Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 08:40 AM EDT

PDB ID	:	2R5I
Title	:	Pentamer Structure of Major Capsid Protein L1 of Human Papilloma Virus type 18
Authors	:	Bishop, B.; Dasgupta, J.; Chen, X.S.
Deposited on	:	2007-09-03
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

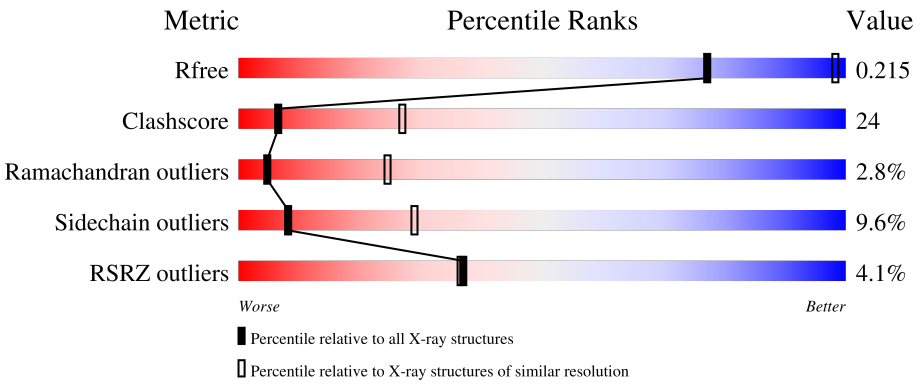
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	428	5% 46% 38% 14% • •
1	B	428	4% 46% 39% 13% • •
1	C	428	5% 48% 38% 12% • •
1	D	428	2% 46% 40% 11% • •
1	E	428	2% 46% 39% 13% • •

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Mol	Chain	Length	Quality of chain
1	F	428	6% 41% 44% 14%
1	G	428	5% 41% 45% 11%
1	H	428	3% 43% 42% 12%
1	I	428	3% 49% 37% 12%
1	J	428	4% 43% 42% 13%
1	K	428	3% 47% 38% 13%
1	L	428	5% 48% 37% 12%
1	M	428	5% 45% 41% 12%
1	N	428	4% 46% 36% 15%
1	O	428	4% 48% 37% 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 49845 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 L1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	423	3323	2098	562	643	20	0	0	0
1	B	423	3323	2098	562	643	20	0	0	0
1	C	423	3323	2098	562	643	20	0	0	0
1	D	423	3323	2098	562	643	20	0	0	0
1	E	423	3323	2098	562	643	20	0	0	0
1	F	423	3323	2098	562	643	20	0	0	0
1	G	423	3323	2098	562	643	20	0	0	0
1	H	423	3323	2098	562	643	20	0	0	0
1	I	423	3323	2098	562	643	20	0	0	0
1	J	423	3323	2098	562	643	20	0	0	0
1	K	423	3323	2098	562	643	20	0	0	0
1	L	423	3323	2098	562	643	20	0	0	0
1	M	423	3323	2098	562	643	20	0	0	0
1	N	423	3323	2098	562	643	20	0	0	0
1	O	423	3323	2098	562	643	20	0	0	0

There are 135 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	expression tag	UNP Q80B70
A	47	ASP	ASN	engineered mutation	UNP Q80B70
A	175	SER	CYS	engineered mutation	UNP Q80B70
A	393	GLN	HIS	engineered mutation	UNP Q80B70
A	405	GLY	-	linker	UNP Q80B70
A	406	GLY	-	linker	UNP Q80B70
A	407	SER	-	linker	UNP Q80B70
A	408	GLY	-	linker	UNP Q80B70
A	409	GLY	-	linker	UNP Q80B70
B	20	ALA	-	expression tag	UNP Q80B70
B	47	ASP	ASN	engineered mutation	UNP Q80B70
B	175	SER	CYS	engineered mutation	UNP Q80B70
B	393	GLN	HIS	engineered mutation	UNP Q80B70
B	405	GLY	-	linker	UNP Q80B70
B	406	GLY	-	linker	UNP Q80B70
B	407	SER	-	linker	UNP Q80B70
B	408	GLY	-	linker	UNP Q80B70
B	409	GLY	-	linker	UNP Q80B70
C	20	ALA	-	expression tag	UNP Q80B70
C	47	ASP	ASN	engineered mutation	UNP Q80B70
C	175	SER	CYS	engineered mutation	UNP Q80B70
C	393	GLN	HIS	engineered mutation	UNP Q80B70
C	405	GLY	-	linker	UNP Q80B70
C	406	GLY	-	linker	UNP Q80B70
C	407	SER	-	linker	UNP Q80B70
C	408	GLY	-	linker	UNP Q80B70
C	409	GLY	-	linker	UNP Q80B70
D	20	ALA	-	expression tag	UNP Q80B70
D	47	ASP	ASN	engineered mutation	UNP Q80B70
D	175	SER	CYS	engineered mutation	UNP Q80B70
D	393	GLN	HIS	engineered mutation	UNP Q80B70
D	405	GLY	-	linker	UNP Q80B70
D	406	GLY	-	linker	UNP Q80B70
D	407	SER	-	linker	UNP Q80B70
D	408	GLY	-	linker	UNP Q80B70
D	409	GLY	-	linker	UNP Q80B70
E	20	ALA	-	expression tag	UNP Q80B70
E	47	ASP	ASN	engineered mutation	UNP Q80B70
E	175	SER	CYS	engineered mutation	UNP Q80B70
E	393	GLN	HIS	engineered mutation	UNP Q80B70
E	405	GLY	-	linker	UNP Q80B70
E	406	GLY	-	linker	UNP Q80B70
E	407	SER	-	linker	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
E	408	GLY	-	linker	UNP Q80B70
E	409	GLY	-	linker	UNP Q80B70
F	20	ALA	-	expression tag	UNP Q80B70
F	47	ASP	ASN	engineered mutation	UNP Q80B70
F	175	SER	CYS	engineered mutation	UNP Q80B70
F	393	GLN	HIS	engineered mutation	UNP Q80B70
F	405	GLY	-	linker	UNP Q80B70
F	406	GLY	-	linker	UNP Q80B70
F	407	SER	-	linker	UNP Q80B70
F	408	GLY	-	linker	UNP Q80B70
F	409	GLY	-	linker	UNP Q80B70
G	20	ALA	-	expression tag	UNP Q80B70
G	47	ASP	ASN	engineered mutation	UNP Q80B70
G	175	SER	CYS	engineered mutation	UNP Q80B70
G	393	GLN	HIS	engineered mutation	UNP Q80B70
G	405	GLY	-	linker	UNP Q80B70
G	406	GLY	-	linker	UNP Q80B70
G	407	SER	-	linker	UNP Q80B70
G	408	GLY	-	linker	UNP Q80B70
G	409	GLY	-	linker	UNP Q80B70
H	20	ALA	-	expression tag	UNP Q80B70
H	47	ASP	ASN	engineered mutation	UNP Q80B70
H	175	SER	CYS	engineered mutation	UNP Q80B70
H	393	GLN	HIS	engineered mutation	UNP Q80B70
H	405	GLY	-	linker	UNP Q80B70
H	406	GLY	-	linker	UNP Q80B70
H	407	SER	-	linker	UNP Q80B70
H	408	GLY	-	linker	UNP Q80B70
H	409	GLY	-	linker	UNP Q80B70
I	20	ALA	-	expression tag	UNP Q80B70
I	47	ASP	ASN	engineered mutation	UNP Q80B70
I	175	SER	CYS	engineered mutation	UNP Q80B70
I	393	GLN	HIS	engineered mutation	UNP Q80B70
I	405	GLY	-	linker	UNP Q80B70
I	406	GLY	-	linker	UNP Q80B70
I	407	SER	-	linker	UNP Q80B70
I	408	GLY	-	linker	UNP Q80B70
I	409	GLY	-	linker	UNP Q80B70
J	20	ALA	-	expression tag	UNP Q80B70
J	47	ASP	ASN	engineered mutation	UNP Q80B70
J	175	SER	CYS	engineered mutation	UNP Q80B70
J	393	GLN	HIS	engineered mutation	UNP Q80B70

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Chain	Residue	Modelled	Actual	Comment	Reference
J	405	GLY	-	linker	UNP Q80B70
J	406	GLY	-	linker	UNP Q80B70
J	407	SER	-	linker	UNP Q80B70
J	408	GLY	-	linker	UNP Q80B70
J	409	GLY	-	linker	UNP Q80B70
K	20	ALA	-	expression tag	UNP Q80B70
K	47	ASP	ASN	engineered mutation	UNP Q80B70
K	175	SER	CYS	engineered mutation	UNP Q80B70
K	393	GLN	HIS	engineered mutation	UNP Q80B70
K	405	GLY	-	linker	UNP Q80B70
K	406	GLY	-	linker	UNP Q80B70
K	407	SER	-	linker	UNP Q80B70
K	408	GLY	-	linker	UNP Q80B70
K	409	GLY	-	linker	UNP Q80B70
L	20	ALA	-	expression tag	UNP Q80B70
L	47	ASP	ASN	engineered mutation	UNP Q80B70
L	175	SER	CYS	engineered mutation	UNP Q80B70
L	393	GLN	HIS	engineered mutation	UNP Q80B70
L	405	GLY	-	linker	UNP Q80B70
L	406	GLY	-	linker	UNP Q80B70
L	407	SER	-	linker	UNP Q80B70
L	408	GLY	-	linker	UNP Q80B70
L	409	GLY	-	linker	UNP Q80B70
M	20	ALA	-	expression tag	UNP Q80B70
M	47	ASP	ASN	engineered mutation	UNP Q80B70
M	175	SER	CYS	engineered mutation	UNP Q80B70
M	393	GLN	HIS	engineered mutation	UNP Q80B70
M	405	GLY	-	linker	UNP Q80B70
M	406	GLY	-	linker	UNP Q80B70
M	407	SER	-	linker	UNP Q80B70
M	408	GLY	-	linker	UNP Q80B70
M	409	GLY	-	linker	UNP Q80B70
N	20	ALA	-	expression tag	UNP Q80B70
N	47	ASP	ASN	engineered mutation	UNP Q80B70
N	175	SER	CYS	engineered mutation	UNP Q80B70
N	393	GLN	HIS	engineered mutation	UNP Q80B70
N	405	GLY	-	linker	UNP Q80B70
N	406	GLY	-	linker	UNP Q80B70
N	407	SER	-	linker	UNP Q80B70
N	408	GLY	-	linker	UNP Q80B70
N	409	GLY	-	linker	UNP Q80B70
O	20	ALA	-	expression tag	UNP Q80B70

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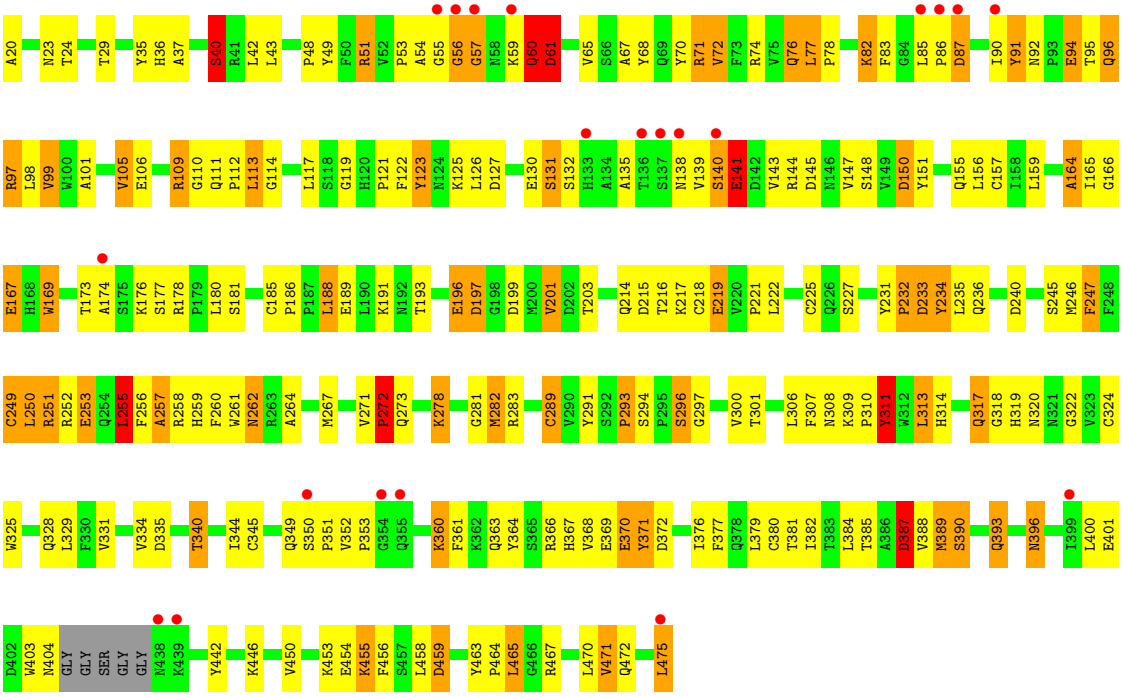
Chain	Residue	Modelled	Actual	Comment	Reference
O	47	ASP	ASN	engineered mutation	UNP Q80B70
O	175	SER	CYS	engineered mutation	UNP Q80B70
O	393	GLN	HIS	engineered mutation	UNP Q80B70
O	405	GLY	-	linker	UNP Q80B70
O	406	GLY	-	linker	UNP Q80B70
O	407	SER	-	linker	UNP Q80B70
O	408	GLY	-	linker	UNP Q80B70
O	409	GLY	-	linker	UNP Q80B70

3 Residue-property plots (i)

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

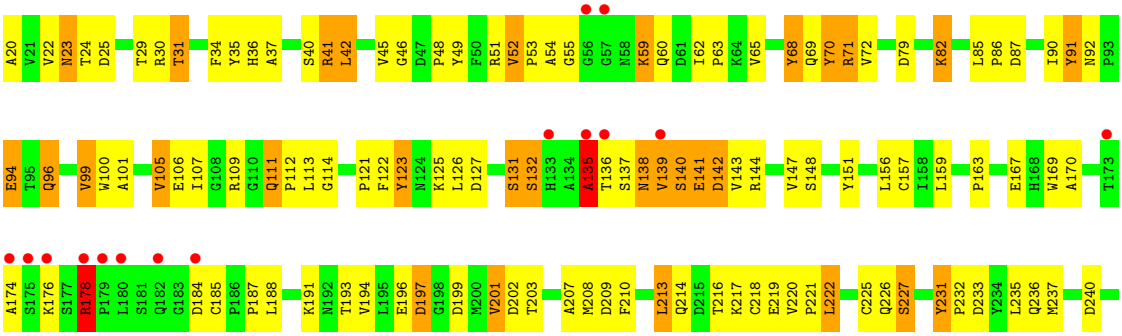
• Molecule 1: L1 protein

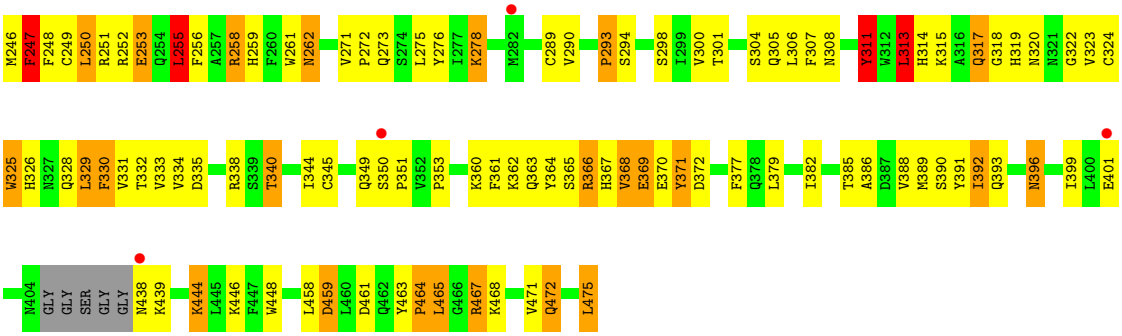
Chain A:



• Molecule 1: L1 protein

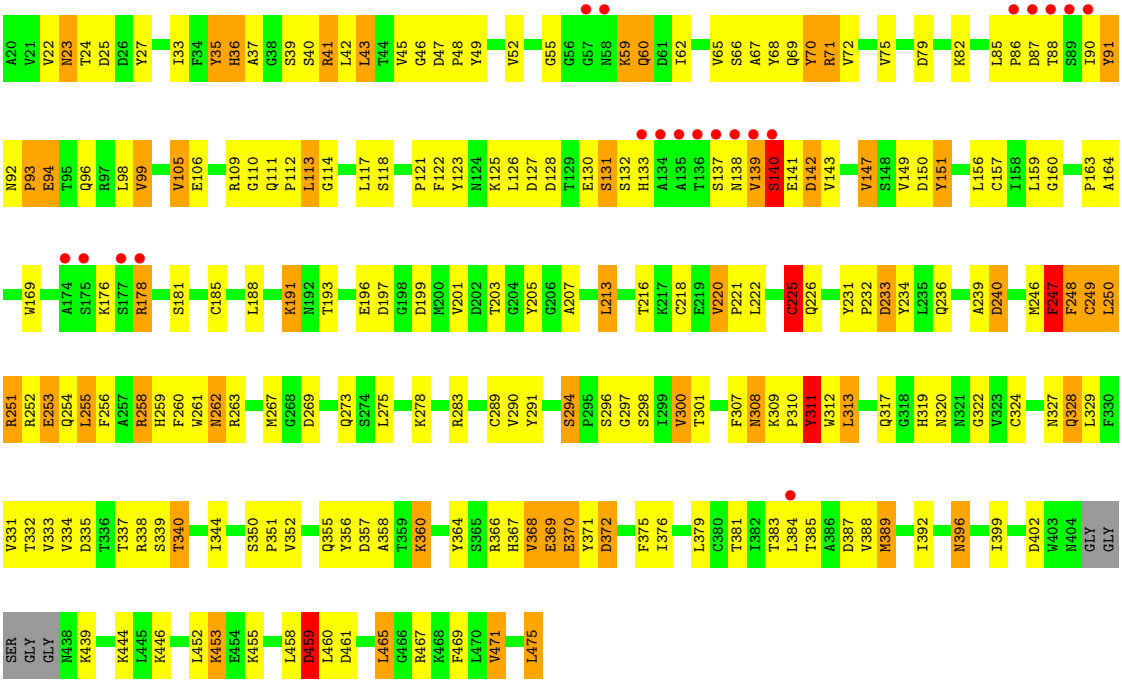
Chain B:





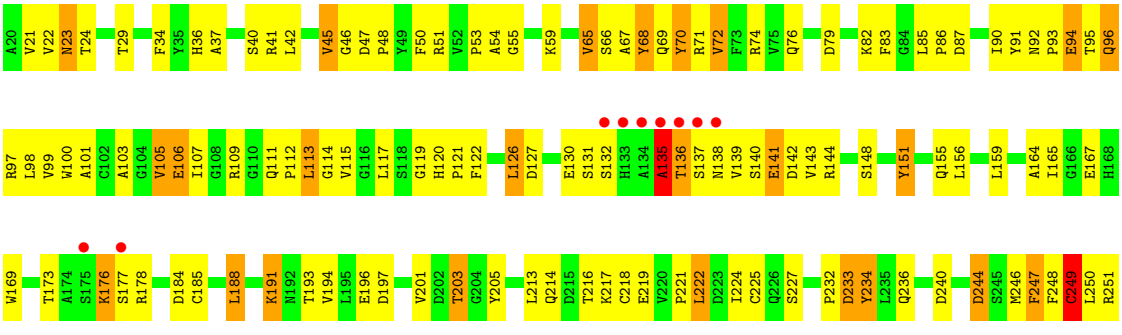
• Molecule 1: L1 protein

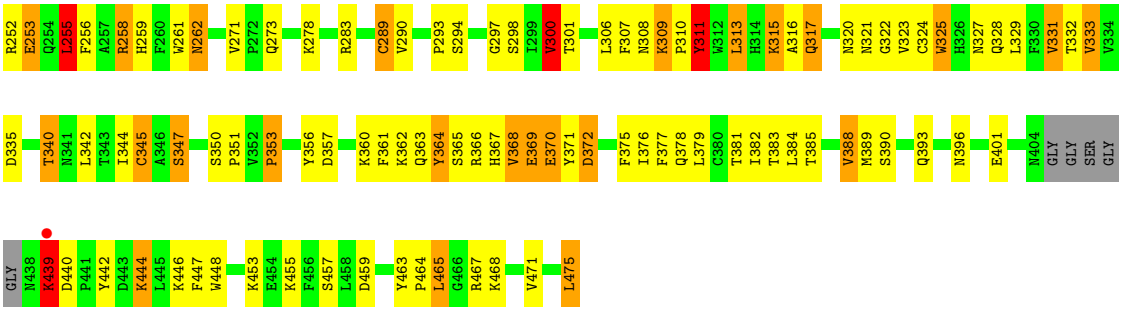
Chain C:



