



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:46 am BST

PDB ID : 5KZF
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

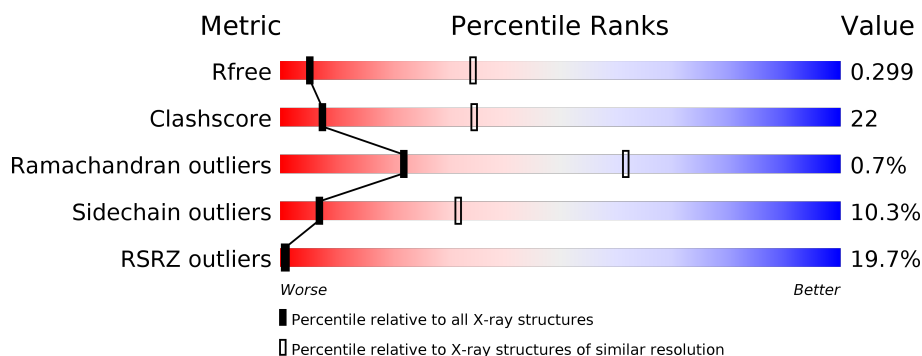
1 Overall quality at a glance

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>21%</div> <div>57%</div> <div>31%</div> <div>6%</div> </div>
1	B	513	<div> <div>19%</div> <div>60%</div> <div>29%</div> <div>7%</div> </div>
1	C	513	<div> <div>19%</div> <div>60%</div> <div>27%</div> <div>8%</div> </div>
1	D	513	<div> <div>22%</div> <div>56%</div> <div>29%</div> <div>5%</div> <div>10%</div> </div>
1	E	513	<div> <div>27%</div> <div>59%</div> <div>26%</div> <div>5%</div> <div>10%</div> </div>
1	F	513	<div> <div>18%</div> <div>55%</div> <div>29%</div> <div>5%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	513	<div><div></div><div>17%</div><div>56%</div><div>28%</div><div>5%</div><div>10%</div></div>
1	H	513	<div><div></div><div>16%</div><div>61%</div><div>28%</div><div></div><div>7%</div></div>
1	I	513	<div><div></div><div>13%</div><div>56%</div><div>31%</div><div>6%</div><div>7%</div></div>
1	J	513	<div><div></div><div>12%</div><div>59%</div><div>30%</div><div></div><div>6%</div></div>
1	K	513	<div><div></div><div>10%</div><div>58%</div><div>32%</div><div>6%</div><div></div></div>
1	L	513	<div><div></div><div>23%</div><div>56%</div><div>31%</div><div>5%</div><div>8%</div></div>

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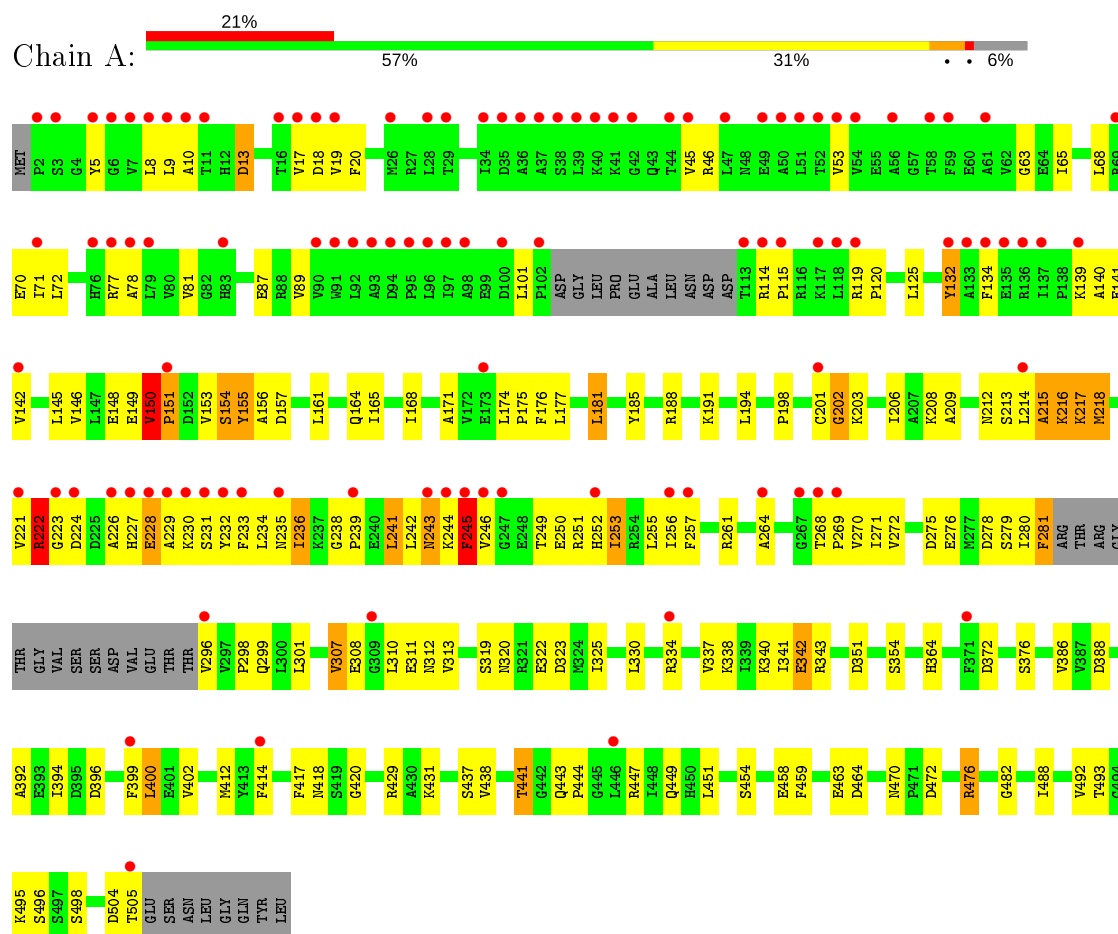
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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	initiating methionine	UNP A5U4E1
G	1	MET	-	initiating methionine	UNP A5U4E1
H	1	MET	-	initiating methionine	UNP A5U4E1
I	1	MET	-	initiating methionine	UNP A5U4E1
J	1	MET	-	initiating methionine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

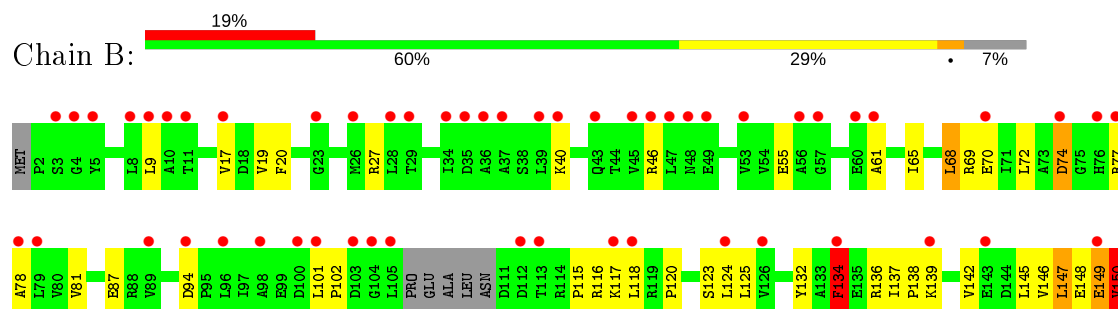
3 Residue-property plots [i](#)

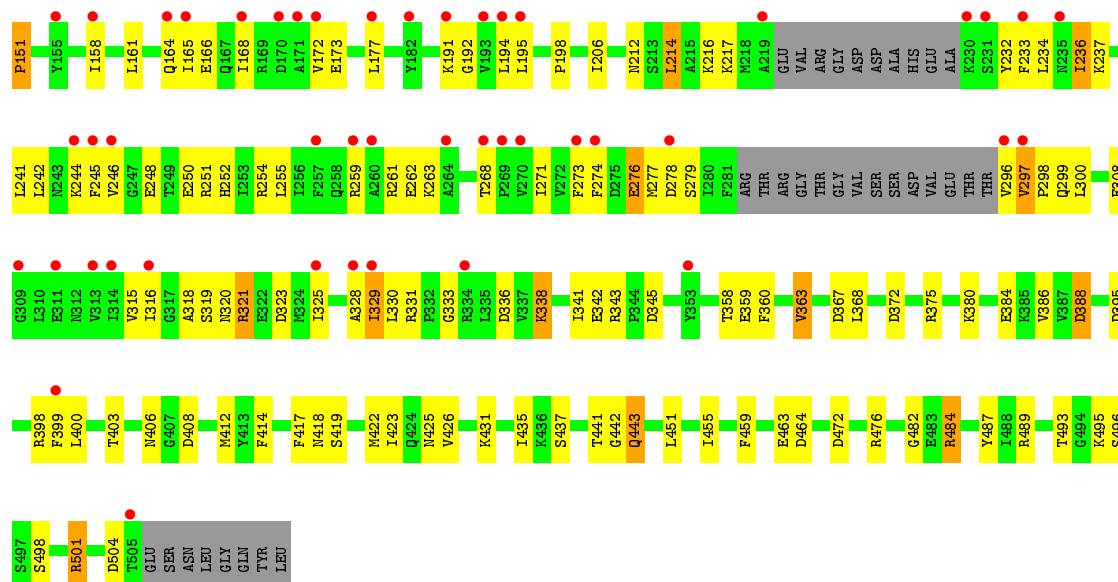
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

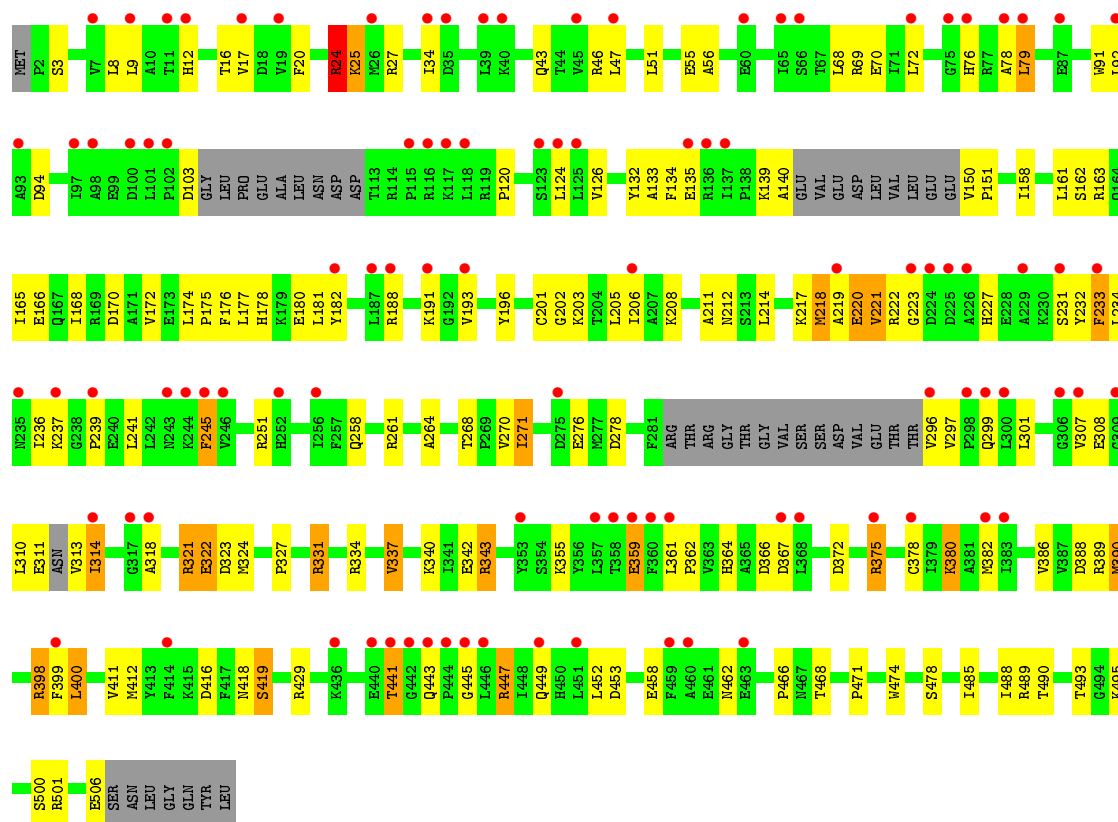


• Molecule 1: Proteasome-associated ATPase



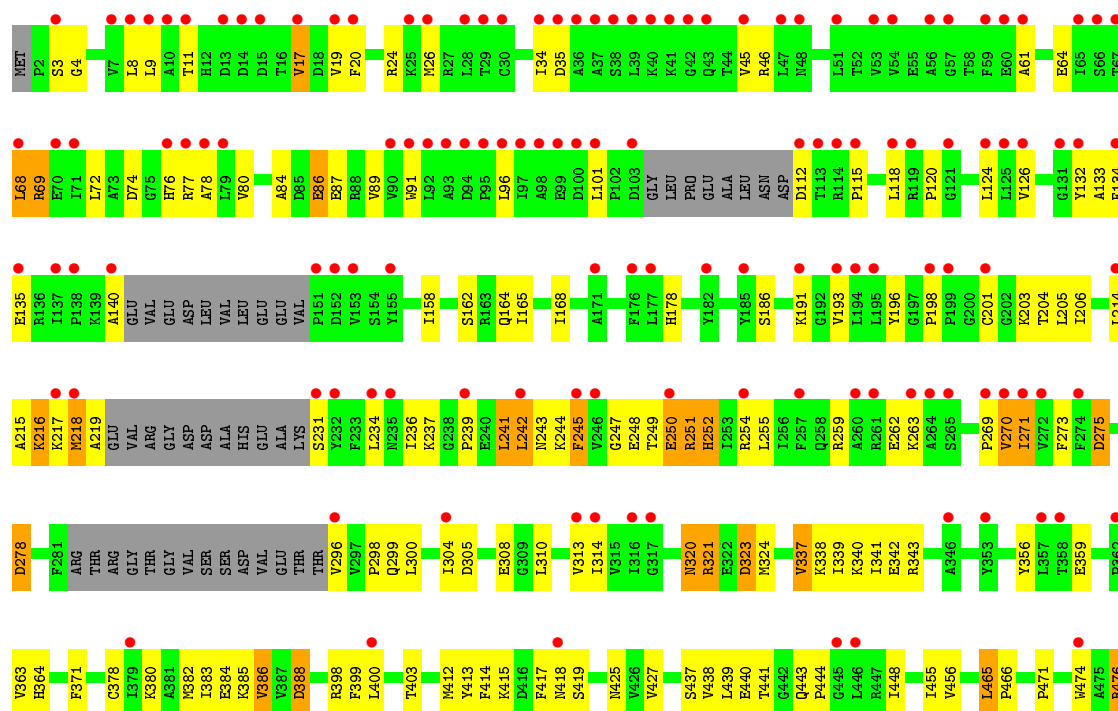


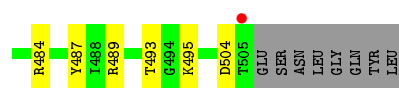
• Molecule 1: Proteasome-associated ATPase



