



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:01 AM UTC

PDB ID : 5KZF / pdb_00005kzf
Title : Crystal structure of near full-length hexameric Mycobacterium tuberculosis proteasomal ATPase Mpa in apo form
Authors : Li, H.; Hu, K.; Yang, S.; Bai, L.
Deposited on : 2016-07-25
Resolution : 3.49 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

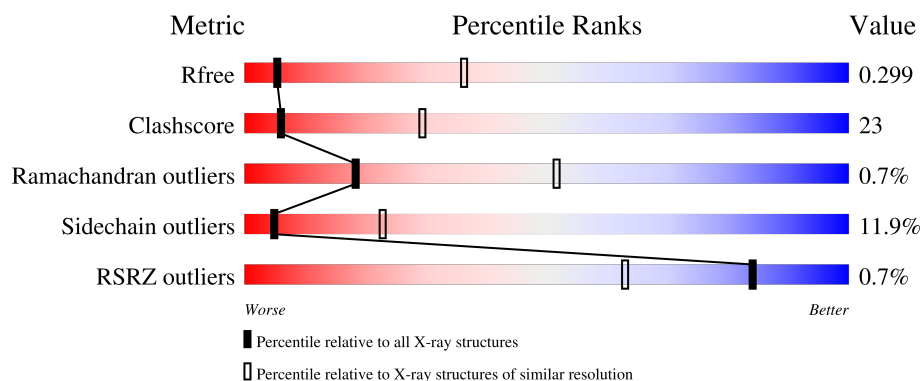
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	513	% 55% 33% 6% • 6%
1	B	513	59% 28% 5% • 7%
1	C	513	% 58% 28% 5% • 8%
1	D	513	% 54% 29% 5% • 10%
1	E	513	% 58% 26% 6% • 10%

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Mol	Chain	Length	Quality of chain
1	F	513	54%29%6% • 10%
1	G	513	% 54%29%6% • 10%
1	H	513	% 59%27%6% • 7%
1	I	513	% 55%30%7% • 7%
1	J	513	% 57%30%7% • 6%
1	K	513	% 55%33%8% • •
1	L	513	55%30%6% • 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 44298 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 Proteasome-associated ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3747	2360	647	729	11			
1	B	475	Total	C	N	O	S	0	0	0
			3707	2337	637	722	11			
1	C	472	Total	C	N	O	S	0	0	0
			3649	2300	632	706	11			
1	D	460	Total	C	N	O	S	0	0	0
			3593	2266	621	695	11			
1	E	461	Total	C	N	O	S	0	0	0
			3597	2268	622	696	11			
1	F	460	Total	C	N	O	S	0	0	0
			3589	2267	615	696	11			
1	G	461	Total	C	N	O	S	0	0	0
			3595	2270	615	698	12			
1	H	478	Total	C	N	O	S	0	0	0
			3729	2351	639	727	12			
1	I	478	Total	C	N	O	S	0	0	0
			3735	2352	645	726	12			
1	J	484	Total	C	N	O	S	0	0	0
			3775	2377	646	740	12			
1	K	498	Total	C	N	O	S	0	0	0
			3887	2442	672	761	12			
1	L	473	Total	C	N	O	S	0	0	0
			3695	2329	635	720	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A5U4E1
B	1	MET	-	initiating methionine	UNP A5U4E1
C	1	MET	-	initiating methionine	UNP A5U4E1
D	1	MET	-	initiating methionine	UNP A5U4E1
E	1	MET	-	initiating methionine	UNP A5U4E1

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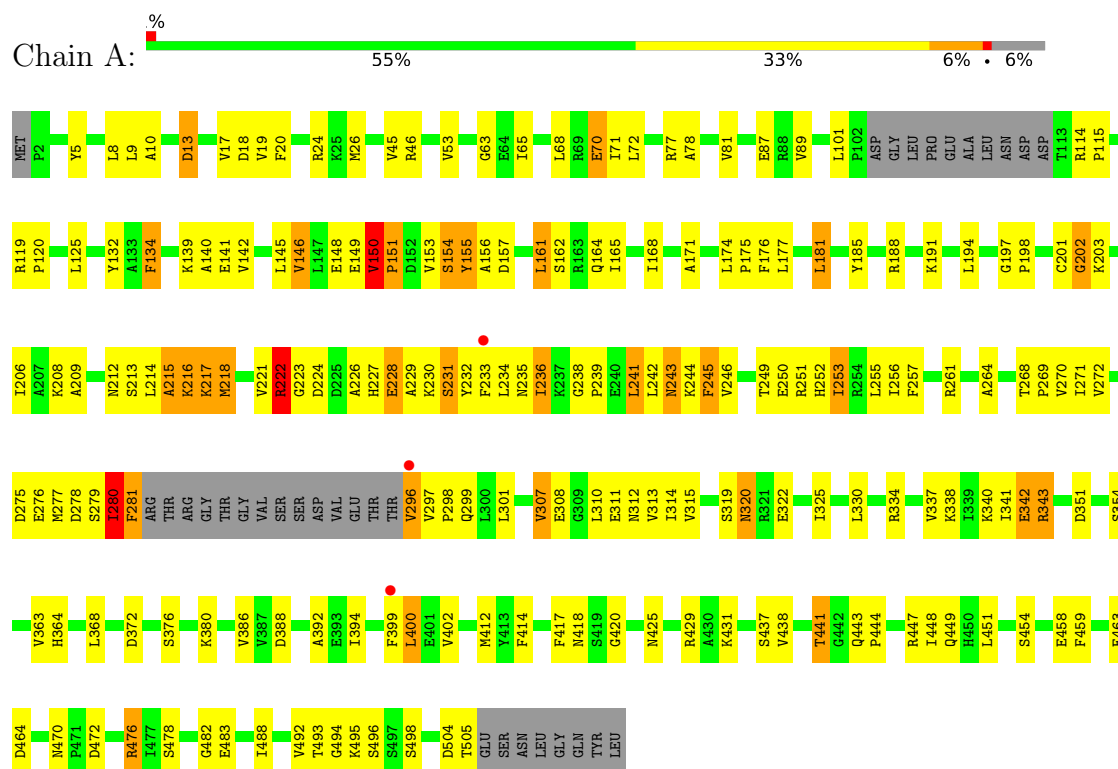
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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	initiating methionine	UNP A5U4E1
G	1	MET	-	initiating methionine	UNP A5U4E1
H	1	MET	-	initiating methionine	UNP A5U4E1
I	1	MET	-	initiating methionine	UNP A5U4E1
J	1	MET	-	initiating methionine	UNP A5U4E1
K	1	MET	-	initiating methionine	UNP A5U4E1
L	1	MET	-	initiating methionine	UNP A5U4E1

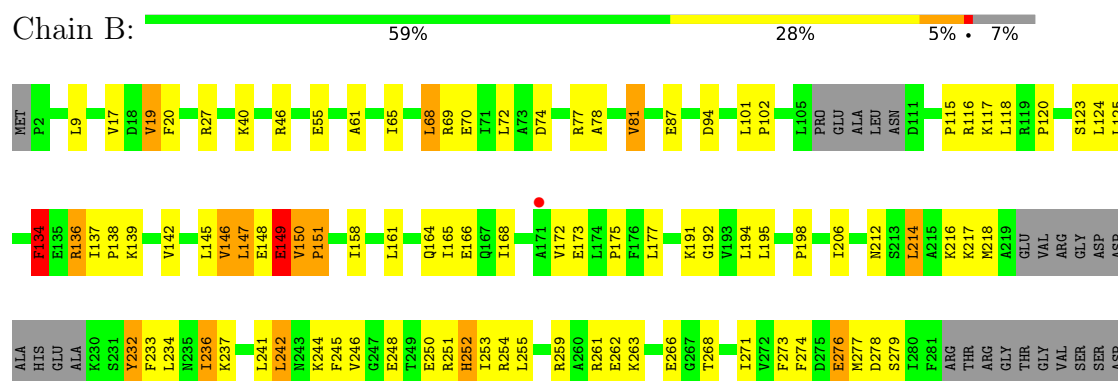
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Proteasome-associated ATPase

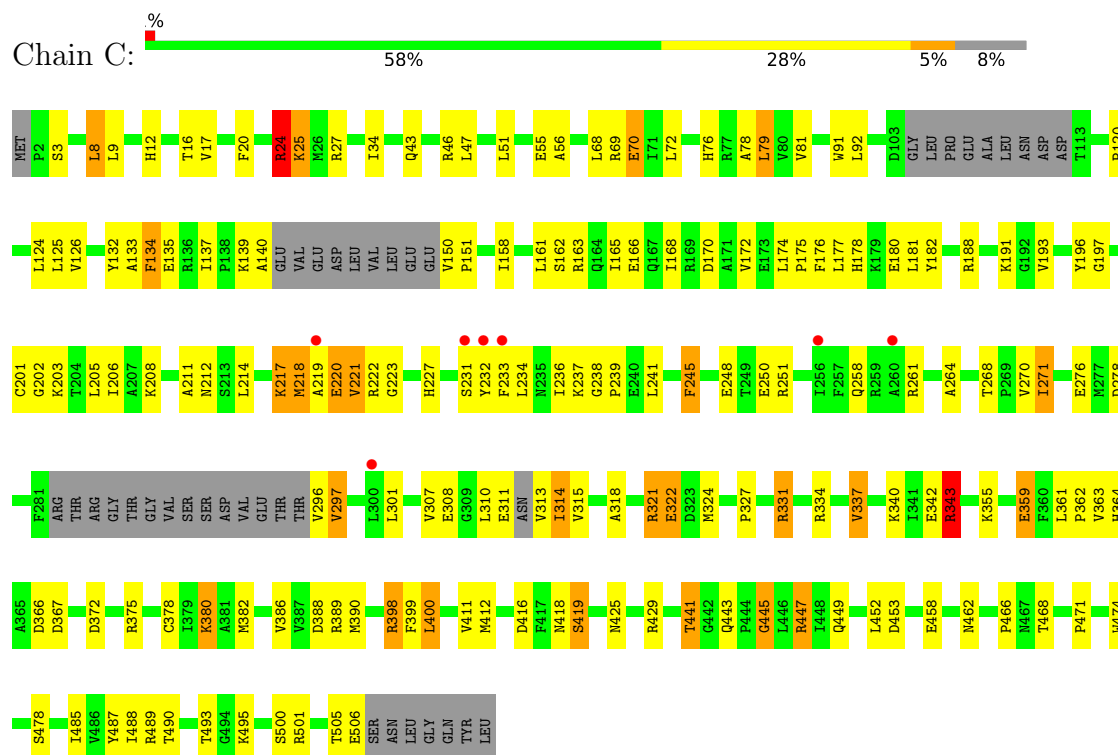


• Molecule 1: Proteasome-associated ATPase

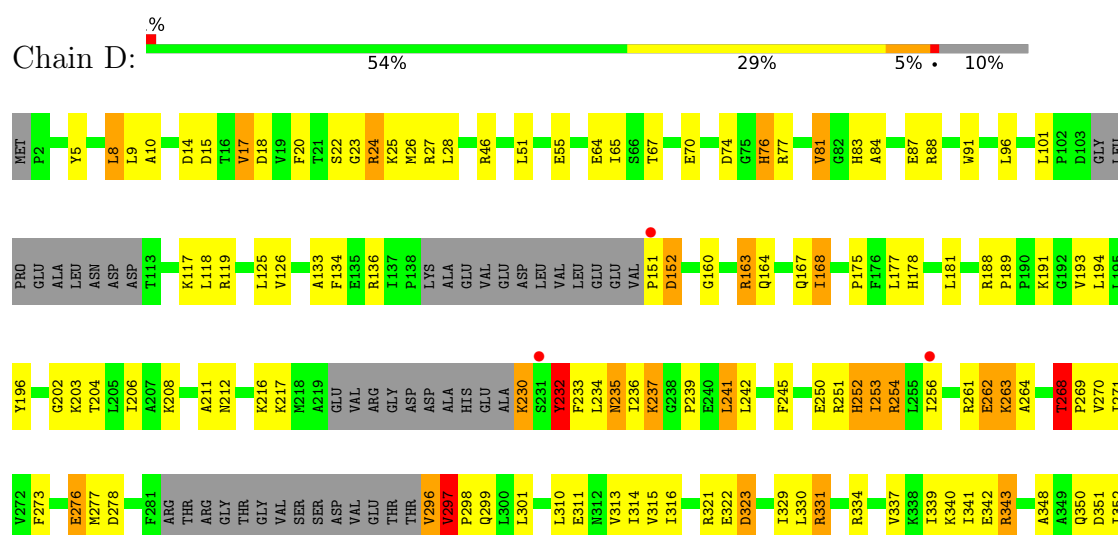


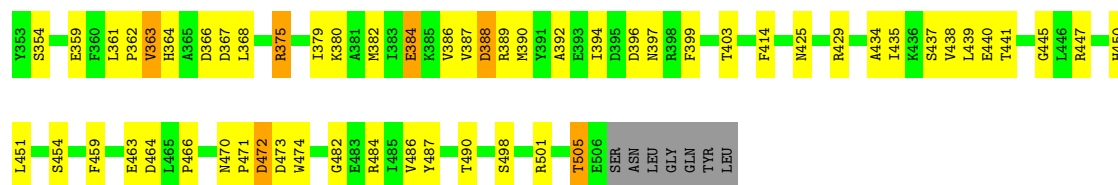


• Molecule 1: Proteasome-associated ATPase

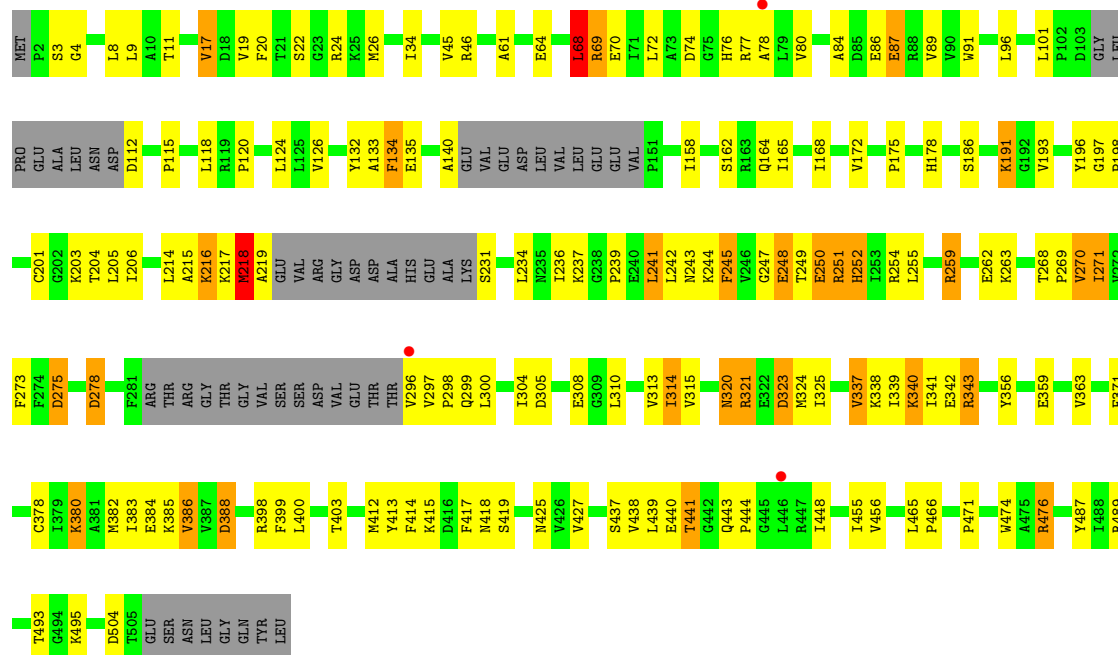


• Molecule 1: Proteasome-associated ATPase

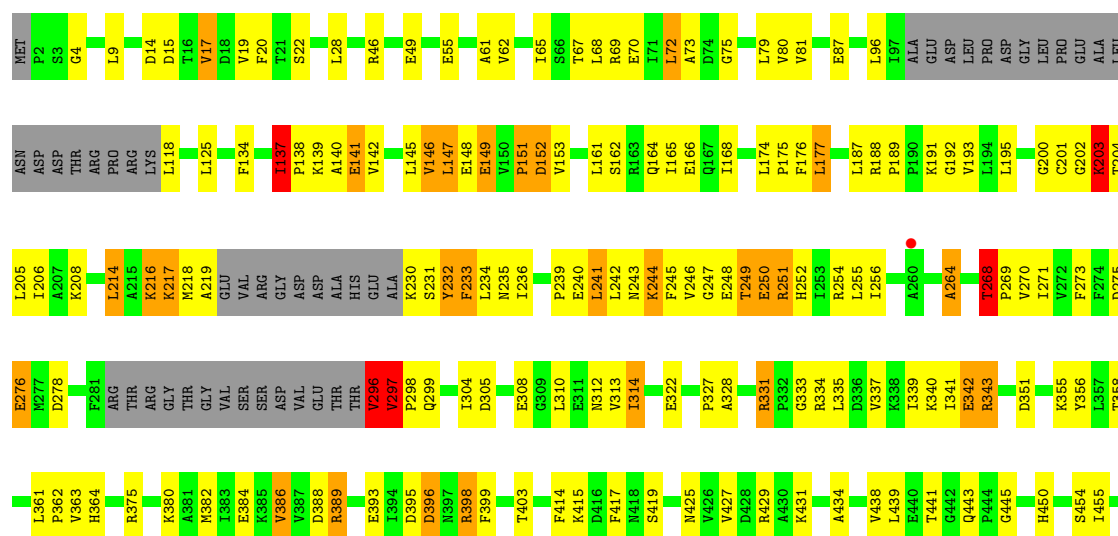




• Molecule 1: Proteasome-associated ATPase

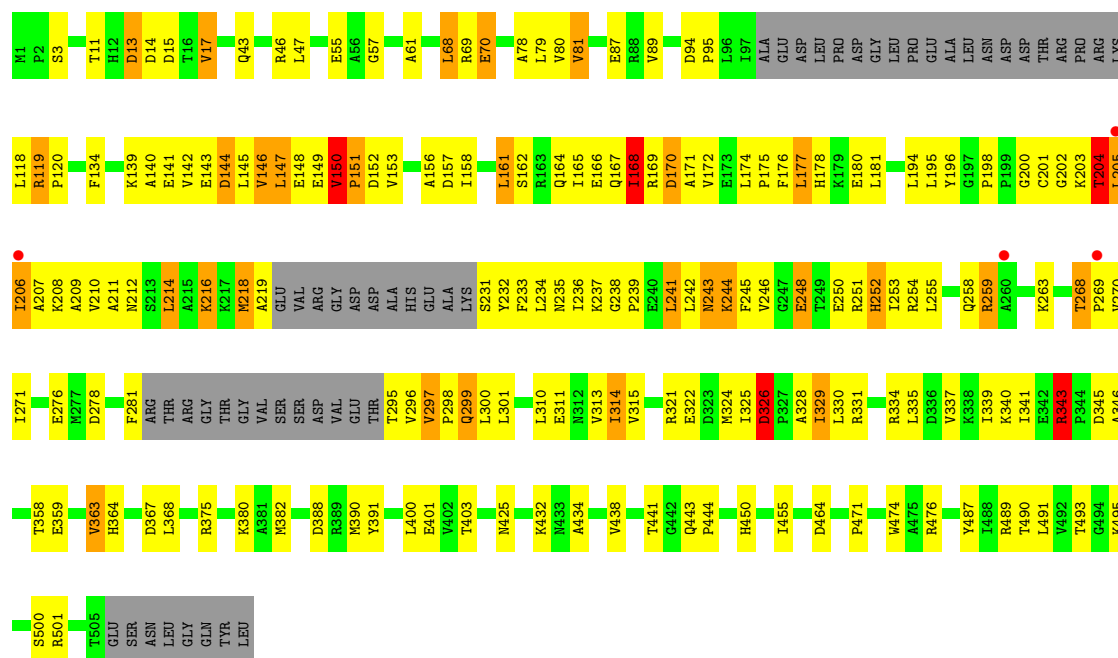


• Molecule 1: Proteasome-associated ATPase

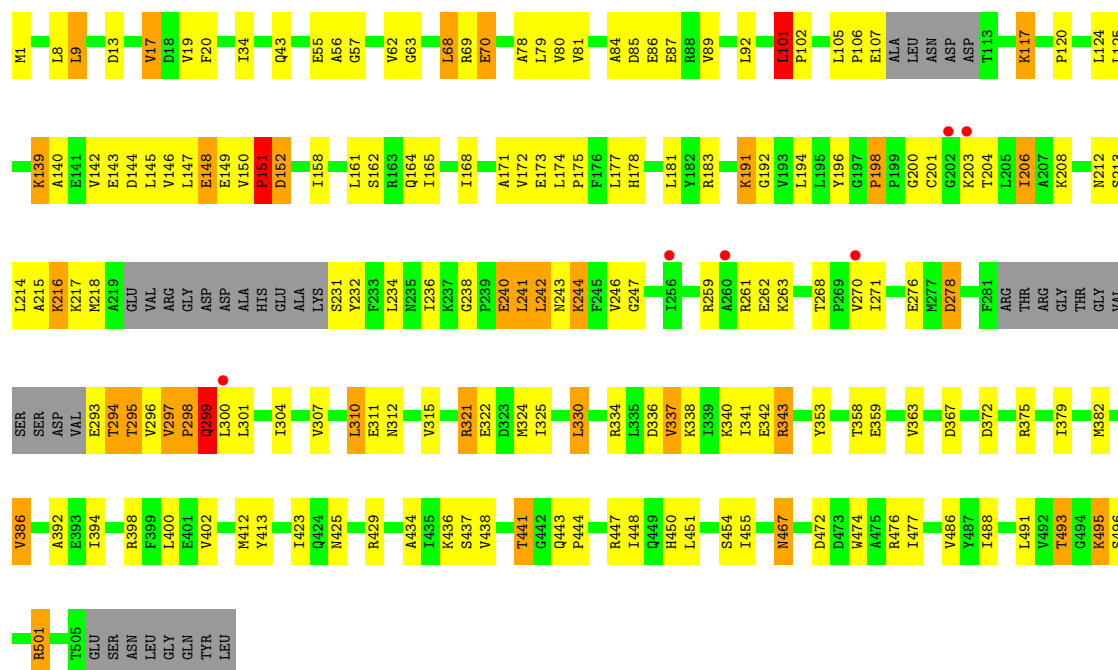




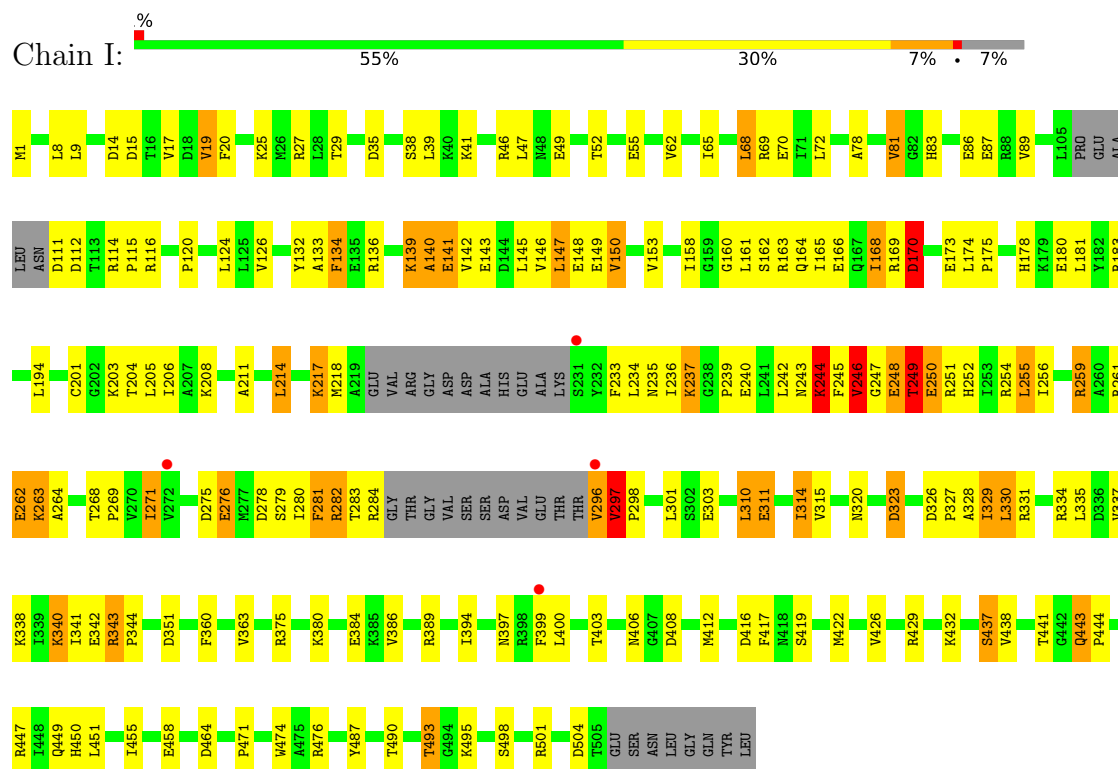
• Molecule 1: Proteasome-associated ATPase



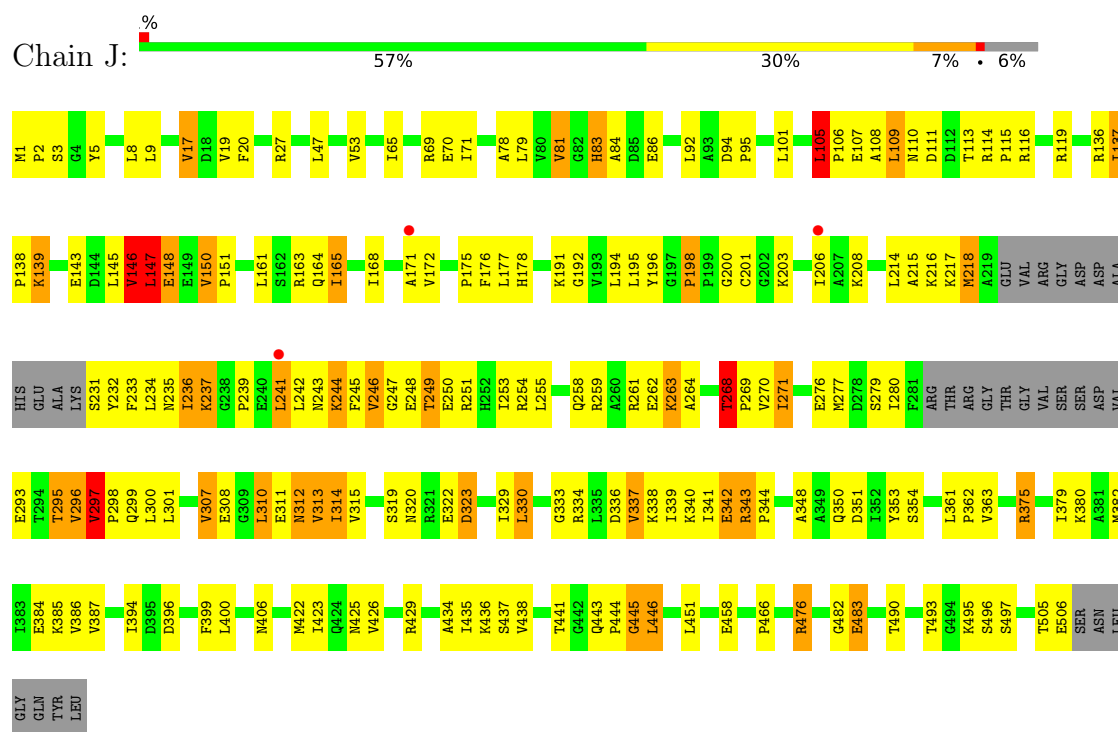
• Molecule 1: Proteasome-associated ATPase