• Molecule 1: L1 protein

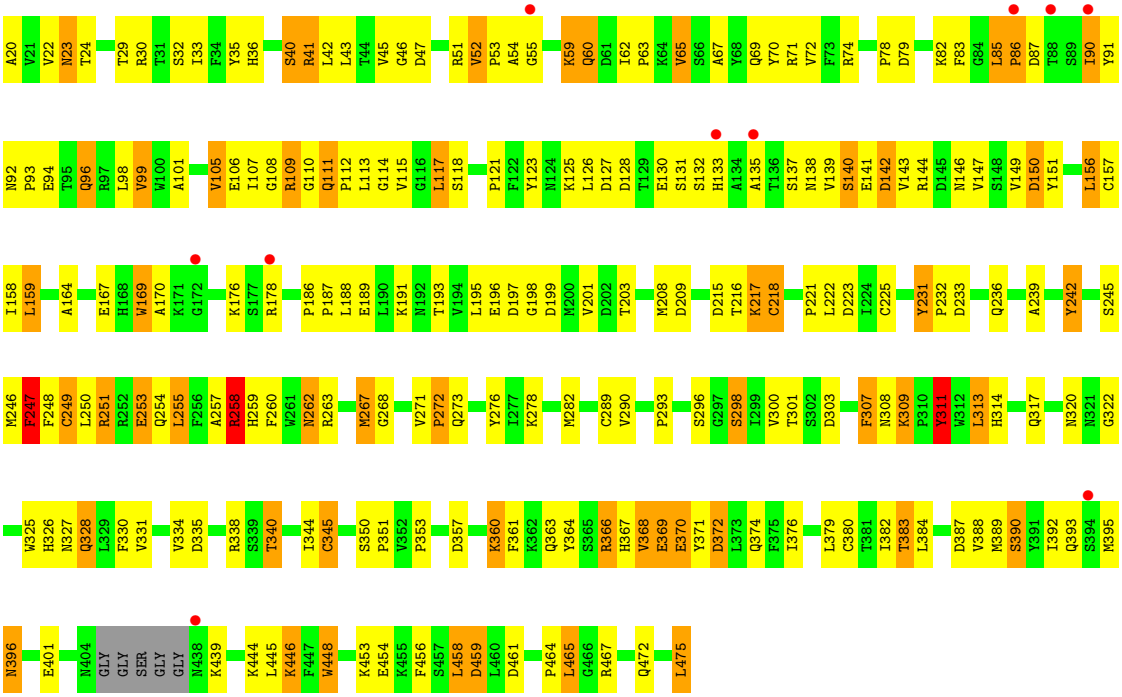
Chain D:





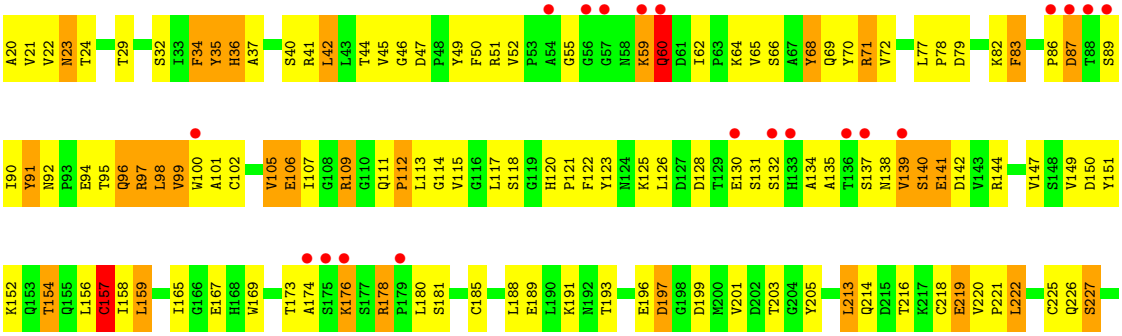
• Molecule 1: L1 protein

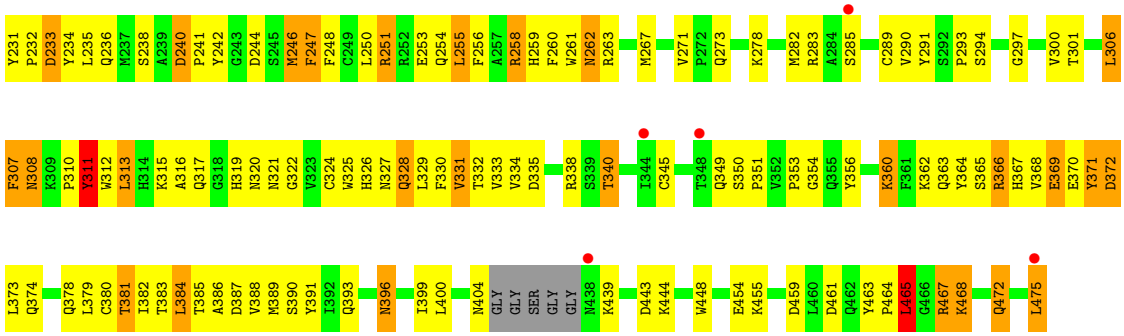
Chain E:



• Molecule 1: L1 protein

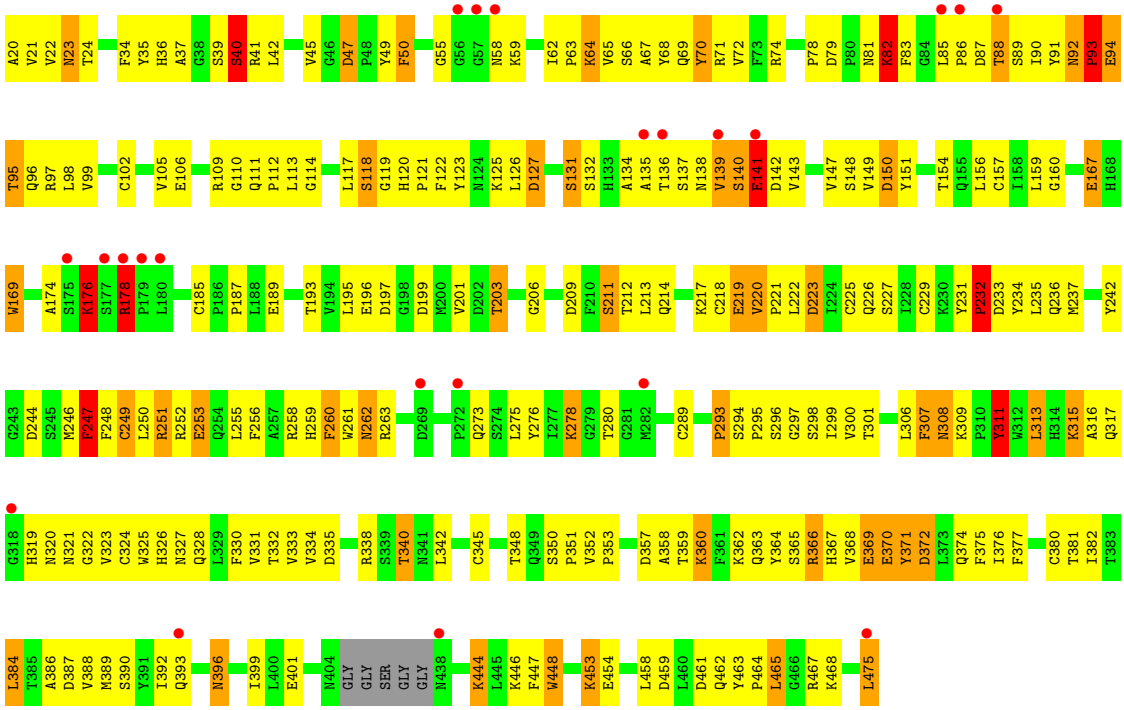
Chain F:





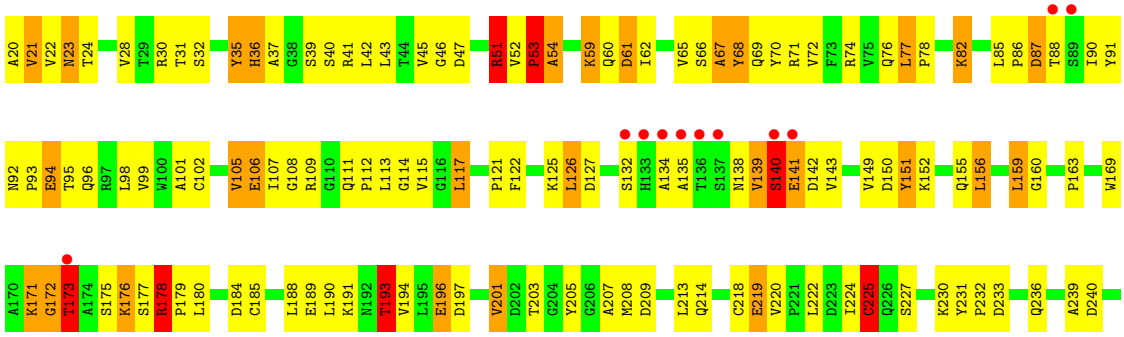
• Molecule 1: L1 protein

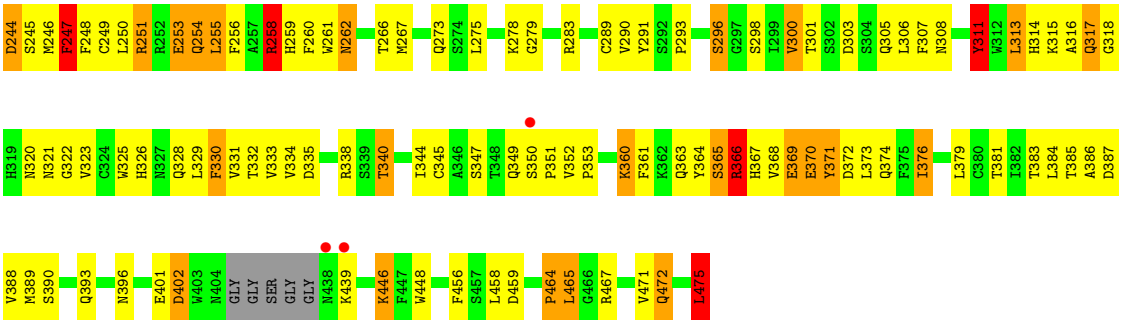
Chain G:



• Molecule 1: L1 protein

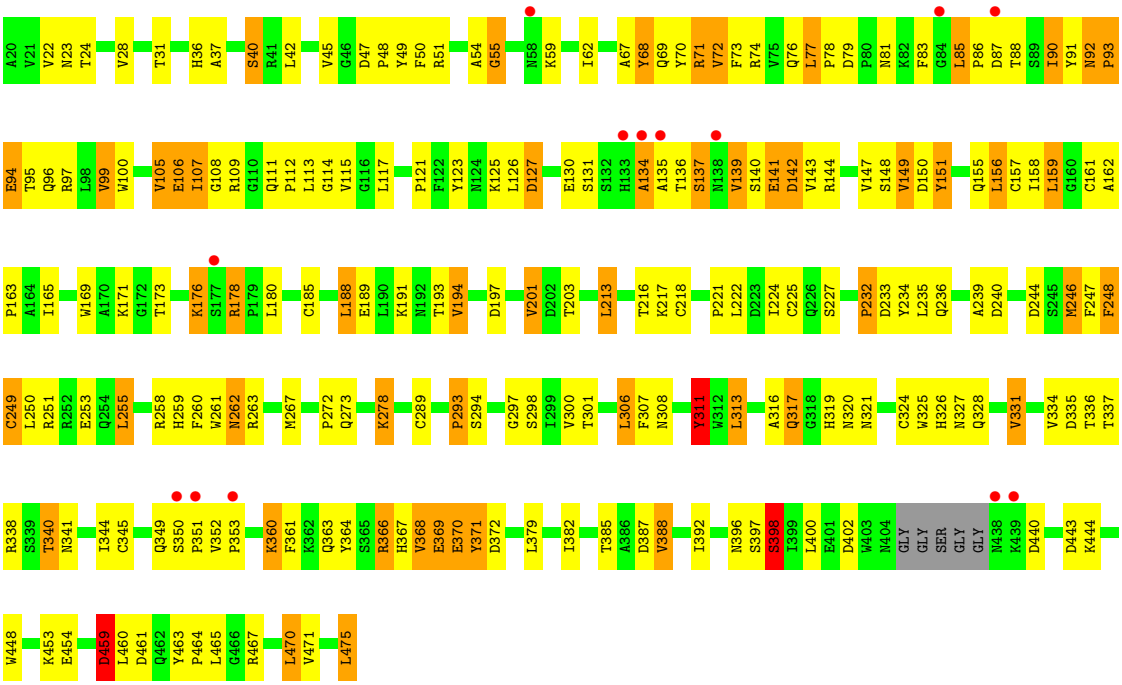
Chain H:





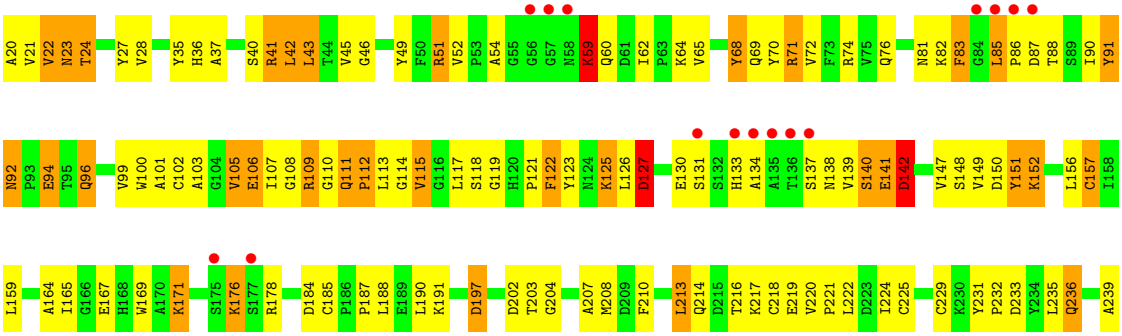
- Molecule 1: L1 protein

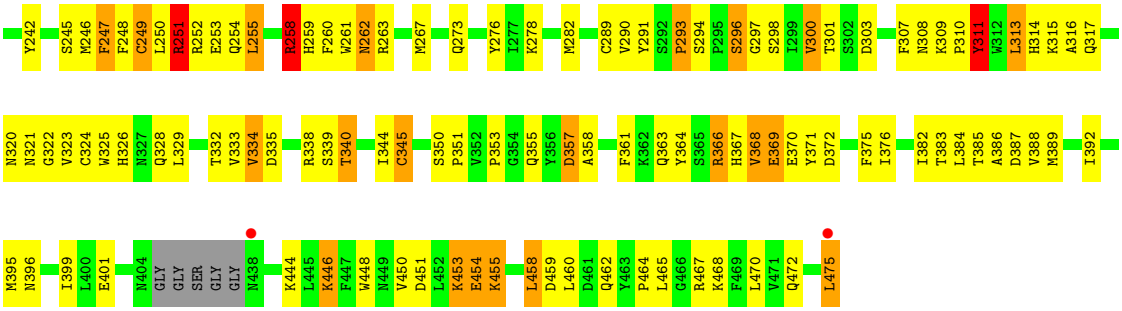
Chain I:



- Molecule 1: L1 protein

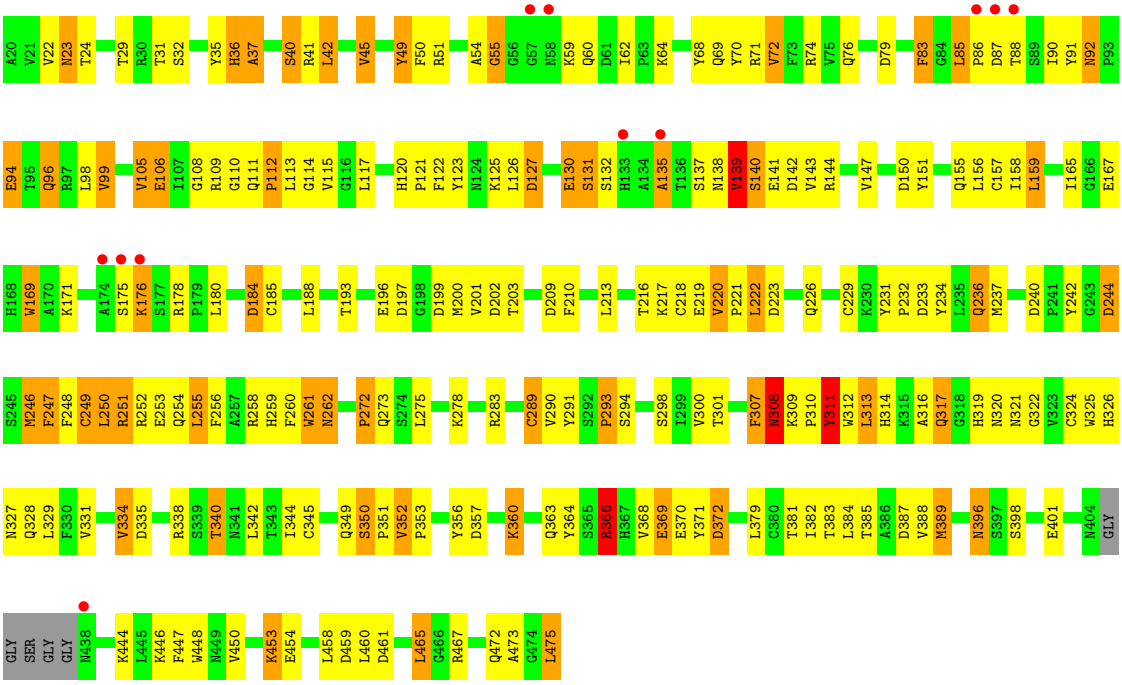
Chain J:





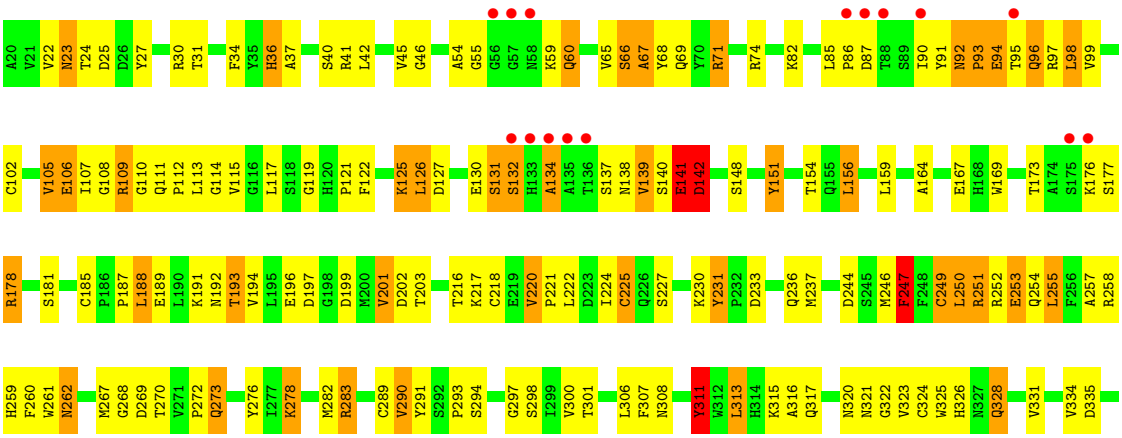
• Molecule 1: L1 protein

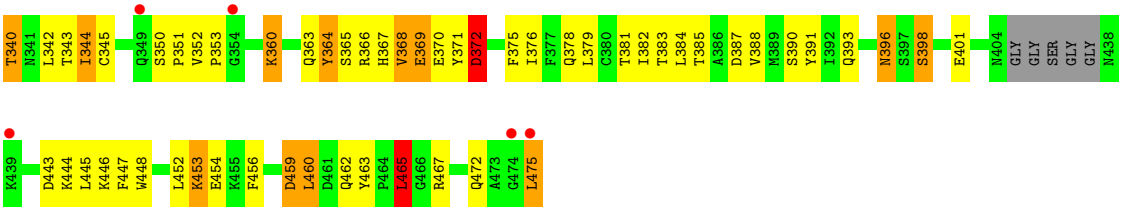
Chain K:



• Molecule 1: L1 protein

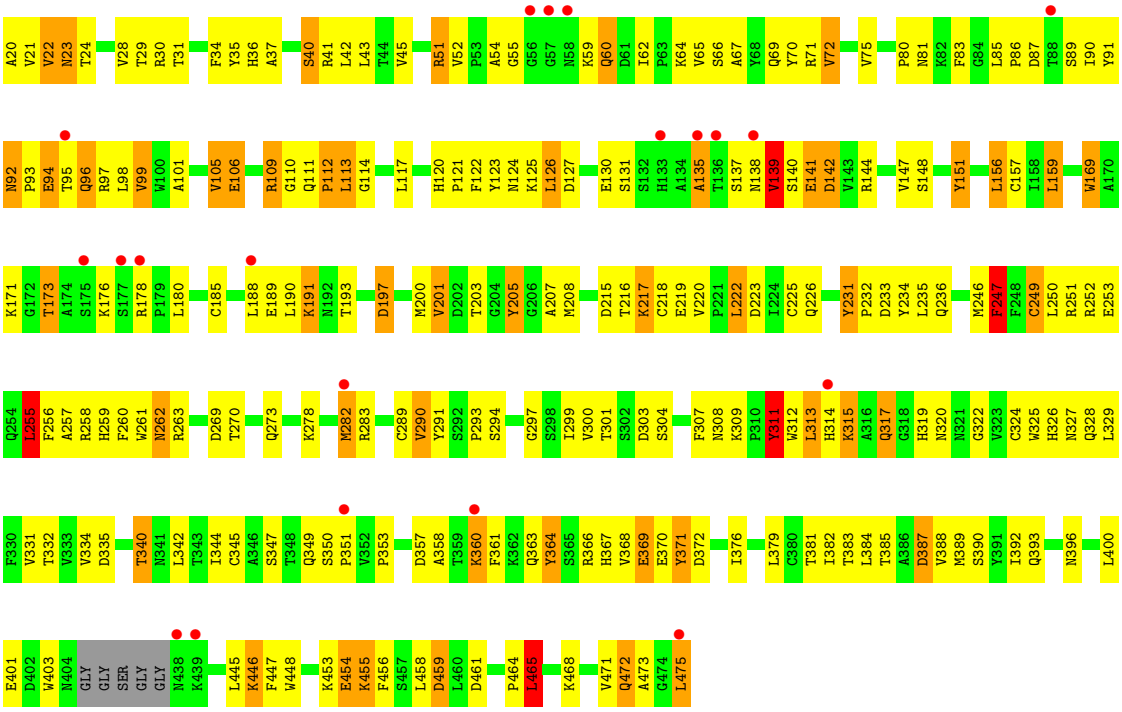
Chain L:





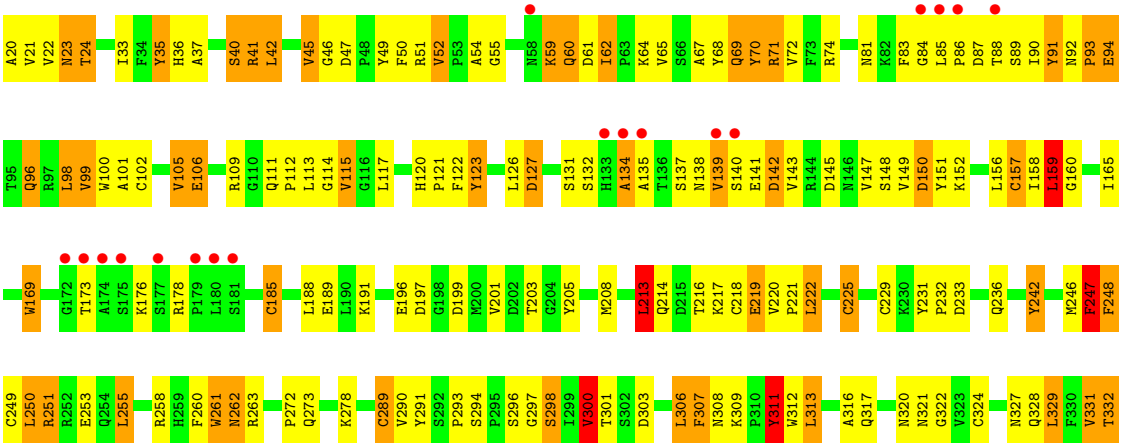
• Molecule 1: L1 protein

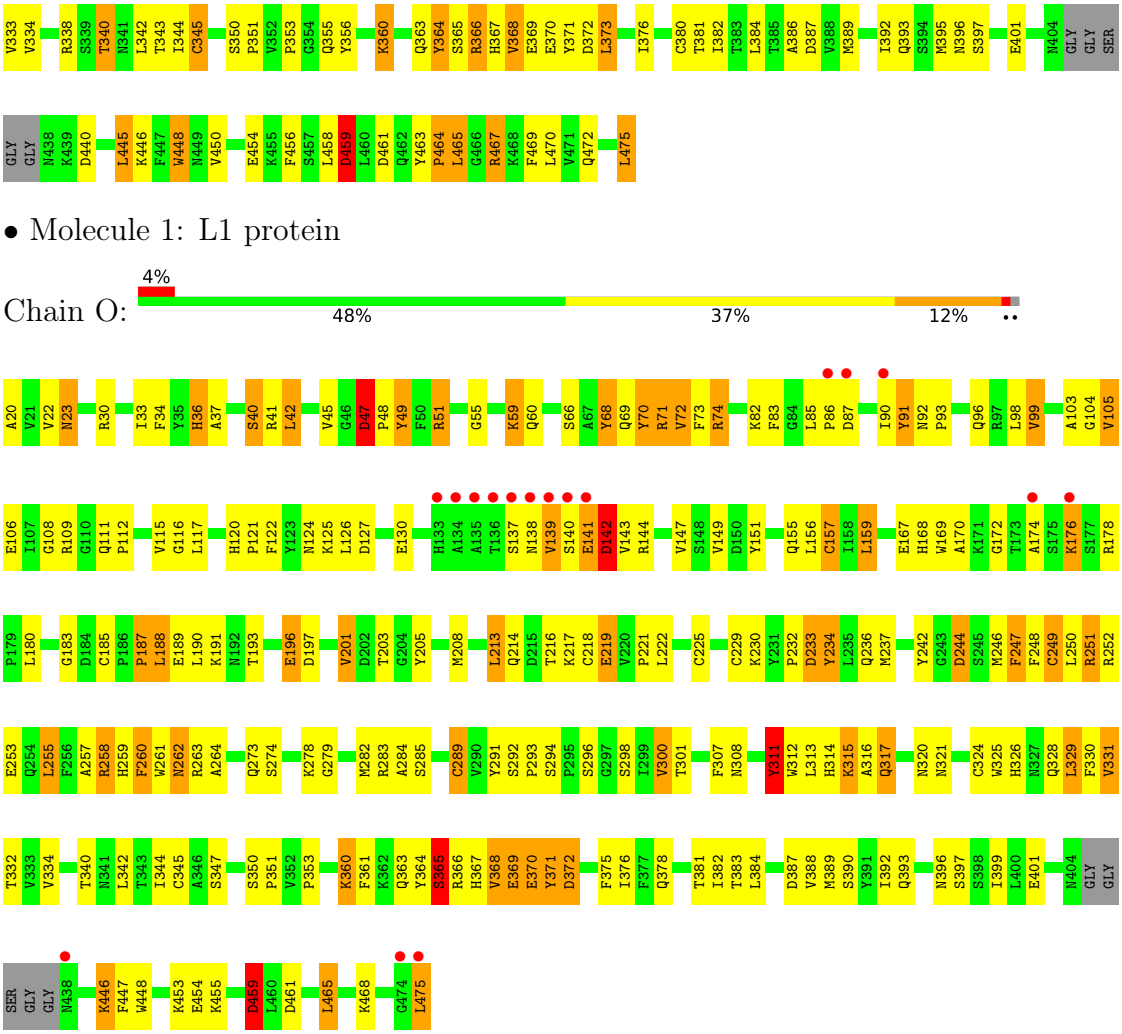
Chain M:



• Molecule 1: L1 protein

Chain N:




V333 V334 R338 S339 T340 N341 L342 T343 I344 C345 S350 P351 V352 P353 G354 Q355 Y356 K360 Q363 Y364 S365 R366 H367 V368 E369 E370 Y371 D372 L373 I376 C380 T381 I382 T383 L384 T385 A386 D387 V388 M389 I392 Q393 S394 M395 N396 S397 E401 N404 GLY GLY SER
GLY GLY N438 K439 D440 L445 K446 F447 W448 N449 V450 E454 K455 F456 S457 L458 D459 L460 D461 Q462 Y463 P464 L465 G466 R467 K468 F469 L470 V471 Q472 L475
• Molecule 1: L1 protein
Chain O:
4%
48%
37%
12%
A20 V21 V22 N23 R30 I33 F34 Y35 H36 A37 S40 R41 L42 V45 G46 D47 P48 Y49 F50 R51 G55 K59 Q60 S66 A67 Y68 Q69 Y70 R71 V72 F73 R74 K82 F83 G84 L85 P86 D87 I90 Y91 N92 P93 Q96 R97 L98 V99 A103 G104 V105
E106 I107 G108 R109 G110 Q111 P112 V115 G116 L117 H120 P121 F122 Y123 N124 K125 L126 D127 E130 H133 A134 A135 T136 S137 N138 V139 S140 E141 D142 V143 R144 V147 S148 V149 D150 Y151 Q155 L156 C157 I158 L159 E167 H168 W169 A170 K171 G172 T173 A174 S175 K176 S177 R178
P179 L180 G183 D184 C185 P186 P187 L188 E189 L190 K191 N192 T193 E196 D197 V201 D202 T203 G204 Y205 M208 L213 Q214 D215 T216 K217 C218 E219 V220 P221 L222 C225 C229 K230 Y231 P232 D233 Y234 L235 Q236 M237 Y242 G243 D244 S245 M246 F247 F248 C249 L250 R251 R252
E253 Q254 L255 F256 A257 R258 H259 F260 W261 N262 R263 A264 Q273 S274 K278 G279 M282 R283 A284 S285 C289 V290 Y291 S292 P293 S294 P295 S296 G297 S298 I299 V300 T301 F307 N308 Y311 W312 L313 H314 K315 A316 Q317 N320 N321 C324 W325 H326 N327 Q328 L329 F330 V331
T332 V333 V334 T340 N341 L342 T343 I344 C345 A346 S347 S350 P351 V352 P353 K360 F361 K362 Q363 Y364 S365 R366 H367 V368 E369 E370 Y371 D372 F375 I376 F377 Q378 T381 I382 T383 L384 D387 V388 M389 S390 Y391 I392 Q393 N396 S397 S398 I399 L400 E401 N404 GLY GLY
SER GLY GLY N438 K446 F447 W448 K453 E454 K455 D459 L460 D461 L465 K468 G474 L475

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.16Å 105.04Å 235.75Å 87.56° 85.66° 68.16°	Depositor
Resolution (Å)	40.00 – 3.40 51.09 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-3.40) 99.3 (51.09-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	19.60	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.260 0.204 , 0.215	Depositor DCC
R_{free} test set	11857 reflections (7.47%)	wwPDB-VP
Wilson B-factor (Å^2)	63.4	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,-h+k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	49845	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.92	72/3408 (2.1%)	1.47	35/4633 (0.8%)
1	B	1.93	78/3408 (2.3%)	1.44	36/4633 (0.8%)
1	C	1.89	64/3408 (1.9%)	1.47	38/4633 (0.8%)
1	D	1.96	79/3408 (2.3%)	1.44	29/4633 (0.6%)
1	E	1.99	80/3408 (2.3%)	1.47	41/4633 (0.9%)
1	F	2.02	90/3408 (2.6%)	1.46	34/4633 (0.7%)
1	G	2.03	90/3408 (2.6%)	1.48	33/4633 (0.7%)
1	H	1.93	71/3408 (2.1%)	1.52	46/4633 (1.0%)
1	I	1.84	46/3408 (1.3%)	1.42	34/4633 (0.7%)
1	J	1.94	71/3408 (2.1%)	1.50	41/4633 (0.9%)
1	K	1.89	66/3408 (1.9%)	1.45	41/4633 (0.9%)
1	L	1.99	81/3408 (2.4%)	1.51	42/4633 (0.9%)
1	M	1.91	70/3408 (2.1%)	1.44	33/4633 (0.7%)
1	N	1.90	72/3408 (2.1%)	1.43	31/4633 (0.7%)
1	O	1.95	80/3408 (2.3%)	1.51	37/4633 (0.8%)
All	All	1.94	1110/51120 (2.2%)	1.47	551/69495 (0.8%)

