:250:GLN:HE21	1.86	0.41
1:E:443:ILE:HG22	1:E:444:LEU:N	2.35	0.41
2:G:24:ASN:O	2:R:161:VAL:HG22	2.21	0.41
2:H:6:VAL:CG1	2:H:7:ARG:N	2.84	0.41
2:H:155:ILE:O	2:H:159:ILE:HG13	2.21	0.41
2:I:1:THR:HG23	2:I:33:LYS:HD3	2.03	0.41
2:I:115:PRO:HG3	2:I:121:LEU:HD11	2.03	0.41
2:I:134:ALA:O	2:I:138:VAL:HG23	2.20	0.41
2:J:1:THR:HG22	2:J:2:THR:H	1.85	0.41
2:J:6:VAL:HG12	2:J:7:ARG:N	2.35	0.41
2:J:72:LEU:HD13	2:J:72:LEU:C	2.46	0.41
2:K:164:ASN:ND2	2:K:164:ASN:H	2.18	0.41
2:M:137:LEU:O	2:M:138:VAL:C	2.64	0.41
2:N:127:GLY:O	2:N:128:ASN:C	2.64	0.41
2:N:153:LEU:HD23	2:N:153:LEU:HA	1.90	0.41
2:P:20:VAL:CG2	1:W:444:LEU:HD21	2.51	0.41
2:Q:4:VAL:HG12	2:Q:153:LEU:CD2	2.50	0.41
2:Q:43:LEU:O	2:Q:97:VAL:HA	2.21	0.41
1:S:69:ARG:HG2	1:S:69:ARG:HH11	1.85	0.41
1:S:260:ASP:C	1:S:262:ILE:H	2.29	0.41
1:S:343:ARG:C	1:S:345:LEU:N	2.78	0.41
1:T:53:ILE:HG12	1:T:329:ILE:HB	2.02	0.41
1:T:233:LYS:C	1:T:235:ILE:HG12	2.46	0.41
1:T:265:LYS:H	1:T:269:SER:CB	2.33	0.41
1:W:369:PHE:HZ	1:W:404:MET:HE1	1.86	0.41
1:X:17:ILE:CD1	1:X:66:ILE:HG12	2.51	0.41
1:A:48:VAL:HA	1:F:355:GLN:OE1	2.21	0.40
1:B:416:GLY:O	1:B:417:GLN:O	2.39	0.40
1:D:111:VAL:HG21	1:D:244:ALA:N	2.36	0.40
1:E:362:THR:HG21	1:F:39:GLN:HG2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:67:HIS:C	2:H:69:GLY:N	2.79	0.40
2:I:72:LEU:O	2:I:73:LYS:C	2.64	0.40
2:J:99:ASP:HA	2:J:172:LEU:CD1	2.51	0.40
2:L:4:VAL:HG23	2:L:122:ALA:HB2	2.03	0.40
2:O:64:LEU:HD23	2:O:64:LEU:HA	1.94	0.40
1:S:17:ILE:HG23	3:S:456:ATP:HN61	1.85	0.40
1:T:421:ILE:HG12	1:T:425:TYR:CD1	2.56	0.40
1:U:17:ILE:HD11	1:U:65:GLU:C	2.46	0.40
1:W:283:LEU:HD21	1:W:322:GLU:HG2	2.02	0.40
1:X:13:LEU:C	1:X:15:GLN:H	2.29	0.40
1:X:20:GLN:O	1:X:21:ALA:CB	2.67	0.40
1:X:260:ASP:HB3	1:X:311:PHE:HD2	1.76	0.40
1:X:289:SER:H	1:X:300:THR:HG1	1.69	0.40
1:A:436:ASN:HB3	1:A:439:LEU:HD12	2.03	0.40
1:B:241:LYS:HD3	1:B:295:HIS:HA	2.03	0.40
1:B:353:THR:C	1:B:355:GLN:N	2.79	0.40
1:C:337:SER:O	1:C:338:ALA:C	2.63	0.40
1:C:339:ALA:O	1:C:342:GLU:HB2	2.22	0.40
1:C:407:ILE:CD1	1:C:419:VAL:HG11	2.51	0.40
1:D:54:LEU:HG	1:D:56:ILE:CD1	2.51	0.40
1:D:340:ASP:O	1:D:344:ILE:HD11	2.22	0.40
1:E:52:ASN:HD21	1:E:305:PHE:H	1.55	0.40
1:E:78:PHE:CD2	1:E:79:ILE:N	2.89	0.40
1:E:435:GLU:OE1	1:E:435:GLU:N	2.54	0.40
1:F:86:PHE:CE2	1:F:96:VAL:HA	2.56	0.40
1:F:321:PRO:HA	1:F:324:GLN:HB3	2.02	0.40
2:G:1:THR:HG23	2:G:33:LYS:HD3	2.03	0.40
2:H:82:TRP:CE2	2:H:108:GLY:O	2.74	0.40
2:J:42:VAL:HG21	2:J:64:LEU:HD13	2.02	0.40
2:J:52:ASP:O	2:J:53:ALA:C	2.62	0.40
2:J:172:LEU:HA	2:J:172:LEU:HD23	1.78	0.40
2:M:54:PHE:HA	2:M:57:PHE:HB3	2.03	0.40
2:P:115:PRO:HG3	2:P:121:LEU:HG	2.03	0.40
2:R:54:PHE:HA	2:R:57:PHE:HB3	2.04	0.40
1:S:441:ARG:HA	1:S:441:ARG:HD3	1.80	0.40
1:T:322:GLU:HG3	1:U:394:ARG:HH12	1.86	0.40
1:T:366:ASN:HD22	1:T:366:ASN:HA	1.63	0.40
1:U:262:ILE:HD12	1:U:279:GLN:HB2	2.03	0.40
1:U:414:MET:HE2	1:U:417:GLN:HE22	1.86	0.40
1:V:37:ARG:HG3	1:V:48:VAL:HG11	2.03	0.40
1:X:18:ILE:HG22	1:X:344:ILE:CG1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:361:ALA:C	1:X:363:GLU:N	2.78	0.40
1:A:262:ILE:HD13	1:A:262:ILE:HG21	1.85	0.40
1:B:439:LEU:O	1:B:440:SER:C	2.64	0.40
1:C:380:ALA:O	1:C:381:ALA:C	2.64	0.40
1:D:378:ALA:O	1:D:379:GLU:C	2.64	0.40
1:E:238:GLU:CD	1:E:238:GLU:H	2.27	0.40
1:E:250:GLN:NE2	1:E:250:GLN:CA	2.84	0.40
1:E:416:GLY:O	1:E:417:GLN:O	2.40	0.40
1:F:6:PRO:HD3	1:F:32:ARG:CD	2.51	0.40
1:F:241:LYS:C	1:F:243:LYS:N	2.77	0.40
2:H:17:ASP:CG	2:H:163:THR:HG23	2.45	0.40
2:H:67:HIS:CD2	2:H:73:LYS:HD3	2.56	0.40
2:J:60:PHE:HZ	2:J:71:LEU:HD22	1.87	0.40
2:M:47:ALA:HB3	2:M:123:ILE:HD12	2.04	0.40
2:M:75:ALA:O	2:M:78:LEU:HB3	2.21	0.40
2:M:112:VAL:O	1:S:444:LEU:HD13	2.22	0.40
2:N:37:LEU:HD23	1:U:441:ARG:NH2	2.36	0.40
2:P:78:LEU:O	2:P:81:ASP:HB2	2.20	0.40
2:P:91:LEU:HB2	2:P:108:GLY:HA3	2.04	0.40
2:Q:149:VAL:O	2:Q:153:LEU:HG	2.21	0.40
2:R:7:ARG:CZ	2:R:12:VAL:CG2	2.99	0.40
1:T:15:GLN:O	1:T:349:HIS:N	2.50	0.40
1:T:55:MET:HE2	1:T:306:ILE:HG21	2.02	0.40
1:U:265:LYS:H	1:U:269:SER:CB	2.33	0.40
1:U:283:LEU:HD21	1:U:322:GLU:HG2	2.04	0.40
1:V:36:ARG:HA	1:V:36:ARG:NE	2.32	0.40
1:V:370:THR:HG21	1:V:422:ASP:CB	2.51	0.40
1:W:343:ARG:C	1:W:345:LEU:N	2.77	0.40
1:X:36:ARG:HE	1:X:36:ARG:CA	2.30	0.40
1:A:381:ALA:O	1:A:382:PHE:C	2.63	0.40
1:A:421:ILE:HG23	1:A:425:TYR:HD1	1.80	0.40
1:B:71:ALA:CB	1:B:78:PHE:HB2	2.52	0.40
1:B:279:GLN:HB3	1:B:320:ILE:CD1	2.52	0.40
1:C:41:GLN:NE2	1:C:41:GLN:CA	2.82	0.40
1:C:115:GLU:C	1:C:117:ALA:N	2.80	0.40
1:C:300:THR:O	1:C:301:ASP:C	2.63	0.40
1:D:352:LEU:HD23	1:D:352:LEU:HA	1.74	0.40
1:D:394:ARG:O	1:D:396:LEU:N	2.55	0.40
1:D:439:LEU:CD2	2:J:72:LEU:HG	2.52	0.40
1:F:283:LEU:HD23	1:F:283:LEU:HA	1.88	0.40
2:M:98:ALA:CB	2:M:103:SER:HA	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:51:ALA:C	2:O:53:ALA:N	2.78	0.40
2:O:115:PRO:HG3	2:O:121:LEU:HG	2.03	0.40
2:Q:19:GLN:HB2	2:Q:164:ASN:CG	2.47	0.40
1:S:259:ILE:O	1:S:260:ASP:C	2.64	0.40
1:S:331:VAL:HG13	1:S:331:VAL:O	2.21	0.40
1:S:407:ILE:HG23	1:S:408:SER:N	2.36	0.40
1:T:279:GLN:O	1:T:320:ILE:HD11	2.21	0.40
1:T:315:ARG:HH22	1:U:436:ASN:ND2	2.19	0.40
1:U:259:ILE:O	1:U:260:ASP:C	2.63	0.40
1:U:322:GLU:HG3	1:V:394:ARG:HH12	1.87	0.40
1:U:407:ILE:HG23	1:U:408:SER:N	2.36	0.40
1:V:27:VAL:CG1	1:V:70:LEU:HD22	2.51	0.40
1:V:108:MET:SD	1:V:244:ALA:HB3	2.61	0.40
1:V:391:ILE:H	1:V:391:ILE:HG12	1.57	0.40
1:V:393:ALA:C	1:V:395:ARG:N	2.80	0.40
1:W:278:VAL:C	1:W:280:ARG:N	2.79	0.40
1:A:441:ARG:HG3	1:A:441:ARG:HH11	1.87	0.40
1:B:25:ARG:O	1:B:28:ALA:N	2.55	0.40
1:C:270:GLY:C	1:C:272:ASP:H	2.30	0.40
1:C:440:SER:O	1:C:441:ARG:C	2.65	0.40
1:D:36:ARG:C	1:D:37:ARG:O	2.61	0.40
1:D:323:LEU:C	1:D:325:GLY:H	2.29	0.40
1:D:380:ALA:O	1:D:383:ARG:HB3	2.22	0.40
1:E:5:THR:O	1:E:6:PRO:C	2.65	0.40
1:E:17:ILE:HG22	1:E:18:ILE:N	2.36	0.40
1:E:17:ILE:HG23	3:E:454:ATP:C6	2.57	0.40
1:E:100:ILE:CD1	1:E:300:THR:HG22	2.52	0.40
1:F:108:MET:HE1	1:F:240:LEU:HG	2.03	0.40
1:F:320:ILE:O	1:F:320:ILE:HG13	2.21	0.40
1:F:343:ARG:C	1:F:345:LEU:N	2.78	0.40
1:F:389:GLU:O	1:F:395:ARG:NH2	2.54	0.40
2:G:34:VAL:HG13	2:G:44:ALA:O	2.22	0.40
2:G:63:LYS:HE2	2:G:78:LEU:HA	2.03	0.40
2:G:79:ALA:C	2:G:81:ASP:N	2.77	0.40
2:H:18:GLY:N	2:H:164:ASN:HD21	2.06	0.40
2:H:95:LEU:HD23	2:H:95:LEU:HA	1.93	0.40
2:I:80:LYS:C	2:I:82:TRP:H	2.29	0.40
2:J:46:PHE:HB3	2:J:95:LEU:HD23	2.02	0.40
2:J:68:GLN:HE21	2:J:68:GLN:HB3	1.72	0.40
2:J:72:LEU:C	2:J:72:LEU:CD1	2.95	0.40
2:P:54:PHE:HA	2:P:57:PHE:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:78:LEU:O	2:Q:81:ASP:HB2	2.22	0.40
2:R:43:LEU:O	2:R:97:VAL:HA	2.22	0.40
2:R:73:LYS:O	2:R:74:SER:C	2.64	0.40
1:S:62:GLY:HA3	3:S:456:ATP:C8	2.57	0.40
1:T:79:ILE:CG2	1:T:103:LEU:HD13	2.49	0.40
1:U:64:THR:OG1	1:U:255:PHE:HE2	2.03	0.40
1:U:390:ASN:C	1:U:390:ASN:ND2	2.80	0.40
1:U:393:ALA:C	1:U:395:ARG:N	2.79	0.40
1:U:439:LEU:O	1:U:440:SER:C	2.64	0.40
1:V:83:ALA:HB1	1:V:262:ILE:HG21	2.02	0.40
1:V:259:ILE:O	1:V:260:ASP:C	2.64	0.40
1:V:345:LEU:HD21	1:V:377:ILE:CG2	2.51	0.40
1:W:32:ARG:O	1:W:36:ARG:HG2	2.22	0.40
1:X:237:PRO:C	1:X:239:GLU:H	2.29	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:7:ARG:NH2	1:X:7:ARG:NH2[2_765]	2.08	0.12