● Molecule 1: Proteasome-associated ATPase

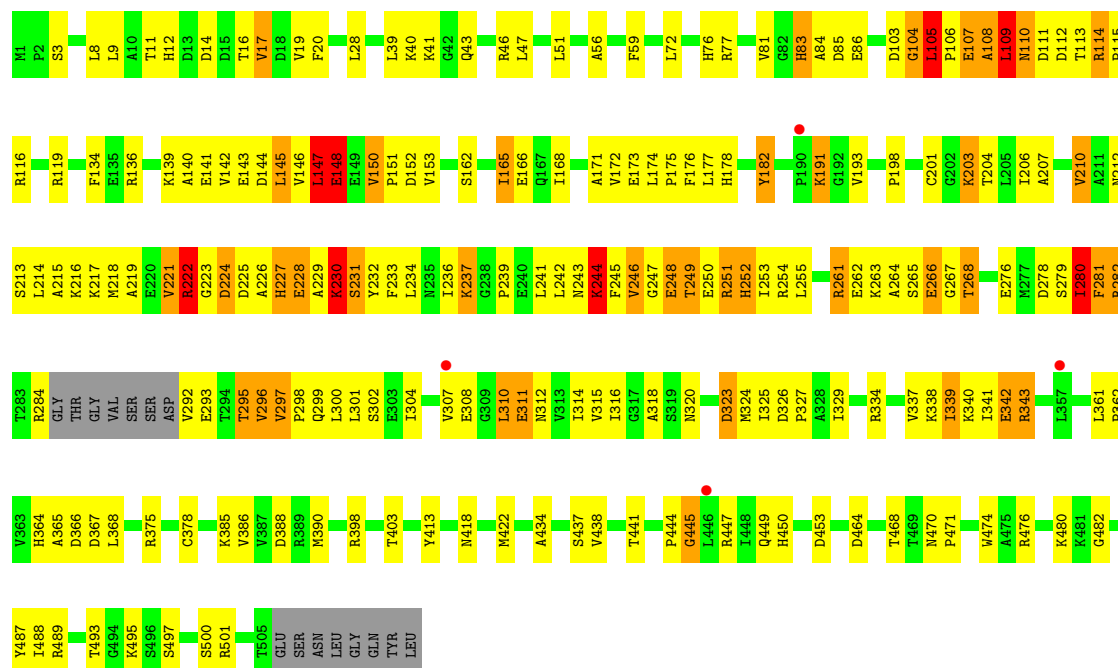


● Molecule 1: Proteasome-associated ATPase



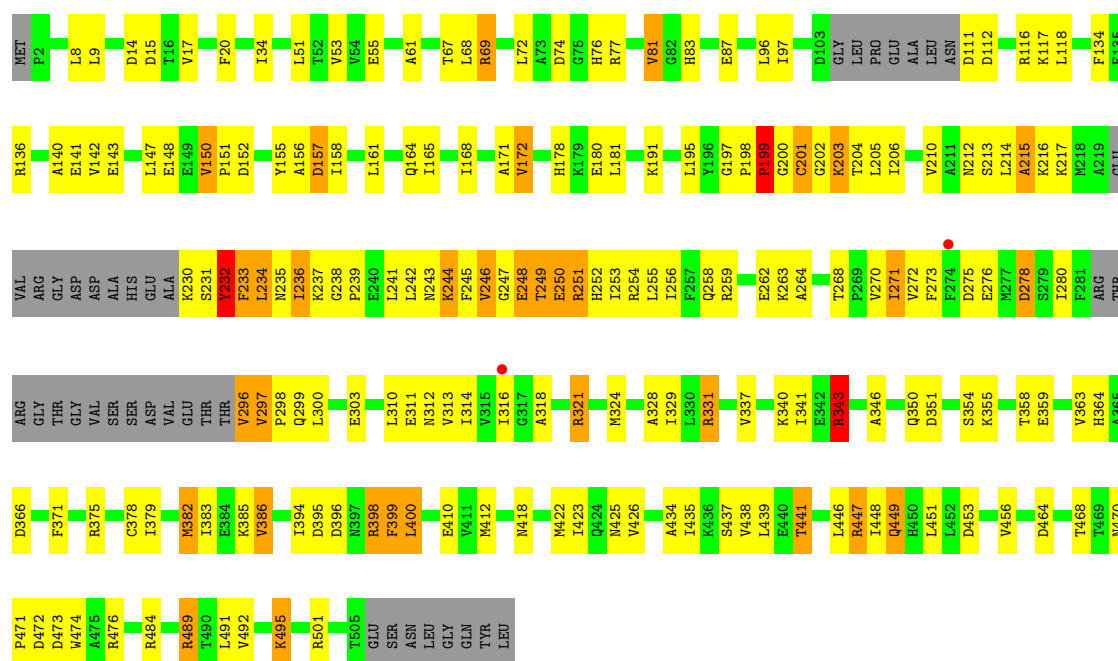
● Molecule 1: Proteasome-associated ATPase





• Molecule 1: Proteasome-associated ATPase

Chain L: 55% 30% 6% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.27Å 202.59Å 303.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.13 – 3.49 71.13 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.4 (71.13-3.49) 99.4 (71.13-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.268 , 0.306 0.262 , 0.299	Depositor DCC
R_{free} test set	1996 reflections (2.19%)	wwPDB-VP
Wilson B-factor (Å ²)	119.4	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 97.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	44298	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.48	2/3808 (0.1%)	0.96	13/5150 (0.3%)
1	B	0.44	0/3766	0.90	9/5092 (0.2%)
1	C	0.44	0/3706	0.91	15/5011 (0.3%)
1	D	0.41	0/3651	0.87	10/4933 (0.2%)
1	E	0.41	1/3655 (0.0%)	0.95	14/4939 (0.3%)
1	F	0.44	0/3646	0.93	16/4929 (0.3%)
1	G	0.50	2/3652 (0.1%)	0.93	17/4939 (0.3%)
1	H	0.47	1/3789 (0.0%)	0.99	15/5126 (0.3%)
1	I	0.46	0/3794	0.99	18/5130 (0.4%)
1	J	0.44	0/3836	0.95	18/5192 (0.3%)
1	K	0.51	0/3950	1.02	22/5346 (0.4%)
1	L	0.41	0/3754	0.94	12/5076 (0.2%)
All	All	0.45	6/45007 (0.0%)	0.95	179/60863 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	1
1	D	0	1
1	F	0	1
1	G	0	2
1	H	0	3
1	I	0	2
1	J	0	1
1	K	0	4
1	L	0	2
All	All	0	21

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	150	VAL	C-N	6.12	1.40	1.33
1	E	466	PRO	N-CD	5.45	1.55	1.47
1	A	151	PRO	N-CD	5.27	1.55	1.47
1	H	298	PRO	N-CD	5.25	1.55	1.47
1	A	150	VAL	C-N	5.24	1.41	1.34
1	G	151	PRO	N-CD	5.15	1.54	1.47

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	150	VAL	CA-C-N	15.53	139.25	119.84
1	H	150	VAL	C-N-CA	15.53	139.25	119.84
1	E	251	ARG	N-CA-C	14.77	130.66	111.75
1	I	140	ALA	N-CA-C	13.39	125.88	111.28
1	E	252	HIS	N-CA-C	13.11	125.56	111.28
1	F	149	GLU	N-CA-C	13.08	125.07	111.07
1	B	441	THR	N-CA-C	11.32	123.69	111.36
1	I	150	VAL	CA-C-N	-11.13	109.50	120.52
1	I	150	VAL	C-N-CA	-11.13	109.50	120.52
1	C	25	LYS	N-CA-C	9.99	125.17	111.39
1	L	399	PHE	N-CA-C	9.86	121.79	111.14
1	K	83	HIS	N-CA-C	9.83	121.99	111.28
1	L	172	VAL	N-CA-C	9.69	119.89	111.56
1	D	76	HIS	N-CA-C	9.56	124.64	111.74
1	K	148	GLU	N-CA-C	9.54	131.12	110.80
1	K	308	GLU	N-CA-C	9.50	121.63	111.28
1	K	251	ARG	N-CA-C	-9.39	95.53	109.62
1	K	110	ASN	N-CA-C	-9.20	98.66	110.53
1	L	232	TYR	N-CA-C	9.00	122.94	110.24
1	H	117	LYS	N-CA-C	8.94	123.73	111.39
1	J	139	LYS	N-CA-C	8.73	120.41	111.07
1	B	134	PHE	N-CA-C	8.72	124.53	112.93
1	K	280	ILE	N-CA-C	8.55	118.56	110.53
1	E	22	SER	N-CA-C	8.48	123.39	111.52
1	L	343	ARG	N-CA-C	8.47	120.40	109.64
1	A	280	ILE	N-CA-C	-8.20	104.49	113.43
1	E	197	GLY	CA-C-N	7.93	125.45	119.66
1	E	197	GLY	C-N-CA	7.93	125.45	119.66
1	K	150	VAL	CA-C-N	7.92	127.98	119.90
1	K	150	VAL	C-N-CA	7.92	127.98	119.90
1	H	336	ASP	N-CA-C	7.92	119.70	111.14
1	K	114	ARG	N-CA-C	-7.91	101.01	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	313	VAL	N-CA-C	7.88	119.14	108.11
1	A	162	SER	N-CA-C	7.67	120.31	111.11
1	H	198	PRO	CA-C-N	7.63	129.38	119.84
1	H	198	PRO	C-N-CA	7.63	129.38	119.84
1	J	147	LEU	CA-C-N	7.49	135.18	121.70
1	J	147	LEU	C-N-CA	7.49	135.18	121.70
1	F	134	PHE	N-CA-C	7.47	122.61	112.68
1	K	343	ARG	N-CA-C	7.41	118.12	109.60
1	F	245	PHE	N-CA-C	-7.40	103.34	112.88
1	K	134	PHE	N-CA-C	7.30	122.40	112.68
1	C	505	THR	N-CA-C	7.29	119.01	111.14
1	G	204	THR	N-CA-C	7.05	119.02	108.31
1	F	296	VAL	CA-C-N	7.04	124.67	120.24
1	F	296	VAL	C-N-CA	7.04	124.67	120.24
1	H	201	CYS	N-CA-C	-6.96	104.53	113.16
1	E	70	GLU	N-CA-C	6.95	118.74	108.60
1	J	83	HIS	N-CA-C	6.91	118.46	111.07
1	C	238	GLY	CA-C-N	-6.87	111.43	119.05
1	C	238	GLY	C-N-CA	-6.87	111.43	119.05
1	J	295	THR	CB-CA-C	-6.84	107.65	115.79
1	G	134	PHE	N-CA-C	6.82	121.74	112.68
1	I	249	THR	CA-C-N	6.78	133.91	121.70
1	I	249	THR	C-N-CA	6.78	133.91	121.70
1	G	146	VAL	N-CA-C	6.76	117.63	107.75
1	G	168	ILE	CB-CA-C	-6.71	103.23	112.02
1	H	191	LYS	N-CA-C	6.67	118.63	111.36
1	G	150	VAL	CA-C-N	-6.63	112.94	119.90
1	G	150	VAL	C-N-CA	-6.63	112.94	119.90
1	F	343	ARG	N-CA-C	6.56	117.97	109.64
1	J	296	VAL	N-CA-C	6.48	119.12	112.90
1	L	197	GLY	CA-C-N	6.33	126.90	120.38
1	L	197	GLY	C-N-CA	6.33	126.90	120.38
1	F	297	VAL	CB-CA-C	-6.32	107.65	114.35
1	F	137	ILE	CA-C-N	-6.32	111.95	119.84
1	F	137	ILE	C-N-CA	-6.32	111.95	119.84
1	G	297	VAL	N-CA-C	6.30	122.50	108.88
1	H	1	MET	CA-C-N	-6.30	111.97	119.84
1	H	1	MET	C-N-CA	-6.30	111.97	119.84
1	A	231	SER	N-CA-C	6.28	117.69	108.14
1	D	268	THR	CA-C-N	6.27	126.23	119.78
1	D	268	THR	C-N-CA	6.27	126.23	119.78
1	D	134	PHE	N-CA-C	6.25	120.99	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	147	LEU	N-CA-C	6.20	119.28	107.75
1	A	134	PHE	N-CA-C	6.17	120.89	112.68
1	J	198	PRO	CA-C-N	-6.16	113.59	121.91
1	J	198	PRO	C-N-CA	-6.16	113.59	121.91
1	F	264	ALA	N-CA-C	6.15	117.78	111.14
1	K	445	GLY	N-CA-C	6.13	117.78	111.95
1	C	343	ARG	CA-C-N	-6.09	113.67	119.76
1	C	343	ARG	C-N-CA	-6.09	113.67	119.76
1	H	101	LEU	CA-C-N	6.07	127.43	119.84
1	H	101	LEU	C-N-CA	6.07	127.43	119.84
1	I	141	GLU	N-CA-C	6.05	122.69	113.61
1	B	297	VAL	N-CA-C	6.04	121.92	108.88
1	I	134	PHE	N-CA-C	6.03	121.15	113.55
1	C	297	VAL	N-CA-C	6.03	121.91	108.88
1	A	197	GLY	CA-C-N	6.03	126.59	120.38
1	A	197	GLY	C-N-CA	6.03	126.59	120.38
1	G	70	GLU	N-CA-C	6.01	117.99	108.79
1	H	70	GLU	N-CA-C	6.00	117.97	108.79
1	A	146	VAL	N-CA-C	5.99	121.79	109.34
1	L	233	PHE	N-CA-C	5.95	118.20	110.53
1	L	134	PHE	N-CA-C	5.92	120.80	112.93
1	E	218	MET	CA-C-N	5.91	132.34	121.70
1	E	218	MET	C-N-CA	5.91	132.34	121.70
1	A	297	VAL	N-CA-C	5.87	121.56	108.88
1	J	297	VAL	N-CA-C	5.87	121.56	108.88
1	C	134	PHE	N-CA-C	5.86	120.72	112.93
1	I	343	ARG	CA-C-N	-5.85	113.73	119.76
1	I	343	ARG	C-N-CA	-5.85	113.73	119.76
1	B	232	TYR	N-CA-C	5.84	116.12	107.88
1	I	170	ASP	N-CA-C	-5.83	104.84	111.14
1	J	445	GLY	N-CA-C	5.81	117.47	111.95
1	E	68	LEU	N-CA-C	5.80	117.75	108.41
1	D	84	ALA	N-CA-C	-5.77	106.22	113.20
1	E	134	PHE	N-CA-C	5.74	120.56	112.93
1	K	109	LEU	N-CA-C	-5.71	104.97	111.07
1	D	22	SER	CB-CA-C	-5.70	109.98	116.54
1	E	297	VAL	N-CA-C	5.70	121.19	108.88
1	D	232	TYR	N-CA-C	5.66	117.07	108.07
1	I	168	ILE	O-C-N	5.65	127.45	121.91
1	B	146	VAL	N-CA-C	5.64	121.07	109.34
1	J	343	ARG	CA-C-N	-5.61	114.20	120.14
1	J	343	ARG	C-N-CA	-5.61	114.20	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	297	VAL	N-CA-C	5.57	120.69	112.61
1	F	268	THR	CA-C-N	5.57	125.51	119.78
1	F	268	THR	C-N-CA	5.57	125.51	119.78
1	G	326	ASP	CA-C-N	5.57	125.24	119.56
1	G	326	ASP	C-N-CA	5.57	125.24	119.56
1	E	343	ARG	N-CA-C	5.56	115.99	109.60
1	L	51	LEU	N-CA-C	5.54	119.22	111.74
1	D	297	VAL	N-CA-C	5.54	120.85	108.88
1	I	244	LYS	N-CA-C	5.53	121.91	113.51
1	F	343	ARG	CA-C-N	-5.51	114.29	119.85
1	F	343	ARG	C-N-CA	-5.51	114.29	119.85
1	K	295	THR	CA-C-N	5.49	131.58	121.70
1	K	295	THR	C-N-CA	5.49	131.58	121.70
1	C	24	ARG	N-CA-C	5.48	117.16	108.67
1	I	297	VAL	N-CA-C	5.44	120.63	108.88
1	E	343	ARG	CA-C-N	-5.43	114.16	119.76
1	E	343	ARG	C-N-CA	-5.43	114.16	119.76
1	A	343	ARG	CA-C-N	-5.43	114.37	119.85
1	A	343	ARG	C-N-CA	-5.43	114.37	119.85
1	D	343	ARG	CA-C-N	-5.41	114.38	119.85
1	D	343	ARG	C-N-CA	-5.41	114.38	119.85
1	B	149	GLU	N-CA-C	5.41	117.85	110.55
1	A	150	VAL	CA-C-N	-5.36	113.10	119.05
1	A	150	VAL	C-N-CA	-5.36	113.10	119.05
1	L	249	THR	CA-C-N	5.36	131.35	121.70
1	L	249	THR	C-N-CA	5.36	131.35	121.70
1	I	139	LYS	CA-C-N	5.35	127.45	120.28
1	I	139	LYS	C-N-CA	5.35	127.45	120.28
1	C	137	ILE	N-CA-C	5.34	113.31	107.60
1	L	297	VAL	N-CA-C	5.29	120.32	108.88
1	G	343	ARG	CA-C-N	-5.28	114.32	119.76
1	G	343	ARG	C-N-CA	-5.28	114.32	119.76
1	B	343	ARG	CA-C-N	-5.27	114.53	119.85
1	B	343	ARG	C-N-CA	-5.27	114.53	119.85
1	B	252	HIS	N-CA-C	5.27	117.03	111.28
1	A	70	GLU	N-CA-C	5.26	116.84	108.79
1	G	313	VAL	N-CA-C	5.21	115.41	108.11
1	H	343	ARG	CA-C-N	-5.21	114.59	119.85
1	H	343	ARG	C-N-CA	-5.21	114.59	119.85
1	F	244	LYS	N-CA-C	5.20	116.86	108.34
1	K	105	LEU	CA-C-N	-5.19	113.57	119.28
1	K	105	LEU	C-N-CA	-5.19	113.57	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	445	GLY	N-CA-C	5.18	118.51	111.72
1	G	119	ARG	CA-C-N	-5.17	115.40	120.52
1	G	119	ARG	C-N-CA	-5.17	115.40	120.52
1	G	171	ALA	CA-C-N	-5.17	117.85	123.08
1	G	171	ALA	C-N-CA	-5.17	117.85	123.08
1	J	178	HIS	N-CA-C	5.15	119.25	112.92
1	I	52	THR	CA-C-N	-5.14	116.06	122.48
1	I	52	THR	C-N-CA	-5.14	116.06	122.48
1	J	312	ASN	N-CA-C	5.12	116.86	111.28
1	C	250	GLU	N-CA-C	5.12	116.54	111.07
1	C	70	GLU	N-CA-C	5.09	116.58	108.79
1	J	268	THR	CA-C-N	5.08	124.84	119.76
1	J	268	THR	C-N-CA	5.08	124.84	119.76
1	K	232	TYR	N-CA-C	5.08	117.03	108.96
1	J	343	ARG	N-CA-C	5.06	115.80	109.57
1	I	244	LYS	N-CA-CB	-5.06	109.04	114.10
1	K	244	LYS	N-CA-C	5.04	121.17	113.51
1	C	197	GLY	CA-C-N	5.01	123.32	119.66
1	C	197	GLY	C-N-CA	5.01	123.32	119.66
1	K	266	GLU	N-CA-C	5.01	116.75	108.49
1	K	244	LYS	N-CA-CB	-5.01	109.09	114.10

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	GLY	Peptide
1	A	215	ALA	Peptide
1	A	222	ARG	Peptide
1	B	297	VAL	Peptide
1	C	24	ARG	Peptide
1	D	232	TYR	Peptide
1	F	151	PRO	Peptide
1	G	177	LEU	Peptide
1	G	297	VAL	Peptide
1	H	139	LYS	Peptide
1	H	151	PRO	Peptide
1	H	299	GLN	Mainchain
1	I	111	ASP	Peptide
1	I	201	CYS	Peptide
1	J	105	LEU	Peptide
1	K	103	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	K	147	LEU	Peptide
1	K	201	CYS	Peptide
1	K	222	ARG	Peptide
1	L	199	PRO	Peptide
1	L	215	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3747	0	3755	198	0
1	B	3707	0	3718	148	0
1	C	3649	0	3644	138	3
1	D	3593	0	3607	124	0
1	E	3597	0	3610	134	0
1	F	3589	0	3606	144	0
1	G	3595	0	3611	223	0
1	H	3729	0	3741	186	0
1	I	3735	0	3749	206	0
1	J	3775	0	3778	216	0
1	K	3887	0	3888	280	3
1	L	3695	0	3704	171	0
All	All	44298	0	44411	2017	3

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 23.