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	D	0	1

All (1110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	439	LYS	CE-NZ	16.04	1.89	1.49
1	L	311	TYR	CE2-CZ	15.05	1.58	1.38
1	O	311	TYR	CE2-CZ	15.03	1.58	1.38
1	E	311	TYR	CE2-CZ	14.64	1.57	1.38
1	I	311	TYR	CE2-CZ	14.61	1.57	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	311	TYR	CE2-CZ	13.73	1.56	1.38
1	L	453	LYS	CD-CE	13.42	1.84	1.51
1	A	245	SER	CB-OG	12.74	1.58	1.42
1	K	311	TYR	CE2-CZ	12.49	1.54	1.38
1	B	140	SER	CB-OG	12.38	1.58	1.42
1	B	141	GLU	CB-CG	12.28	1.75	1.52
1	A	311	TYR	CE2-CZ	12.16	1.54	1.38
1	C	311	TYR	CE2-CZ	12.16	1.54	1.38
1	G	311	TYR	CE2-CZ	12.04	1.54	1.38
1	G	64	LYS	CD-CE	11.88	1.80	1.51
1	F	311	TYR	CE2-CZ	11.63	1.53	1.38
1	G	315	LYS	CD-CE	11.38	1.79	1.51
1	O	365	SER	CB-OG	11.25	1.56	1.42
1	M	311	TYR	CE2-CZ	11.07	1.52	1.38
1	E	446	LYS	CD-CE	11.06	1.78	1.51
1	L	360	LYS	CD-CE	10.93	1.78	1.51
1	J	311	TYR	CE2-CZ	10.72	1.52	1.38
1	D	311	TYR	CE2-CZ	10.60	1.52	1.38
1	N	149	VAL	CB-CG1	-10.59	1.30	1.52
1	J	248	PHE	CE2-CZ	10.59	1.57	1.37
1	O	315	LYS	CE-NZ	10.52	1.75	1.49
1	N	311	TYR	CE2-CZ	10.52	1.52	1.38
1	F	189	GLU	CD-OE1	10.45	1.37	1.25
1	F	369	GLU	CD-OE2	10.41	1.37	1.25
1	L	106	GLU	CD-OE1	10.19	1.36	1.25
1	L	139	VAL	CB-CG2	10.17	1.74	1.52
1	C	191	LYS	CD-CE	10.16	1.76	1.51
1	K	401	GLU	CD-OE1	10.15	1.36	1.25
1	L	94	GLU	CG-CD	10.12	1.67	1.51
1	D	191	LYS	CE-NZ	10.09	1.74	1.49
1	G	34	PHE	CE1-CZ	10.07	1.56	1.37
1	M	191	LYS	CD-CE	10.05	1.76	1.51
1	N	20	ALA	CA-CB	10.05	1.73	1.52
1	F	311	TYR	CG-CD2	9.97	1.52	1.39
1	C	164	ALA	CA-CB	-9.84	1.31	1.52
1	H	248	PHE	CE2-CZ	9.78	1.55	1.37
1	L	177	SER	CB-OG	9.74	1.54	1.42
1	D	101	ALA	CA-CB	-9.62	1.32	1.52
1	H	248	PHE	CD1-CE1	9.55	1.58	1.39
1	I	454	GLU	CD-OE2	9.52	1.36	1.25
1	F	167	GLU	CD-OE2	9.49	1.36	1.25
1	B	311	TYR	CE2-CZ	9.47	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	40	SER	CB-OG	9.38	1.54	1.42
1	C	453	LYS	CE-NZ	9.37	1.72	1.49
1	F	248	PHE	CE2-CZ	9.35	1.55	1.37
1	L	94	GLU	CD-OE2	9.29	1.35	1.25
1	M	472	GLN	CG-CD	9.27	1.72	1.51
1	C	207	ALA	CA-CB	-9.27	1.32	1.52
1	H	370	GLU	CD-OE2	9.25	1.35	1.25
1	E	390	SER	CB-OG	9.16	1.54	1.42
1	F	35	TYR	CE1-CZ	9.16	1.50	1.38
1	D	252	ARG	CZ-NH2	9.12	1.45	1.33
1	K	115	VAL	CB-CG1	-9.01	1.33	1.52
1	J	125	LYS	CE-NZ	9.00	1.71	1.49
1	D	106	GLU	CG-CD	8.99	1.65	1.51
1	I	189	GLU	CD-OE1	8.99	1.35	1.25
1	B	401	GLU	CD-OE1	8.94	1.35	1.25
1	G	160	GLY	C-O	8.92	1.38	1.23
1	L	225	CYS	CB-SG	-8.90	1.67	1.82
1	L	323	VAL	CB-CG2	-8.89	1.34	1.52
1	E	189	GLU	CD-OE1	8.88	1.35	1.25
1	L	191	LYS	CD-CE	8.87	1.73	1.51
1	G	377	PHE	CE1-CZ	8.87	1.54	1.37
1	J	72	VAL	CB-CG1	-8.86	1.34	1.52
1	J	453	LYS	CD-CE	8.79	1.73	1.51
1	L	454	GLU	CD-OE1	8.73	1.35	1.25
1	M	72	VAL	CB-CG1	-8.73	1.34	1.52
1	E	189	GLU	CD-OE2	8.69	1.35	1.25
1	O	191	LYS	CD-CE	8.68	1.73	1.51
1	H	191	LYS	CD-CE	8.66	1.73	1.51
1	L	252	ARG	CG-CD	8.66	1.73	1.51
1	A	141	GLU	CD-OE2	8.58	1.35	1.25
1	F	248	PHE	CD1-CE1	8.57	1.56	1.39
1	C	248	PHE	CE2-CZ	8.56	1.53	1.37
1	L	375	PHE	CE2-CZ	8.55	1.53	1.37
1	E	20	ALA	N-CA	8.52	1.63	1.46
1	C	311	TYR	CG-CD2	8.50	1.50	1.39
1	D	41	ARG	CZ-NH1	8.49	1.44	1.33
1	D	167	GLU	CG-CD	8.49	1.64	1.51
1	D	439	LYS	CD-CE	8.49	1.72	1.51
1	E	366	ARG	CZ-NH1	8.49	1.44	1.33
1	F	285	SER	CB-OG	8.48	1.53	1.42
1	B	446	LYS	CD-CE	8.48	1.72	1.51
1	E	311	TYR	CG-CD1	8.48	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	271	VAL	CB-CG2	-8.44	1.35	1.52
1	E	380	CYS	CB-SG	-8.44	1.68	1.82
1	L	366	ARG	CZ-NH1	8.44	1.44	1.33
1	D	249	CYS	CB-SG	-8.42	1.68	1.82
1	E	360	LYS	CD-CE	8.41	1.72	1.51
1	K	55	GLY	C-O	8.41	1.37	1.23
1	M	51	ARG	CG-CD	8.40	1.73	1.51
1	E	82	LYS	CD-CE	8.39	1.72	1.51
1	L	194	VAL	CB-CG1	-8.38	1.35	1.52
1	D	191	LYS	CD-CE	8.35	1.72	1.51
1	O	170	ALA	CA-CB	-8.34	1.34	1.52
1	M	257	ALA	CA-CB	-8.34	1.34	1.52
1	L	189	GLU	CD-OE1	8.30	1.34	1.25
1	L	453	LYS	CG-CD	8.28	1.80	1.52
1	N	40	SER	CB-OG	8.27	1.53	1.42
1	G	360	LYS	CD-CE	8.26	1.72	1.51
1	A	177	SER	CB-OG	8.25	1.52	1.42
1	G	189	GLU	CD-OE1	8.23	1.34	1.25
1	D	45	VAL	CB-CG2	-8.20	1.35	1.52
1	N	189	GLU	CD-OE2	8.19	1.34	1.25
1	B	248	PHE	CD1-CE1	8.17	1.55	1.39
1	O	248	PHE	CE2-CZ	8.16	1.52	1.37
1	J	164	ALA	CA-CB	-8.15	1.35	1.52
1	H	82	LYS	CE-NZ	8.14	1.69	1.49
1	E	164	ALA	CA-CB	-8.14	1.35	1.52
1	L	106	GLU	CG-CD	8.13	1.64	1.51
1	A	219	GLU	CG-CD	8.11	1.64	1.51
1	N	345	CYS	CB-SG	-8.11	1.68	1.82
1	K	366	ARG	CZ-NH1	8.09	1.43	1.33
1	O	401	GLU	CG-CD	8.09	1.64	1.51
1	F	89	SER	C-O	8.07	1.38	1.23
1	A	278	LYS	CD-CE	8.06	1.71	1.51
1	L	364	TYR	CE1-CZ	8.04	1.49	1.38
1	G	242	TYR	CE2-CZ	8.03	1.49	1.38
1	J	22	VAL	CB-CG2	-8.03	1.35	1.52
1	G	82	LYS	CE-NZ	8.03	1.69	1.49
1	K	130	GLU	CB-CG	8.03	1.67	1.52
1	O	189	GLU	CD-OE2	8.01	1.34	1.25
1	H	67	ALA	CA-CB	-8.00	1.35	1.52
1	N	248	PHE	CE2-CZ	8.00	1.52	1.37
1	O	368	VAL	CB-CG1	-7.96	1.36	1.52
1	O	453	LYS	CD-CE	7.96	1.71	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	196	GLU	CD-OE2	7.95	1.34	1.25
1	J	147	VAL	CB-CG2	-7.94	1.36	1.52
1	L	453	LYS	CE-NZ	7.92	1.68	1.49
1	L	278	LYS	CE-NZ	7.91	1.68	1.49
1	E	225	CYS	CB-SG	-7.91	1.68	1.82
1	J	276	TYR	CB-CG	7.89	1.63	1.51
1	O	196	GLU	CD-OE1	7.89	1.34	1.25
1	M	453	LYS	CD-CE	7.88	1.71	1.51
1	B	147	VAL	CB-CG2	-7.87	1.36	1.52
1	G	330	PHE	CE1-CZ	7.85	1.52	1.37
1	F	139	VAL	CB-CG2	7.84	1.69	1.52
1	B	20	ALA	CA-CB	7.83	1.69	1.52
1	G	444	LYS	CD-CE	7.83	1.70	1.51
1	F	371	TYR	CE1-CZ	7.83	1.48	1.38
1	H	99	VAL	CB-CG2	-7.83	1.36	1.52
1	G	229	CYS	CB-SG	7.82	1.95	1.82
1	H	94	GLU	CG-CD	7.82	1.63	1.51
1	L	102	CYS	CB-SG	-7.82	1.69	1.82
1	A	20	ALA	CA-CB	7.80	1.68	1.52
1	D	106	GLU	CD-OE2	7.80	1.34	1.25
1	F	370	GLU	CG-CD	7.80	1.63	1.51
1	E	369	GLU	CG-CD	7.80	1.63	1.51
1	I	22	VAL	CB-CG2	-7.80	1.36	1.52
1	B	101	ALA	CA-CB	-7.77	1.36	1.52
1	D	315	LYS	CG-CD	7.77	1.78	1.52
1	M	22	VAL	CB-CG2	-7.77	1.36	1.52
1	A	67	ALA	CA-CB	-7.76	1.36	1.52
1	M	40	SER	CB-OG	7.76	1.52	1.42
1	F	157	CYS	CB-SG	7.74	1.95	1.82
1	K	252	ARG	CZ-NH1	7.74	1.43	1.33
1	C	453	LYS	CD-CE	7.73	1.70	1.51
1	J	171	LYS	CE-NZ	7.73	1.68	1.49
1	N	365	SER	CB-OG	7.73	1.52	1.42
1	E	141	GLU	CD-OE1	7.71	1.34	1.25
1	J	125	LYS	CD-CE	7.70	1.70	1.51
1	O	189	GLU	CD-OE1	7.70	1.34	1.25
1	G	97	ARG	CZ-NH1	7.69	1.43	1.33
1	K	334	VAL	CA-CB	-7.69	1.38	1.54
1	K	356	TYR	CD1-CE1	-7.68	1.27	1.39
1	N	189	GLU	CD-OE1	7.67	1.34	1.25
1	L	401	GLU	CG-CD	7.67	1.63	1.51
1	I	360	LYS	CE-NZ	7.66	1.68	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	147	VAL	CB-CG1	-7.66	1.36	1.52
1	D	271	VAL	CB-CG1	-7.64	1.36	1.52
1	A	147	VAL	CB-CG2	-7.64	1.36	1.52
1	E	309	LYS	CE-NZ	7.61	1.68	1.49
1	N	360	LYS	CD-CE	7.58	1.70	1.51
1	L	282	MET	CG-SD	7.58	2.00	1.81
1	K	312	TRP	CE3-CZ3	-7.58	1.25	1.38
1	F	369	GLU	CG-CD	7.57	1.63	1.51
1	I	368	VAL	CB-CG1	-7.56	1.36	1.52
1	M	371	TYR	CE2-CZ	-7.55	1.28	1.38
1	N	69	GLN	C-O	-7.54	1.09	1.23
1	G	252	ARG	CZ-NH1	7.53	1.42	1.33
1	M	207	ALA	CA-CB	-7.53	1.36	1.52
1	E	248	PHE	CE2-CZ	7.51	1.51	1.37
1	B	49	TYR	CE2-CZ	-7.51	1.28	1.38
1	J	118	SER	CB-OG	7.50	1.51	1.42
1	A	105	VAL	CB-CG1	-7.49	1.37	1.52
1	H	219	GLU	CD-OE2	7.46	1.33	1.25
1	K	253	GLU	CD-OE2	7.46	1.33	1.25
1	H	189	GLU	CD-OE1	7.45	1.33	1.25
1	H	446	LYS	CD-CE	7.45	1.69	1.51
1	G	468	LYS	CD-CE	7.45	1.69	1.51
1	D	68	TYR	CD2-CE2	7.45	1.50	1.39
1	O	371	TYR	CG-CD1	-7.45	1.29	1.39
1	L	454	GLU	CG-CD	7.43	1.63	1.51
1	A	471	VAL	CB-CG2	7.41	1.68	1.52
1	D	290	VAL	CB-CG2	-7.41	1.37	1.52
1	J	446	LYS	CD-CE	7.41	1.69	1.51
1	N	35	TYR	CE2-CZ	7.40	1.48	1.38
1	H	105	VAL	CB-CG2	-7.40	1.37	1.52
1	G	206	GLY	C-O	7.38	1.35	1.23
1	A	219	GLU	CD-OE1	7.37	1.33	1.25
1	L	66	SER	CB-OG	7.37	1.51	1.42
1	D	444	LYS	CD-CE	7.36	1.69	1.51
1	F	219	GLU	CD-OE1	7.35	1.33	1.25
1	C	157	CYS	CB-SG	7.35	1.94	1.82
1	K	290	VAL	CB-CG2	-7.34	1.37	1.52
1	B	135	ALA	CA-CB	7.33	1.67	1.52
1	C	369	GLU	CD-OE2	7.33	1.33	1.25
1	F	191	LYS	CD-CE	7.32	1.69	1.51
1	N	370	GLU	CG-CD	7.32	1.62	1.51
1	M	454	GLU	CG-CD	7.32	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	189	GLU	CD-OE2	7.31	1.33	1.25
1	M	317	GLN	CG-CD	7.30	1.67	1.51
1	H	365	SER	CB-OG	7.30	1.51	1.42
1	J	71	ARG	CZ-NH1	7.29	1.42	1.33
1	K	70	TYR	CD1-CE1	7.28	1.50	1.39
1	K	291	TYR	CE2-CZ	-7.28	1.29	1.38
1	G	20	ALA	CA-CB	7.27	1.67	1.52
1	O	103	ALA	CA-CB	-7.27	1.37	1.52
1	L	370	GLU	CG-CD	7.27	1.62	1.51
1	E	446	LYS	CE-NZ	7.26	1.67	1.49
1	D	457	SER	CB-OG	7.25	1.51	1.42
1	M	135	ALA	CA-CB	7.25	1.67	1.52
1	G	139	VAL	CB-CG1	7.25	1.68	1.52
1	I	331	VAL	CB-CG2	-7.25	1.37	1.52
1	A	370	GLU	CG-CD	7.25	1.62	1.51
1	F	311	TYR	CE1-CZ	7.24	1.48	1.38
1	O	191	LYS	CE-NZ	7.24	1.67	1.49
1	K	37	ALA	CA-CB	-7.23	1.37	1.52
1	M	446	LYS	CD-CE	7.23	1.69	1.51
1	O	369	GLU	CD-OE2	7.22	1.33	1.25
1	L	391	TYR	CD1-CE1	7.21	1.50	1.39
1	N	380	CYS	CB-SG	-7.20	1.70	1.82
1	D	471	VAL	CB-CG1	-7.19	1.37	1.52
1	E	118	SER	CB-OG	7.19	1.51	1.42
1	O	370	GLU	CG-CD	7.19	1.62	1.51
1	B	253	GLU	CD-OE2	7.18	1.33	1.25
1	M	401	GLU	CG-CD	7.17	1.62	1.51
1	H	140	SER	CB-OG	7.16	1.51	1.42
1	L	446	LYS	CD-CE	7.16	1.69	1.51
1	I	189	GLU	CG-CD	7.16	1.62	1.51
1	O	468	LYS	CE-NZ	7.15	1.67	1.49
1	H	471	VAL	CB-CG1	-7.14	1.37	1.52
1	N	134	ALA	CA-CB	7.13	1.67	1.52
1	O	70	TYR	CD2-CE2	-7.13	1.28	1.39
1	J	106	GLU	CG-CD	7.12	1.62	1.51
1	J	122	PHE	CE2-CZ	-7.12	1.23	1.37
1	J	468	LYS	CD-CE	7.12	1.69	1.51
1	O	397	SER	CB-OG	7.12	1.51	1.42
1	F	189	GLU	CD-OE2	7.11	1.33	1.25
1	O	401	GLU	CD-OE1	7.11	1.33	1.25
1	C	105	VAL	CB-CG1	-7.11	1.38	1.52
1	G	102	CYS	CB-SG	7.10	1.94	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	381	THR	C-O	7.10	1.36	1.23
1	A	94	GLU	CB-CG	7.10	1.65	1.52
1	M	34	PHE	CE2-CZ	-7.10	1.23	1.37
1	J	101	ALA	CA-CB	-7.09	1.37	1.52
1	G	94	GLU	CG-CD	7.09	1.62	1.51
1	H	189	GLU	CD-OE2	7.09	1.33	1.25
1	E	32	SER	CB-OG	7.09	1.51	1.42
1	M	446	LYS	CG-CD	7.08	1.76	1.52
1	D	446	LYS	CD-CE	7.08	1.69	1.51
1	H	141	GLU	CD-OE1	7.07	1.33	1.25
1	N	467	ARG	CZ-NH2	7.05	1.42	1.33
1	L	71	ARG	CZ-NH1	7.05	1.42	1.33
1	O	147	VAL	CB-CG1	-7.04	1.38	1.52
1	E	169	TRP	CG-CD1	-7.04	1.26	1.36
1	D	362	LYS	CE-NZ	7.04	1.66	1.49
1	C	356	TYR	CE1-CZ	-7.02	1.29	1.38
1	J	245	SER	CB-OG	7.02	1.51	1.42
1	E	147	VAL	CB-CG2	-7.02	1.38	1.52
1	M	75	VAL	CB-CG2	-7.02	1.38	1.52
1	H	151	TYR	CD1-CE1	-7.01	1.28	1.39
1	I	161	CYS	CB-SG	-7.01	1.70	1.82
1	K	454	GLU	CD-OE1	7.00	1.33	1.25
1	F	256	PHE	CD2-CE2	6.99	1.53	1.39
1	M	217	LYS	CD-CE	6.99	1.68	1.51
1	M	371	TYR	CD1-CE1	-6.99	1.28	1.39
1	H	370	GLU	CG-CD	6.99	1.62	1.51
1	M	171	LYS	CD-CE	6.99	1.68	1.51
1	N	311	TYR	CE1-CZ	6.99	1.47	1.38
1	A	49	TYR	CG-CD2	-6.98	1.30	1.39
1	B	247	PHE	CE1-CZ	6.98	1.50	1.37
1	J	450	VAL	CB-CG2	-6.96	1.38	1.52
1	B	99	VAL	CB-CG2	-6.96	1.38	1.52
1	C	147	VAL	CB-CG1	-6.96	1.38	1.52
1	D	252	ARG	CZ-NH1	6.94	1.42	1.33
1	I	370	GLU	CD-OE2	6.94	1.33	1.25
1	K	312	TRP	CG-CD1	-6.92	1.27	1.36
1	B	147	VAL	CB-CG1	-6.92	1.38	1.52
1	G	453	LYS	CD-CE	6.91	1.68	1.51
1	F	196	GLU	CD-OE1	6.91	1.33	1.25
1	N	143	VAL	CB-CG2	-6.90	1.38	1.52
1	G	219	GLU	CG-CD	6.89	1.62	1.51
1	D	100	TRP	CE3-CZ3	6.89	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	40	SER	CB-OG	6.89	1.51	1.42
1	J	248	PHE	CD1-CE1	6.88	1.53	1.39
1	F	68	TYR	CG-CD1	-6.87	1.30	1.39
1	C	149	VAL	CB-CG1	-6.86	1.38	1.52
1	C	94	GLU	CD-OE2	6.86	1.33	1.25
1	I	369	GLU	CG-CD	6.86	1.62	1.51
1	E	20	ALA	CA-CB	6.85	1.66	1.52
1	E	401	GLU	CD-OE2	6.84	1.33	1.25
1	K	289	CYS	CB-SG	-6.83	1.70	1.82
1	D	105	VAL	CB-CG1	-6.82	1.38	1.52
1	B	201	VAL	CB-CG1	-6.82	1.38	1.52
1	O	249	CYS	CB-SG	6.82	1.93	1.82
1	J	446	LYS	CG-CD	6.81	1.75	1.52
1	K	248	PHE	CE2-CZ	6.81	1.50	1.37
1	L	368	VAL	CB-CG1	-6.81	1.38	1.52
1	F	331	VAL	CB-CG2	-6.80	1.38	1.52
1	E	83	PHE	C-O	6.79	1.36	1.23
1	O	116	GLY	C-O	6.79	1.34	1.23
1	G	70	TYR	CB-CG	-6.79	1.41	1.51
1	C	220	VAL	CB-CG1	-6.78	1.38	1.52
1	H	248	PHE	CB-CG	-6.78	1.39	1.51
1	A	140	SER	CB-OG	6.77	1.51	1.42
1	O	141	GLU	CB-CG	6.77	1.65	1.52
1	K	83	PHE	CD1-CE1	6.77	1.52	1.39
1	M	169	TRP	CG-CD1	-6.76	1.27	1.36
1	K	141	GLU	CG-CD	6.76	1.62	1.51
1	A	393	GLN	CB-CG	6.76	1.70	1.52
1	E	401	GLU	CD-OE1	6.75	1.33	1.25
1	F	227	SER	CB-OG	6.75	1.51	1.42
1	D	106	GLU	CD-OE1	6.73	1.33	1.25
1	C	300	VAL	CB-CG1	-6.73	1.38	1.52
1	G	365	SER	CB-OG	6.73	1.50	1.42
1	C	471	VAL	CB-CG1	6.72	1.67	1.52
1	O	147	VAL	CB-CG2	-6.72	1.38	1.52
1	J	467	ARG	CZ-NH1	6.72	1.41	1.33
1	L	369	GLU	CD-OE2	6.71	1.33	1.25
1	H	139	VAL	CB-CG2	6.70	1.67	1.52
1	J	27	TYR	CD2-CE2	-6.70	1.29	1.39
1	D	401	GLU	CD-OE1	6.70	1.33	1.25
1	D	65	VAL	CB-CG1	-6.69	1.38	1.52
1	F	20	ALA	N-CA	6.69	1.59	1.46
1	F	139	VAL	CB-CG1	6.69	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	193	THR	CB-CG2	6.69	1.74	1.52
1	F	106	GLU	CD-OE2	6.68	1.32	1.25
1	N	71	ARG	CZ-NH1	6.67	1.41	1.33
1	J	20	ALA	N-CA	6.67	1.59	1.46
1	I	99	VAL	CB-CG1	-6.67	1.38	1.52
1	O	40	SER	CB-OG	6.67	1.50	1.42
1	K	350	SER	CB-OG	6.66	1.50	1.42
1	D	115	VAL	CB-CG1	-6.66	1.38	1.52
1	E	231	TYR	CD2-CE2	-6.66	1.29	1.39
1	K	32	SER	CB-OG	6.65	1.50	1.42
1	B	30	ARG	CZ-NH1	6.64	1.41	1.33
1	B	248	PHE	CE2-CZ	6.64	1.50	1.37
1	M	364	TYR	CG-CD1	-6.63	1.30	1.39
1	L	106	GLU	CD-OE2	6.62	1.32	1.25
1	D	196	GLU	CD-OE1	6.62	1.32	1.25
1	N	123	TYR	CD1-CE1	6.62	1.49	1.39
1	B	91	TYR	CE1-CZ	-6.61	1.29	1.38
1	C	248	PHE	CB-CG	-6.60	1.40	1.51
1	M	219	GLU	CD-OE2	6.60	1.32	1.25
1	B	401	GLU	CD-OE2	6.60	1.32	1.25
1	N	448	TRP	CB-CG	-6.59	1.38	1.50
1	F	32	SER	CB-OG	6.59	1.50	1.42
1	O	247	PHE	CE1-CZ	6.59	1.49	1.37
1	E	72	VAL	CB-CG1	-6.58	1.39	1.52
1	C	247	PHE	CG-CD1	-6.58	1.28	1.38