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	318/444 (72%)	244 (77%)	57 (18%)	17 (5%)	1	10
1	B	318/444 (72%)	241 (76%)	58 (18%)	19 (6%)	1	8
1	C	311/444 (70%)	234 (75%)	60 (19%)	17 (6%)	1	10
1	D	310/444 (70%)	235 (76%)	56 (18%)	19 (6%)	1	8
1	E	309/444 (70%)	238 (77%)	51 (16%)	20 (6%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	312/444 (70%)	240 (77%)	54 (17%)	18 (6%)	1	9
1	S	309/444 (70%)	227 (74%)	57 (18%)	25 (8%)	1	4
1	T	323/444 (73%)	236 (73%)	63 (20%)	24 (7%)	1	5
1	U	314/444 (71%)	237 (76%)	54 (17%)	23 (7%)	1	5
1	V	305/444 (69%)	228 (75%)	54 (18%)	23 (8%)	1	5
1	W	304/444 (68%)	223 (73%)	57 (19%)	24 (8%)	1	5
1	X	314/444 (71%)	235 (75%)	56 (18%)	23 (7%)	1	5
2	G	171/174 (98%)	141 (82%)	28 (16%)	2 (1%)	10	35
2	H	171/174 (98%)	139 (81%)	26 (15%)	6 (4%)	3	16
2	I	171/174 (98%)	136 (80%)	30 (18%)	5 (3%)	3	19
2	J	171/174 (98%)	136 (80%)	28 (16%)	7 (4%)	2	14
2	K	171/174 (98%)	138 (81%)	26 (15%)	7 (4%)	2	14
2	L	171/174 (98%)	137 (80%)	27 (16%)	7 (4%)	2	14
2	M	171/174 (98%)	128 (75%)	34 (20%)	9 (5%)	1	10
2	N	171/174 (98%)	129 (75%)	34 (20%)	8 (5%)	2	12
2	O	171/174 (98%)	130 (76%)	32 (19%)	9 (5%)	1	10
2	P	171/174 (98%)	128 (75%)	34 (20%)	9 (5%)	1	10
2	Q	171/174 (98%)	130 (76%)	32 (19%)	9 (5%)	1	10
2	R	171/174 (98%)	128 (75%)	33 (19%)	10 (6%)	1	9
All	All	5799/7416 (78%)	4418 (76%)	1041 (18%)	340 (6%)	1	9

All (340) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	235	ILE
1	A	417	GLN
1	A	436	ASN
1	A	438	ASP
1	A	441	ARG
1	B	52	ASN
1	B	231	ALA
1	B	417	GLN
1	B	438	ASP
1	B	440	SER

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Mol	Chain	Res	Type
1	B	441	ARG
1	C	52	ASN
1	C	417	GLN
1	C	436	ASN
1	C	438	ASP
1	C	440	SER
1	C	441	ARG
1	D	52	ASN
1	D	435	GLU
1	D	440	SER
1	D	441	ARG
1	E	52	ASN
1	E	417	GLN
1	E	432	GLU
1	E	433	VAL
1	E	436	ASN
1	E	438	ASP
1	E	441	ARG
1	F	417	GLN
1	F	436	ASN
1	F	438	ASP
1	F	441	ARG
2	H	86	ARG
2	H	89	ARG
2	I	87	ALA
2	I	90	LYS
2	J	87	ALA
2	J	88	LEU
2	J	119	GLN
2	K	92	GLU
2	L	87	ALA
2	L	90	LYS
2	M	119	GLN
2	N	50	THR
2	N	71	LEU
2	P	71	LEU
2	Q	50	THR
2	Q	119	GLN
2	R	71	LEU
1	S	21	ALA
1	S	41	GLN
1	S	48	VAL

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Mol	Chain	Res	Type
1	S	58	PRO
1	S	74	ALA
1	S	75	ASN
1	S	235	ILE
1	S	436	ASN
1	S	437	GLU
1	S	438	ASP
1	S	440	SER
1	T	21	ALA
1	T	41	GLN
1	T	58	PRO
1	T	74	ALA
1	T	75	ASN
1	T	235	ILE
1	T	436	ASN
1	T	440	SER
1	T	442	PHE
1	U	21	ALA
1	U	41	GLN
1	U	58	PRO
1	U	74	ALA
1	U	75	ASN
1	U	235	ILE
1	U	242	GLN
1	U	442	PHE
1	V	21	ALA
1	V	41	GLN
1	V	58	PRO
1	V	74	ALA
1	V	75	ASN
1	V	440	SER
1	V	442	PHE
1	W	21	ALA
1	W	41	GLN
1	W	58	PRO
1	W	74	ALA
1	W	75	ASN
1	W	442	PHE
1	X	21	ALA
1	X	58	PRO
1	X	74	ALA
1	X	75	ASN

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Mol	Chain	Res	Type
1	X	236	ASN
1	X	237	PRO
1	X	435	GLU
1	A	113	GLN
1	A	276	GLU
1	A	405	ASP
1	A	415	ASN
1	A	429	ALA
1	B	237	PRO
1	B	405	ASP
1	B	429	ALA
1	C	405	ASP
1	D	276	GLU
1	D	405	ASP
1	D	429	ALA
1	D	438	ASP
1	E	113	GLN
1	E	405	ASP
1	E	429	ALA
1	E	437	GLU
1	F	52	ASN
1	F	276	GLU
1	F	405	ASP
1	F	429	ALA
1	F	439	LEU
1	F	440	SER
2	J	89	ARG
2	K	86	ARG
2	L	86	ARG
2	M	17	ASP
2	M	50	THR
2	M	71	LEU
2	M	127	GLY
2	M	128	ASN
2	N	17	ASP
2	N	72	LEU
2	N	127	GLY
2	N	128	ASN
2	O	17	ASP
2	O	50	THR
2	O	71	LEU
2	O	72	LEU

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Mol	Chain	Res	Type
2	O	127	GLY
2	O	128	ASN
2	P	17	ASP
2	P	50	THR
2	P	72	LEU
2	P	127	GLY
2	P	128	ASN
2	Q	17	ASP
2	Q	71	LEU
2	Q	72	LEU
2	Q	127	GLY
2	Q	128	ASN
2	R	17	ASP
2	R	50	THR
2	R	72	LEU
2	R	127	GLY
2	R	128	ASN
1	S	301	ASP
1	T	48	VAL
1	T	301	ASP
1	U	48	VAL
1	U	301	ASP
1	U	440	SER
1	V	48	VAL
1	V	301	ASP
1	W	48	VAL
1	W	119	ASN
1	W	301	ASP
1	W	439	LEU
1	X	41	GLN
1	X	48	VAL
1	X	301	ASP
1	X	440	SER
1	A	112	ARG
1	A	317	SER
1	B	42	GLU
1	B	294	LYS
1	B	350	ALA
1	B	411	ALA
1	C	390	ASN
1	C	429	ALA
1	D	42	GLU

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Mol	Chain	Res	Type
1	D	240	LEU
1	D	317	SER
1	D	417	GLN
1	E	276	GLU
1	E	390	ASN
1	E	411	ALA
1	F	415	ASN
2	H	17	ASP
2	H	119	GLN
2	J	50	THR
2	K	81	ASP
2	K	89	ARG
2	M	72	LEU
2	M	117	GLU
2	N	117	GLU
2	O	117	GLU
2	P	117	GLU
2	R	117	GLU
1	S	43	PRO
1	S	44	LEU
1	S	258	GLU
1	S	439	LEU
1	T	14	ASP
1	T	43	PRO
1	T	44	LEU
1	T	233	LYS
1	T	258	GLU
1	T	394	ARG
1	U	43	PRO
1	U	44	LEU
1	U	258	GLU
1	V	43	PRO
1	V	44	LEU
1	V	435	GLU
1	V	439	LEU
1	W	43	PRO
1	W	44	LEU
1	W	258	GLU
1	W	440	SER
1	X	43	PRO
1	X	258	GLU
1	A	42	GLU

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Mol	Chain	Res	Type
1	B	324	GLN
1	B	415	ASN
1	D	113	GLN
1	D	415	ASN
1	E	237	PRO
1	E	294	LYS
1	E	317	SER
1	F	4	MET
1	F	42	GLU
1	F	240	LEU
2	G	92	GLU
2	H	50	THR
2	I	17	ASP
2	I	89	ARG
2	J	91	LEU
2	K	50	THR
2	K	116	GLU
2	L	17	ASP
2	Q	117	GLU
1	S	14	ASP
1	S	20	GLN
1	S	261	LYS
1	S	313	VAL
1	S	394	ARG
1	T	20	GLN
1	T	313	VAL
1	T	438	ASP
1	U	14	ASP
1	U	20	GLN
1	U	23	ALA
1	U	313	VAL
1	U	394	ARG
1	V	14	ASP
1	V	20	GLN
1	V	23	ALA
1	V	258	GLU
1	W	14	ASP
1	W	20	GLN
1	W	313	VAL
1	W	394	ARG
1	X	14	ASP
1	X	20	GLN

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Mol	Chain	Res	Type
1	X	23	ALA
1	X	44	LEU
1	X	313	VAL
1	X	394	ARG
1	A	6	PRO
1	B	317	SER
1	B	390	ASN
1	C	42	GLU
1	C	276	GLU
1	C	350	ALA
1	D	294	LYS
1	D	324	GLN
1	E	42	GLU
1	F	236	ASN
1	F	404	MET
2	H	71	LEU
2	I	50	THR
2	J	17	ASP
2	K	17	ASP
2	L	52	ASP
1	S	23	ALA
1	S	29	ILE
1	S	388	THR
1	T	23	ALA
1	T	388	THR
1	V	313	VAL
1	W	23	ALA
1	W	29	ILE
1	W	242	GLN
1	W	388	THR
1	A	440	SER
1	C	109	LYS
1	C	236	ASN
1	D	439	LEU
1	E	404	MET
2	G	9	ASN
2	L	9	ASN
2	L	50	THR
2	N	90	LYS
2	O	39	ASN
2	P	115	PRO
2	R	90	LYS