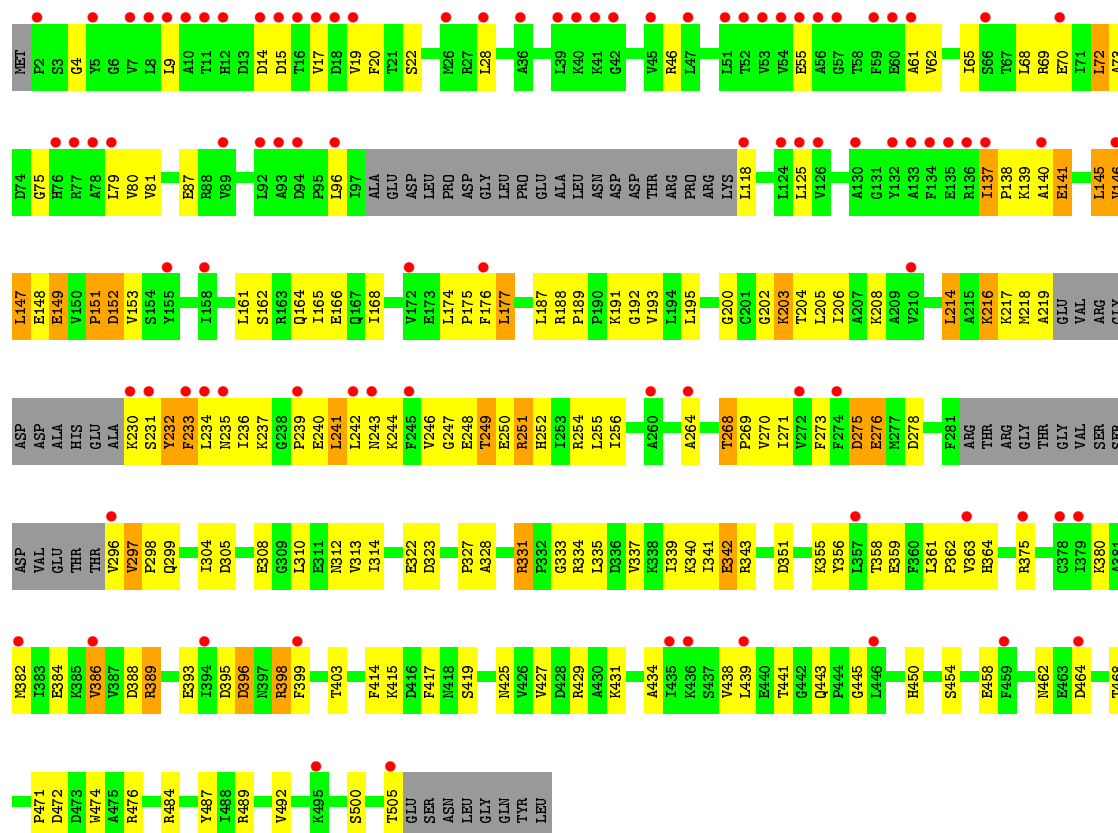
• Molecule 1: Proteasome-associated ATPase



