



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2017 – 01:37 AM EDT

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 : unknown
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

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

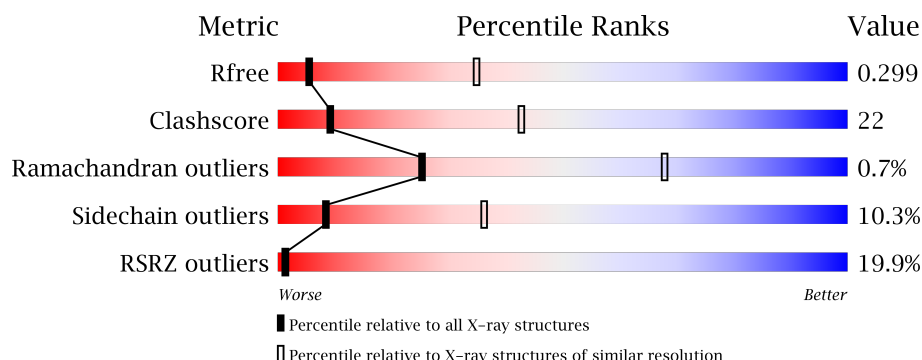
1 Overall quality at a glance ⓘ

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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (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. 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>20%</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>

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Mol	Chain	Length	Quality of chain
1	F	513	<div><div>18%</div><div><div></div><div>55%</div><div>29%</div><div>5%</div><div>10%</div></div></div>
1	G	513	<div><div>17%</div><div><div></div><div>56%</div><div>28%</div><div>5%</div><div>10%</div></div></div>
1	H	513	<div><div>16%</div><div><div></div><div>61%</div><div>28%</div><div><div></div><div>•</div></div><div>7%</div></div></div>
1	I	513	<div><div>14%</div><div><div></div><div>56%</div><div>31%</div><div>6%</div><div>7%</div></div></div>
1	J	513	<div><div>12%</div><div><div></div><div>59%</div><div>30%</div><div><div></div><div>•</div></div><div>6%</div></div></div>
1	K	513	<div><div>10%</div><div><div></div><div>58%</div><div>32%</div><div>6%</div><div><div></div><div>•</div></div></div></div>
1	L	513	<div><div>23%</div><div><div></div><div>56%</div><div>31%</div><div>5%</div><div>8%</div></div></div>

2 Entry composition [i](#)

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			

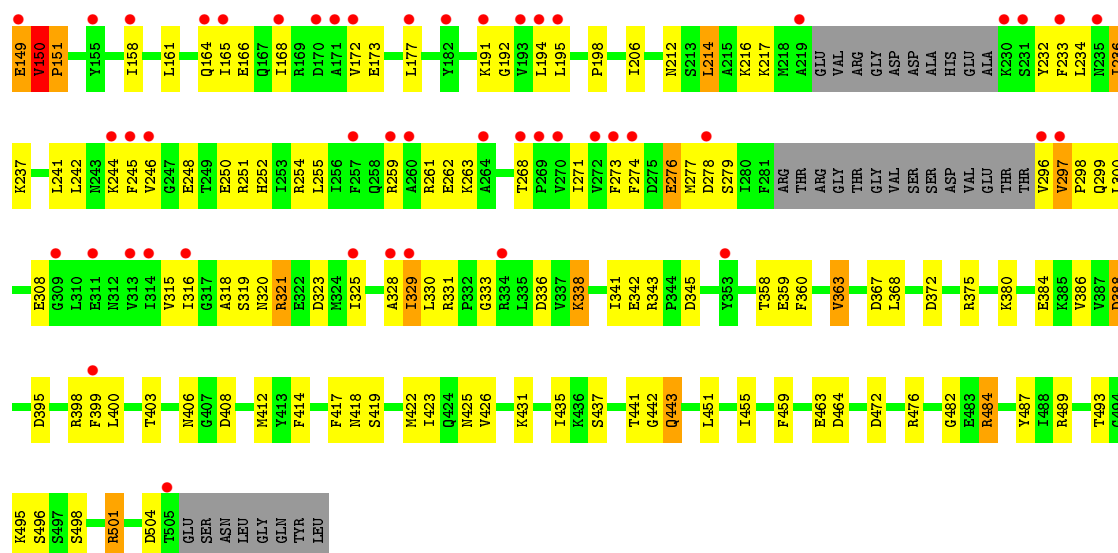
There are 12 discrepancies between the modelled and reference sequences:

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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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