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Mol	Chain	Res	Type
1	T	29	ILE
1	U	237	PRO
1	U	388	THR
1	V	237	PRO
1	V	261	LYS
1	W	261	LYS
1	X	29	ILE
1	X	261	LYS
1	X	388	THR
1	B	6	PRO
1	D	262	ILE
1	E	6	PRO
1	F	262	ILE
2	Q	115	PRO
1	S	79	ILE
1	T	79	ILE
1	U	29	ILE
1	U	79	ILE
1	V	29	ILE
1	W	79	ILE
1	X	79	ILE
1	B	50	PRO
1	D	6	PRO
2	M	115	PRO
2	O	138	VAL
2	P	138	VAL
1	V	79	ILE
1	A	116	ILE
1	C	248	VAL
2	R	115	PRO
1	C	6	PRO
1	C	237	PRO
1	F	284	PRO
1	V	443	ILE
2	R	138	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/373 (74%)	244 (89%)	30 (11%)	6	22
1	B	274/373 (74%)	242 (88%)	32 (12%)	5	20
1	C	268/373 (72%)	231 (86%)	37 (14%)	3	14
1	D	267/373 (72%)	234 (88%)	33 (12%)	4	18
1	E	264/373 (71%)	232 (88%)	32 (12%)	5	18
1	F	269/373 (72%)	235 (87%)	34 (13%)	4	17
1	S	267/373 (72%)	250 (94%)	17 (6%)	16	41
1	T	276/373 (74%)	261 (95%)	15 (5%)	20	46
1	U	270/373 (72%)	254 (94%)	16 (6%)	18	43
1	V	263/373 (70%)	251 (95%)	12 (5%)	24	49
1	W	262/373 (70%)	249 (95%)	13 (5%)	22	48
1	X	270/373 (72%)	258 (96%)	12 (4%)	25	50
2	G	130/140 (93%)	117 (90%)	13 (10%)	7	25
2	H	130/140 (93%)	116 (89%)	14 (11%)	6	22
2	I	133/140 (95%)	122 (92%)	11 (8%)	10	34
2	J	130/140 (93%)	118 (91%)	12 (9%)	8	29
2	K	130/140 (93%)	119 (92%)	11 (8%)	10	32
2	L	133/140 (95%)	123 (92%)	10 (8%)	12	37
2	M	125/140 (89%)	118 (94%)	7 (6%)	19	45
2	N	125/140 (89%)	117 (94%)	8 (6%)	16	41
2	O	124/140 (89%)	117 (94%)	7 (6%)	19	45
2	P	124/140 (89%)	117 (94%)	7 (6%)	19	45
2	Q	125/140 (89%)	118 (94%)	7 (6%)	19	45
2	R	124/140 (89%)	117 (94%)	7 (6%)	19	45
All	All	4757/6156 (77%)	4360 (92%)	397 (8%)	10	34

All (397) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	6	PRO
1	A	20	GLN
1	A	34	ARG

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Mol	Chain	Res	Type
1	A	41	GLN
1	A	46	HIS
1	A	96	VAL
1	A	105	ASP
1	A	114	GLN
1	A	234	LEU
1	A	251	ASN
1	A	264	LYS
1	A	301	ASP
1	A	313	VAL
1	A	326	ARG
1	A	336	LEU
1	A	344	ILE
1	A	345	LEU
1	A	362	THR
1	A	370	THR
1	A	371	THR
1	A	379	GLU
1	A	382	PHE
1	A	384	VAL
1	A	398	THR
1	A	403	LEU
1	A	410	SER
1	A	421	ILE
1	A	428	ASP
1	A	444	LEU
1	B	5	THR
1	B	6	PRO
1	B	20	GLN
1	B	37	ARG
1	B	39	GLN
1	B	41	GLN
1	B	46	HIS
1	B	56	ILE
1	B	96	VAL
1	B	105	ASP
1	B	114	GLN
1	B	120	ARG
1	B	251	ASN
1	B	263	CYS
1	B	264	LYS
1	B	301	ASP

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Mol	Chain	Res	Type
1	B	313	VAL
1	B	326	ARG
1	B	336	LEU
1	B	344	ILE
1	B	345	LEU
1	B	359	LEU
1	B	362	THR
1	B	370	THR
1	B	379	GLU
1	B	382	PHE
1	B	384	VAL
1	B	398	THR
1	B	403	LEU
1	B	410	SER
1	B	421	ILE
1	B	440	SER
1	C	4	MET
1	C	5	THR
1	C	6	PRO
1	C	20	GLN
1	C	34	ARG
1	C	39	GLN
1	C	46	HIS
1	C	56	ILE
1	C	82	GLU
1	C	96	VAL
1	C	111	VAL
1	C	118	LYS
1	C	119	ASN
1	C	251	ASN
1	C	263	CYS
1	C	264	LYS
1	C	301	ASP
1	C	308	SER
1	C	312	GLN
1	C	313	VAL
1	C	326	ARG
1	C	336	LEU
1	C	337	SER
1	C	344	ILE
1	C	345	LEU
1	C	359	LEU

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Mol	Chain	Res	Type
1	C	362	THR
1	C	370	THR
1	C	379	GLU
1	C	382	PHE
1	C	384	VAL
1	C	398	THR
1	C	403	LEU
1	C	428	ASP
1	C	432	GLU
1	C	434	VAL
1	C	441	ARG
1	D	5	THR
1	D	6	PRO
1	D	17	ILE
1	D	20	GLN
1	D	25	ARG
1	D	39	GLN
1	D	41	GLN
1	D	46	HIS
1	D	82	GLU
1	D	96	VAL
1	D	105	ASP
1	D	108	MET
1	D	110	LEU
1	D	113	GLN
1	D	251	ASN
1	D	264	LYS
1	D	301	ASP
1	D	313	VAL
1	D	326	ARG
1	D	336	LEU
1	D	344	ILE
1	D	345	LEU
1	D	362	THR
1	D	379	GLU
1	D	382	PHE
1	D	384	VAL
1	D	398	THR
1	D	403	LEU
1	D	410	SER
1	D	421	ILE
1	D	432	GLU

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Mol	Chain	Res	Type
1	D	434	VAL
1	D	437	GLU
1	E	5	THR
1	E	6	PRO
1	E	20	GLN
1	E	34	ARG
1	E	41	GLN
1	E	46	HIS
1	E	96	VAL
1	E	105	ASP
1	E	251	ASN
1	E	263	CYS
1	E	264	LYS
1	E	291	VAL
1	E	301	ASP
1	E	313	VAL
1	E	326	ARG
1	E	336	LEU
1	E	337	SER
1	E	344	ILE
1	E	345	LEU
1	E	362	THR
1	E	379	GLU
1	E	382	PHE
1	E	384	VAL
1	E	398	THR
1	E	402	ARG
1	E	403	LEU
1	E	419	VAL
1	E	421	ILE
1	E	428	ASP
1	E	434	VAL
1	E	435	GLU
1	E	441	ARG
1	F	5	THR
1	F	17	ILE
1	F	20	GLN
1	F	34	ARG
1	F	39	GLN
1	F	46	HIS
1	F	82	GLU
1	F	96	VAL

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Mol	Chain	Res	Type
1	F	105	ASP
1	F	119	ASN
1	F	251	ASN
1	F	253	ILE
1	F	264	LYS
1	F	278	VAL
1	F	291	VAL
1	F	301	ASP
1	F	313	VAL
1	F	319	LEU
1	F	321	PRO
1	F	326	ARG
1	F	336	LEU
1	F	344	ILE
1	F	345	LEU
1	F	362	THR
1	F	370	THR
1	F	379	GLU
1	F	382	PHE
1	F	384	VAL
1	F	398	THR
1	F	403	LEU
1	F	421	ILE
1	F	433	VAL
1	F	437	GLU
1	F	440	SER
2	G	7	ARG
2	G	55	THR
2	G	56	LEU
2	G	68	GLN
2	G	72	LEU
2	G	84	THR
2	G	85	ASP
2	G	104	LEU
2	G	135	ARG
2	G	137	LEU
2	G	141	THR
2	G	164	ASN
2	G	168	THR
2	H	7	ARG
2	H	55	THR
2	H	56	LEU

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Mol	Chain	Res	Type
2	H	68	GLN
2	H	72	LEU
2	H	84	THR
2	H	85	ASP
2	H	88	LEU
2	H	91	LEU
2	H	104	LEU
2	H	135	ARG
2	H	141	THR
2	H	164	ASN
2	H	168	THR
2	I	55	THR
2	I	56	LEU
2	I	68	GLN
2	I	72	LEU
2	I	88	LEU
2	I	104	LEU
2	I	119	GLN
2	I	135	ARG
2	I	141	THR
2	I	164	ASN
2	I	168	THR
2	J	55	THR
2	J	56	LEU
2	J	68	GLN
2	J	72	LEU
2	J	85	ASP
2	J	91	LEU
2	J	104	LEU
2	J	119	GLN
2	J	135	ARG
2	J	141	THR
2	J	164	ASN
2	J	168	THR
2	K	55	THR
2	K	56	LEU
2	K	68	GLN
2	K	72	LEU
2	K	88	LEU
2	K	91	LEU
2	K	104	LEU
2	K	135	ARG

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Mol	Chain	Res	Type
2	K	141	THR
2	K	164	ASN
2	K	168	THR
2	L	55	THR
2	L	56	LEU
2	L	68	GLN
2	L	72	LEU
2	L	85	ASP
2	L	91	LEU
2	L	135	ARG
2	L	141	THR
2	L	164	ASN
2	L	168	THR
2	M	8	ARG
2	M	13	VAL
2	M	95	LEU
2	M	96	ILE
2	M	137	LEU
2	M	164	ASN
2	M	167	PHE
2	N	8	ARG
2	N	13	VAL
2	N	95	LEU
2	N	96	ILE
2	N	119	GLN
2	N	137	LEU
2	N	164	ASN
2	N	167	PHE
2	O	8	ARG
2	O	13	VAL
2	O	95	LEU
2	O	96	ILE
2	O	137	LEU
2	O	164	ASN
2	O	167	PHE
2	P	8	ARG
2	P	13	VAL
2	P	95	LEU
2	P	96	ILE
2	P	137	LEU
2	P	164	ASN
2	P	167	PHE

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Mol	Chain	Res	Type
2	Q	8	ARG
2	Q	13	VAL
2	Q	95	LEU
2	Q	96	ILE
2	Q	137	LEU
2	Q	164	ASN
2	Q	167	PHE
2	R	8	ARG
2	R	13	VAL
2	R	95	LEU
2	R	96	ILE
2	R	137	LEU
2	R	164	ASN
2	R	167	PHE
1	S	75	ASN
1	S	114	GLN
1	S	116	ILE
1	S	241	LYS
1	S	260	ASP
1	S	282	LEU
1	S	322	GLU
1	S	326	ARG
1	S	333	LEU
1	S	366	ASN
1	S	388	THR
1	S	391	ILE
1	S	430	LEU
1	S	439	LEU
1	S	441	ARG
1	S	442	PHE
1	S	444	LEU
1	T	75	ASN
1	T	120	ARG
1	T	125	ASP
1	T	246	ASP
1	T	260	ASP
1	T	282	LEU
1	T	322	GLU
1	T	326	ARG
1	T	333	LEU
1	T	366	ASN
1	T	388	THR