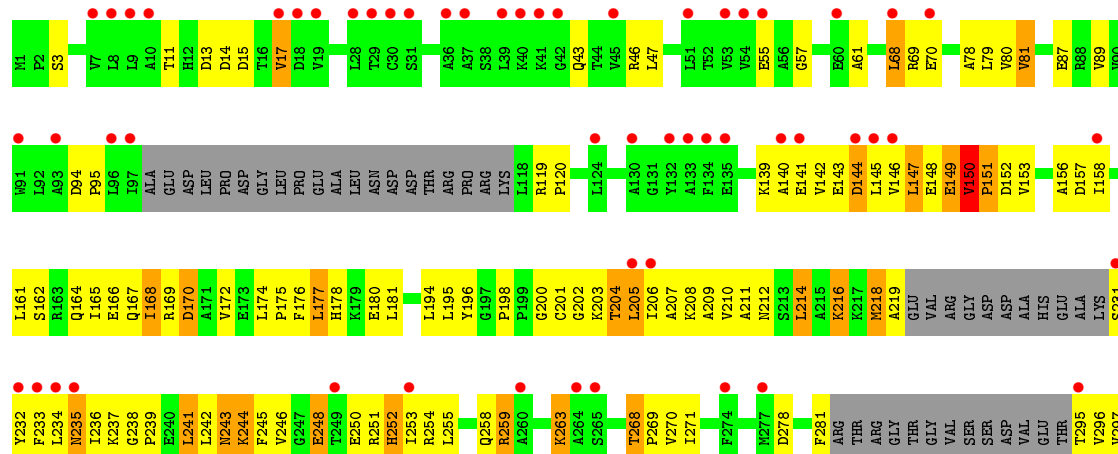


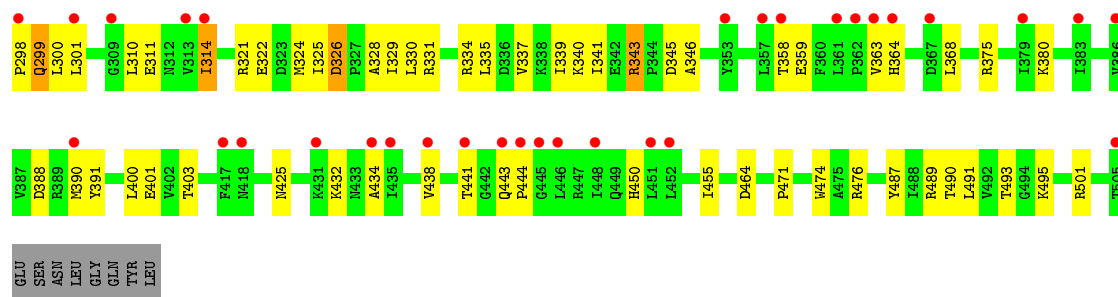


● Molecule 1: Proteasome-associated ATPase

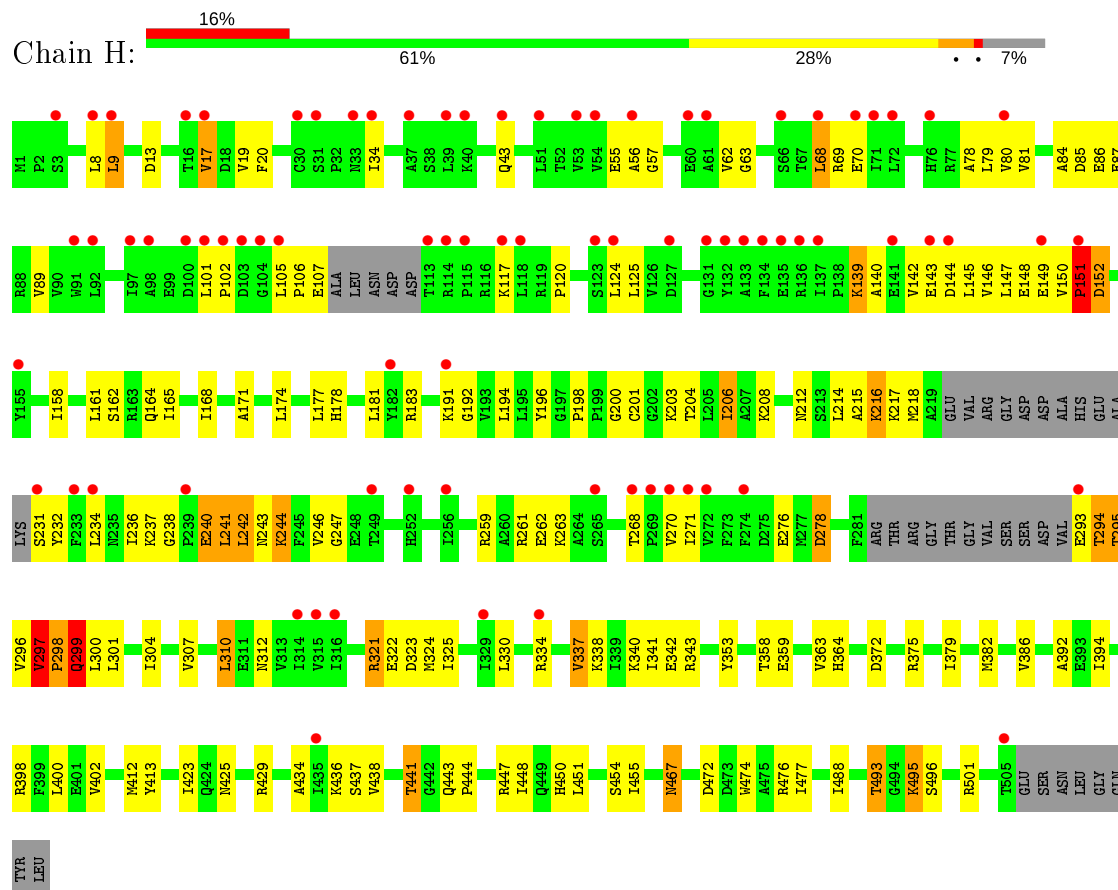


● Molecule 1: Proteasome-associated ATPase

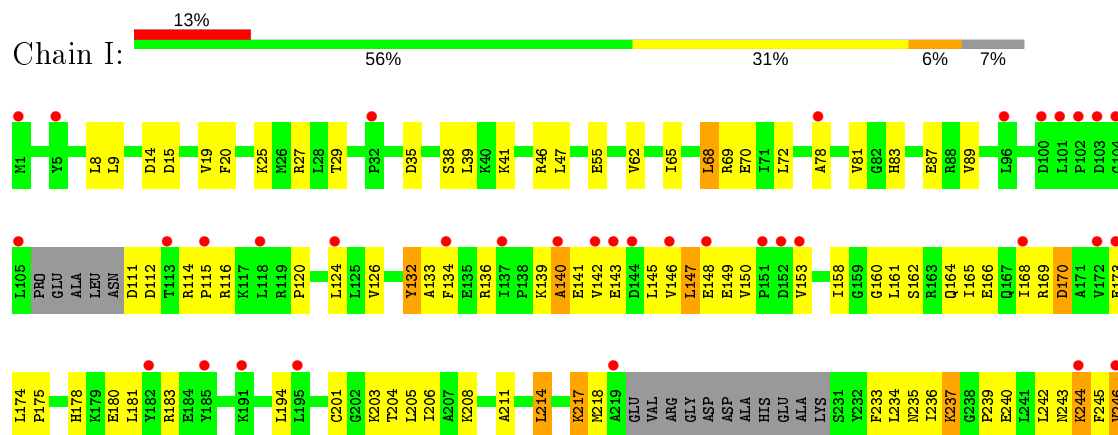


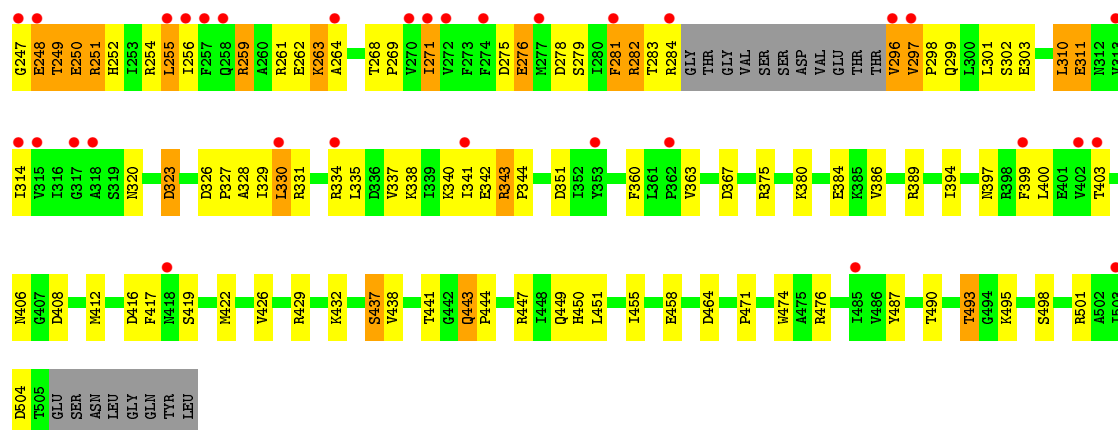


• Molecule 1: Proteasome-associated ATPase

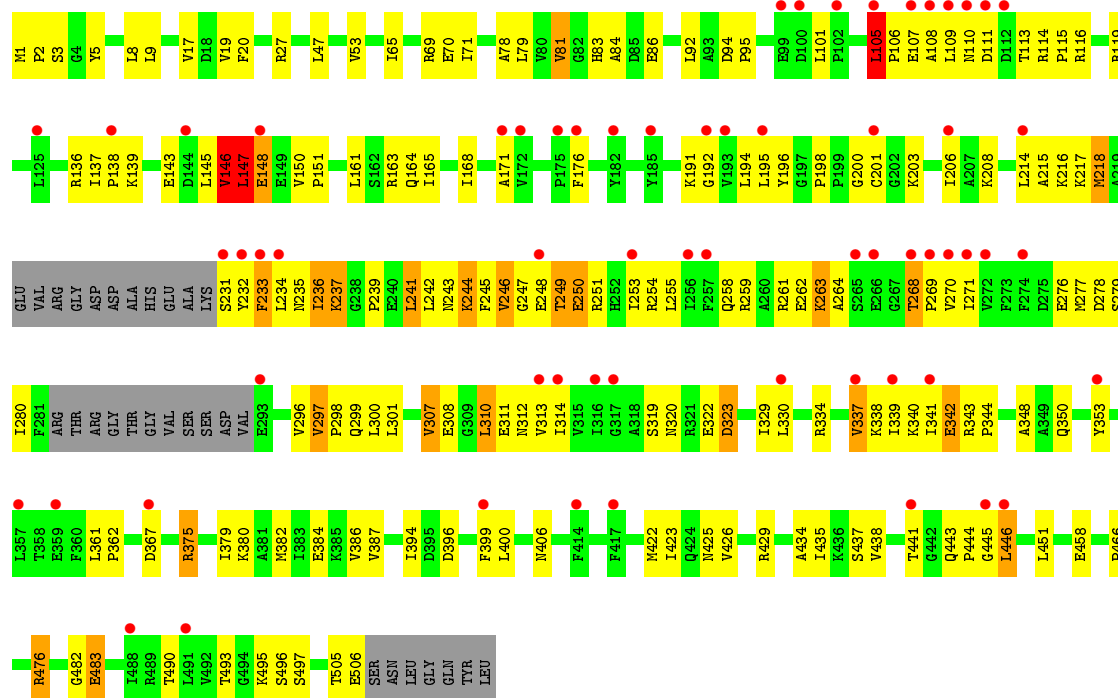


• Molecule 1: Proteasome-associated ATPase

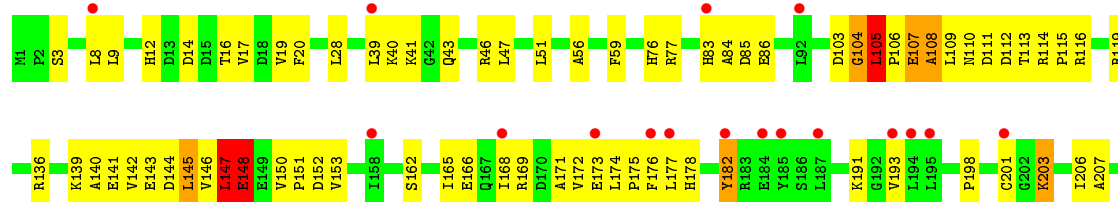


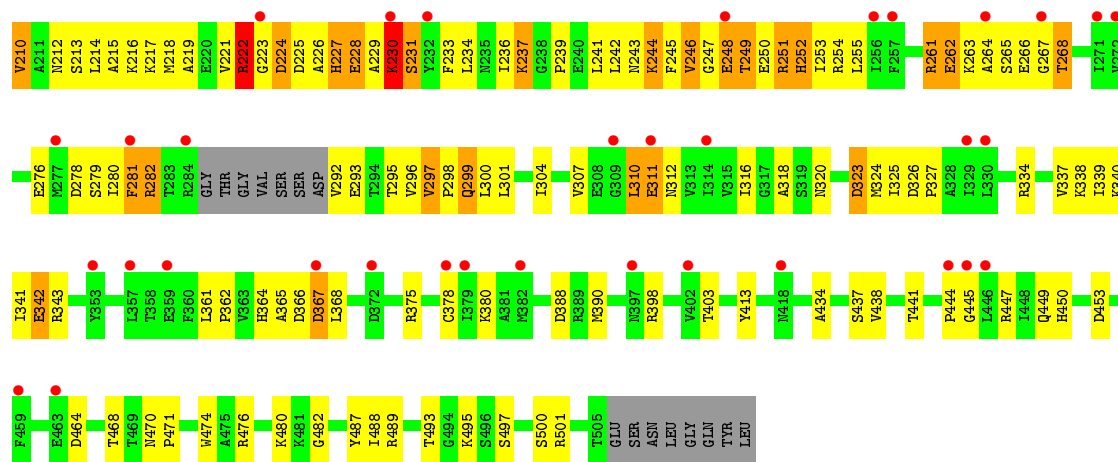


• Molecule 1: Proteasome-associated ATPase

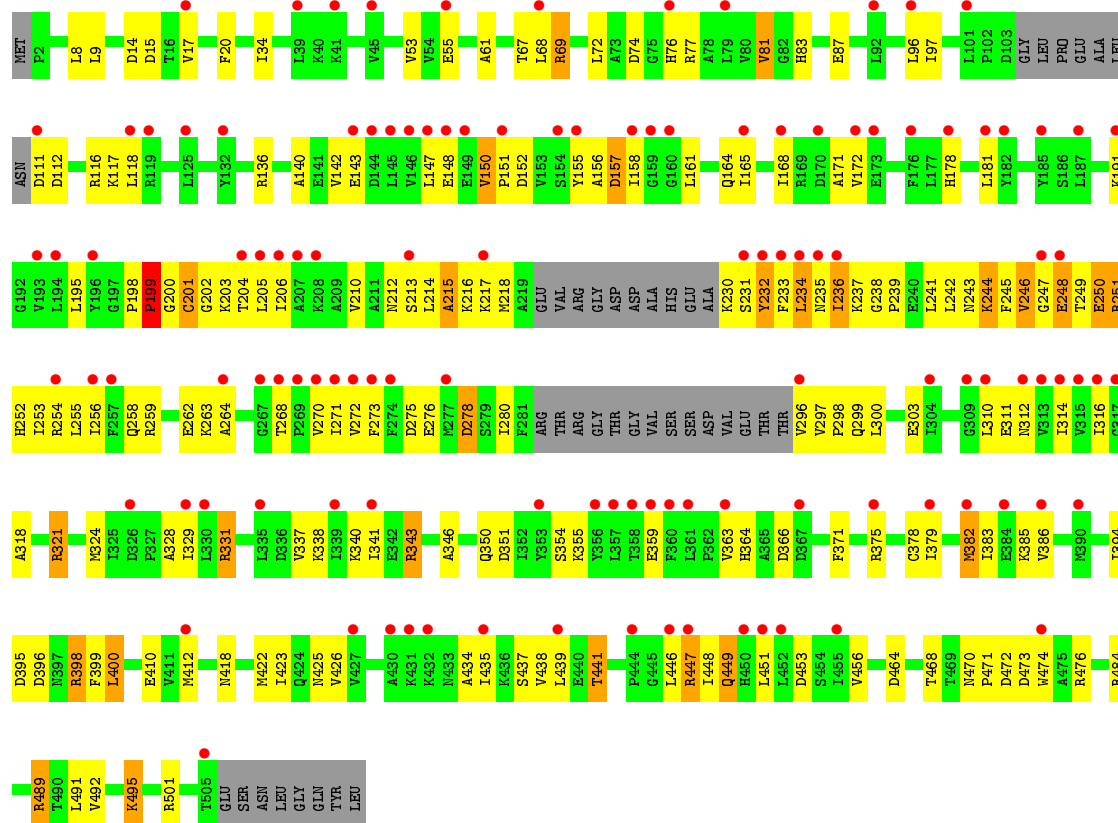


• Molecule 1: Proteasome-associated ATPase





• Molecule 1: Proteasome-associated ATPase



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 (2.21%)	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)	0.36 , 92.7	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	0.35	1/3808 (0.0%)	0.60	1/5150 (0.0%)
1	B	0.32	0/3766	0.56	3/5092 (0.1%)
1	C	0.31	0/3706	0.56	1/5011 (0.0%)
1	D	0.30	0/3651	0.53	1/4933 (0.0%)
1	E	0.31	1/3655 (0.0%)	0.55	3/4939 (0.1%)
1	F	0.32	0/3646	0.57	2/4929 (0.0%)
1	G	0.35	1/3652 (0.0%)	0.56	1/4939 (0.0%)
1	H	0.35	1/3789 (0.0%)	0.58	2/5126 (0.0%)
1	I	0.34	0/3794	0.60	1/5130 (0.0%)
1	J	0.32	0/3836	0.58	2/5192 (0.0%)
1	K	0.37	0/3950	0.62	3/5346 (0.1%)
1	L	0.31	0/3754	0.56	0/5076
All	All	0.33	4/45007 (0.0%)	0.57	20/60863 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	466	PRO	N-CD	5.37	1.55	1.47
1	A	151	PRO	N-CD	5.20	1.55	1.47
1	H	298	PRO	N-CD	5.18	1.55	1.47
1	G	151	PRO	N-CD	5.08	1.54	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	148	GLU	N-CA-C	7.45	131.12	111.00
1	E	251	ARG	N-CA-C	7.28	130.66	111.00
1	H	150	VAL	C-N-CD	-6.30	106.75	120.60
1	K	251	ARG	N-CA-C	-5.73	95.53	111.00
1	G	150	VAL	C-N-CD	5.69	140.36	128.40
1	E	465	LEU	C-N-CD	5.62	140.21	128.40
1	A	150	VAL	C-N-CD	5.61	140.19	128.40
1	J	105	LEU	CA-CB-CG	5.61	128.20	115.30
1	H	297	VAL	C-N-CD	5.53	140.00	128.40
1	I	140	ALA	N-CA-C	5.51	125.88	111.00
1	E	252	HIS	N-CA-C	5.39	125.56	111.00
1	J	147	LEU	C-N-CA	5.39	135.18	121.70
1	K	105	LEU	C-N-CD	5.27	139.47	128.40
1	C	25	LYS	N-CA-C	5.25	125.17	111.00
1	F	149	GLU	N-CA-C	5.21	125.07	111.00
1	B	150	VAL	C-N-CD	-5.19	109.17	120.60
1	F	145	LEU	CA-CB-CG	5.06	126.94	115.30
1	D	76	HIS	N-CA-C	5.05	124.64	111.00
1	B	134	PHE	N-CA-C	5.01	124.53	111.00
1	B	400	LEU	CA-CB-CG	5.00	126.81	115.30

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

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Mol	Chain	Res	Type	Group
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
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	190	0
1	B	3707	0	3718	145	0
1	C	3649	0	3644	136	3
1	D	3593	0	3607	120	0
1	E	3597	0	3610	131	0
1	F	3589	0	3606	137	0
1	G	3595	0	3611	219	0
1	H	3729	0	3741	180	0
1	I	3735	0	3749	205	0
1	J	3775	0	3778	206	0
1	K	3887	0	3888	270	3
1	L	3695	0	3704	166	0
All	All	44298	0	44411	1957	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 22.