All (2017) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:CG2	1:A:231:SER:HA	1.52	1.38
1:H:296:VAL:CG2	1:I:242:LEU:HD21	1.51	1.38
1:K:153:VAL:O	1:K:212:ASN:ND2	1.57	1.38
1:G:148:GLU:CG	1:G:150:VAL:HG13	1.54	1.34
1:K:140:ALA:O	1:K:141:GLU:HG2	1.25	1.32
1:F:149:GLU:O	1:F:233:PHE:CB	1.78	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:GLU:OE1	1:G:150:VAL:HG11	1.23	1.31
1:A:150:VAL:CG1	1:A:232:TYR:N	1.93	1.30
1:K:229:ALA:CA	1:K:230:LYS:HB2	1.46	1.30
1:K:229:ALA:HA	1:K:230:LYS:CB	1.54	1.30
1:A:150:VAL:HG13	1:A:232:TYR:N	0.97	1.27
1:A:151:PRO:CG	1:A:212:ASN:HB2	1.65	1.25
1:K:249:THR:CA	1:K:250:GLU:HB3	1.66	1.24
1:E:244:LYS:HZ2	1:E:248:GLU:CB	1.48	1.24
1:K:173:GLU:OE2	1:K:213:SER:OG	1.56	1.23
1:H:70:GLU:OE2	1:I:140:ALA:HB2	1.11	1.22
1:C:132:TYR:HB3	1:C:134:PHE:CE1	1.74	1.22
1:C:150:VAL:HG11	1:C:231:SER:CB	1.70	1.21
1:J:270:VAL:O	1:J:313:VAL:HG13	1.08	1.21
1:A:150:VAL:HG13	1:A:231:SER:C	1.65	1.20
1:I:166:GLU:O	1:I:170:ASP:OD1	1.58	1.19
1:J:84:ALA:O	1:K:83:HIS:NE2	1.74	1.18
1:G:148:GLU:HG3	1:G:150:VAL:HG13	1.26	1.18
1:H:68:LEU:CD1	1:H:78:ALA:HB1	1.72	1.18
1:H:298:PRO:CD	1:I:242:LEU:HD22	1.72	1.18
1:H:299:GLN:OE1	1:H:300:LEU:HD12	1.41	1.17
1:K:109:LEU:HD12	1:K:148:GLU:OE2	1.40	1.16
1:L:233:PHE:CE2	1:L:234:LEU:O	1.98	1.16
1:K:249:THR:HA	1:K:250:GLU:CB	1.62	1.16
1:A:150:VAL:HG12	1:A:232:TYR:CB	1.74	1.16
1:G:158:ILE:HG12	1:G:206:ILE:HG12	1.18	1.15
1:J:86:GLU:HB3	1:K:83:HIS:CD2	1.80	1.15
1:A:151:PRO:HG2	1:A:212:ASN:CB	1.77	1.14
1:G:68:LEU:CD1	1:G:78:ALA:HB1	1.79	1.12
1:H:296:VAL:HG23	1:I:242:LEU:HD21	1.22	1.12
1:F:149:GLU:O	1:F:233:PHE:HB2	1.44	1.12
1:K:109:LEU:HD12	1:K:148:GLU:CD	1.73	1.12
1:K:222:ARG:HB2	1:K:223:GLY:HA2	1.31	1.11
1:G:158:ILE:CG1	1:G:206:ILE:HG12	1.76	1.11
1:G:139:LYS:NZ	1:G:142:VAL:HG21	1.65	1.11
1:H:296:VAL:CB	1:I:242:LEU:HD11	1.81	1.11
1:A:150:VAL:CG1	1:A:232:TYR:CB	2.29	1.10
1:A:150:VAL:HG21	1:A:231:SER:HA	1.14	1.10
1:A:150:VAL:HG22	1:A:231:SER:OG	1.51	1.10
1:G:147:LEU:HB3	1:G:148:GLU:HB2	1.21	1.10
1:H:298:PRO:HD2	1:I:242:LEU:HD22	1.34	1.10
1:A:150:VAL:HG22	1:A:231:SER:CB	1.80	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:LYS:NZ	1:E:248:GLU:HB2	1.65	1.10
1:K:250:GLU:OE1	1:K:299:GLN:HG3	1.46	1.09
1:A:150:VAL:CG2	1:A:231:SER:CA	2.29	1.09
1:G:68:LEU:HD11	1:G:78:ALA:HB1	1.30	1.09
1:K:110:ASN:HB3	1:K:111:ASP:HB3	1.13	1.08
1:J:150:VAL:HG22	1:J:232:TYR:HB2	1.32	1.08
1:I:249:THR:HA	1:I:250:GLU:HB3	1.31	1.08
1:J:270:VAL:O	1:J:313:VAL:CG1	2.01	1.08
1:A:150:VAL:HG12	1:A:232:TYR:HB3	1.09	1.08
1:K:230:LYS:HE2	1:K:230:LYS:HA	1.30	1.07
1:A:148:GLU:HB3	1:A:149:GLU:HB3	1.36	1.07
1:I:141:GLU:O	1:I:145:LEU:HB2	1.53	1.07
1:A:150:VAL:HG13	1:A:232:TYR:CA	1.84	1.07
1:C:132:TYR:CB	1:C:134:PHE:HE1	1.67	1.07
1:B:149:GLU:HB2	1:B:233:PHE:O	1.55	1.06
1:A:150:VAL:CG1	1:A:231:SER:C	2.26	1.06
1:J:86:GLU:HB3	1:K:83:HIS:HD2	0.92	1.06
1:H:68:LEU:HD11	1:H:78:ALA:HB1	1.38	1.05
1:A:151:PRO:HG3	1:A:208:LYS:O	1.54	1.05
1:H:298:PRO:CG	1:I:242:LEU:HD22	1.87	1.05
1:B:147:LEU:HB2	1:B:148:GLU:CD	1.81	1.05
1:H:70:GLU:OE2	1:I:140:ALA:CB	2.03	1.05
1:E:244:LYS:HZ3	1:E:248:GLU:HG3	1.17	1.04
1:F:149:GLU:O	1:F:233:PHE:HB3	1.55	1.03
1:H:296:VAL:HB	1:I:242:LEU:HD11	1.07	1.03
1:J:109:LEU:HB2	1:J:110:ASN:HB3	1.38	1.03
1:G:148:GLU:OE1	1:G:150:VAL:CG1	2.06	1.03
1:B:437:SER:O	1:B:441:THR:HG22	1.58	1.02
1:K:219:ALA:O	1:K:225:ASP:HA	1.57	1.02
1:K:250:GLU:OE1	1:K:299:GLN:CG	2.08	1.01
1:G:148:GLU:CG	1:G:150:VAL:CG1	2.38	1.01
1:K:219:ALA:C	1:K:226:ALA:H	1.68	1.01
1:G:166:GLU:O	1:G:170:ASP:OD1	1.78	1.01
1:H:296:VAL:CG2	1:I:242:LEU:CD2	2.38	1.00
1:C:132:TYR:HB3	1:C:134:PHE:HE1	0.87	1.00
1:J:176:PHE:CZ	1:J:311:GLU:O	2.15	1.00
1:J:176:PHE:HZ	1:J:311:GLU:O	1.43	1.00
1:G:164:GLN:O	1:G:168:ILE:CD1	2.08	0.99
1:H:296:VAL:HB	1:I:242:LEU:CD1	1.91	0.99
1:K:107:GLU:N	1:K:107:GLU:OE2	1.95	0.99
1:L:233:PHE:CZ	1:L:234:LEU:O	2.14	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:400:LEU:CD1	1:L:412:MET:HB2	1.92	0.98
1:L:69:ARG:HG2	1:L:69:ARG:HH11	1.29	0.98
1:J:86:GLU:CB	1:K:83:HIS:HD2	1.77	0.98
1:A:243:ASN:OD1	1:A:251:ARG:NH1	1.97	0.97
1:H:298:PRO:CD	1:I:242:LEU:CD2	2.42	0.97
1:K:251:ARG:O	1:K:252:HIS:CD2	2.16	0.97
1:H:296:VAL:HG21	1:I:242:LEU:HD21	1.47	0.97
1:L:400:LEU:HD11	1:L:412:MET:HB2	1.42	0.97
1:J:83:HIS:ND1	1:J:86:GLU:OE1	1.98	0.97
1:J:119:ARG:NH2	1:J:262:GLU:OE1	1.96	0.97
1:E:244:LYS:HZ2	1:E:248:GLU:HB2	0.80	0.97
1:L:68:LEU:HD12	1:L:69:ARG:H	1.30	0.96
1:G:148:GLU:HG2	1:G:150:VAL:HG13	1.43	0.96
1:E:244:LYS:NZ	1:E:248:GLU:CB	2.23	0.95
1:G:170:ASP:O	1:G:175:PRO:HD3	1.66	0.95
1:G:158:ILE:HG12	1:G:206:ILE:CG1	1.96	0.95
1:G:207:ALA:O	1:G:210:VAL:HG12	1.66	0.95
1:G:139:LYS:HZ2	1:G:142:VAL:HG21	1.28	0.95
1:B:441:THR:HG23	1:B:443:GLN:H	1.32	0.95
1:E:244:LYS:HZ3	1:E:248:GLU:CG	1.80	0.95
1:L:69:ARG:NH1	1:L:87:GLU:OE2	1.98	0.94
1:K:219:ALA:O	1:K:226:ALA:N	1.99	0.94
1:H:299:GLN:CD	1:H:300:LEU:HD12	1.92	0.94
1:K:9:LEU:HD11	1:K:20:PHE:HB2	1.46	0.94
1:K:221:VAL:CB	1:K:222:ARG:HD2	1.97	0.94
1:A:150:VAL:CG1	1:A:232:TYR:HB3	1.93	0.94
1:L:68:LEU:HD12	1:L:69:ARG:N	1.83	0.93
1:I:399:PHE:CE2	1:I:417:PHE:CG	2.55	0.93
1:B:149:GLU:CB	1:B:233:PHE:O	2.16	0.93
1:A:229:ALA:HB1	1:A:230:LYS:HA	1.51	0.93
1:E:244:LYS:NZ	1:E:248:GLU:CG	2.31	0.93
1:J:242:LEU:HG	1:J:243:ASN:HA	1.51	0.92
1:H:298:PRO:HD2	1:I:242:LEU:CD2	1.99	0.92
1:H:298:PRO:HG2	1:I:242:LEU:HD22	1.50	0.92
1:L:156:ALA:O	1:L:355:LYS:NZ	2.03	0.92
1:L:249:THR:HA	1:L:250:GLU:HG3	1.50	0.92
1:E:244:LYS:NZ	1:E:248:GLU:HG3	1.83	0.92
1:A:150:VAL:HG22	1:A:231:SER:CA	1.94	0.92
1:H:296:VAL:HG21	1:I:242:LEU:CD2	2.00	0.92
1:I:399:PHE:HE2	1:I:417:PHE:CD2	1.88	0.92
1:J:310:LEU:HD21	1:J:312:ASN:HB2	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:153:VAL:C	1:K:212:ASN:ND2	2.28	0.91
1:A:150:VAL:HG13	1:A:232:TYR:H	1.22	0.91
1:D:177:LEU:HD21	1:D:217:LYS:HE2	1.52	0.91
1:J:109:LEU:CB	1:J:110:ASN:HB3	2.00	0.91
1:H:299:GLN:OE1	1:H:300:LEU:N	2.04	0.91
1:K:221:VAL:HB	1:K:222:ARG:HD2	1.52	0.91
1:K:301:LEU:HD23	1:K:334:ARG:HH12	1.34	0.91
1:K:218:MET:O	1:K:221:VAL:HG23	1.70	0.90
1:J:264:ALA:HA	1:J:312:ASN:HD22	1.35	0.90
1:B:77:ARG:NH1	1:C:135:GLU:OE1	2.03	0.90
1:A:72:LEU:HD13	1:B:139:LYS:HE3	1.52	0.90
1:L:233:PHE:HD1	1:L:271:ILE:HD13	1.34	0.90
1:I:399:PHE:HE2	1:I:417:PHE:CG	1.88	0.90
1:K:301:LEU:HD23	1:K:334:ARG:NH1	1.86	0.90
1:G:231:SER:HB2	1:G:268:THR:HB	1.53	0.89
1:K:219:ALA:O	1:K:225:ASP:CA	2.21	0.89
1:A:165:ILE:HA	1:A:168:ILE:HD12	1.53	0.89
1:K:227:HIS:C	1:K:228:GLU:OE2	2.15	0.89
1:K:110:ASN:HB3	1:K:111:ASP:CB	2.02	0.88
1:K:144:ASP:O	1:K:147:LEU:HD23	1.74	0.88
1:C:458:GLU:O	1:C:462:ASN:ND2	2.05	0.88
1:K:104:GLY:C	1:K:106:PRO:CD	2.47	0.88
1:A:218:MET:SD	1:A:218:MET:N	2.46	0.88
1:E:252:HIS:HA	1:E:255:LEU:HD23	1.56	0.88
1:C:150:VAL:CG1	1:C:231:SER:CB	2.52	0.88
1:A:154:SER:O	1:A:156:ALA:N	2.06	0.87
1:A:150:VAL:CG2	1:A:231:SER:OG	2.21	0.87
1:J:147:LEU:HA	1:J:148:GLU:HB2	1.57	0.87
1:L:233:PHE:CE2	1:L:234:LEU:C	2.51	0.87
1:A:476:ARG:NH2	1:B:464:ASP:OD2	2.07	0.87
1:K:106:PRO:HB2	1:K:107:GLU:OE2	1.72	0.87
1:L:203:LYS:HZ3	1:L:318:ALA:HB1	1.38	0.87
1:G:168:ILE:H	1:G:168:ILE:HD12	1.38	0.86
1:L:202:GLY:HA3	1:L:205:LEU:HG	1.55	0.86
1:G:202:GLY:O	1:G:204:THR:OG1	1.92	0.86
1:K:111:ASP:OD2	1:K:113:THR:OG1	1.92	0.86
1:H:242:LEU:HD12	1:H:242:LEU:H	1.39	0.86
1:H:298:PRO:CG	1:I:242:LEU:HD13	2.05	0.86
1:I:68:LEU:CD1	1:I:78:ALA:HB1	2.05	0.86
1:K:140:ALA:O	1:K:141:GLU:CG	2.18	0.86
1:K:110:ASN:CB	1:K:111:ASP:HB3	2.01	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:221:VAL:CG1	1:K:222:ARG:HD2	2.06	0.85
1:J:110:ASN:N	1:J:111:ASP:HA	1.89	0.85
1:A:150:VAL:HG21	1:A:231:SER:CA	1.98	0.84
1:L:434:ALA:O	1:L:438:VAL:HG23	1.77	0.84
1:G:148:GLU:O	1:G:233:PHE:HB3	1.76	0.84
1:K:150:VAL:HG13	1:K:231:SER:O	1.78	0.84
1:F:9:LEU:HD11	1:F:20:PHE:HB2	1.58	0.84
1:K:250:GLU:OE2	1:K:253:ILE:HD13	1.78	0.84
1:H:295:THR:HG22	1:H:296:VAL:H	1.42	0.84
1:I:139:LYS:HG2	1:I:140:ALA:H	1.41	0.84
1:K:223:GLY:H	1:K:224:ASP:HB2	1.41	0.83
1:K:207:ALA:O	1:K:210:VAL:HG13	1.77	0.83
1:F:393:GLU:OE2	1:F:415:LYS:NZ	2.11	0.83
1:G:69:ARG:O	1:G:70:GLU:HG3	1.79	0.83
1:J:70:GLU:HG2	1:J:71:ILE:N	1.93	0.82
1:E:68:LEU:HD11	1:E:78:ALA:HB1	1.59	0.82
1:A:399:PHE:HE2	1:A:417:PHE:CG	1.97	0.82
1:A:151:PRO:HB2	1:A:153:VAL:HG12	1.62	0.82
1:G:139:LYS:HZ3	1:G:142:VAL:HG21	1.41	0.82
1:I:146:VAL:HG21	1:I:256:ILE:HG22	1.62	0.82
1:B:147:LEU:HD23	1:B:147:LEU:O	1.79	0.82
1:A:399:PHE:CE2	1:A:417:PHE:CG	2.66	0.81
1:C:208:LYS:HG2	1:C:233:PHE:HE2	1.44	0.81
1:K:267:GLY:O	1:K:312:ASN:OD1	1.95	0.81
1:G:151:PRO:HD3	1:G:233:PHE:HB2	1.61	0.81
1:G:298:PRO:HG2	1:H:242:LEU:HB3	1.62	0.81
1:E:248:GLU:OE2	1:E:249:THR:OG1	1.98	0.81
1:F:254:ARG:NH1	1:F:299:GLN:HB2	1.95	0.81
1:H:69:ARG:O	1:H:120:PRO:HG3	1.79	0.81
1:H:300:LEU:HD12	1:H:300:LEU:H	1.44	0.81
1:C:237:LYS:HB2	1:C:239:PRO:HD2	1.63	0.81
1:H:293:GLU:HG3	1:H:294:THR:OG1	1.80	0.81
1:G:400:LEU:CD2	1:G:490:THR:HG22	2.10	0.81
1:H:299:GLN:OE1	1:H:300:LEU:CD1	2.28	0.81
1:K:177:LEU:HD21	1:K:217:LYS:CB	2.10	0.81
1:K:198:PRO:HG2	1:K:343:ARG:HG3	1.62	0.81
1:B:68:LEU:CD1	1:B:78:ALA:HB1	2.11	0.81
1:K:222:ARG:HB2	1:K:223:GLY:CA	2.11	0.80
1:K:222:ARG:O	1:K:225:ASP:HA	1.82	0.80
1:E:68:LEU:CD1	1:E:78:ALA:HB1	2.10	0.80
1:G:205:LEU:HD13	1:G:206:ILE:HG13	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HD11	1:A:20:PHE:HB2	1.61	0.80
1:K:177:LEU:HD11	1:K:217:LYS:HB3	1.64	0.80
1:G:147:LEU:CB	1:G:148:GLU:HB2	2.08	0.80
1:K:215:ALA:HB2	1:K:231:SER:HB2	1.63	0.80
1:J:264:ALA:HA	1:J:312:ASN:ND2	1.97	0.79
1:A:151:PRO:HG2	1:A:212:ASN:HB2	0.83	0.79
1:H:243:ASN:OD1	1:H:244:LYS:HG2	1.81	0.79
1:H:191:LYS:NZ	1:H:304:ILE:HG23	1.97	0.79
1:C:219:ALA:H	1:C:220:GLU:HA	1.48	0.79
1:H:68:LEU:HD13	1:H:78:ALA:HB1	1.64	0.79
1:F:241:LEU:HD12	1:F:242:LEU:H	1.48	0.79
1:G:148:GLU:CD	1:G:150:VAL:CG1	2.55	0.79
1:K:173:GLU:CD	1:K:213:SER:OG	2.26	0.79
1:A:150:VAL:CG1	1:A:232:TYR:CA	2.54	0.79
1:H:299:GLN:O	1:H:300:LEU:C	2.23	0.78
1:H:321:ARG:HH11	1:H:321:ARG:HB2	1.48	0.78
1:G:164:GLN:O	1:G:168:ILE:HG13	1.82	0.78
1:G:248:GLU:HB2	1:G:252:HIS:HB2	1.65	0.78
1:I:112:ASP:OD2	1:I:116:ARG:NH1	2.16	0.78
1:K:104:GLY:C	1:K:106:PRO:HD3	2.08	0.78
1:L:233:PHE:CD2	1:L:234:LEU:N	2.51	0.78
1:K:221:VAL:HG12	1:K:222:ARG:HD2	1.65	0.78
1:A:154:SER:O	1:A:155:TYR:C	2.27	0.78
1:A:150:VAL:CG1	1:A:231:SER:HA	2.13	0.78
1:A:399:PHE:CE2	1:A:417:PHE:CB	2.67	0.78
1:H:299:GLN:O	1:H:301:LEU:N	2.17	0.78
1:I:142:VAL:HG11	1:I:255:LEU:HB3	1.66	0.77
1:C:220:GLU:HG2	1:C:227:HIS:CB	2.14	0.77
1:A:250:GLU:HB2	1:A:253:ILE:HD11	1.67	0.77
1:B:437:SER:O	1:B:441:THR:CG2	2.31	0.77
1:A:151:PRO:HB3	1:A:208:LYS:HB3	1.66	0.77
1:G:254:ARG:HH12	1:G:299:GLN:HB2	1.49	0.77
1:C:400:LEU:HD12	1:C:412:MET:HG3	1.66	0.76
1:L:69:ARG:HG2	1:L:69:ARG:NH1	1.96	0.76
1:H:105:LEU:HD22	1:H:106:PRO:HD3	1.66	0.76
1:E:386:VAL:HG23	1:E:455:ILE:HD11	1.67	0.76
1:K:177:LEU:HD21	1:K:217:LYS:HB2	1.65	0.76
1:I:147:LEU:HD13	1:I:148:GLU:HB3	1.68	0.76
1:G:164:GLN:O	1:G:168:ILE:CG1	2.34	0.76
1:A:176:PHE:HD2	1:A:177:LEU:HD12	1.49	0.75
1:K:109:LEU:HD22	1:K:110:ASN:OD1	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:112:ASP:HB3	1:K:136:ARG:NH1	2.02	0.75
1:A:223:GLY:N	1:A:224:ASP:HB2	2.02	0.75
1:B:150:VAL:H	1:B:233:PHE:HB3	1.51	0.75
1:D:254:ARG:HH22	1:D:299:GLN:HB3	1.52	0.75
1:J:116:ARG:NH1	1:J:119:ARG:NE	2.35	0.75
1:B:150:VAL:CA	1:B:233:PHE:HB3	2.17	0.75
1:K:268:THR:O	1:K:312:ASN:ND2	2.19	0.75
1:G:149:GLU:HB3	1:G:232:TYR:HB3	1.67	0.75
1:I:141:GLU:HB3	1:I:145:LEU:HD13	1.67	0.75
1:K:145:LEU:HD22	1:K:146:VAL:H	1.51	0.75
1:K:214:LEU:O	1:K:214:LEU:HD23	1.87	0.75
1:H:298:PRO:HG2	1:I:242:LEU:HD13	1.67	0.74
1:B:118:LEU:HD22	1:B:136:ARG:HG3	1.67	0.74
1:G:400:LEU:HD21	1:G:490:THR:HG22	1.67	0.74
1:D:270:VAL:HB	1:D:313:VAL:HG22	1.69	0.74
1:J:254:ARG:HH12	1:J:299:GLN:HB3	1.53	0.74
1:B:191:LYS:HE2	1:B:308:GLU:HG3	1.70	0.74
1:G:205:LEU:O	1:G:209:ALA:N	2.19	0.74
1:K:112:ASP:HB3	1:K:136:ARG:HH12	1.53	0.74
1:G:148:GLU:O	1:G:233:PHE:C	2.31	0.74
1:G:204:THR:O	1:G:208:LYS:HG3	1.88	0.74
1:G:205:LEU:HD12	1:G:205:LEU:N	2.01	0.74
1:A:154:SER:O	1:A:157:ASP:N	2.17	0.74
1:H:298:PRO:HG2	1:I:242:LEU:CD2	2.17	0.74
1:I:146:VAL:HG21	1:I:256:ILE:CG2	2.17	0.74
1:A:194:LEU:HD22	1:A:330:LEU:HD11	1.69	0.74
1:B:150:VAL:N	1:B:233:PHE:HB3	2.01	0.73
1:B:147:LEU:HB2	1:B:148:GLU:OE1	1.87	0.73
1:J:194:LEU:HD22	1:J:330:LEU:HD11	1.70	0.73
1:K:249:THR:HA	1:K:250:GLU:HB3	0.82	0.73
1:G:202:GLY:C	1:G:204:THR:OG1	2.32	0.73
1:K:207:ALA:O	1:K:210:VAL:CG1	2.37	0.73
1:E:241:LEU:HD12	1:E:242:LEU:H	1.54	0.73
1:H:295:THR:HG22	1:H:296:VAL:N	2.03	0.72
1:H:296:VAL:CG1	1:I:242:LEU:HD11	2.18	0.72
1:K:106:PRO:C	1:K:107:GLU:OE2	2.32	0.72
1:L:400:LEU:HD11	1:L:412:MET:CB	2.17	0.72
1:B:165:ILE:HA	1:B:168:ILE:HD12	1.70	0.72
1:C:69:ARG:O	1:C:70:GLU:HG3	1.89	0.72
1:G:299:GLN:HB3	1:H:242:LEU:HD23	1.70	0.72
1:F:254:ARG:HH12	1:F:299:GLN:HB2	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:CG1	1:A:231:SER:CA	2.67	0.72
1:D:20:PHE:CD1	1:D:25:LYS:HD3	2.24	0.72
1:F:202:GLY:O	1:F:205:LEU:N	2.22	0.72
1:J:264:ALA:CA	1:J:312:ASN:HD22	2.01	0.72
1:A:150:VAL:CG1	1:A:232:TYR:HB2	2.20	0.72
1:F:147:LEU:HD12	1:F:147:LEU:N	2.04	0.72
1:G:148:GLU:CD	1:G:150:VAL:HG11	2.11	0.72
1:G:153:VAL:HG11	1:G:205:LEU:HB2	1.72	0.72
1:G:168:ILE:HD12	1:G:168:ILE:N	2.05	0.72
1:I:217:LYS:HZ3	1:I:269:PRO:HG3	1.54	0.72
1:A:244:LYS:NZ	1:A:249:THR:HG23	2.03	0.72
1:G:148:GLU:HG2	1:G:150:VAL:CG1	2.14	0.72
1:G:206:ILE:O	1:G:209:ALA:HB3	1.90	0.72
1:I:194:LEU:HD22	1:I:330:LEU:HD11	1.72	0.72
1:A:150:VAL:CB	1:A:231:SER:HA	2.18	0.71
1:A:234:LEU:HD22	1:A:272:VAL:HA	1.70	0.71
1:G:205:LEU:CD1	1:G:206:ILE:HG13	2.19	0.71
1:A:151:PRO:CB	1:A:208:LYS:HB3	2.18	0.71
1:B:296:VAL:HG12	1:B:297:VAL:H	1.54	0.71
1:G:194:LEU:HB2	1:G:335:LEU:HD23	1.72	0.71
1:G:68:LEU:HD12	1:G:80:VAL:HG12	1.70	0.71
1:H:194:LEU:HD22	1:H:330:LEU:HD11	1.72	0.71
1:J:108:ALA:HB1	1:J:111:ASP:O	1.89	0.71
1:A:241:LEU:HD12	1:A:242:LEU:H	1.56	0.71
1:I:244:LYS:N	1:I:245:PHE:HA	2.05	0.71
1:I:400:LEU:CD2	1:I:490:THR:HG22	2.20	0.71
1:D:434:ALA:O	1:D:438:VAL:HG23	1.91	0.71
1:E:198:PRO:HG2	1:E:343:ARG:HG3	1.72	0.71
1:J:109:LEU:H	1:J:110:ASN:C	1.97	0.71
1:A:151:PRO:CG	1:A:208:LYS:O	2.35	0.71
1:G:201:CYS:HB3	1:G:202:GLY:HA2	1.73	0.71
1:F:177:LEU:HD11	1:F:217:LYS:HE3	1.73	0.71
1:J:191:LYS:HE2	1:J:308:GLU:HA	1.71	0.71
1:L:233:PHE:HE2	1:L:235:ASN:HB2	1.54	0.71
1:H:242:LEU:HD12	1:H:242:LEU:N	2.05	0.71
1:J:263:LYS:HZ3	1:J:263:LYS:H	1.39	0.71
1:K:230:LYS:HA	1:K:230:LYS:CE	2.06	0.70
1:H:191:LYS:HZ2	1:H:304:ILE:HG23	1.56	0.70
1:K:223:GLY:N	1:K:224:ASP:HB2	2.05	0.70
1:L:198:PRO:CB	1:L:343:ARG:HE	2.04	0.70
1:C:364:HIS:NE2	1:C:366:ASP:OD2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:TYR:HB3	1:E:134:PHE:CZ	2.26	0.70
1:F:340:LYS:HE2	1:F:342:GLU:HB3	1.72	0.70
1:I:169:ARG:O	1:I:173:GLU:HB2	1.92	0.70
1:J:298:PRO:HA	1:J:301:LEU:HD13	1.72	0.70
1:A:244:LYS:HZ3	1:A:249:THR:HG23	1.56	0.70
1:H:191:LYS:HE3	1:H:304:ILE:O	1.91	0.70
1:H:296:VAL:CB	1:I:242:LEU:HD21	2.19	0.70
1:I:147:LEU:HB2	1:I:148:GLU:HA	1.74	0.70
1:I:297:VAL:HG13	1:I:298:PRO:HD3	1.72	0.70
1:L:233:PHE:CG	1:L:234:LEU:N	2.59	0.70
1:C:132:TYR:CB	1:C:134:PHE:CE1	2.55	0.70
1:G:164:GLN:O	1:G:168:ILE:HD12	1.92	0.70
1:H:140:ALA:H	1:H:142:VAL:HG23	1.56	0.70
1:L:470:ASN:ND2	1:L:472:ASP:HB3	2.06	0.70
1:A:132:TYR:HB3	1:A:134:PHE:CE1	2.27	0.69
1:G:69:ARG:C	1:G:70:GLU:HG3	2.14	0.69
1:A:150:VAL:HG11	1:A:231:SER:C	2.12	0.69
1:H:299:GLN:HE22	1:H:300:LEU:CD1	2.05	0.69
1:J:105:LEU:O	1:J:108:ALA:N	2.20	0.69
1:B:9:LEU:HD11	1:B:20:PHE:HB2	1.74	0.69
1:G:148:GLU:HG2	1:G:150:VAL:HG22	1.73	0.69
1:K:109:LEU:CD1	1:K:148:GLU:OE2	2.32	0.69
1:F:191:LYS:HZ1	1:F:304:ILE:HG22	1.58	0.69
1:L:250:GLU:HA	1:L:253:ILE:HD13	1.73	0.69
1:C:191:LYS:HE2	1:C:308:GLU:HG3	1.74	0.69
1:A:140:ALA:C	1:A:142:VAL:H	2.01	0.69
1:F:162:SER:HA	1:F:165:ILE:HG12	1.75	0.69
1:G:231:SER:OG	1:G:232:TYR:N	2.25	0.69
1:I:399:PHE:CD2	1:I:417:PHE:CG	2.81	0.69
1:J:147:LEU:HA	1:J:148:GLU:CB	2.22	0.69
1:K:215:ALA:HB2	1:K:231:SER:CB	2.23	0.69
1:K:219:ALA:C	1:K:226:ALA:N	2.46	0.69
1:K:14:ASP:OD2	1:K:16:THR:OG1	2.07	0.69
1:K:340:LYS:HE2	1:K:342:GLU:HB3	1.73	0.69
1:B:68:LEU:O	1:B:120:PRO:HA	1.93	0.69
1:K:109:LEU:CD1	1:K:148:GLU:CD	2.62	0.69
1:J:108:ALA:HB1	1:J:111:ASP:C	2.17	0.68
1:J:116:ARG:NH1	1:J:119:ARG:CZ	2.55	0.68
1:L:470:ASN:HD21	1:L:472:ASP:HB3	1.58	0.68
1:C:24:ARG:HH11	1:C:25:LYS:HD2	1.56	0.68
1:G:147:LEU:HD23	1:G:148:GLU:OE2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:116:ARG:HD2	1:J:119:ARG:NH2	2.09	0.68
1:C:165:ILE:HA	1:C:168:ILE:HD12	1.76	0.68
1:H:299:GLN:NE2	1:H:300:LEU:HD12	2.07	0.68
1:J:438:VAL:HG22	1:J:444:PRO:HA	1.75	0.68
1:L:400:LEU:HD12	1:L:412:MET:HB2	1.74	0.68
1:H:165:ILE:HA	1:H:168:ILE:HD12	1.74	0.68
1:L:81:VAL:HG23	1:L:87:GLU:HG2	1.75	0.68
1:K:109:LEU:HG	1:K:148:GLU:HB3	1.76	0.68
1:D:254:ARG:HH11	1:D:254:ARG:CG	2.05	0.68
1:L:418:ASN:HD21	1:L:423:ILE:HD11	1.59	0.68
1:A:429:ARG:NH2	1:A:458:GLU:OE1	2.25	0.68
1:H:147:LEU:HD23	1:H:148:GLU:OE2	1.93	0.68
1:E:438:VAL:HG22	1:E:444:PRO:HA	1.76	0.68
1:K:218:MET:C	1:K:221:VAL:HG23	2.18	0.68
1:A:146:VAL:HG22	1:A:148:GLU:O	1.94	0.68
1:G:146:VAL:O	1:G:147:LEU:HG	1.94	0.68
1:J:69:ARG:HD2	1:J:81:VAL:HG23	1.76	0.68
1:E:418:ASN:OD1	1:E:419:SER:N	2.27	0.67
1:J:105:LEU:HD12	1:J:262:GLU:HG2	1.76	0.67
1:H:243:ASN:OD1	1:H:244:LYS:N	2.27	0.67
1:K:111:ASP:HB2	1:K:143:GLU:OE1	1.95	0.67
1:I:399:PHE:HD2	1:I:417:PHE:CD1	2.12	0.67
1:G:143:GLU:O	1:G:144:ASP:CB	2.43	0.67
1:J:362:PRO:O	1:J:445:GLY:HA2	1.95	0.67
1:C:400:LEU:HD12	1:C:412:MET:HB2	1.75	0.67
1:C:400:LEU:HD12	1:C:412:MET:CG	2.24	0.67
1:K:111:ASP:CA	1:K:143:GLU:OE1	2.43	0.67
1:A:149:GLU:N	1:A:149:GLU:OE1	2.28	0.67
1:K:340:LYS:HD2	1:L:464:ASP:OD2	1.94	0.67
1:J:429:ARG:NH2	1:J:458:GLU:OE1	2.27	0.67
1:K:171:ALA:HB1	1:K:337:VAL:HG21	1.76	0.67
1:K:191:LYS:HD2	1:K:307:VAL:HG13	1.75	0.66
1:E:201:CYS:SG	1:E:343:ARG:HA	2.34	0.66
1:F:145:LEU:HD21	1:F:256:ILE:HG22	1.76	0.66
1:F:152:ASP:OD1	1:F:153:VAL:N	2.28	0.66
1:I:165:ILE:HA	1:I:168:ILE:HD12	1.78	0.66
1:E:298:PRO:HB2	1:F:243:ASN:HB3	1.76	0.66
1:G:438:VAL:HG22	1:G:444:PRO:HA	1.75	0.66
1:A:252:HIS:HA	1:A:255:LEU:HD23	1.78	0.66
1:J:301:LEU:HD23	1:J:334:ARG:HH12	1.58	0.66
1:D:254:ARG:HH11	1:D:254:ARG:HG3	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:84:ALA:O	1:K:83:HIS:CD2	2.48	0.66
1:C:311:GLU:O	1:C:313:VAL:N	2.28	0.66
1:K:245:PHE:N	1:K:249:THR:O	2.28	0.66
1:G:148:GLU:O	1:G:233:PHE:CB	2.43	0.66
1:A:399:PHE:C	1:A:400:LEU:HG	2.21	0.66
1:C:24:ARG:NH1	1:C:25:LYS:HD2	2.11	0.66
1:K:268:THR:O	1:K:312:ASN:CG	2.39	0.66
1:C:196:TYR:HB2	1:C:322:GLU:HG2	1.78	0.66
1:B:399:PHE:CD1	1:B:414:PHE:CE1	2.84	0.65
1:J:244:LYS:NZ	1:J:246:VAL:O	2.22	0.65
1:K:295:THR:HB	1:K:296:VAL:HA	1.78	0.65
1:B:149:GLU:OE1	1:B:150:VAL:HG23	1.96	0.65
1:D:234:LEU:O	1:D:235:ASN:ND2	2.28	0.65
1:E:72:LEU:HD11	1:E:77:ARG:HB2	1.79	0.65
1:G:148:GLU:O	1:G:233:PHE:CA	2.44	0.65
1:J:109:LEU:HB2	1:J:110:ASN:CB	2.22	0.65
1:J:310:LEU:HD13	1:J:310:LEU:C	2.21	0.65
1:J:310:LEU:HD11	1:J:312:ASN:CB	2.25	0.65
1:K:268:THR:O	1:K:312:ASN:OD1	2.14	0.65
1:L:198:PRO:HG3	1:L:343:ARG:HG3	1.78	0.65
1:C:72:LEU:HD23	1:C:79:LEU:HB2	1.78	0.65
1:G:148:GLU:CD	1:G:150:VAL:HG13	2.18	0.65
1:B:437:SER:C	1:B:441:THR:HG22	2.20	0.65
1:J:69:ARG:HH21	1:K:139:LYS:NZ	1.94	0.65
1:A:154:SER:C	1:A:156:ALA:N	2.54	0.65
1:K:109:LEU:HD23	1:K:109:LEU:C	2.21	0.65
1:H:81:VAL:HG22	1:H:87:GLU:HG2	1.78	0.65
1:H:298:PRO:HG2	1:I:242:LEU:CG	2.27	0.65
1:H:298:PRO:HG3	1:I:242:LEU:HD13	1.79	0.65
1:L:233:PHE:CD1	1:L:271:ILE:HD13	2.25	0.65
1:C:400:LEU:CD1	1:C:412:MET:HG3	2.26	0.65
1:F:188:ARG:HD3	1:F:189:PRO:HD2	1.77	0.65
1:I:147:LEU:HB2	1:I:148:GLU:CA	2.27	0.65
1:A:188:ARG:HH12	1:G:219:ALA:HB2	1.62	0.65
1:E:231:SER:OG	1:E:269:PRO:O	2.14	0.65
1:G:243:ASN:ND2	1:L:299:GLN:OE1	2.30	0.64
1:L:470:ASN:OD1	1:L:473:ASP:OD2	2.14	0.64
1:I:437:SER:O	1:I:441:THR:HG22	1.98	0.64
1:K:222:ARG:CB	1:K:223:GLY:HA2	2.15	0.64
1:H:151:PRO:HB2	1:H:212:ASN:HB3	1.77	0.64
1:I:139:LYS:HG2	1:I:140:ALA:N	2.07	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:250:GLU:OE2	1:J:253:ILE:N	2.30	0.64
1:K:109:LEU:HG	1:K:148:GLU:CB	2.27	0.64
1:L:96:LEU:HD22	1:L:118:LEU:HD11	1.79	0.64
1:A:399:PHE:CD1	1:A:414:PHE:CZ	2.86	0.64
1:I:329:ILE:HG23	1:I:335:LEU:HD13	1.78	0.64
1:I:399:PHE:CE2	1:I:417:PHE:CD2	2.79	0.64
1:E:248:GLU:CD	1:E:249:THR:H	2.05	0.64
1:B:150:VAL:HG12	1:B:151:PRO:N	2.13	0.64
1:F:232:TYR:OH	1:F:271:ILE:O	2.16	0.64
1:I:243:ASN:C	1:I:245:PHE:HA	2.22	0.64
1:I:343:ARG:HD2	1:I:416:ASP:O	1.98	0.64
1:I:422:MET:HG3	1:I:458:GLU:OE2	1.97	0.64
1:J:340:LYS:HD2	1:K:464:ASP:OD2	1.98	0.64
1:K:221:VAL:HG12	1:K:222:ARG:CD	2.28	0.64
1:L:204:THR:HG22	1:L:273:PHE:CE2	2.33	0.64
1:C:449:GLN:NE2	1:C:453:ASP:OD2	2.30	0.64
1:E:271:ILE:HG23	1:E:314:ILE:HG22	1.79	0.63
1:J:296:VAL:O	1:J:299:GLN:NE2	2.30	0.63
1:J:168:ILE:HG12	1:J:339:ILE:HD13	1.80	0.63
1:L:9:LEU:HD11	1:L:20:PHE:HB2	1.79	0.63
1:L:69:ARG:HH12	1:L:87:GLU:CD	2.04	0.63
1:G:205:LEU:HD12	1:G:205:LEU:H	1.62	0.63
1:I:298:PRO:HA	1:I:301:LEU:HD13	1.79	0.63
1:J:108:ALA:O	1:J:109:LEU:HD12	1.99	0.63
1:C:177:LEU:HD21	1:C:218:MET:HB2	1.79	0.63
1:A:13:ASP:OD1	1:A:13:ASP:N	2.31	0.63
1:C:321:ARG:HG2	1:C:324:MET:HG2	1.79	0.63
1:C:367:ASP:OD2	1:C:447:ARG:HA	1.99	0.63
1:F:239:PRO:HD3	1:F:276:GLU:HG3	1.80	0.63
1:G:146:VAL:C	1:G:147:LEU:HD12	2.22	0.63
1:K:310:LEU:O	1:K:312:ASN:N	2.31	0.63
1:G:158:ILE:CG2	1:G:206:ILE:HG12	2.27	0.63
1:H:215:ALA:HA	1:H:231:SER:HB3	1.81	0.63
1:J:83:HIS:CE1	1:J:86:GLU:OE1	2.51	0.63
1:K:244:LYS:O	1:K:250:GLU:N	2.32	0.63
1:L:262:GLU:HB3	1:L:263:LYS:HZ2	1.63	0.63
1:B:248:GLU:HG2	1:B:250:GLU:HB3	1.80	0.63
1:F:434:ALA:O	1:F:438:VAL:HG23	1.98	0.63
1:H:242:LEU:CD1	1:H:246:VAL:HG11	2.29	0.63
1:B:149:GLU:HA	1:B:234:LEU:HA	1.81	0.63
1:G:143:GLU:O	1:G:144:ASP:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:441:THR:HG23	1:I:443:GLN:HG3	1.81	0.63
1:G:158:ILE:HG21	1:G:206:ILE:HG21	1.81	0.62
1:G:205:LEU:CD1	1:G:206:ILE:H	2.12	0.62
1:G:244:LYS:HA	1:G:244:LYS:NZ	2.14	0.62
1:J:297:VAL:HG13	1:J:298:PRO:HD3	1.80	0.62
1:A:72:LEU:HB2	1:B:139:LYS:HZ1	1.64	0.62
1:D:241:LEU:HD12	1:D:242:LEU:H	1.64	0.62
1:G:149:GLU:HA	1:G:233:PHE:H	1.64	0.62
1:K:144:ASP:O	1:K:147:LEU:CD2	2.46	0.62
1:G:170:ASP:OD1	1:G:170:ASP:N	2.32	0.62
1:H:298:PRO:HG2	1:I:242:LEU:CD1	2.29	0.62
1:J:119:ARG:HD2	1:J:258:GLN:NE2	2.15	0.62
1:K:251:ARG:O	1:K:252:HIS:CG	2.52	0.62
1:J:109:LEU:HG	1:J:232:TYR:OH	1.99	0.62
1:E:398:ARG:HG2	1:E:413:TYR:HE1	1.64	0.62
1:H:198:PRO:O	1:H:200:GLY:HA2	1.99	0.62
1:I:399:PHE:CD2	1:I:417:PHE:CD1	2.88	0.62
1:K:227:HIS:O	1:K:228:GLU:OE2	2.17	0.62
1:L:398:ARG:HG3	1:L:491:LEU:HD12	1.79	0.62
1:B:68:LEU:HD13	1:B:78:ALA:HB1	1.82	0.62
1:J:108:ALA:C	1:J:109:LEU:HD12	2.24	0.62
1:K:248:GLU:OE1	1:K:248:GLU:N	2.33	0.62
1:C:203:LYS:HD2	1:C:318:ALA:HB1	1.81	0.62
1:I:142:VAL:HG12	1:I:259:ARG:HD2	1.82	0.62
1:E:299:GLN:HG3	1:F:243:ASN:HB2	1.82	0.62
1:I:165:ILE:O	1:I:169:ARG:HG3	1.99	0.62
1:I:239:PRO:HD3	1:I:276:GLU:HG3	1.82	0.62
1:I:283:THR:OG1	1:I:284:ARG:N	2.33	0.62
1:K:229:ALA:CB	1:K:230:LYS:HB2	2.27	0.62
1:G:400:LEU:HD23	1:G:490:THR:HA	1.81	0.62
1:L:150:VAL:HG22	1:L:151:PRO:HD2	1.82	0.62
1:L:398:ARG:HG3	1:L:491:LEU:CD1	2.30	0.62
1:E:191:LYS:HD2	1:E:308:GLU:HA	1.80	0.61
1:G:493:THR:HG23	1:G:495:LYS:H	1.65	0.61
1:E:234:LEU:HB3	1:E:271:ILE:O	2.00	0.61
1:I:344:PRO:HD2	1:I:419:SER:HA	1.82	0.61
1:I:399:PHE:CE2	1:I:417:PHE:CB	2.82	0.61
1:C:490:THR:O	1:C:500:SER:OG	2.15	0.61
1:I:149:GLU:CG	1:I:150:VAL:H	2.13	0.61
1:K:250:GLU:OE2	1:K:253:ILE:CD1	2.48	0.61
1:J:476:ARG:NH2	1:K:464:ASP:OD1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:244:LYS:N	1:K:245:PHE:HA	2.14	0.61
1:L:278:ASP:N	1:L:278:ASP:OD1	2.23	0.61
1:G:205:LEU:O	1:G:209:ALA:HB2	2.00	0.61
1:J:236:ILE:HA	1:J:237:LYS:HZ1	1.66	0.61
1:J:244:LYS:N	1:J:245:PHE:HA	2.15	0.61
1:F:79:LEU:HD21	1:F:87:GLU:HB3	1.83	0.61
1:I:149:GLU:HG2	1:I:150:VAL:H	1.66	0.61
1:L:198:PRO:HG3	1:L:343:ARG:CG	2.31	0.61
1:A:146:VAL:O	1:A:148:GLU:O	2.18	0.61
1:E:298:PRO:HB3	1:F:239:PRO:O	2.00	0.61
1:F:232:TYR:CG	1:F:233:PHE:N	2.68	0.61
1:G:148:GLU:H	1:G:234:LEU:HA	1.66	0.61
1:I:164:GLN:HG2	1:I:341:ILE:HD13	1.82	0.61
1:I:170:ASP:O	1:I:175:PRO:HD3	2.00	0.61
1:J:215:ALA:O	1:J:231:SER:N	2.34	0.61
1:L:242:LEU:HA	1:L:243:ASN:C	2.25	0.61
1:B:46:ARG:NH1	1:B:55:GLU:OE1	2.33	0.61
1:G:464:ASP:OD2	1:L:340:LYS:HD3	2.00	0.61
1:H:177:LEU:HD11	1:H:217:LYS:HE2	1.83	0.61
1:F:191:LYS:NZ	1:F:304:ILE:HG22	2.15	0.61
1:H:300:LEU:H	1:H:300:LEU:CD1	2.13	0.61
1:K:141:GLU:O	1:K:145:LEU:N	2.29	0.61
1:K:221:VAL:C	1:K:222:ARG:HD2	2.25	0.61
1:L:262:GLU:HB3	1:L:263:LYS:NZ	2.15	0.61
1:F:151:PRO:HB3	1:F:233:PHE:CE2	2.35	0.60
1:I:142:VAL:HG11	1:I:255:LEU:HD12	1.83	0.60
1:E:252:HIS:O	1:E:255:LEU:N	2.30	0.60
1:F:244:LYS:HB3	1:F:247:GLY:H	1.65	0.60
1:L:244:LYS:N	1:L:245:PHE:HA	2.16	0.60
1:K:264:ALA:HA	1:K:312:ASN:HD22	1.65	0.60
1:E:471:PRO:HA	1:E:474:TRP:CD1	2.37	0.60
1:G:326:ASP:OD1	1:G:326:ASP:N	2.25	0.60
1:I:1:MET:HE2	1:I:49:GLU:HB2	1.83	0.60
1:I:69:ARG:O	1:I:120:PRO:HG3	2.01	0.60
1:K:146:VAL:O	1:K:146:VAL:HG22	2.02	0.60
1:K:217:LYS:O	1:K:221:VAL:CG2	2.50	0.60
1:H:467:ASN:H	1:H:467:ASN:HD22	1.49	0.60
1:A:399:PHE:CD2	1:A:417:PHE:CG	2.90	0.60
1:B:145:LEU:O	1:B:146:VAL:HG12	2.02	0.60
1:D:474:TRP:CD1	1:D:505:THR:HG1	2.20	0.60
1:E:68:LEU:O	1:E:120:PRO:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:PHE:HD2	1:B:417:PHE:CD1	2.19	0.60
1:G:141:GLU:HG3	1:G:141:GLU:O	2.00	0.60
1:J:69:ARG:HB2	1:J:79:LEU:O	2.01	0.60
1:L:238:GLY:HA3	1:L:276:GLU:HB2	1.83	0.60
1:D:399:PHE:HB2	1:D:414:PHE:CD2	2.37	0.60
1:E:203:LYS:HB3	1:E:205:LEU:HG	1.84	0.60
1:H:296:VAL:HG23	1:I:242:LEU:CD2	2.14	0.60
1:K:206:ILE:O	1:K:210:VAL:HG12	2.01	0.60
1:D:164:GLN:HG2	1:D:341:ILE:HD13	1.83	0.60
1:G:295:THR:N	1:H:243:ASN:HD22	2.00	0.60
1:K:176:PHE:CD2	1:K:214:LEU:HD11	2.37	0.60
1:E:84:ALA:HB3	1:E:86:GLU:OE2	2.01	0.59
1:H:296:VAL:HG21	1:I:242:LEU:CG	2.32	0.59
1:B:147:LEU:HD23	1:B:147:LEU:C	2.25	0.59
1:F:270:VAL:HB	1:F:313:VAL:HG22	1.84	0.59
1:A:233:PHE:CG	1:A:234:LEU:N	2.71	0.59
1:D:8:LEU:HD13	1:D:17:VAL:HG13	1.83	0.59
1:I:158:ILE:HD13	1:I:206:ILE:HD13	1.82	0.59
1:J:139:LYS:HE2	1:J:259:ARG:HH21	1.68	0.59
1:K:226:ALA:HB1	1:K:227:HIS:HA	1.83	0.59
1:K:295:THR:CB	1:K:296:VAL:HA	2.32	0.59
1:L:264:ALA:HB1	1:L:310:LEU:HD21	1.84	0.59
1:J:310:LEU:HD11	1:J:312:ASN:HB3	1.83	0.59
1:K:111:ASP:CB	1:K:143:GLU:OE1	2.50	0.59
1:K:247:GLY:C	1:K:248:GLU:OE1	2.44	0.59
1:C:201:CYS:O	1:C:203:LYS:HG2	2.02	0.59
1:E:249:THR:O	1:E:250:GLU:HG3	2.02	0.59
1:G:149:GLU:C	1:G:151:PRO:HD2	2.28	0.59
1:K:111:ASP:HA	1:K:143:GLU:OE1	2.03	0.59
1:A:17:VAL:HG12	1:A:19:VAL:HG23	1.84	0.59
1:A:301:LEU:HD23	1:A:334:ARG:HH12	1.67	0.59
1:G:153:VAL:HG23	1:G:157:ASP:OD2	2.02	0.59
1:H:164:GLN:HG2	1:H:341:ILE:HD13	1.85	0.59
1:J:203:LYS:NZ	1:J:320:ASN:HA	2.17	0.59
1:E:9:LEU:HD21	1:E:20:PHE:HB2	1.82	0.59
1:D:203:LYS:HA	1:D:206:ILE:HD13	1.85	0.59
1:E:168:ILE:HG12	1:E:339:ILE:HD13	1.83	0.59
1:F:231:SER:O	1:F:232:TYR:HD2	1.86	0.59
1:K:292:VAL:N	1:K:293:GLU:HA	2.17	0.59
1:A:151:PRO:CG	1:A:212:ASN:CB	2.58	0.59
1:G:11:THR:HA	1:G:17:VAL:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:LEU:HD13	1:J:146:VAL:HB	1.84	0.59
1:J:231:SER:OG	1:J:269:PRO:O	2.16	0.59
1:A:399:PHE:HE2	1:A:417:PHE:CD2	2.19	0.59
1:J:119:ARG:HD2	1:J:258:GLN:HE21	1.67	0.59
1:J:237:LYS:H	1:J:237:LYS:NZ	2.01	0.59
1:J:496:SER:OG	1:J:497:SER:N	2.35	0.59
1:G:401:GLU:OE1	1:G:489:ARG:NE	2.31	0.58
1:K:9:LEU:HD11	1:K:20:PHE:CB	2.27	0.58
1:K:219:ALA:O	1:K:225:ASP:C	2.45	0.58
1:G:203:LYS:HD2	1:G:203:LYS:N	2.18	0.58
1:I:68:LEU:HD11	1:I:78:ALA:HB1	1.85	0.58
1:J:110:ASN:HA	1:J:143:GLU:OE2	2.03	0.58
1:A:65:ILE:HB	1:F:87:GLU:HB2	1.86	0.58
1:C:400:LEU:HD12	1:C:412:MET:CB	2.32	0.58
1:E:198:PRO:HG2	1:E:343:ARG:CG	2.32	0.58
1:H:173:GLU:OE2	1:H:213:SER:OG	2.18	0.58
1:J:270:VAL:HG12	1:J:313:VAL:HG22	1.84	0.58
1:K:203:LYS:HG2	1:K:318:ALA:HB1	1.85	0.58
1:L:147:LEU:HB2	1:L:148:GLU:HB2	1.85	0.58
1:C:202:GLY:HA2	1:C:203:LYS:HB2	1.85	0.58
1:C:322:GLU:OE1	1:D:501:ARG:NH2	2.31	0.58
1:H:242:LEU:O	1:H:242:LEU:HD13	2.03	0.58
1:L:72:LEU:HD12	1:L:74:ASP:H	1.66	0.58
1:C:163:ARG:NH1	1:C:342:GLU:OE2	2.36	0.58
1:E:203:LYS:HG2	1:E:204:THR:H	1.68	0.58
1:J:195:LEU:HD22	1:J:341:ILE:HD11	1.85	0.58
1:B:493:THR:HG23	1:B:495:LYS:H	1.68	0.58
1:J:69:ARG:HH21	1:K:139:LYS:HZ3	1.49	0.58
1:J:114:ARG:O	1:J:136:ARG:NH2	2.36	0.58
1:K:105:LEU:HD12	1:K:105:LEU:O	2.04	0.58
1:A:280:ILE:HG22	1:A:281:PHE:CD2	2.39	0.58
1:D:232:TYR:OH	1:D:234:LEU:HB3	2.04	0.58
1:H:299:GLN:NE2	1:H:300:LEU:CD1	2.66	0.58
1:B:276:GLU:O	1:B:279:SER:OG	2.21	0.58
1:I:301:LEU:HD23	1:I:334:ARG:HH12	1.69	0.58
1:J:406:ASN:HB3	1:J:483:GLU:OE2	2.04	0.58
1:K:214:LEU:HD23	1:K:214:LEU:C	2.28	0.58
1:C:211:ALA:HB2	1:C:271:ILE:HD11	1.85	0.58
1:C:362:PRO:O	1:C:445:GLY:HA2	2.04	0.58
1:G:244:LYS:HZ1	1:L:299:GLN:HA	1.68	0.58
1:I:323:ASP:OD1	1:I:323:ASP:N	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:109:LEU:HB2	1:K:148:GLU:HG3	1.86	0.58
1:D:254:ARG:HG3	1:D:254:ARG:NH1	2.18	0.57
1:G:148:GLU:HG3	1:G:150:VAL:CG1	2.18	0.57
1:I:141:GLU:HB3	1:I:145:LEU:HD22	1.85	0.57
1:K:8:LEU:HD21	1:K:39:LEU:HB3	1.86	0.57