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Mol	Chain	Res	Type
1	T	391	ILE
1	T	430	LEU
1	T	439	LEU
1	T	442	PHE
1	U	75	ASN
1	U	119	ASN
1	U	120	ARG
1	U	260	ASP
1	U	282	LEU
1	U	322	GLU
1	U	326	ARG
1	U	333	LEU
1	U	366	ASN
1	U	388	THR
1	U	391	ILE
1	U	430	LEU
1	U	432	GLU
1	U	438	ASP
1	U	439	LEU
1	U	442	PHE
1	V	75	ASN
1	V	260	ASP
1	V	282	LEU
1	V	322	GLU
1	V	326	ARG
1	V	333	LEU
1	V	366	ASN
1	V	388	THR
1	V	391	ILE
1	V	430	LEU
1	V	432	GLU
1	V	442	PHE
1	W	75	ASN
1	W	246	ASP
1	W	260	ASP
1	W	282	LEU
1	W	322	GLU
1	W	326	ARG
1	W	333	LEU
1	W	366	ASN
1	W	388	THR
1	W	391	ILE

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Mol	Chain	Res	Type
1	W	430	LEU
1	W	436	ASN
1	W	442	PHE
1	X	75	ASN
1	X	114	GLN
1	X	260	ASP
1	X	282	LEU
1	X	322	GLU
1	X	326	ARG
1	X	333	LEU
1	X	366	ASN
1	X	388	THR
1	X	391	ILE
1	X	430	LEU
1	X	442	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (164) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	39	GLN
1	A	41	GLN
1	A	75	ASN
1	A	114	GLN
1	A	119	ASN
1	A	236	ASN
1	A	250	GLN
1	A	279	GLN
1	A	295	HIS
1	A	324	GLN
1	A	417	GLN
1	A	436	ASN
1	B	15	GLN
1	B	16	HIS
1	B	20	GLN
1	B	39	GLN
1	B	41	GLN
1	B	236	ASN
1	B	250	GLN
1	B	279	GLN
1	B	324	GLN
1	B	397	HIS

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Mol	Chain	Res	Type
1	B	417	GLN
1	B	436	ASN
1	C	15	GLN
1	C	20	GLN
1	C	39	GLN
1	C	41	GLN
1	C	52	ASN
1	C	75	ASN
1	C	119	ASN
1	C	250	GLN
1	C	279	GLN
1	C	295	HIS
1	C	324	GLN
1	C	349	HIS
1	C	397	HIS
1	C	417	GLN
1	D	16	HIS
1	D	39	GLN
1	D	41	GLN
1	D	114	GLN
1	D	250	GLN
1	D	279	GLN
1	D	295	HIS
1	D	324	GLN
1	D	397	HIS
1	D	417	GLN
1	D	436	ASN
1	E	20	GLN
1	E	39	GLN
1	E	41	GLN
1	E	52	ASN
1	E	75	ASN
1	E	114	GLN
1	E	236	ASN
1	E	250	GLN
1	E	279	GLN
1	E	324	GLN
1	E	397	HIS
1	E	417	GLN
1	F	20	GLN
1	F	39	GLN
1	F	41	GLN

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Mol	Chain	Res	Type
1	F	114	GLN
1	F	250	GLN
1	F	279	GLN
1	F	295	HIS
1	F	324	GLN
1	F	397	HIS
1	F	417	GLN
2	G	24	ASN
2	G	164	ASN
2	H	24	ASN
2	H	67	HIS
2	H	140	ASN
2	H	164	ASN
2	H	166	ASN
2	I	24	ASN
2	I	30	ASN
2	I	67	HIS
2	I	70	HIS
2	I	164	ASN
2	J	24	ASN
2	J	67	HIS
2	J	164	ASN
2	K	24	ASN
2	K	119	GLN
2	K	164	ASN
2	L	24	ASN
2	L	164	ASN
2	M	164	ASN
2	N	24	ASN
2	N	119	GLN
2	N	164	ASN
2	O	114	GLN
2	O	164	ASN
2	P	164	ASN
2	Q	164	ASN
2	R	68	GLN
2	R	164	ASN
1	S	41	GLN
1	S	75	ASN
1	S	236	ASN
1	S	251	ASN
1	S	279	GLN

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Mol	Chain	Res	Type
1	S	312	GLN
1	S	366	ASN
1	S	385	ASN
1	S	390	ASN
1	S	397	HIS
1	S	417	GLN
1	S	436	ASN
1	T	41	GLN
1	T	75	ASN
1	T	119	ASN
1	T	279	GLN
1	T	324	GLN
1	T	366	ASN
1	T	385	ASN
1	T	390	ASN
1	T	417	GLN
1	T	436	ASN
1	U	41	GLN
1	U	119	ASN
1	U	279	GLN
1	U	302	HIS
1	U	324	GLN
1	U	366	ASN
1	U	385	ASN
1	U	390	ASN
1	U	417	GLN
1	U	436	ASN
1	V	41	GLN
1	V	75	ASN
1	V	119	ASN
1	V	236	ASN
1	V	251	ASN
1	V	279	GLN
1	V	366	ASN
1	V	385	ASN
1	V	390	ASN
1	V	417	GLN
1	W	41	GLN
1	W	75	ASN
1	W	113	GLN
1	W	114	GLN
1	W	119	ASN

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Mol	Chain	Res	Type
1	W	279	GLN
1	W	324	GLN
1	W	366	ASN
1	W	385	ASN
1	W	390	ASN
1	W	417	GLN
1	X	41	GLN
1	X	75	ASN
1	X	119	ASN
1	X	251	ASN
1	X	279	GLN
1	X	366	ASN
1	X	385	ASN
1	X	390	ASN
1	X	417	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	C	452	-	32,33,33	1.02	1 (3%)	48,52,52	0.89	2 (4%)
3	ATP	W	460	-	32,33,33	0.69	1 (3%)	48,52,52	0.74	1 (2%)
3	ATP	D	453	-	32,33,33	0.91	1 (3%)	48,52,52	0.93	1 (2%)
3	ATP	A	450	-	32,33,33	0.74	1 (3%)	48,52,52	0.91	3 (6%)
3	ATP	E	454	-	32,33,33	1.05	3 (9%)	48,52,52	0.91	3 (6%)
3	ATP	U	458	-	32,33,33	0.82	3 (9%)	48,52,52	0.73	1 (2%)
3	ATP	F	455	-	32,33,33	0.87	1 (3%)	48,52,52	0.91	2 (4%)
3	ATP	S	456	-	32,33,33	0.77	1 (3%)	48,52,52	0.74	1 (2%)
3	ATP	B	451	-	32,33,33	0.83	1 (3%)	48,52,52	0.81	2 (4%)
3	ATP	X	461	-	32,33,33	0.55	0	48,52,52	0.74	1 (2%)
3	ATP	V	459	-	32,33,33	0.74	1 (3%)	48,52,52	0.72	1 (2%)
3	ATP	T	457	-	32,33,33	0.72	1 (3%)	48,52,52	0.72	1 (2%)

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	ATP	C	452	-	-	4/22/38/38	0/3/3/3
3	ATP	W	460	-	-	4/22/38/38	0/3/3/3
3	ATP	D	453	-	-	3/22/38/38	0/3/3/3
3	ATP	A	450	-	-	2/22/38/38	0/3/3/3
3	ATP	E	454	-	-	4/22/38/38	0/3/3/3
3	ATP	U	458	-	-	4/22/38/38	0/3/3/3
3	ATP	F	455	-	-	4/22/38/38	0/3/3/3
3	ATP	S	456	-	-	6/22/38/38	0/3/3/3
3	ATP	B	451	-	-	0/22/38/38	0/3/3/3
3	ATP	X	461	-	-	6/22/38/38	0/3/3/3
3	ATP	V	459	-	-	3/22/38/38	0/3/3/3
3	ATP	T	457	-	-	4/22/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	452	ATP	PB-O3B	5.21	1.65	1.59
3	D	453	ATP	PB-O3B	4.25	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	454	ATP	PB-O3B	4.19	1.64	1.59
3	B	451	ATP	PB-O3B	3.71	1.63	1.59
3	F	455	ATP	PB-O3B	3.35	1.63	1.59
3	S	456	ATP	PB-O3B	3.27	1.63	1.59
3	V	459	ATP	PB-O3B	2.90	1.62	1.59
3	U	458	ATP	PB-O3B	2.73	1.62	1.59
3	W	460	ATP	PB-O3B	2.62	1.62	1.59
3	T	457	ATP	PB-O3B	2.54	1.62	1.59
3	U	458	ATP	PB-O3A	2.32	1.62	1.59
3	A	450	ATP	PB-O3B	2.31	1.62	1.59
3	U	458	ATP	PA-O3A	2.20	1.61	1.59
3	E	454	ATP	PB-O3A	2.19	1.61	1.59
3	E	454	ATP	PA-O3A	2.02	1.61	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	453	ATP	O2A-PA-O3A	-2.76	99.82	107.27
3	E	454	ATP	C2'-C1'-N9	-2.52	107.05	113.30
3	E	454	ATP	O3B-PG-O1G	-2.42	98.29	111.04
3	F	455	ATP	O3G-PG-O2G	2.34	116.56	107.80
3	W	460	ATP	O3G-PG-O2G	2.33	116.53	107.80
3	X	461	ATP	O3G-PG-O2G	2.32	116.51	107.80
3	U	458	ATP	O3G-PG-O2G	2.31	116.45	107.80
3	F	455	ATP	O3B-PG-O1G	-2.30	98.92	111.04
3	T	457	ATP	O3G-PG-O2G	2.29	116.38	107.80
3	S	456	ATP	O3G-PG-O2G	2.28	116.36	107.80
3	C	452	ATP	O3A-PA-O1A	-2.27	103.87	110.70
3	V	459	ATP	O3G-PG-O2G	2.26	116.29	107.80
3	B	451	ATP	O3G-PG-O2G	2.22	116.13	107.80
3	C	452	ATP	O3G-PG-O2G	2.18	115.96	107.80
3	E	454	ATP	O3G-PG-O2G	2.17	115.92	107.80
3	B	451	ATP	O3B-PG-O1G	-2.12	99.89	111.04
3	A	450	ATP	O3B-PG-O1G	-2.07	100.14	111.04
3	A	450	ATP	O3G-PG-O2G	2.05	115.50	107.80
3	A	450	ATP	O2A-PA-O3A	2.03	112.77	107.27

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	453	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	D	453	ATP	C5'-O5'-PA-O2A
3	D	453	ATP	C5'-O5'-PA-O3A
3	F	455	ATP	C5'-O5'-PA-O1A
3	F	455	ATP	C5'-O5'-PA-O2A
3	F	455	ATP	C5'-O5'-PA-O3A
3	T	457	ATP	O4'-C4'-C5'-O5'
3	U	458	ATP	C5'-O5'-PA-O1A
3	V	459	ATP	C5'-O5'-PA-O1A
3	W	460	ATP	C5'-O5'-PA-O1A
3	T	457	ATP	C3'-C4'-C5'-O5'
3	U	458	ATP	O4'-C4'-C5'-O5'
3	U	458	ATP	C3'-C4'-C5'-O5'
3	X	461	ATP	O4'-C4'-C5'-O5'
3	U	458	ATP	C4'-C5'-O5'-PA
3	X	461	ATP	C3'-C4'-C5'-O5'
3	S	456	ATP	O4'-C4'-C5'-O5'
3	S	456	ATP	C3'-C4'-C5'-O5'
3	W	460	ATP	C3'-C4'-C5'-O5'
3	W	460	ATP	O4'-C4'-C5'-O5'
3	V	459	ATP	C3'-C4'-C5'-O5'
3	A	450	ATP	PA-O3A-PB-O1B
3	C	452	ATP	PA-O3A-PB-O1B
3	E	454	ATP	PB-O3B-PG-O1G
3	V	459	ATP	O4'-C4'-C5'-O5'
3	X	461	ATP	PG-O3B-PB-O2B
3	S	456	ATP	C4'-C5'-O5'-PA
3	C	452	ATP	C5'-O5'-PA-O3A
3	S	456	ATP	C5'-O5'-PA-O1A
3	X	461	ATP	C5'-O5'-PA-O1A
3	W	460	ATP	C4'-C5'-O5'-PA
3	E	454	ATP	PA-O3A-PB-O2B
3	X	461	ATP	C4'-C5'-O5'-PA
3	C	452	ATP	PA-O3A-PB-O2B
3	S	456	ATP	PA-O3A-PB-O1B
3	T	457	ATP	PG-O3B-PB-O2B
3	X	461	ATP	PG-O3B-PB-O1B
3	E	454	ATP	PB-O3B-PG-O2G
3	E	454	ATP	PB-O3B-PG-O3G
3	A	450	ATP	PA-O3A-PB-O2B
3	F	455	ATP	PB-O3A-PA-O2A
3	C	452	ATP	PG-O3B-PB-O1B
3	S	456	ATP	PG-O3B-PB-O1B