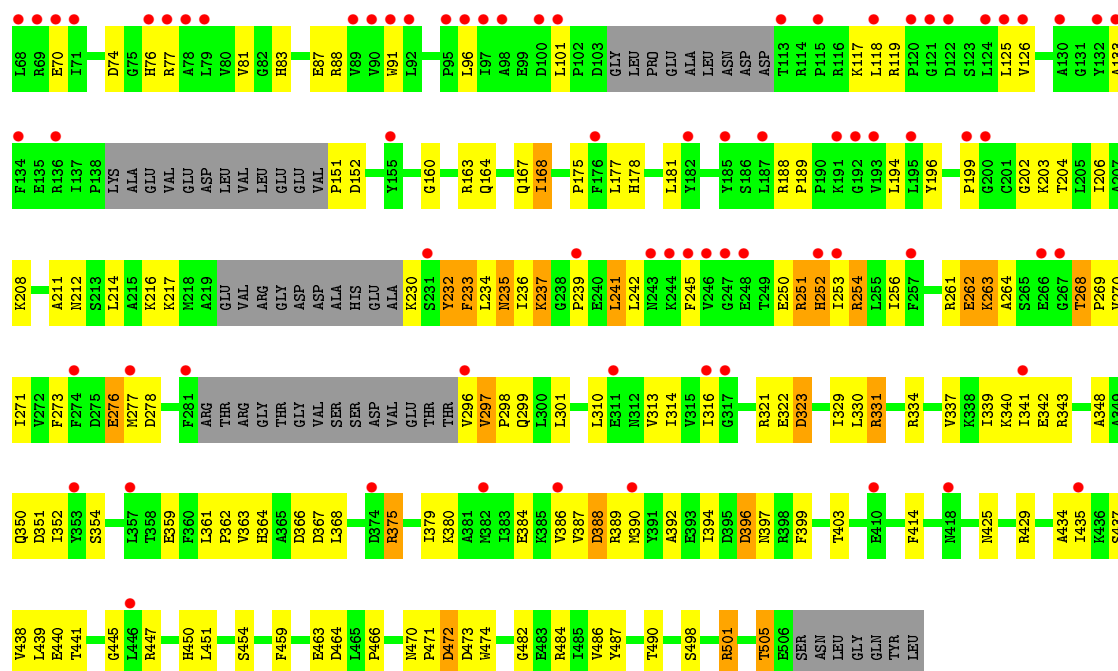


• Molecule 1: Proteasome-associated ATPase

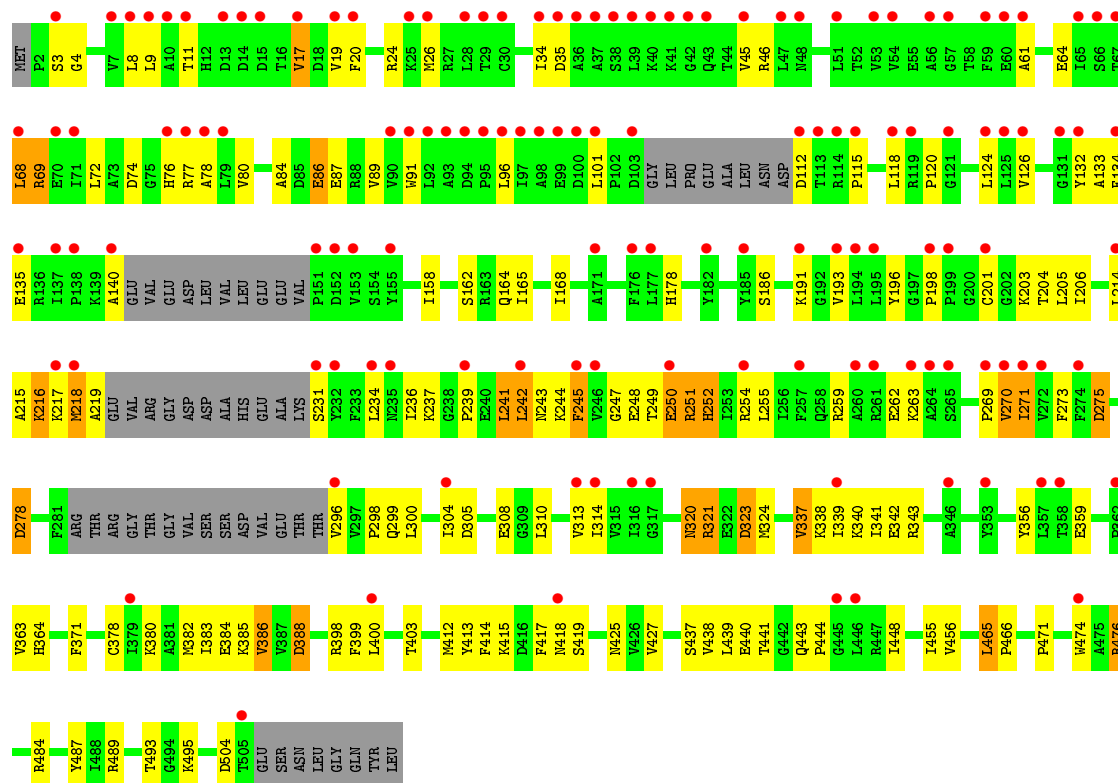


• Molecule 1: Proteasome-associated ATPase



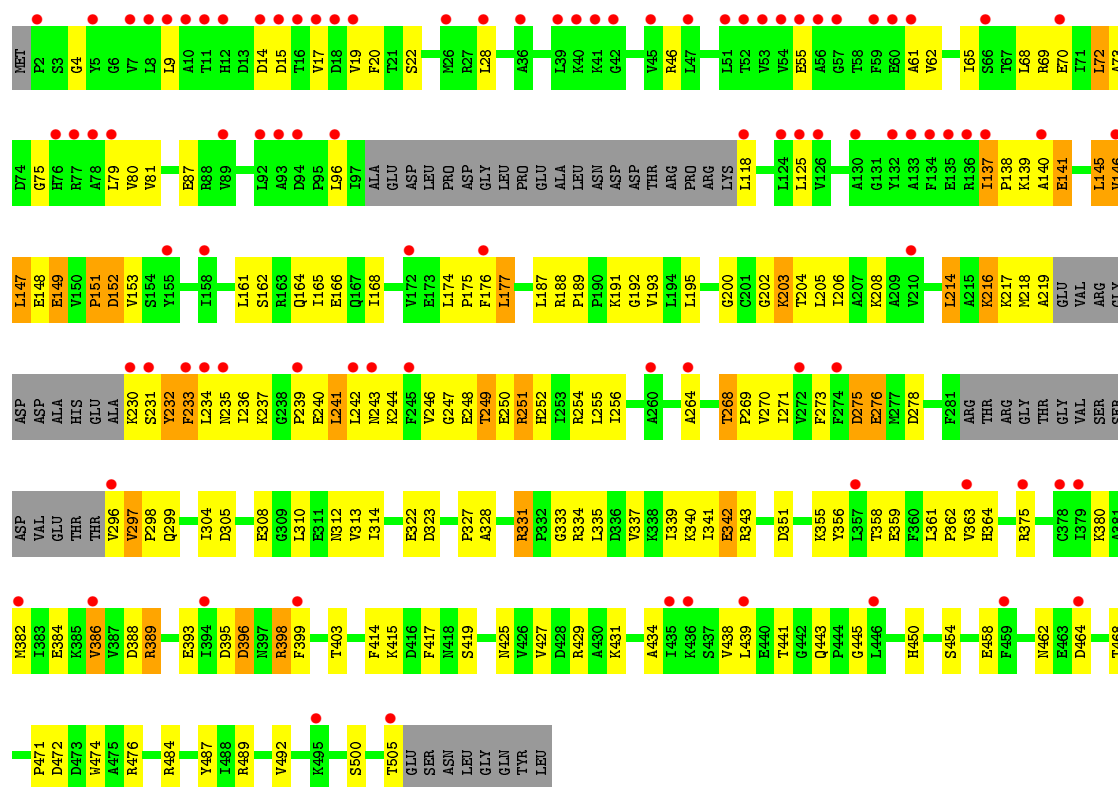


• Molecule 1: Proteasome-associated ATPase

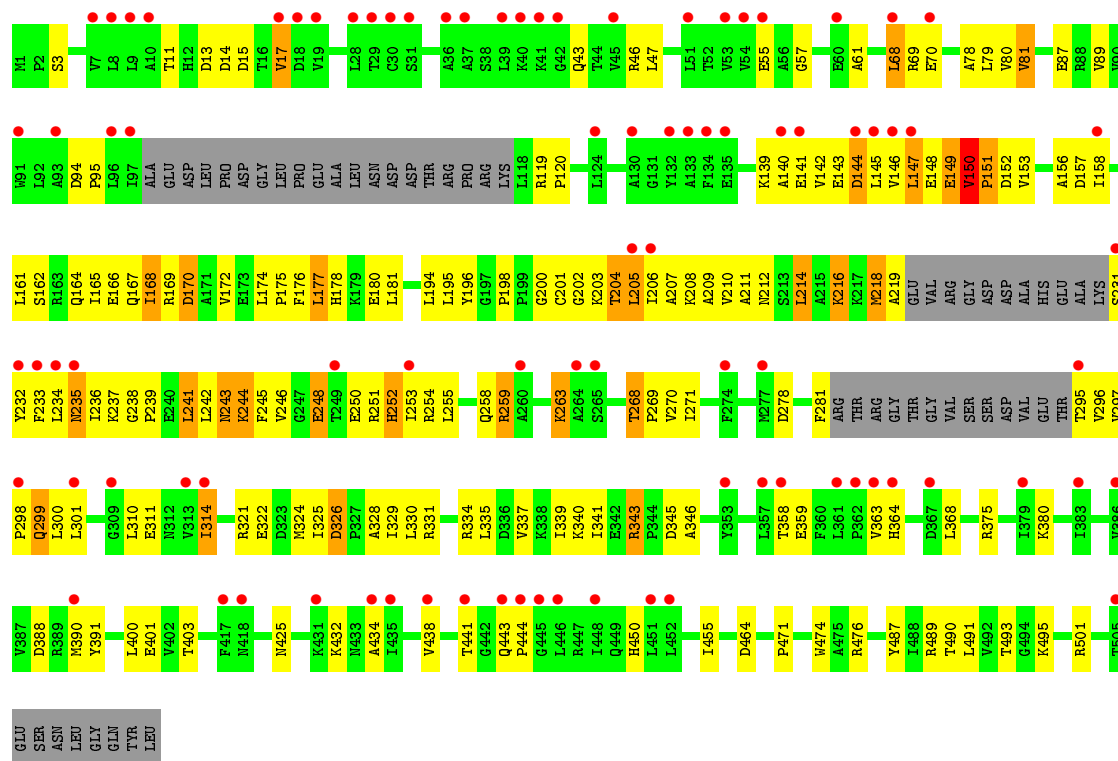


• Molecule 1: Proteasome-associated ATPase





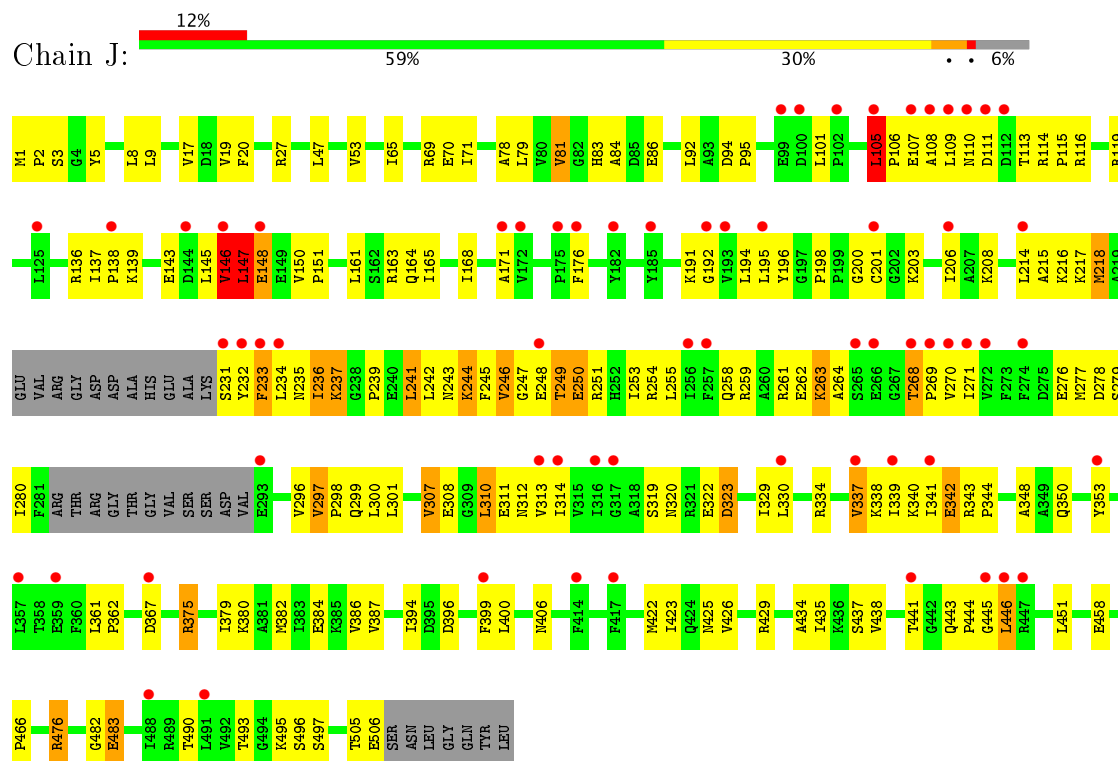
• Molecule 1: Proteasome-associated ATPase