1:A:402:VAL:HG22	1:A:488:ILE:HG12	1.85	0.57
1:J:1:MET:HG3	1:J:2:PRO:HA	1.86	0.57
1:K:104:GLY:C	1:K:106:PRO:HD2	2.28	0.57
1:A:87:GLU:HB2	1:B:65:ILE:HB	1.86	0.57
1:G:68:LEU:HB2	1:G:80:VAL:HG12	1.86	0.57
1:K:242:LEU:HG	1:K:243:ASN:HA	1.86	0.57
1:F:191:LYS:NZ	1:F:304:ILE:O	2.30	0.57
1:K:249:THR:CB	1:K:250:GLU:HB3	2.33	0.57
1:A:146:VAL:HG22	1:A:146:VAL:O	2.04	0.57
1:A:399:PHE:HD2	1:A:417:PHE:CD1	2.22	0.57
1:C:301:LEU:HG	1:C:334:ARG:NH1	2.19	0.57
1:G:148:GLU:HG2	1:G:150:VAL:CG2	2.35	0.57
1:H:300:LEU:HD12	1:H:300:LEU:N	2.15	0.57
1:I:271:ILE:HG23	1:I:314:ILE:HG22	1.85	0.57
1:A:148:GLU:CB	1:A:149:GLU:HB3	2.25	0.57
1:B:161:LEU:HB3	1:B:164:GLN:HB2	1.87	0.57
1:C:220:GLU:OE2	1:C:227:HIS:CB	2.52	0.57
1:F:492:VAL:HG22	1:F:500:SER:HB3	1.86	0.57
1:H:198:PRO:O	1:H:203:LYS:NZ	2.38	0.57
1:I:147:LEU:CD1	1:I:148:GLU:HB3	2.35	0.57
1:K:243:ASN:C	1:K:245:PHE:HA	2.30	0.57
1:E:3:SER:OG	1:E:46:ARG:NH1	2.36	0.57
1:E:4:GLY:O	1:E:46:ARG:HG3	2.04	0.57
1:G:244:LYS:HA	1:G:244:LYS:HZ2	1.69	0.57
1:I:145:LEU:O	1:I:146:VAL:HG12	2.04	0.57
1:G:471:PRO:HA	1:G:474:TRP:CD1	2.39	0.57
1:I:68:LEU:O	1:I:120:PRO:HA	2.05	0.57
1:J:105:LEU:HD22	1:J:106:PRO:HA	1.86	0.57
1:K:217:LYS:O	1:K:221:VAL:HG23	2.04	0.57
1:A:226:ALA:HB3	1:A:227:HIS:HA	1.87	0.57
1:A:330:LEU:HG	1:A:338:LYS:HE2	1.86	0.57
1:C:188:ARG:HD3	1:C:191:LYS:NZ	2.20	0.57
1:F:146:VAL:HB	1:F:234:LEU:HD12	1.86	0.57
1:K:298:PRO:HA	1:K:301:LEU:HD13	1.86	0.57
1:B:437:SER:O	1:B:441:THR:N	2.36	0.57
1:D:23:GLY:C	1:D:24:ARG:CG	2.78	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:301:LEU:HD23	1:I:334:ARG:NH1	2.20	0.57
1:K:227:HIS:C	1:K:228:GLU:CD	2.73	0.57
1:A:24:ARG:HH11	1:A:26:MET:HE3	1.70	0.56
1:D:250:GLU:HG2	1:D:251:ARG:N	2.20	0.56
1:J:441:THR:HG23	1:J:443:GLN:H	1.70	0.56
1:K:207:ALA:HA	1:K:210:VAL:CG1	2.35	0.56
1:A:228:GLU:OE2	1:A:229:ALA:N	2.38	0.56
1:D:237:LYS:HB2	1:D:239:PRO:HD2	1.87	0.56
1:E:164:GLN:O	1:E:168:ILE:HG13	2.04	0.56
1:J:3:SER:HB2	1:J:47:LEU:O	2.06	0.56
1:K:493:THR:HG23	1:K:495:LYS:H	1.70	0.56
1:A:399:PHE:HE2	1:A:417:PHE:CB	2.13	0.56
1:D:46:ARG:HG2	1:D:55:GLU:HB3	1.85	0.56
1:D:168:ILE:HG13	1:D:339:ILE:HD12	1.87	0.56
1:E:87:GLU:HG3	1:F:65:ILE:HB	1.85	0.56
1:E:262:GLU:HG3	1:E:263:LYS:HZ2	1.70	0.56
1:F:46:ARG:NH1	1:F:55:GLU:OE2	2.38	0.56
1:F:140:ALA:O	1:F:141:GLU:HG3	2.06	0.56
1:F:328:ALA:O	1:F:334:ARG:NH1	2.39	0.56
1:G:403:THR:HB	1:G:487:TYR:HB3	1.86	0.56
1:L:140:ALA:C	1:L:142:VAL:H	2.14	0.56
1:A:216:LYS:HZ3	1:A:216:LYS:N	2.03	0.56
1:G:198:PRO:HG2	1:G:343:ARG:CG	2.36	0.56
1:K:224:ASP:OD2	1:K:224:ASP:N	2.38	0.56
1:H:43:GLN:NE2	1:H:56:ALA:HB1	2.21	0.56
1:J:8:LEU:HD13	1:J:17:VAL:HG13	1.87	0.56
1:A:89:VAL:HG23	1:B:65:ILE:HD11	1.87	0.56
1:F:203:LYS:HA	1:F:206:ILE:HD12	1.86	0.56
1:G:231:SER:HB3	1:G:269:PRO:O	2.05	0.56
1:I:68:LEU:HD12	1:I:78:ALA:HB1	1.88	0.56
1:K:104:GLY:O	1:K:106:PRO:HD2	2.06	0.56
1:K:250:GLU:OE1	1:K:299:GLN:CB	2.53	0.56
1:B:399:PHE:CE2	1:B:417:PHE:CG	2.94	0.56
1:C:418:ASN:OD1	1:C:419:SER:N	2.32	0.56
1:D:343:ARG:NH2	1:D:473:ASP:OD2	2.38	0.56
1:C:219:ALA:N	1:C:220:GLU:HA	2.18	0.56
1:C:343:ARG:HD2	1:C:416:ASP:O	2.06	0.56
1:I:438:VAL:HG22	1:I:444:PRO:HA	1.88	0.56
1:H:296:VAL:C	1:H:298:PRO:HD3	2.31	0.56
1:I:399:PHE:O	1:I:400:LEU:HD23	2.06	0.56
1:J:386:VAL:HG11	1:J:451:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG11	1:A:231:SER:HA	1.87	0.56
1:D:175:PRO:HB3	1:D:189:PRO:HB3	1.88	0.56
1:D:363:VAL:HG13	1:D:368:LEU:HD11	1.88	0.56
1:F:147:LEU:HD12	1:F:147:LEU:H	1.70	0.56
1:H:191:LYS:NZ	1:H:307:VAL:CG1	2.68	0.56
1:H:398:ARG:HG2	1:H:413:TYR:CE1	2.41	0.56
1:J:245:PHE:N	1:J:249:THR:O	2.39	0.56
1:L:395:ASP:O	1:L:398:ARG:HD3	2.06	0.56
1:C:68:LEU:CD1	1:C:78:ALA:HB1	2.35	0.55
1:D:23:GLY:C	1:D:24:ARG:HG2	2.31	0.55
1:F:399:PHE:CD1	1:F:414:PHE:CZ	2.94	0.55
1:H:240:GLU:O	1:H:242:LEU:HG	2.06	0.55
1:K:112:ASP:N	1:K:143:GLU:OE1	2.37	0.55
1:D:70:GLU:OE2	1:E:140:ALA:N	2.37	0.55
1:F:165:ILE:HA	1:F:168:ILE:HD12	1.89	0.55
1:G:206:ILE:HA	1:G:209:ALA:HB3	1.88	0.55
1:H:298:PRO:CG	1:I:242:LEU:CD2	2.68	0.55
1:I:14:ASP:O	1:I:15:ASP:HB2	2.05	0.55
1:I:233:PHE:CG	1:I:234:LEU:N	2.73	0.55
1:J:243:ASN:C	1:J:245:PHE:HA	2.32	0.55
1:K:114:ARG:HG2	1:K:115:PRO:HD2	1.87	0.55
1:E:237:LYS:HG3	1:E:239:PRO:HD2	1.88	0.55
1:E:270:VAL:HG12	1:E:313:VAL:HG22	1.89	0.55
1:H:43:GLN:HE21	1:H:57:GLY:H	1.55	0.55
1:H:196:TYR:CZ	1:H:340:LYS:HB2	2.41	0.55
1:H:438:VAL:HG22	1:H:444:PRO:HA	1.88	0.55
1:L:232:TYR:O	1:L:270:VAL:HG23	2.05	0.55
1:C:251:ARG:HA	1:C:251:ARG:HH11	1.71	0.55
1:G:68:LEU:O	1:G:120:PRO:HA	2.07	0.55
1:G:146:VAL:O	1:G:146:VAL:HG23	2.06	0.55
1:J:232:TYR:CE2	1:J:263:LYS:HD3	2.40	0.55
1:K:237:LYS:HB2	1:K:239:PRO:HD2	1.87	0.55
1:L:418:ASN:HA	1:L:422:MET:HE2	1.89	0.55
1:F:191:LYS:NZ	1:F:305:ASP:HA	2.21	0.55
1:G:3:SER:OG	1:G:47:LEU:O	2.24	0.55
1:C:307:VAL:HG21	1:C:313:VAL:HG11	1.89	0.55
1:D:362:PRO:O	1:D:445:GLY:HA2	2.07	0.55
1:F:204:THR:HG22	1:F:208:LYS:HE2	1.89	0.55
1:H:246:VAL:HG22	1:H:247:GLY:H	1.71	0.55
1:I:183:ARG:HG2	1:I:183:ARG:HH11	1.72	0.55
1:J:264:ALA:C	1:J:312:ASN:HD22	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:471:PRO:HA	1:L:474:TRP:CD1	2.42	0.55
1:C:27:ARG:HB2	1:D:5:TYR:HE2	1.70	0.55
1:G:147:LEU:HD12	1:G:147:LEU:N	2.21	0.55
1:G:329:ILE:HG22	1:G:330:LEU:HD12	1.89	0.55
1:H:242:LEU:HD12	1:H:246:VAL:HG11	1.88	0.55
1:J:246:VAL:HG12	1:J:247:GLY:H	1.72	0.55
1:C:220:GLU:CG	1:C:227:HIS:CB	2.84	0.55
1:G:168:ILE:CD1	1:G:168:ILE:H	2.03	0.55
1:K:229:ALA:CA	1:K:230:LYS:CB	2.37	0.55
1:G:158:ILE:HG21	1:G:206:ILE:CG2	2.37	0.55
1:J:203:LYS:NZ	1:J:319:SER:O	2.40	0.55
1:B:252:HIS:HA	1:B:255:LEU:HG	1.89	0.55
1:C:191:LYS:HE3	1:C:308:GLU:O	2.07	0.55
1:C:232:TYR:C	1:C:270:VAL:HG12	2.32	0.55
1:E:247:GLY:O	1:E:250:GLU:HB2	2.07	0.55
1:G:296:VAL:HG12	1:G:298:PRO:HD3	1.88	0.55
1:H:278:ASP:OD1	1:H:278:ASP:N	2.35	0.55
1:J:9:LEU:HD11	1:J:20:PHE:HB2	1.89	0.55
1:B:173:GLU:HG2	1:B:214:LEU:HB2	1.89	0.54
1:D:194:LEU:HD22	1:D:330:LEU:HD11	1.89	0.54
1:G:296:VAL:HG23	1:H:243:ASN:HB2	1.88	0.54
1:I:145:LEU:C	1:I:146:VAL:HG12	2.32	0.54
1:J:296:VAL:HB	1:J:299:GLN:HE22	1.73	0.54
1:K:214:LEU:CD2	1:K:218:MET:CE	2.85	0.54
1:A:114:ARG:HB3	1:A:115:PRO:HD2	1.90	0.54
1:J:164:GLN:O	1:J:168:ILE:HG13	2.08	0.54
1:K:203:LYS:N	1:K:206:ILE:HD13	2.22	0.54
1:K:296:VAL:HG23	1:K:298:PRO:HD2	1.88	0.54
1:A:198:PRO:HG3	1:A:343:ARG:HG3	1.89	0.54
1:B:328:ALA:HA	1:B:331:ARG:HD2	1.89	0.54
1:D:474:TRP:NE1	1:D:505:THR:OG1	2.41	0.54
1:D:482:GLY:HA2	1:E:489:ARG:HD3	1.89	0.54
1:I:164:GLN:O	1:I:168:ILE:HG13	2.08	0.54
1:K:268:THR:C	1:K:312:ASN:OD1	2.51	0.54
1:F:165:ILE:HG13	1:F:166:GLU:N	2.22	0.54
1:F:275:ASP:C	1:F:276:GLU:HG2	2.33	0.54
1:G:206:ILE:HA	1:G:209:ALA:CB	2.37	0.54
1:G:244:LYS:NZ	1:L:299:GLN:HA	2.22	0.54
1:L:203:LYS:NZ	1:L:318:ALA:HB1	2.18	0.54
1:A:238:GLY:N	1:A:275:ASP:O	2.40	0.54
1:B:300:LEU:H	1:B:300:LEU:HD12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:223:GLY:CA	1:K:224:ASP:CB	2.85	0.54
1:A:340:LYS:HE3	1:A:342:GLU:HB3	1.89	0.54
1:C:8:LEU:HD13	1:C:17:VAL:HG13	1.88	0.54
1:F:164:GLN:O	1:F:168:ILE:HG13	2.07	0.54
1:G:210:VAL:HG13	1:G:211:ALA:N	2.22	0.54
1:H:441:THR:HG23	1:H:443:GLN:H	1.72	0.54
1:I:161:LEU:HD22	1:I:206:ILE:HD11	1.90	0.54
1:J:151:PRO:HB3	1:J:208:LYS:HB3	1.89	0.54
1:J:237:LYS:H	1:J:237:LYS:HZ2	1.55	0.54
1:K:218:MET:CA	1:K:221:VAL:HG23	2.38	0.54
1:B:333:GLY:N	1:B:336:ASP:OD1	2.38	0.54
1:C:126:VAL:HG12	1:C:133:ALA:HA	1.90	0.54
1:D:323:ASP:OD1	1:D:323:ASP:N	2.41	0.54
1:L:400:LEU:CD1	1:L:412:MET:CB	2.76	0.54
1:A:140:ALA:O	1:A:142:VAL:N	2.36	0.54
1:B:403:THR:HB	1:B:487:TYR:HB3	1.89	0.54
1:F:69:ARG:HG3	1:F:81:VAL:HG23	1.90	0.54
1:G:255:LEU:O	1:G:259:ARG:HG2	2.08	0.54
1:I:217:LYS:NZ	1:I:269:PRO:HG3	2.21	0.54
1:K:105:LEU:N	1:K:106:PRO:CD	2.71	0.54
1:L:321:ARG:HG2	1:L:324:MET:HG2	1.90	0.54
1:B:69:ARG:C	1:B:70:GLU:HG3	2.33	0.54
1:F:149:GLU:O	1:F:233:PHE:CA	2.53	0.54
1:J:237:LYS:NZ	1:J:237:LYS:N	2.56	0.54
1:L:198:PRO:CG	1:L:343:ARG:CG	2.86	0.54
1:A:148:GLU:HB3	1:A:149:GLU:CB	2.25	0.54
1:B:125:LEU:HB2	1:B:137:ILE:HD11	1.90	0.54
1:B:149:GLU:HB3	1:B:233:PHE:O	2.04	0.54
1:E:68:LEU:HD22	1:E:124:LEU:HD11	1.90	0.54
1:E:254:ARG:HH22	1:E:299:GLN:HB3	1.73	0.54
1:E:437:SER:O	1:E:441:THR:HG22	2.08	0.54
1:I:249:THR:CA	1:I:250:GLU:HB3	2.19	0.54
1:I:403:THR:HB	1:I:487:TYR:HB3	1.89	0.54
1:J:145:LEU:O	1:J:146:VAL:HG12	2.07	0.54
1:L:253:ILE:O	1:L:256:ILE:HG12	2.08	0.54
1:C:68:LEU:O	1:C:120:PRO:HA	2.08	0.53
1:D:271:ILE:HA	1:D:314:ILE:O	2.08	0.53
1:J:263:LYS:HZ3	1:J:263:LYS:N	2.05	0.53
1:K:140:ALA:C	1:K:141:GLU:HG2	2.22	0.53
1:L:238:GLY:N	1:L:239:PRO:HD2	2.22	0.53
1:B:137:ILE:HG22	1:B:139:LYS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:ARG:HG2	1:B:484:ARG:HH11	1.72	0.53
1:D:164:GLN:O	1:D:168:ILE:HD12	2.08	0.53
1:L:69:ARG:HH11	1:L:69:ARG:CG	2.10	0.53
1:A:278:ASP:HB3	1:A:319:SER:OG	2.09	0.53
1:B:437:SER:O	1:B:441:THR:CB	2.56	0.53
1:D:392:ALA:HB1	1:D:394:ILE:HG23	1.91	0.53
1:H:467:ASN:HD22	1:H:467:ASN:N	2.05	0.53
1:L:310:LEU:HD22	1:L:311:GLU:H	1.72	0.53
1:D:88:ARG:HD3	1:E:64:GLU:HG2	1.90	0.53
1:E:320:ASN:HD22	1:E:320:ASN:N	2.05	0.53
1:F:278:ASP:OD1	1:F:278:ASP:N	2.35	0.53
1:H:89:VAL:HG23	1:I:65:ILE:HD11	1.91	0.53
1:K:212:ASN:O	1:K:216:LYS:HG3	2.08	0.53
1:B:146:VAL:O	1:B:146:VAL:HG13	2.08	0.53
1:H:429:ARG:HB3	1:H:454:SER:OG	2.09	0.53
1:K:105:LEU:N	1:K:106:PRO:HD3	2.21	0.53
1:D:296:VAL:HG12	1:D:297:VAL:H	1.73	0.53
1:G:139:LYS:HZ2	1:G:142:VAL:CG2	2.11	0.53
1:G:205:LEU:HD13	1:G:206:ILE:N	2.24	0.53
1:G:232:TYR:N	1:G:232:TYR:CD1	2.77	0.53
1:L:150:VAL:HG23	1:L:232:TYR:HB3	1.90	0.53
1:A:77:ARG:NH1	1:B:61:ALA:O	2.39	0.53
1:D:96:LEU:HD22	1:D:118:LEU:HD11	1.90	0.53
1:E:89:VAL:HG23	1:F:65:ILE:HD11	1.90	0.53
1:E:193:VAL:HA	1:E:337:VAL:HG23	1.90	0.53
1:F:96:LEU:HD22	1:F:118:LEU:HD11	1.90	0.53
1:I:147:LEU:HD22	1:I:148:GLU:HB3	1.90	0.53
1:J:151:PRO:HD3	1:J:233:PHE:HB2	1.91	0.53
1:K:246:VAL:HG12	1:K:247:GLY:H	1.73	0.53
1:A:441:THR:HG23	1:A:443:GLN:H	1.74	0.53
1:G:68:LEU:CD1	1:G:78:ALA:CB	2.70	0.53
1:G:363:VAL:HG13	1:G:368:LEU:HD11	1.91	0.53
1:K:173:GLU:OE2	1:K:213:SER:CB	2.54	0.53
1:K:223:GLY:HA3	1:K:224:ASP:CG	2.33	0.53
1:A:399:PHE:CD1	1:A:414:PHE:CE1	2.96	0.53
1:A:437:SER:O	1:A:441:THR:HG22	2.09	0.53
1:C:9:LEU:HD11	1:C:20:PHE:HB2	1.91	0.53
1:H:298:PRO:CG	1:I:242:LEU:CD1	2.81	0.53
1:H:434:ALA:HA	1:H:450:HIS:CE1	2.42	0.53
1:I:165:ILE:HG13	1:I:166:GLU:N	2.23	0.53
1:A:139:LYS:NZ	1:A:246:VAL:HG13	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:PHE:CE1	1:A:325:ILE:HA	2.44	0.53
1:B:150:VAL:H	1:B:233:PHE:CB	2.21	0.53
1:I:298:PRO:HB2	1:J:242:LEU:HD22	1.90	0.53
1:J:109:LEU:HD21	1:J:232:TYR:CE1	2.44	0.53
1:A:245:PHE:CE1	1:F:254:ARG:HG3	2.43	0.52
1:A:399:PHE:N	1:A:412:MET:O	2.36	0.52
1:B:399:PHE:HE2	1:B:417:PHE:CG	2.27	0.52
1:D:464:ASP:HB2	1:D:498:SER:HB2	1.90	0.52
1:G:195:LEU:HD23	1:G:339:ILE:HB	1.91	0.52
1:H:322:GLU:HA	1:H:325:ILE:HG13	1.90	0.52
1:L:195:LEU:HD22	1:L:341:ILE:HD11	1.90	0.52
1:L:312:ASN:N	1:L:312:ASN:OD1	2.42	0.52
1:B:72:LEU:HD23	1:B:74:ASP:H	1.73	0.52
1:F:200:GLY:H	1:F:419:SER:HB2	1.73	0.52
1:H:69:ARG:O	1:H:120:PRO:CG	2.55	0.52
1:I:147:LEU:CG	1:I:148:GLU:HB3	2.39	0.52
1:A:101:LEU:HD22	1:A:115:PRO:HB3	1.90	0.52
1:B:399:PHE:CD1	1:B:414:PHE:CZ	2.97	0.52
1:B:399:PHE:CD2	1:B:417:PHE:CD1	2.97	0.52
1:C:359:GLU:HG3	1:C:375:ARG:HG2	1.91	0.52
1:E:476:ARG:NH2	1:F:464:ASP:OD1	2.43	0.52
1:K:437:SER:O	1:K:441:THR:HG22	2.10	0.52
1:L:198:PRO:CG	1:L:343:ARG:HG3	2.39	0.52
1:L:399:PHE:CD1	1:L:399:PHE:C	2.85	0.52
1:D:211:ALA:HA	1:D:271:ILE:HD12	1.90	0.52
1:E:218:MET:HA	1:E:219:ALA:HB3	1.92	0.52
1:G:205:LEU:O	1:G:209:ALA:CB	2.58	0.52
1:I:237:LYS:HD3	1:I:240:GLU:HG3	1.92	0.52
1:J:113:THR:HA	1:J:136:ARG:HH12	1.75	0.52
1:L:351:ASP:O	1:L:354:SER:OG	2.27	0.52
1:A:392:ALA:HB1	1:A:394:ILE:HG23	1.91	0.52
1:F:70:GLU:HG2	1:F:72:LEU:H	1.74	0.52
1:G:158:ILE:CB	1:G:206:ILE:HG12	2.39	0.52
1:G:205:LEU:HD12	1:G:206:ILE:H	1.73	0.52
1:I:204:THR:CG2	1:I:275:ASP:OD2	2.58	0.52
1:J:255:LEU:O	1:J:259:ARG:HG3	2.09	0.52
1:D:118:LEU:O	1:D:119:ARG:HG3	2.10	0.52
1:E:204:THR:HG23	1:E:273:PHE:CE2	2.45	0.52
1:F:68:LEU:HA	1:F:80:VAL:HG12	1.92	0.52
1:I:9:LEU:HD11	1:I:20:PHE:HB2	1.91	0.52
1:J:27:ARG:HD3	1:K:46:ARG:HD2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG13	1:A:209:ALA:HA	1.89	0.52
1:E:26:MET:HA	1:F:4:GLY:HA2	1.91	0.52
1:F:271:ILE:HG23	1:F:314:ILE:HG22	1.91	0.52
1:G:46:ARG:HB3	1:G:55:GLU:HB3	1.91	0.52
1:I:132:TYR:HB3	1:I:134:PHE:CZ	2.45	0.52
1:K:109:LEU:HD23	1:K:109:LEU:O	2.10	0.52
1:K:295:THR:OG1	1:L:242:LEU:HG	2.09	0.52
1:K:297:VAL:HG13	1:K:298:PRO:HD3	1.91	0.52
1:L:204:THR:HG22	1:L:273:PHE:CZ	2.44	0.52
1:E:8:LEU:HA	1:E:19:VAL:HG22	1.92	0.52
1:G:170:ASP:O	1:G:175:PRO:CD	2.48	0.52
1:C:150:VAL:CB	1:C:231:SER:CB	2.88	0.52
1:D:254:ARG:HH11	1:D:254:ARG:CB	2.22	0.52
1:D:301:LEU:HG	1:D:334:ARG:NH1	2.25	0.52
1:F:191:LYS:HZ2	1:F:304:ILE:C	2.17	0.52
1:F:248:GLU:HB2	1:F:250:GLU:OE2	2.09	0.52
1:I:142:VAL:HG12	1:I:142:VAL:O	2.10	0.52
1:I:399:PHE:C	1:I:400:LEU:HG	2.35	0.52
1:K:221:VAL:HB	1:K:222:ARG:CD	2.34	0.52
1:K:403:THR:HB	1:K:487:TYR:HB3	1.91	0.52
1:L:199:PRO:O	1:L:201:CYS:N	2.35	0.52
1:A:8:LEU:HD13	1:A:17:VAL:HG13	1.92	0.52
1:A:399:PHE:CD2	1:A:417:PHE:HB2	2.44	0.52
1:C:172:VAL:C	1:C:175:PRO:HD2	2.35	0.52
1:D:151:PRO:O	1:D:212:ASN:ND2	2.43	0.52
1:D:152:ASP:OD1	1:D:152:ASP:N	2.33	0.52
1:G:68:LEU:CD1	1:G:80:VAL:HG12	2.39	0.52
1:J:322:GLU:OE2	1:K:501:ARG:NH1	2.39	0.52
1:J:422:MET:O	1:J:426:VAL:HG23	2.10	0.52
1:L:252:HIS:O	1:L:256:ILE:HG23	2.10	0.52
1:B:150:VAL:CG1	1:B:151:PRO:N	2.73	0.51
1:F:471:PRO:HA	1:F:474:TRP:CD1	2.45	0.51
1:G:46:ARG:HH11	1:G:55:GLU:CD	2.19	0.51
1:H:168:ILE:HD13	1:H:206:ILE:HG12	1.91	0.51
1:H:298:PRO:CD	1:I:242:LEU:HD21	2.36	0.51
1:I:160:GLY:N	1:I:351:ASP:OD2	2.36	0.51
1:I:255:LEU:O	1:I:259:ARG:HG2	2.10	0.51
1:I:386:VAL:HG11	1:I:451:LEU:HD13	1.92	0.51
1:K:41:LYS:NZ	1:K:76:HIS:HD2	2.07	0.51
1:B:150:VAL:HA	1:B:233:PHE:HB3	1.90	0.51
1:G:158:ILE:HG23	1:G:206:ILE:HG12	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:TYR:CZ	1:G:340:LYS:HB2	2.45	0.51
1:G:271:ILE:HG23	1:G:314:ILE:HG22	1.93	0.51
1:J:382:MET:O	1:J:386:VAL:HG13	2.10	0.51
1:K:304:ILE:O	1:K:307:VAL:HG12	2.10	0.51
1:L:198:PRO:HB3	1:L:343:ARG:HE	1.75	0.51
1:A:191:LYS:HE2	1:A:308:GLU:HG3	1.92	0.51
1:A:239:PRO:O	1:F:298:PRO:HB3	2.09	0.51
1:B:254:ARG:HH12	1:B:299:GLN:HB3	1.75	0.51
1:B:262:GLU:HB3	1:B:263:LYS:HZ2	1.75	0.51
1:G:172:VAL:HG12	1:G:214:LEU:HD13	1.92	0.51
1:H:68:LEU:HB2	1:H:124:LEU:HD12	1.92	0.51
1:H:295:THR:CG2	1:H:296:VAL:H	2.19	0.51
1:K:152:ASP:C	1:K:212:ASN:HD21	2.19	0.51
1:A:176:PHE:HZ	1:A:217:LYS:HZ2	1.57	0.51
1:D:241:LEU:HD12	1:D:242:LEU:N	2.26	0.51
1:G:359:GLU:HG3	1:G:375:ARG:HD2	1.93	0.51
1:I:116:ARG:HG2	1:I:136:ARG:NH2	2.24	0.51
1:J:147:LEU:O	1:J:235:ASN:HB3	2.11	0.51
1:K:298:PRO:HB3	1:L:239:PRO:HB3	1.92	0.51
1:A:139:LYS:HZ2	1:A:246:VAL:HG13	1.75	0.51
1:C:161:LEU:HD13	1:C:206:ILE:HD11	1.93	0.51
1:E:343:ARG:NH1	1:E:417:PHE:O	2.43	0.51
1:I:20:PHE:HD1	1:I:25:LYS:HG3	1.75	0.51
1:K:77:ARG:HD3	1:L:61:ALA:HB1	1.92	0.51
1:K:295:THR:HG1	1:L:242:LEU:HG	1.75	0.51
1:A:81:VAL:HG22	1:A:87:GLU:HG2	1.93	0.51
1:A:151:PRO:HB2	1:A:208:LYS:HB3	1.92	0.51
1:A:343:ARG:HD3	1:A:418:ASN:O	2.11	0.51
1:D:77:ARG:HH22	1:E:135:GLU:CD	2.18	0.51
1:G:390:MET:HG3	1:G:455:ILE:HD13	1.92	0.51
1:I:262:GLU:HG2	1:I:263:LYS:NZ	2.26	0.51
1:J:171:ALA:HB1	1:J:337:VAL:HG21	1.92	0.51
1:J:255:LEU:O	1:J:258:GLN:HG2	2.10	0.51
1:L:399:PHE:HD1	1:L:399:PHE:O	1.94	0.51
1:A:493:THR:HG23	1:A:495:LYS:H	1.76	0.51
1:C:493:THR:HG23	1:C:495:LYS:H	1.75	0.51
1:E:380:LYS:O	1:E:384:GLU:HG2	2.10	0.51
1:H:262:GLU:HB3	1:H:263:LYS:NZ	2.25	0.51
1:I:330:LEU:HG	1:I:338:LYS:HE3	1.92	0.51
1:J:101:LEU:HD22	1:J:115:PRO:HB3	1.93	0.51
1:J:145:LEU:HD22	1:J:146:VAL:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:263:LYS:H	1:J:263:LYS:NZ	2.07	0.51
1:L:198:PRO:CB	1:L:343:ARG:NE	2.74	0.51
1:L:202:GLY:HA2	1:L:203:LYS:HB2	1.92	0.51
1:C:220:GLU:HG3	1:C:221:VAL:N	2.24	0.51
1:C:441:THR:HG23	1:C:443:GLN:H	1.74	0.51
1:E:24:ARG:HH22	1:F:22:SER:HB2	1.76	0.51
1:E:254:ARG:HH12	1:E:299:GLN:HB3	1.74	0.51
1:I:406:ASN:ND2	1:I:408:ASP:OD2	2.41	0.51
1:K:177:LEU:HD21	1:K:217:LYS:HB3	1.92	0.51
1:L:236:ILE:HG23	1:L:273:PHE:O	2.11	0.51
1:L:398:ARG:O	1:L:398:ARG:HG2	2.10	0.51
1:B:101:LEU:HB3	1:B:115:PRO:O	2.10	0.51
1:B:149:GLU:O	1:B:150:VAL:HB	2.11	0.51
1:D:81:VAL:HG22	1:D:87:GLU:HG2	1.92	0.51
1:E:398:ARG:HG2	1:E:413:TYR:CE1	2.43	0.51
1:F:395:ASP:O	1:F:398:ARG:HD3	2.11	0.51
1:F:396:ASP:OD2	1:F:396:ASP:N	2.43	0.51
1:G:252:HIS:HA	1:G:255:LEU:HD23	1.92	0.51
1:H:386:VAL:HG11	1:H:451:LEU:HD13	1.92	0.51
1:H:392:ALA:HB1	1:H:394:ILE:HG23	1.93	0.51
1:J:69:ARG:HE	1:K:139:LYS:HE3	1.76	0.51
1:J:301:LEU:CD2	1:J:334:ARG:HH12	2.24	0.51
1:K:203:LYS:H	1:K:206:ILE:HD13	1.75	0.51
1:B:172:VAL:HG12	1:B:214:LEU:HD13	1.92	0.51
1:B:299:GLN:CD	1:B:299:GLN:H	2.17	0.51
1:C:264:ALA:HB1	1:C:310:LEU:HD21	1.93	0.51
1:D:278:ASP:OD1	1:D:278:ASP:N	2.43	0.51
1:E:340:LYS:HD2	1:E:342:GLU:HB3	1.92	0.51
1:F:149:GLU:C	1:F:233:PHE:HB3	2.32	0.51
1:G:148:GLU:N	1:G:234:LEU:HA	2.26	0.51
1:H:298:PRO:HG2	1:I:242:LEU:HB3	1.93	0.51
1:J:109:LEU:H	1:J:111:ASP:N	2.08	0.51
1:K:241:LEU:HD22	1:K:280:ILE:HD13	1.92	0.51
1:L:364:HIS:NE2	1:L:366:ASP:OD2	2.43	0.51
1:F:216:LYS:O	1:F:217:LYS:HD2	2.11	0.50
1:J:263:LYS:O	1:J:312:ASN:ND2	2.44	0.50
1:J:340:LYS:HG2	1:J:342:GLU:HB3	1.93	0.50
1:A:164:GLN:O	1:A:168:ILE:HG13	2.11	0.50
1:B:343:ARG:HD3	1:B:418:ASN:O	2.11	0.50
1:E:101:LEU:HD22	1:E:115:PRO:HB2	1.93	0.50
1:G:301:LEU:HD23	1:G:334:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:295:THR:CG2	1:H:296:VAL:N	2.74	0.50
1:J:109:LEU:CB	1:J:110:ASN:CB	2.85	0.50
1:J:262:GLU:HB3	1:J:263:LYS:NZ	2.26	0.50
1:K:145:LEU:HD13	1:K:146:VAL:HB	1.93	0.50
1:A:478:SER:OG	1:A:483:GLU:O	2.26	0.50
1:K:107:GLU:O	1:K:108:ALA:HB3	2.11	0.50
1:D:470:ASN:HD21	1:D:472:ASP:HB2	1.76	0.50
1:E:255:LEU:O	1:E:259:ARG:HG2	2.11	0.50
1:E:299:GLN:CD	1:E:299:GLN:H	2.18	0.50
1:G:205:LEU:CD1	1:G:206:ILE:N	2.73	0.50
1:I:132:TYR:HB3	1:I:134:PHE:CE1	2.46	0.50
1:J:105:LEU:HD11	1:J:263:LYS:HG3	1.93	0.50
1:J:437:SER:O	1:J:441:THR:HG22	2.11	0.50
1:K:198:PRO:O	1:K:203:LYS:NZ	2.45	0.50
1:L:234:LEU:HD22	1:L:272:VAL:HG22	1.94	0.50
1:A:399:PHE:CD2	1:A:417:PHE:CD1	2.99	0.50
1:C:219:ALA:HB3	1:C:220:GLU:C	2.37	0.50
1:D:466:PRO:HG3	1:D:490:THR:HG21	1.93	0.50
1:E:74:ASP:OD2	1:E:76:HIS:HB2	2.11	0.50
1:F:174:LEU:HB3	1:F:175:PRO:HD3	1.94	0.50
1:G:322:GLU:OE1	1:G:322:GLU:N	2.43	0.50
1:A:68:LEU:HD13	1:A:78:ALA:HB1	1.94	0.50
1:B:406:ASN:ND2	1:B:408:ASP:OD2	2.41	0.50
1:I:245:PHE:CE1	1:I:251:ARG:HB3	2.47	0.50
1:J:196:TYR:HE2	1:J:338:LYS:HB3	1.77	0.50
1:K:141:GLU:CG	1:K:142:VAL:N	2.73	0.50
1:K:203:LYS:O	1:K:206:ILE:N	2.43	0.50
1:K:207:ALA:HA	1:K:210:VAL:HG12	1.94	0.50
1:B:386:VAL:HB	1:B:455:ILE:HD11	1.94	0.50
1:F:341:ILE:HG22	1:F:341:ILE:O	2.11	0.50
1:F:429:ARG:HB3	1:F:454:SER:OG	2.11	0.50
1:G:149:GLU:CB	1:G:232:TYR:HB3	2.39	0.50
1:H:152:ASP:H	1:H:212:ASN:ND2	2.10	0.50
1:J:109:LEU:HB3	1:J:110:ASN:HB3	1.91	0.50
1:J:113:THR:C	1:J:136:ARG:HH22	2.20	0.50
1:J:262:GLU:HB3	1:J:263:LYS:HZ2	1.76	0.50
1:E:248:GLU:CG	1:E:249:THR:H	2.25	0.50
1:F:193:VAL:HA	1:F:337:VAL:HG23	1.94	0.50
1:F:364:HIS:HA	1:F:445:GLY:HA3	1.94	0.50
1:F:458:GLU:O	1:F:462:ASN:ND2	2.38	0.50
1:J:310:LEU:HD13	1:J:312:ASN:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:362:PRO:O	1:K:445:GLY:HA2	2.12	0.50
1:L:164:GLN:O	1:L:168:ILE:HG13	2.12	0.50
1:A:150:VAL:HG11	1:A:231:SER:CA	2.40	0.50
1:B:146:VAL:O	1:B:146:VAL:HG22	2.11	0.50
1:C:182:TYR:CD1	1:D:435:ILE:HD13	2.47	0.50
1:E:72:LEU:HD22	1:F:137:ILE:HG21	1.94	0.50
1:E:162:SER:O	1:E:165:ILE:HG13	2.12	0.50
1:E:403:THR:HB	1:E:487:TYR:HB3	1.93	0.50
1:G:152:ASP:C	1:G:212:ASN:ND2	2.69	0.50
1:H:191:LYS:CE	1:H:304:ILE:O	2.59	0.50
1:I:170:ASP:HA	1:I:174:LEU:HB2	1.93	0.50
1:L:364:HIS:HD2	1:L:447:ARG:NH1	2.09	0.50
1:B:248:GLU:HB3	1:B:250:GLU:HG2	1.93	0.49
1:D:46:ARG:CG	1:D:55:GLU:HB3	2.41	0.49
1:J:244:LYS:O	1:J:250:GLU:N	2.25	0.49
1:K:221:VAL:C	1:K:222:ARG:CD	2.85	0.49
1:B:147:LEU:CB	1:B:148:GLU:CD	2.71	0.49
1:B:149:GLU:C	1:B:150:VAL:HG23	2.36	0.49
1:C:429:ARG:NH2	1:C:458:GLU:OE1	2.38	0.49
1:G:158:ILE:HG23	1:G:206:ILE:CD1	2.41	0.49
1:H:86:GLU:HB3	1:I:83:HIS:CD2	2.47	0.49
1:I:380:LYS:O	1:I:384:GLU:HG3	2.13	0.49
1:J:394:ILE:HG13	1:J:396:ASP:H	1.77	0.49
1:K:364:HIS:HD2	1:K:447:ARG:HH11	1.60	0.49
1:C:399:PHE:C	1:C:399:PHE:CD1	2.90	0.49
1:D:264:ALA:HB1	1:D:310:LEU:HG	1.95	0.49
1:E:296:VAL:HG12	1:E:298:PRO:HD3	1.93	0.49
1:H:232:TYR:O	1:H:270:VAL:HA	2.12	0.49
1:H:299:GLN:C	1:H:301:LEU:N	2.68	0.49
1:H:400:LEU:HB2	1:H:412:MET:HB2	1.94	0.49
1:J:203:LYS:HZ2	1:J:320:ASN:HD22	1.58	0.49
1:K:243:ASN:O	1:K:246:VAL:N	2.43	0.49
1:B:233:PHE:CG	1:B:234:LEU:N	2.79	0.49
1:C:233:PHE:HE1	1:C:271:ILE:HG12	1.77	0.49
1:G:69:ARG:C	1:G:70:GLU:CG	2.86	0.49
1:K:223:GLY:N	1:K:224:ASP:CB	2.73	0.49
1:A:399:PHE:CE2	1:A:417:PHE:HB3	2.48	0.49
1:B:198:PRO:HG2	1:B:343:ARG:HG3	1.93	0.49
1:C:76:HIS:O	1:C:92:LEU:HG	2.12	0.49
1:E:384:GLU:O	1:E:388:ASP:HB2	2.13	0.49
1:F:403:THR:HB	1:F:487:TYR:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:TYR:N	1:G:232:TYR:HD1	2.09	0.49
1:G:400:LEU:HD23	1:G:490:THR:HG22	1.94	0.49
1:J:71:ILE:O	1:J:71:ILE:HG13	2.12	0.49
1:B:359:GLU:HG3	1:G:156:ALA:HB2	1.93	0.49
1:D:160:GLY:N	1:D:351:ASP:OD2	2.30	0.49
1:E:132:TYR:O	1:E:134:PHE:CE2	2.66	0.49
1:I:89:VAL:HG23	1:J:65:ILE:HD11	1.93	0.49
1:J:109:LEU:HD23	1:J:148:GLU:O	2.12	0.49
1:A:216:LYS:N	1:A:216:LYS:NZ	2.60	0.49
1:A:322:GLU:OE2	1:A:472:ASP:OD2	2.31	0.49
1:B:102:PRO:C	1:B:116:ARG:HD2	2.37	0.49
1:B:158:ILE:HD13	1:B:206:ILE:HG13	1.94	0.49
1:D:367:ASP:OD2	1:D:382:MET:HE2	2.13	0.49
1:F:14:ASP:O	1:F:15:ASP:HB2	2.13	0.49
1:G:328:ALA:O	1:G:334:ARG:NH1	2.43	0.49
1:H:243:ASN:CG	1:H:244:LYS:HE2	2.38	0.49
1:J:270:VAL:C	1:J:313:VAL:HG13	2.16	0.49
1:L:382:MET:O	1:L:386:VAL:HG13	2.13	0.49
1:C:162:SER:O	1:C:165:ILE:HG13	2.12	0.49
1:D:151:PRO:HB3	1:D:233:PHE:HB2	1.95	0.49
1:D:342:GLU:O	1:D:343:ARG:C	2.54	0.49
1:D:471:PRO:HA	1:D:474:TRP:CD1	2.47	0.49
1:H:68:LEU:HD13	1:H:78:ALA:CB	2.39	0.49
1:H:297:VAL:HG13	1:H:297:VAL:O	2.12	0.49
1:K:227:HIS:ND1	1:K:227:HIS:N	2.60	0.49
1:A:145:LEU:O	1:A:146:VAL:HG12	2.13	0.49
1:A:235:ASN:OD1	1:A:236:ILE:N	2.45	0.49
1:H:144:ASP:O	1:H:147:LEU:HG	2.12	0.49
1:J:108:ALA:C	1:J:109:LEU:CD1	2.86	0.49
1:J:150:VAL:CG2	1:J:232:TYR:HB2	2.23	0.49
1:K:28:LEU:HD22	1:K:51:LEU:HB3	1.95	0.49
1:G:203:LYS:HD2	1:G:203:LYS:H	1.76	0.49
1:H:212:ASN:HA	1:H:215:ALA:HB3	1.95	0.49
1:J:310:LEU:CD1	1:J:312:ASN:H	2.26	0.49
1:B:151:PRO:HG2	1:B:212:ASN:HB2	1.94	0.48
1:B:482:GLY:HA2	1:C:489:ARG:HD3	1.95	0.48
1:H:117:LYS:HG3	1:H:117:LYS:O	2.13	0.48
1:H:191:LYS:NZ	1:H:307:VAL:HG12	2.27	0.48
1:B:118:LEU:HD13	1:B:124:LEU:HD21	1.95	0.48
1:E:69:ARG:O	1:E:120:PRO:HG3	2.13	0.48
1:E:262:GLU:HG3	1:E:263:LYS:NZ	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:ILE:C	1:G:209:ALA:HB3	2.38	0.48
1:I:8:LEU:HD21	1:I:39:LEU:HB3	1.95	0.48
1:J:236:ILE:CA	1:J:237:LYS:HZ1	2.25	0.48
1:K:86:GLU:HG3	1:L:83:HIS:CG	2.47	0.48
1:K:227:HIS:O	1:K:228:GLU:CD	2.56	0.48
1:A:212:ASN:O	1:A:216:LYS:NZ	2.37	0.48
1:A:242:LEU:HD23	1:F:296:VAL:HG21	1.95	0.48
1:B:69:ARG:C	1:B:70:GLU:CG	2.86	0.48
1:C:219:ALA:H	1:C:220:GLU:CA	2.23	0.48
1:F:271:ILE:HA	1:F:314:ILE:O	2.13	0.48
1:D:188:ARG:HD3	1:D:189:PRO:HD2	1.96	0.48
1:D:348:ALA:O	1:D:352:ILE:HG13	2.12	0.48
1:G:299:GLN:HG2	1:G:300:LEU:HD12	1.96	0.48
1:K:226:ALA:CB	1:K:227:HIS:HA	2.41	0.48
1:L:112:ASP:OD2	1:L:112:ASP:N	2.46	0.48
1:L:233:PHE:CD2	1:L:234:LEU:C	2.91	0.48
1:A:201:CYS:HA	1:A:202:GLY:HA2	1.59	0.48
1:B:395:ASP:HA	1:B:398:ARG:HG3	1.96	0.48
1:J:146:VAL:HG22	1:J:234:LEU:HD11	1.93	0.48
1:K:111:ASP:OD2	1:K:113:THR:N	2.47	0.48
1:A:140:ALA:C	1:A:142:VAL:N	2.71	0.48
1:A:464:ASP:OD2	1:F:340:LYS:HD2	2.14	0.48
1:C:134:PHE:N	1:C:134:PHE:CD1	2.75	0.48
1:D:28:LEU:HD22	1:D:51:LEU:HB3	1.95	0.48
1:J:263:LYS:N	1:J:263:LYS:NZ	2.60	0.48
1:A:399:PHE:CE1	1:A:414:PHE:CE1	3.01	0.48
1:B:236:ILE:HD13	1:B:274:PHE:HE1	1.78	0.48
1:D:27:ARG:HD3	1:E:46:ARG:CD	2.44	0.48
1:D:101:LEU:O	1:D:117:LYS:HD3	2.14	0.48
1:D:322:GLU:HG3	1:E:465:LEU:HD13	1.95	0.48
1:E:321:ARG:HG2	1:E:324:MET:HG2	1.96	0.48
1:H:493:THR:OG1	1:H:495:LYS:HE3	2.14	0.48
1:I:399:PHE:N	1:I:412:MET:O	2.37	0.48
1:J:310:LEU:HD13	1:J:312:ASN:H	1.79	0.48
1:K:109:LEU:C	1:K:109:LEU:CD2	2.85	0.48
1:K:250:GLU:OE2	1:K:250:GLU:HA	2.13	0.48
1:A:310:LEU:HD13	1:A:312:ASN:H	1.78	0.48
1:B:151:PRO:HD3	1:B:233:PHE:HB2	1.96	0.48
1:D:299:GLN:H	1:D:299:GLN:CD	2.21	0.48
1:F:244:LYS:HD2	1:F:247:GLY:C	2.39	0.48
1:I:146:VAL:O	1:I:146:VAL:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:231:SER:HB3	1:J:268:THR:HB	1.96	0.48
1:L:172:VAL:HG13	1:L:314:ILE:HG13	1.96	0.48
1:L:449:GLN:O	1:L:453:ASP:HB2	2.14	0.48
1:A:232:TYR:CG	1:A:233:PHE:N	2.80	0.48
1:B:399:PHE:CE1	1:B:414:PHE:CE1	3.02	0.48
1:C:24:ARG:HG3	1:C:25:LYS:HB2	1.95	0.48
1:D:384:GLU:O	1:D:388:ASP:HB2	2.14	0.48
1:E:278:ASP:OD1	1:E:278:ASP:N	2.39	0.48
1:G:177:LEU:HD12	1:G:178:HIS:CE1	2.49	0.48
1:G:204:THR:HB	1:G:205:LEU:H	1.52	0.48
1:G:239:PRO:O	1:L:298:PRO:HB3	2.14	0.48
1:G:296:VAL:CG2	1:H:243:ASN:HB2	2.43	0.48
1:K:250:GLU:OE1	1:K:299:GLN:CD	2.57	0.48
1:L:171:ALA:HB1	1:L:337:VAL:HG21	1.96	0.48
1:A:24:ARG:HD2	1:A:26:MET:HE3	1.95	0.48
1:B:69:ARG:O	1:B:120:PRO:HG3	2.14	0.48
1:G:79:LEU:HD11	1:G:87:GLU:HB3	1.95	0.48
1:G:298:PRO:HG3	1:H:241:LEU:O	2.14	0.48
1:G:434:ALA:HA	1:G:450:HIS:CE1	2.49	0.48
1:I:81:VAL:HG22	1:I:87:GLU:HG2	1.94	0.48
1:J:116:ARG:CD	1:J:119:ARG:NH2	2.77	0.48
1:K:323:ASP:OD1	1:K:323:ASP:N	2.47	0.48
1:A:241:LEU:HD12	1:A:242:LEU:N	2.28	0.47
1:C:3:SER:HB3	1:C:47:LEU:O	2.14	0.47
1:D:204:THR:O	1:D:208:LYS:HG2	2.14	0.47
1:F:382:MET:O	1:F:386:VAL:HG12	2.14	0.47
1:B:40:LYS:HB2	1:B:94:ASP:HB2	1.95	0.47
1:G:161:LEU:HD23	1:G:161:LEU:HA	1.69	0.47
1:I:261:ARG:HG3	1:I:310:LEU:HD11	1.95	0.47
1:J:296:VAL:HB	1:J:299:GLN:NE2	2.29	0.47
1:L:67:THR:OG1	1:L:81:VAL:HG12	2.14	0.47
1:L:296:VAL:HG12	1:L:297:VAL:H	1.78	0.47
1:L:364:HIS:CD2	1:L:447:ARG:NH1	2.82	0.47
1:B:134:PHE:N	1:B:134:PHE:CD2	2.81	0.47
1:D:298:PRO:HB3	1:E:239:PRO:O	2.13	0.47
1:F:147:LEU:HA	1:F:148:GLU:HA	1.76	0.47
1:I:247:GLY:HA2	1:I:248:GLU:HA	1.70	0.47
1:K:218:MET:HA	1:K:221:VAL:CG2	2.44	0.47
1:K:223:GLY:N	1:K:224:ASP:C	2.73	0.47
1:K:434:ALA:HA	1:K:450:HIS:CE1	2.50	0.47
1:L:206:ILE:O	1:L:210:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:TYR:HE1	1:A:269:PRO:O	1.96	0.47
1:A:299:GLN:H	1:A:299:GLN:CD	2.20	0.47
1:B:216:LYS:C	1:B:217:LYS:HD2	2.40	0.47
1:E:158:ILE:HD13	1:E:206:ILE:HG13	1.96	0.47
1:E:244:LYS:O	1:E:245:PHE:HB2	2.13	0.47
1:J:17:VAL:HG12	1:J:19:VAL:HG23	1.95	0.47
1:K:214:LEU:C	1:K:214:LEU:CD2	2.88	0.47
1:K:296:VAL:HB	1:L:242:LEU:CB	2.45	0.47
1:A:171:ALA:HB1	1:A:337:VAL:HG21	1.96	0.47
1:B:255:LEU:O	1:B:259:ARG:HG2	2.14	0.47
1:D:321:ARG:NH1	1:D:471:PRO:HG2	2.29	0.47
1:D:359:GLU:HG2	1:D:379:ILE:HD12	1.96	0.47
1:E:96:LEU:HD22	1:E:118:LEU:HD11	1.96	0.47
1:F:191:LYS:HD3	1:F:308:GLU:HA	1.96	0.47
1:G:181:LEU:HD12	1:G:181:LEU:HA	1.72	0.47
1:G:345:ASP:CG	1:G:346:ALA:H	2.22	0.47
1:J:271:ILE:HG23	1:J:314:ILE:HG22	1.95	0.47
1:E:399:PHE:HB2	1:E:414:PHE:CD2	2.49	0.47
1:G:244:LYS:HE3	1:G:245:PHE:CE1	2.50	0.47
1:L:217:LYS:HD3	1:L:217:LYS:HA	1.51	0.47
1:L:379:ILE:HA	1:L:382:MET:HB2	1.95	0.47
1:C:43:GLN:NE2	1:C:56:ALA:HB1	2.30	0.47
1:D:239:PRO:HD3	1:D:276:GLU:HB2	1.96	0.47
1:E:132:TYR:CB	1:E:134:PHE:CZ	2.97	0.47
1:E:305:ASP:HA	1:E:308:GLU:HB2	1.96	0.47
1:F:232:TYR:CE2	1:F:270:VAL:HA	2.50	0.47
1:F:441:THR:HG22	1:F:443:GLN:HG2	1.95	0.47
1:G:81:VAL:HG23	1:G:87:GLU:HG2	1.97	0.47
1:G:198:PRO:HG2	1:G:343:ARG:HG3	1.96	0.47
1:H:192:GLY:O	1:H:337:VAL:HG23	2.14	0.47
1:I:386:VAL:HB	1:I:455:ILE:HD11	1.96	0.47
1:J:70:GLU:HG2	1:J:71:ILE:H	1.74	0.47
1:J:198:PRO:HG3	1:J:343:ARG:CG	2.45	0.47
1:K:106:PRO:CB	1:K:107:GLU:OE2	2.54	0.47
1:K:151:PRO:HD3	1:K:233:PHE:HB2	1.96	0.47
1:K:438:VAL:HG22	1:K:444:PRO:HA	1.95	0.47
1:K:447:ARG:HD3	1:K:450:HIS:CE1	2.49	0.47
1:L:165:ILE:HA	1:L:168:ILE:HD12	1.95	0.47
1:L:215:ALA:HB1	1:L:231:SER:H	1.79	0.47
1:L:275:ASP:OD1	1:L:276:GLU:N	2.48	0.47
1:L:400:LEU:HD12	1:L:400:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:PHE:CE2	1:A:417:PHE:HB2	2.47	0.47
1:A:463:GLU:OE1	1:A:492:VAL:HA	2.14	0.47
1:B:464:ASP:OD1	1:B:498:SER:HA	2.14	0.47
1:C:398:ARG:HG2	1:C:411:VAL:CG1	2.44	0.47
1:D:474:TRP:NE1	1:D:505:THR:HG1	2.13	0.47
1:H:216:LYS:O	1:H:217:LYS:HD2	2.14	0.47
1:I:142:VAL:O	1:I:259:ARG:NE	2.47	0.47
1:I:311:GLU:H	1:I:311:GLU:HG3	1.48	0.47
1:K:139:LYS:HE2	1:K:141:GLU:OE2	2.15	0.47
1:L:111:ASP:HB2	1:L:143:GLU:HB2	1.97	0.47
1:L:152:ASP:O	1:L:212:ASN:ND2	2.48	0.47
1:L:437:SER:O	1:L:441:THR:HG22	2.15	0.47
1:A:45:VAL:HB	1:A:53:VAL:HG13	1.96	0.47
1:C:133:ALA:C	1:C:134:PHE:CD1	2.93	0.47
1:E:204:THR:OG1	1:E:275:ASP:OD2	2.32	0.47
1:G:301:LEU:HD23	1:G:334:ARG:HH12	1.80	0.47
1:H:297:VAL:N	1:H:298:PRO:HD3	2.30	0.47
1:H:382:MET:O	1:H:386:VAL:HG13	2.15	0.47
1:I:72:LEU:HD22	1:J:138:PRO:HG2	1.96	0.47
1:J:310:LEU:HD22	1:J:311:GLU:N	2.30	0.47
1:J:380:LYS:O	1:J:384:GLU:HG2	2.15	0.47
1:D:459:PHE:O	1:D:463:GLU:HG3	2.15	0.47
1:F:310:LEU:HG	1:F:312:ASN:H	1.80	0.47
1:H:340:LYS:HE2	1:H:342:GLU:HB3	1.96	0.47