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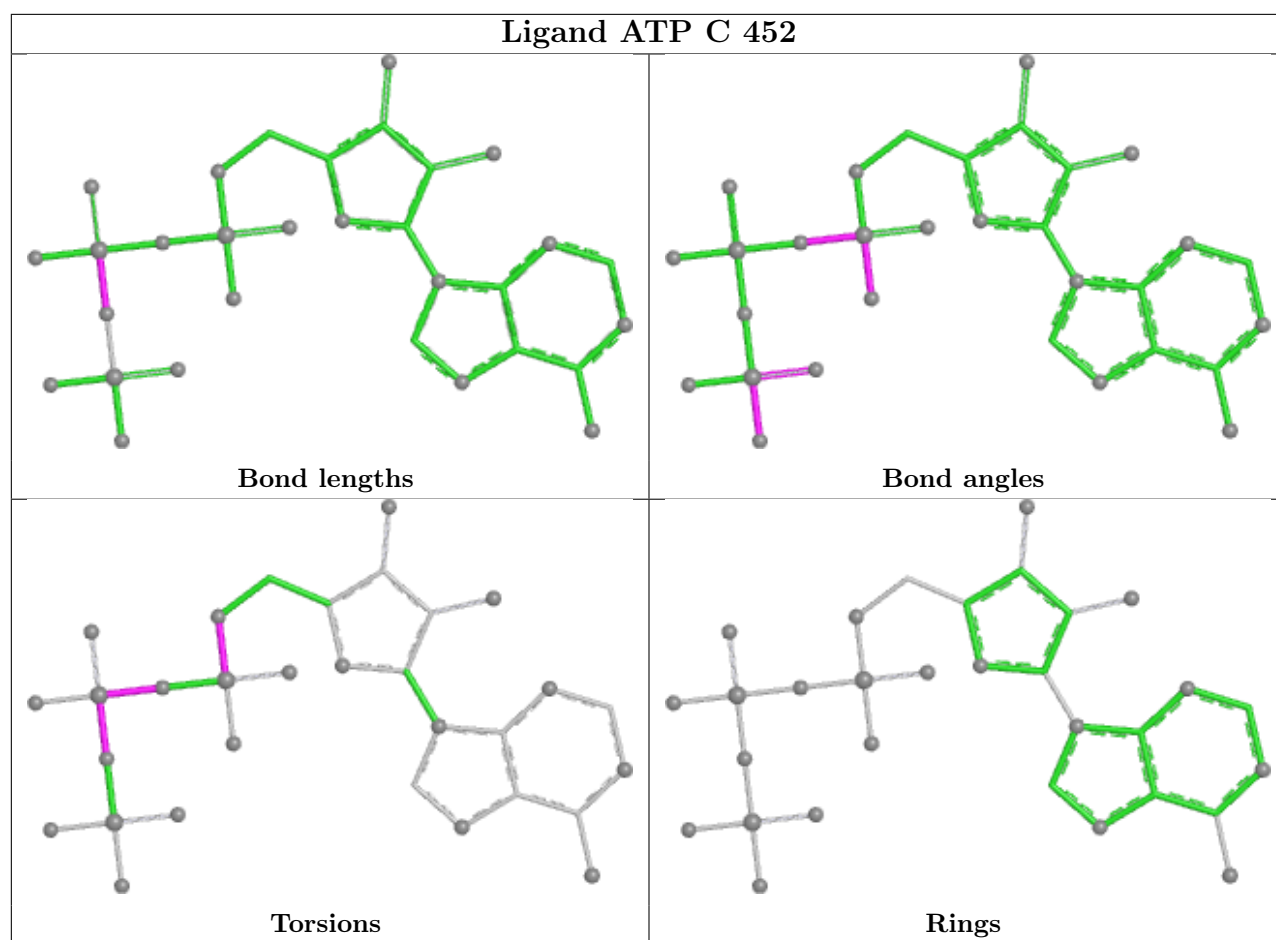
Mol	Chain	Res	Type	Atoms
3	T	457	ATP	PG-O3B-PB-O1B

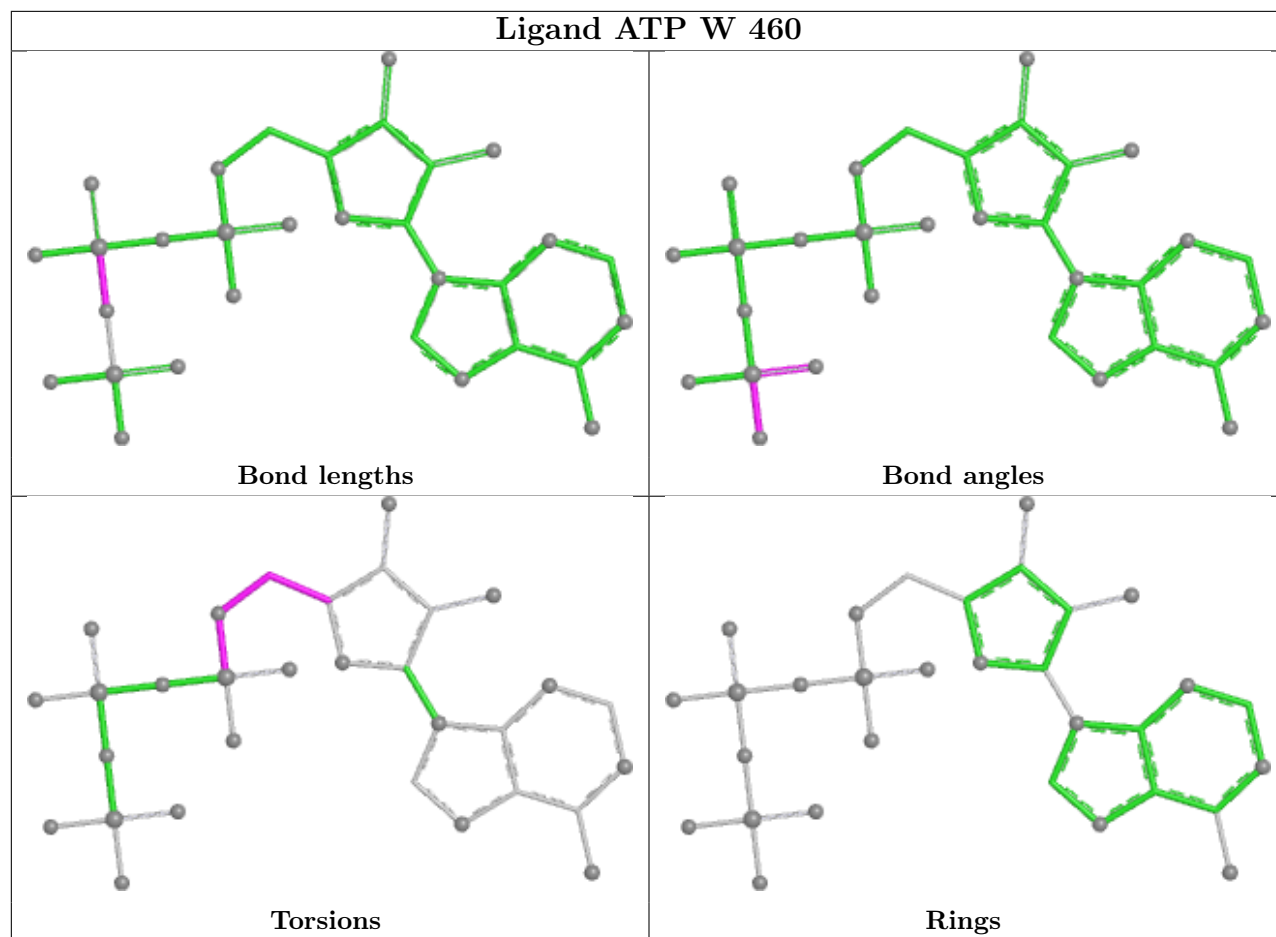
There are no ring outliers.

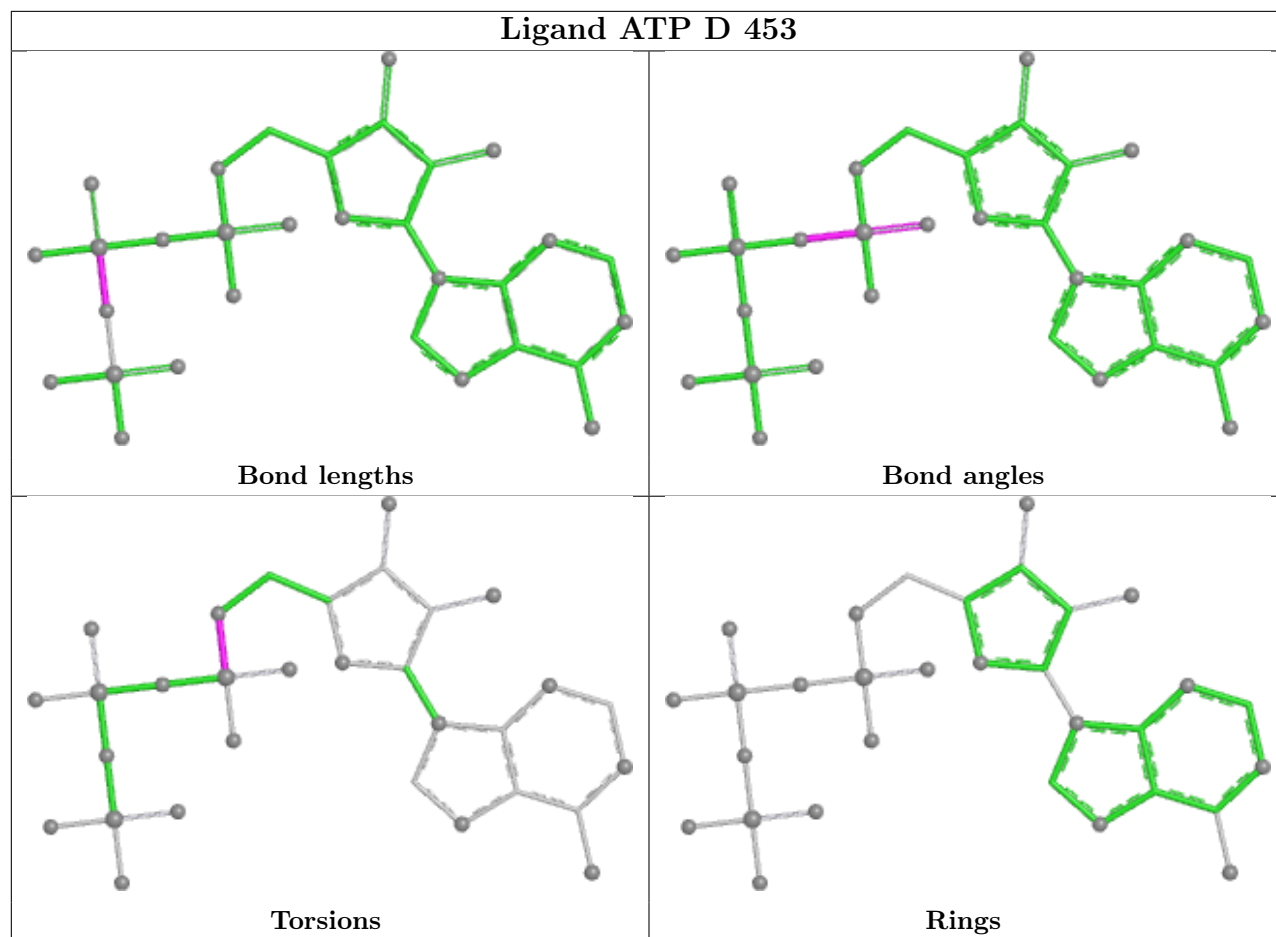
12 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	452	ATP	5	0
3	W	460	ATP	8	0
3	D	453	ATP	4	0
3	A	450	ATP	2	0
3	E	454	ATP	9	0
3	U	458	ATP	12	0
3	F	455	ATP	8	0
3	S	456	ATP	14	0
3	B	451	ATP	5	0
3	X	461	ATP	9	0
3	V	459	ATP	3	0
3	T	457	ATP	3	0