1	C	99	VAL	CB-CG2	-6.58	1.39	1.52
1	D	347	SER	CB-OG	-6.57	1.33	1.42
1	N	450	VAL	CB-CG2	-6.57	1.39	1.52
1	D	176	LYS	CD-CE	6.56	1.67	1.51
1	O	20	ALA	CA-CB	6.56	1.66	1.52
1	L	454	GLU	CB-CG	6.55	1.64	1.52
1	H	402	ASP	CB-CG	6.55	1.65	1.51
1	C	141	GLU	CB-CG	6.55	1.64	1.52
1	L	311	TYR	CG-CD2	6.55	1.47	1.39
1	L	94	GLU	CD-OE1	6.55	1.32	1.25
1	L	454	GLU	CD-OE2	6.55	1.32	1.25
1	L	253	GLU	CG-CD	6.54	1.61	1.51
1	N	106	GLU	CG-CD	6.54	1.61	1.51
1	E	453	LYS	CE-NZ	6.54	1.65	1.49
1	F	20	ALA	CA-CB	6.54	1.66	1.52
1	L	391	TYR	CD2-CE2	6.54	1.49	1.39
1	A	83	PHE	CE2-CZ	6.53	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	106	GLU	CG-CD	6.53	1.61	1.51
1	H	205	TYR	CD1-CE1	6.52	1.49	1.39
1	O	174	ALA	CA-CB	6.52	1.66	1.52
1	O	248	PHE	CE1-CZ	6.52	1.49	1.37
1	E	40	SER	CB-OG	6.51	1.50	1.42
1	E	83	PHE	CD1-CE1	6.51	1.52	1.39
1	G	454	GLU	CD-OE1	6.50	1.32	1.25
1	L	401	GLU	CD-OE1	6.50	1.32	1.25
1	D	94	GLU	CB-CG	6.49	1.64	1.52
1	G	94	GLU	CD-OE2	6.49	1.32	1.25
1	G	174	ALA	CA-CB	6.48	1.66	1.52
1	G	309	LYS	CE-NZ	6.47	1.65	1.49
1	E	140	SER	CB-OG	6.47	1.50	1.42
1	L	257	ALA	CA-CB	-6.47	1.38	1.52
1	L	401	GLU	CD-OE2	6.46	1.32	1.25
1	E	99	VAL	CB-CG2	-6.46	1.39	1.52
1	N	100	TRP	CE3-CZ3	6.46	1.49	1.38
1	B	70	TYR	CD2-CE2	-6.46	1.29	1.39
1	H	76	GLN	CG-CD	6.45	1.65	1.51
1	E	370	GLU	CG-CD	6.44	1.61	1.51
1	G	260	PHE	CE1-CZ	6.44	1.49	1.37
1	O	369	GLU	CD-OE1	6.44	1.32	1.25
1	N	70	TYR	CE1-CZ	6.43	1.47	1.38
1	K	94	GLU	CD-OE1	6.42	1.32	1.25
1	K	99	VAL	CB-CG2	-6.42	1.39	1.52
1	D	94	GLU	CG-CD	6.42	1.61	1.51
1	F	454	GLU	CD-OE1	6.42	1.32	1.25
1	D	234	TYR	CG-CD2	-6.42	1.30	1.39
1	G	40	SER	CB-OG	6.42	1.50	1.42
1	L	27	TYR	CE2-CZ	-6.42	1.30	1.38
1	J	334	VAL	CB-CG2	-6.41	1.39	1.52
1	M	312	TRP	CE2-CZ2	-6.41	1.28	1.39
1	M	304	SER	CB-OG	6.41	1.50	1.42
1	D	135	ALA	CA-CB	6.40	1.65	1.52
1	I	388	VAL	CB-CG2	-6.40	1.39	1.52
1	I	201	VAL	CB-CG1	-6.40	1.39	1.52
1	B	276	TYR	CG-CD1	6.39	1.47	1.39
1	L	276	TYR	CD2-CE2	-6.39	1.29	1.39
1	A	174	ALA	CA-CB	6.39	1.65	1.52
1	A	371	TYR	CZ-OH	6.39	1.48	1.37
1	M	456	PHE	CD2-CE2	-6.39	1.26	1.39
1	A	253	GLU	CG-CD	6.39	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	139	VAL	CA-CB	6.38	1.68	1.54
1	J	167	GLU	CG-CD	6.38	1.61	1.51
1	K	309	LYS	CE-NZ	6.38	1.65	1.49
1	O	311	TYR	CG-CD2	6.38	1.47	1.39
1	O	242	TYR	CE2-CZ	6.38	1.46	1.38
1	O	139	VAL	CB-CG1	6.37	1.66	1.52
1	B	123	TYR	CB-CG	-6.37	1.42	1.51
1	B	202	ASP	CB-CG	6.36	1.65	1.51
1	N	115	VAL	CB-CG1	-6.36	1.39	1.52
1	O	183	GLY	C-O	-6.35	1.13	1.23
1	A	404	ASN	C-O	6.34	1.35	1.23
1	C	312	TRP	CE2-CZ2	-6.33	1.28	1.39
1	A	56	GLY	N-CA	6.33	1.55	1.46
1	C	370	GLU	CG-CD	6.32	1.61	1.51
1	F	71	ARG	CZ-NH1	6.32	1.41	1.33
1	A	257	ALA	CA-CB	-6.31	1.39	1.52
1	G	468	LYS	CE-NZ	6.31	1.64	1.49
1	G	135	ALA	CA-CB	6.30	1.65	1.52
1	I	370	GLU	CG-CD	6.30	1.61	1.51
1	F	468	LYS	CE-NZ	6.30	1.64	1.49
1	F	40	SER	CB-OG	6.30	1.50	1.42
1	B	256	PHE	CD1-CE1	-6.29	1.26	1.39
1	D	151	TYR	CE1-CZ	-6.29	1.30	1.38
1	B	167	GLU	CB-CG	-6.29	1.40	1.52
1	G	401	GLU	CD-OE1	6.29	1.32	1.25
1	A	232	PRO	N-CD	-6.29	1.39	1.47
1	H	311	TYR	CD1-CE1	6.28	1.48	1.39
1	G	149	VAL	CB-CG2	-6.28	1.39	1.52
1	G	371	TYR	CE1-CZ	6.28	1.46	1.38
1	O	252	ARG	CZ-NH1	6.28	1.41	1.33
1	E	253	GLU	CD-OE2	6.28	1.32	1.25
1	C	252	ARG	CZ-NH1	6.27	1.41	1.33
1	I	176	LYS	CD-CE	6.27	1.67	1.51
1	C	249	CYS	CB-SG	6.27	1.93	1.82
1	A	219	GLU	CD-OE2	6.26	1.32	1.25
1	M	139	VAL	CB-CG2	6.25	1.66	1.52
1	B	377	PHE	CG-CD2	6.25	1.48	1.38
1	D	455	LYS	CE-NZ	6.25	1.64	1.49
1	H	88	THR	CA-CB	6.25	1.69	1.53
1	N	298	SER	CB-OG	6.25	1.50	1.42
1	A	147	VAL	CB-CG1	-6.24	1.39	1.52
1	B	225	CYS	CB-SG	-6.24	1.71	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	115	VAL	CB-CG1	-6.24	1.39	1.52
1	B	34	PHE	CD1-CE1	-6.24	1.26	1.39
1	D	333	VAL	CB-CG2	-6.24	1.39	1.52
1	E	248	PHE	CB-CG	-6.24	1.40	1.51
1	I	134	ALA	CA-CB	6.24	1.65	1.52
1	C	181	SER	CB-OG	6.24	1.50	1.42
1	C	163	PRO	CB-CG	-6.23	1.18	1.50
1	O	219	GLU	CD-OE2	6.23	1.32	1.25
1	D	177	SER	CA-CB	6.23	1.62	1.52
1	J	20	ALA	CA-CB	6.23	1.65	1.52
1	E	141	GLU	CD-OE2	6.22	1.32	1.25
1	M	189	GLU	CG-CD	6.22	1.61	1.51
1	N	191	LYS	CD-CE	6.21	1.66	1.51
1	I	366	ARG	CZ-NH2	6.20	1.41	1.33
1	M	369	GLU	CD-OE2	6.20	1.32	1.25
1	M	447	PHE	CE1-CZ	-6.20	1.25	1.37
1	C	446	LYS	CD-CE	6.19	1.66	1.51
1	N	331	VAL	CB-CG2	-6.19	1.39	1.52
1	H	360	LYS	CD-CE	6.18	1.66	1.51
1	D	325	TRP	CG-CD1	-6.18	1.28	1.36
1	K	401	GLU	CD-OE2	6.17	1.32	1.25
1	I	317	GLN	CG-CD	6.17	1.65	1.51
1	K	338	ARG	CZ-NH1	6.17	1.41	1.33
1	O	141	GLU	CD-OE2	6.17	1.32	1.25
1	J	103	ALA	CA-CB	-6.16	1.39	1.52
1	L	82	LYS	CD-CE	6.16	1.66	1.51
1	A	278	LYS	CE-NZ	6.16	1.64	1.49
1	G	21	VAL	CB-CG2	6.16	1.65	1.52
1	N	290	VAL	CB-CG1	-6.16	1.40	1.52
1	B	311	TYR	CZ-OH	6.15	1.48	1.37
1	G	137	SER	CB-OG	6.15	1.50	1.42
1	B	369	GLU	CG-CD	6.14	1.61	1.51
1	N	247	PHE	CE2-CZ	-6.14	1.25	1.37
1	D	94	GLU	CD-OE1	6.13	1.32	1.25
1	F	334	VAL	CB-CG1	-6.13	1.40	1.52
1	J	54	ALA	CA-CB	6.13	1.65	1.52
1	E	253	GLU	CG-CD	6.12	1.61	1.51
1	A	371	TYR	CE2-CZ	6.12	1.46	1.38
1	F	465	LEU	CG-CD1	6.12	1.74	1.51
1	J	49	TYR	CZ-OH	6.12	1.48	1.37
1	O	168	HIS	C-O	-6.12	1.11	1.23
1	M	94	GLU	CD-OE1	6.12	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	454	GLU	CD-OE2	6.12	1.32	1.25
1	A	311	TYR	CG-CD2	6.10	1.47	1.39
1	G	401	GLU	CB-CG	6.10	1.63	1.52
1	H	369	GLU	CG-CD	6.10	1.61	1.51
1	F	369	GLU	CD-OE1	6.10	1.32	1.25
1	G	276	TYR	CD2-CE2	6.10	1.48	1.39
1	K	300	VAL	CB-CG1	-6.10	1.40	1.52
1	E	85	LEU	C-O	6.09	1.34	1.23
1	G	189	GLU	CG-CD	6.09	1.61	1.51
1	H	106	GLU	CD-OE1	6.08	1.32	1.25
1	F	315	LYS	CG-CD	6.08	1.73	1.52
1	L	125	LYS	CE-NZ	6.08	1.64	1.49
1	C	151	TYR	CE1-CZ	-6.08	1.30	1.38
1	G	93	PRO	C-O	6.08	1.35	1.23
1	O	71	ARG	CZ-NH1	6.08	1.41	1.33
1	B	304	SER	CB-OG	6.07	1.50	1.42
1	J	345	CYS	CB-SG	6.06	1.92	1.82
1	A	20	ALA	N-CA	6.06	1.58	1.46
1	B	123	TYR	CG-CD2	-6.06	1.31	1.39
1	I	40	SER	CB-OG	6.06	1.50	1.42
1	K	72	VAL	C-O	-6.06	1.11	1.23
1	N	360	LYS	CE-NZ	6.06	1.64	1.49
1	L	315	LYS	CD-CE	6.06	1.66	1.51
1	K	453	LYS	CE-NZ	6.05	1.64	1.49
1	I	73	PHE	CE1-CZ	-6.05	1.25	1.37
1	C	247	PHE	CE2-CZ	-6.05	1.25	1.37
1	H	376	ILE	CB-CG2	-6.05	1.34	1.52
1	O	149	VAL	CB-CG2	-6.05	1.40	1.52
1	N	469	PHE	CE2-CZ	-6.04	1.25	1.37
1	L	151	TYR	CE2-CZ	6.04	1.46	1.38
1	A	101	ALA	CA-CB	-6.04	1.39	1.52
1	A	401	GLU	CG-CD	6.04	1.61	1.51
1	C	70	TYR	CD2-CE2	-6.04	1.30	1.39
1	D	353	PRO	CB-CG	6.03	1.80	1.50
1	G	278	LYS	CE-NZ	6.03	1.64	1.49
1	I	248	PHE	CD1-CE1	6.03	1.51	1.39
1	M	94	GLU	CD-OE2	6.03	1.32	1.25
1	A	272	PRO	N-CA	-6.03	1.37	1.47
1	F	307	PHE	CE2-CZ	6.03	1.48	1.37
1	C	294	SER	CA-CB	-6.02	1.44	1.52
1	C	311	TYR	CG-CD1	6.02	1.47	1.39
1	A	40	SER	CB-OG	6.02	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	444	LYS	CD-CE	6.01	1.66	1.51
1	J	220	VAL	CB-CG2	-6.01	1.40	1.52
1	G	401	GLU	CG-CD	6.00	1.60	1.51
1	G	118	SER	CB-OG	6.00	1.50	1.42
1	G	149	VAL	CB-CG1	-5.99	1.40	1.52
1	O	368	VAL	CB-CG2	-5.99	1.40	1.52
1	L	167	GLU	CG-CD	5.98	1.60	1.51
1	M	65	VAL	CB-CG2	-5.98	1.40	1.52
1	M	123	TYR	CD2-CE2	5.98	1.48	1.39
1	H	225	CYS	CB-SG	-5.98	1.72	1.81
1	H	151	TYR	CD2-CE2	-5.98	1.30	1.39
1	F	82	LYS	CE-NZ	5.97	1.64	1.49
1	B	401	GLU	CB-CG	5.96	1.63	1.52
1	G	82	LYS	CD-CE	5.96	1.66	1.51
1	K	450	VAL	CB-CG1	-5.96	1.40	1.52
1	O	331	VAL	CB-CG1	-5.96	1.40	1.52
1	C	339	SER	CB-OG	5.96	1.50	1.42
1	N	219	GLU	CD-OE1	5.96	1.32	1.25
1	J	455	LYS	CE-NZ	5.96	1.64	1.49
1	K	307	PHE	C-O	-5.96	1.12	1.23
1	I	371	TYR	CG-CD2	-5.96	1.31	1.39
1	O	312	TRP	CE3-CZ3	-5.96	1.28	1.38
1	K	220	VAL	CB-CG1	-5.96	1.40	1.52
1	A	53	PRO	N-CD	5.95	1.56	1.47
1	E	248	PHE	CD1-CE1	5.95	1.51	1.39
1	M	299	ILE	CA-CB	-5.95	1.41	1.54
1	N	45	VAL	CB-CG2	-5.95	1.40	1.52
1	J	311	TYR	CG-CD2	5.95	1.46	1.39
1	I	158	ILE	CB-CG2	-5.94	1.34	1.52
1	C	178	ARG	CZ-NH1	5.94	1.40	1.33
1	F	191	LYS	CG-CD	5.94	1.72	1.52
1	M	225	CYS	CB-SG	-5.94	1.72	1.81
1	H	134	ALA	CA-CB	5.94	1.65	1.52
1	F	167	GLU	CG-CD	5.93	1.60	1.51
1	H	106	GLU	CG-CD	5.93	1.60	1.51
1	E	86	PRO	C-O	5.93	1.35	1.23
1	H	251	ARG	NE-CZ	5.92	1.40	1.33
1	B	231	TYR	CD2-CE2	-5.92	1.30	1.39
1	A	325	TRP	CG-CD1	-5.92	1.28	1.36
1	I	248	PHE	CB-CG	-5.92	1.41	1.51
1	O	446	LYS	CD-CE	5.91	1.66	1.51
1	B	278	LYS	CD-CE	5.90	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	164	ALA	CA-CB	-5.90	1.40	1.52
1	L	220	VAL	CB-CG2	-5.90	1.40	1.52
1	L	278	LYS	CD-CE	5.90	1.66	1.51
1	L	291	TYR	CE2-CZ	5.90	1.46	1.38
1	N	106	GLU	CD-OE1	5.89	1.32	1.25
1	J	468	LYS	CE-NZ	5.88	1.63	1.49
1	A	446	LYS	CD-CE	5.88	1.66	1.51
1	N	289	CYS	CB-SG	5.88	1.92	1.82
1	G	446	LYS	CD-CE	5.87	1.66	1.51
1	G	330	PHE	C-O	5.86	1.34	1.23
1	L	181	SER	CB-OG	5.86	1.49	1.42
1	I	225	CYS	CB-SG	-5.86	1.72	1.81
1	N	89	SER	C-O	5.85	1.34	1.23
1	E	282	MET	CG-SD	5.85	1.96	1.81
1	E	65	VAL	CB-CG1	-5.85	1.40	1.52
1	E	369	GLU	CD-OE2	5.85	1.32	1.25
1	G	248	PHE	CE2-CZ	5.85	1.48	1.37
1	B	197	ASP	C-O	-5.84	1.12	1.23
1	H	101	ALA	CA-CB	-5.84	1.40	1.52
1	O	51	ARG	CZ-NH2	5.84	1.40	1.33
1	J	21	VAL	CB-CG1	-5.84	1.40	1.52
1	F	91	TYR	CE2-CZ	5.84	1.46	1.38
1	N	401	GLU	CG-CD	5.84	1.60	1.51
1	E	67	ALA	CA-CB	-5.83	1.40	1.52
1	O	342	LEU	C-O	5.83	1.34	1.23
1	O	453	LYS	CG-CD	5.83	1.72	1.52
1	A	215	ASP	CB-CG	5.83	1.64	1.51
1	H	401	GLU	CD-OE1	5.83	1.32	1.25
1	K	135	ALA	CA-CB	5.83	1.64	1.52
1	O	300	VAL	CB-CG1	-5.82	1.40	1.52
1	B	472	GLN	C-O	5.82	1.34	1.23
1	F	366	ARG	CZ-NH1	5.81	1.40	1.33
1	G	20	ALA	N-CA	5.81	1.57	1.46
1	K	401	GLU	CG-CD	5.81	1.60	1.51
1	L	456	PHE	CD2-CE2	-5.80	1.27	1.39
1	N	456	PHE	CB-CG	-5.80	1.41	1.51
1	F	34	PHE	CE1-CZ	5.79	1.48	1.37
1	K	94	GLU	CB-CG	5.79	1.63	1.52
1	B	401	GLU	CG-CD	5.79	1.60	1.51
1	F	137	SER	CB-OG	5.79	1.49	1.42
1	M	468	LYS	CE-NZ	5.78	1.63	1.49
1	D	196	GLU	CD-OE2	5.78	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	207	ALA	CA-CB	-5.77	1.40	1.52
1	C	337	THR	CB-CG2	-5.77	1.33	1.52
1	M	290	VAL	CB-CG2	-5.77	1.40	1.52
1	B	276	TYR	CE2-CZ	5.77	1.46	1.38
1	D	103	ALA	CA-CB	-5.77	1.40	1.52
1	G	454	GLU	CG-CD	5.77	1.60	1.51
1	N	185	CYS	CB-SG	-5.77	1.72	1.81
1	F	360	LYS	CD-CE	5.76	1.65	1.51
1	A	82	LYS	CD-CE	5.76	1.65	1.51
1	O	213	LEU	CG-CD1	-5.75	1.30	1.51
1	O	49	TYR	CD1-CE1	-5.75	1.30	1.39
1	B	100	TRP	CG-CD1	-5.75	1.28	1.36
1	C	205	TYR	CG-CD2	-5.75	1.31	1.39
1	B	210	PHE	CB-CG	-5.75	1.41	1.51
1	G	64	LYS	CG-CD	5.75	1.72	1.52
1	H	323	VAL	CB-CG1	-5.74	1.40	1.52
1	B	368	VAL	CB-CG1	-5.74	1.40	1.52
1	H	253	GLU	CG-CD	5.74	1.60	1.51
1	J	204	GLY	N-CA	-5.74	1.37	1.46
1	N	364	TYR	CD2-CE2	5.74	1.48	1.39
1	G	34	PHE	CG-CD2	5.73	1.47	1.38
1	J	83	PHE	CE2-CZ	5.73	1.48	1.37
1	M	454	GLU	CD-OE1	5.73	1.31	1.25
1	F	463	TYR	CD2-CE2	5.73	1.48	1.39
1	O	446	LYS	CG-CD	5.73	1.72	1.52
1	I	141	GLU	CD-OE2	5.73	1.31	1.25
1	A	83	PHE	CG-CD1	5.72	1.47	1.38
1	B	444	LYS	CD-CE	5.72	1.65	1.51
1	E	90	ILE	C-O	5.71	1.34	1.23
1	B	191	LYS	CD-CE	5.70	1.65	1.51
1	I	398	SER	CB-OG	5.70	1.49	1.42
1	B	290	VAL	CB-CG1	-5.70	1.40	1.52
1	L	139	VAL	CB-CG1	5.70	1.64	1.52
1	I	366	ARG	CZ-NH1	5.70	1.40	1.33
1	K	311	TYR	CZ-OH	5.70	1.47	1.37
1	O	167	GLU	CG-CD	5.70	1.60	1.51
1	D	444	LYS	CE-NZ	5.69	1.63	1.49
1	B	370	GLU	CG-CD	5.69	1.60	1.51
1	F	94	GLU	CD-OE2	5.69	1.31	1.25
1	J	149	VAL	CB-CG1	-5.69	1.41	1.52
1	D	70	TYR	CD1-CE1	-5.69	1.30	1.39
1	N	300	VAL	CB-CG1	-5.69	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	52	VAL	CA-CB	-5.68	1.42	1.54
1	D	47	ASP	C-O	5.68	1.34	1.23
1	C	118	SER	CB-OG	5.68	1.49	1.42
1	C	231	TYR	CD1-CE1	5.68	1.47	1.39
1	K	360	LYS	CD-CE	5.67	1.65	1.51
1	O	453	LYS	CE-NZ	5.67	1.63	1.49
1	A	371	TYR	CD1-CE1	-5.67	1.30	1.39
1	A	442	TYR	CD2-CE2	5.67	1.47	1.39
1	D	256	PHE	CD1-CE1	5.67	1.50	1.39
1	F	106	GLU	CD-OE1	5.67	1.31	1.25
1	N	229	CYS	CB-SG	5.67	1.91	1.82
1	J	366	ARG	CZ-NH1	5.66	1.40	1.33
1	G	189	GLU	CD-OE2	5.66	1.31	1.25
1	O	189	GLU	CG-CD	5.66	1.60	1.51
1	E	149	VAL	CB-CG1	-5.66	1.41	1.52
1	G	65	VAL	CB-CG1	-5.66	1.41	1.52
1	A	377	PHE	CE2-CZ	5.65	1.48	1.37
1	B	42	LEU	C-O	-5.65	1.12	1.23
1	D	368	VAL	CB-CG1	-5.65	1.41	1.52
1	I	191	LYS	CD-CE	5.65	1.65	1.51
1	J	309	LYS	CD-CE	5.64	1.65	1.51
1	E	170	ALA	CA-CB	-5.64	1.40	1.52
1	E	247	PHE	CE1-CZ	5.64	1.48	1.37
1	J	91	TYR	CE2-CZ	5.64	1.45	1.38
1	N	50	PHE	CB-CG	-5.64	1.41	1.51
1	O	115	VAL	CB-CG1	-5.64	1.41	1.52
1	D	82	LYS	CE-NZ	5.64	1.63	1.49
1	K	446	LYS	CD-CE	5.64	1.65	1.51
1	L	463	TYR	CD2-CE2	5.63	1.47	1.39
1	B	362	LYS	CE-NZ	5.63	1.63	1.49
1	G	311	TYR	CG-CD2	5.63	1.46	1.39
1	H	172	GLY	N-CA	-5.63	1.37	1.46
1	L	194	VAL	CA-CB	-5.63	1.43	1.54
1	N	307	PHE	CB-CG	-5.62	1.41	1.51
1	A	72	VAL	CB-CG1	-5.62	1.41	1.52
1	C	94	GLU	CD-OE1	5.62	1.31	1.25
1	L	444	LYS	CE-NZ	5.62	1.63	1.49
1	H	251	ARG	CZ-NH1	5.62	1.40	1.33
1	A	167	GLU	CG-CD	5.62	1.60	1.51
1	G	362	LYS	CE-NZ	5.62	1.63	1.49
1	I	360	LYS	CD-CE	5.62	1.65	1.51
1	O	205	TYR	CE2-CZ	-5.62	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	99	VAL	CB-CG2	-5.62	1.41	1.52
1	B	167	GLU	CG-CD	5.62	1.60	1.51
1	D	446	LYS	CE-NZ	5.61	1.63	1.49
1	J	191	LYS	CD-CE	5.61	1.65	1.51
1	C	253	GLU	CD-OE1	5.61	1.31	1.25
1	O	317	GLN	CG-CD	5.60	1.64	1.51
1	F	115	VAL	CB-CG1	-5.60	1.41	1.52
1	F	242	TYR	C-O	5.60	1.33	1.23
1	F	189	GLU	CG-CD	5.59	1.60	1.51
1	K	461	ASP	CB-CG	5.59	1.63	1.51
1	N	169	TRP	CB-CG	-5.58	1.40	1.50
1	F	312	TRP	CB-CG	-5.58	1.40	1.50
1	L	443	ASP	CB-CG	5.58	1.63	1.51
1	G	253	GLU	CB-CG	5.58	1.62	1.52
1	C	446	LYS	CG-CD	5.58	1.71	1.52
1	C	312	TRP	CG-CD1	-5.57	1.28	1.36
1	G	220	VAL	CB-CG1	-5.57	1.41	1.52
1	F	271	VAL	CB-CG2	-5.57	1.41	1.52