1:J:105:LEU:O	1:J:107:GLU:N	2.48	0.47
1:J:254:ARG:NH1	1:J:299:GLN:HB3	2.25	0.47
1:K:252:HIS:O	1:K:255:LEU:N	2.48	0.47
1:L:249:THR:HB	1:L:251:ARG:HB2	1.97	0.47
1:A:399:PHE:HB3	1:A:412:MET:O	2.15	0.46
1:B:217:LYS:HB2	1:B:218:MET:HE2	1.96	0.46
1:C:139:LYS:HG3	1:C:140:ALA:H	1.80	0.46
1:D:470:ASN:ND2	1:D:472:ASP:HB2	2.30	0.46
1:E:19:VAL:HG21	1:E:45:VAL:HG21	1.97	0.46
1:E:216:LYS:O	1:E:216:LYS:HD3	2.15	0.46
1:B:147:LEU:CB	1:B:148:GLU:OE1	2.60	0.46
1:B:102:PRO:O	1:B:116:ARG:HB2	2.15	0.46
1:E:323:ASP:OD1	1:E:323:ASP:N	2.44	0.46
1:H:296:VAL:HG21	1:I:242:LEU:HG	1.96	0.46
1:J:94:ASP:N	1:J:95:PRO:HD2	2.29	0.46
1:D:10:ALA:H	1:D:18:ASP:HB2	1.81	0.46
1:D:202:GLY:C	1:D:204:THR:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:ASP:O	1:G:15:ASP:HB2	2.15	0.46
1:G:180:GLU:CD	1:G:180:GLU:H	2.23	0.46
1:G:328:ALA:O	1:G:331:ARG:HG2	2.15	0.46
1:J:165:ILE:HG22	1:J:206:ILE:HD11	1.96	0.46
1:K:230:LYS:CE	1:K:230:LYS:CA	2.87	0.46
1:K:449:GLN:NE2	1:K:453:ASP:OD2	2.48	0.46
1:A:181:LEU:HD23	1:B:435:ILE:HG23	1.98	0.46
1:A:281:PHE:HE1	1:A:325:ILE:HA	1.80	0.46
1:C:221:VAL:O	1:C:221:VAL:HG12	2.15	0.46
1:D:252:HIS:O	1:D:256:ILE:HG12	2.16	0.46
1:G:89:VAL:HG12	1:H:62:VAL:HG12	1.98	0.46
1:J:243:ASN:O	1:J:246:VAL:N	2.49	0.46
1:K:217:LYS:O	1:K:221:VAL:HG22	2.16	0.46
1:K:221:VAL:O	1:K:222:ARG:NE	2.48	0.46
1:L:150:VAL:CG2	1:L:232:TYR:HB3	2.45	0.46
1:C:176:PHE:CZ	1:C:314:ILE:HD13	2.50	0.46
1:C:478:SER:HB2	1:C:485:ILE:HG13	1.97	0.46
1:F:9:LEU:HD11	1:F:20:PHE:CB	2.39	0.46
1:F:389:ARG:HG2	1:F:389:ARG:HH11	1.80	0.46
1:H:191:LYS:HZ1	1:H:307:VAL:HG12	1.80	0.46
1:I:298:PRO:HB3	1:J:239:PRO:HB3	1.98	0.46
1:K:145:LEU:C	1:K:146:VAL:HG12	2.41	0.46
1:K:249:THR:HB	1:K:250:GLU:C	2.40	0.46
1:K:261:ARG:HA	1:K:264:ALA:HB3	1.98	0.46
1:L:69:ARG:CZ	1:L:87:GLU:OE2	2.63	0.46
1:D:273:PHE:HA	1:D:316:ILE:O	2.16	0.46
1:D:331:ARG:NH1	1:E:203:LYS:HE3	2.31	0.46
1:E:69:ARG:O	1:E:120:PRO:HB3	2.16	0.46
1:H:68:LEU:O	1:H:120:PRO:HA	2.15	0.46
1:H:86:GLU:HA	1:I:83:HIS:HB3	1.96	0.46
1:H:89:VAL:HG12	1:I:62:VAL:HG12	1.98	0.46
1:H:296:VAL:CB	1:I:242:LEU:CD1	2.69	0.46
1:I:261:ARG:HA	1:I:264:ALA:HB3	1.98	0.46
1:B:123:SER:HB2	1:B:137:ILE:O	2.16	0.46
1:B:149:GLU:O	1:B:150:VAL:CB	2.63	0.46
1:B:192:GLY:HA2	1:B:315:VAL:O	2.16	0.46
1:B:386:VAL:HG11	1:B:451:LEU:HD13	1.98	0.46
1:D:24:ARG:O	1:D:26:MET:HG3	2.15	0.46
1:F:192:GLY:HA3	1:F:335:LEU:HD12	1.98	0.46
1:F:268:THR:HA	1:F:269:PRO:HD3	1.78	0.46
1:G:363:VAL:HG12	1:G:375:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3:SER:HB2	1:K:47:LEU:O	2.15	0.46
1:K:168:ILE:HG12	1:K:339:ILE:HD13	1.97	0.46
1:K:178:HIS:CE1	1:L:439:LEU:HD13	2.51	0.46
1:L:34:ILE:HD11	1:L:55:GLU:HA	1.98	0.46
1:A:261:ARG:HA	1:A:264:ALA:CB	2.46	0.46
1:B:319:SER:OG	1:B:321:ARG:O	2.33	0.46
1:D:9:LEU:HD21	1:D:20:PHE:HB2	1.98	0.46
1:E:340:LYS:CD	1:E:342:GLU:HB3	2.46	0.46
1:G:364:HIS:CE1	1:G:443:GLN:HG3	2.51	0.46
1:H:296:VAL:HB	1:H:298:PRO:HD3	1.97	0.46
1:I:141:GLU:CB	1:I:145:LEU:HD13	2.43	0.46
1:I:422:MET:O	1:I:426:VAL:HG23	2.15	0.46
1:J:323:ASP:N	1:J:323:ASP:OD1	2.49	0.46
1:K:267:GLY:C	1:K:312:ASN:OD1	2.59	0.46
1:A:213:SER:HA	1:A:216:LYS:HE3	1.98	0.46
1:C:178:HIS:CD2	1:D:439:LEU:HD21	2.51	0.46
1:C:220:GLU:HG3	1:C:222:ARG:N	2.31	0.46
1:H:68:LEU:HB2	1:H:80:VAL:HG12	1.97	0.46
1:H:144:ASP:OD2	1:H:145:LEU:N	2.49	0.46
1:H:451:LEU:O	1:H:455:ILE:HG13	2.16	0.46
1:K:182:TYR:CD1	1:L:435:ILE:HD13	2.51	0.46
1:L:346:ALA:O	1:L:350:GLN:HG3	2.16	0.46
1:A:261:ARG:HA	1:A:264:ALA:HB3	1.98	0.45
1:A:399:PHE:CD2	1:A:417:PHE:CB	2.99	0.45
1:B:212:ASN:O	1:B:216:LYS:HG2	2.16	0.45
1:C:208:LYS:HG2	1:C:233:PHE:CE2	2.36	0.45
1:E:441:THR:HG23	1:E:443:GLN:HG2	1.98	0.45
1:F:254:ARG:CZ	1:F:299:GLN:HB2	2.46	0.45
1:I:281:PHE:CD1	1:I:297:VAL:HB	2.51	0.45
1:J:147:LEU:CA	1:J:148:GLU:HB2	2.38	0.45
1:B:195:LEU:O	1:B:318:ALA:HA	2.16	0.45
1:D:434:ALA:HA	1:D:450:HIS:CE1	2.50	0.45
1:I:328:ALA:HA	1:I:331:ARG:HG3	1.97	0.45
1:K:40:LYS:HD2	1:K:59:PHE:HZ	1.81	0.45
1:K:229:ALA:HA	1:K:230:LYS:HB2	0.59	0.45
1:L:470:ASN:ND2	1:L:472:ASP:CB	2.77	0.45
1:F:393:GLU:CD	1:F:415:LYS:HZ3	2.16	0.45
1:I:464:ASP:HB2	1:I:498:SER:HB2	1.98	0.45
1:J:203:LYS:NZ	1:J:320:ASN:HD22	2.14	0.45
1:K:214:LEU:CD2	1:K:218:MET:HE3	2.46	0.45
1:K:223:GLY:N	1:K:224:ASP:CA	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ASN:HD22	1:A:320:ASN:N	2.14	0.45
1:E:68:LEU:HB2	1:E:80:VAL:HG12	1.98	0.45
1:E:216:LYS:C	1:E:217:LYS:HD2	2.42	0.45
1:F:195:LEU:HD23	1:F:339:ILE:HB	1.99	0.45
1:G:198:PRO:HD2	1:G:341:ILE:O	2.16	0.45
1:H:242:LEU:HA	1:H:243:ASN:HA	1.67	0.45
1:J:310:LEU:HD13	1:J:310:LEU:O	2.16	0.45
1:K:207:ALA:CA	1:K:210:VAL:HG12	2.47	0.45
1:L:157:ASP:N	1:L:157:ASP:OD1	2.48	0.45
1:L:273:PHE:HD1	1:L:316:ILE:HB	1.81	0.45
1:A:154:SER:C	1:A:156:ALA:H	2.23	0.45
1:A:201:CYS:CB	1:A:420:GLY:H	2.29	0.45
1:C:151:PRO:HD3	1:C:233:PHE:CD2	2.51	0.45
1:D:343:ARG:HH21	1:D:473:ASP:CG	2.22	0.45
1:G:170:ASP:HA	1:G:174:LEU:HB2	1.97	0.45
1:I:141:GLU:HB3	1:I:145:LEU:CD1	2.42	0.45
1:K:218:MET:HA	1:K:221:VAL:HG23	1.97	0.45
1:K:418:ASN:HA	1:K:422:MET:HE2	1.97	0.45
1:L:76:HIS:CD2	1:L:97:ILE:HD13	2.51	0.45
1:A:139:LYS:NZ	1:F:69:ARG:NH2	2.65	0.45
1:A:215:ALA:HA	1:A:217:LYS:HG3	1.99	0.45
1:B:65:ILE:HD12	1:B:137:ILE:HD13	1.99	0.45
1:F:145:LEU:HG	1:F:146:VAL:H	1.82	0.45
1:G:490:THR:O	1:G:500:SER:OG	2.34	0.45
1:H:204:THR:HB	1:H:208:LYS:NZ	2.31	0.45
1:I:143:GLU:N	1:I:143:GLU:OE2	2.49	0.45
1:I:340:LYS:HE3	1:I:342:GLU:HB3	1.99	0.45
1:J:466:PRO:HG3	1:J:490:THR:HG21	1.99	0.45
1:K:215:ALA:HB1	1:K:229:ALA:HB1	1.98	0.45
1:A:214:LEU:HD12	1:A:271:ILE:HD11	1.99	0.45
1:A:351:ASP:O	1:A:354:SER:OG	2.23	0.45
1:B:418:ASN:HD21	1:B:423:ILE:HD11	1.82	0.45
1:G:69:ARG:O	1:G:120:PRO:HB3	2.16	0.45
1:G:172:VAL:C	1:G:175:PRO:HD2	2.42	0.45
1:H:299:GLN:CD	1:H:299:GLN:N	2.73	0.45
1:H:367:ASP:OD2	1:H:382:MET:HE2	2.16	0.45
1:I:145:LEU:O	1:I:146:VAL:CG1	2.65	0.45
1:J:250:GLU:HG2	1:J:253:ILE:HD12	1.99	0.45
1:K:43:GLN:NE2	1:K:56:ALA:HB1	2.31	0.45
1:L:280:ILE:HG21	1:L:300:LEU:HD11	1.99	0.45
1:B:27:ARG:HD3	1:C:46:ARG:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:VAL:HG22	1:B:87:GLU:HG2	1.99	0.45
1:D:271:ILE:HG12	1:D:314:ILE:HB	1.98	0.45
1:F:73:ALA:C	1:F:75:GLY:H	2.23	0.45
1:F:399:PHE:HD1	1:F:414:PHE:CZ	2.33	0.45
1:G:206:ILE:HG13	1:G:206:ILE:H	1.59	0.45
1:G:238:GLY:N	1:G:239:PRO:HD2	2.32	0.45
1:H:148:GLU:HG3	1:H:149:GLU:H	1.82	0.45
1:H:322:GLU:HG2	1:I:501:ARG:HH22	1.82	0.45
1:I:429:ARG:NH2	1:I:458:GLU:OE1	2.43	0.45
1:K:375:ARG:HA	1:K:378:CYS:HB3	1.99	0.45
1:L:371:PHE:CD2	1:L:378:CYS:HA	2.51	0.45
1:A:202:GLY:H	1:A:341:ILE:HG21	1.81	0.45
1:C:68:LEU:HB2	1:C:124:LEU:CD1	2.46	0.45
1:E:300:LEU:O	1:E:304:ILE:HG13	2.17	0.45
1:G:147:LEU:O	1:G:234:LEU:HA	2.17	0.45
1:H:34:ILE:HD11	1:H:55:GLU:HA	1.99	0.45
1:H:162:SER:O	1:H:165:ILE:HG13	2.17	0.45
1:I:8:LEU:HA	1:I:19:VAL:HG22	1.99	0.45
1:J:217:LYS:HA	1:J:218:MET:HA	1.82	0.45
1:L:259:ARG:O	1:L:263:LYS:NZ	2.50	0.45
1:A:146:VAL:O	1:A:146:VAL:HG13	2.16	0.45
1:C:485:ILE:HG21	1:C:488:ILE:HD11	1.99	0.45
1:E:259:ARG:O	1:E:263:LYS:NZ	2.50	0.45
1:I:242:LEU:HD23	1:I:243:ASN:HD22	1.82	0.45
1:J:116:ARG:HH12	1:J:119:ARG:CG	2.30	0.45
1:L:399:PHE:CD1	1:L:399:PHE:O	2.70	0.45
1:A:459:PHE:O	1:A:463:GLU:HG3	2.17	0.44
1:B:262:GLU:HB3	1:B:263:LYS:NZ	2.32	0.44
1:C:386:VAL:O	1:C:390:MET:HB2	2.18	0.44
1:F:147:LEU:O	1:F:147:LEU:HD13	2.18	0.44
1:G:149:GLU:O	1:G:151:PRO:HD2	2.16	0.44
1:H:298:PRO:HG2	1:I:242:LEU:CB	2.46	0.44
1:H:343:ARG:HG2	1:H:343:ARG:HH11	1.81	0.44
1:J:139:LYS:NZ	1:J:143:GLU:HA	2.32	0.44
1:J:191:LYS:HG3	1:J:308:GLU:HG3	1.99	0.44
1:K:174:LEU:HB3	1:K:175:PRO:HD3	1.99	0.44
1:L:116:ARG:HG3	1:L:117:LYS:O	2.17	0.44
1:A:270:VAL:HG12	1:A:313:VAL:HG22	2.00	0.44
1:C:251:ARG:HA	1:C:251:ARG:NH1	2.33	0.44
1:E:382:MET:O	1:E:386:VAL:HG12	2.18	0.44
1:F:201:CYS:O	1:F:203:LYS:NZ	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:297:VAL:HG13	1:F:298:PRO:HD3	1.97	0.44
1:H:437:SER:O	1:H:441:THR:HG22	2.17	0.44
1:I:68:LEU:HB2	1:I:124:LEU:HD12	1.99	0.44
1:I:279:SER:O	1:I:282:ARG:NH1	2.50	0.44
1:L:8:LEU:HD12	1:L:9:LEU:N	2.32	0.44
1:L:161:LEU:HD23	1:L:161:LEU:HA	1.80	0.44
1:C:398:ARG:HG2	1:C:411:VAL:HG11	1.99	0.44
1:G:198:PRO:HG2	1:G:343:ARG:HG2	2.00	0.44
1:I:493:THR:OG1	1:I:495:LYS:HD3	2.16	0.44
1:J:110:ASN:HB2	1:J:148:GLU:CD	2.42	0.44
1:K:228:GLU:CD	1:K:228:GLU:N	2.73	0.44
1:L:14:ASP:O	1:L:15:ASP:HB2	2.17	0.44
1:L:328:ALA:HA	1:L:331:ARG:HD3	2.00	0.44
1:B:363:VAL:HG13	1:B:368:LEU:HD11	1.99	0.44
1:B:422:MET:O	1:B:426:VAL:HG23	2.17	0.44
1:C:258:GLN:O	1:C:261:ARG:HB2	2.18	0.44
1:D:399:PHE:O	1:D:399:PHE:CD1	2.71	0.44
1:G:148:GLU:HG3	1:G:149:GLU:N	2.32	0.44
1:H:143:GLU:O	1:H:146:VAL:HG22	2.17	0.44
1:K:223:GLY:CA	1:K:224:ASP:HB2	2.47	0.44
1:A:438:VAL:HG22	1:A:444:PRO:HA	2.00	0.44
1:B:116:ARG:HG2	1:B:117:LYS:H	1.82	0.44
1:C:151:PRO:HB3	1:C:208:LYS:HB3	1.99	0.44
1:C:331:ARG:H	1:C:331:ARG:HG2	1.50	0.44
1:D:126:VAL:HG12	1:D:133:ALA:HB2	1.98	0.44
1:E:186:SER:O	1:F:431:LYS:NZ	2.49	0.44
1:G:200:GLY:HA3	1:G:201:CYS:HB2	1.99	0.44
1:H:84:ALA:O	1:H:85:ASP:HB2	2.15	0.44
1:H:101:LEU:HA	1:H:102:PRO:HD3	1.66	0.44
1:J:237:LYS:HZ1	1:J:237:LYS:N	2.16	0.44
1:J:277:MET:HA	1:J:280:ILE:HD13	2.00	0.44
1:J:353:TYR:CZ	1:J:423:ILE:HG23	2.53	0.44
1:A:198:PRO:O	1:A:203:LYS:NZ	2.51	0.44
1:E:383:ILE:O	1:E:386:VAL:HG13	2.18	0.44
1:G:61:ALA:HB1	1:L:77:ARG:HD3	1.98	0.44
1:G:206:ILE:CA	1:G:209:ALA:HB3	2.47	0.44
1:I:249:THR:HG23	1:I:251:ARG:N	2.33	0.44
1:I:296:VAL:HG12	1:I:297:VAL:H	1.82	0.44
1:J:200:GLY:HA2	1:J:201:CYS:HB2	1.99	0.44
1:J:244:LYS:NZ	1:J:247:GLY:HA2	2.33	0.44
1:J:263:LYS:HD2	1:J:270:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:322:GLU:OE1	1:J:322:GLU:N	2.48	0.44
1:K:298:PRO:HB3	1:L:239:PRO:CB	2.47	0.44
1:L:233:PHE:CE1	1:L:271:ILE:HB	2.53	0.44
1:L:246:VAL:HG22	1:L:247:GLY:H	1.83	0.44
1:L:251:ARG:HB3	1:L:252:HIS:H	1.68	0.44
1:L:254:ARG:HH11	1:L:303:GLU:HG2	1.82	0.44
1:A:9:LEU:HD11	1:A:20:PHE:CB	2.41	0.44
1:A:261:ARG:H	1:A:261:ARG:HG2	1.68	0.44
1:E:172:VAL:C	1:E:175:PRO:HD2	2.43	0.44
1:G:140:ALA:O	1:G:141:GLU:HG2	2.17	0.44
1:G:218:MET:HG3	1:G:219:ALA:N	2.33	0.44
1:G:367:ASP:OD2	1:G:382:MET:HE2	2.17	0.44
1:K:172:VAL:C	1:K:175:PRO:HD2	2.42	0.44
1:K:207:ALA:C	1:K:210:VAL:HG12	2.42	0.44
1:B:138:PRO:HD2	1:B:139:LYS:HA	1.99	0.44
1:C:150:VAL:HG21	1:C:231:SER:CB	2.47	0.44
1:D:178:HIS:O	1:D:181:LEU:N	2.41	0.44
1:E:69:ARG:O	1:E:120:PRO:CB	2.66	0.44
1:F:191:LYS:HE2	1:F:333:GLY:O	2.17	0.44
1:F:241:LEU:O	1:F:249:THR:OG1	2.21	0.44
1:G:151:PRO:HD3	1:G:233:PHE:CB	2.39	0.44
1:G:170:ASP:OD2	1:H:436:LYS:HD2	2.18	0.44
1:I:181:LEU:HD23	1:J:435:ILE:HG23	2.00	0.44
1:B:241:LEU:HD12	1:B:242:LEU:N	2.33	0.44
1:B:273:PHE:HA	1:B:316:ILE:O	2.18	0.44
1:B:419:SER:O	1:B:423:ILE:HG12	2.18	0.44
1:C:158:ILE:CG2	1:C:161:LEU:HD12	2.48	0.44
1:C:217:LYS:O	1:C:219:ALA:HA	2.18	0.44
1:F:140:ALA:C	1:F:142:VAL:H	2.25	0.44
1:F:384:GLU:O	1:F:388:ASP:HB2	2.17	0.44
1:J:137:ILE:HD13	1:J:137:ILE:HA	1.82	0.44
1:K:111:ASP:HB2	1:K:113:THR:HG23	2.00	0.44
1:K:281:PHE:HA	1:K:282:ARG:HB3	2.00	0.44
1:L:310:LEU:HD22	1:L:311:GLU:N	2.33	0.44
1:A:150:VAL:CG2	1:A:231:SER:CB	2.63	0.43
1:A:301:LEU:HD12	1:A:301:LEU:H	1.83	0.43
1:B:399:PHE:HE2	1:B:417:PHE:CD2	2.35	0.43
1:C:380:LYS:HE3	1:C:380:LYS:HB2	1.84	0.43
1:F:218:MET:HA	1:F:219:ALA:HA	1.57	0.43
1:G:263:LYS:H	1:G:263:LYS:HD2	1.83	0.43
1:H:140:ALA:C	1:H:142:VAL:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:402:VAL:HG22	1:H:488:ILE:HG12	1.98	0.43
1:B:236:ILE:HG23	1:B:273:PHE:O	2.18	0.43
1:D:254:ARG:HH11	1:D:254:ARG:CA	2.31	0.43
1:G:148:GLU:O	1:G:233:PHE:O	2.36	0.43
1:I:114:ARG:HA	1:I:115:PRO:HD3	1.76	0.43
1:I:447:ARG:HG2	1:I:450:HIS:CE1	2.52	0.43
1:K:367:ASP:OD1	1:K:367:ASP:N	2.51	0.43
1:K:398:ARG:HG2	1:K:413:TYR:CE1	2.54	0.43
1:L:155:TYR:OH	1:L:210:VAL:HG23	2.18	0.43
1:L:343:ARG:HG3	1:L:343:ARG:H	1.54	0.43
1:A:464:ASP:HB2	1:A:498:SER:HB2	2.00	0.43
1:B:150:VAL:H	1:B:233:PHE:C	2.26	0.43
1:B:150:VAL:HA	1:B:151:PRO:HD3	1.58	0.43
1:C:46:ARG:HD3	1:C:55:GLU:HG2	1.99	0.43
1:C:92:LEU:CD2	1:C:133:ALA:HB3	2.48	0.43
1:D:268:THR:HA	1:D:269:PRO:HD3	1.81	0.43
1:E:493:THR:HG23	1:E:495:LYS:H	1.84	0.43
1:K:141:GLU:CG	1:K:142:VAL:H	2.31	0.43
1:B:165:ILE:HG13	1:B:166:GLU:N	2.31	0.43
1:B:412:MET:HE3	1:B:412:MET:HB3	1.86	0.43
1:D:380:LYS:O	1:D:384:GLU:HG2	2.18	0.43
1:G:13:ASP:OD1	1:G:13:ASP:N	2.31	0.43
1:G:149:GLU:HB3	1:G:232:TYR:CD2	2.52	0.43
1:H:353:TYR:CE1	1:H:423:ILE:HG23	2.54	0.43
1:I:254:ARG:NH1	1:I:303:GLU:HG2	2.34	0.43
1:K:213:SER:O	1:K:217:LYS:HG2	2.18	0.43
1:K:214:LEU:HD21	1:K:218:MET:CE	2.49	0.43
1:K:296:VAL:HB	1:L:242:LEU:HB2	2.00	0.43
1:C:166:GLU:OE2	1:C:170:ASP:OD2	2.37	0.43
1:C:177:LEU:CD2	1:C:218:MET:HB2	2.46	0.43
1:C:389:ARG:HG2	1:C:452:LEU:HD22	2.00	0.43
1:D:74:ASP:C	1:D:76:HIS:H	2.25	0.43
1:E:441:THR:HG23	1:E:443:GLN:H	1.83	0.43
1:F:429:ARG:NH2	1:F:458:GLU:OE1	2.42	0.43
1:I:8:LEU:CD2	1:I:39:LEU:HB3	2.49	0.43
1:K:365:ALA:HA	1:K:368:LEU:HD12	2.01	0.43
1:L:422:MET:O	1:L:426:VAL:HG23	2.18	0.43
1:A:10:ALA:HB3	1:A:18:ASP:HB2	2.00	0.43
1:A:229:ALA:HB1	1:A:230:LYS:CA	2.36	0.43
1:C:68:LEU:HD13	1:C:78:ALA:HB1	2.01	0.43
1:C:327:PRO:O	1:C:331:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:GLN:HG2	1:E:341:ILE:HD13	2.00	0.43
1:F:147:LEU:H	1:F:147:LEU:CD1	2.30	0.43
1:F:176:PHE:CD2	1:F:214:LEU:HD11	2.53	0.43
1:G:255:LEU:O	1:G:258:GLN:HB3	2.18	0.43
1:I:27:ARG:HD2	1:J:5:TYR:OH	2.18	0.43
1:I:29:THR:OG1	1:J:1:MET:HG2	2.18	0.43
1:J:109:LEU:N	1:J:110:ASN:C	2.73	0.43
1:L:410:GLU:HG2	1:L:412:MET:SD	2.59	0.43
1:B:177:LEU:HD11	1:B:217:LYS:HE2	2.00	0.43
1:C:217:LYS:HE2	1:C:217:LYS:HB2	1.71	0.43
1:C:487:TYR:C	1:C:488:ILE:HG13	2.44	0.43
1:D:196:TYR:CZ	1:D:340:LYS:HB2	2.52	0.43
1:D:364:HIS:CD2	1:D:366:ASP:HB2	2.54	0.43
1:G:208:LYS:O	1:G:211:ALA:HB3	2.19	0.43
1:H:178:HIS:HB3	1:H:181:LEU:HD12	1.99	0.43
1:I:147:LEU:HD13	1:I:148:GLU:CB	2.43	0.43
1:I:214:LEU:HD21	1:I:269:PRO:HB2	2.01	0.43
1:J:47:LEU:HD23	1:J:53:VAL:HA	1.99	0.43
1:J:261:ARG:HA	1:J:264:ALA:HB3	2.01	0.43
1:K:278:ASP:OD1	1:K:320:ASN:N	2.51	0.43
1:A:70:GLU:HG2	1:A:71:ILE:N	2.33	0.43
1:H:161:LEU:HD23	1:H:161:LEU:HA	1.79	0.43
1:I:145:LEU:O	1:I:146:VAL:C	2.61	0.43
1:I:249:THR:OG1	1:I:250:GLU:OE1	2.25	0.43
1:I:360:PHE:CD1	1:I:360:PHE:N	2.86	0.43
1:I:400:LEU:O	1:I:412:MET:N	2.47	0.43
1:K:17:VAL:HG12	1:K:19:VAL:HG23	2.01	0.43
1:K:112:ASP:OD2	1:K:116:ARG:NE	2.52	0.43
1:K:471:PRO:HA	1:K:474:TRP:CD1	2.53	0.43
1:L:254:ARG:HH11	1:L:303:GLU:CG	2.32	0.43
1:B:384:GLU:O	1:B:388:ASP:HB2	2.18	0.43
1:C:133:ALA:C	1:C:134:PHE:HD1	2.27	0.43
1:C:151:PRO:HD3	1:C:233:PHE:CB	2.48	0.43
1:D:396:ASP:OD2	1:D:396:ASP:N	2.51	0.43
1:F:240:GLU:HA	1:F:243:ASN:OD1	2.18	0.43
1:I:203:LYS:HE2	1:I:320:ASN:ND2	2.33	0.43
1:J:116:ARG:HH12	1:J:119:ARG:HG2	1.83	0.43
1:J:399:PHE:O	1:J:400:LEU:HD23	2.19	0.43
1:L:249:THR:HA	1:L:250:GLU:CG	2.35	0.43
1:L:394:ILE:HG13	1:L:396:ASP:H	1.84	0.43
1:A:226:ALA:CB	1:A:228:GLU:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:PRO:HG2	1:C:212:ASN:HB2	2.01	0.43
1:D:350:GLN:HG2	1:D:387:VAL:HG21	2.00	0.43
1:D:429:ARG:HB3	1:D:454:SER:OG	2.19	0.43
1:F:161:LEU:HD23	1:F:161:LEU:HA	1.73	0.43
1:G:68:LEU:HD12	1:G:80:VAL:CG1	2.43	0.43
1:G:232:TYR:O	1:G:270:VAL:HG23	2.19	0.43
1:H:321:ARG:HG2	1:H:324:MET:HG3	2.01	0.43
1:J:249:THR:HB	1:J:251:ARG:HB2	2.01	0.43
1:A:176:PHE:CD2	1:A:177:LEU:HD12	2.40	0.42
1:A:256:ILE:HG13	1:A:257:PHE:H	1.84	0.42
1:A:307:VAL:HG21	1:A:313:VAL:HG11	2.00	0.42
1:A:429:ARG:HB3	1:A:454:SER:OG	2.19	0.42
1:D:202:GLY:O	1:D:204:THR:N	2.51	0.42
1:E:69:ARG:O	1:E:120:PRO:CG	2.67	0.42
1:E:215:ALA:HB1	1:E:231:SER:N	2.34	0.42
1:G:210:VAL:CG1	1:G:211:ALA:N	2.82	0.42
1:H:472:ASP:O	1:H:476:ARG:HG3	2.19	0.42
1:I:147:LEU:HB2	1:I:148:GLU:HB3	2.01	0.42
1:I:178:HIS:HB3	1:I:180:GLU:OE2	2.19	0.42
1:I:432:LYS:HE2	1:I:432:LYS:HB3	1.87	0.42
1:J:307:VAL:O	1:J:310:LEU:O	2.37	0.42
1:K:251:ARG:O	1:K:251:ARG:HG2	2.19	0.42
1:K:470:ASN:OD1	1:K:470:ASN:N	2.52	0.42
1:L:400:LEU:HD11	1:L:412:MET:CG	2.48	0.42
1:A:482:GLY:HA2	1:B:489:ARG:HD3	2.00	0.42
1:B:27:ARG:CD	1:C:46:ARG:HD2	2.48	0.42
1:C:471:PRO:HA	1:C:474:TRP:CD1	2.54	0.42
1:D:14:ASP:O	1:D:15:ASP:HB2	2.19	0.42
1:E:252:HIS:O	1:E:255:LEU:HB2	2.19	0.42
1:F:176:PHE:HE2	1:F:269:PRO:HB3	1.84	0.42
1:F:254:ARG:HH22	1:F:299:GLN:HB3	1.84	0.42
1:F:399:PHE:CE2	1:F:417:PHE:CD2	3.07	0.42
1:G:46:ARG:NH1	1:G:55:GLU:OE1	2.52	0.42
1:G:176:PHE:CZ	1:G:314:ILE:HD13	2.55	0.42
1:G:208:LYS:HG3	1:G:208:LYS:H	1.63	0.42
1:H:298:PRO:HD3	1:I:242:LEU:CD2	2.42	0.42
1:J:198:PRO:HG3	1:J:343:ARG:HG2	2.00	0.42
1:J:482:GLY:HA2	1:K:489:ARG:HD3	2.01	0.42
1:L:247:GLY:HA2	1:L:248:GLU:HA	1.55	0.42
1:A:119:ARG:HB2	1:A:120:PRO:HD2	2.01	0.42
1:A:296:VAL:HG12	1:A:298:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ARG:NH1	1:C:46:ARG:HH11	2.18	0.42
1:B:254:ARG:HG3	1:C:245:PHE:CZ	2.54	0.42
1:E:77:ARG:HH11	1:F:61:ALA:HB1	1.83	0.42
1:F:17:VAL:HG12	1:F:19:VAL:HG23	2.01	0.42
1:F:264:ALA:HB1	1:F:310:LEU:CD2	2.49	0.42
1:G:43:GLN:HG3	1:G:57:GLY:O	2.20	0.42
1:G:119:ARG:HG3	1:G:120:PRO:O	2.19	0.42
1:H:17:VAL:HG12	1:H:19:VAL:HG23	2.00	0.42
1:H:79:LEU:HD21	1:H:87:GLU:HB3	2.01	0.42
1:H:238:GLY:O	1:H:240:GLU:N	2.45	0.42
1:H:299:GLN:CD	1:H:300:LEU:N	2.73	0.42
1:I:389:ARG:NH1	1:I:397:ASN:OD1	2.52	0.42
1:J:233:PHE:CG	1:J:234:LEU:N	2.86	0.42
1:L:158:ILE:HD11	1:L:206:ILE:HA	1.99	0.42
1:L:203:LYS:HZ2	1:L:203:LYS:HB3	1.84	0.42
1:L:242:LEU:HD13	1:L:244:LYS:N	2.34	0.42
1:A:8:LEU:HD13	1:A:17:VAL:CG1	2.49	0.42
1:C:202:GLY:HA3	1:C:205:LEU:HB2	2.01	0.42
1:C:205:LEU:HD23	1:C:205:LEU:HA	1.88	0.42
1:C:301:LEU:HG	1:C:334:ARG:HH12	1.82	0.42
1:D:88:ARG:NH1	1:E:64:GLU:HG3	2.35	0.42
1:E:382:MET:HG2	1:E:448:ILE:HD13	2.01	0.42
1:J:105:LEU:CD1	1:J:105:LEU:H	2.32	0.42
1:K:222:ARG:O	1:K:225:ASP:CA	2.61	0.42
1:K:242:LEU:HA	1:K:244:LYS:N	2.34	0.42
1:K:482:GLY:HA2	1:L:489:ARG:HD3	2.01	0.42
1:B:194:LEU:HD23	1:B:338:LYS:HB3	2.02	0.42
1:B:232:TYR:OH	1:B:263:LYS:HB3	2.19	0.42
1:D:91:TRP:CZ2	1:E:61:ALA:HB3	2.55	0.42
1:D:230:LYS:HE2	1:D:230:LYS:HB2	1.82	0.42
1:D:403:THR:HB	1:D:487:TYR:HB3	2.01	0.42
1:G:205:LEU:HD13	1:G:206:ILE:H	1.78	0.42
1:I:147:LEU:HB2	1:I:148:GLU:CB	2.49	0.42
1:J:351:ASP:O	1:J:354:SER:OG	2.27	0.42
1:K:141:GLU:HG2	1:K:142:VAL:H	1.84	0.42
1:K:341:ILE:O	1:K:341:ILE:HG22	2.20	0.42
1:D:81:VAL:CG2	1:D:87:GLU:HG2	2.49	0.42
1:F:203:LYS:HA	1:F:206:ILE:CD1	2.50	0.42
1:G:14:ASP:OD1	1:G:14:ASP:N	2.36	0.42
1:H:63:GLY:N	1:H:125:LEU:HD11	2.35	0.42
1:J:111:ASP:HB3	1:J:143:GLU:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:310:LEU:CD1	1:J:312:ASN:N	2.83	0.42
1:K:84:ALA:O	1:K:85:ASP:HB2	2.19	0.42
1:K:247:GLY:HA2	1:K:248:GLU:HA	1.81	0.42
1:L:341:ILE:HG22	1:L:341:ILE:O	2.19	0.42
1:L:400:LEU:HD12	1:L:400:LEU:C	2.43	0.42
1:A:63:GLY:N	1:A:125:LEU:HD11	2.35	0.42
1:C:340:LYS:HD3	1:D:464:ASP:OD2	2.20	0.42
1:G:148:GLU:O	1:G:233:PHE:N	2.53	0.42
1:H:172:VAL:C	1:H:175:PRO:HD2	2.45	0.42
1:H:191:LYS:HZ3	1:H:307:VAL:CG1	2.31	0.42
1:J:344:PRO:HB2	1:J:348:ALA:HB3	2.02	0.42
1:L:213:SER:OG	1:L:214:LEU:N	2.52	0.42
1:A:5:TYR:CE1	1:A:46:ARG:HG3	2.55	0.42
1:A:139:LYS:HZ3	1:F:69:ARG:NH2	2.18	0.42
1:A:151:PRO:HB3	1:A:208:LYS:CB	2.43	0.42
1:C:188:ARG:HD3	1:C:191:LYS:HZ3	1.85	0.42
1:C:193:VAL:HA	1:C:337:VAL:HG23	2.02	0.42
1:D:361:LEU:HA	1:D:362:PRO:HD3	1.75	0.42
1:E:126:VAL:HG12	1:E:133:ALA:HA	2.00	0.42
1:F:246:VAL:HG13	1:F:251:ARG:NH1	2.34	0.42
1:G:149:GLU:HB3	1:G:232:TYR:CB	2.45	0.42
1:G:242:LEU:HD11	1:G:250:GLU:HG2	2.02	0.42
1:H:140:ALA:O	1:H:142:VAL:HG23	2.20	0.42
1:K:104:GLY:CA	1:K:106:PRO:HD3	2.49	0.42
1:K:193:VAL:HB	1:K:316:ILE:HG12	2.00	0.42
1:K:222:ARG:C	1:K:224:ASP:C	2.88	0.42
1:K:367:ASP:OD2	1:K:447:ARG:HA	2.19	0.42
1:L:151:PRO:HG2	1:L:212:ASN:HB2	2.01	0.42
1:B:360:PHE:HE2	1:G:216:LYS:HE3	1.84	0.42
1:C:174:LEU:HB3	1:C:175:PRO:HD3	2.01	0.42
1:C:378:CYS:O	1:C:382:MET:HG3	2.20	0.42
1:E:24:ARG:HE	1:E:26:MET:HE2	1.85	0.42
1:F:195:LEU:HD22	1:F:341:ILE:HD11	2.01	0.42
1:F:434:ALA:HA	1:F:450:HIS:CE1	2.54	0.42
1:G:251:ARG:O	1:G:253:ILE:N	2.53	0.42
1:I:170:ASP:OD1	1:I:170:ASP:N	2.47	0.42
1:L:255:LEU:HA	1:L:258:GLN:HB3	2.01	0.42
1:A:185:TYR:O	1:B:431:LYS:HD3	2.19	0.42
1:A:431:LYS:HB2	1:F:187:LEU:HD13	2.01	0.42
1:B:17:VAL:HG12	1:B:19:VAL:HG23	2.02	0.42
1:C:296:VAL:HG12	1:C:297:VAL:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:PHE:HB2	1:D:414:PHE:CE2	2.55	0.42
1:E:343:ARG:NH1	1:E:417:PHE:C	2.78	0.42
1:F:341:ILE:HD12	1:F:341:ILE:HG23	1.86	0.42
1:G:205:LEU:HA	1:G:208:LYS:HD3	2.01	0.42
1:H:232:TYR:CZ	1:H:263:LYS:HD2	2.54	0.42
1:H:299:GLN:CD	1:H:300:LEU:H	2.27	0.42
1:I:149:GLU:CG	1:I:150:VAL:N	2.82	0.42
1:J:493:THR:HG23	1:J:495:LYS:H	1.85	0.42
1:K:162:SER:O	1:K:165:ILE:HG13	2.20	0.42
1:K:221:VAL:CG1	1:K:222:ARG:CD	2.85	0.42
1:L:383:ILE:O	1:L:386:VAL:HG22	2.19	0.42
1:C:12:HIS:HB2	1:C:16:THR:O	2.20	0.41
1:C:361:LEU:HA	1:C:362:PRO:HD3	1.75	0.41
1:D:178:HIS:CD2	1:E:439:LEU:HD21	2.56	0.41
1:G:252:HIS:HA	1:G:255:LEU:HB2	2.02	0.41
1:H:301:LEU:HG	1:H:334:ARG:NH1	2.35	0.41
1:I:47:LEU:O	1:I:47:LEU:HD12	2.20	0.41
1:I:211:ALA:HB1	1:I:271:ILE:HD13	2.01	0.41
1:L:118:LEU:HD22	1:L:136:ARG:HD3	2.02	0.41
1:C:278:ASP:OD1	1:C:278:ASP:N	2.53	0.41
1:E:196:TYR:OH	1:F:464:ASP:OD2	2.31	0.41
1:J:340:LYS:HE2	1:J:342:GLU:HB3	2.02	0.41
1:K:146:VAL:O	1:K:146:VAL:HG13	2.20	0.41
1:L:386:VAL:HG11	1:L:451:LEU:HD13	2.02	0.41
1:B:459:PHE:O	1:B:463:GLU:HG3	2.19	0.41
1:D:27:ARG:HD3	1:E:46:ARG:HD2	2.02	0.41
1:D:351:ASP:O	1:D:354:SER:OG	2.38	0.41
1:E:356:TYR:HB3	1:E:427:VAL:HG21	2.01	0.41
1:E:371:PHE:CD2	1:E:378:CYS:HA	2.56	0.41
1:F:177:LEU:HD12	1:F:177:LEU:HA	1.76	0.41
1:G:281:PHE:HD2	1:G:324:MET:O	2.02	0.41
1:H:174:LEU:HD12	1:H:178:HIS:HD2	1.85	0.41
1:H:242:LEU:O	1:H:246:VAL:HB	2.21	0.41
1:H:382:MET:HG2	1:H:448:ILE:HD13	2.02	0.41
1:J:208:LYS:HG2	1:J:233:PHE:CE1	2.55	0.41
1:K:361:LEU:HA	1:K:362:PRO:HD3	1.77	0.41
1:A:364:HIS:NE2	1:A:447:ARG:NH1	2.68	0.41
1:C:271:ILE:HG22	1:C:314:ILE:H	1.85	0.41
1:G:198:PRO:HB3	1:G:343:ARG:CZ	2.49	0.41
1:G:244:LYS:HZ1	1:L:299:GLN:CA	2.33	0.41
1:I:360:PHE:N	1:I:360:PHE:HD1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:109:LEU:CD2	1:J:232:TYR:CE1	3.03	0.41
1:K:12:HIS:HB2	1:K:16:THR:O	2.21	0.41
1:K:104:GLY:O	1:K:106:PRO:CD	2.61	0.41
1:K:281:PHE:CZ	1:K:300:LEU:HD22	2.55	0.41
1:B:101:LEU:O	1:B:116:ARG:HG3	2.21	0.41
1:G:205:LEU:CD1	1:G:205:LEU:H	2.28	0.41
1:H:262:GLU:HB3	1:H:263:LYS:HZ2	1.84	0.41
1:H:296:VAL:HB	1:I:242:LEU:HD21	1.99	0.41
1:J:111:ASP:HB3	1:J:143:GLU:OE2	2.20	0.41
1:K:177:LEU:CD1	1:K:217:LYS:HB3	2.42	0.41
1:K:242:LEU:HA	1:K:243:ASN:C	2.46	0.41
1:K:250:GLU:HG3	1:K:250:GLU:O	2.20	0.41
1:A:264:ALA:HB1	1:A:310:LEU:HG	2.02	0.41
1:A:494:GLY:C	1:A:495:LYS:HE2	2.45	0.41
1:B:138:PRO:CD	1:B:139:LYS:HA	2.50	0.41
1:B:149:GLU:CA	1:B:234:LEU:HA	2.50	0.41
1:D:163:ARG:HE	1:D:167:GLN:NE2	2.19	0.41
1:G:216:LYS:NZ	1:G:216:LYS:HB2	2.34	0.41
1:H:232:TYR:CE2	1:H:263:LYS:HD2	2.55	0.41
1:I:243:ASN:CB	1:I:246:VAL:H	2.33	0.41
1:I:252:HIS:O	1:I:256:ILE:HG23	2.20	0.41
1:I:275:ASP:HB3	1:I:276:GLU:HG2	2.03	0.41
1:I:327:PRO:O	1:I:331:ARG:HG2	2.20	0.41
1:I:399:PHE:CD2	1:I:417:PHE:CB	3.04	0.41
1:J:109:LEU:CD1	1:J:109:LEU:N	2.83	0.41
1:J:249:THR:HA	1:J:250:GLU:CB	2.51	0.41
1:L:180:GLU:CD	1:L:180:GLU:H	2.28	0.41
1:L:243:ASN:HB2	1:L:245:PHE:CD1	2.55	0.41
1:B:138:PRO:HB2	1:B:139:LYS:O	2.21	0.41
1:B:232:TYR:OH	1:B:268:THR:HB	2.20	0.41
1:B:297:VAL:N	1:B:298:PRO:HD3	2.36	0.41
1:B:320:ASN:HD22	1:B:320:ASN:N	2.18	0.41
1:C:301:LEU:CD2	1:C:334:ARG:HH12	2.32	0.41
1:D:168:ILE:HG13	1:D:339:ILE:CD1	2.49	0.41
1:D:471:PRO:HA	1:D:474:TRP:HD1	1.86	0.41
1:E:91:TRP:CD1	1:F:62:VAL:HG11	2.56	0.41
1:F:147:LEU:N	1:F:147:LEU:CD1	2.72	0.41
1:H:105:LEU:HA	1:H:105:LEU:HD23	1.77	0.41
1:H:436:LYS:HE2	1:H:436:LYS:HB3	1.91	0.41
1:I:41:LYS:HB3	1:I:132:TYR:OH	2.21	0.41
1:J:250:GLU:HG3	1:J:299:GLN:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:203:LYS:O	1:K:204:THR:C	2.63	0.41
1:K:222:ARG:HE	1:K:222:ARG:HB3	1.80	0.41
1:A:188:ARG:NH2	1:G:219:ALA:H	2.18	0.41
1:C:91:TRP:O	1:C:133:ALA:N	2.53	0.41
1:C:355:LYS:HA	1:C:355:LYS:HD3	1.63	0.41
1:D:74:ASP:OD1	1:D:74:ASP:N	2.50	0.41
1:F:470:ASN:HD21	1:F:472:ASP:CG	2.27	0.41
1:G:234:LEU:HD23	1:G:235:ASN:N	2.36	0.41
1:H:9:LEU:HD11	1:H:20:PHE:HB2	2.03	0.41
1:I:147:LEU:CD2	1:I:148:GLU:HB3	2.50	0.41
1:I:153:VAL:HG21	1:I:205:LEU:HD11	2.02	0.41
1:K:105:LEU:HB3	1:K:262:GLU:OE2	2.21	0.41
1:K:474:TRP:CZ3	1:K:488:ILE:HD13	2.55	0.41
1:L:178:HIS:O	1:L:181:LEU:N	2.53	0.41
1:A:310:LEU:HD13	1:A:312:ASN:N	2.36	0.41
1:A:320:ASN:O	1:A:470:ASN:ND2	2.54	0.41
1:C:178:HIS:O	1:C:181:LEU:N	2.51	0.41
1:C:239:PRO:HD3	1:C:276:GLU:HB2	2.02	0.41
1:C:399:PHE:CD1	1:C:399:PHE:O	2.73	0.41
1:D:206:ILE:HD12	1:D:206:ILE:H	1.86	0.41
1:E:341:ILE:HG22	1:E:341:ILE:O	2.21	0.41
1:E:400:LEU:HB2	1:E:412:MET:HB2	2.02	0.41
1:E:415:LYS:HB3	1:E:415:LYS:HE3	1.95	0.41
1:F:72:LEU:HD12	1:F:73:ALA:H	1.84	0.41
1:F:356:TYR:HB3	1:F:427:VAL:HG11	2.03	0.41
1:G:94:ASP:N	1:G:95:PRO:HD2	2.35	0.41
1:G:234:LEU:HB3	1:G:271:ILE:O	2.21	0.41
1:G:244:LYS:HE3	1:G:245:PHE:CZ	2.56	0.41
1:G:345:ASP:O	1:G:391:TYR:CE2	2.74	0.41
1:H:330:LEU:HG	1:H:338:LYS:HE2	2.02	0.41
1:H:474:TRP:CE3	1:H:477:ILE:HD12	2.55	0.41
1:I:126:VAL:HG12	1:I:133:ALA:HA	2.03	0.41
1:I:162:SER:HA	1:I:165:ILE:HG12	2.03	0.41
1:I:244:LYS:HE2	1:I:296:VAL:N	2.36	0.41
1:I:441:THR:HG23	1:I:443:GLN:H	1.86	0.41
1:J:172:VAL:C	1:J:175:PRO:HD2	2.45	0.41
1:J:192:GLY:N	1:J:334:ARG:O	2.53	0.41
1:J:350:GLN:HG2	1:J:387:VAL:HG21	2.02	0.41
1:J:361:LEU:HA	1:J:362:PRO:HD3	1.77	0.41
1:K:11:THR:C	1:K:12:HIS:HD2	2.28	0.41
1:K:105:LEU:O	1:K:105:LEU:CG	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:116:ARG:HG2	1:K:136:ARG:NH2	2.36	0.41
1:K:207:ALA:C	1:K:210:VAL:CG1	2.94	0.41
1:L:17:VAL:HG11	1:L:53:VAL:HG21	2.03	0.41
1:L:246:VAL:O	1:L:249:THR:N	2.54	0.41
1:L:495:LYS:H	1:L:495:LYS:HG2	1.63	0.41
1:A:139:LYS:HZ3	1:F:69:ARG:HH21	1.70	0.41
1:A:174:LEU:HB3	1:A:175:PRO:HD3	2.03	0.41
1:A:229:ALA:CB	1:A:230:LYS:HA	2.34	0.41
1:D:253:ILE:H	1:D:253:ILE:HG13	1.51	0.41
1:D:375:ARG:HE	1:D:375:ARG:HB2	1.69	0.41
1:D:386:VAL:HG11	1:D:451:LEU:HB3	2.03	0.41
1:H:8:LEU:HD13	1:H:17:VAL:HG13	2.02	0.41
1:H:13:ASP:OD1	1:H:13:ASP:N	2.45	0.41
1:I:283:THR:HB	1:I:326:ASP:OD2	2.21	0.41
1:I:471:PRO:HA	1:I:474:TRP:CD1	2.56	0.41
1:J:241:LEU:HD12	1:J:241:LEU:HA	1.76	0.41
1:J:434:ALA:HB2	1:J:446:LEU:HB2	2.02	0.41
1:B:329:ILE:HG22	1:B:330:LEU:HD12	2.03	0.40
1:B:441:THR:HG23	1:B:442:GLY:N	2.36	0.40
1:C:188:ARG:HD3	1:C:191:LYS:HZ1	1.86	0.40
1:D:65:ILE:HD13	1:D:125:LEU:HA	2.02	0.40
1:F:232:TYR:OH	1:F:271:ILE:N	2.51	0.40
1:F:399:PHE:HE2	1:F:417:PHE:CD2	2.39	0.40
1:I:142:VAL:CG1	1:I:255:LEU:HB3	2.44	0.40
1:I:259:ARG:O	1:I:263:LYS:NZ	2.54	0.40
1:K:165:ILE:HG13	1:K:166:GLU:N	2.36	0.40
1:K:172:VAL:O	1:K:175:PRO:HD2	2.21	0.40
1:A:139:LYS:HE2	1:F:87:GLU:OE2	2.21	0.40
1:A:168:ILE:HD13	1:A:206:ILE:HG23	2.03	0.40
1:A:386:VAL:HG11	1:A:451:LEU:HD13	2.03	0.40
1:B:172:VAL:C	1:B:175:PRO:HD2	2.46	0.40
1:C:208:LYS:HA	1:C:233:PHE:CE2	2.56	0.40
1:C:219:ALA:HB3	1:C:221:VAL:N	2.36	0.40
1:D:83:HIS:O	1:D:83:HIS:ND1	2.54	0.40
1:E:248:GLU:OE2	1:E:249:THR:HG23	2.21	0.40
1:F:235:ASN:HB2	1:F:273:PHE:HD2	1.86	0.40
1:F:322:GLU:OE1	1:F:322:GLU:N	2.42	0.40
1:F:361:LEU:HA	1:F:362:PRO:HD3	1.83	0.40
1:G:241:LEU:HD11	1:L:298:PRO:HG2	2.03	0.40
1:H:171:ALA:HB1	1:H:337:VAL:HG21	2.04	0.40
1:I:46:ARG:NE	1:I:55:GLU:OE2	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:208:LYS:HG2	1:I:233:PHE:CZ	2.55	0.40
1:J:375:ARG:O	1:J:379:ILE:HG12	2.21	0.40
1:L:243:ASN:C	1:L:245:PHE:HA	2.45	0.40
1:L:400:LEU:CD1	1:L:400:LEU:C	2.94	0.40
1:A:161:LEU:CD1	1:A:206:ILE:HD11	2.51	0.40
1:B:216:LYS:O	1:B:217:LYS:HD2	2.20	0.40
1:B:341:ILE:O	1:B:341:ILE:HG22	2.21	0.40
1:C:343:ARG:CD	1:C:416:ASP:O	2.69	0.40
1:D:262:GLU:HG2	1:D:263:LYS:NZ	2.36	0.40
1:F:152:ASP:CG	1:F:153:VAL:N	2.79	0.40
1:F:327:PRO:O	1:F:331:ARG:HG2	2.22	0.40
1:G:167:GLN:N	1:G:168:ILE:HD12	2.36	0.40
1:G:194:LEU:HD22	1:G:330:LEU:HD11	2.03	0.40
1:H:358:THR:O	1:H:379:ILE:HD13	2.21	0.40
1:J:78:ALA:HB2	1:J:92:LEU:HD21	2.03	0.40
1:J:243:ASN:HB2	1:J:245:PHE:CD1	2.57	0.40
1:J:293:GLU:C	1:J:295:THR:H	2.29	0.40
1:K:107:GLU:O	1:K:108:ALA:CB	2.69	0.40
1:K:326:ASP:HA	1:K:327:PRO:HD3	1.96	0.40
1:L:150:VAL:HG23	1:L:232:TYR:CB	2.50	0.40
1:D:389:ARG:NH1	1:D:397:ASN:OD1	2.53	0.40
1:E:11:THR:HA	1:E:17:VAL:HG22	2.02	0.40
1:G:162:SER:O	1:G:165:ILE:HG13	2.22	0.40
1:G:322:GLU:CD	1:H:501:ARG:HH12	2.30	0.40
1:H:310:LEU:HD11	1:H:312:ASN:HB3	2.03	0.40
1:J:163:ARG:NH1	1:K:497:SER:HB3	2.36	0.40
1:J:239:PRO:HD3	1:J:276:GLU:HB2	2.04	0.40
1:J:242:LEU:HA	1:J:243:ASN:C	2.46	0.40
1:J:300:LEU:H	1:J:300:LEU:HD12	1.86	0.40
1:L:204:THR:HG21	1:L:275:ASP:OD2	2.21	0.40
1:B:464:ASP:O	1:B:501:ARG:HD2	2.21	0.40
1:B:484:ARG:HH11	1:B:484:ARG:CG	2.33	0.40
1:E:178:HIS:CE1	1:F:439:LEU:HD13	2.56	0.40
1:F:145:LEU:O	1:F:146:VAL:HG22	2.21	0.40
1:F:351:ASP:OD1	1:F:355:LYS:HE2	2.21	0.40
1:G:401:GLU:HB2	1:G:491:LEU:HD21	2.04	0.40
1:H:158:ILE:CD1	1:H:206:ILE:HA	2.51	0.40
1:I:35:ASP:O	1:I:38:SER:OG	2.38	0.40
1:I:343:ARG:CD	1:I:416:ASP:O	2.67	0.40
1:J:161:LEU:HD23	1:J:161:LEU:HA	1.79	0.40
1:J:298:PRO:HB3	1:K:239:PRO:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:333:GLY:H	1:J:336:ASP:CG	2.30	0.40
1:K:215:ALA:HB1	1:K:229:ALA:CB	2.52	0.40