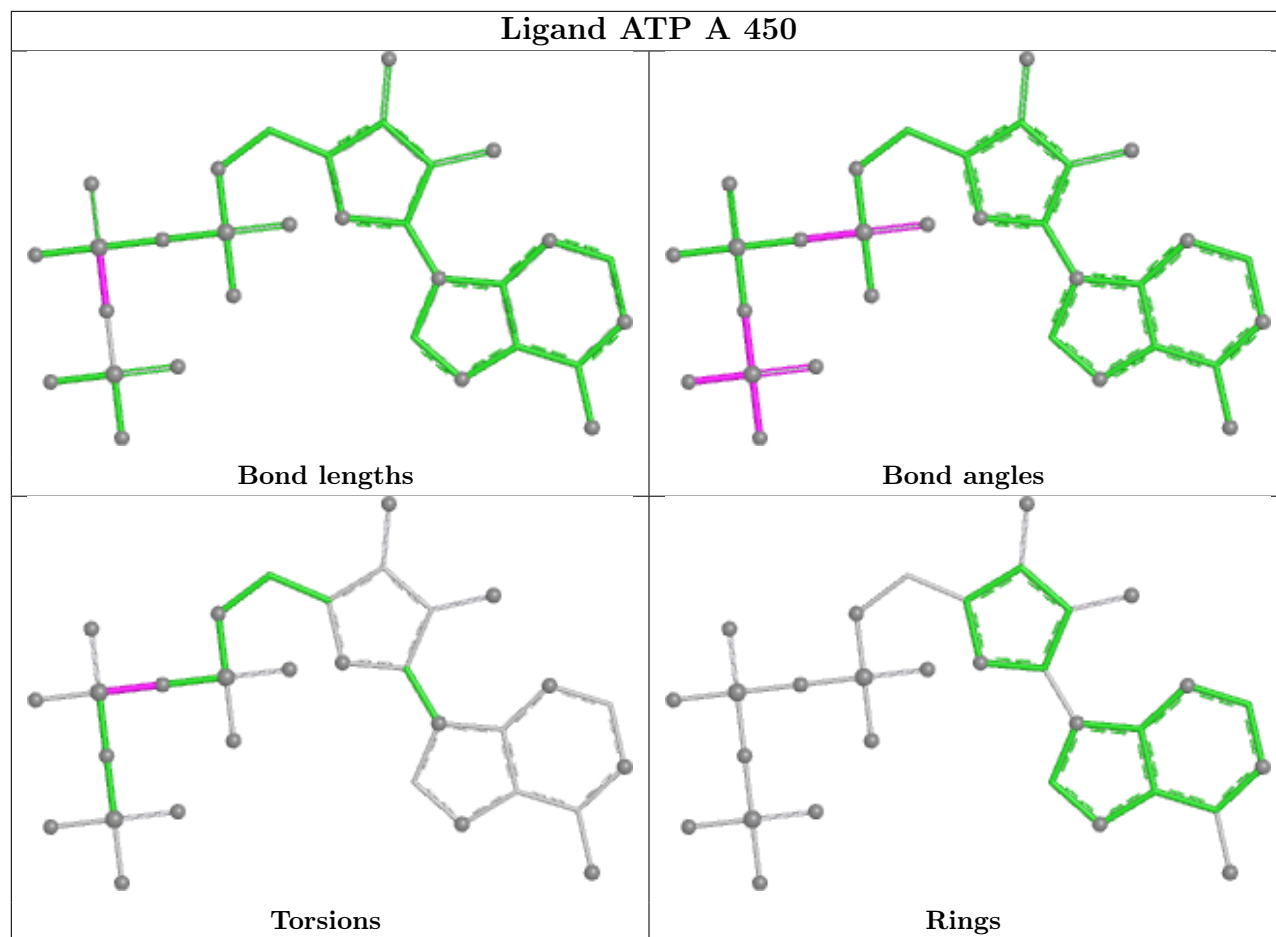
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