1	K	369	GLU	CD-OE2	5.57	1.31	1.25
1	O	72	VAL	CA-CB	-5.57	1.43	1.54
1	H	245	SER	CB-OG	5.57	1.49	1.42
1	L	463	TYR	CD1-CE1	5.57	1.47	1.39
1	E	51	ARG	CG-CD	5.57	1.65	1.51
1	G	88	THR	CB-CG2	5.57	1.70	1.52
1	I	72	VAL	CA-CB	-5.57	1.43	1.54
1	L	369	GLU	CG-CD	5.56	1.60	1.51
1	C	139	VAL	CB-CG1	5.56	1.64	1.52
1	D	240	ASP	C-O	5.56	1.33	1.23
1	J	137	SER	CA-CB	5.55	1.61	1.52
1	F	141	GLU	CB-CG	5.55	1.62	1.52
1	E	63	PRO	CB-CG	-5.55	1.22	1.50
1	I	336	THR	CB-CG2	-5.55	1.34	1.52
1	O	242	TYR	CG-CD1	5.55	1.46	1.39
1	F	176	LYS	CE-NZ	5.55	1.62	1.49
1	J	207	ALA	CA-CB	-5.55	1.40	1.52
1	L	231	TYR	CD1-CE1	5.54	1.47	1.39
1	D	194	VAL	CB-CG1	-5.54	1.41	1.52
1	G	242	TYR	CG-CD2	5.54	1.46	1.39
1	B	139	VAL	CB-CG1	5.54	1.64	1.52
1	N	105	VAL	CB-CG2	-5.53	1.41	1.52
1	F	105	VAL	CB-CG2	-5.52	1.41	1.52
1	C	469	PHE	CE2-CZ	5.52	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	404	ASN	CB-CG	5.51	1.63	1.51
1	E	189	GLU	CG-CD	5.51	1.60	1.51
1	E	239	ALA	CA-CB	-5.51	1.40	1.52
1	J	251	ARG	CZ-NH2	5.51	1.40	1.33
1	E	242	TYR	CZ-OH	5.50	1.47	1.37
1	I	77	LEU	CG-CD1	-5.50	1.31	1.51
1	A	97	ARG	CZ-NH2	5.50	1.40	1.33
1	O	401	GLU	CD-OE2	5.50	1.31	1.25
1	I	149	VAL	CB-CG2	-5.50	1.41	1.52
1	I	278	LYS	CD-CE	5.49	1.65	1.51
1	L	247	PHE	CE2-CZ	-5.49	1.26	1.37
1	K	106	GLU	CG-CD	5.49	1.60	1.51
1	K	155	GLN	C-O	-5.49	1.12	1.23
1	M	106	GLU	CD-OE1	5.49	1.31	1.25
1	M	219	GLU	CD-OE1	5.49	1.31	1.25
1	B	227	SER	CB-OG	5.49	1.49	1.42
1	H	28	VAL	CB-CG1	5.49	1.64	1.52
1	M	360	LYS	CG-CD	5.49	1.71	1.52
1	A	155	GLN	CB-CG	-5.48	1.37	1.52
1	N	368	VAL	C-O	-5.48	1.12	1.23
1	D	369	GLU	CG-CD	5.48	1.60	1.51
1	F	461	ASP	CG-OD2	5.47	1.38	1.25
1	O	83	PHE	CG-CD2	5.47	1.47	1.38
1	H	472	GLN	CG-CD	5.47	1.63	1.51
1	F	134	ALA	CA-CB	5.47	1.64	1.52
1	G	307	PHE	CE1-CZ	5.47	1.47	1.37
1	F	330	PHE	CE1-CZ	5.46	1.47	1.37
1	C	94	GLU	CB-CG	5.46	1.62	1.52
1	E	307	PHE	CB-CG	-5.46	1.42	1.51
1	A	401	GLU	CD-OE1	5.46	1.31	1.25
1	E	52	VAL	CA-CB	-5.46	1.43	1.54
1	F	455	LYS	CD-CE	5.46	1.64	1.51
1	F	468	LYS	CD-CE	5.45	1.64	1.51
1	M	94	GLU	CG-CD	5.45	1.60	1.51
1	B	105	VAL	CA-CB	-5.45	1.43	1.54
1	I	94	GLU	CG-CD	5.45	1.60	1.51
1	K	169	TRP	CG-CD1	-5.45	1.29	1.36
1	M	173	THR	C-O	5.45	1.33	1.23
1	G	366	ARG	CZ-NH1	5.44	1.40	1.33
1	B	68	TYR	CB-CG	-5.44	1.43	1.51
1	D	136	THR	C-O	5.44	1.33	1.23
1	L	67	ALA	CA-CB	-5.44	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	GLU	CD-OE1	5.43	1.31	1.25
1	B	178	ARG	CZ-NH1	5.43	1.40	1.33
1	D	248	PHE	CB-CG	-5.43	1.42	1.51
1	F	137	SER	CA-CB	5.43	1.61	1.52
1	H	311	TYR	CG-CD2	5.43	1.46	1.39
1	M	189	GLU	CD-OE2	5.43	1.31	1.25
1	C	369	GLU	CD-OE1	5.42	1.31	1.25
1	A	76	GLN	CG-CD	5.42	1.63	1.51
1	E	368	VAL	CB-CG1	-5.42	1.41	1.52
1	E	454	GLU	CD-OE1	5.42	1.31	1.25
1	C	27	TYR	CG-CD2	-5.42	1.32	1.39
1	F	176	LYS	CD-CE	5.42	1.64	1.51
1	A	196	GLU	CD-OE1	5.42	1.31	1.25
1	G	369	GLU	CD-OE2	5.42	1.31	1.25
1	K	473	ALA	CA-CB	-5.42	1.41	1.52
1	L	141	GLU	CG-CD	5.42	1.60	1.51
1	D	401	GLU	CG-CD	5.41	1.60	1.51
1	F	391	TYR	CD1-CE1	5.41	1.47	1.39
1	B	52	VAL	CA-CB	-5.40	1.43	1.54
1	J	338	ARG	CZ-NH2	5.40	1.40	1.33
1	G	247	PHE	CE1-CZ	5.39	1.47	1.37
1	N	59	LYS	CG-CD	5.39	1.70	1.52
1	F	311	TYR	CZ-OH	5.39	1.47	1.37
1	L	192	ASN	C-O	-5.39	1.13	1.23
1	L	467	ARG	CZ-NH2	5.39	1.40	1.33
1	E	157	CYS	CB-SG	5.39	1.91	1.82
1	F	101	ALA	C-O	5.38	1.33	1.23
1	B	100	TRP	CE2-CZ2	-5.38	1.30	1.39
1	B	438	ASN	N-CA	5.38	1.57	1.46
1	D	252	ARG	NE-CZ	5.38	1.40	1.33
1	G	293	PRO	N-CA	-5.38	1.38	1.47
1	O	141	GLU	CG-CD	5.38	1.60	1.51
1	M	197	ASP	C-O	-5.38	1.13	1.23
1	H	59	LYS	CE-NZ	5.38	1.62	1.49
1	M	40	SER	CA-CB	5.37	1.61	1.52
1	D	311	TYR	CG-CD2	5.37	1.46	1.39
1	K	308	ASN	C-O	-5.37	1.13	1.23
1	A	189	GLU	CD-OE1	5.36	1.31	1.25
1	J	151	TYR	CG-CD2	5.36	1.46	1.39
1	N	101	ALA	CA-CB	-5.36	1.41	1.52
1	C	140	SER	C-O	5.36	1.33	1.23
1	E	439	LYS	CG-CD	5.36	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	404	ASN	C-O	5.36	1.33	1.23
1	G	187	PRO	C-O	5.36	1.33	1.23
1	I	99	VAL	CB-CG2	-5.36	1.41	1.52
1	D	72	VAL	CB-CG1	-5.35	1.41	1.52
1	D	132	SER	C-O	5.35	1.33	1.23
1	H	207	ALA	CA-CB	-5.35	1.41	1.52
1	G	256	PHE	CE1-CZ	-5.35	1.27	1.37
1	N	454	GLU	CG-CD	5.35	1.59	1.51
1	G	348	THR	CB-CG2	5.35	1.70	1.52
1	H	152	LYS	CD-CE	5.35	1.64	1.51
1	D	135	ALA	C-O	5.35	1.33	1.23
1	M	64	LYS	CE-NZ	5.35	1.62	1.49
1	O	311	TYR	CZ-OH	5.35	1.47	1.37
1	G	211	SER	CB-OG	5.34	1.49	1.42
1	K	74	ARG	CZ-NH1	5.34	1.40	1.33
1	H	196	GLU	CD-OE1	5.34	1.31	1.25
1	C	455	LYS	CE-NZ	5.34	1.62	1.49
1	J	339	SER	CB-OG	5.34	1.49	1.42
1	N	331	VAL	CA-CB	-5.34	1.43	1.54
1	D	447	PHE	CB-CG	-5.34	1.42	1.51
1	E	448	TRP	CB-CG	-5.34	1.40	1.50
1	C	253	GLU	C-O	-5.33	1.13	1.23
1	M	130	GLU	CB-CG	5.33	1.62	1.52
1	B	278	LYS	CE-NZ	5.33	1.62	1.49
1	G	232	PRO	CG-CD	5.33	1.68	1.50
1	N	311	TYR	CG-CD1	5.33	1.46	1.39
1	O	292	SER	CA-CB	5.33	1.60	1.52
1	G	169	TRP	C-O	5.33	1.33	1.23
1	A	169	TRP	CE3-CZ3	-5.32	1.29	1.38
1	B	471	VAL	CB-CG2	5.32	1.64	1.52
1	N	309	LYS	CD-CE	5.32	1.64	1.51
1	O	315	LYS	CD-CE	5.32	1.64	1.51
1	E	472	GLN	CG-CD	5.32	1.63	1.51
1	K	158	ILE	CB-CG2	-5.32	1.36	1.52
1	A	234	TYR	CD2-CE2	5.32	1.47	1.39
1	E	218	CYS	CB-SG	5.32	1.91	1.82
1	H	132	SER	CB-OG	5.32	1.49	1.42
1	B	371	TYR	CD1-CE1	-5.31	1.31	1.39
1	C	94	GLU	CG-CD	5.31	1.59	1.51
1	F	174	ALA	CA-CB	5.31	1.63	1.52
1	H	175	SER	CB-OG	5.31	1.49	1.42
1	J	202	ASP	CB-CG	5.31	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	361	PHE	CE1-CZ	5.31	1.47	1.37
1	K	139	VAL	N-CA	5.31	1.56	1.46
1	O	99	VAL	CB-CG2	-5.31	1.41	1.52
1	E	101	ALA	CA-CB	-5.31	1.41	1.52
1	E	446	LYS	CG-CD	5.31	1.70	1.52
1	F	167	GLU	CD-OE1	5.31	1.31	1.25
1	H	247	PHE	CE2-CZ	-5.31	1.27	1.37
1	B	392	ILE	CA-CB	-5.30	1.42	1.54
1	E	191	LYS	CD-CE	5.30	1.64	1.51
1	I	106	GLU	CG-CD	5.30	1.59	1.51
1	B	468	LYS	CD-CE	5.30	1.64	1.51
1	A	390	SER	CB-OG	5.30	1.49	1.42
1	N	191	LYS	CG-CD	5.30	1.70	1.52
1	E	63	PRO	N-CA	-5.30	1.38	1.47
1	H	32	SER	CB-OG	5.29	1.49	1.42
1	M	28	VAL	CB-CG2	-5.29	1.41	1.52
1	N	242	TYR	CE1-CZ	5.29	1.45	1.38
1	I	68	TYR	CZ-OH	5.29	1.46	1.37
1	D	234	TYR	CZ-OH	5.29	1.46	1.37
1	M	147	VAL	CB-CG1	-5.28	1.41	1.52
1	G	176	LYS	CD-CE	5.28	1.64	1.51
1	H	330	PHE	CE1-CZ	5.28	1.47	1.37
1	A	68	TYR	CE1-CZ	-5.27	1.31	1.38
1	M	309	LYS	CE-NZ	5.27	1.62	1.49
1	I	162	ALA	CA-CB	-5.27	1.41	1.52
1	M	101	ALA	CA-CB	-5.27	1.41	1.52
1	O	51	ARG	CG-CD	5.27	1.65	1.51
1	F	439	LYS	CE-NZ	5.27	1.62	1.49
1	C	71	ARG	CZ-NH1	5.26	1.39	1.33
1	E	245	SER	CB-OG	5.26	1.49	1.42
1	F	109	ARG	CZ-NH2	5.26	1.39	1.33
1	G	370	GLU	CD-OE2	5.26	1.31	1.25
1	J	106	GLU	CD-OE1	5.26	1.31	1.25
1	K	45	VAL	CB-CG2	-5.26	1.41	1.52
1	M	369	GLU	CD-OE1	5.26	1.31	1.25
1	N	397	SER	CB-OG	5.26	1.49	1.42
1	J	239	ALA	CA-CB	-5.26	1.41	1.52
1	B	187	PRO	CG-CD	5.25	1.68	1.50
1	N	71	ARG	CG-CD	-5.25	1.38	1.51
1	J	152	LYS	CG-CD	5.25	1.70	1.52
1	O	73	PHE	CE2-CZ	-5.25	1.27	1.37
1	D	370	GLU	CD-OE1	5.25	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	68	TYR	CG-CD1	-5.24	1.32	1.39
1	M	453	LYS	CE-NZ	5.24	1.62	1.49
1	N	94	GLU	CD-OE1	5.24	1.31	1.25
1	H	456	PHE	C-O	-5.24	1.13	1.23
1	N	312	TRP	CG-CD1	-5.24	1.29	1.36
1	A	360	LYS	CD-CE	5.24	1.64	1.51
1	M	401	GLU	CD-OE1	5.23	1.31	1.25
1	E	167	GLU	CG-CD	5.23	1.59	1.51
1	L	151	TYR	CD2-CE2	-5.23	1.31	1.39
1	L	311	TYR	CZ-OH	5.23	1.46	1.37
1	D	253	GLU	CG-CD	5.23	1.59	1.51
1	F	132	SER	CB-OG	5.22	1.49	1.42
1	L	251	ARG	CG-CD	5.22	1.65	1.51
1	A	311	TYR	CZ-OH	5.22	1.46	1.37
1	G	167	GLU	CD-OE2	5.22	1.31	1.25
1	G	447	PHE	CE2-CZ	-5.22	1.27	1.37
1	L	273	GLN	CG-CD	5.22	1.63	1.51
1	N	160	GLY	C-O	5.22	1.31	1.23
1	E	345	CYS	CB-SG	-5.21	1.73	1.81
1	O	234	TYR	CZ-OH	5.21	1.46	1.37
1	D	377	PHE	CD1-CE1	-5.21	1.28	1.39
1	J	297	GLY	C-O	-5.21	1.15	1.23
1	H	21	VAL	CB-CG2	-5.20	1.42	1.52
1	G	95	THR	C-O	5.20	1.33	1.23
1	K	447	PHE	CD1-CE1	-5.20	1.28	1.39
1	D	388	VAL	CB-CG1	-5.20	1.42	1.52
1	J	368	VAL	CB-CG2	-5.20	1.42	1.52
1	A	252	ARG	CZ-NH1	5.20	1.39	1.33
1	B	94	GLU	CG-CD	5.20	1.59	1.51
1	H	94	GLU	CD-OE2	5.19	1.31	1.25
1	F	205	TYR	CD2-CE2	-5.19	1.31	1.39
1	H	446	LYS	CG-CD	5.19	1.70	1.52
1	K	49	TYR	CG-CD1	-5.19	1.32	1.39
1	I	388	VAL	CB-CG1	-5.18	1.42	1.52
1	K	217	LYS	CD-CE	5.18	1.64	1.51
1	B	139	VAL	CA-CB	5.18	1.65	1.54
1	B	170	ALA	CA-CB	-5.18	1.41	1.52
1	O	105	VAL	CB-CG1	-5.18	1.42	1.52
1	L	154	THR	CA-CB	5.18	1.66	1.53
1	L	253	GLU	CD-OE2	5.18	1.31	1.25
1	B	252	ARG	CZ-NH1	5.17	1.39	1.33
1	F	248	PHE	CB-CG	-5.17	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	467	ARG	CZ-NH1	5.17	1.39	1.33
1	B	439	LYS	N-CA	5.17	1.56	1.46
1	G	252	ARG	CG-CD	5.17	1.64	1.51
1	C	191	LYS	CG-CD	5.17	1.70	1.52
1	F	354	GLY	C-O	5.17	1.31	1.23
1	K	83	PHE	CE2-CZ	5.17	1.47	1.37
1	C	151	TYR	CG-CD1	-5.17	1.32	1.39
1	G	256	PHE	CE2-CZ	5.16	1.47	1.37
1	M	217	LYS	CE-NZ	5.16	1.61	1.49
1	M	231	TYR	CB-CG	-5.16	1.44	1.51
1	A	455	LYS	CD-CE	5.16	1.64	1.51
1	D	463	TYR	CD2-CE2	5.16	1.47	1.39
1	E	186	PRO	CA-C	-5.16	1.42	1.52
1	D	309	LYS	CE-NZ	5.16	1.61	1.49
1	M	189	GLU	CD-OE1	5.16	1.31	1.25
1	M	360	LYS	CD-CE	5.16	1.64	1.51
1	B	68	TYR	CG-CD1	-5.16	1.32	1.39
1	D	205	TYR	CD1-CE1	-5.16	1.31	1.39
1	K	242	TYR	CD2-CE2	-5.16	1.31	1.39
1	J	260	PHE	CG-CD1	-5.16	1.31	1.38
1	A	87	ASP	C-O	5.15	1.33	1.23
1	N	251	ARG	CG-CD	5.15	1.64	1.51
1	J	76	GLN	CD-OE1	5.15	1.35	1.24
1	L	344	ILE	CB-CG2	-5.15	1.36	1.52
1	C	370	GLU	CD-OE2	5.15	1.31	1.25
1	L	447	PHE	CE1-CZ	-5.15	1.27	1.37
1	C	309	LYS	CE-NZ	5.14	1.61	1.49
1	F	472	GLN	CG-CD	5.14	1.62	1.51
1	A	311	TYR	CD1-CE1	5.14	1.47	1.39
1	E	198	GLY	N-CA	-5.14	1.38	1.46
1	E	276	TYR	CB-CG	-5.14	1.44	1.51
1	O	360	LYS	CD-CE	5.14	1.64	1.51
1	F	94	GLU	CG-CD	5.14	1.59	1.51
1	F	238	SER	CB-OG	-5.14	1.35	1.42
1	H	371	TYR	CD1-CE1	-5.14	1.31	1.39
1	J	94	GLU	CB-CG	5.14	1.61	1.52
1	D	40	SER	CA-CB	5.13	1.60	1.52
1	H	439	LYS	CG-CD	5.13	1.70	1.52
1	A	49	TYR	CB-CG	-5.13	1.44	1.51
1	H	20	ALA	N-CA	5.13	1.56	1.46
1	H	254	GLN	CD-NE2	5.13	1.45	1.32
1	N	205	TYR	CG-CD2	-5.13	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	272	PRO	N-CA	-5.13	1.38	1.47
1	K	472	GLN	CG-CD	5.13	1.62	1.51
1	C	439	LYS	CD-CE	5.12	1.64	1.51
1	K	83	PHE	CG-CD2	5.12	1.46	1.38
1	N	261	TRP	CG-CD1	-5.12	1.29	1.36
1	F	150	ASP	CB-CG	5.12	1.62	1.51
1	J	35	TYR	CG-CD1	5.12	1.45	1.39
1	A	164	ALA	CA-CB	-5.11	1.41	1.52
1	C	35	TYR	CE2-CZ	-5.11	1.31	1.38
1	J	28	VAL	CB-CG2	-5.11	1.42	1.52
1	A	191	LYS	CD-CE	5.11	1.64	1.51
1	K	105	VAL	CA-CB	-5.11	1.44	1.54
1	M	247	PHE	CE1-CZ	5.11	1.47	1.37
1	F	219	GLU	CD-OE2	5.11	1.31	1.25
1	O	176	LYS	CD-CE	5.11	1.64	1.51
1	A	309	LYS	CE-NZ	5.11	1.61	1.49
1	C	368	VAL	CB-CG1	-5.11	1.42	1.52
1	B	368	VAL	CB-CG2	-5.10	1.42	1.52
1	D	248	PHE	CD1-CE1	5.10	1.49	1.39
1	H	253	GLU	CD-OE2	5.10	1.31	1.25
1	G	315	LYS	CB-CG	5.10	1.66	1.52
1	G	338	ARG	CZ-NH1	5.10	1.39	1.33
1	K	444	LYS	CD-CE	5.10	1.64	1.51
1	O	260	PHE	CG-CD2	-5.10	1.31	1.38
1	D	317	GLN	CG-CD	5.09	1.62	1.51
1	D	364	TYR	CD2-CE2	-5.09	1.31	1.39
1	B	361	PHE	CB-CG	-5.09	1.42	1.51
1	E	251	ARG	CG-CD	5.09	1.64	1.51
1	I	28	VAL	CB-CG2	-5.09	1.42	1.52
1	O	285	SER	CB-OG	5.09	1.48	1.42
1	H	94	GLU	CD-OE1	5.09	1.31	1.25
1	F	248	PHE	CD2-CE2	5.09	1.49	1.39
1	H	39	SER	CB-OG	-5.09	1.35	1.42
1	B	325	TRP	CE3-CZ3	5.08	1.47	1.38
1	L	134	ALA	CA-CB	5.08	1.63	1.52
1	N	24	THR	CB-CG2	-5.08	1.35	1.52
1	E	242	TYR	CE1-CZ	5.08	1.45	1.38
1	D	468	LYS	CE-NZ	5.08	1.61	1.49
1	G	444	LYS	CG-CD	5.08	1.69	1.52
1	K	175	SER	CB-OG	5.08	1.48	1.42
1	G	252	ARG	CZ-NH2	5.08	1.39	1.33
1	E	231	TYR	CD1-CE1	-5.07	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	257	ALA	CA-CB	-5.07	1.41	1.52
1	G	140	SER	N-CA	-5.07	1.36	1.46
1	A	291	TYR	CD1-CE1	-5.07	1.31	1.39
1	J	22	VAL	CB-CG1	-5.07	1.42	1.52
1	J	82	LYS	CE-NZ	5.07	1.61	1.49
1	L	446	LYS	CG-CD	5.07	1.69	1.52
1	B	330	PHE	CG-CD2	5.07	1.46	1.38
1	G	50	PHE	CB-CG	-5.06	1.42	1.51
1	J	59	LYS	CD-CE	5.06	1.63	1.51
1	N	366	ARG	CZ-NH1	5.06	1.39	1.33
1	B	323	VAL	CB-CG2	-5.05	1.42	1.52
1	G	134	ALA	CA-CB	5.05	1.63	1.52
1	N	67	ALA	CA-CB	-5.05	1.41	1.52
1	M	315	LYS	CE-NZ	5.05	1.61	1.49
1	A	450	VAL	CB-CG2	-5.05	1.42	1.52
1	N	446	LYS	CD-CE	5.05	1.63	1.51
1	F	356	TYR	CB-CG	5.04	1.59	1.51
1	A	252	ARG	NE-CZ	5.04	1.39	1.33
1	F	109	ARG	CZ-NH1	5.04	1.39	1.33
1	G	88	THR	CB-OG1	5.04	1.53	1.43
1	J	24	THR	CB-CG2	-5.04	1.35	1.52
1	E	108	GLY	C-O	-5.04	1.15	1.23
1	M	369	GLU	CG-CD	5.04	1.59	1.51
1	M	110	GLY	N-CA	-5.04	1.38	1.46
1	A	225	CYS	CB-SG	-5.04	1.73	1.81
1	G	39	SER	CB-OG	-5.04	1.35	1.42
1	F	454	GLU	CD-OE2	5.03	1.31	1.25
1	J	133	HIS	C-O	5.03	1.32	1.23
1	L	290	VAL	CB-CG2	-5.03	1.42	1.52
1	C	225	CYS	CB-SG	-5.03	1.73	1.81
1	O	219	GLU	CD-OE1	5.03	1.31	1.25
1	N	139	VAL	CB-CG1	5.03	1.63	1.52
1	O	229	CYS	CB-SG	5.03	1.90	1.82
1	G	323	VAL	CB-CG2	-5.02	1.42	1.52
1	K	352	VAL	CB-CG1	-5.02	1.42	1.52
1	B	174	ALA	CA-CB	5.02	1.62	1.52
1	A	446	LYS	CG-CD	5.02	1.69	1.52
1	K	465	LEU	CG-CD2	-5.02	1.33	1.51
1	M	151	TYR	CD1-CE1	-5.02	1.31	1.39
1	F	83	PHE	CE1-CZ	5.01	1.46	1.37
1	H	35	TYR	CD2-CE2	-5.01	1.31	1.39
1	K	261	TRP	CB-CG	-5.01	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	123	TYR	CB-CG	-5.01	1.44	1.51
1	O	190	LEU	C-O	-5.01	1.13	1.23
1	I	139	VAL	CB-CG1	5.01	1.63	1.52
1	H	141	GLU	CB-CG	5.01	1.61	1.52
1	J	68	TYR	C-O	-5.01	1.13	1.23
1	J	369	GLU	CD-OE2	5.01	1.31	1.25
1	M	20	ALA	N-CA	5.01	1.56	1.46
1	J	64	LYS	CE-NZ	-5.01	1.36	1.49
1	C	312	TRP	CB-CG	-5.00	1.41	1.50
1	O	447	PHE	CE1-CZ	-5.00	1.27	1.37
1	H	201	VAL	CB-CG2	-5.00	1.42	1.52
1	I	151	TYR	CG-CD1	-5.00	1.32	1.39
1	M	112	PRO	CG-CD	5.00	1.67	1.50