All (1957) 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:K:229:ALA:CA	1:K:230:LYS:HB2	1.46	1.45
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
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: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: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:298:PRO:CD	1:I:242:LEU:HD22	1.72	1.18
1:H:68:LEU:CD1	1:H:78:ALA:HB1	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:A:150:VAL:HG13	1:A:231:SER:C	1.65	1.15
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:VAL:HG22	1:A:231:SER:OG	1.51	1.10
1:H:298:PRO:HD2	1:I:242:LEU:HD22	1.34	1.10
1:G:147:LEU:HB3	1:G:148:GLU:HB2	1.21	1.10
1:E:244:LYS:NZ	1:E:248:GLU:HB2	1.65	1.10
1:A:150:VAL:HG22	1:A:231:SER:CB	1.80	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:HA	1:K:230:LYS:HE2	1.30	1.07
1:I:141:GLU:O	1:I:145:LEU:HB2	1.53	1.07
1:A:148:GLU:HB3	1:A:149:GLU:HB3	1.36	1.07
1:K:109:LEU:HD12	1:K:148:GLU:CD	1.73	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: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: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:A:150:VAL:CG1	1:A:231:SER:C	2.26	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: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:B:147:LEU:HB2	1:B:148:GLU:CD	1.81	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:K:219:ALA:C	1:K:226:ALA:H	1.68	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:K:221:VAL:CB	1:K:222:ARG:HD2	1.97	0.94
1:K:9:LEU:HD11	1:K:20:PHE:HB2	1.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:299:GLN:CD	1:H:300:LEU:HD12	1.92	0.89
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: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: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: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:K:153:VAL:C	1:K:212:ASN:ND2	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:110:ASN:CB	1:K:111:ASP:HB3	2.01	0.86
1:K:227:HIS:C	1:K:228:GLU:OE2	2.15	0.85
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:K:104:GLY:C	1:K:106:PRO:CD	2.47	0.83
1:L:203:LYS:HZ3	1:L:318:ALA:HB1	1.43	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:L:233:PHE:CE2	1:L:234:LEU:C	2.51	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:F:254:ARG:NH1	1:F:299:GLN:HB2	1.95	0.81
1:E:248:GLU:OE2	1:E:249:THR:OG1	1.98	0.81
1:H:300:LEU:HD12	1:H:300:LEU:H	1.44	0.81
1:H:69:ARG:O	1:H:120:PRO:HG3	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:150:VAL:CG1	1:A:232:TYR:CA	2.54	0.79
1:H:321:ARG:HB2	1:H:321:ARG:HH11	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: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: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:HD23	1:K:214:LEU:O	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:148:GLU:CD	1:G:150:VAL:CG1	2.55	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:K:173:GLU:CD	1:K:213:SER:OG	2.26	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:H:299:GLN:O	1:H:300:LEU:C	2.23	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:K:104:GLY:C	1:K:106:PRO:HD3	2.08	0.73
1:J:194:LEU:HD22	1:J:330:LEU:HD11	1.70	0.73
1:A:154:SER:O	1:A:155:TYR:C	2.27	0.73
1:K:249:THR:HA	1:K:250:GLU:HB3	0.82	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	1:F:147:LEU:HD12	2.04	0.72
1:G:153:VAL:HG11	1:G:205:LEU:HB2	1.72	0.72
1:G:168:ILE:N	1:G:168:ILE:HD12	2.05	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: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: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:F:191:LYS:HZ1	1:F:304:ILE:HG22	1.57	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
1:E:132:TYR:HB3	1:E:134:PHE:CZ	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:147:LEU:HB2	1:I:148:GLU:HA	1.74	0.70
1:H:296:VAL:CB	1:I:242:LEU:HD21	2.19	0.70
1:I:297:VAL:HG13	1:I:298:PRO:HD3	1.72	0.70
1:J:244:LYS:NZ	1:J:246:VAL:O	2.22	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:I:139:LYS:HG2	1:I:140:ALA:N	2.07	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: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: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:J:147:LEU:HA	1:J:148:GLU:CB	2.22	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:K:215:ALA:HB2	1:K:231:SER:CB	2.23	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: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
1:G:148:GLU:O	1:G:233:PHE:C	2.31	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:237:LYS:H	1:J:237:LYS:HZ2	1.41	0.68
1:K:109:LEU:HG	1:K:148:GLU:HB3	1.76	0.68
1:D:254:ARG:CG	1:D:254:ARG:HH11	2.05	0.68
1:K:106:PRO:C	1:K:107:GLU:OE2	2.32	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: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:J:109:LEU:H	1:J:110:ASN:C	1.97	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:OE1	1:A:149:GLU:N	2.28	0.67
1:K:340:LYS:HD2	1:L:464:ASP:OD2	1.94	0.67
1:G:202:GLY:C	1:G:204:THR:OG1	2.32	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:HG3	1:D:254:ARG:HH11	1.59	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:24:ARG:NH1	1:C:25:LYS:HD2	2.11	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:K:295:THR:HB	1:K:296:VAL:HA	1.78	0.65
1:A:150:VAL:HG11	1:A:231:SER:C	2.12	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: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:J:108:ALA:HB1	1:J:111:ASP:C	2.17	0.65
1:J:69:ARG:HH21	1:K:139:LYS:NZ	1.94	0.65
1:G:69:ARG:C	1:G:70:GLU:HG3	2.14	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: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:140:ALA:C	1:A:142:VAL:H	2.01	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:B:150:VAL:HG12	1:B:151:PRO:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:232:TYR:OH	1:F:271:ILE:O	2.16	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:K:221:VAL:HG12	1:K:222:ARG:CD	2.28	0.64
1:J:340:LYS:HD2	1:K:464:ASP:OD2	1.98	0.64
1:K:219:ALA:C	1:K:226:ALA:N	2.46	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: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:N	1:A:13:ASP:OD1	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:K:218:MET:C	1:K:221:VAL:HG23	2.18	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: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
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: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:N	1:G:170:ASP:OD1	2.32	0.62
1:H:298:PRO:HG2	1:I:242:LEU:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:109:LEU:CD1	1:K:148:GLU:CD	2.62	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
1:K:244:LYS:N	1:K:245:PHE:HA	2.14	0.61
1:K:268:THR:O	1:K:312:ASN:CG	2.39	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: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:F:232:TYR:CG	1:F:233:PHE:N	2.68	0.61
1:E:298:PRO:HB3	1:F:239:PRO:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:GLU:H	1:G:234:LEU:HA	1.66	0.61
1:I:170:ASP:O	1:I:175:PRO:HD3	2.00	0.61
1:I:164:GLN:HG2	1:I:341:ILE:HD13	1.82	0.61
1:J:215:ALA:O	1:J:231:SER:N	2.34	0.61
1:B:46:ARG:NH1	1:B:55:GLU:OE1	2.33	0.61
1:H:177:LEU:HD11	1:H:217:LYS:HE2	1.83	0.61
1:G:464:ASP:OD2	1:L:340:LYS:HD3	2.00	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:J:310:LEU:HD13	1:J:310:LEU:C	2.21	0.61
1:K:141:GLU:O	1:K:145:LEU:N	2.29	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:G:148:GLU:CD	1:G:150:VAL:HG13	2.18	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:B:437:SER:C	1:B:441:THR:HG22	2.20	0.60
1:E:471:PRO:HA	1:E:474:TRP:CD1	2.37	0.60
1:A:154:SER:C	1:A:156:ALA:N	2.54	0.60
1:A:399:PHE:C	1:A:400:LEU:HG	2.21	0.60
1:G:326:ASP:OD1	1:G:326:ASP:N	2.25	0.60
1:I:69:ARG:O	1:I:120:PRO:HG3	2.01	0.60
1:K:109:LEU:HD23	1:K:109:LEU:C	2.21	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:E:68:LEU:O	1:E:120:PRO:HA	2.02	0.60
1:B:399:PHE:HD2	1:B:417:PHE:CD1	2.19	0.60
1:G:141:GLU:O	1:G:141:GLU:HG3	2.00	0.60
1:I:243:ASN:C	1:I:245:PHE:HA	2.22	0.60
1:J:69:ARG:HB2	1:J:79:LEU:O	2.01	0.60
1:L:262:GLU:HB3	1:L:263:LYS:HZ2	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:248:GLU:CD	1:E:249:THR:H	2.05	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:263:LYS:H	1:J:263:LYS:HZ3	1.50	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: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: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
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:236:ILE:HA	1:J:237:LYS:HZ1	1.67	0.59
1:J:496:SER:OG	1:J:497:SER:N	2.35	0.59
1:A:139:LYS:HZ2	1:A:246:VAL:HG13	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:G:146:VAL:C	1:G:147:LEU:HD12	2.22	0.58
1:H:242:LEU:HD13	1:H:242:LEU:O	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:114:ARG:O	1:J:136:ARG:NH2	2.36	0.58
1:K:105:LEU:O	1:K:105:LEU:HD12	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: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:I:323:ASP:N	1:I:323:ASP:OD1	2.27	0.58
1:K:109:LEU:HB2	1:K:148:GLU:HG3	1.86	0.58
1:G:244:LYS:HZ1	1:L:299:GLN:HA	1.68	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:146:VAL:HG22	1:A:146:VAL:O	2.04	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:A:87:GLU:HB2	1:B:65:ILE:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:J:108:ALA:C	1:J:109:LEU:HD12	2.24	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: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:I:301:LEU:HD23	1:I:334:ARG:NH1	2.20	0.57
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:L:203:LYS:NZ	1:L:318:ALA:HB1	2.18	0.56
1:D:46:ARG:HG2	1:D:55:GLU:HB3	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:87:GLU:HG3	1:F:65:ILE:HB	1.85	0.56
1:L:242:LEU:HA	1:L:243:ASN:C	2.25	0.56
1:A:399:PHE:HE2	1:A:417:PHE:CB	2.13	0.56
1:D:168:ILE:HG13	1:D:339:ILE:HD12	1.87	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: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:217:LYS:HZ3	1:I:269:PRO:HG3	1.70	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:221:VAL:C	1:K:222:ARG:HD2	2.25	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: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
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:H	1:F:147:LEU:HD12	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:I:233:PHE:CG	1:I:234:LEU:N	2.73	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:14:ASP:O	1:I:15:ASP:HB2	2.05	0.55
1:H:298:PRO:CG	1:I:242:LEU:CD2	2.68	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:196:TYR:CZ	1:H:340:LYS:HB2	2.41	0.55
1:H:43:GLN:HE21	1:H:57:GLY:H	1.55	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:HH11	1:C:251:ARG:HA	1.71	0.55
1:G:146:VAL:HG23	1:G:146:VAL:O	2.06	0.55
1:G:147:LEU:HD12	1:G:147:LEU:N	2.21	0.55
1:G:68:LEU:O	1:G:120:PRO:HA	2.07	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:F:191:LYS:NZ	1:F:305:ASP:HA	2.21	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:I:217:LYS:NZ	1:I:269:PRO:HG3	2.21	0.55
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: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:L:69:ARG:HH12	1:L:87:GLU:CD	2.04	0.55
1:B:147:LEU:HD23	1:B:147:LEU:C	2.25	0.55
1:C:220:GLU:CG	1:C:227:HIS:CB	2.84	0.55
1:G:168:ILE:H	1:G:168:ILE:CD1	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:E:247:GLY:O	1:E:250:GLU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:ILE:HG13	1:F:166:GLU:N	2.22	0.55
1:G:296:VAL:HG12	1:G:298:PRO:HD3	1.88	0.55
1:H:278:ASP:N	1:H:278:ASP:OD1	2.35	0.55
1:J:9:LEU:HD11	1:J:20:PHE:HB2	1.89	0.55
1:K:247:GLY:C	1:K:248:GLU:OE1	2.44	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:149:GLU:C	1:G:151:PRO:HD2	2.28	0.54
1:G:296:VAL:HG23	1:H:243:ASN:HB2	1.88	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:482:GLY:HA2	1:E:489:ARG:HD3	1.89	0.54
1:D:474:TRP:NE1	1:D:505:THR:OG1	2.41	0.54
1:I:164:GLN:O	1:I:168:ILE:HG13	2.08	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:A:238:GLY:N	1:A:275:ASP:O	2.40	0.54
1:B:300:LEU:HD12	1:B:300:LEU:H	1.72	0.54
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: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:N	1:D:323:ASP:OD1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:149:GLU:O	1:F:233:PHE:CA	2.53	0.54
1:J:237:LYS:N	1:J:237:LYS:NZ	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: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:E:68:LEU:HD22	1:E:124:LEU:HD11	1.90	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: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
1:B:484:ARG:HH11	1:B:484:ARG:HG2	1.72	0.53
1:D:164:GLN:O	1:D:168:ILE:HD12	2.08	0.53
1:G:3:SER:OG	1:G:47:LEU:O	2.24	0.53
1:K:219:ALA:O	1:K:225:ASP:C	2.45	0.53
1:L:69:ARG:CG	1:L:69:ARG:HH11	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:N	1:H:467:ASN:HD22	2.05	0.53
1:L:310:LEU:HD22	1:L:311:GLU:H	1.72	0.53
1:E:320:ASN:N	1:E:320:ASN:HD22	2.05	0.53
1:D:88:ARG:HD3	1:E:64:GLU:HG2	1.90	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:K:214:LEU:HD23	1:K:214:LEU:C	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:TYR:CD1	1:G:232:TYR:N	2.77	0.53
1:K:104:GLY:C	1:K:106:PRO:HD2	2.28	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:193:VAL:HA	1:E:337:VAL:HG23	1.90	0.53
1:E:89:VAL:HG23	1:F:65:ILE:HD11	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:363:VAL:HG13	1:G:368:LEU:HD11	1.91	0.53
1:G:68:LEU:CD1	1:G:78:ALA:CB	2.70	0.53
1:K:173:GLU:OE2	1:K:213:SER:CB	2.54	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: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:H:298:PRO:CG	1:I:242:LEU:CD1	2.81	0.53
1:A:139:LYS:NZ	1:A:246:VAL:HG13	2.24	0.53
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:J:109:LEU:HD21	1:J:232:TYR:CE1	2.44	0.53
1:I:298:PRO:HB2	1:J:242:LEU:HD22	1.90	0.53
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:A:245:PHE:CE1	1:F:254:ARG:HG3	2.43	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:312:ASN:OD1	1:L:312:ASN:N	2.42	0.52
1:L:195:LEU:HD22	1:L:341:ILE:HD11	1.90	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:K:243:ASN:C	1:K:245:PHE:HA	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:205:LEU:HD12	1:G:206:ILE:H	1.73	0.52
1:G:158:ILE:CB	1:G:206:ILE:HG12	2.39	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:D:23:GLY:C	1:D:24:ARG:CG	2.78	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
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:297:VAL:HG13	1:K:298:PRO:HD3	1.91	0.52
1:K:295:THR:OG1	1:L:242:LEU:HG	2.09	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:CB	1:D:254:ARG:HH11	2.22	0.52
1:D:301:LEU:HG	1:D:334:ARG:NH1	2.25	0.52
1:F:248:GLU:HB2	1:F:250:GLU:OE2	2.09	0.52
1:I:142:VAL:O	1:I:142:VAL:HG12	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:199:PRO:O	1:L:201:CYS:N	2.35	0.52
1:A:399:PHE:CD2	1:A:417:PHE:HB2	2.44	0.52
1:A:8:LEU:HD13	1:A:17:VAL:HG13	1.92	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:422:MET:O	1:J:426:VAL:HG23	2.10	0.52
1:J:322:GLU:OE2	1:K:501:ARG:NH1	2.39	0.52
1:L:140:ALA:C	1:L:142:VAL:H	2.14	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: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:255:LEU:O	1:I:259:ARG:HG2	2.10	0.51
1:I:160:GLY:N	1:I:351:ASP:OD2	2.36	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:196:TYR:CZ	1:G:340:LYS:HB2	2.45	0.51
1:G:158:ILE:HG23	1:G:206:ILE:HG12	1.90	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:G:172:VAL:HG12	1:G:214:LEU:HD13	1.92	0.51
1:H:295:THR:CG2	1:H:296:VAL:H	2.19	0.51
1:H:68:LEU:HB2	1:H:124:LEU:HD12	1.92	0.51
1:J:263:LYS:NZ	1:J:263:LYS:H	2.07	0.51
1:L:398:ARG:O	1:L:398:ARG:HG2	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:PHE:HD1	1:I:25:LYS:HG3	1.75	0.51
1:K:295:THR:HG1	1:L:242:LEU:HG	1.75	0.51
1:K:77:ARG:HD3	1:L:61:ALA:HB1	1.92	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:A:81:VAL:HG22	1:A:87:GLU:HG2	1.93	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:255:LEU:O	1:J:258:GLN:HG2	2.10	0.51
1:J:171:ALA:HB1	1:J:337:VAL:HG21	1.92	0.51
1:L:399:PHE:O	1:L:399:PHE:HD1	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:F:396:ASP:N	1:F:396:ASP:OD2	2.43	0.51
1:H:262:GLU:HB3	1:H:263:LYS:NZ	2.25	0.51
1:H:296:VAL:C	1:H:298:PRO:HD3	2.31	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
1:L:202:GLY:HA2	1:L:203:LYS:HB2	1.92	0.51
1:L:198:PRO:CB	1:L:343:ARG:NE	2.74	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:254:ARG:HH12	1:E:299:GLN:HB3	1.74	0.51
1:E:24:ARG:HH22	1:F:22:SER:HB2	1.76	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: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: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:301:LEU:CD2	1:J:334:ARG:HH12	2.24	0.51
1:J:69:ARG:HE	1:K:139:LYS:HE3	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ALA:HB1	1:C:310:LEU:HD21	1.93	0.51
1:D:278:ASP:N	1:D:278:ASP:OD1	2.43	0.51
1:E:340:LYS:HD2	1:E:342:GLU:HB3	1.92	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:107:GLU:O	1:K:108:ALA:HB3	2.11	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:D:23:GLY:C	1:D:24:ARG:HG2	2.31	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
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: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: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:264:ALA:C	1:J:312:ASN:HD22	2.15	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: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:N	1:G:322:GLU:OE1	2.43	0.50
1:A:72:LEU:HB2	1:B:139:LYS:HZ1	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:232:TYR:C	1:C:270:VAL:HG12	2.32	0.50
1:F:341:ILE:O	1:F:341:ILE:HG22	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:I:145:LEU:C	1:I:146:VAL:HG12	2.32	0.50
1:J:109:LEU:HB3	1:J:110:ASN:HB3	1.91	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
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: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:E:72:LEU:HD22	1:F:137:ILE:HG21	1.94	0.50
1:F:275:ASP:C	1:F:276:GLU:HG2	2.33	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:268:THR:C	1:K:312:ASN:OD1	2.51	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: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:400:LEU:HB2	1:H:412:MET:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:243:ASN:C	1:J:245:PHE:HA	2.32	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
1:G:232:TYR:HD1	1:G:232:TYR:N	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: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:B:359:GLU:HG3	1:G:156:ALA:HB2	1.93	0.49
1:J:109:LEU:HD23	1:J:148:GLU:O	2.12	0.49
1:I:89:VAL:HG23	1:J:65:ILE:HD11	1.93	0.49
1:K:214:LEU:HD21	1:K:218:MET:HE1	1.94	0.49
1:A:216:LYS:N	1:A:216:LYS:NZ	2.60	0.49
1:A:232:TYR:CG	1:A:233:PHE:N	2.80	0.49
1:A:322:GLU:OE2	1:A:472:ASP:OD2	2.31	0.49
1:B:158:ILE:HD13	1:B:206:ILE:HG13	1.94	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: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:471:PRO:HA	1:D:474:TRP:CD1	2.47	0.49
1:H:297:VAL:O	1:H:297:VAL:HG13	2.12	0.49