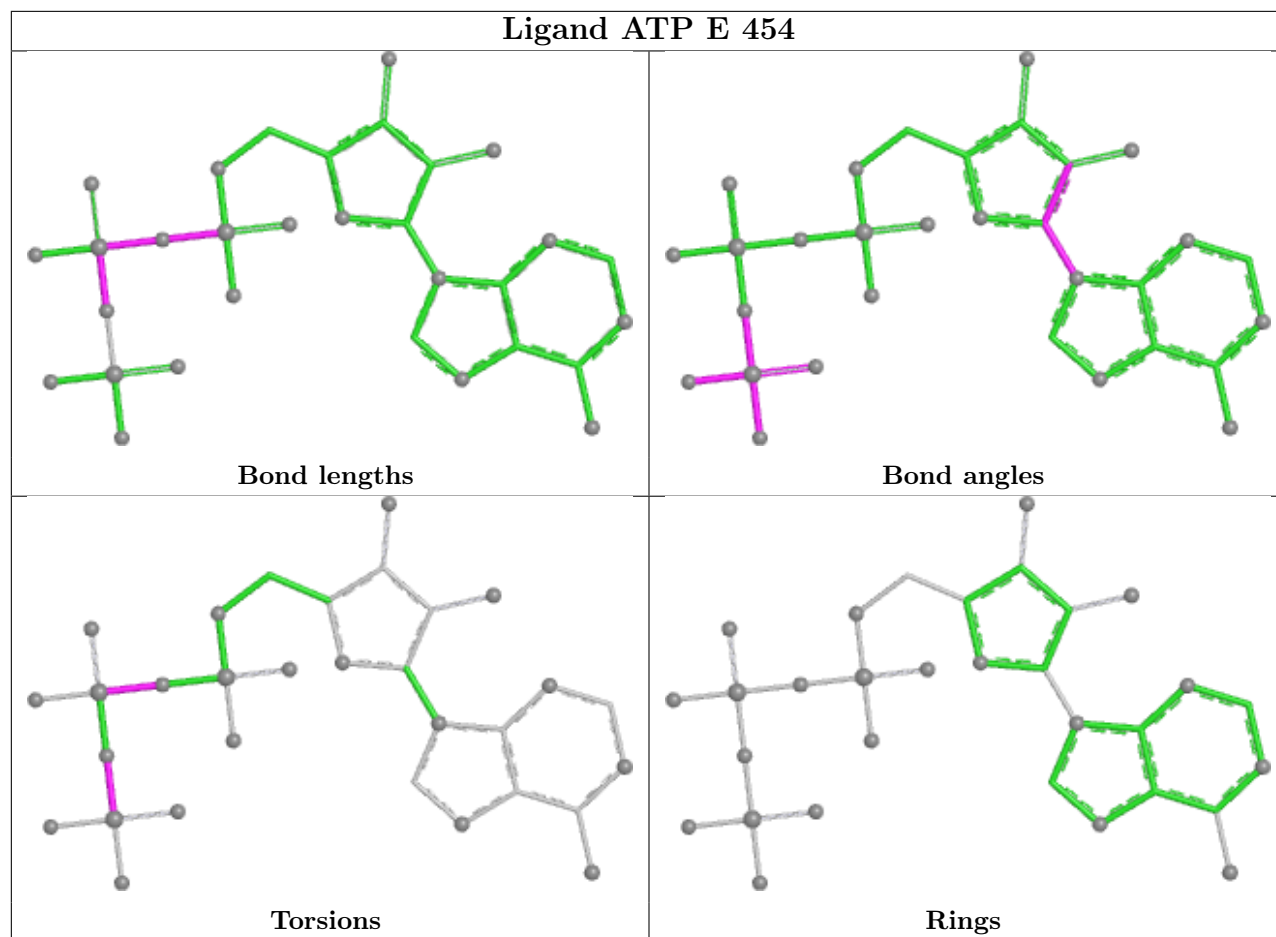




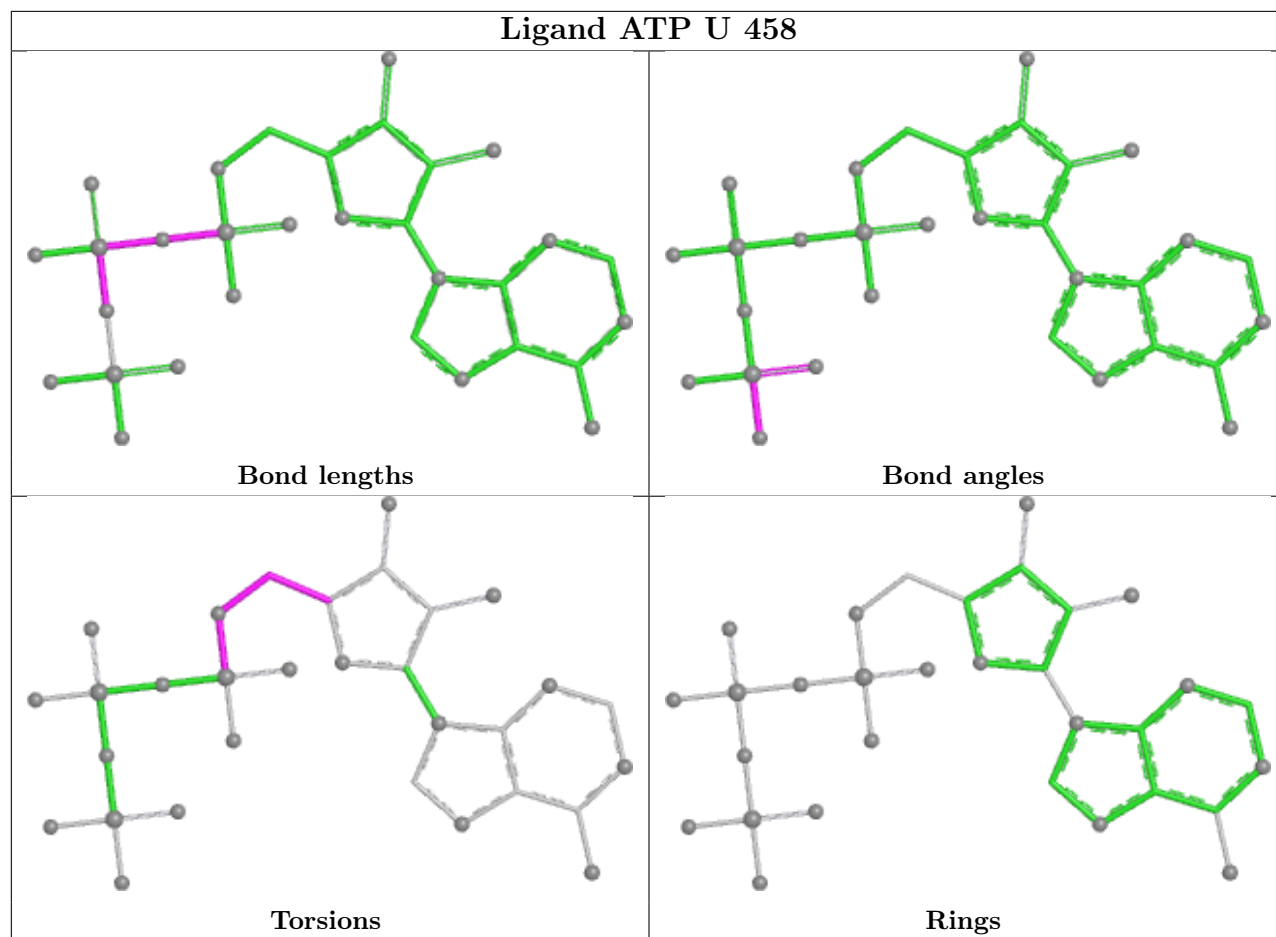
Ligand ATP A 450



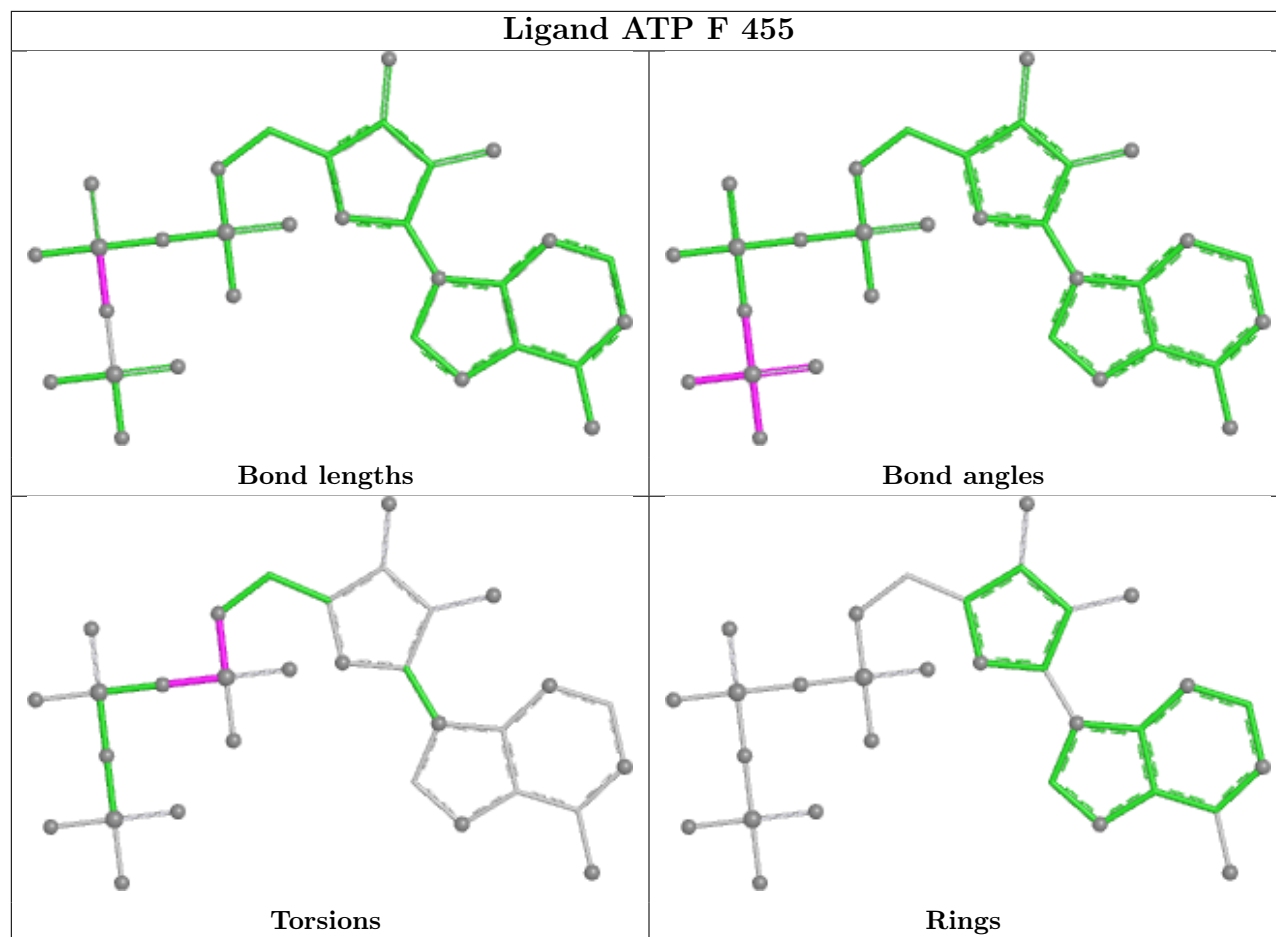
Ligand ATP E 454



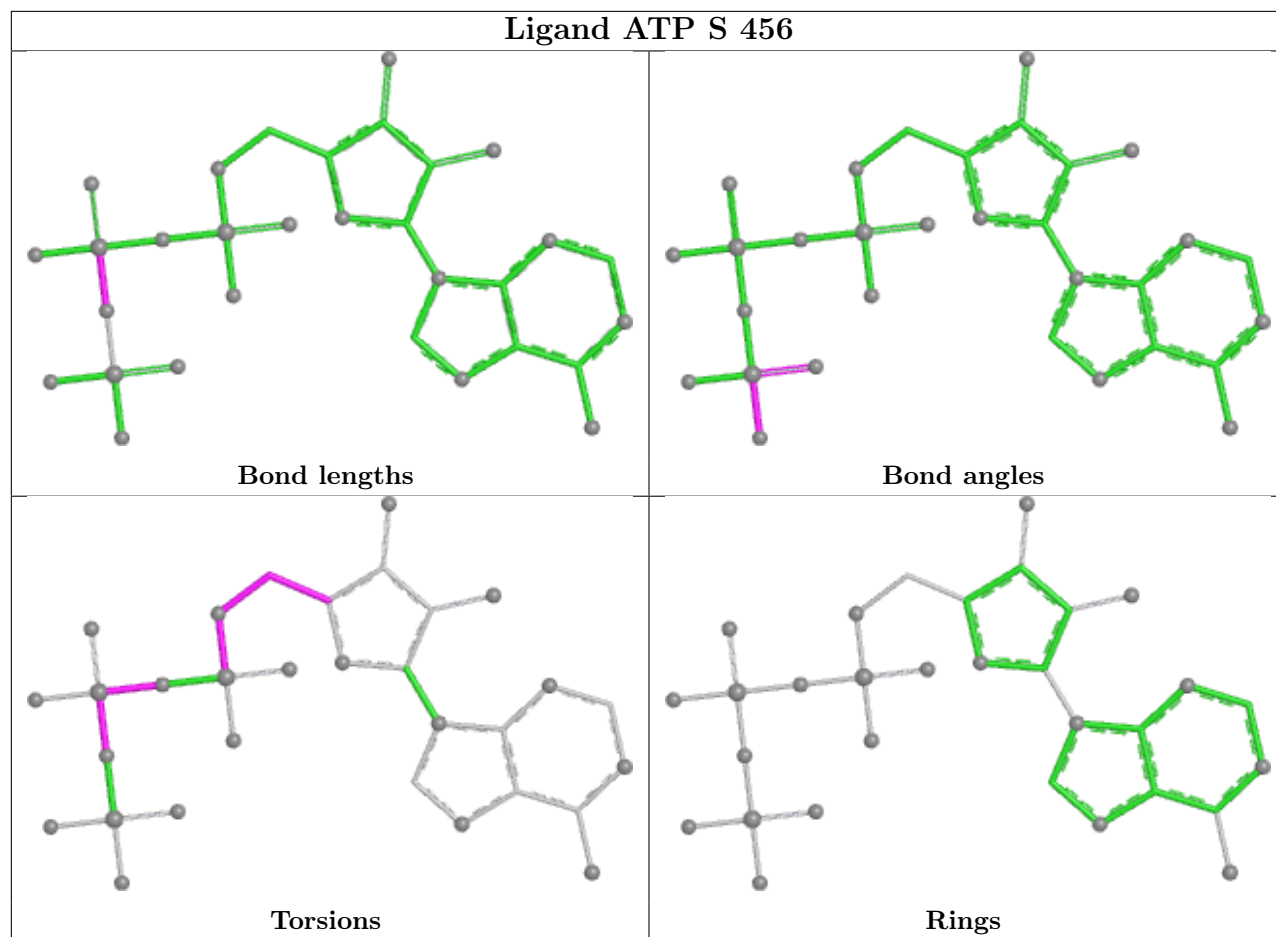
Ligand ATP U 458



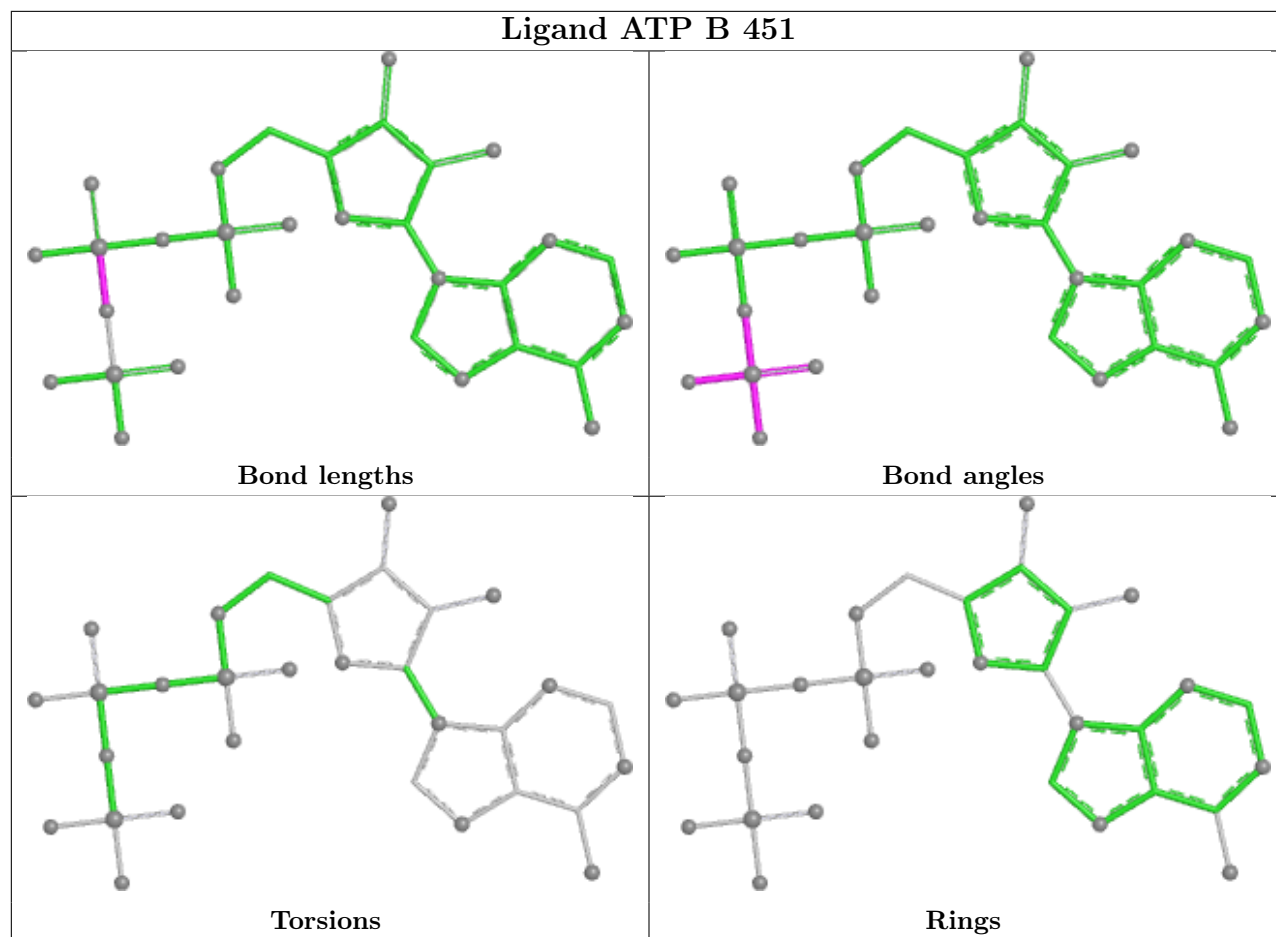
Ligand ATP F 455