All (551) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	109	ARG	NE-CZ-NH1	-17.51	111.55	120.30
1	F	263	ARG	NE-CZ-NH2	-16.83	111.89	120.30
1	L	109	ARG	NE-CZ-NH2	16.15	128.38	120.30
1	L	366	ARG	NE-CZ-NH2	-13.69	113.45	120.30
1	O	252	ARG	NE-CZ-NH2	-13.15	113.72	120.30
1	K	252	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	O	263	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	E	366	ARG	NE-CZ-NH2	-12.37	114.11	120.30
1	J	252	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	A	252	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	O	252	ARG	NE-CZ-NH1	11.17	125.89	120.30
1	O	461	ASP	CB-CG-OD1	-11.02	108.38	118.30
1	M	263	ARG	NE-CZ-NH2	-10.95	114.82	120.30
1	C	338	ARG	NE-CZ-NH1	-10.73	114.94	120.30
1	C	240	ASP	CB-CG-OD1	-10.59	108.77	118.30
1	F	338	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	G	197	ASP	CB-CG-OD1	-10.32	109.01	118.30
1	G	140	SER	C-N-CA	-10.23	96.11	121.70
1	F	263	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	N	98	LEU	CB-CG-CD1	-9.96	94.08	111.00
1	C	178	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	D	167	GLU	OE1-CD-OE2	-9.91	111.41	123.30
1	H	467	ARG	NE-CZ-NH2	9.89	125.25	120.30
1	J	258	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	J	41	ARG	NE-CZ-NH2	9.63	125.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	251	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	C	41	ARG	NE-CZ-NH1	-9.52	115.54	120.30
1	K	85	LEU	CB-CG-CD1	-9.40	95.03	111.00
1	C	128	ASP	CB-CG-OD2	-9.33	109.90	118.30
1	I	71	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	B	329	LEU	CB-CG-CD2	-9.16	95.43	111.00
1	A	150	ASP	CB-CG-OD1	-9.10	110.11	118.30
1	H	41	ARG	NE-CZ-NH2	9.10	124.85	120.30
1	H	251	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	H	51	ARG	NE-CZ-NH1	-8.95	115.83	120.30
1	H	61	ASP	N-CA-CB	-8.94	94.51	110.60
1	F	233	ASP	CB-CG-OD1	-8.94	110.26	118.30
1	O	315	LYS	CD-CE-NZ	-8.83	91.39	111.70
1	J	197	ASP	CB-CG-OD2	8.80	126.22	118.30
1	J	252	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	K	342	LEU	CB-CG-CD2	-8.67	96.26	111.00
1	L	453	LYS	CD-CE-NZ	-8.64	91.82	111.70
1	B	467	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	B	311	TYR	CB-CG-CD1	-8.60	115.84	121.00
1	O	311	TYR	CB-CG-CD1	-8.55	115.87	121.00
1	H	366	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	C	251	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	L	311	TYR	CB-CG-CD1	-8.42	115.95	121.00
1	A	233	ASP	CB-CG-OD1	-8.39	110.75	118.30
1	O	244	ASP	CB-CG-OD1	8.37	125.83	118.30
1	M	453	LYS	CD-CE-NZ	-8.37	92.45	111.70
1	N	42	LEU	CA-CB-CG	-8.34	96.13	115.30
1	N	373	LEU	CB-CG-CD2	-8.33	96.84	111.00
1	M	41	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	C	263	ARG	NE-CZ-NH1	-8.29	116.15	120.30
1	L	41	ARG	NE-CZ-NH1	-8.23	116.18	120.30
1	J	85	LEU	CB-CG-CD1	-8.23	97.01	111.00
1	B	366	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	G	338	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	L	30	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	A	197	ASP	CB-CG-OD2	8.10	125.59	118.30
1	J	142	ASP	CB-CG-OD2	8.09	125.58	118.30
1	G	252	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	E	142	ASP	CB-CG-OD2	8.04	125.54	118.30
1	E	195	LEU	CB-CG-CD2	-8.01	97.38	111.00
1	B	141	GLU	N-CA-C	7.99	132.57	111.00
1	O	41	ARG	NE-CZ-NH1	-7.98	116.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	ASP	CB-CG-OD2	7.95	125.45	118.30
1	H	159	LEU	CB-CG-CD1	-7.93	97.52	111.00
1	K	240	ASP	CB-CG-OD1	-7.92	111.17	118.30
1	D	74	ARG	NE-CZ-NH1	-7.91	116.34	120.30
1	J	74	ARG	NE-CZ-NH1	-7.91	116.35	120.30
1	J	127	ASP	CB-CG-OD1	-7.90	111.19	118.30
1	G	251	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	D	184	ASP	CB-CG-OD2	7.88	125.39	118.30
1	N	51	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	L	41	ARG	NE-CZ-NH2	7.87	124.23	120.30
1	B	25	ASP	CB-CG-OD1	7.87	125.38	118.30
1	E	258	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C	25	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	G	384	LEU	CB-CG-CD2	-7.85	97.65	111.00
1	K	251	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	N	338	ARG	NE-CZ-NH1	-7.81	116.39	120.30
1	H	102	CYS	CA-CB-SG	-7.77	100.02	114.00
1	K	387	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	C	233	ASP	CB-CG-OD1	-7.70	111.37	118.30
1	F	71	ARG	NE-CZ-NH1	-7.63	116.48	120.30
1	G	223	ASP	CB-CG-OD2	7.61	125.15	118.30
1	J	357	ASP	CB-CG-OD1	-7.61	111.45	118.30
1	I	311	TYR	CB-CG-CD1	-7.61	116.44	121.00
1	B	41	ARG	NE-CZ-NH2	7.54	124.07	120.30
1	J	311	TYR	CB-CG-CD1	-7.53	116.48	121.00
1	N	263	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	M	30	ARG	NE-CZ-NH2	7.51	124.06	120.30
1	J	366	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	387	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	D	439	LYS	CD-CE-NZ	-7.47	94.52	111.70
1	L	156	LEU	CB-CG-CD1	-7.47	98.31	111.00
1	F	102	CYS	CA-CB-SG	-7.46	100.57	114.00
1	B	258	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	N	306	LEU	CB-CG-CD2	-7.43	98.37	111.00
1	B	142	ASP	N-CA-C	-7.42	90.96	111.00
1	K	159	LEU	CB-CG-CD2	-7.42	98.39	111.00
1	C	113	LEU	CB-CG-CD2	-7.42	98.39	111.00
1	N	297	GLY	N-CA-C	-7.39	94.63	113.10
1	O	30	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	J	125	LYS	CD-CE-NZ	-7.38	94.73	111.70
1	L	252	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	E	311	TYR	CB-CG-CD1	-7.37	116.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	387	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	N	102	CYS	CA-CB-SG	-7.34	100.78	114.00
1	J	141	GLU	CA-CB-CG	-7.34	97.25	113.40
1	B	25	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	I	366	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	F	467	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	E	458	LEU	CB-CG-CD2	-7.27	98.64	111.00
1	F	159	LEU	CB-CG-CD2	-7.27	98.63	111.00
1	E	109	ARG	NE-CZ-NH1	-7.27	116.67	120.30
1	J	142	ASP	CB-CG-OD1	-7.26	111.77	118.30
1	M	144	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	H	248	PHE	CD1-CE1-CZ	-7.21	111.45	120.10
1	G	102	CYS	CA-CB-SG	-7.20	101.04	114.00
1	D	379	LEU	CB-CG-CD2	-7.16	98.83	111.00
1	K	252	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	E	209	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	J	282	MET	CG-SD-CE	7.15	111.64	100.20
1	G	209	ASP	CB-CG-OD1	-7.15	111.86	118.30
1	J	467	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	O	263	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	K	74	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	I	366	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	A	56	GLY	N-CA-C	7.10	130.85	113.10
1	D	311	TYR	CB-CG-CD1	-7.10	116.74	121.00
1	A	387	ASP	CB-CG-OD1	7.07	124.67	118.30
1	O	47	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	B	167	GLU	OE1-CD-OE2	-7.06	114.83	123.30
1	F	180	LEU	CB-CG-CD2	-7.06	99.00	111.00
1	L	366	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	J	224	ILE	CG1-CB-CG2	-7.03	95.92	111.40
1	O	251	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	M	113	LEU	CB-CG-CD2	-7.00	99.10	111.00
1	D	233	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	C	252	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	C	357	ASP	CB-CG-OD1	-6.95	112.05	118.30
1	C	402	ASP	CB-CG-OD1	-6.94	112.05	118.30
1	O	251	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	N	41	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	C	178	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	E	251	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	H	373	LEU	CB-CG-CD2	-6.92	99.23	111.00
1	F	128	ASP	CB-CG-OD1	6.92	124.52	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	453	LYS	CG-CD-CE	-6.91	91.17	111.90
1	C	338	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	N	303	ASP	CB-CG-OD1	6.89	124.50	118.30
1	C	47	ASP	CB-CG-OD2	6.89	124.50	118.30
1	M	311	TYR	CB-CG-CD1	-6.88	116.87	121.00
1	D	141	GLU	N-CA-C	6.87	129.55	111.00
1	I	263	ARG	NE-CZ-NH1	-6.87	116.87	120.30
1	K	335	ASP	CB-CG-OD1	6.87	124.48	118.30
1	E	141	GLU	N-CA-C	6.86	129.53	111.00
1	M	109	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	I	402	ASP	CB-CG-OD1	-6.84	112.14	118.30
1	H	311	TYR	CB-CG-CD1	-6.84	116.89	121.00
1	A	53	PRO	N-CD-CG	-6.84	92.95	103.20
1	L	178	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	K	283	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	O	74	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	60	GLN	O-C-N	6.81	133.60	122.70
1	A	255	LEU	CA-CB-CG	6.80	130.95	115.30
1	J	202	ASP	CB-CG-OD1	6.80	124.42	118.30
1	H	172	GLY	CA-C-N	-6.80	102.25	117.20
1	K	366	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	77	LEU	CB-CG-CD2	-6.78	99.47	111.00
1	K	246	MET	CG-SD-CE	6.77	111.03	100.20
1	E	445	LEU	CB-CG-CD2	-6.73	99.55	111.00
1	F	141	GLU	N-CA-C	6.73	129.18	111.00
1	J	43	LEU	CB-CG-CD1	-6.73	99.56	111.00
1	O	68	TYR	CB-CG-CD2	6.73	125.04	121.00
1	H	156	LEU	CB-CG-CD1	-6.73	99.56	111.00
1	A	311	TYR	CB-CG-CD1	-6.72	116.97	121.00
1	A	60	GLN	CA-C-N	-6.72	102.42	117.20
1	B	240	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	K	389	MET	CG-SD-CE	6.68	110.90	100.20
1	B	446	LYS	CD-CE-NZ	-6.68	96.33	111.70
1	K	311	TYR	CB-CG-CD1	-6.68	116.99	121.00
1	D	283	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	G	311	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	J	109	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	338	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	J	458	LEU	CB-CG-CD2	-6.65	99.69	111.00
1	L	251	ARG	NH1-CZ-NH2	-6.65	112.08	119.40
1	F	42	LEU	CA-CB-CG	-6.65	100.01	115.30
1	K	240	ASP	CB-CG-OD2	6.64	124.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	306	LEU	CB-CG-CD2	-6.64	99.72	111.00
1	H	178	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	O	47	ASP	CB-CG-OD1	6.59	124.23	118.30
1	L	452	LEU	CB-CG-CD1	-6.58	99.81	111.00
1	C	128	ASP	CB-CG-OD1	6.55	124.19	118.30
1	E	303	ASP	CB-CG-OD2	6.53	124.18	118.30
1	K	180	LEU	CB-CG-CD2	-6.53	99.90	111.00
1	A	145	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	O	115	VAL	CG1-CB-CG2	-6.53	100.46	110.90
1	G	263	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	K	251	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	F	98	LEU	CB-CG-CD2	6.50	122.04	111.00
1	D	97	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	I	188	LEU	CB-CG-CD1	-6.49	99.97	111.00
1	C	461	ASP	CB-CG-OD2	6.48	124.13	118.30
1	M	215	ASP	CB-CG-OD1	6.48	124.13	118.30
1	D	178	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	K	64	LYS	CD-CE-NZ	-6.44	96.89	111.70
1	M	144	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	G	74	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	141	GLU	N-CA-C	6.41	128.31	111.00
1	C	252	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	D	144	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	A	61	ASP	N-CA-CB	-6.38	99.11	110.60
1	B	389	MET	CG-SD-CE	6.38	110.41	100.20
1	J	467	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	389	MET	CG-SD-CE	6.36	110.38	100.20
1	F	87	ASP	CB-CG-OD1	-6.35	112.58	118.30
1	F	199	ASP	CB-CG-OD2	6.35	124.01	118.30
1	I	338	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	K	62	ILE	CG1-CB-CG2	-6.34	97.45	111.40
1	O	105	VAL	CA-CB-CG2	-6.34	101.39	110.90
1	G	332	THR	CA-CB-CG2	-6.33	103.53	112.40
1	M	156	LEU	CB-CG-CD1	-6.33	100.23	111.00
1	E	263	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	J	42	LEU	CA-CB-CG	-6.33	100.74	115.30
1	G	203	THR	CA-CB-CG2	-6.33	103.54	112.40
1	G	212	THR	CA-CB-CG2	-6.32	103.55	112.40
1	K	387	ASP	CB-CG-OD1	6.32	123.99	118.30
1	N	289	CYS	CA-CB-SG	-6.32	102.63	114.00
1	E	282	MET	CG-SD-CE	6.31	110.30	100.20
1	N	329	LEU	CB-CG-CD2	-6.31	100.28	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	297	GLY	N-CA-C	-6.30	97.34	113.10
1	L	343	THR	N-CA-C	-6.30	94.00	111.00
1	C	42	LEU	CA-CB-CG	-6.29	100.83	115.30
1	O	159	LEU	CB-CG-CD1	-6.28	100.32	111.00
1	H	77	LEU	CB-CG-CD2	-6.28	100.33	111.00
1	B	222	LEU	CB-CG-CD2	-6.27	100.33	111.00
1	L	282	MET	CG-SD-CE	6.27	110.24	100.20
1	N	98	LEU	CB-CG-CD2	6.27	121.67	111.00
1	I	22	VAL	CG1-CB-CG2	-6.27	100.87	110.90
1	E	47	ASP	CB-CG-OD2	6.26	123.94	118.30
1	N	459	ASP	CB-CG-OD1	6.25	123.92	118.30
1	G	297	GLY	N-CA-C	-6.24	97.50	113.10
1	H	300	VAL	CG1-CB-CG2	-6.22	100.94	110.90
1	G	47	ASP	CB-CG-OD1	6.22	123.90	118.30
1	F	240	ASP	CB-CG-OD1	-6.21	112.72	118.30
1	M	282	MET	CG-SD-CE	6.20	110.12	100.20
1	I	165	ILE	CG1-CB-CG2	-6.20	97.76	111.40
1	F	297	GLY	N-CA-C	-6.19	97.62	113.10
1	N	62	ILE	CG1-CB-CG2	-6.19	97.78	111.40
1	N	105	VAL	CB-CA-C	-6.19	99.64	111.40
1	I	331	VAL	CG1-CB-CG2	-6.19	101.00	110.90
1	L	142	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	C	311	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	H	258	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	126	LEU	CB-CG-CD2	-6.17	100.50	111.00
1	G	315	LYS	CD-CE-NZ	-6.16	97.53	111.70
1	C	269	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	H	47	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	E	338	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	459	ASP	CB-CG-OD1	6.13	123.82	118.30
1	F	311	TYR	CZ-CE2-CD2	-6.12	114.30	119.80
1	K	357	ASP	CB-CG-OD2	6.10	123.79	118.30
1	L	126	LEU	CB-CG-CD1	6.10	121.37	111.00
1	L	372	ASP	CB-CG-OD1	6.10	123.79	118.30
1	G	47	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	J	357	ASP	CB-CG-OD2	6.09	123.78	118.30
1	D	331	VAL	CG1-CB-CG2	-6.08	101.17	110.90
1	E	158	ILE	CG1-CB-CG2	-6.08	98.03	111.40
1	E	357	ASP	CB-CG-OD2	6.08	123.77	118.30
1	D	54	ALA	N-CA-C	6.04	127.31	111.00
1	B	41	ARG	NE-CZ-NH1	-6.03	117.28	120.30
1	A	251	ARG	NE-CZ-NH1	6.03	123.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	448	TRP	N-CA-C	-6.03	94.73	111.00
1	N	290	VAL	CG1-CB-CG2	-6.03	101.26	110.90
1	I	62	ILE	CG1-CB-CG2	-6.02	98.16	111.40
1	J	51	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	L	465	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	I	159	LEU	CA-CB-CG	6.01	129.12	115.30
1	E	41	ARG	NE-CZ-NH2	6.01	123.30	120.30
1	C	258	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	G	70	TYR	CD1-CE1-CZ	-5.97	114.42	119.80
1	D	188	LEU	CA-CB-CG	5.97	129.04	115.30
1	J	184	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	K	105	VAL	CB-CA-C	-5.96	100.07	111.40
1	L	459	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	71	ARG	N-CA-C	-5.95	94.93	111.00
1	E	109	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	B	313	LEU	CB-CG-CD1	-5.94	100.90	111.00
1	K	150	ASP	CB-CG-OD1	-5.94	112.96	118.30
1	E	150	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	A	289	CYS	CA-CB-SG	-5.92	103.35	114.00
1	N	343	THR	N-CA-C	-5.91	95.05	111.00
1	F	384	LEU	CB-CG-CD1	-5.91	100.96	111.00
1	M	459	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	H	303	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	J	102	CYS	CA-CB-SG	-5.89	103.40	114.00
1	K	167	GLU	OE1-CD-OE2	-5.88	116.24	123.30
1	A	252	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	I	471	VAL	CG1-CB-CG2	-5.88	101.50	110.90
1	K	42	LEU	CA-CB-CG	-5.88	101.78	115.30
1	L	370	GLU	OE1-CD-OE2	-5.88	116.25	123.30
1	M	400	LEU	CB-CG-CD2	-5.87	101.02	111.00
1	D	297	GLY	N-CA-C	-5.86	98.44	113.10
1	G	280	THR	CA-CB-CG2	-5.85	104.20	112.40
1	G	141	GLU	N-CA-C	5.85	126.78	111.00
1	L	269	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	I	297	GLY	N-CA-C	-5.83	98.52	113.10
1	J	313	LEU	CB-CG-CD1	-5.83	101.08	111.00
1	C	105	VAL	CG1-CB-CG2	-5.82	101.59	110.90
1	G	64	LYS	CD-CE-NZ	-5.82	98.32	111.70
1	H	30	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	H	258	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	O	68	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	H	68	TYR	CZ-CE2-CD2	-5.80	114.58	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	282	MET	CG-SD-CE	5.79	109.46	100.20
1	E	225	CYS	N-CA-CB	-5.79	100.18	110.60
1	O	180	LEU	CB-CG-CD2	-5.78	101.17	111.00
1	K	283	ARG	NE-CZ-NH1	-5.77	117.41	120.30
1	F	197	ASP	CB-CG-OD1	-5.77	113.11	118.30
1	H	209	ASP	CB-CG-OD1	-5.76	113.11	118.30
1	G	197	ASP	CB-CG-OD2	5.76	123.49	118.30
1	M	97	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	42	LEU	CA-CB-CG	-5.76	102.06	115.30
1	H	141	GLU	CA-CB-CG	-5.76	100.73	113.40
1	B	370	GLU	OE1-CD-OE2	-5.76	116.39	123.30
1	H	244	ASP	CB-CG-OD1	-5.75	113.12	118.30
1	H	61	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	G	142	ASP	CB-CG-OD2	5.75	123.47	118.30
1	O	142	ASP	CB-CG-OD2	5.74	123.47	118.30
1	H	105	VAL	CB-CA-C	-5.74	100.49	111.40
1	K	244	ASP	CB-CG-OD1	5.74	123.47	118.30
1	N	213	LEU	CB-CG-CD1	-5.74	101.25	111.00
1	H	175	SER	CA-C-N	-5.73	104.59	117.20
1	M	465	LEU	CB-CG-CD1	-5.73	101.25	111.00
1	L	188	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	J	208	MET	CG-SD-CE	5.72	109.35	100.20
1	A	113	LEU	CB-CG-CD2	-5.72	101.28	111.00
1	F	362	LYS	CD-CE-NZ	-5.71	98.56	111.70
1	E	251	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	H	171	LYS	N-CA-C	-5.70	95.61	111.00
1	E	47	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	H	190	LEU	CB-CG-CD1	-5.68	101.34	111.00
1	B	82	LYS	CB-CG-CD	-5.67	96.84	111.60
1	L	71	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	F	144	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	O	371	TYR	CZ-CE2-CD2	-5.67	114.70	119.80
1	L	105	VAL	CB-CA-C	-5.66	100.64	111.40
1	M	97	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	255	LEU	CA-CB-CG	5.65	128.30	115.30
1	I	337	THR	CA-CB-CG2	-5.65	104.49	112.40
1	J	338	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	K	216	THR	CA-CB-CG2	-5.64	104.50	112.40
1	I	144	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	J	297	GLY	N-CA-C	-5.64	99.00	113.10
1	O	370	GLU	OE1-CD-OE2	-5.64	116.54	123.30
1	K	467	ARG	NE-CZ-NH1	5.62	123.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	99	VAL	CB-CA-C	-5.62	100.72	111.40
1	M	252	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	J	115	VAL	CG1-CB-CG2	-5.61	101.93	110.90
1	B	306	LEU	CB-CG-CD2	-5.60	101.47	111.00
1	K	41	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	D	255	LEU	CA-CB-CG	5.59	128.16	115.30
1	M	387	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	E	117	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	A	55	GLY	N-CA-C	5.58	127.06	113.10
1	B	311	TYR	CB-CG-CD2	5.58	124.35	121.00
1	B	311	TYR	CE1-CZ-OH	-5.58	105.03	120.10
1	L	97	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	M	282	MET	CB-CG-SD	-5.58	95.67	112.40
1	O	329	LEU	CB-CG-CD2	-5.58	101.52	111.00
1	H	87	ASP	CB-CG-OD1	-5.56	113.29	118.30
1	M	201	VAL	CB-CA-C	-5.56	100.84	111.40
1	B	208	MET	CG-SD-CE	5.55	109.08	100.20
1	O	242	TYR	CD1-CE1-CZ	-5.54	114.81	119.80
1	L	372	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	282	MET	CG-SD-CE	5.54	109.06	100.20
1	L	291	TYR	CD1-CE1-CZ	-5.54	114.82	119.80
1	E	223	ASP	CB-CG-OD2	5.53	123.28	118.30
1	G	223	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	A	366	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	B	105	VAL	CB-CA-C	-5.53	100.89	111.40
1	K	313	LEU	CB-CG-CD1	-5.53	101.61	111.00
1	E	215	ASP	CB-CG-OD2	5.52	123.27	118.30
1	E	360	LYS	N-CA-CB	-5.52	100.67	110.60
1	B	459	ASP	CB-CG-OD2	-5.52	113.34	118.30
1	N	332	THR	CA-CB-CG2	-5.51	104.68	112.40
1	O	331	VAL	CG1-CB-CG2	-5.51	102.09	110.90
1	E	267	MET	CG-SD-CE	5.49	108.98	100.20
1	M	222	LEU	CB-CG-CD2	-5.48	101.68	111.00
1	D	345	CYS	CA-CB-SG	-5.47	104.16	114.00
1	N	448	TRP	N-CA-C	-5.46	96.25	111.00
1	L	25	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	N	338	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	J	300	VAL	CG1-CB-CG2	-5.46	102.17	110.90
1	K	202	ASP	CB-CG-OD2	5.46	123.21	118.30
1	D	289	CYS	CA-CB-SG	-5.46	104.18	114.00
1	K	311	TYR	CE1-CZ-OH	-5.46	105.37	120.10
1	B	311	TYR	OH-CZ-CE2	5.45	134.82	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	156	LEU	CB-CG-CD1	-5.45	101.74	111.00
1	L	384	LEU	CB-CG-CD1	-5.44	101.74	111.00
1	F	98	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	E	461	ASP	CB-CG-OD2	5.44	123.19	118.30
1	H	126	LEU	CB-CG-CD2	-5.44	101.75	111.00
1	O	311	TYR	CE1-CZ-OH	-5.43	105.43	120.10
1	A	123	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	O	188	LEU	CA-CB-CG	5.43	127.79	115.30
1	H	149	VAL	CG1-CB-CG2	-5.42	102.22	110.90
1	B	209	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	C	402	ASP	CB-CG-OD2	5.42	123.18	118.30
1	F	311	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	H	117	LEU	CB-CG-CD2	-5.40	101.81	111.00
1	I	105	VAL	CB-CA-C	-5.40	101.14	111.40
1	K	74	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	M	303	ASP	CB-CG-OD1	5.40	123.16	118.30
1	F	105	VAL	CA-CB-CG2	-5.40	102.80	110.90
1	H	201	VAL	CB-CA-C	-5.40	101.14	111.40
1	J	171	LYS	CD-CE-NZ	-5.40	99.28	111.70
1	H	107	ILE	CG1-CB-CG2	-5.40	99.52	111.40
1	J	105	VAL	CG1-CB-CG2	-5.40	102.27	110.90
1	M	255	LEU	CA-CB-CG	5.39	127.71	115.30
1	I	85	LEU	CA-CB-CG	-5.39	102.90	115.30
1	H	467	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	M	455	LYS	CD-CE-NZ	5.38	124.08	111.70
1	F	176	LYS	CD-CE-NZ	5.38	124.08	111.70
1	H	188	LEU	CB-CG-CD2	-5.38	101.85	111.00
1	K	311	TYR	CB-CG-CD2	5.38	124.23	121.00
1	A	297	GLY	N-CA-C	-5.37	99.67	113.10
1	L	167	GLU	OE1-CD-OE2	-5.37	116.86	123.30
1	N	306	LEU	CB-CG-CD1	5.37	120.12	111.00
1	D	105	VAL	CB-CA-C	-5.36	101.22	111.40
1	C	47	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	I	127	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	M	215	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	M	105	VAL	CB-CA-C	-5.35	101.23	111.40
1	A	366	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	H	279	GLY	N-CA-C	-5.35	99.73	113.10
1	F	97	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	G	263	ARG	NH1-CZ-NH2	5.34	125.28	119.40
1	B	144	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	J	71	ARG	NE-CZ-NH2	-5.34	117.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	225	CYS	N-CA-CB	-5.34	100.99	110.60
1	E	383	THR	CA-CB-CG2	-5.34	104.92	112.40
1	J	263	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	O	188	LEU	CB-CG-CD2	-5.34	101.93	111.00
1	O	289	CYS	CA-CB-SG	-5.34	104.40	114.00
1	I	90	ILE	CB-CA-C	-5.32	100.96	111.60
1	G	71	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	E	461	ASP	CB-CG-OD1	-5.32	113.52	118.30
1	N	71	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	F	443	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	H	275	LEU	CB-CG-CD1	-5.30	101.98	111.00
1	A	71	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	C	297	GLY	N-CA-C	-5.29	99.86	113.10
1	C	39	SER	N-CA-C	-5.29	96.71	111.00
1	E	30	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	A	105	VAL	CB-CA-C	-5.29	101.35	111.40
1	H	338	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	L	460	LEU	CA-CB-CG	-5.28	103.15	115.30
1	N	159	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	C	368	VAL	CB-CA-C	-5.28	101.38	111.40
1	O	453	LYS	CB-CG-CD	-5.28	97.88	111.60
1	C	43	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	C	453	LYS	CD-CE-NZ	-5.27	99.57	111.70
1	F	258	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	M	445	LEU	CA-CB-CG	-5.27	103.17	115.30
1	L	283	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	H	171	LYS	C-N-CA	-5.26	111.24	122.30
1	O	459	ASP	CB-CG-OD1	5.26	123.04	118.30
1	D	365	SER	N-CA-CB	-5.26	102.61	110.50
1	N	150	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	G	263	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	L	202	ASP	CB-CG-OD2	5.24	123.02	118.30
1	G	150	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	A	42	LEU	CA-CB-CG	-5.23	103.26	115.30
1	E	144	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	F	142	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	J	176	LYS	CD-CE-NZ	5.23	123.74	111.70
1	I	235	LEU	CB-CG-CD2	5.23	119.89	111.00
1	A	379	LEU	CA-CB-CG	-5.22	103.29	115.30
1	K	311	TYR	OH-CZ-CE2	5.21	134.17	120.10
1	M	142	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	O	41	ARG	NE-CZ-NH2	5.21	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	360	LYS	CD-CE-NZ	-5.20	99.73	111.70
1	E	311	TYR	CD1-CE1-CZ	-5.20	115.12	119.80
1	N	445	LEU	CB-CG-CD1	5.20	119.83	111.00
1	E	159	LEU	CA-CB-CG	5.19	127.24	115.30
1	C	337	THR	CA-CB-CG2	-5.18	105.14	112.40
1	L	25	ASP	CB-CG-OD1	5.18	122.97	118.30
1	D	357	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	109	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	M	269	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	31	THR	CA-CB-CG2	-5.17	105.16	112.40
1	D	244	ASP	CB-CG-OD1	5.16	122.94	118.30
1	M	205	TYR	CG-CD2-CE2	5.16	125.43	121.30
1	O	42	LEU	CA-CB-CG	-5.16	103.44	115.30
1	B	105	VAL	CA-CB-CG2	-5.15	103.17	110.90
1	E	51	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	F	300	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	M	28	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	E	156	LEU	CB-CG-CD2	-5.14	102.26	111.00
1	K	105	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	K	165	ILE	CG1-CB-CG2	-5.14	100.09	111.40
1	C	105	VAL	CB-CA-C	-5.14	101.64	111.40
1	D	113	LEU	CB-CG-CD1	5.14	119.73	111.00
1	H	283	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	I	149	VAL	CA-CB-CG2	-5.13	103.20	110.90
1	O	233	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	E	105	VAL	CB-CA-C	-5.13	101.65	111.40
1	E	311	TYR	CE1-CZ-OH	-5.12	106.26	120.10
1	G	178	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	389	MET	CG-SD-CE	5.12	108.39	100.20
1	B	231	TYR	CD1-CE1-CZ	-5.12	115.19	119.80
1	D	203	THR	CA-CB-CG2	-5.12	105.23	112.40
1	D	54	ALA	C-N-CA	-5.12	111.56	122.30
1	F	158	ILE	CB-CA-C	-5.11	101.39	111.60
1	I	470	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	K	184	ASP	CB-CG-OD2	5.11	122.90	118.30
1	N	311	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	O	282	MET	CG-SD-CE	5.11	108.37	100.20
1	H	53	PRO	CA-C-N	-5.10	105.99	117.20
1	I	107	ILE	CG1-CB-CG2	-5.10	100.19	111.40
1	H	184	ASP	CB-CG-OD2	5.09	122.88	118.30
1	I	194	VAL	CG1-CB-CG2	5.08	119.02	110.90
1	H	475	LEU	CA-CB-CG	5.07	126.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	300	VAL	CG1-CB-CG2	-5.06	102.81	110.90
1	I	225	CYS	N-CA-CB	-5.06	101.50	110.60
1	J	468	LYS	CD-CE-NZ	-5.06	100.07	111.70
1	I	55	GLY	N-CA-C	5.05	125.73	113.10
1	J	303	ASP	CB-CG-OD1	5.05	122.85	118.30
1	L	323	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	F	306	LEU	CA-CB-CG	-5.05	103.69	115.30
1	B	141	GLU	CA-CB-CG	-5.05	102.30	113.40
1	I	97	ARG	NE-CZ-NH2	5.05	122.82	120.30
1	C	42	LEU	CB-CG-CD1	-5.04	102.43	111.00
1	M	159	LEU	CA-CB-CG	5.04	126.89	115.30
1	D	97	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	I	246	MET	CB-CG-SD	5.04	127.51	112.40
1	D	300	VAL	CA-CB-CG1	-5.03	103.35	110.90
1	L	251	ARG	NE-CZ-NH2	5.03	122.82	120.30
1	N	41	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
1	N	145	ASP	CB-CG-OD1	-5.03	113.78	118.30
1	A	255	LEU	CB-CG-CD2	5.02	119.54	111.00
1	L	98	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	I	459	ASP	CB-CG-OD1	5.02	122.82	118.30
1	G	251	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
1	A	201	VAL	CB-CA-C	-5.00	101.90	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	53	PRO	Peptide