All (3) 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:C:180:GLU:CG	1:K:230:LYS:CD[3_444]	1.97	0.23
1:C:180:GLU:CG	1:K:230:LYS:CE[3_444]	2.05	0.15
1:C:180:GLU:CG	1:K:230:LYS:NZ[3_444]	2.11	0.09

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	474/513 (92%)	440 (93%)	29 (6%)	5 (1%)	11	43
1	B	467/513 (91%)	441 (94%)	23 (5%)	3 (1%)	21	54
1	C	462/513 (90%)	429 (93%)	30 (6%)	3 (1%)	21	54
1	D	450/513 (88%)	433 (96%)	17 (4%)	0	100	100
1	E	451/513 (88%)	431 (96%)	19 (4%)	1 (0%)	43	74
1	F	452/513 (88%)	424 (94%)	24 (5%)	4 (1%)	14	47
1	G	453/513 (88%)	428 (94%)	21 (5%)	4 (1%)	14	47
1	H	470/513 (92%)	442 (94%)	24 (5%)	4 (1%)	14	47
1	I	470/513 (92%)	446 (95%)	23 (5%)	1 (0%)	43	74
1	J	478/513 (93%)	442 (92%)	33 (7%)	3 (1%)	21	54
1	K	494/513 (96%)	457 (92%)	29 (6%)	8 (2%)	7	36
1	L	465/513 (91%)	434 (93%)	27 (6%)	4 (1%)	14	47
All	All	5586/6156 (91%)	5247 (94%)	299 (5%)	40 (1%)	18	51