• 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 (2.26%)	DCC
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 , 92.9	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:68:LEU:CD1	1:H:78:ALA:HB1	1.72	1.18
1:H:298:PRO:CD	1:I:242:LEU:HD22	1.72	1.18
1:H:299:GLN:OE1	1:H:300:LEU:HD12	1.41	1.17
1:K:109:LEU:HD12	1:K:148:GLU:OE2	1.40	1.16
1:L:233:PHE:CE2	1:L:234:LEU:O	1.98	1.16
1:K:249:THR:HA	1:K:250:GLU:CB	1.62	1.16
1:A:150:VAL:HG12	1:A:232:TYR:CB	1.74	1.16
1: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:69:ARG:O	1:H:120:PRO:HG3	1.79	0.81
1:H:300:LEU:HD12	1:H:300:LEU:H	1.44	0.81
1:C:237:LYS:HB2	1:C:239:PRO:HD2	1.63	0.81
1:H:293:GLU:HG3	1:H:294:THR:OG1	1.80	0.81
1:G:400:LEU:CD2	1:G:490:THR:HG22	2.10	0.81
1:H:299:GLN:OE1	1:H:300:LEU:CD1	2.28	0.81
1:K:177:LEU:HD21	1:K:217:LYS:CB	2.10	0.81
1:K:198:PRO:HG2	1:K:343:ARG:HG3	1.62	0.81

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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:298:PRO:HG3	1:I:242:LEU:HD13	1.79	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: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:E:231:SER:OG	1:E:269:PRO:O	2.14	0.65
1:A:188:ARG:HH12	1:G:219:ALA:HB2	1.62	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:399:PHE:CE2	1:I:417:PHE:CB	2.82	0.61
1:I:344:PRO:HD2	1:I:419:SER:HA	1.82	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: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:J:476:ARG:NH2	1:K:464:ASP:OD1	2.33	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:164:GLN:HG2	1:I:341:ILE:HD13	1.82	0.61
1:I:170:ASP:O	1:I:175:PRO:HD3	2.00	0.61
1:J:215:ALA:O	1:J:231:SER:N	2.34	0.61
1: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:238:GLY:HA3	1:L:276:GLU:HB2	1.83	0.60
1:L:262:GLU:HB3	1:L:263:LYS:HZ2	1.66	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:236:ILE:HA	1:J:237:LYS:HZ1	1.67	0.59
1:J:237:LYS:H	1:J:237:LYS:NZ	2.01	0.59
1:J:119:ARG:HD2	1:J:258:GLN:HE21	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:E:87:GLU:HG3	1:F:65:ILE:HB	1.85	0.56
1:F:46:ARG:NH1	1:F:55:GLU:OE2	2.38	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:68:LEU:O	1:G:120:PRO:HA	2.07	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: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:474:TRP:NE1	1:D:505:THR:OG1	2.41	0.54
1:D:482:GLY:HA2	1:E:489:ARG:HD3	1.89	0.54
1:I:164:GLN:O	1:I:168:ILE:HG13	2.08	0.54
1: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:68:LEU:HD22	1:E:124:LEU:HD11	1.90	0.54
1:E:254:ARG:HH22	1:E:299:GLN:HB3	1.73	0.54
1:E:437:SER:O	1:E:441:THR:HG22	2.08	0.54
1:I:249:THR:CA	1:I:250:GLU:HB3	2.19	0.54
1:I:403:THR:HB	1:I:487:TYR:HB3	1.89	0.54
1:J:145:LEU:O	1:J:146:VAL:HG12	2.07	0.54
1:L:253:ILE:O	1:L:256:ILE:HG12	2.08	0.54
1:C:68:LEU:O	1:C:120:PRO:HA	2.08	0.53
1:D:271:ILE:HA	1:D:314:ILE:O	2.08	0.53
1: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:D:88:ARG:HD3	1:E:64:GLU:HG2	1.90	0.53
1:E:320:ASN:N	1:E:320:ASN:HD22	2.05	0.53
1:F:278:ASP:OD1	1:F:278:ASP:N	2.35	0.53
1:H:89:VAL:HG23	1:I:65:ILE:HD11	1.91	0.53
1:K:212:ASN:O	1:K:216:LYS:HG3	2.08	0.53
1:B:146:VAL:O	1:B:146:VAL:HG13	2.08	0.53
1:H:429:ARG:HB3	1:H:454:SER:OG	2.09	0.53
1:K:105:LEU:N	1:K:106:PRO:HD3	2.21	0.53
1: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:F:96:LEU:HD22	1:F:118:LEU:HD11	1.90	0.53
1:E:89:VAL:HG23	1:F:65:ILE: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:245:PHE:CE1	1:F:254:ARG:HG3	2.43	0.52
1:A:399:PHE:N	1:A:412:MET:O	2.36	0.52
1:B:399:PHE:HE2	1:B:417:PHE:CG	2.27	0.52
1:D:464:ASP:HB2	1:D:498:SER:HB2	1.90	0.52
1:G:195:LEU:HD23	1:G:339:ILE:HB	1.91	0.52
1:H:322:GLU:HA	1:H:325:ILE:HG13	1.90	0.52
1:L:195:LEU:HD22	1:L:341:ILE:HD11	1.90	0.52
1:L:312:ASN:OD1	1:L:312:ASN:N	2.42	0.52
1:B:72:LEU:HD23	1:B:74:ASP:H	1.73	0.52
1:F:200:GLY:H	1:F:419:SER:HB2	1.73	0.52
1:H:69:ARG:O	1:H:120:PRO:CG	2.55	0.52
1:I:147:LEU:CG	1:I:148:GLU:HB3	2.39	0.52
1: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:158:ILE:CB	1:G:206:ILE:HG12	2.39	0.52
1:G:205:LEU:HD12	1:G:206:ILE:H	1.73	0.52
1:I:204:THR:CG2	1:I:275:ASP:OD2	2.58	0.52
1:J:255:LEU:O	1:J:259:ARG:HG3	2.09	0.52
1:D:118:LEU:O	1:D:119:ARG:HG3	2.10	0.52
1: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:8:LEU:HD13	1:A:17:VAL:HG13	1.92	0.52
1:A:399:PHE:CD2	1:A:417:PHE:HB2	2.44	0.52
1:D:151:PRO:O	1:D:212:ASN:ND2	2.43	0.52
1:D:152:ASP:OD1	1:D:152:ASP:N	2.33	0.52
1:G:68:LEU:CD1	1:G:80:VAL:HG12	2.39	0.52
1:J:322:GLU:OE2	1:K:501:ARG:NH1	2.39	0.52
1:J:422:MET:O	1:J:426:VAL:HG23	2.10	0.52
1:L: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: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:G:196:TYR:CZ	1:G:340:LYS:HB2	2.45	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:239:PRO:O	1:F:298:PRO:HB3	2.09	0.51
1:A:191:LYS:HE2	1:A:308:GLU:HG3	1.92	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:24:ARG:HH22	1:F:22:SER:HB2	1.76	0.51
1:E:254:ARG:HH12	1:E:299:GLN:HB3	1.74	0.51
1:I:406:ASN:ND2	1:I:408:ASP:OD2	2.41	0.51
1:K:177:LEU:HD21	1:K:217:LYS:HB3	1.92	0.51
1:L:236:ILE:HG23	1:L:273:PHE:O	2.11	0.51
1: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:392:ALA:HB1	1:H:394:ILE:HG23	1.93	0.51
1:H:386:VAL:HG11	1:H:451:LEU:HD13	1.92	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:B:359:GLU:HG3	1:G:156:ALA:HB2	1.93	0.49
1:D:160:GLY:N	1:D:351:ASP:OD2	2.30	0.49
1:E:132:TYR:O	1:E:134:PHE:CE2	2.66	0.49
1: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:69:ARG:O	1:E:120:PRO:HG3	2.13	0.48
1:E:262:GLU:HG3	1:E:263:LYS:NZ	2.28	0.48
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: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:A:242:LEU:HD23	1:F:296:VAL:HG21	1.95	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:E:321:ARG:HG2	1:E:324:MET:HG2	1.96	0.48
1:D:322:GLU:HG3	1:E:465:LEU:HD13	1.95	0.48
1:D:27:ARG:HD3	1:E:46:ARG:CD	2.44	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:L:171:ALA:HB1	1:L:337:VAL:HG21	1.96	0.48
1:G:239:PRO:O	1:L:298:PRO:HB3	2.14	0.48
1:B:69:ARG:O	1:B:120:PRO:HG3	2.14	0.48
1:G:298:PRO:HG3	1:H:241:LEU:O	2.14	0.48
1:G:434:ALA:HA	1:G:450:HIS:CE1	2.49	0.48
1:G:79:LEU:HD11	1:G:87:GLU:HB3	1.95	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:216:LYS:O	1:E:216:LYS:HD3	2.15	0.46
1:E:19:VAL:HG21	1:E:45:VAL:HG21	1.97	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:86:GLU:HA	1:I:83:HIS:HB3	1.96	0.46
1:H:89:VAL:HG12	1:I:62:VAL:HG12	1.98	0.46
1:I:261:ARG:HA	1:I:264:ALA:HB3	1.98	0.46
1:B:123:SER:HB2	1:B:137:ILE:O	2.16	0.46
1:B:149:GLU:O	1:B:150:VAL:CB	2.63	0.46
1:B:192:GLY:HA2	1:B:315:VAL:O	2.16	0.46
1:B:386:VAL:HG11	1:B:451:LEU:HD13	1.98	0.46
1:D:24:ARG:O	1:D:26:MET:HG3	2.15	0.46
1:F:192:GLY:HA3	1:F:335:LEU:HD12	1.98	0.46
1:F:268:THR:HA	1:F:269:PRO:HD3	1.78	0.46
1:G:363:VAL:HG12	1:G:375:ARG:NH1	2.31	0.46
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:178:HIS:CE1	1:L:439:LEU:HD13	2.51	0.46
1:K:168:ILE:HG12	1:K:339:ILE:HD13	1.97	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:9:LEU:HD21	1:D:20:PHE:HB2	1.98	0.46
1:D:342:GLU:O	1:D:343:ARG:C	2.54	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:L:346:ALA:O	1:L:350:GLN:HG3	2.16	0.46
1:K:182:TYR:CD1	1:L:435:ILE:HD13	2.51	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:81:VAL:HG22	1:B:87:GLU:HG2	1.99	0.45
1:B:27:ARG:HD3	1:C:46:ARG:HD2	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:H:322:GLU:HG2	1:I:501:ARG:HH22	1.82	0.45
1:I:429:ARG:NH2	1:I:458:GLU:OE1	2.43	0.45
1:K:375:ARG:HA	1:K:378:CYS:HB3	1.99	0.45
1:L:371:PHE:CD2	1:L:378:CYS:HA	2.51	0.45
1:A:202:GLY:H	1:A:341:ILE:HG21	1.81	0.45
1:C:68:LEU:HB2	1:C:124:LEU:CD1	2.46	0.45
1:E:300:LEU:O	1:E:304:ILE:HG13	2.17	0.45
1:G:147:LEU:O	1:G:234:LEU:HA	2.17	0.45
1:H: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:298:PRO:HG2	1:I:242:LEU:CB	2.46	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:J:139:LYS:NZ	1:J:143:GLU:HA	2.32	0.44
1:J:259:ARG:O	1:J:263:LYS:NZ	2.46	0.44
1:J:191:LYS:HG3	1:J:308:GLU:HG3	1.99	0.44
1:K:174:LEU:HB3	1:K:175:PRO:HD3	1.99	0.44
1: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:G:61:ALA:HB1	1:L:77:ARG:HD3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:251:ARG:HB3	1:L:252:HIS:H	1.68	0.44
1:L:254:ARG:HH11	1:L:303:GLU:HG2	1.82	0.44
1:L:233:PHE:CE1	1:L:271:ILE:HB	2.53	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:191:LYS:HE2	1:F:333:GLY:O	2.17	0.44
1:F:241:LEU:O	1:F:249:THR:OG1	2.21	0.44
1:G:151:PRO:HD3	1:G:233:PHE:CB	2.39	0.44
1:G:170:ASP:OD2	1:H:436:LYS:HD2	2.18	0.44
1:G:206:ILE:C	1:G:209:ALA:HB3	2.38	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:46:ARG:HD3	1:C:55:GLU:HG2	1.99	0.43
1:C:92:LEU:CD2	1:C:133:ALA:HB3	2.48	0.43
1:D:268:THR:HA	1:D:269:PRO:HD3	1.81	0.43
1:E:493:THR:HG23	1:E:495:LYS:H	1.84	0.43
1:K:141:GLU:CG	1:K:142:VAL:H	2.31	0.43
1: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:27:ARG:HD2	1:J:5:TYR:OH	2.18	0.43
1:I:29:THR:OG1	1:J:1:MET:HG2	2.18	0.43