1:H:68:LEU:HD13	1:H:78:ALA:CB	2.39	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:GLY:HA2	1:C:489:ARG:HD3	1.95	0.48
1:H:117:LYS:O	1:H:117:LYS:HG3	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:262:GLU:HG3	1:E:263:LYS:NZ	2.28	0.48
1:E:69:ARG:O	1:E:120:PRO:HG3	2.13	0.48
1:I:8:LEU:HD21	1:I:39:LEU:HB3	1.95	0.48
1:K:86:GLU:HG3	1:L:83:HIS:CG	2.47	0.48
1:A:242:LEU:HD23	1:F:296:VAL:HG21	1.95	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:J:263:LYS:NZ	1:J:263:LYS:N	2.60	0.48
1:K:226:ALA:CB	1:K:227:HIS:HA	2.41	0.48
1:L:112:ASP:N	1:L:112:ASP:OD2	2.46	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: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:A:464:ASP:OD2	1:F:340:LYS:HD2	2.14	0.48
1:K:223:GLY:HA3	1:K:224:ASP:CG	2.33	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:B:69:ARG:C	1:B:70:GLU:HG3	2.33	0.48
1:D:101:LEU:O	1:D:117:LYS:HD3	2.14	0.48
1:D:27:ARG:HD3	1:E:46:ARG:CD	2.44	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: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:I:146:VAL:O	1:I:146:VAL:HG22	2.13	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:449:GLN:O	1:L:453:ASP:HB2	2.14	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:296:VAL:CG2	1:H:243:ASN:HB2	2.43	0.48
1:G:239:PRO:O	1:L:298:PRO:HB3	2.14	0.48
1:L:171:ALA:HB1	1:L:337:VAL:HG21	1.96	0.48
1:B:69:ARG:O	1:B:120:PRO:HG3	2.14	0.48
1:G:434:ALA:HA	1:G:450:HIS:CE1	2.49	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: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:N	1:K:323:ASP:OD1	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:L:399:PHE:CD1	1:L:399:PHE:C	2.85	0.47
1:B:40:LYS:HB2	1:B:94:ASP:HB2	1.95	0.47
1:G:161:LEU:HA	1:G:161:LEU:HD23	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: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:L:67:THR:OG1	1:L:81:VAL:HG12	2.14	0.47
1:B:134:PHE:CD2	1:B:134:PHE:N	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: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
1:A:232:TYR:HE1	1:A:269:PRO:O	1.96	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:296:VAL:HB	1:L:242:LEU:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:G:181:LEU:HD12	1.72	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:K:227:HIS:C	1:K:228:GLU:CD	2.73	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: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:198:PRO:HG2	1:G:343:ARG:HG3	1.96	0.47
1:G:81:VAL:HG23	1:G:87:GLU:HG2	1.97	0.47
1:J:70:GLU:HG2	1:J:71:ILE:H	1.74	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:215:ALA:HB1	1:L:231:SER:H	1.79	0.47
1:C:43:GLN:NE2	1:C:56:ALA:HB1	2.30	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: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:L:165:ILE:HA	1:L:168:ILE:HD12	1.95	0.47
1:L:275:ASP:OD1	1:L:276:GLU:N	2.48	0.47
1:L:400:LEU:O	1:L:400:LEU:HD12	2.14	0.47
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:172:VAL:C	1:C:175:PRO:HD2	2.35	0.47
1:C:398:ARG:HG2	1:C:411:VAL:CG1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:69:ARG:HH21	1:K:139:LYS:HZ3	1.61	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:221:VAL:O	1:C:221:VAL:HG12	2.15	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:J:203:LYS:HZ2	1:J:320:ASN:HD22	1.61	0.47
1:K:152:ASP:C	1:K:212:ASN:HD21	2.19	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: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:I:399:PHE:C	1:I:400:LEU:HG	2.35	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:D:77:ARG:HH22	1:E:135:GLU:CD	2.18	0.46
1:E:323:ASP:N	1:E:323:ASP:OD1	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:G:14:ASP:O	1:G:15:ASP:HB2	2.15	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:CA	1:K:230:LYS:CE	2.87	0.46
1:K:449:GLN:NE2	1:K:453:ASP:OD2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:299:GLN:H	1:B:299:GLN:CD	2.17	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:389:ARG:HG2	1:F:389:ARG:HH11	1.80	0.46
1:F:9:LEU:HD11	1:F:20:PHE:CB	2.39	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: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:F:149:GLU:C	1:F:233:PHE:HB3	2.32	0.46
1:H:296:VAL:CB	1:I:242:LEU:CD1	2.69	0.46
1:H:68:LEU:O	1:H:120:PRO:HA	2.15	0.46
1:H:89:VAL:HG12	1:I:62:VAL:HG12	1.98	0.46
1:I:261:ARG:HA	1:I:264:ALA:HB3	1.98	0.46
1:H:86:GLU:HA	1:I:83:HIS:HB3	1.96	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
1:G:46:ARG:HH11	1:G:55:GLU:CD	2.19	0.46
1:J:236:ILE:CA	1:J:237:LYS:HZ1	2.28	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:K:3:SER:HB2	1:K:47:LEU:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:SER:OG	1:B:321:ARG:O	2.33	0.46
1:D:342:GLU:O	1:D:343:ARG:C	2.54	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:L:203:LYS:HB3	1:L:203:LYS:HZ2	1.80	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: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:H:68:LEU:HB2	1:H:80:VAL:HG12	1.97	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:299:GLN:H	1:E:299:GLN:CD	2.18	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:C:219:ALA:HB3	1:C:220:GLU:C	2.37	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:229:ALA:HA	1:K:230:LYS:HB2	0.59	0.45
1:K:40:LYS:HD2	1:K:59:PHE:HZ	1.81	0.45
1:L:470:ASN:ND2	1:L:472:ASP:CB	2.77	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:104:GLY:O	1:K:106:PRO:CD	2.61	0.45
1:K:223:GLY:N	1:K:224:ASP:CA	2.79	0.45
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:F:195:LEU:HD23	1:F:339:ILE:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:THR:C	1:J:136:ARG:HH22	2.20	0.45
1:J:310:LEU:O	1:J:310:LEU:HD13	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: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:G:170:ASP:HA	1:G:174:LEU:HB2	1.97	0.45
1:H:84:ALA:O	1:H:85:ASP:HB2	2.15	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: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:152:ASP:C	1:G:212:ASN:ND2	2.69	0.45
1:H:204:THR:HB	1:H:208:LYS:NZ	2.31	0.45
1:I:143:GLU:OE2	1:I:143:GLU:N	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:102:PRO:C	1:B:116:ARG:HD2	2.37	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: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:262:GLU:HB3	1:B:263:LYS:HZ2	1.82	0.45
1:B:27:ARG:HD3	1:C:46:ARG:HD2	1.99	0.45
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:429:ARG:NH2	1:I:458:GLU:OE1	2.43	0.45
1:H:322:GLU:HG2	1:I:501:ARG:HH22	1.82	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:162:SER:O	1:H:165:ILE:HG13	2.17	0.45
1:H:34:ILE:HD11	1:H:55:GLU:HA	1.99	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:HG13	1:A:146:VAL:O	2.16	0.45
1:C:399:PHE:C	1:C:399:PHE:CD1	2.90	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:G:149:GLU:O	1:G:151:PRO:HD2	2.16	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:H:299:GLN:C	1:H:301:LEU:N	2.68	0.44
1:H:343:ARG:HG2	1:H:343:ARG:HH11	1.81	0.44
1:H:298:PRO:HG2	1:I:242:LEU:CB	2.46	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:J:259:ARG:O	1:J:263:LYS:NZ	2.46	0.44
1:K:174:LEU:HB3	1:K:175:PRO:HD3	1.99	0.44
1:K:221:VAL:C	1:K:222:ARG:CD	2.85	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:NH1	1:C:251:ARG:HA	2.33	0.44
1:E:382:MET:O	1:E:386:VAL:HG12	2.18	0.44
1:F:297:VAL:HG13	1:F:298:PRO:HD3	1.97	0.44
1:H:243:ASN:CG	1:H:244:LYS:HE2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:279:SER:O	1:I:282:ARG:NH1	2.50	0.44
1:K:367:ASP:N	1:K:367:ASP:OD1	2.51	0.44
1:L:161:LEU:HD23	1:L:161:LEU:HA	1.80	0.44
1:L:8:LEU:HD12	1:L:9:LEU:N	2.32	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: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:CD1	1:D:399:PHE:O	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:B:149:GLU:C	1:B:150:VAL:HG23	2.36	0.44
1:B:165:ILE:HG13	1:B:166:GLU:N	2.31	0.44
1:C:151:PRO:HB3	1:C:208:LYS:HB3	1.99	0.44
1:C:331:ARG:HG2	1:C:331:ARG:H	1.50	0.44
1:D:126:VAL:HG12	1:D:133:ALA:HB2	1.98	0.44
1:G:200:GLY:HA3	1:G:201:CYS:HB2	1.99	0.44
1:G:69:ARG:C	1:G:70:GLU:CG	2.86	0.44
1:H:101:LEU:HA	1:H:102:PRO:HD3	1.66	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: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:108:ALA:C	1:J:109:LEU:CD1	2.86	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:254:ARG:HH11	1:L:303:GLU:HG2	1.82	0.44
1:L:233:PHE:CE1	1:L:271:ILE:HB	2.53	0.44
1:G:61:ALA:HB1	1:L:77:ARG:HD3	1.98	0.44
1:A:261:ARG:H	1:A:261:ARG:HG2	1.68	0.44
1:A:9:LEU:HD11	1:A:20:PHE:CB	2.41	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: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:241:LEU:O	1:F:249:THR:OG1	2.21	0.44
1:F:191:LYS:HE2	1:F:333:GLY:O	2.17	0.44
1:G:151:PRO:HD3	1:G:233:PHE:CB	2.39	0.44
1:G:206:ILE:C	1:G:209:ALA:HB3	2.38	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:K:227:HIS:O	1:K:228:GLU:CD	2.56	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:B:69:ARG:C	1:B:70:GLU:CG	2.86	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:384:GLU:O	1:F:388:ASP:HB2	2.17	0.44
1:J:137:ILE:HA	1:J:137:ILE:HD13	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:233:PHE:CD2	1:L:234:LEU:C	2.91	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:H	1:A:301:LEU:HD12	1.83	0.43
1:B:399:PHE:HE2	1:B:417:PHE:CD2	2.35	0.43
1:C:380:LYS:HB2	1:C:380:LYS:HE3	1.84	0.43
1:D:299:GLN:H	1:D:299:GLN:CD	2.21	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: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:F:191:LYS:HZ2	1:F:304:ILE:C	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:140:ALA:C	1:K:141:GLU:HG2	2.22	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:HA	1:B:151:PRO:HD3	1.58	0.43
1:C:92:LEU:CD2	1:C:133:ALA:HB3	2.48	0.43
1:C:46:ARG:HD3	1:C:55:GLU:HG2	1.99	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: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:E:441:THR:HG23	1:E:443:GLN:H	1.83	0.43
1:F:244:LYS:HD2	1:F:247:GLY:C	2.39	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:327:PRO:O	1:C:331:ARG:HG2	2.19	0.43
1:C:68:LEU:HD13	1:C:78:ALA:HB1	2.01	0.43
1:E:164:GLN:HG2	1:E:341:ILE:HD13	2.00	0.43
1:F:147:LEU:CD1	1:F:147:LEU:H	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:29:THR:OG1	1:J:1:MET:HG2	2.18	0.43
1:I:27:ARG:HD2	1:J:5:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:250:GLU:OE1	1:K:299:GLN:CD	2.57	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: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:261:ARG:HA	1:J:264:ALA:HB3	2.01	0.43
1:J:47:LEU:HD23	1:J:53:VAL:HA	1.99	0.43
1:K:278:ASP:OD1	1:K:320:ASN:N	2.51	0.43
1:A:299:GLN:CD	1:A:299:GLN:H	2.20	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:249:THR:OG1	1:I:250:GLU:OE1	2.25	0.43
1:I:299:GLN:O	1:I:302:SER:OG	2.32	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:112:ASP:OD2	1:K:116:ARG:NE	2.52	0.43
1:K:17:VAL:HG12	1:K:19:VAL:HG23	2.01	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: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
1:B:147:LEU:CB	1:B:148:GLU:CD	2.71	0.43
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:232:TYR:O	1:G:270:VAL:HG23	2.19	0.43
1:G:68:LEU:HD12	1:G:80:VAL:CG1	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:223:GLY:N	1:K:224:ASP:C	2.73	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:B:216:LYS:C	1:B:217:LYS:HD2	2.40	0.42
1:D:202:GLY:O	1:D:204:THR:N	2.51	0.42
1:E:215:ALA:HB1	1:E:231:SER:N	2.34	0.42
1:E:69:ARG:O	1:E:120:PRO:CG	2.67	0.42
1:G:210:VAL:CG1	1:G:211:ALA:N	2.82	0.42
1:G:345:ASP:CG	1:G:346:ALA:H	2.22	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:HB3	1:I:432:LYS:HE2	1.87	0.42
1:J:307:VAL:O	1:J:310:LEU:O	2.37	0.42
1:K:214:LEU:CD2	1:K:214:LEU:C	2.88	0.42
1:K:251:ARG:HG2	1:K:251:ARG:O	2.19	0.42
1:K:470:ASN:N	1:K:470:ASN:OD1	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:254:ARG:HH22	1:F:299:GLN:HB3	1.84	0.42
1:F:176:PHE:HE2	1:F:269:PRO:HB3	1.84	0.42
1:F:399:PHE:CE2	1:F:417:PHE:CD2	3.07	0.42
1:G:208:LYS:H	1:G:208:LYS:HG3	1.63	0.42
1:G:176:PHE:CZ	1:G:314:ILE:HD13	2.55	0.42
1:G:46:ARG:NH1	1:G:55:GLU:OE1	2.52	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:K:109:LEU:CD2	1:K:109:LEU:C	2.85	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
1:B:254:ARG:HG3	1:C:245:PHE:CZ	2.54	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: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:E:77:ARG:HH11	1:F:61:ALA:HB1	1.83	0.42
1:G:119:ARG:HG3	1:G:120:PRO:O	2.19	0.42
1:G:43:GLN:HG3	1:G:57:GLY:O	2.20	0.42
1:H:17:VAL:HG12	1:H:19:VAL:HG23	2.00	0.42
1:H:238:GLY:O	1:H:240:GLU:N	2.45	0.42
1:H:79:LEU:HD21	1:H:87:GLU:HB3	2.01	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: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:H	1:J:105:LEU:CD1	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:232:TYR:OH	1:B:263:LYS:HB3	2.19	0.42
1:B:194:LEU:HD23	1:B:338:LYS:HB3	2.02	0.42
1:D:230:LYS:HB2	1:D:230:LYS:HE2	1.82	0.42
1:D:403:THR:HB	1:D:487:TYR:HB3	2.01	0.42
1:D:91:TRP:CZ2	1:E:61:ALA:HB3	2.55	0.42
1:E:186:SER:O	1:F:431:LYS:NZ	2.49	0.42
1:G:180:GLU:H	1:G:180:GLU:CD	2.23	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: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:A:140:ALA:C	1:A:142:VAL:N	2.71	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:N	1:G:14:ASP:OD1	2.36	0.42
1:H:63:GLY:N	1:H:125:LEU:HD11	2.35	0.42
1:J:310:LEU:CD1	1:J:312:ASN:N	2.83	0.42
1:K:247:GLY:HA2	1:K:248:GLU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:84:ALA:O	1:K:85:ASP:HB2	2.19	0.42
1:L:341:ILE:HG22	1:L:341:ILE:O	2.19	0.42
1:A:63:GLY:N	1:A:125:LEU:HD11	2.35	0.42
1:C:133:ALA:C	1:C:134:PHE:CD1	2.93	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:191:LYS:HZ3	1:H:307:VAL:CG1	2.31	0.42
1:H:293:GLU:HG3	1:H:294:THR:HG1	1.82	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:151:PRO:HB3	1:A:208:LYS:CB	2.43	0.42
1:A:5:TYR:CE1	1:A:46:ARG:HG3	2.55	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: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: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: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:B:360:PHE:HE2	1:G:216:LYS:HE3	1.84	0.42
1:G:251:ARG:O	1:G:253:ILE:N	2.53	0.42
1:I:170:ASP:N	1:I:170:ASP:OD1	2.47	0.42
1:L:255:LEU:HA	1:L:258:GLN:HB3	2.01	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:A:185:TYR:O	1:B:431:LYS:HD3	2.19	0.42
1:C:296:VAL:HG12	1:C:297:VAL:H	1.84	0.42
1:D:399:PHE:HB2	1:D:414:PHE:CE2	2.55	0.42
1:F:341:ILE:HG23	1:F:341:ILE:HD12	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:I:149:GLU:CG	1:I:150:VAL:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:211:ALA:HB1	1:I:271:ILE:HD13	2.01	0.41
1:I:47:LEU:O	1:I:47:LEU:HD12	2.20	0.41
1:L:118:LEU:HD22	1:L:136:ARG:HD3	2.02	0.41
1:B:412:MET:HE2	1:B:417:PHE:HE1	1.86	0.41
1:C:278:ASP:N	1:C:278:ASP:OD1	2.53	0.41
1:D:202:GLY:C	1:D:204:THR:H	2.23	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: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:HD1	1:I:360:PHE:N	2.18	0.41
1:J:109:LEU:CD2	1:J:232:TYR:CE1	3.03	0.41
1:K:145:LEU:C	1:K:146:VAL:HG12	2.41	0.41
1:K:12:HIS:HB2	1:K:16:THR:O	2.21	0.41
1:K:249:THR:HB	1:K:250:GLU:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:250:GLU:O	1:K:250:GLU:HG3	2.20	0.41
1:A:264:ALA:HB1	1:A:310:LEU:HG	2.02	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: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:F:147:LEU:CD1	1:F:147:LEU:N	2.72	0.41
1:E:91:TRP:CD1	1:F:62:VAL:HG11	2.56	0.41
1:H:105:LEU:HA	1:H:105:LEU:HD23	1.77	0.41
1:H:436:LYS:HB3	1:H:436:LYS:HE2	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
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:355:LYS:HD3	1:C:355:LYS:HA	1.63	0.41
1:C:91:TRP:O	1:C:133:ALA:N	2.53	0.41
1:D:74:ASP:OD1	1:D:74:ASP:N	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:351:ASP:O	1:D:354:SER:OG	2.38	0.41
1:E:341:ILE:O	1:E:341:ILE:HG22	2.21	0.41
1:E:400:LEU:HB2	1:E:412:MET:HB2	2.02	0.41
1:F:72:LEU:HD12	1:F:73:ALA:H	1.84	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: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:A:320:ASN:O	1:A:470:ASN:ND2	2.54	0.41
1:C:399:PHE:O	1:C:399:PHE:CD1	2.73	0.41
1:D:206:ILE:HD12	1:D:206:ILE:H	1.86	0.41
1:E:415:LYS:HE3	1:E:415:LYS:HB3	1.95	0.41
1:F:356:TYR:HB3	1:F:427:VAL:HG11	2.03	0.41
1:G:244:LYS:HE3	1:G:245:PHE:CZ	2.56	0.41
1:G:234:LEU:HB3	1:G:271:ILE:O	2.21	0.41
1:G:345:ASP:O	1:G:391:TYR:CE2	2.74	0.41
1:G:94:ASP:N	1:G:95:PRO:HD2	2.35	0.41
1:H:330:LEU:HG	1:H:338:LYS:HE2	2.02	0.41
1:J:361:LEU:HA	1:J:362:PRO:HD3	1.77	0.41
1:K:105:LEU:O	1:K:105:LEU:CG	2.69	0.41
1:K:116:ARG:HG2	1:K:136:ARG:NH2	2.36	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:154:SER:C	1:A:156:ALA:H	2.23	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:HG13	1:D:253:ILE:H	1.51	0.41
1:D:375:ARG:HB2	1:D:375:ARG:HE	1.69	0.41
1:D:386:VAL:HG11	1:D:451:LEU:HB3	2.03	0.41
1:H:13:ASP:N	1:H:13:ASP:OD1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:LEU:HD13	1:H:17:VAL:HG13	2.02	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:HA	1:J:241:LEU:HD12	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:E:216:LYS:C	1:E:217:LYS:HD2	2.42	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: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:343:ARG:HH21	1:D:473:ASP:CG	2.22	0.40
1:D:83:HIS:ND1	1:D:83:HIS:O	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:H:171:ALA:HB1	1:H:337:VAL:HG21	2.04	0.40
1:I:208:LYS:HG2	1:I:233:PHE:CZ	2.55	0.40
1:I:46:ARG:NE	1:I:55:GLU:OE2	2.41	0.40
1:J:375:ARG:O	1:J:379:ILE:HG12	2.21	0.40
1:G:241:LEU:HD11	1:L:298:PRO:HG2	2.03	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:HG22	1:B:341:ILE:O	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:110:ASN:HB2	1:J:148:GLU:CD	2.42	0.40
1:J:243:ASN:HB2	1:J:245:PHE:CD1	2.57	0.40
1:J:78:ALA:HB2	1:J:92:LEU:HD21	2.03	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:172:VAL:C	1:G:175:PRO:HD2	2.42	0.40
1:H:299:GLN:CD	1:H:299:GLN:N	2.73	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:300:LEU:HD12	1:J:300:LEU:H	1.86	0.40
1:L:204:THR:HG21	1:L:275:ASP:OD2	2.21	0.40
1:B:484:ARG:HH11	1:B:484:ARG:CG	2.33	0.40
1:B:464:ASP:O	1:B:501:ARG:HD2	2.21	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:F:73:ALA:C	1:F:75:GLY:H	2.23	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:HA	1:J:161:LEU:HD23	1.79	0.40
1:K:215:ALA:HB1	1:K:229:ALA:CB	2.52	0.40
1:J:298:PRO:HB3	1:K:239:PRO:HB2	2.03	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%)	14	52
1	B	467/513 (91%)	441 (94%)	23 (5%)	3 (1%)	25	64
1	C	462/513 (90%)	429 (93%)	30 (6%)	3 (1%)	25	64
1	D	450/513 (88%)	433 (96%)	17 (4%)	0	100	100
1	E	451/513 (88%)	431 (96%)	19 (4%)	1 (0%)	47	81
1	F	452/513 (88%)	424 (94%)	24 (5%)	4 (1%)	17	56
1	G	453/513 (88%)	428 (94%)	21 (5%)	4 (1%)	17	56
1	H	470/513 (92%)	442 (94%)	24 (5%)	4 (1%)	17	56
1	I	470/513 (92%)	446 (95%)	23 (5%)	1 (0%)	47	81
1	J	478/513 (93%)	442 (92%)	33 (7%)	3 (1%)	25	64
1	K	494/513 (96%)	457 (92%)	29 (6%)	8 (2%)	9	43
1	L	465/513 (91%)	434 (93%)	27 (6%)	4 (1%)	17	56
All	All	5586/6156 (91%)	5247 (94%)	299 (5%)	40 (1%)	22	61