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	PRO
1	E	250	GLU
1	H	151	PRO
1	H	152	ASP
1	K	222	ARG
1	A	155	TYR
1	G	144	ASP
1	G	246	VAL
1	I	246	VAL
1	J	146	VAL
1	J	246	VAL
1	K	230	LYS
1	K	246	VAL
1	K	311	GLU
1	L	200	GLY
1	A	141	GLU
1	A	342	GLU
1	F	138	PRO
1	J	148	GLU
1	K	105	LEU
1	K	108	ALA
1	F	203	LYS
1	G	252	HIS
1	H	295	THR
1	K	252	HIS
1	A	222	ARG
1	A	245	PHE
1	B	150	VAL
1	B	342	GLU
1	F	139	LYS
1	G	150	VAL
1	L	199	PRO
1	L	201	CYS
1	C	221	VAL
1	C	466	PRO
1	K	104	GLY
1	C	223	GLY
1	F	146	VAL
1	H	297	VAL
1	L	246	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	405/433 (94%)	363 (90%)	42 (10%)	7	27
1	B	402/433 (93%)	356 (89%)	46 (11%)	5	24
1	C	389/433 (90%)	350 (90%)	39 (10%)	7	28
1	D	389/433 (90%)	339 (87%)	50 (13%)	4	21
1	E	389/433 (90%)	345 (89%)	44 (11%)	5	25
1	F	389/433 (90%)	341 (88%)	48 (12%)	4	22
1	G	390/433 (90%)	342 (88%)	48 (12%)	4	22
1	H	405/433 (94%)	357 (88%)	48 (12%)	5	23
1	I	405/433 (94%)	354 (87%)	51 (13%)	4	21
1	J	410/433 (95%)	367 (90%)	43 (10%)	6	27
1	K	421/433 (97%)	359 (85%)	62 (15%)	3	17
1	L	401/433 (93%)	351 (88%)	50 (12%)	4	22
All	All	4795/5196 (92%)	4224 (88%)	571 (12%)	5	23