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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:176:PHE:HE2	1:F:269:PRO:HB3	1.84	0.42
1:F:254:ARG:HH22	1:F:299:GLN:HB3	1.84	0.42
1:F:399:PHE:CE2	1:F:417:PHE:CD2	3.07	0.42
1:G: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:E:382:MET:HG2	1:E:448:ILE:HD13	2.01	0.42
1:D:88:ARG:NH1	1:E:64:GLU:HG3	2.35	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:194:LEU:HD23	1:B:338:LYS:HB3	2.02	0.42
1:B:232:TYR:OH	1:B:263:LYS:HB3	2.19	0.42
1:D: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:293:GLU:HG3	1:H:294:THR:HG1	1.82	0.42
1:H:191:LYS:HZ3	1:H:307:VAL:CG1	2.31	0.42
1:J:344:PRO:HB2	1:J:348:ALA:HB3	2.02	0.42
1:L:213:SER:OG	1:L:214:LEU:N	2.52	0.42
1:A: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:B:360:PHE:HE2	1:G:216:LYS:HE3	1.84	0.42
1:C:174:LEU:HB3	1:C:175:PRO:HD3	2.01	0.42
1:C:378:CYS:O	1:C:382:MET:HG3	2.20	0.42
1:F:195:LEU:HD22	1:F:341:ILE:HD11	2.01	0.42
1:F:434:ALA:HA	1:F:450:HIS:CE1	2.54	0.42
1:G:251:ARG:O	1:G:253:ILE:N	2.53	0.42
1:I:170:ASP: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:185:TYR:O	1:B:431:LYS:HD3	2.19	0.42
1:B:17:VAL:HG12	1:B:19:VAL:HG23	2.02	0.42
1:C:296:VAL:HG12	1:C:297:VAL:H	1.84	0.42
1:D:399:PHE:HB2	1:D:414:PHE:CE2	2.55	0.42
1:A:431:LYS:HB2	1:F:187:LEU:HD13	2.01	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:371:PHE:CD2	1:E:378:CYS:HA	2.56	0.41
1:E:356:TYR:HB3	1:E:427:VAL:HG21	2.01	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:244:LYS:HZ1	1:L:299:GLN:CA	2.33	0.41
1:G:198:PRO:HB3	1:G:343:ARG:CZ	2.49	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: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:A:139:LYS:HE2	1:F:87:GLU:OE2	2.21	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%)	17	59
1	B	467/513 (91%)	441 (94%)	23 (5%)	3 (1%)	28	70
1	C	462/513 (90%)	429 (93%)	30 (6%)	3 (1%)	28	70
1	D	450/513 (88%)	433 (96%)	17 (4%)	0	100	100
1	E	451/513 (88%)	431 (96%)	19 (4%)	1 (0%)	51	85
1	F	452/513 (88%)	424 (94%)	24 (5%)	4 (1%)	20	63
1	G	453/513 (88%)	428 (94%)	21 (5%)	4 (1%)	20	63
1	H	470/513 (92%)	442 (94%)	24 (5%)	4 (1%)	20	63
1	I	470/513 (92%)	446 (95%)	23 (5%)	1 (0%)	51	85
1	J	478/513 (93%)	442 (92%)	33 (7%)	3 (1%)	28	70
1	K	494/513 (96%)	457 (92%)	29 (6%)	8 (2%)	11	50
1	L	465/513 (91%)	434 (93%)	27 (6%)	4 (1%)	20	63
All	All	5586/6156 (91%)	5247 (94%)	299 (5%)	40 (1%)	25	68

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%)	13	46
1	B	402/433 (93%)	362 (90%)	40 (10%)	9	37
1	C	389/433 (90%)	351 (90%)	38 (10%)	9	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	389/433 (90%)	346 (89%)	43 (11%)	7	32
1	E	389/433 (90%)	351 (90%)	38 (10%)	9	38
1	F	389/433 (90%)	345 (89%)	44 (11%)	7	31
1	G	390/433 (90%)	347 (89%)	43 (11%)	7	33
1	H	405/433 (94%)	362 (89%)	43 (11%)	8	35
1	I	405/433 (94%)	362 (89%)	43 (11%)	8	35
1	J	410/433 (95%)	376 (92%)	34 (8%)	13	46
1	K	421/433 (97%)	371 (88%)	50 (12%)	6	28
1	L	401/433 (93%)	356 (89%)	45 (11%)	7	32
All	All	4795/5196 (92%)	4300 (90%)	495 (10%)	8	36

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	108 (22%)  	56, 117, 190, 215	0
1	B	475/513 (92%)	1.19	102 (21%)  	57, 133, 189, 213	0
1	C	472/513 (92%)	1.13	100 (21%)  	55, 134, 193, 231	0
1	D	460/513 (89%)	1.33	114 (24%)  	66, 127, 215, 230	0
1	E	461/513 (89%)	1.61	137 (29%)  	71, 149, 212, 231	0
1	F	460/513 (89%)	1.14	93 (20%)  	66, 136, 191, 226	0
1	G	461/513 (89%)	1.11	89 (19%)  	69, 128, 195, 223	0
1	H	478/513 (93%)	1.10	80 (16%)  	61, 107, 191, 209	0
1	I	478/513 (93%)	0.93	70 (14%)  	62, 107, 176, 217	0
1	J	484/513 (94%)	0.89	64 (13%)  	70, 120, 191, 215	0
1	K	498/513 (97%)	0.78	52 (10%)  	67, 114, 164, 191	0
1	L	473/513 (92%)	1.36	119 (25%)  	64, 146, 205, 219	0
All	All	5680/6156 (92%)	1.14	1128 (19%)  	55, 125, 200, 231	0