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

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Mol	Chain	Res	Type
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%)	371 (92%)	34 (8%)	11	40
1	B	402/433 (93%)	362 (90%)	40 (10%)	7	32
1	C	389/433 (90%)	351 (90%)	38 (10%)	8	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	389/433 (90%)	346 (89%)	43 (11%)	6	28
1	E	389/433 (90%)	351 (90%)	38 (10%)	8	33
1	F	389/433 (90%)	345 (89%)	44 (11%)	6	27
1	G	390/433 (90%)	347 (89%)	43 (11%)	6	29
1	H	405/433 (94%)	362 (89%)	43 (11%)	6	30
1	I	405/433 (94%)	362 (89%)	43 (11%)	6	30
1	J	410/433 (95%)	376 (92%)	34 (8%)	11	40
1	K	421/433 (97%)	371 (88%)	50 (12%)	5	25
1	L	401/433 (93%)	356 (89%)	45 (11%)	6	27
All	All	4795/5196 (92%)	4300 (90%)	495 (10%)	7	32

All (495) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	132	TYR
1	A	150	VAL
1	A	154	SER
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
1	A	245	PHE
1	A	253	ILE
1	A	268	THR
1	A	276	GLU
1	A	279	SER
1	A	281	PHE
1	A	307	VAL
1	A	311	GLU
1	A	323	ASP
1	A	372	ASP
1	A	376	SER

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Mol	Chain	Res	Type
1	A	388	ASP
1	A	396	ASP
1	A	400	LEU
1	A	441	THR
1	A	449	GLN
1	A	476	ARG
1	A	496	SER
1	A	504	ASP
1	A	505	THR
1	B	68	LEU
1	B	74	ASP
1	B	132	TYR
1	B	134	PHE
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	244	LYS
1	B	245	PHE
1	B	246	VAL
1	B	251	ARG
1	B	261	ARG
1	B	271	ILE
1	B	276	GLU
1	B	277	MET
1	B	278	ASP
1	B	321	ARG
1	B	323	ASP
1	B	325	ILE
1	B	329	ILE
1	B	338	LYS
1	B	345	ASP
1	B	358	THR
1	B	363	VAL
1	B	367	ASP
1	B	372	ASP
1	B	375	ARG
1	B	380	LYS
1	B	388	ASP
1	B	425	ASN

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Mol	Chain	Res	Type
1	B	443	GLN
1	B	472	ASP
1	B	476	ARG
1	B	484	ARG
1	B	496	SER
1	B	501	ARG
1	B	504	ASP
1	C	24	ARG
1	C	34	ILE
1	C	51	LEU
1	C	79	LEU
1	C	94	ASP
1	C	103	ASP
1	C	214	LEU
1	C	218	MET
1	C	220	GLU
1	C	233	PHE
1	C	234	LEU
1	C	236	ILE
1	C	241	LEU
1	C	245	PHE
1	C	268	THR
1	C	271	ILE
1	C	299	GLN
1	C	314	ILE
1	C	321	ARG
1	C	322	GLU
1	C	323	ASP
1	C	331	ARG
1	C	337	VAL
1	C	343	ARG
1	C	359	GLU
1	C	372	ASP
1	C	375	ARG
1	C	380	LYS
1	C	388	ASP
1	C	390	MET
1	C	398	ARG
1	C	400	LEU
1	C	419	SER
1	C	441	THR
1	C	447	ARG

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Mol	Chain	Res	Type
1	C	468	THR
1	C	501	ARG
1	C	506	GLU
1	D	17	VAL
1	D	24	ARG
1	D	64	GLU
1	D	67	THR
1	D	168	ILE
1	D	199	PRO
1	D	214	LEU
1	D	216	LYS
1	D	233	PHE
1	D	235	ASN
1	D	236	ILE
1	D	237	LYS
1	D	241	LEU
1	D	245	PHE
1	D	251	ARG
1	D	252	HIS
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	297	VAL
1	D	323	ASP
1	D	329	ILE
1	D	331	ARG
1	D	337	VAL
1	D	367	ASP
1	D	375	ARG
1	D	388	ASP
1	D	390	MET
1	D	396	ASP
1	D	425	ASN
1	D	437	SER
1	D	440	GLU
1	D	441	THR
1	D	447	ARG
1	D	472	ASP

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Mol	Chain	Res	Type
1	D	484	ARG
1	D	486	VAL
1	D	501	ARG
1	D	505	THR
1	E	17	VAL
1	E	34	ILE
1	E	35	ASP
1	E	68	LEU
1	E	69	ARG
1	E	86	GLU
1	E	112	ASP
1	E	214	LEU
1	E	216	LYS
1	E	218	MET
1	E	236	ILE
1	E	241	LEU
1	E	242	LEU
1	E	243	ASN
1	E	245	PHE
1	E	251	ARG
1	E	270	VAL
1	E	271	ILE
1	E	275	ASP
1	E	278	ASP
1	E	310	LEU
1	E	320	ASN
1	E	321	ARG
1	E	323	ASP
1	E	337	VAL
1	E	338	LYS
1	E	359	GLU
1	E	363	VAL
1	E	364	HIS
1	E	385	LYS
1	E	386	VAL
1	E	388	ASP
1	E	425	ASN
1	E	440	GLU
1	E	456	VAL
1	E	476	ARG
1	E	484	ARG
1	E	504	ASP

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Mol	Chain	Res	Type
1	F	28	LEU
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	214	LEU
1	F	216	LYS
1	F	230	LYS
1	F	232	TYR
1	F	233	PHE
1	F	236	ILE
1	F	237	LYS
1	F	241	LEU
1	F	249	THR
1	F	251	ARG
1	F	252	HIS
1	F	255	LEU
1	F	268	THR
1	F	275	ASP
1	F	276	GLU
1	F	297	VAL
1	F	323	ASP
1	F	331	ARG
1	F	342	GLU
1	F	343	ARG
1	F	358	THR
1	F	359	GLU
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	468	THR
1	F	472	ASP
1	F	476	ARG
1	F	484	ARG

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Mol	Chain	Res	Type
1	F	489	ARG
1	F	505	THR
1	G	17	VAL
1	G	68	LEU
1	G	81	VAL
1	G	145	LEU
1	G	147	LEU
1	G	149	GLU
1	G	150	VAL
1	G	168	ILE
1	G	169	ARG
1	G	170	ASP
1	G	204	THR
1	G	205	LEU
1	G	214	LEU
1	G	216	LYS
1	G	218	MET
1	G	235	ASN
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	263	LYS
1	G	268	THR
1	G	278	ASP
1	G	299	GLN
1	G	310	LEU
1	G	311	GLU
1	G	314	ILE
1	G	321	ARG
1	G	325	ILE
1	G	326	ASP
1	G	337	VAL
1	G	343	ARG
1	G	358	THR
1	G	380	LYS
1	G	388	ASP
1	G	425	ASN
1	G	432	LYS

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Mol	Chain	Res	Type
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	107	GLU
1	H	139	LYS
1	H	183	ARG
1	H	201	CYS
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	237	LYS
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	321	ARG
1	H	323	ASP
1	H	337	VAL
1	H	359	GLU
1	H	363	VAL
1	H	364	HIS
1	H	372	ASP
1	H	375	ARG
1	H	425	ASN
1	H	441	THR
1	H	447	ARG
1	H	467	ASN

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Mol	Chain	Res	Type
1	H	493	THR
1	H	495	LYS
1	H	496	SER
1	H	501	ARG
1	I	68	LEU
1	I	70	GLU
1	I	132	TYR
1	I	147	LEU
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	248	GLU
1	I	249	THR
1	I	250	GLU
1	I	251	ARG
1	I	255	LEU
1	I	259	ARG
1	I	263	LYS
1	I	268	THR
1	I	271	ILE
1	I	276	GLU
1	I	278	ASP
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	323	ASP
1	I	330	LEU
1	I	337	VAL
1	I	343	ARG
1	I	363	VAL
1	I	367	ASP
1	I	375	ARG
1	I	394	ILE
1	I	437	SER

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Mol	Chain	Res	Type
1	I	443	GLN
1	I	449	GLN
1	I	476	ARG
1	I	493	THR
1	I	504	ASP
1	J	81	VAL
1	J	105	LEU
1	J	146	VAL
1	J	147	LEU
1	J	214	LEU
1	J	216	LYS
1	J	218	MET
1	J	233	PHE
1	J	236	ILE
1	J	237	LYS
1	J	241	LEU
1	J	244	LYS
1	J	248	GLU
1	J	249	THR
1	J	250	GLU
1	J	263	LYS
1	J	268	THR
1	J	278	ASP
1	J	279	SER
1	J	297	VAL
1	J	307	VAL
1	J	310	LEU
1	J	323	ASP
1	J	329	ILE
1	J	337	VAL
1	J	342	GLU
1	J	367	ASP
1	J	375	ARG
1	J	425	ASN
1	J	446	LEU
1	J	476	ARG
1	J	483	GLU
1	J	505	THR
1	J	506	GLU
1	K	107	GLU
1	K	119	ARG
1	K	145	LEU

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Mol	Chain	Res	Type
1	K	147	LEU
1	K	148	GLU
1	K	169	ARG
1	K	182	TYR
1	K	203	LYS
1	K	210	VAL
1	K	222	ARG
1	K	224	ASP
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	262	GLU
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	281	PHE
1	K	282	ARG
1	K	297	VAL
1	K	299	GLN
1	K	310	LEU
1	K	311	GLU
1	K	323	ASP
1	K	324	MET
1	K	325	ILE
1	K	338	LYS
1	K	342	GLU
1	K	366	ASP
1	K	367	ASP
1	K	380	LYS
1	K	388	ASP

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Mol	Chain	Res	Type
1	K	390	MET
1	K	468	THR
1	K	476	ARG
1	K	480	LYS
1	K	500	SER
1	L	69	ARG
1	L	81	VAL
1	L	150	VAL
1	L	157	ASP
1	L	191	LYS
1	L	216	LYS
1	L	218	MET
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	278	ASP
1	L	321	ARG
1	L	329	ILE
1	L	331	ARG
1	L	338	LYS
1	L	343	ARG
1	L	359	GLU
1	L	363	VAL
1	L	375	ARG
1	L	382	MET
1	L	385	LYS
1	L	398	ARG
1	L	400	LEU
1	L	425	ASN
1	L	441	THR
1	L	446	LEU
1	L	447	ARG
1	L	448	ILE
1	L	449	GLN

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	364	HIS
1	C	76	HIS
1	C	235	ASN
1	C	449	GLN
1	C	462	ASN
1	D	167	GLN
1	E	243	ASN
1	E	252	HIS
1	E	320	ASN
1	F	212	ASN
1	F	312	ASN
1	F	470	ASN
1	G	243	ASN
1	G	299	GLN
1	G	364	HIS
1	H	43	GLN
1	H	178	HIS
1	H	450	HIS
1	H	467	ASN
1	I	243	ASN
1	I	320	ASN
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	K	76	HIS
1	K	243	ASN
1	K	252	HIS

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Mol	Chain	Res	Type
1	K	364	HIS
1	L	76	HIS
1	L	212	ASN
1	L	252	HIS
1	L	320	ASN
1	L	443	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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%)	1.17	107 (22%) 0 0	56, 117, 190, 215	0
1	B	475/513 (92%)	1.19	100 (21%) 1 1	57, 133, 189, 213	0
1	C	472/513 (92%)	1.13	100 (21%) 0 1	55, 134, 193, 231	0
1	D	460/513 (89%)	1.33	111 (24%) 0 0	66, 127, 215, 230	0
1	E	461/513 (89%)	1.61	136 (29%) 0 0	71, 149, 212, 231	0
1	F	460/513 (89%)	1.14	93 (20%) 1 1	66, 136, 191, 226	0
1	G	461/513 (89%)	1.11	88 (19%) 1 1	69, 128, 195, 223	0
1	H	478/513 (93%)	1.10	81 (16%) 1 2	61, 107, 191, 209	0
1	I	478/513 (93%)	0.93	68 (14%) 2 3	62, 107, 176, 217	0
1	J	484/513 (94%)	0.88	63 (13%) 3 4	70, 120, 191, 215	0
1	K	498/513 (97%)	0.78	51 (10%) 6 7	67, 114, 164, 191	0
1	L	473/513 (92%)	1.36	119 (25%) 0 0	64, 146, 205, 219	0
All	All	5680/6156 (92%)	1.14	1117 (19%) 1 1	55, 125, 200, 231	0

All (1117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	231	SER	11.2
1	D	78	ALA	11.2
1	C	231	SER	10.9
1	L	146	VAL	10.4
1	L	232	TYR	10.1
1	E	78	ALA	10.0
1	I	103	ASP	9.4
1	L	247	GLY	9.2
1	E	96	LEU	8.9
1	E	118	LEU	8.8
1	E	134	PHE	8.7

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Mol	Chain	Res	Type	RSRZ
1	L	248	GLU	8.4
1	L	269	PRO	8.3
1	L	314	ILE	8.2
1	J	270	VAL	8.2
1	E	36	ALA	8.0
1	L	316	ILE	8.0
1	E	35	ASP	7.9
1	D	97	ILE	7.7
1	L	272	VAL	7.6
1	E	59	PHE	7.5
1	D	96	LEU	7.5
1	D	77	ARG	7.4
1	H	118	LEU	7.4
1	E	264	ALA	7.3
1	C	243	ASN	7.3
1	G	446	LEU	7.2
1	A	223	GLY	6.9
1	D	92	LEU	6.9
1	A	39	LEU	6.8
1	E	152	ASP	6.8
1	J	109	LEU	6.8
1	E	265	SER	6.8
1	F	42	GLY	6.7
1	E	39	LEU	6.7
1	I	104	GLY	6.6
1	L	315	VAL	6.6
1	A	36	ALA	6.6
1	F	243	ASN	6.6
1	J	232	TYR	6.5
1	E	30	CYS	6.4
1	G	8	LEU	6.4
1	J	313	VAL	6.3
1	B	244	LYS	6.3
1	E	269	PRO	6.2
1	B	246	VAL	6.1
1	D	56	ALA	6.0
1	L	233	PHE	6.0
1	A	224	ASP	5.9
1	G	36	ALA	5.9
1	D	244	LYS	5.9
1	C	233	PHE	5.9
1	L	155	TYR	5.9