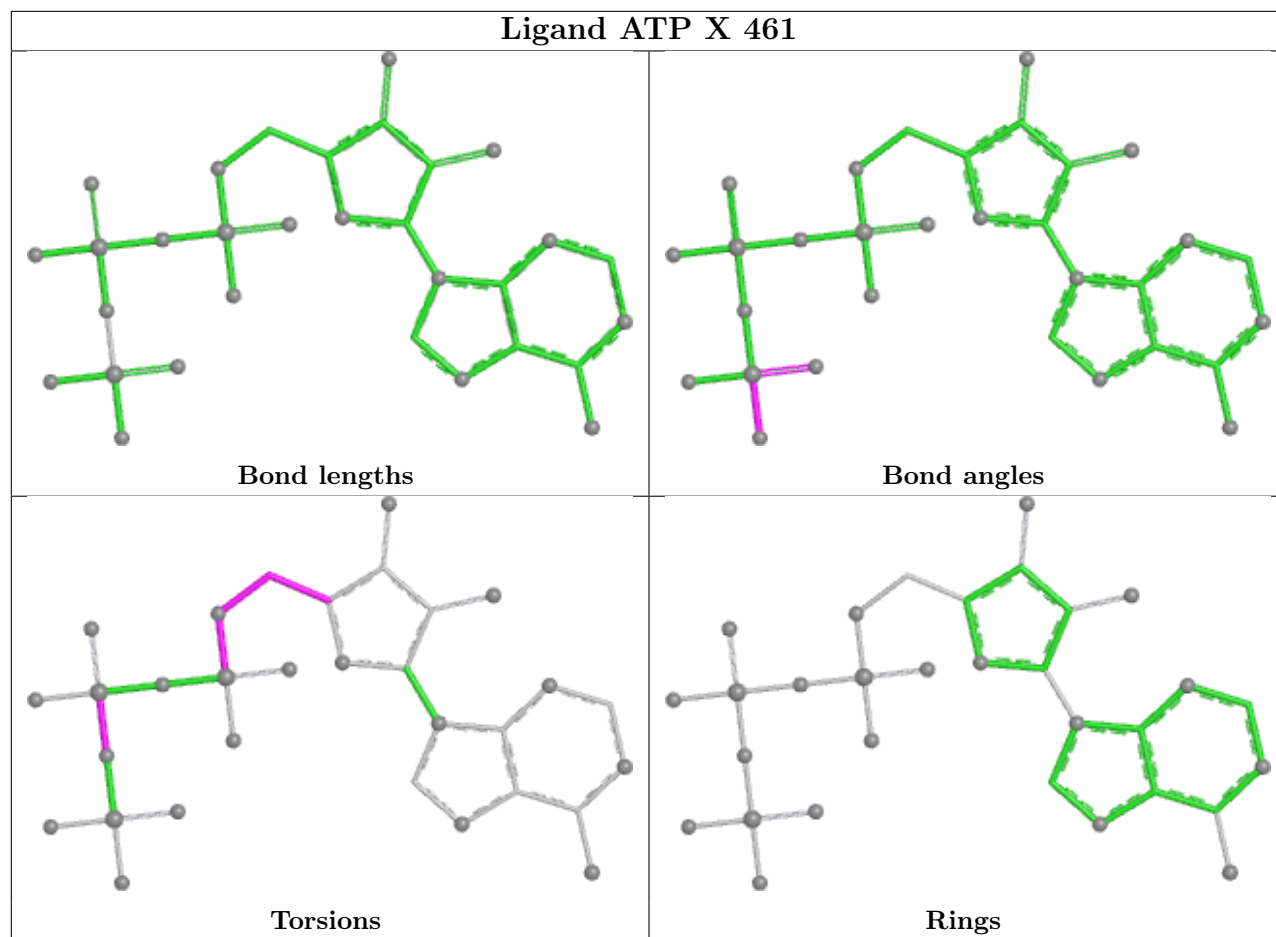


Ligand ATP S 456

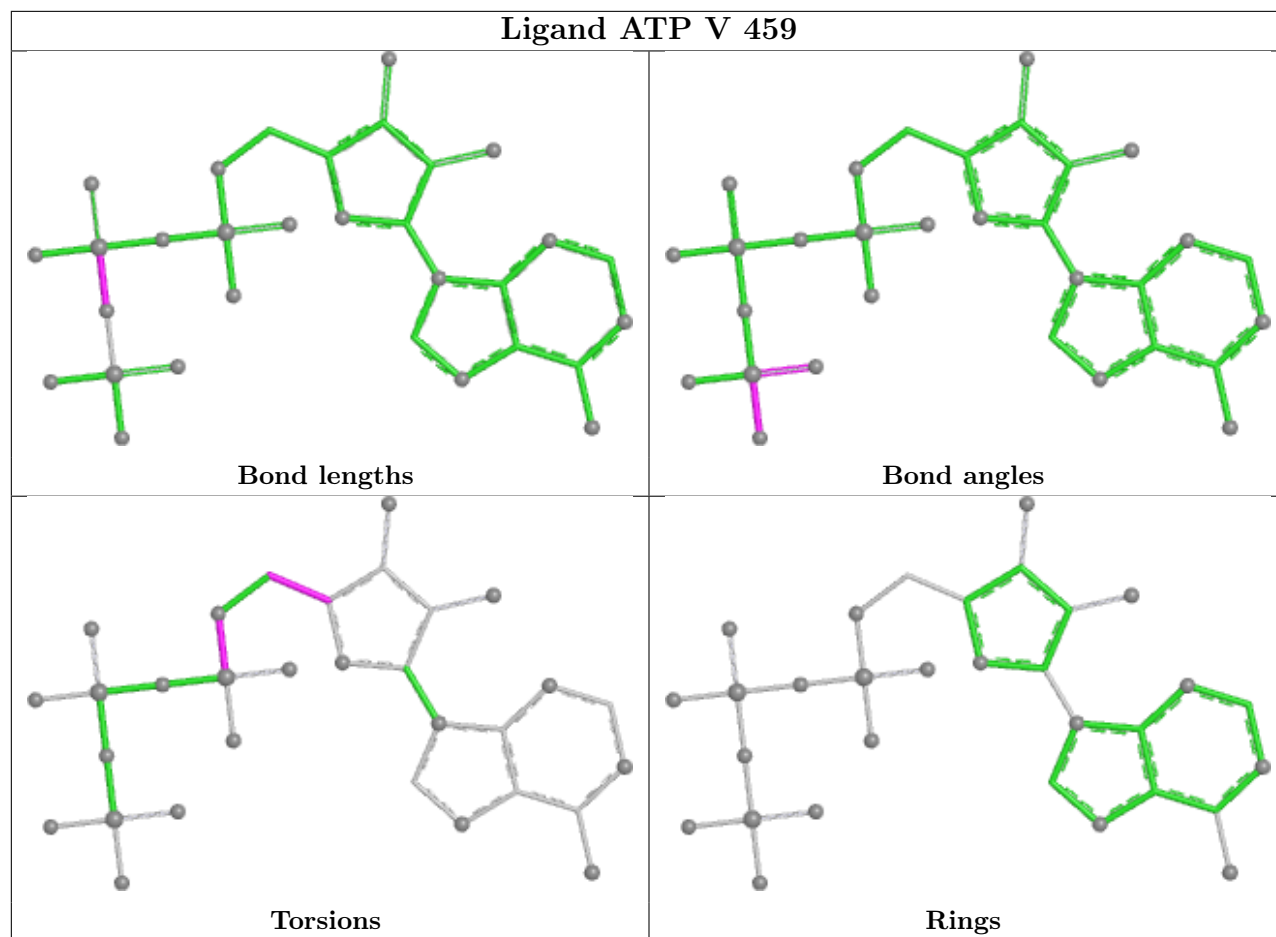


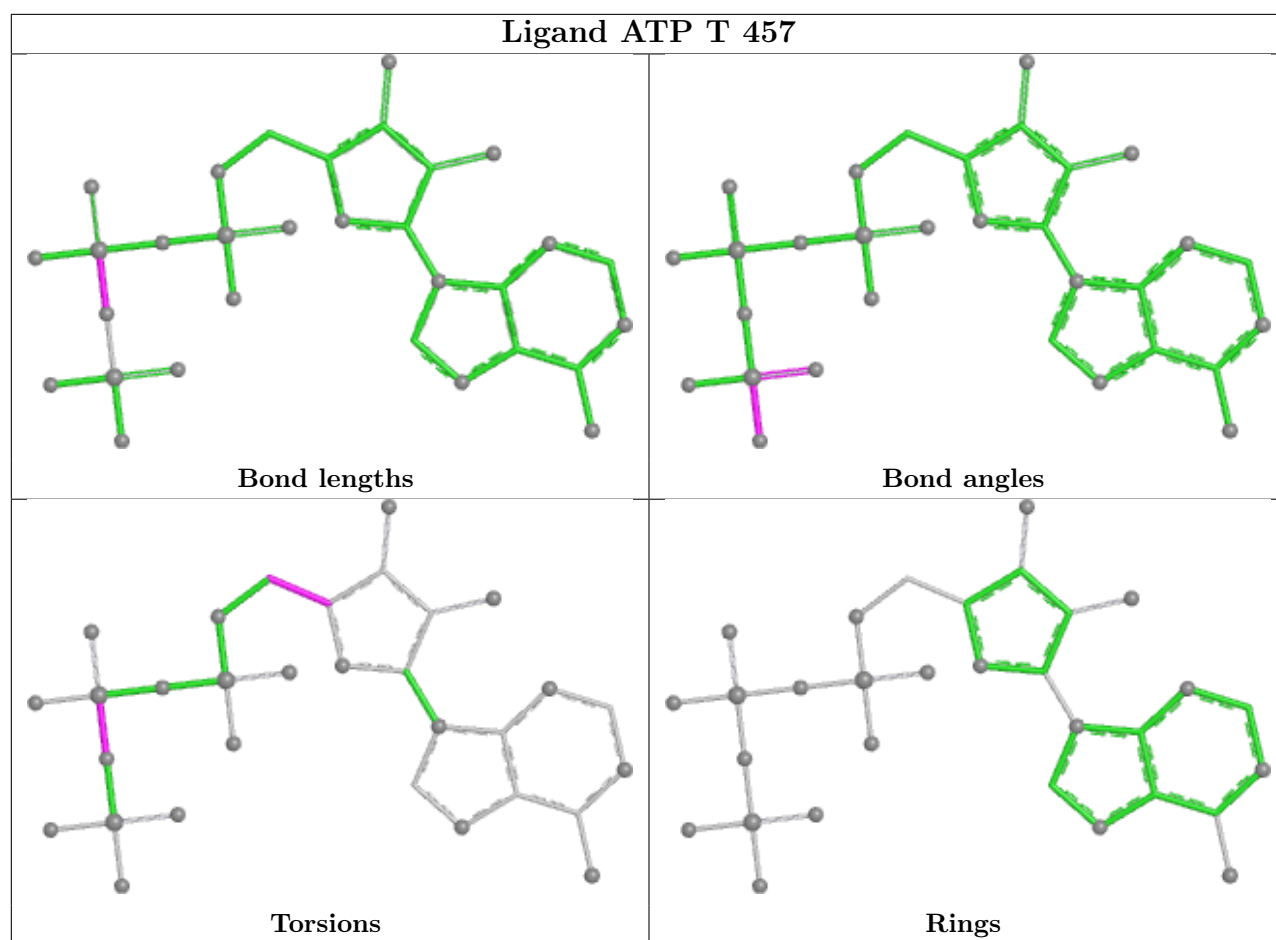
Ligand ATP B 451





Ligand ATP V 459





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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.