All (1128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	231	SER	11.3
1	D	78	ALA	11.2
1	C	231	SER	10.9
1	L	146	VAL	10.5
1	L	232	TYR	10.1
1	E	78	ALA	10.0
1	I	103	ASP	9.4
1	L	247	GLY	9.0
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	8.6
1	L	269	PRO	8.3
1	L	314	ILE	8.1
1	J	270	VAL	8.1
1	E	36	ALA	8.0
1	L	316	ILE	7.9
1	E	35	ASP	7.8
1	D	97	ILE	7.7
1	L	272	VAL	7.7
1	E	59	PHE	7.5
1	D	96	LEU	7.5
1	H	118	LEU	7.4
1	E	264	ALA	7.3
1	D	77	ARG	7.3
1	C	243	ASN	7.2
1	G	446	LEU	7.2
1	D	92	LEU	7.0
1	A	223	GLY	6.9
1	A	39	LEU	6.8
1	E	265	SER	6.8
1	I	104	GLY	6.7
1	J	109	LEU	6.7
1	E	39	LEU	6.7
1	E	152	ASP	6.7
1	F	42	GLY	6.7
1	L	315	VAL	6.7
1	J	232	TYR	6.6
1	A	36	ALA	6.6
1	F	243	ASN	6.5
1	B	244	LYS	6.4
1	E	30	CYS	6.4
1	G	8	LEU	6.4
1	E	269	PRO	6.3
1	J	313	VAL	6.3
1	B	246	VAL	6.2
1	L	233	PHE	6.0
1	D	56	ALA	6.0
1	D	244	LYS	6.0
1	G	36	ALA	6.0
1	A	224	ASP	6.0
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	L	257	PHE	5.8
1	L	313	VAL	5.8
1	B	139	LYS	5.7
1	E	11	THR	5.7
1	F	61	ALA	5.7
1	E	153	VAL	5.7
1	F	135	GLU	5.6
1	A	47	LEU	5.6
1	F	11	THR	5.6
1	E	53	VAL	5.6
1	H	141	GLU	5.5
1	G	39	LEU	5.5
1	E	446	LEU	5.5
1	I	219	ALA	5.5
1	C	11	THR	5.5
1	D	26	MET	5.5
1	E	239	PRO	5.5
1	D	45	VAL	5.5
1	E	271	ILE	5.5
1	E	40	LYS	5.4
1	H	233	PHE	5.4
1	E	13	ASP	5.4
1	A	96	LEU	5.4
1	B	118	LEU	5.4
1	D	248	GLU	5.4
1	J	233	PHE	5.4
1	B	171	ALA	5.4
1	D	40	LYS	5.4
1	H	132	TYR	5.3
1	H	102	PRO	5.3
1	E	28	LEU	5.3
1	B	314	ILE	5.3
1	D	41	LYS	5.3
1	D	17	VAL	5.2
1	E	56	ALA	5.2
1	D	28	LEU	5.2
1	E	68	LEU	5.2
1	L	234	LEU	5.2
1	G	42	GLY	5.2
1	L	151	PRO	5.2
1	C	39	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	9	LEU	5.2
1	B	47	LEU	5.2
1	G	60	GLU	5.1
1	H	39	LEU	5.1
1	D	76	HIS	5.1
1	F	134	PHE	5.1
1	E	61	ALA	5.1
1	H	133	ALA	5.1
1	K	201	CYS	5.1
1	I	142	VAL	5.1
1	C	76	HIS	5.1
1	G	253	ILE	5.0
1	H	105	LEU	5.0
1	F	28	LEU	5.0
1	E	10	ALA	5.0
1	A	56	ALA	5.0
1	A	118	LEU	5.0
1	I	144	ASP	5.0
1	I	146	VAL	5.0
1	D	101	LEU	5.0
1	L	274	PHE	5.0
1	A	151	PRO	5.0
1	C	79	LEU	4.9
1	E	42	GLY	4.9
1	F	56	ALA	4.9
1	F	375	ARG	4.9
1	A	92	LEU	4.9
1	L	176	PHE	4.9
1	F	231	SER	4.9
1	D	71	ILE	4.9
1	G	265	SER	4.9
1	E	232	TYR	4.8
1	H	16	THR	4.8
1	F	439	LEU	4.8
1	H	53	VAL	4.8
1	E	97	ILE	4.8
1	K	182	TYR	4.8
1	B	260	ALA	4.8
1	D	118	LEU	4.8
1	D	100	ASP	4.8
1	C	446	LEU	4.8
1	A	51	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	103	ASP	4.8
1	J	314	ILE	4.7
1	F	55	GLU	4.7
1	G	264	ALA	4.7
1	B	117	LYS	4.7
1	L	145	LEU	4.7
1	A	132	TYR	4.7
1	L	446	LEU	4.7
1	E	54	VAL	4.7
1	E	260	ALA	4.7
1	H	113	THR	4.7
1	H	134	PHE	4.7
1	B	60	GLU	4.7
1	E	313	VAL	4.7
1	G	134	PHE	4.7
1	D	91	TRP	4.7
1	E	38	SER	4.7
1	G	53	VAL	4.7
1	E	51	LEU	4.7
1	J	172	VAL	4.7
1	E	92	LEU	4.7
1	A	246	VAL	4.7
1	L	148	GLU	4.6
1	E	60	GLU	4.6
1	E	3	SER	4.6
1	F	378	CYS	4.6
1	B	45	VAL	4.6
1	G	441	THR	4.6
1	H	269	PRO	4.6
1	L	231	SER	4.6
1	J	176	PHE	4.6
1	G	41	LYS	4.6
1	D	24	ARG	4.5
1	B	56	ALA	4.5
1	G	295	THR	4.5
1	F	17	VAL	4.5
1	K	445	GLY	4.5
1	C	445	GLY	4.5
1	A	78	ALA	4.5
1	I	314	ILE	4.5
1	E	70	GLU	4.5
1	D	245	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	8	LEU	4.5
1	C	359	GLU	4.5
1	G	367	ASP	4.5
1	L	193	VAL	4.4
1	E	185	TYR	4.4
1	E	15	ASP	4.4
1	L	271	ILE	4.4
1	B	219	ALA	4.4
1	E	100	ASP	4.4
1	E	112	ASP	4.4
1	B	191	LYS	4.4
1	B	257	PHE	4.4
1	J	293	GLU	4.4
1	E	25	LYS	4.4
1	J	357	LEU	4.4
1	A	93	ALA	4.4
1	B	36	ALA	4.4
1	H	265	SER	4.3
1	K	446	LEU	4.3
1	L	204	THR	4.3
1	J	271	ILE	4.3
1	B	5	TYR	4.3
1	A	6	GLY	4.3
1	A	137	ILE	4.3
1	G	205	LEU	4.3
1	A	244	LYS	4.3
1	F	79	LEU	4.3
1	A	41	LYS	4.3
1	E	79	LEU	4.3
1	G	206	ILE	4.3
1	E	90	VAL	4.3
1	L	172	VAL	4.3
1	G	357	LEU	4.3
1	K	187	LEU	4.3
1	B	313	VAL	4.3
1	D	53	VAL	4.3
1	D	239	PRO	4.3
1	B	35	ASP	4.3
1	J	269	PRO	4.2
1	C	252	HIS	4.2
1	B	230	LYS	4.2
1	H	270	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	L	270	VAL	4.2
1	A	76	HIS	4.2
1	D	418	ASN	4.2
1	C	40	LYS	4.2
1	D	98	ALA	4.2
1	A	94	ASP	4.2
1	E	115	PRO	4.2
1	A	53	VAL	4.2
1	L	235	ASN	4.2
1	E	314	ILE	4.2
1	B	273	PHE	4.2
1	E	67	THR	4.2
1	A	117	LYS	4.1
1	E	29	THR	4.1
1	A	61	ALA	4.1
1	H	70	GLU	4.1
1	E	14	ASP	4.1
1	C	246	VAL	4.1
1	F	7	VAL	4.1
1	B	268	THR	4.1
1	A	38	SER	4.1
1	I	115	PRO	4.1
1	E	76	HIS	4.1
1	F	26	MET	4.1
1	I	318	ALA	4.1
1	F	137	ILE	4.1
1	G	68	LEU	4.1
1	G	9	LEU	4.1
1	D	43	GLN	4.1
1	E	135	GLU	4.1
1	L	359	GLU	4.1
1	H	314	ILE	4.1
1	C	124	LEU	4.1
1	F	52	THR	4.0
1	L	273	PHE	4.0
1	A	239	PRO	4.0
1	E	137	ILE	4.0
1	F	118	LEU	4.0
1	C	75	GLY	4.0
1	I	313	VAL	4.0
1	B	70	GLU	4.0
1	H	293	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	260	ALA	4.0
1	A	139	LYS	4.0
1	D	113	THR	4.0
1	A	11	THR	4.0
1	C	98	ALA	4.0
1	F	10	ALA	4.0
1	F	59	PHE	4.0
1	K	353	TYR	4.0
1	D	231	SER	4.0
1	F	446	LEU	4.0
1	E	245	PHE	4.0
1	D	55	GLU	4.0
1	H	54	VAL	4.0
1	E	357	LEU	4.0
1	D	39	LEU	4.0
1	E	218	MET	4.0
1	B	98	ALA	4.0
1	D	317	GLY	3.9
1	L	158	ILE	3.9
1	F	60	GLU	3.9
1	C	306	GLY	3.9
1	B	78	ALA	3.9