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Mol	Chain	Res	Type	RSRZ
1	G	29	THR	5.8
1	E	11	THR	5.8
1	L	313	VAL	5.8
1	L	257	PHE	5.8
1	B	139	LYS	5.7
1	I	219	ALA	5.7
1	F	61	ALA	5.7
1	F	11	THR	5.6
1	E	153	VAL	5.6
1	A	47	LEU	5.6
1	F	135	GLU	5.6
1	E	53	VAL	5.6
1	C	11	THR	5.5
1	G	39	LEU	5.5
1	H	141	GLU	5.5
1	E	446	LEU	5.5
1	D	45	VAL	5.4
1	E	239	PRO	5.4
1	H	233	PHE	5.4
1	D	26	MET	5.4
1	D	40	LYS	5.4
1	D	248	GLU	5.4
1	E	13	ASP	5.4
1	A	96	LEU	5.4
1	B	171	ALA	5.4
1	E	271	ILE	5.4
1	E	40	LYS	5.4
1	H	132	TYR	5.3
1	J	233	PHE	5.3
1	B	118	LEU	5.3
1	D	41	LYS	5.3
1	B	314	ILE	5.3
1	E	28	LEU	5.3
1	H	102	PRO	5.3
1	C	39	LEU	5.2
1	E	68	LEU	5.2
1	L	234	LEU	5.2
1	D	17	VAL	5.2
1	L	151	PRO	5.2
1	E	56	ALA	5.2
1	G	42	GLY	5.2
1	D	28	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	47	LEU	5.2
1	D	76	HIS	5.2
1	E	9	LEU	5.2
1	F	134	PHE	5.2
1	H	39	LEU	5.1
1	G	60	GLU	5.1
1	F	28	LEU	5.1
1	I	144	ASP	5.1
1	C	76	HIS	5.1
1	K	201	CYS	5.1
1	H	133	ALA	5.1
1	G	253	ILE	5.1
1	I	142	VAL	5.1
1	E	61	ALA	5.0
1	H	105	LEU	5.0
1	C	79	LEU	5.0
1	L	274	PHE	5.0
1	A	56	ALA	5.0
1	F	56	ALA	5.0
1	A	118	LEU	5.0
1	A	92	LEU	4.9
1	E	42	GLY	4.9
1	I	146	VAL	4.9
1	F	375	ARG	4.9
1	A	151	PRO	4.9
1	E	10	ALA	4.9
1	D	101	LEU	4.9
1	E	232	TYR	4.9
1	F	231	SER	4.9
1	E	97	ILE	4.9
1	G	265	SER	4.9
1	F	439	LEU	4.8
1	H	53	VAL	4.8
1	K	182	TYR	4.8
1	L	176	PHE	4.8
1	C	446	LEU	4.8
1	D	100	ASP	4.8
1	E	103	ASP	4.8
1	D	71	ILE	4.8
1	H	16	THR	4.8
1	J	314	ILE	4.8
1	A	51	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	260	ALA	4.8
1	E	260	ALA	4.7
1	G	264	ALA	4.7
1	F	55	GLU	4.7
1	B	117	LYS	4.7
1	D	118	LEU	4.7
1	E	51	LEU	4.7
1	L	145	LEU	4.7
1	E	38	SER	4.7
1	D	91	TRP	4.7
1	A	132	TYR	4.7
1	H	113	THR	4.7
1	L	446	LEU	4.7
1	E	54	VAL	4.7
1	G	53	VAL	4.7
1	J	172	VAL	4.7
1	H	134	PHE	4.7
1	G	134	PHE	4.7
1	B	60	GLU	4.7
1	L	148	GLU	4.7
1	E	313	VAL	4.7
1	E	92	LEU	4.6
1	B	45	VAL	4.6
1	E	60	GLU	4.6
1	F	378	CYS	4.6
1	A	246	VAL	4.6
1	L	231	SER	4.6
1	B	219	ALA	4.6
1	E	3	SER	4.6
1	H	269	PRO	4.6
1	J	176	PHE	4.5
1	G	441	THR	4.5
1	B	56	ALA	4.5
1	G	41	LYS	4.5
1	E	112	ASP	4.5
1	A	8	LEU	4.5
1	D	24	ARG	4.5
1	C	359	GLU	4.5
1	E	70	GLU	4.5
1	E	185	TYR	4.5
1	I	314	ILE	4.5
1	G	295	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	15	ASP	4.4
1	F	17	VAL	4.4
1	K	445	GLY	4.4
1	L	193	VAL	4.4
1	G	367	ASP	4.4
1	C	445	GLY	4.4
1	A	78	ALA	4.4
1	D	245	PHE	4.4
1	E	25	LYS	4.4
1	E	100	ASP	4.4
1	L	271	ILE	4.4
1	B	191	LYS	4.4
1	J	293	GLU	4.4
1	B	257	PHE	4.4
1	A	137	ILE	4.3
1	F	79	LEU	4.3
1	J	357	LEU	4.3
1	B	36	ALA	4.3
1	A	41	LYS	4.3
1	A	244	LYS	4.3
1	J	271	ILE	4.3
1	B	5	TYR	4.3
1	A	93	ALA	4.3
1	G	205	LEU	4.3
1	K	446	LEU	4.3
1	L	172	VAL	4.3
1	A	6	GLY	4.3
1	L	204	THR	4.3
1	H	265	SER	4.3
1	E	79	LEU	4.3
1	D	53	VAL	4.3
1	B	35	ASP	4.3
1	K	187	LEU	4.3
1	L	270	VAL	4.3
1	B	230	LYS	4.2
1	G	357	LEU	4.2
1	B	313	VAL	4.2
1	E	90	VAL	4.2
1	G	206	ILE	4.2
1	E	67	THR	4.2
1	D	418	ASN	4.2
1	H	270	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	J	269	PRO	4.2
1	A	94	ASP	4.2
1	L	235	ASN	4.2
1	A	76	HIS	4.2
1	A	117	LYS	4.2
1	C	40	LYS	4.2
1	C	252	HIS	4.2
1	E	14	ASP	4.2
1	C	246	VAL	4.2
1	E	314	ILE	4.2
1	D	98	ALA	4.2
1	D	239	PRO	4.2
1	A	61	ALA	4.2
1	E	115	PRO	4.2
1	A	53	VAL	4.1
1	F	7	VAL	4.1
1	A	38	SER	4.1
1	B	273	PHE	4.1
1	B	268	THR	4.1
1	F	52	THR	4.1
1	E	76	HIS	4.1
1	I	318	ALA	4.1
1	E	245	PHE	4.1
1	H	70	GLU	4.1
1	G	9	LEU	4.1
1	G	68	LEU	4.1
1	I	115	PRO	4.1
1	E	29	THR	4.1
1	L	359	GLU	4.1
1	H	314	ILE	4.1
1	F	26	MET	4.1
1	C	124	LEU	4.1
1	D	113	THR	4.1
1	F	118	LEU	4.1
1	F	137	ILE	4.1
1	A	11	THR	4.0
1	B	70	GLU	4.0
1	F	10	ALA	4.0
1	D	43	GLN	4.0
1	A	139	LYS	4.0
1	B	98	ALA	4.0
1	A	239	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	75	GLY	4.0
1	C	98	ALA	4.0
1	G	260	ALA	4.0
1	E	137	ILE	4.0
1	E	135	GLU	4.0
1	H	293	GLU	4.0
1	I	313	VAL	4.0
1	E	357	LEU	4.0
1	L	273	PHE	4.0
1	H	54	VAL	4.0
1	D	317	GLY	4.0
1	D	231	SER	4.0
1	K	353	TYR	4.0
1	F	60	GLU	4.0
1	L	158	ILE	4.0
1	D	55	GLU	3.9
1	C	306	GLY	3.9
1	F	446	LEU	3.9
1	E	218	MET	3.9
1	E	113	THR	3.9
1	F	59	PHE	3.9
1	L	173	GLU	3.9
1	D	39	LEU	3.9
1	G	445	GLY	3.9
1	G	30	CYS	3.9
1	L	367	ASP	3.9
1	C	444	PRO	3.9
1	D	70	GLU	3.9
1	B	78	ALA	3.9
1	D	89	VAL	3.9
1	E	77	ARG	3.8
1	G	232	TYR	3.8
1	L	304	ILE	3.8
1	B	39	LEU	3.8
1	F	39	LEU	3.8
1	K	185	TYR	3.8
1	H	72	LEU	3.8
1	L	45	VAL	3.8
1	D	20	PHE	3.8
1	D	191	LYS	3.8
1	I	134	PHE	3.8
1	B	297	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	132	TYR	3.8
1	H	135	GLU	3.8
1	A	45	VAL	3.8
1	F	495	LYS	3.8
1	H	60	GLU	3.8
1	L	182	TYR	3.8
1	F	51	LEU	3.8
1	L	147	LEU	3.8
1	E	217	LYS	3.7
1	J	102	PRO	3.7
1	G	145	LEU	3.7
1	F	296	VAL	3.7
1	H	151	PRO	3.7
1	A	35	ASP	3.7
1	F	53	VAL	3.7
1	B	245	PHE	3.7
1	F	245	PHE	3.7
1	H	30	CYS	3.7
1	C	382	MET	3.7
1	E	124	LEU	3.7
1	H	68	LEU	3.7
1	L	358	THR	3.7
1	I	105	LEU	3.7
1	K	264	ALA	3.7
1	D	126	VAL	3.7
1	G	28	LEU	3.7
1	D	311	GLU	3.7
1	A	91	TRP	3.6
1	L	361	LEU	3.6
1	D	130	ALA	3.6
1	E	94	ASP	3.6
1	E	191	LYS	3.6
1	L	357	LEU	3.6
1	F	233	PHE	3.6
1	E	250	GLU	3.6
1	L	144	ASP	3.6
1	F	92	LEU	3.6
1	G	235	ASN	3.6
1	D	124	LEU	3.6
1	D	10	ALA	3.6
1	C	441	THR	3.6
1	F	78	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	37	ALA	3.6
1	E	47	LEU	3.6
1	L	439	LEU	3.6
1	D	247	GLY	3.6
1	B	329	ILE	3.5
1	E	418	ASN	3.5
1	D	446	LEU	3.5
1	H	124	LEU	3.5
1	H	144	ASP	3.5
1	E	17	VAL	3.5
1	C	9	LEU	3.5
1	E	231	SER	3.5
1	E	7	VAL	3.5
1	A	221	VAL	3.5
1	F	260	ALA	3.5
1	I	257	PHE	3.5
1	G	313	VAL	3.5
1	D	357	LEU	3.5
1	C	298	PRO	3.5
1	B	274	PHE	3.5
1	A	505	THR	3.5
1	A	201	CYS	3.5
1	F	76	HIS	3.5
1	A	54	VAL	3.5
1	D	42	GLY	3.5
1	K	267	GLY	3.5
1	H	103	ASP	3.4
1	H	115	PRO	3.4
1	E	37	ALA	3.4
1	L	310	LEU	3.4
1	B	4	GLY	3.4
1	I	78	ALA	3.4
1	C	235	ASN	3.4
1	G	363	VAL	3.4
1	A	113	THR	3.4
1	K	357	LEU	3.4
1	A	5	TYR	3.4
1	F	125	LEU	3.4
1	G	443	GLN	3.4
1	J	182	TYR	3.4
1	A	9	LEU	3.4
1	C	296	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	155	TYR	3.4
1	F	140	ALA	3.4
1	J	193	VAL	3.4
1	L	268	THR	3.4
1	C	97	ILE	3.4
1	J	195	LEU	3.4
1	B	34	ILE	3.4
1	B	233	PHE	3.4
1	F	41	LYS	3.4
1	G	233	PHE	3.4
1	L	379	ILE	3.4
1	D	6	GLY	3.4
1	L	317	GLY	3.4
1	I	296	VAL	3.3
1	D	382	MET	3.3
1	J	446	LEU	3.3
1	B	155	TYR	3.3
1	F	132	TYR	3.3
1	F	242	LEU	3.3
1	I	153	VAL	3.3
1	L	390	MET	3.3
1	F	239	PRO	3.3
1	E	57	GLY	3.3
1	B	296	VAL	3.3
1	A	136	ARG	3.3
1	B	325	ILE	3.3
1	D	18	ASP	3.3
1	D	16	THR	3.3
1	H	34	ILE	3.3
1	E	151	PRO	3.3
1	I	272	VAL	3.3
1	A	134	PHE	3.3
1	H	56	ALA	3.3
1	I	143	GLU	3.3
1	D	5	TYR	3.3
1	C	436	LYS	3.3
1	E	41	LYS	3.3
1	L	181	LEU	3.3
1	A	79	LEU	3.3
1	G	361	LEU	3.3
1	A	296	VAL	3.3
1	C	443	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	132	TYR	3.3
1	I	118	LEU	3.3
1	I	297	VAL	3.3
1	H	505	THR	3.3
1	A	90	VAL	3.3
1	A	233	PHE	3.3
1	C	244	LYS	3.3
1	E	8	LEU	3.3
1	E	182	TYR	3.3
1	F	94	ASP	3.3
1	C	17	VAL	3.3
1	G	40	LYS	3.3
1	C	360	PHE	3.2
1	C	357	LEU	3.2
1	F	40	LYS	3.2
1	D	122	ASP	3.2
1	J	111	ASP	3.2
1	C	135	GLU	3.2
1	L	450	HIS	3.2
1	C	117	LYS	3.2
1	I	191	LYS	3.2
1	D	30	CYS	3.2
1	E	214	LEU	3.2
1	E	445	GLY	3.2
1	L	309	GLY	3.2
1	G	448	ILE	3.2
1	A	37	ALA	3.2
1	E	48	ASN	3.2
1	H	315	VAL	3.2
1	E	242	LEU	3.2
1	H	101	LEU	3.2
1	A	399	PHE	3.2
1	D	115	PRO	3.2
1	E	272	VAL	3.2
1	F	230	LYS	3.2
1	B	48	ASN	3.2
1	C	123	SER	3.2
1	H	100	ASP	3.2
1	L	207	ALA	3.2
1	A	7	VAL	3.2
1	K	177	LEU	3.2
1	E	270	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	168	ILE	3.2
1	D	31	SER	3.2
1	A	34	ILE	3.2
1	A	17	VAL	3.2
1	J	441	THR	3.2
1	A	309	GLY	3.1
1	B	8	LEU	3.1
1	H	91	TRP	3.1
1	D	243	ASN	3.1
1	L	264	ALA	3.1
1	G	353	TYR	3.1
1	L	196	TYR	3.1
1	C	118	LEU	3.1
1	D	38	SER	3.1
1	D	68	LEU	3.1
1	A	95	PRO	3.1
1	L	360	PHE	3.1
1	B	100	ASP	3.1
1	E	34	ILE	3.1
1	G	19	VAL	3.1
1	C	300	LEU	3.1
1	H	131	GLY	3.1
1	E	119	ARG	3.1
1	A	40	LYS	3.1
1	G	274	PHE	3.1
1	C	449	GLN	3.1
1	D	200	GLY	3.1
1	L	375	ARG	3.1
1	I	248	GLU	3.1
1	B	79	LEU	3.1
1	E	121	GLY	3.1
1	E	125	LEU	3.1
1	H	92	LEU	3.1
1	D	66	SER	3.1
1	G	31	SER	3.1
1	L	111	ASP	3.1
1	H	191	LYS	3.1
1	J	337	VAL	3.1
1	F	133	ALA	3.1
1	F	379	ILE	3.0
1	D	90	VAL	3.0
1	K	248	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	382	MET	3.0
1	B	269	PRO	3.0
1	H	239	PRO	3.0
1	E	199	PRO	3.0
1	C	367	ASP	3.0
1	I	315	VAL	3.0
1	J	445	GLY	3.0
1	J	112	ASP	3.0
1	D	267	GLY	3.0
1	B	235	ASN	3.0
1	L	447	ARG	3.0
1	L	505	THR	3.0
1	K	359	GLU	3.0
1	E	379	ILE	3.0
1	L	159	GLY	3.0
1	D	19	VAL	3.0
1	C	47	LEU	3.0
1	B	57	GLY	3.0
1	E	505	THR	3.0
1	I	246	VAL	3.0
1	I	101	LEU	3.0
1	I	195	LEU	3.0
1	G	140	ALA	3.0
1	H	271	ILE	3.0
1	G	135	GLU	3.0
1	B	182	TYR	3.0
1	D	23	GLY	3.0
1	E	171	ALA	3.0
1	G	18	ASP	3.0
1	D	390	MET	3.0
1	D	69	ARG	2.9
1	G	158	ILE	2.9
1	H	114	ARG	2.9
1	G	124	LEU	2.9
1	G	132	TYR	2.9
1	L	356	TYR	2.9
1	D	27	ARG	2.9
1	J	316	ILE	2.9
1	D	386	VAL	2.9
1	E	263	LYS	2.9
1	K	367	ASP	2.9
1	J	266	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	127	ASP	2.9
1	B	309	GLY	2.9
1	A	226	ALA	2.9
1	D	62	VAL	2.9
1	D	95	PRO	2.9
1	E	198	PRO	2.9
1	I	353	TYR	2.9
1	K	309	GLY	2.9
1	L	382	MET	2.9
1	F	12	HIS	2.9
1	F	210	VAL	2.9
1	C	237	LYS	2.9
1	F	124	LEU	2.9
1	G	234	LEU	2.9
1	J	206	ILE	2.9
1	F	274	PHE	2.9
1	L	143	GLU	2.9
1	D	61	ALA	2.9
1	E	358	THR	2.9
1	H	149	GLU	2.9
1	J	268	THR	2.9
1	E	26	MET	2.9
1	H	97	ILE	2.9
1	J	256	ILE	2.9
1	L	118	LEU	2.9
1	C	309	GLY	2.9
1	B	124	LEU	2.9
1	B	165	ILE	2.9
1	E	234	LEU	2.9
1	G	383	ILE	2.9
1	G	451	LEU	2.9