All (571) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	150	VAL
1	A	154	SER
1	A	161	LEU
1	A	181	LEU
1	A	216	LYS
1	A	217	LYS
1	A	218	MET
1	A	221	VAL
1	A	222	ARG
1	A	228	GLU
1	A	236	ILE
1	A	241	LEU
1	A	243	ASN

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Mol	Chain	Res	Type
1	A	253	ILE
1	A	268	THR
1	A	276	GLU
1	A	277	MET
1	A	279	SER
1	A	280	ILE
1	A	281	PHE
1	A	296	VAL
1	A	307	VAL
1	A	311	GLU
1	A	314	ILE
1	A	315	VAL
1	A	320	ASN
1	A	363	VAL
1	A	368	LEU
1	A	372	ASP
1	A	376	SER
1	A	380	LYS
1	A	388	ASP
1	A	400	LEU
1	A	425	ASN
1	A	441	THR
1	A	448	ILE
1	A	449	GLN
1	A	476	ARG
1	A	496	SER
1	A	504	ASP
1	A	505	THR
1	B	19	VAL
1	B	68	LEU
1	B	81	VAL
1	B	134	PHE
1	B	136	ARG
1	B	142	VAL
1	B	147	LEU
1	B	149	GLU
1	B	214	LEU
1	B	236	ILE
1	B	237	LYS
1	B	242	LEU
1	B	244	LYS
1	B	245	PHE

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Mol	Chain	Res	Type
1	B	246	VAL
1	B	251	ARG
1	B	253	ILE
1	B	261	ARG
1	B	266	GLU
1	B	271	ILE
1	B	276	GLU
1	B	277	MET
1	B	278	ASP
1	B	315	VAL
1	B	320	ASN
1	B	323	ASP
1	B	325	ILE
1	B	329	ILE
1	B	337	VAL
1	B	338	LYS
1	B	345	ASP
1	B	358	THR
1	B	363	VAL
1	B	372	ASP
1	B	375	ARG
1	B	380	LYS
1	B	388	ASP
1	B	400	LEU
1	B	425	ASN
1	B	443	GLN
1	B	449	GLN
1	B	472	ASP
1	B	476	ARG
1	B	484	ARG
1	B	496	SER
1	B	501	ARG
1	C	8	LEU
1	C	24	ARG
1	C	34	ILE
1	C	51	LEU
1	C	79	LEU
1	C	81	VAL
1	C	125	LEU
1	C	214	LEU
1	C	217	LYS
1	C	218	MET

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Mol	Chain	Res	Type
1	C	220	GLU
1	C	234	LEU
1	C	236	ILE
1	C	241	LEU
1	C	245	PHE
1	C	248	GLU
1	C	268	THR
1	C	271	ILE
1	C	314	ILE
1	C	315	VAL
1	C	321	ARG
1	C	322	GLU
1	C	331	ARG
1	C	337	VAL
1	C	343	ARG
1	C	359	GLU
1	C	363	VAL
1	C	372	ASP
1	C	380	LYS
1	C	388	ASP
1	C	398	ARG
1	C	400	LEU
1	C	419	SER
1	C	425	ASN
1	C	441	THR
1	C	447	ARG
1	C	468	THR
1	C	501	ARG
1	C	506	GLU
1	D	8	LEU
1	D	17	VAL
1	D	24	ARG
1	D	64	GLU
1	D	67	THR
1	D	81	VAL
1	D	136	ARG
1	D	152	ASP
1	D	163	ARG
1	D	168	ILE
1	D	191	LYS
1	D	193	VAL
1	D	216	LYS

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Mol	Chain	Res	Type
1	D	230	LYS
1	D	235	ASN
1	D	236	ILE
1	D	237	LYS
1	D	241	LEU
1	D	245	PHE
1	D	252	HIS
1	D	253	ILE
1	D	254	ARG
1	D	261	ARG
1	D	262	GLU
1	D	263	LYS
1	D	268	THR
1	D	276	GLU
1	D	277	MET
1	D	296	VAL
1	D	297	VAL
1	D	311	GLU
1	D	315	VAL
1	D	323	ASP
1	D	329	ILE
1	D	331	ARG
1	D	337	VAL
1	D	363	VAL
1	D	375	ARG
1	D	384	GLU
1	D	388	ASP
1	D	390	MET
1	D	425	ASN
1	D	437	SER
1	D	440	GLU
1	D	441	THR
1	D	447	ARG
1	D	472	ASP
1	D	484	ARG
1	D	486	VAL
1	D	505	THR
1	E	17	VAL
1	E	34	ILE
1	E	68	LEU
1	E	69	ARG
1	E	87	GLU

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Mol	Chain	Res	Type
1	E	112	ASP
1	E	191	LYS
1	E	214	LEU
1	E	216	LYS
1	E	218	MET
1	E	236	ILE
1	E	241	LEU
1	E	243	ASN
1	E	245	PHE
1	E	248	GLU
1	E	251	ARG
1	E	259	ARG
1	E	268	THR
1	E	270	VAL
1	E	271	ILE
1	E	275	ASP
1	E	278	ASP
1	E	310	LEU
1	E	314	ILE
1	E	315	VAL
1	E	320	ASN
1	E	321	ARG
1	E	323	ASP
1	E	325	ILE
1	E	337	VAL
1	E	338	LYS
1	E	340	LYS
1	E	359	GLU
1	E	363	VAL
1	E	380	LYS
1	E	385	LYS
1	E	386	VAL
1	E	388	ASP
1	E	425	ASN
1	E	440	GLU
1	E	441	THR
1	E	456	VAL
1	E	476	ARG
1	E	504	ASP
1	F	17	VAL
1	F	28	LEU
1	F	49	GLU

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Mol	Chain	Res	Type
1	F	67	THR
1	F	72	LEU
1	F	125	LEU
1	F	137	ILE
1	F	141	GLU
1	F	147	LEU
1	F	152	ASP
1	F	177	LEU
1	F	203	LYS
1	F	214	LEU
1	F	216	LYS
1	F	217	LYS
1	F	230	LYS
1	F	232	TYR
1	F	233	PHE
1	F	236	ILE
1	F	241	LEU
1	F	249	THR
1	F	250	GLU
1	F	251	ARG
1	F	252	HIS
1	F	255	LEU
1	F	268	THR
1	F	276	GLU
1	F	296	VAL
1	F	297	VAL
1	F	314	ILE
1	F	331	ARG
1	F	342	GLU
1	F	343	ARG
1	F	358	THR
1	F	363	VAL
1	F	375	ARG
1	F	380	LYS
1	F	386	VAL
1	F	389	ARG
1	F	396	ASP
1	F	398	ARG
1	F	425	ASN
1	F	455	ILE
1	F	468	THR
1	F	476	ARG

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Mol	Chain	Res	Type
1	F	489	ARG
1	F	503	ILE
1	F	505	THR
1	G	13	ASP
1	G	17	VAL
1	G	68	LEU
1	G	81	VAL
1	G	118	LEU
1	G	145	LEU
1	G	147	LEU
1	G	150	VAL
1	G	161	LEU
1	G	168	ILE
1	G	169	ARG
1	G	170	ASP
1	G	204	THR
1	G	205	LEU
1	G	206	ILE
1	G	214	LEU
1	G	216	LYS
1	G	218	MET
1	G	236	ILE
1	G	237	LYS
1	G	241	LEU
1	G	243	ASN
1	G	244	LYS
1	G	248	GLU
1	G	259	ARG
1	G	268	THR
1	G	276	GLU
1	G	278	ASP
1	G	299	GLN
1	G	310	LEU
1	G	311	GLU
1	G	314	ILE
1	G	315	VAL
1	G	321	ARG
1	G	325	ILE
1	G	326	ASP
1	G	329	ILE
1	G	337	VAL
1	G	343	ARG

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Mol	Chain	Res	Type
1	G	358	THR
1	G	363	VAL
1	G	380	LYS
1	G	388	ASP
1	G	425	ASN
1	G	432	LYS
1	G	441	THR
1	G	476	ARG
1	G	501	ARG
1	H	9	LEU
1	H	17	VAL
1	H	68	LEU
1	H	92	LEU
1	H	101	LEU
1	H	107	GLU
1	H	139	LYS
1	H	148	GLU
1	H	183	ARG
1	H	206	ILE
1	H	214	LEU
1	H	216	LYS
1	H	218	MET
1	H	234	LEU
1	H	236	ILE
1	H	240	GLU
1	H	241	LEU
1	H	242	LEU
1	H	244	LYS
1	H	259	ARG
1	H	261	ARG
1	H	268	THR
1	H	271	ILE
1	H	276	GLU
1	H	278	ASP
1	H	294	THR
1	H	299	GLN
1	H	310	LEU
1	H	311	GLU
1	H	315	VAL
1	H	321	ARG
1	H	330	LEU
1	H	337	VAL

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Mol	Chain	Res	Type
1	H	359	GLU
1	H	363	VAL
1	H	372	ASP
1	H	375	ARG
1	H	386	VAL
1	H	425	ASN
1	H	441	THR
1	H	447	ARG
1	H	467	ASN
1	H	486	VAL
1	H	491	LEU
1	H	493	THR
1	H	495	LYS
1	H	496	SER
1	H	501	ARG
1	I	17	VAL
1	I	19	VAL
1	I	68	LEU
1	I	70	GLU
1	I	81	VAL
1	I	86	GLU
1	I	147	LEU
1	I	163	ARG
1	I	170	ASP
1	I	214	LEU
1	I	217	LYS
1	I	218	MET
1	I	235	ASN
1	I	236	ILE
1	I	237	LYS
1	I	244	LYS
1	I	246	VAL
1	I	248	GLU
1	I	249	THR
1	I	250	GLU
1	I	255	LEU
1	I	259	ARG
1	I	262	GLU
1	I	263	LYS
1	I	268	THR
1	I	271	ILE
1	I	276	GLU

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Mol	Chain	Res	Type
1	I	278	ASP
1	I	280	ILE
1	I	281	PHE
1	I	282	ARG
1	I	296	VAL
1	I	297	VAL
1	I	310	LEU
1	I	311	GLU
1	I	314	ILE
1	I	315	VAL
1	I	323	ASP
1	I	329	ILE
1	I	330	LEU
1	I	337	VAL
1	I	340	LYS
1	I	363	VAL
1	I	375	ARG
1	I	394	ILE
1	I	437	SER
1	I	443	GLN
1	I	449	GLN
1	I	476	ARG
1	I	493	THR
1	I	504	ASP
1	J	17	VAL
1	J	81	VAL
1	J	105	LEU
1	J	109	LEU
1	J	137	ILE
1	J	146	VAL
1	J	147	LEU
1	J	150	VAL
1	J	165	ILE
1	J	177	LEU
1	J	214	LEU
1	J	216	LYS
1	J	218	MET
1	J	236	ILE
1	J	237	LYS
1	J	241	LEU
1	J	244	LYS
1	J	248	GLU

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Mol	Chain	Res	Type
1	J	249	THR
1	J	263	LYS
1	J	268	THR
1	J	271	ILE
1	J	279	SER
1	J	297	VAL
1	J	307	VAL
1	J	310	LEU
1	J	314	ILE
1	J	315	VAL
1	J	323	ASP
1	J	329	ILE
1	J	330	LEU
1	J	337	VAL
1	J	342	GLU
1	J	363	VAL
1	J	375	ARG
1	J	385	LYS
1	J	425	ASN
1	J	436	LYS
1	J	446	LEU
1	J	476	ARG
1	J	483	GLU
1	J	505	THR
1	J	506	GLU
1	K	17	VAL
1	K	72	LEU
1	K	81	VAL
1	K	107	GLU
1	K	109	LEU
1	K	119	ARG
1	K	145	LEU
1	K	147	LEU
1	K	148	GLU
1	K	165	ILE
1	K	182	TYR
1	K	191	LYS
1	K	203	LYS
1	K	210	VAL
1	K	221	VAL
1	K	222	ARG
1	K	224	ASP

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Mol	Chain	Res	Type
1	K	227	HIS
1	K	228	GLU
1	K	230	LYS
1	K	231	SER
1	K	234	LEU
1	K	236	ILE
1	K	237	LYS
1	K	244	LYS
1	K	248	GLU
1	K	249	THR
1	K	254	ARG
1	K	261	ARG
1	K	263	LYS
1	K	265	SER
1	K	266	GLU
1	K	268	THR
1	K	276	GLU
1	K	279	SER
1	K	280	ILE
1	K	281	PHE
1	K	282	ARG
1	K	284	ARG
1	K	296	VAL
1	K	297	VAL
1	K	302	SER
1	K	310	LEU
1	K	311	GLU
1	K	314	ILE
1	K	315	VAL
1	K	323	ASP
1	K	324	MET
1	K	325	ILE
1	K	329	ILE
1	K	338	LYS
1	K	339	ILE
1	K	342	GLU
1	K	366	ASP
1	K	385	LYS
1	K	386	VAL
1	K	388	ASP
1	K	390	MET
1	K	468	THR

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Mol	Chain	Res	Type
1	K	476	ARG
1	K	480	LYS
1	K	500	SER
1	L	69	ARG
1	L	81	VAL
1	L	141	GLU
1	L	150	VAL
1	L	157	ASP
1	L	191	LYS
1	L	203	LYS
1	L	216	LYS
1	L	230	LYS
1	L	232	TYR
1	L	234	LEU
1	L	236	ILE
1	L	237	LYS
1	L	241	LEU
1	L	244	LYS
1	L	248	GLU
1	L	250	GLU
1	L	251	ARG
1	L	268	THR
1	L	271	ILE
1	L	278	ASP
1	L	296	VAL
1	L	313	VAL
1	L	321	ARG
1	L	329	ILE
1	L	331	ARG
1	L	343	ARG
1	L	358	THR
1	L	359	GLU
1	L	363	VAL
1	L	375	ARG
1	L	382	MET
1	L	385	LYS
1	L	386	VAL
1	L	398	ARG
1	L	400	LEU
1	L	425	ASN
1	L	441	THR
1	L	446	LEU

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Mol	Chain	Res	Type
1	L	447	ARG
1	L	448	ILE
1	L	449	GLN
1	L	456	VAL
1	L	468	THR
1	L	476	ARG
1	L	484	ARG
1	L	489	ARG
1	L	492	VAL
1	L	495	LYS
1	L	501	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	ASN
1	B	364	HIS
1	C	76	HIS
1	C	235	ASN
1	C	449	GLN
1	C	450	HIS
1	C	470	ASN
1	D	167	GLN
1	D	470	ASN
1	E	43	GLN
1	E	243	ASN
1	E	252	HIS
1	E	320	ASN
1	E	450	HIS
1	F	212	ASN
1	F	235	ASN
1	F	312	ASN
1	F	320	ASN
1	F	470	ASN
1	G	178	HIS
1	G	243	ASN
1	G	299	GLN
1	G	364	HIS
1	H	43	GLN
1	H	178	HIS
1	H	424	GLN
1	H	450	HIS

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Mol	Chain	Res	Type
1	H	467	ASN
1	I	235	ASN
1	I	243	ASN
1	J	12	HIS
1	J	110	ASN
1	J	243	ASN
1	J	252	HIS
1	J	258	GLN
1	J	312	ASN
1	J	320	ASN
1	J	462	ASN
1	K	76	HIS
1	K	178	HIS
1	K	243	ASN
1	K	252	HIS
1	K	462	ASN
1	L	212	ASN
1	L	252	HIS
1	L	320	ASN
1	L	406	ASN
1	L	418	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	480/513 (93%)	-0.24	3 (0%) 85 65	56, 117, 190, 215	0
1	B	475/513 (92%)	-0.18	1 (0%) 91 82	57, 133, 189, 213	0
1	C	472/513 (92%)	-0.12	7 (1%) 72 47	55, 134, 193, 231	0
1	D	460/513 (89%)	-0.20	3 (0%) 84 63	66, 127, 215, 230	0
1	E	461/513 (89%)	-0.17	3 (0%) 84 63	71, 149, 212, 231	0
1	F	460/513 (89%)	-0.12	1 (0%) 91 82	66, 136, 191, 226	0
1	G	461/513 (89%)	-0.10	4 (0%) 81 58	69, 128, 195, 223	0
1	H	478/513 (93%)	-0.18	6 (1%) 75 50	61, 107, 191, 209	0
1	I	478/513 (93%)	-0.21	4 (0%) 82 60	62, 107, 176, 217	0
1	J	484/513 (94%)	-0.21	3 (0%) 85 65	70, 120, 191, 215	0
1	K	498/513 (97%)	-0.23	4 (0%) 82 60	67, 114, 164, 191	0
1	L	473/513 (92%)	-0.17	2 (0%) 88 72	64, 146, 205, 219	0
All	All	5680/6156 (92%)	-0.18	41 (0%) 84 63	55, 125, 200, 231	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	260	ALA	4.8
1	L	274	PHE	4.7
1	C	231	SER	4.4
1	G	206	ILE	4.3
1	A	399	PHE	4.0
1	C	233	PHE	3.8
1	G	205	LEU	3.5
1	E	78	ALA	3.3
1	K	307	VAL	3.1
1	C	256	ILE	3.1
1	I	272	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	296	VAL	2.9
1	H	300	LEU	2.9
1	H	202	GLY	2.8
1	C	219	ALA	2.7
1	D	256	ILE	2.6
1	L	316	ILE	2.6
1	D	231	SER	2.4
1	I	231	SER	2.4
1	D	151	PRO	2.4
1	H	203	LYS	2.4
1	A	296	VAL	2.4
1	K	190	PRO	2.3
1	I	399	PHE	2.3
1	H	270	VAL	2.3
1	K	357	LEU	2.2
1	K	446	LEU	2.2
1	J	206	ILE	2.2
1	E	446	LEU	2.2
1	G	260	ALA	2.2
1	C	232	TYR	2.2
1	H	256	ILE	2.2
1	J	171	ALA	2.2
1	H	260	ALA	2.1
1	G	269	PRO	2.1
1	E	296	VAL	2.1
1	C	300	LEU	2.1
1	B	171	ALA	2.1
1	A	233	PHE	2.1
1	C	260	ALA	2.0
1	J	241	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.