1	G	445	GLY	3.9
1	C	444	PRO	3.9
1	E	113	THR	3.9
1	L	173	GLU	3.9
1	D	70	GLU	3.9
1	L	304	ILE	3.9
1	D	20	PHE	3.9
1	G	30	CYS	3.9
1	B	297	VAL	3.8
1	F	39	LEU	3.8
1	H	72	LEU	3.8
1	I	134	PHE	3.8
1	E	77	ARG	3.8
1	L	367	ASP	3.8
1	H	135	GLU	3.8
1	D	132	TYR	3.8
1	F	495	LYS	3.8
1	L	45	VAL	3.8
1	K	185	TYR	3.8
1	B	39	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	J	102	PRO	3.8
1	D	89	VAL	3.8
1	G	232	TYR	3.8
1	D	191	LYS	3.8
1	A	45	VAL	3.8
1	L	182	TYR	3.8
1	E	217	LYS	3.8
1	I	105	LEU	3.8
1	H	60	GLU	3.8
1	F	51	LEU	3.8
1	F	245	PHE	3.8
1	G	145	LEU	3.7
1	H	151	PRO	3.7
1	F	53	VAL	3.7
1	L	358	THR	3.7
1	A	35	ASP	3.7
1	F	296	VAL	3.7
1	H	68	LEU	3.7
1	B	245	PHE	3.7
1	L	147	LEU	3.7
1	C	382	MET	3.7
1	E	94	ASP	3.7
1	E	124	LEU	3.7
1	L	361	LEU	3.7
1	D	126	VAL	3.7
1	H	30	CYS	3.7
1	D	10	ALA	3.7
1	F	233	PHE	3.7
1	A	91	TRP	3.6
1	G	28	LEU	3.6
1	C	441	THR	3.6
1	D	311	GLU	3.6
1	E	250	GLU	3.6
1	D	124	LEU	3.6
1	L	357	LEU	3.6
1	L	144	ASP	3.6
1	E	191	LYS	3.6
1	K	264	ALA	3.6
1	E	47	LEU	3.6
1	D	37	ALA	3.6
1	D	130	ALA	3.6
1	E	231	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	439	LEU	3.6
1	F	92	LEU	3.6
1	G	235	ASN	3.6
1	B	329	ILE	3.6
1	E	17	VAL	3.6
1	A	221	VAL	3.6
1	F	78	ALA	3.6
1	H	124	LEU	3.6
1	D	247	GLY	3.6
1	D	357	LEU	3.6
1	E	418	ASN	3.5
1	D	446	LEU	3.5
1	F	260	ALA	3.5
1	G	313	VAL	3.5
1	C	9	LEU	3.5
1	H	144	ASP	3.5
1	B	274	PHE	3.5
1	C	298	PRO	3.5
1	A	201	CYS	3.5
1	E	7	VAL	3.5
1	A	113	THR	3.5
1	I	257	PHE	3.5
1	F	140	ALA	3.5
1	K	267	GLY	3.5
1	C	235	ASN	3.4
1	A	54	VAL	3.4
1	D	42	GLY	3.4
1	F	76	HIS	3.4
1	I	78	ALA	3.4
1	J	182	TYR	3.4
1	C	97	ILE	3.4
1	G	363	VAL	3.4
1	G	443	GLN	3.4
1	K	357	LEU	3.4
1	H	103	ASP	3.4
1	A	505	THR	3.4
1	E	37	ALA	3.4
1	B	4	GLY	3.4
1	A	9	LEU	3.4
1	L	310	LEU	3.4
1	D	6	GLY	3.4
1	E	57	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	239	PRO	3.4
1	L	317	GLY	3.4
1	C	296	VAL	3.4
1	A	5	TYR	3.4
1	E	155	TYR	3.4
1	B	233	PHE	3.4
1	A	136	ARG	3.4
1	F	132	TYR	3.4
1	I	296	VAL	3.4
1	J	195	LEU	3.4
1	B	34	ILE	3.4
1	F	41	LYS	3.4
1	F	125	LEU	3.4
1	B	325	ILE	3.4
1	L	379	ILE	3.4
1	L	268	THR	3.4
1	D	382	MET	3.4
1	F	242	LEU	3.3
1	J	193	VAL	3.3
1	J	446	LEU	3.3
1	L	181	LEU	3.3
1	B	155	TYR	3.3
1	I	297	VAL	3.3
1	L	390	MET	3.3
1	H	115	PRO	3.3
1	D	18	ASP	3.3
1	D	5	TYR	3.3
1	G	233	PHE	3.3
1	C	443	GLN	3.3
1	E	41	LYS	3.3
1	I	153	VAL	3.3
1	I	272	VAL	3.3
1	G	361	LEU	3.3
1	E	132	TYR	3.3
1	A	79	LEU	3.3
1	D	16	THR	3.3
1	I	118	LEU	3.3
1	A	296	VAL	3.3
1	E	8	LEU	3.3
1	C	117	LYS	3.3
1	I	143	GLU	3.3
1	E	182	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	134	PHE	3.3
1	H	34	ILE	3.3
1	A	233	PHE	3.3
1	B	296	VAL	3.3
1	C	17	VAL	3.3
1	C	436	LYS	3.3
1	H	505	THR	3.3
1	H	56	ALA	3.3
1	C	357	LEU	3.3
1	C	244	LYS	3.3
1	L	309	GLY	3.2
1	C	360	PHE	3.2
1	C	135	GLU	3.2
1	E	151	PRO	3.2
1	E	445	GLY	3.2
1	F	230	LYS	3.2
1	A	37	ALA	3.2
1	C	123	SER	3.2
1	D	68	LEU	3.2
1	D	30	CYS	3.2
1	H	315	VAL	3.2
1	J	441	THR	3.2
1	G	448	ILE	3.2
1	E	214	LEU	3.2
1	A	90	VAL	3.2
1	J	111	ASP	3.2
1	E	242	LEU	3.2
1	E	48	ASN	3.2
1	G	40	LYS	3.2
1	I	191	LYS	3.2
1	F	94	ASP	3.2
1	H	100	ASP	3.2
1	A	17	VAL	3.2
1	H	101	LEU	3.2
1	A	399	PHE	3.2
1	E	270	VAL	3.2
1	L	264	ALA	3.2
1	L	450	HIS	3.2
1	A	34	ILE	3.2
1	F	40	LYS	3.2
1	L	168	ILE	3.2
1	D	31	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	122	ASP	3.2
1	E	272	VAL	3.2
1	K	177	LEU	3.2
1	D	243	ASN	3.2
1	A	7	VAL	3.2
1	G	19	VAL	3.2
1	B	100	ASP	3.2
1	G	353	TYR	3.2
1	I	248	GLU	3.2
1	A	309	GLY	3.1
1	C	118	LEU	3.1
1	H	91	TRP	3.1
1	L	360	PHE	3.1
1	L	207	ALA	3.1
1	A	40	LYS	3.1
1	B	8	LEU	3.1
1	L	196	TYR	3.1
1	E	34	ILE	3.1
1	C	449	GLN	3.1
1	A	95	PRO	3.1
1	B	79	LEU	3.1
1	E	121	GLY	3.1
1	D	115	PRO	3.1
1	G	274	PHE	3.1
1	J	337	VAL	3.1
1	L	505	THR	3.1
1	H	191	LYS	3.1
1	B	48	ASN	3.1
1	E	125	LEU	3.1
1	C	300	LEU	3.1
1	E	119	ARG	3.1
1	H	131	GLY	3.1
1	D	38	SER	3.1
1	J	112	ASP	3.1
1	D	200	GLY	3.1
1	D	267	GLY	3.1
1	H	92	LEU	3.1
1	I	101	LEU	3.1
1	B	269	PRO	3.0
1	F	379	ILE	3.0
1	I	315	VAL	3.0
1	K	248	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	375	ARG	3.0
1	B	57	GLY	3.0
1	D	90	VAL	3.0
1	E	505	THR	3.0
1	E	199	PRO	3.0
1	H	239	PRO	3.0
1	B	235	ASN	3.0
1	C	367	ASP	3.0
1	D	66	SER	3.0
1	D	23	GLY	3.0
1	L	111	ASP	3.0
1	G	140	ALA	3.0
1	J	445	GLY	3.0
1	E	198	PRO	3.0
1	G	31	SER	3.0
1	K	382	MET	3.0
1	F	133	ALA	3.0
1	E	379	ILE	3.0
1	I	195	LEU	3.0
1	L	447	ARG	3.0
1	K	359	GLU	3.0
1	B	182	TYR	3.0
1	C	47	LEU	3.0
1	G	18	ASP	3.0
1	H	271	ILE	3.0
1	D	19	VAL	3.0
1	G	124	LEU	3.0
1	H	114	ARG	3.0
1	D	95	PRO	3.0
1	B	309	GLY	3.0
1	G	135	GLU	3.0
1	D	69	ARG	3.0
1	G	158	ILE	3.0
1	K	367	ASP	3.0
1	L	356	TYR	3.0
1	K	309	GLY	2.9
1	L	159	GLY	2.9
1	I	246	VAL	2.9
1	D	390	MET	2.9
1	D	61	ALA	2.9
1	D	62	VAL	2.9
1	E	171	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	316	ILE	2.9
1	D	27	ARG	2.9
1	J	266	GLU	2.9
1	E	263	LYS	2.9
1	F	12	HIS	2.9
1	H	127	ASP	2.9
1	J	144	ASP	2.9
1	L	382	MET	2.9
1	F	210	VAL	2.9