1	K	379	ILE	2.9
1	C	459	PHE	2.9
1	B	334	ARG	2.9
1	A	446	LEU	2.9
1	E	235	ASN	2.9
1	J	105	LEU	2.9
1	L	206	ILE	2.9
1	L	256	ILE	2.8
1	D	281	PHE	2.8
1	F	15	ASP	2.8
1	F	47	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	104	GLY	2.8
1	J	144	ASP	2.8
1	H	272	VAL	2.8
1	H	61	ALA	2.8
1	A	77	ARG	2.8
1	K	168	ILE	2.8
1	A	50	ALA	2.8
1	A	44	THR	2.8
1	J	234	LEU	2.8
1	F	45	VAL	2.8
1	I	168	ILE	2.8
1	L	386	VAL	2.8
1	A	10	ALA	2.8
1	E	43	GLN	2.8
1	C	101	LEU	2.8
1	E	177	LEU	2.8
1	G	97	ILE	2.8
1	L	149	GLU	2.8
1	C	353	TYR	2.8
1	E	93	ALA	2.8
1	G	141	GLU	2.8
1	G	51	LEU	2.8
1	L	41	LYS	2.8
1	D	193	VAL	2.8
1	H	80	VAL	2.8
1	H	274	PHE	2.8
1	B	143	GLU	2.8
1	D	46	ARG	2.8
1	B	193	VAL	2.8
1	E	19	VAL	2.8
1	H	71	ILE	2.8
1	H	37	ALA	2.8
1	L	170	ASP	2.8
1	C	223	GLY	2.8
1	H	17	VAL	2.8
1	E	71	ILE	2.8
1	K	329	ILE	2.8
1	B	311	GLU	2.8
1	G	418	ASN	2.8
1	A	18	ASP	2.8
1	B	316	ILE	2.8
1	D	316	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	438	VAL	2.8
1	C	34	ILE	2.8
1	E	91	TRP	2.8
1	K	314	ILE	2.8
1	C	440	GLU	2.8
1	G	54	VAL	2.8
1	G	146	VAL	2.8
1	D	253	ILE	2.7
1	D	176	PHE	2.7
1	C	12	HIS	2.7
1	D	11	THR	2.7
1	I	244	LYS	2.7
1	C	45	VAL	2.7
1	D	246	VAL	2.7
1	J	265	SER	2.7
1	L	213	SER	2.7
1	K	158	ILE	2.7
1	F	357	LEU	2.7
1	I	113	THR	2.7
1	L	208	LYS	2.7
1	I	96	LEU	2.7
1	G	298	PRO	2.7
1	I	100	ASP	2.7
1	F	93	ALA	2.7
1	F	130	ALA	2.7
1	G	7	VAL	2.7
1	L	451	LEU	2.7
1	I	140	ALA	2.7
1	J	272	VAL	2.7
1	E	201	CYS	2.7
1	D	47	LEU	2.7
1	E	20	PHE	2.7
1	J	108	ALA	2.7
1	E	362	PRO	2.7
1	F	89	VAL	2.7
1	A	264	ALA	2.7
1	G	91	TRP	2.7
1	L	187	LEU	2.7
1	B	505	THR	2.7
1	L	296	VAL	2.7
1	F	234	LEU	2.7
1	J	367	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	432	LYS	2.7
1	B	26	MET	2.7
1	I	270	VAL	2.7
1	A	229	ALA	2.7
1	D	435	ILE	2.7
1	L	431	LYS	2.6
1	D	136	ARG	2.6
1	I	124	LEU	2.6
1	C	442	GLY	2.6
1	F	126	VAL	2.6
1	E	346	ALA	2.6
1	I	284	ARG	2.6
1	J	110	ASN	2.6
1	B	49	GLU	2.6
1	I	271	ILE	2.6
1	A	243	ASN	2.6
1	B	11	THR	2.6
1	G	249	THR	2.6
1	C	115	PRO	2.6
1	C	318	ALA	2.6
1	F	176	PHE	2.6
1	G	364	HIS	2.6
1	L	76	HIS	2.6
1	K	173	GLU	2.6
1	L	17	VAL	2.6
1	L	254	ARG	2.6
1	C	72	LEU	2.6
1	H	268	THR	2.6
1	I	403	THR	2.6
1	B	89	VAL	2.6
1	G	390	MET	2.6
1	B	278	ASP	2.6
1	D	79	LEU	2.6
1	L	185	TYR	2.6
1	B	77	ARG	2.6
1	L	363	VAL	2.6
1	D	195	LEU	2.6
1	L	335	LEU	2.6
1	H	33	ASN	2.6
1	K	444	PRO	2.6
1	F	54	VAL	2.6
1	L	154	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	98	ALA	2.6
1	C	125	LEU	2.6
1	H	9	LEU	2.6
1	A	98	ALA	2.6
1	C	245	PHE	2.6
1	H	182	TYR	2.6
1	J	107	GLU	2.6
1	A	227	HIS	2.6
1	E	274	PHE	2.6
1	J	99	GLU	2.6
1	J	359	GLU	2.6
1	K	378	CYS	2.6
1	G	444	PRO	2.6
1	L	312	ASN	2.6
1	L	178	HIS	2.6
1	J	399	PHE	2.6
1	E	353	TYR	2.6
1	B	103	ASP	2.6
1	I	274	PHE	2.5
1	B	105	LEU	2.5
1	L	412	MET	2.5
1	E	474	TRP	2.5
1	G	10	ALA	2.5
1	A	19	VAL	2.5
1	K	330	LEU	2.5
1	F	399	PHE	2.5
1	H	31	SER	2.5
1	A	268	THR	2.5
1	E	98	ALA	2.5
1	B	40	LYS	2.5
1	D	25	LYS	2.5
1	A	2	PRO	2.5
1	K	372	ASP	2.5
1	K	184	GLU	2.5
1	A	29	THR	2.5
1	J	138	PRO	2.5
1	G	434	ALA	2.5
1	H	234	LEU	2.5
1	C	116	ARG	2.5
1	A	256	ILE	2.5
1	E	66	SER	2.5
1	F	155	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	264	ALA	2.5
1	B	259	ARG	2.5
1	K	418	ASN	2.5
1	L	474	TRP	2.5
1	E	304	ILE	2.5
1	A	42	GLY	2.5
1	C	225	ASP	2.5
1	L	452	LEU	2.5
1	C	399	PHE	2.5
1	D	341	ILE	2.5
1	B	328	ALA	2.5
1	D	63	GLY	2.5
1	B	43	GLN	2.5
1	C	239	PRO	2.5
1	K	39	LEU	2.5
1	D	374	ASP	2.5
1	A	252	HIS	2.5
1	B	231	SER	2.5
1	H	66	SER	2.5
1	H	123	SER	2.5
1	B	37	ALA	2.5
1	G	417	PHE	2.5
1	D	252	HIS	2.5
1	E	400	LEU	2.5
1	L	160	GLY	2.5
1	D	199	PRO	2.5
1	I	173	GLU	2.5
1	C	26	MET	2.4
1	B	10	ALA	2.4
1	E	257	PHE	2.4
1	F	363	VAL	2.4
1	A	114	ARG	2.4
1	D	134	PHE	2.4
1	C	299	GLN	2.4
1	I	258	GLN	2.4
1	A	26	MET	2.4
1	C	191	LYS	2.4
1	F	18	ASP	2.4
1	H	40	LYS	2.4
1	C	193	VAL	2.4
1	D	121	GLY	2.4
1	L	96	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	95	PRO	2.4
1	E	138	PRO	2.4
1	G	277	MET	2.4
1	C	66	SER	2.4
1	E	261	ARG	2.4
1	B	61	ALA	2.4
1	D	133	ALA	2.4
1	F	5	TYR	2.4
1	H	249	THR	2.4
1	A	119	ARG	2.4
1	C	451	LEU	2.4
1	I	1	MET	2.4
1	K	459	PHE	2.4
1	L	455	ILE	2.4
1	A	28	LEU	2.4
1	C	358	THR	2.4
1	I	317	GLY	2.4
1	K	272	VAL	2.4
1	L	101	LEU	2.4
1	L	329	ILE	2.4
1	B	126	VAL	2.4
1	E	296	VAL	2.4
1	G	17	VAL	2.4
1	G	452	LEU	2.4
1	L	194	LEU	2.4
1	J	414	PHE	2.4
1	B	158	ILE	2.4
1	B	168	ILE	2.4
1	A	230	LYS	2.4
1	H	43	GLN	2.4
1	B	23	GLY	2.4
1	G	309	GLY	2.4
1	B	353	TYR	2.4
1	B	177	LEU	2.4
1	C	361	LEU	2.4
1	F	57	GLY	2.4
1	J	317	GLY	2.4
1	C	226	ALA	2.4
1	B	9	LEU	2.4
1	L	92	LEU	2.4
1	C	307	VAL	2.4
1	F	146	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	284	ARG	2.4
1	D	125	LEU	2.4
1	J	417	PHE	2.4
1	A	71	ILE	2.4
1	C	219	ALA	2.4
1	L	353	TYR	2.4
1	H	51	LEU	2.4
1	J	171	ALA	2.3
1	J	353	TYR	2.3
1	D	187	LEU	2.3
1	A	83	HIS	2.3
1	F	19	VAL	2.3
1	F	14	ASP	2.3
1	J	274	PHE	2.3
1	C	102	PRO	2.3
1	F	8	LEU	2.3
1	C	100	ASP	2.3
1	A	267	GLY	2.3
1	K	223	GLY	2.3
1	C	35	ASP	2.3
1	D	34	ILE	2.3
1	F	394	ILE	2.3
1	K	256	ILE	2.3
1	E	99	GLU	2.3
1	H	252	HIS	2.3
1	B	164	GLN	2.3
1	I	418	ASN	2.3
1	H	316	ILE	2.3
1	F	172	VAL	2.3
1	K	193	VAL	2.3
1	C	87	GLU	2.3
1	C	188	ARG	2.3
1	B	170	ASP	2.3
1	C	224	ASP	2.3
1	C	229	ALA	2.3
1	J	339	ILE	2.3
1	A	257	PHE	2.3
1	E	176	PHE	2.3
1	H	136	ARG	2.3
1	G	96	LEU	2.3
1	G	37	ALA	2.3
1	J	100	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	132	TYR	2.3
1	H	143	GLU	2.3
1	C	92	LEU	2.3
1	E	65	ILE	2.3
1	A	334	ARG	2.3
1	F	386	VAL	2.3
1	A	228	GLU	2.3
1	E	194	LEU	2.3
1	I	485	ILE	2.3
1	G	45	VAL	2.3
1	C	187	LEU	2.3
1	E	195	LEU	2.3
1	L	330	LEU	2.3
1	G	314	ILE	2.3
1	B	17	VAL	2.3
1	G	130	ALA	2.3
1	I	182	TYR	2.3
1	F	136	ARG	2.3
1	G	301	LEU	2.3
1	L	119	ARG	2.3
1	A	100	ASP	2.2
1	D	52	THR	2.2
1	K	195	LEU	2.2
1	L	68	LEU	2.2
1	A	245	PHE	2.2
1	B	399	PHE	2.2
1	C	206	ILE	2.2
1	D	274	PHE	2.2
1	F	459	PHE	2.2
1	G	435	ILE	2.2
1	D	296	VAL	2.2
1	I	399	PHE	2.2
1	A	3	SER	2.2
1	B	104	GLY	2.2
1	C	60	GLU	2.2
1	D	60	GLU	2.2
1	L	79	LEU	2.2
1	D	35	ASP	2.2
1	B	134	PHE	2.2
1	H	137	ILE	2.2
1	I	151	PRO	2.2
1	F	66	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	194	LEU	2.2
1	B	74	ASP	2.2
1	G	386	VAL	2.2
1	B	76	HIS	2.2
1	B	194	LEU	2.2
1	C	414	PHE	2.2
1	B	112	ASP	2.2
1	E	193	VAL	2.2
1	F	2	PRO	2.2
1	J	248	GLU	2.2
1	B	96	LEU	2.2
1	B	195	LEU	2.2
1	C	368	LEU	2.2
1	J	257	PHE	2.2
1	B	172	VAL	2.2
1	F	77	ARG	2.2
1	B	264	ALA	2.2
1	F	235	ASN	2.2
1	G	358	THR	2.2
1	H	155	TYR	2.2
1	I	247	GLY	2.2
1	B	28	LEU	2.2
1	J	330	LEU	2.2
1	E	316	ILE	2.2
1	L	217	LYS	2.2
1	L	339	ILE	2.2
1	J	192	GLY	2.2
1	B	46	ARG	2.2
1	K	176	PHE	2.2
1	I	256	ILE	2.2
1	C	182	TYR	2.2
1	I	341	ILE	2.2
1	A	49	GLU	2.2
1	A	269	PRO	2.2
1	E	114	ARG	2.2
1	I	330	LEU	2.2
1	B	29	THR	2.2
1	B	53	VAL	2.2
1	B	149	GLU	2.2
1	C	314	ILE	2.2
1	K	271	ILE	2.2
1	L	277	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	384	GLU	2.2
1	A	231	SER	2.2
1	H	8	LEU	2.2
1	A	59	PHE	2.2
1	K	281	PHE	2.2
1	A	133	ALA	2.2
1	A	232	TYR	2.2
1	L	39	LEU	2.2
1	L	205	LEU	2.2
1	I	102	PRO	2.2
1	A	173	GLU	2.2
1	B	270	VAL	2.2
1	H	435	ILE	2.2
1	I	152	ASP	2.2
1	K	463	GLU	2.2
1	E	131	GLY	2.2
1	D	353	TYR	2.1
1	J	214	LEU	2.1
1	G	133	ALA	2.1
1	B	3	SER	2.1
1	A	102	PRO	2.1
1	E	126	VAL	2.1
1	F	464	ASP	2.1
1	H	256	ILE	2.1
1	I	172	VAL	2.1
1	J	488	ILE	2.1
1	I	185	TYR	2.1
1	C	383	ILE	2.1
1	G	231	SER	2.1
1	I	362	PRO	2.1
1	I	503	ILE	2.1
1	J	175	PRO	2.1
1	G	93	ALA	2.1
1	G	505	THR	2.1
1	J	185	TYR	2.1
1	K	83	HIS	2.1
1	C	256	ILE	2.1
1	J	148	GLU	2.1
1	J	341	ILE	2.1
1	K	232	TYR	2.1
1	H	334	ARG	2.1
1	J	201	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	97	ILE	2.1
1	G	55	GLU	2.1
1	A	214	LEU	2.1
1	D	192	GLY	2.1
1	L	125	LEU	2.1
1	L	444	PRO	2.1
1	B	94	ASP	2.1
1	H	76	HIS	2.1
1	A	16	THR	2.1
1	I	402	VAL	2.1
1	C	378	CYS	2.1
1	J	491	LEU	2.1
1	L	267	GLY	2.1
1	C	136	ARG	2.1
1	K	230	LYS	2.1
1	D	257	PHE	2.1
1	F	36	ALA	2.1
1	F	505	THR	2.1
1	F	9	LEU	2.1
1	I	277	MET	2.1
1	K	8	LEU	2.1
1	I	32	PRO	2.1
1	H	3	SER	2.1
1	D	15	ASP	2.1
1	A	142	VAL	2.1
1	D	266	GLU	2.1
1	D	410	GLU	2.1
1	C	317	GLY	2.1
1	F	436	LYS	2.1
1	F	70	GLU	2.1
1	F	264	ALA	2.1
1	E	45	VAL	2.1
1	K	402	VAL	2.1
1	A	69	ARG	2.1
1	A	414	PHE	2.1
1	G	70	GLU	2.1
1	F	158	ILE	2.1
1	G	379	ILE	2.1
1	K	257	PHE	2.1
1	A	135	GLU	2.1
1	C	78	ALA	2.1
1	L	191	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	272	VAL	2.1
1	E	317	GLY	2.1
1	C	463	GLU	2.1
1	D	155	TYR	2.1
1	I	5	TYR	2.1
1	L	430	ALA	2.1
1	F	435	ILE	2.1
1	K	92	LEU	2.1
1	C	275	ASP	2.1
1	E	254	ARG	2.0
1	G	431	LYS	2.0
1	L	55	GLU	2.0
1	A	115	PRO	2.0
1	D	93	ALA	2.0
1	E	140	ALA	2.0
1	E	246	VAL	2.0
1	C	137	ILE	2.0
1	L	165	ILE	2.0
1	L	435	ILE	2.0
1	A	371	PHE	2.0
1	I	281	PHE	2.0
1	I	334	ARG	2.0
1	L	326	ASP	2.0
1	C	7	VAL	2.0
1	A	52	THR	2.0
1	B	113	THR	2.0
1	E	101	LEU	2.0
1	G	362	PRO	2.0
1	J	125	LEU	2.0
1	K	397	ASN	2.0
1	G	144	ASP	2.0
1	H	231	SER	2.0
1	C	93	ALA	2.0
1	I	255	LEU	2.0
1	L	236	ILE	2.0
1	C	375	ARG	2.0
1	F	16	THR	2.0
1	K	277	MET	2.0
1	D	185	TYR	2.0
1	L	427	VAL	2.0
1	I	137	ILE	2.0
1	A	58	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	382	MET	2.0
1	I	148	GLU	2.0
1	K	311	GLU	2.0
1	C	19	VAL	2.0
1	H	117	LYS	2.0
1	B	101	LEU	2.0
1	C	460	ALA	2.0
1	A	247	GLY	2.0
1	C	65	ILE	2.0
1	F	96	LEU	2.0
1	H	329	ILE	2.0
1	J	253	ILE	2.0
1	L	341	ILE	2.0
1	A	235	ASN	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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.