1	J	206	ILE	2.9
1	C	237	LYS	2.9
1	D	386	VAL	2.9
1	B	334	ARG	2.9
1	F	274	PHE	2.9
1	I	353	TYR	2.9
1	G	234	LEU	2.9
1	H	97	ILE	2.9
1	G	132	TYR	2.9
1	B	165	ILE	2.9
1	J	256	ILE	2.9
1	E	235	ASN	2.9
1	H	104	GLY	2.9
1	E	234	LEU	2.9
1	F	124	LEU	2.9
1	G	451	LEU	2.9
1	K	379	ILE	2.9
1	L	206	ILE	2.9
1	A	226	ALA	2.9
1	H	149	GLU	2.9
1	A	77	ARG	2.9
1	B	124	LEU	2.9
1	J	268	THR	2.9
1	L	118	LEU	2.9
1	C	459	PHE	2.9
1	C	309	GLY	2.9
1	G	383	ILE	2.9
1	L	256	ILE	2.9
1	A	10	ALA	2.9
1	A	446	LEU	2.9
1	H	272	VAL	2.8
1	K	168	ILE	2.8
1	L	386	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	281	PHE	2.8
1	L	143	GLU	2.8
1	L	149	GLU	2.8
1	J	105	LEU	2.8
1	I	168	ILE	2.8
1	E	43	GLN	2.8
1	H	61	ALA	2.8
1	B	193	VAL	2.8
1	D	193	VAL	2.8
1	E	26	MET	2.8
1	B	143	GLU	2.8
1	A	44	THR	2.8
1	E	358	THR	2.8
1	L	41	LYS	2.8
1	F	47	LEU	2.8
1	J	234	LEU	2.8
1	E	177	LEU	2.8
1	G	51	LEU	2.8
1	J	265	SER	2.8
1	F	45	VAL	2.8
1	H	71	ILE	2.8
1	F	15	ASP	2.8
1	H	274	PHE	2.8
1	A	50	ALA	2.8
1	D	46	ARG	2.8
1	L	170	ASP	2.8
1	C	353	TYR	2.8
1	E	93	ALA	2.8
1	C	34	ILE	2.8
1	D	253	ILE	2.8
1	E	71	ILE	2.8
1	H	80	VAL	2.8
1	G	418	ASN	2.8
1	B	311	GLU	2.8
1	C	440	GLU	2.8
1	C	12	HIS	2.8
1	A	18	ASP	2.8
1	H	37	ALA	2.8
1	E	19	VAL	2.8
1	H	17	VAL	2.8
1	B	316	ILE	2.8
1	C	223	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	146	VAL	2.8
1	G	97	ILE	2.8
1	K	314	ILE	2.8
1	K	329	ILE	2.8
1	D	11	THR	2.8
1	D	246	VAL	2.8
1	I	113	THR	2.8
1	D	316	ILE	2.7
1	G	141	GLU	2.7
1	L	213	SER	2.7
1	C	45	VAL	2.7
1	J	272	VAL	2.7
1	B	505	THR	2.7
1	E	91	TRP	2.7
1	C	101	LEU	2.7
1	I	244	LYS	2.7
1	G	54	VAL	2.7
1	E	362	PRO	2.7
1	G	298	PRO	2.7
1	K	158	ILE	2.7
1	G	91	TRP	2.7
1	A	264	ALA	2.7
1	D	176	PHE	2.7
1	G	7	VAL	2.7
1	G	438	VAL	2.7
1	I	100	ASP	2.7
1	E	20	PHE	2.7
1	L	296	VAL	2.7
1	L	208	LYS	2.7
1	F	357	LEU	2.7
1	I	96	LEU	2.7
1	F	89	VAL	2.7
1	I	270	VAL	2.7
1	E	346	ALA	2.7
1	F	130	ALA	2.7
1	I	271	ILE	2.7
1	L	451	LEU	2.7
1	J	110	ASN	2.7
1	D	47	LEU	2.7
1	I	124	LEU	2.7
1	F	93	ALA	2.7
1	C	442	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	140	ALA	2.7
1	J	367	ASP	2.7
1	F	234	LEU	2.7
1	A	243	ASN	2.7
1	L	187	LEU	2.7
1	L	432	LYS	2.7
1	D	435	ILE	2.7
1	B	278	ASP	2.6
1	H	268	THR	2.6
1	J	108	ALA	2.6
1	C	245	PHE	2.6
1	B	26	MET	2.6
1	C	318	ALA	2.6
1	G	364	HIS	2.6
1	G	390	MET	2.6
1	L	17	VAL	2.6
1	L	431	LYS	2.6
1	I	403	THR	2.6
1	A	98	ALA	2.6
1	E	201	CYS	2.6
1	K	444	PRO	2.6
1	L	76	HIS	2.6
1	L	154	SER	2.6
1	F	126	VAL	2.6
1	K	173	GLU	2.6
1	D	79	LEU	2.6
1	C	115	PRO	2.6
1	L	185	TYR	2.6
1	F	176	PHE	2.6
1	D	136	ARG	2.6
1	L	254	ARG	2.6
1	H	33	ASN	2.6
1	L	335	LEU	2.6
1	A	229	ALA	2.6
1	H	182	TYR	2.6
1	J	99	GLU	2.6
1	D	195	LEU	2.6
1	A	227	HIS	2.6
1	B	49	GLU	2.6
1	C	72	LEU	2.6
1	K	378	CYS	2.6
1	B	77	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	98	ALA	2.6
1	B	11	THR	2.6
1	L	178	HIS	2.6
1	H	9	LEU	2.6
1	I	284	ARG	2.6
1	E	274	PHE	2.6
1	E	353	TYR	2.6
1	J	399	PHE	2.6
1	C	125	LEU	2.6
1	B	40	LYS	2.6
1	B	103	ASP	2.6
1	J	107	GLU	2.6
1	G	249	THR	2.6
1	F	54	VAL	2.6
1	A	2	PRO	2.6
1	C	239	PRO	2.6
1	G	444	PRO	2.6
1	L	312	ASN	2.6
1	B	89	VAL	2.5
1	L	363	VAL	2.5
1	K	330	LEU	2.5
1	L	412	MET	2.5
1	I	274	PHE	2.5
1	F	399	PHE	2.5
1	E	474	TRP	2.5
1	A	19	VAL	2.5
1	A	42	GLY	2.5
1	H	31	SER	2.5
1	K	372	ASP	2.5
1	A	268	THR	2.5
1	G	434	ALA	2.5
1	L	474	TRP	2.5
1	A	256	ILE	2.5
1	D	25	LYS	2.5
1	D	63	GLY	2.5
1	F	155	TYR	2.5
1	B	105	LEU	2.5
1	H	234	LEU	2.5
1	E	66	SER	2.5
1	J	138	PRO	2.5
1	J	359	GLU	2.5
1	A	252	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	418	ASN	2.5
1	D	341	ILE	2.5
1	D	374	ASP	2.5
1	G	10	ALA	2.5
1	H	123	SER	2.5
1	I	264	ALA	2.5
1	B	43	GLN	2.5
1	B	10	ALA	2.5
1	B	328	ALA	2.5
1	L	160	GLY	2.5
1	L	452	LEU	2.5
1	I	173	GLU	2.5
1	B	259	ARG	2.5
1	E	98	ALA	2.5
1	E	400	LEU	2.5
1	K	39	LEU	2.5
1	H	40	LYS	2.5
1	E	304	ILE	2.5
1	K	184	GLU	2.5
1	A	29	THR	2.5
1	B	37	ALA	2.5
1	D	121	GLY	2.5
1	C	399	PHE	2.5
1	G	417	PHE	2.5
1	C	225	ASP	2.5
1	H	66	SER	2.5
1	F	363	VAL	2.4
1	E	95	PRO	2.4
1	B	231	SER	2.4
1	D	252	HIS	2.4
1	C	191	LYS	2.4
1	D	134	PHE	2.4
1	F	5	TYR	2.4
1	C	116	ARG	2.4
1	H	249	THR	2.4
1	I	258	GLN	2.4
1	I	1	MET	2.4
1	A	28	LEU	2.4
1	C	193	VAL	2.4
1	I	317	GLY	2.4
1	L	96	LEU	2.4
1	B	126	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	18	ASP	2.4
1	G	277	MET	2.4
1	G	452	LEU	2.4
1	A	114	ARG	2.4
1	C	66	SER	2.4
1	C	358	THR	2.4
1	A	26	MET	2.4
1	C	26	MET	2.4
1	D	199	PRO	2.4
1	L	194	LEU	2.4
1	E	257	PHE	2.4
1	A	119	ARG	2.4
1	B	9	LEU	2.4
1	C	102	PRO	2.4
1	E	261	ARG	2.4
1	H	43	GLN	2.4
1	E	296	VAL	2.4
1	G	309	GLY	2.4
1	K	459	PHE	2.4
1	B	168	ILE	2.4
1	L	455	ILE	2.4
1	C	299	GLN	2.4
1	D	125	LEU	2.4
1	A	230	LYS	2.4
1	B	23	GLY	2.4
1	B	353	TYR	2.4
1	L	329	ILE	2.4
1	B	177	LEU	2.4
1	C	451	LEU	2.4
1	F	8	LEU	2.4
1	K	223	GLY	2.4
1	K	272	VAL	2.4
1	L	101	LEU	2.4
1	J	414	PHE	2.4
1	C	307	VAL	2.4
1	C	361	LEU	2.4
1	E	138	PRO	2.4
1	J	171	ALA	2.4
1	B	158	ILE	2.4
1	F	57	GLY	2.4
1	G	17	VAL	2.4
1	C	226	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	353	TYR	2.4
1	A	71	ILE	2.4
1	F	14	ASP	2.4
1	H	51	LEU	2.4
1	L	92	LEU	2.4
1	J	274	PHE	2.4
1	B	61	ALA	2.4
1	C	219	ALA	2.4
1	A	83	HIS	2.4
1	H	252	HIS	2.4
1	L	330	LEU	2.4
1	A	267	GLY	2.3
1	J	317	GLY	2.3
1	L	353	TYR	2.3
1	F	146	VAL	2.3
1	K	284	ARG	2.3
1	E	99	GLU	2.3
1	H	143	GLU	2.3
1	D	34	ILE	2.3
1	D	133	ALA	2.3
1	J	417	PHE	2.3
1	K	193	VAL	2.3
1	J	100	ASP	2.3
1	F	394	ILE	2.3
1	B	164	GLN	2.3
1	C	224	ASP	2.3
1	H	316	ILE	2.3
1	C	87	GLU	2.3
1	I	418	ASN	2.3
1	C	100	ASP	2.3
1	D	187	LEU	2.3
1	G	37	ALA	2.3
1	G	96	LEU	2.3
1	K	256	ILE	2.3
1	E	176	PHE	2.3
1	F	19	VAL	2.3
1	F	172	VAL	2.3
1	B	104	GLY	2.3
1	B	170	ASP	2.3
1	C	35	ASP	2.3
1	C	229	ALA	2.3
1	A	257	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	386	VAL	2.3
1	C	188	ARG	2.3
1	J	339	ILE	2.3
1	L	79	LEU	2.3
1	D	274	PHE	2.3
1	L	119	ARG	2.3
1	C	92	LEU	2.3
1	E	65	ILE	2.3
1	G	130	ALA	2.3
1	L	132	TYR	2.3
1	E	194	LEU	2.3
1	H	137	ILE	2.3
1	I	485	ILE	2.3
1	B	74	ASP	2.3
1	C	187	LEU	2.3
1	G	301	LEU	2.3
1	A	3	SER	2.3
1	A	334	ARG	2.3
1	G	314	ILE	2.3
1	D	296	VAL	2.3
1	G	45	VAL	2.3
1	I	399	PHE	2.3
1	D	52	THR	2.3
1	F	2	PRO	2.3
1	F	66	SER	2.3
1	F	459	PHE	2.3
1	G	435	ILE	2.3
1	I	182	TYR	2.3
1	A	228	GLU	2.2
1	D	60	GLU	2.2
1	F	77	ARG	2.2
1	F	136	ARG	2.2
1	H	136	ARG	2.2
1	K	195	LEU	2.2
1	C	206	ILE	2.2
1	E	195	LEU	2.2
1	K	194	LEU	2.2
1	D	35	ASP	2.2
1	B	399	PHE	2.2
1	J	257	PHE	2.2
1	B	96	LEU	2.2
1	B	195	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	330	LEU	2.2
1	L	68	LEU	2.2
1	E	316	ILE	2.2
1	B	17	VAL	2.2
1	B	172	VAL	2.2
1	E	193	VAL	2.2
1	C	60	GLU	2.2
1	B	194	LEU	2.2
1	C	414	PHE	2.2
1	A	100	ASP	2.2
1	B	112	ASP	2.2
1	G	386	VAL	2.2
1	B	264	ALA	2.2
1	H	155	TYR	2.2
1	L	217	LYS	2.2
1	C	368	LEU	2.2
1	A	231	SER	2.2
1	L	339	ILE	2.2
1	E	131	GLY	2.2
1	J	248	GLU	2.2
1	I	151	PRO	2.2
1	B	76	HIS	2.2
1	B	134	PHE	2.2
1	E	114	ARG	2.2
1	I	341	ILE	2.2
1	A	49	GLU	2.2
1	J	192	GLY	2.2
1	I	152	ASP	2.2
1	F	235	ASN	2.2
1	K	176	PHE	2.2
1	B	270	VAL	2.2
1	C	314	ILE	2.2
1	I	247	GLY	2.2
1	C	182	TYR	2.2
1	L	205	LEU	2.2
1	B	29	THR	2.2
1	K	281	PHE	2.2
1	I	256	ILE	2.2
1	K	271	ILE	2.2
1	A	173	GLU	2.2
1	L	384	GLU	2.2
1	A	232	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	3	SER	2.2
1	G	133	ALA	2.2
1	I	185	TYR	2.2
1	A	269	PRO	2.2
1	A	245	PHE	2.2
1	A	133	ALA	2.2
1	B	28	LEU	2.2
1	I	330	LEU	2.2
1	I	102	PRO	2.2
1	H	256	ILE	2.2
1	L	277	MET	2.2
1	D	353	TYR	2.2
1	F	36	ALA	2.2
1	H	8	LEU	2.2
1	L	444	PRO	2.2
1	I	172	VAL	2.2
1	J	488	ILE	2.2
1	G	358	THR	2.2
1	J	185	TYR	2.1
1	J	214	LEU	2.1
1	B	46	ARG	2.1
1	B	53	VAL	2.1
1	C	383	ILE	2.1
1	I	503	ILE	2.1
1	J	201	CYS	2.1
1	L	267	GLY	2.1
1	L	125	LEU	2.1
1	E	246	VAL	2.1
1	H	435	ILE	2.1
1	I	362	PRO	2.1
1	K	463	GLU	2.1
1	F	464	ASP	2.1
1	L	39	LEU	2.1
1	H	76	HIS	2.1
1	K	83	HIS	2.1
1	A	59	PHE	2.1
1	A	97	ILE	2.1
1	C	256	ILE	2.1
1	F	70	GLU	2.1
1	J	341	ILE	2.1
1	J	175	PRO	2.1
1	F	9	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	93	ALA	2.1
1	K	232	TYR	2.1
1	A	135	GLU	2.1
1	D	266	GLU	2.1
1	E	126	VAL	2.1
1	G	55	GLU	2.1
1	I	402	VAL	2.1
1	J	148	GLU	2.1
1	G	231	SER	2.1
1	C	136	ARG	2.1
1	D	257	PHE	2.1
1	F	264	ALA	2.1
1	K	230	LYS	2.1
1	B	149	GLU	2.1
1	D	410	GLU	2.1
1	G	505	THR	2.1
1	C	378	CYS	2.1
1	A	102	PRO	2.1
1	A	214	LEU	2.1
1	I	32	PRO	2.1
1	B	94	ASP	2.1
1	E	45	VAL	2.1
1	G	70	GLU	2.1
1	H	334	ARG	2.1
1	J	491	LEU	2.1
1	A	115	PRO	2.1
1	E	140	ALA	2.1
1	A	142	VAL	2.1
1	K	402	VAL	2.1
1	B	113	THR	2.1
1	C	317	GLY	2.1
1	F	436	LYS	2.1
1	F	505	THR	2.1
1	I	277	MET	2.1
1	K	8	LEU	2.1
1	A	414	PHE	2.1
1	K	257	PHE	2.1
1	I	5	TYR	2.1
1	A	247	GLY	2.1
1	E	254	ARG	2.1
1	D	155	TYR	2.1
1	L	430	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	158	ILE	2.1
1	F	272	VAL	2.1
1	H	3	SER	2.1
1	I	334	ARG	2.1
1	L	236	ILE	2.1
1	E	317	GLY	2.1
1	A	69	ARG	2.1
1	C	78	ALA	2.1
1	C	463	GLU	2.1
1	L	435	ILE	2.1
1	D	15	ASP	2.1
1	D	192	GLY	2.1
1	K	92	LEU	2.1
1	K	277	MET	2.1
1	L	55	GLU	2.1
1	L	191	LYS	2.1
1	A	16	THR	2.1
1	D	57	GLY	2.1
1	E	101	LEU	2.1
1	F	96	LEU	2.1
1	G	379	ILE	2.1
1	L	165	ILE	2.1
1	C	375	ARG	2.0
1	A	52	THR	2.0
1	C	130	ALA	2.0
1	C	137	ILE	2.0
1	C	362	PRO	2.0
1	D	120	PRO	2.0
1	J	125	LEU	2.0
1	A	371	PHE	2.0
1	C	275	ASP	2.0
1	F	435	ILE	2.0
1	L	341	ILE	2.0
1	H	117	LYS	2.0
1	D	277	MET	2.0
1	G	144	ASP	2.0
1	L	443	GLN	2.0
1	E	339	ILE	2.0
1	G	147	LEU	2.0
1	I	255	LEU	2.0
1	K	491	LEU	2.0
1	A	58	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	235	ASN	2.0
1	F	16	THR	2.0
1	G	362	PRO	2.0
1	B	272	VAL	2.0
1	D	185	TYR	2.0
1	B	51	LEU	2.0
1	B	101	LEU	2.0
1	G	431	LYS	2.0
1	H	329	ILE	2.0
1	I	137	ILE	2.0
1	I	281	PHE	2.0
1	F	382	MET	2.0
1	K	397	ASN	2.0
1	C	7	VAL	2.0
1	C	80	VAL	2.0
1	C	65	ILE	2.0
1	J	447	ARG	2.0
1	I	202	GLY	2.0
1	I	176	PHE	2.0
1	A	220	GLU	2.0
1	K	311	GLU	2.0
1	L	216	LYS	2.0
1	D	182	TYR	2.0
1	I	214	LEU	2.0
1	J	146	VAL	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.