5.2 Too-close contacts (i)

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	3323	0	3192	188	1
1	B	3323	0	3192	170	0
1	C	3323	0	3192	154	1
1	D	3323	0	3192	151	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3323	0	3192	161	0
1	F	3323	0	3192	199	0
1	G	3323	0	3192	197	0
1	H	3323	0	3192	202	0
1	I	3323	0	3192	165	0
1	J	3323	0	3192	166	0
1	K	3323	0	3192	152	0
1	L	3323	0	3192	175	0
1	M	3323	0	3192	166	0
1	N	3323	0	3192	174	0
1	O	3323	0	3192	157	0
All	All	49845	0	47880	2325	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (2325) 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:J:446:LYS:CG	1:J:446:LYS:CD	1.75	1.63
1:B:141:GLU:CB	1:B:141:GLU:CG	1.75	1.63
1:C:191:LYS:CE	1:C:191:LYS:CD	1.76	1.62
1:L:360:LYS:CD	1:L:360:LYS:CE	1.78	1.61
1:F:465:LEU:CG	1:F:465:LEU:CD1	1.74	1.61
1:D:315:LYS:CG	1:D:315:LYS:CD	1.78	1.60
1:M:446:LYS:CD	1:M:446:LYS:CG	1.76	1.59
1:G:64:LYS:CD	1:G:64:LYS:CE	1.80	1.59
1:M:191:LYS:CD	1:M:191:LYS:CE	1.76	1.59
1:E:446:LYS:CE	1:E:446:LYS:CD	1.78	1.57
1:B:90:ILE:CD1	1:B:90:ILE:CG1	1.75	1.57
1:J:171:LYS:NZ	1:J:171:LYS:CE	1.68	1.57
1:L:453:LYS:CG	1:L:453:LYS:CD	1.80	1.56
1:G:315:LYS:CD	1:G:315:LYS:CE	1.79	1.56
1:G:82:LYS:NZ	1:G:82:LYS:CE	1.69	1.54
1:H:82:LYS:NZ	1:H:82:LYS:CE	1.69	1.53
1:L:453:LYS:NZ	1:L:453:LYS:CE	1.68	1.53
1:L:278:LYS:NZ	1:L:278:LYS:CE	1.68	1.53
1:L:453:LYS:CD	1:L:453:LYS:CE	1.84	1.53
1:E:309:LYS:NZ	1:E:309:LYS:CE	1.68	1.51
1:C:453:LYS:NZ	1:C:453:LYS:CE	1.72	1.50
1:D:191:LYS:NZ	1:D:191:LYS:CE	1.74	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:360:LYS:NZ	1:I:360:LYS:CE	1.68	1.49
1:J:125:LYS:NZ	1:J:125:LYS:CE	1.71	1.49
1:D:353:PRO:CB	1:D:353:PRO:CG	1.80	1.48
1:O:315:LYS:NZ	1:O:315:LYS:CE	1.75	1.48
1:A:267:MET:CE	1:A:267:MET:SD	2.02	1.48
1:B:138:ASN:ND2	1:B:140:SER:HB3	1.28	1.45
1:M:282:MET:CE	1:M:282:MET:SD	2.04	1.45
1:G:58:ASN:HB2	1:H:178:ARG:NH1	1.11	1.39
1:D:439:LYS:NZ	1:D:439:LYS:CE	1.89	1.35
1:A:57:GLY:HA3	1:B:184:ASP:OD2	1.29	1.29
1:B:138:ASN:HD21	1:B:140:SER:CB	1.48	1.24
1:L:353:PRO:CD	1:L:360:LYS:HZ2	1.49	1.24
1:G:58:ASN:CB	1:H:178:ARG:HH12	1.52	1.22
1:L:353:PRO:HD2	1:L:360:LYS:NZ	1.56	1.20
1:G:353:PRO:CD	1:G:360:LYS:HZ2	1.55	1.17
1:F:181:SER:HB2	1:M:89:SER:HB2	1.17	1.16
1:A:353:PRO:HD2	1:A:360:LYS:HZ2	1.11	1.16
1:G:58:ASN:CB	1:H:178:ARG:NH1	2.05	1.14
1:A:57:GLY:CA	1:B:184:ASP:OD2	1.94	1.14
1:N:353:PRO:HG2	1:N:360:LYS:HZ2	1.05	1.13
1:H:273:GLN:HE22	1:H:278:LYS:HE2	1.00	1.12
1:B:273:GLN:HE22	1:B:278:LYS:HE2	1.09	1.09
1:M:273:GLN:HE22	1:M:278:LYS:HE2	1.05	1.09
1:A:282:MET:HG2	1:G:89:SER:HB2	1.27	1.09
1:H:353:PRO:HD2	1:H:360:LYS:HZ2	1.00	1.09
1:L:121:PRO:HG3	1:M:289:CYS:SG	1.93	1.08
1:H:141:GLU:HG2	1:H:142:ASP:N	1.68	1.07
1:L:273:GLN:HE22	1:L:278:LYS:HE2	1.07	1.07
1:C:273:GLN:HE22	1:C:278:LYS:HE2	1.12	1.07
1:E:353:PRO:CD	1:E:360:LYS:HZ2	1.68	1.07
1:J:273:GLN:HE22	1:J:278:LYS:HE2	1.19	1.06
1:D:475:LEU:HD23	1:D:475:LEU:H	1.20	1.05
1:G:353:PRO:HD2	1:G:360:LYS:NZ	1.71	1.05
1:E:353:PRO:HD2	1:E:360:LYS:NZ	1.69	1.05
1:N:475:LEU:H	1:N:475:LEU:HD23	1.16	1.05
1:H:141:GLU:CG	1:H:142:ASP:N	2.18	1.04
1:H:353:PRO:HD2	1:H:360:LYS:NZ	1.71	1.04
1:H:121:PRO:HG3	1:I:289:CYS:SG	1.97	1.04
1:H:51:ARG:NH1	1:H:61:ASP:OD2	1.92	1.03
1:N:273:GLN:HE22	1:N:278:LYS:HE2	1.18	1.03
1:B:353:PRO:HG2	1:B:360:LYS:HZ2	1.24	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:PRO:HG2	1:F:360:LYS:HZ2	1.25	1.01
1:E:353:PRO:HD2	1:E:360:LYS:HZ2	0.88	1.01
1:L:273:GLN:NE2	1:L:278:LYS:HE2	1.76	1.00
1:G:353:PRO:HD2	1:G:360:LYS:HZ2	0.85	1.00
1:A:216:THR:HG22	1:A:218:CYS:HB2	1.44	0.99
1:H:273:GLN:NE2	1:H:278:LYS:HE2	1.76	0.99
1:O:353:PRO:HD2	1:O:360:LYS:HZ1	1.21	0.99
1:H:141:GLU:HG2	1:H:142:ASP:H	1.24	0.99
1:F:273:GLN:HE22	1:F:278:LYS:HE2	1.24	0.99
1:A:353:PRO:HG2	1:A:360:LYS:HZ3	1.27	0.97
1:A:273:GLN:HE22	1:A:278:LYS:HE2	1.30	0.96
1:I:136:THR:O	1:I:137:SER:O	1.83	0.96
1:N:111:GLN:HB3	1:N:112:PRO:HD2	1.44	0.96
1:L:353:PRO:CD	1:L:360:LYS:NZ	2.23	0.95
1:G:58:ASN:HB2	1:H:178:ARG:HH11	1.32	0.94
1:F:289:CYS:SG	1:J:121:PRO:HG3	2.08	0.94
1:N:353:PRO:HG2	1:N:360:LYS:NZ	1.80	0.94
1:A:289:CYS:SG	1:E:121:PRO:HG3	2.07	0.94
1:M:126:LEU:HB3	1:M:262:ASN:HB3	1.48	0.94
1:L:353:PRO:HD2	1:L:360:LYS:HZ2	0.78	0.94
1:I:353:PRO:HD2	1:I:360:LYS:HZ2	1.32	0.94
1:H:353:PRO:CD	1:H:360:LYS:HZ2	1.82	0.93
1:L:126:LEU:HB3	1:L:262:ASN:HB3	1.51	0.93
1:K:353:PRO:HD2	1:K:360:LYS:HZ1	1.31	0.93
1:I:353:PRO:HD2	1:I:360:LYS:NZ	1.84	0.91
1:A:353:PRO:HD2	1:A:360:LYS:NZ	1.86	0.91
1:F:181:SER:CB	1:M:89:SER:HB2	1.99	0.91
1:B:121:PRO:HG3	1:C:289:CYS:SG	2.11	0.90
1:L:111:GLN:HB3	1:L:112:PRO:HD2	1.52	0.90
1:F:475:LEU:H	1:F:475:LEU:HD23	1.35	0.90
1:D:273:GLN:HE22	1:D:278:LYS:HE2	1.35	0.90
1:K:475:LEU:HD23	1:K:475:LEU:H	1.37	0.90
1:E:273:GLN:HE22	1:E:278:LYS:HE2	1.36	0.89
1:H:350:SER:HB3	1:H:351:PRO:HD3	1.55	0.89
1:O:143:VAL:O	1:O:143:VAL:HG12	1.73	0.88
1:E:138:ASN:HD22	1:E:140:SER:HB3	1.38	0.88
1:I:273:GLN:HE22	1:I:278:LYS:HE2	1.37	0.88
1:D:45:VAL:HG12	1:D:368:VAL:HG22	1.52	0.88
1:K:353:PRO:HD2	1:K:360:LYS:NZ	1.88	0.87
1:K:273:GLN:HE22	1:K:278:LYS:HE2	1.38	0.87
1:M:273:GLN:NE2	1:M:278:LYS:HE2	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:353:PRO:HD2	1:O:360:LYS:NZ	1.88	0.87
1:A:353:PRO:CD	1:A:360:LYS:HZ2	1.87	0.87
1:D:121:PRO:HG3	1:E:289:CYS:SG	2.14	0.87
1:O:70:TYR:OH	1:O:232:PRO:HD3	1.75	0.87
1:J:247:PHE:CE2	1:J:322:GLY:HA2	2.10	0.86
1:I:344:ILE:HD11	1:J:188:LEU:HD11	1.56	0.86
1:E:111:GLN:HB3	1:E:112:PRO:HD2	1.56	0.85
1:E:353:PRO:HG2	1:E:360:LYS:HZ3	1.39	0.85
1:B:273:GLN:NE2	1:B:278:LYS:HE2	1.91	0.85
1:M:313:LEU:H	1:M:313:LEU:HD23	1.40	0.84
1:O:329:LEU:HD23	1:O:329:LEU:C	1.98	0.84
1:F:111:GLN:HB3	1:F:112:PRO:HD2	1.58	0.84
1:O:138:ASN:HD22	1:O:140:SER:HB3	1.43	0.84
1:G:353:PRO:CD	1:G:360:LYS:NZ	2.36	0.83
1:A:324:CYS:HB3	1:A:328:GLN:O	1.77	0.83
1:F:126:LEU:HB3	1:F:262:ASN:HB3	1.59	0.83
1:K:353:PRO:HG2	1:K:360:LYS:HZ2	1.42	0.83
1:N:353:PRO:CG	1:N:360:LYS:HZ2	1.90	0.83
1:G:368:VAL:HG11	1:H:169:TRP:CZ2	2.14	0.83
1:B:364:TYR:CD2	1:C:185:CYS:HB2	2.14	0.83
1:G:388:VAL:O	1:G:392:ILE:HG13	1.79	0.83
1:M:105:VAL:HG21	1:M:159:LEU:HD11	1.59	0.83
1:C:273:GLN:NE2	1:C:278:LYS:HE2	1.92	0.83
1:H:353:PRO:HG2	1:H:360:LYS:HZ3	1.43	0.83
1:C:350:SER:HB3	1:C:351:PRO:HD3	1.61	0.82
1:F:313:LEU:HD23	1:F:313:LEU:H	1.43	0.82
1:L:353:PRO:HG2	1:L:360:LYS:HZ3	1.44	0.82
1:E:475:LEU:HD23	1:E:475:LEU:H	1.44	0.82
1:G:350:SER:HB3	1:G:351:PRO:HD3	1.61	0.81
1:O:315:LYS:NZ	1:O:315:LYS:CD	2.43	0.81
1:G:111:GLN:HB3	1:G:112:PRO:HD2	1.62	0.81
1:J:138:ASN:HD22	1:J:140:SER:HB3	1.45	0.81
1:A:51:ARG:NH1	1:A:61:ASP:OD2	2.14	0.81
1:G:105:VAL:HG21	1:G:159:LEU:HD11	1.62	0.81
1:J:171:LYS:NZ	1:J:171:LYS:CD	2.43	0.81
1:B:353:PRO:HG2	1:B:360:LYS:NZ	1.95	0.81
1:H:141:GLU:HG2	1:H:142:ASP:HB2	1.59	0.81
1:C:105:VAL:HG21	1:C:159:LEU:HD11	1.61	0.80
1:D:105:VAL:HG21	1:D:159:LEU:HD11	1.63	0.80
1:J:99:VAL:HG21	1:J:382:ILE:HD11	1.64	0.80
1:B:141:GLU:CG	1:B:141:GLU:CA	2.58	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ILE:HD11	1:C:188:LEU:HD11	1.64	0.80
1:F:384:LEU:HB3	1:F:389:MET:CE	2.11	0.80
1:H:307:PHE:HE1	1:H:335:ASP:HB2	1.46	0.80
1:H:159:LEU:CD2	1:H:331:VAL:HG22	2.11	0.80
1:K:121:PRO:HG3	1:L:289:CYS:SG	2.22	0.80
1:N:368:VAL:HG11	1:O:169:TRP:CZ2	2.16	0.80
1:A:282:MET:HG2	1:G:89:SER:CB	2.09	0.80
1:E:353:PRO:CD	1:E:360:LYS:NZ	2.37	0.80
1:F:105:VAL:HG21	1:F:159:LEU:HD11	1.62	0.80
1:H:45:VAL:HG12	1:H:368:VAL:HG22	1.64	0.80
1:E:345:CYS:HB3	1:E:363:GLN:NE2	1.96	0.80
1:F:141:GLU:HG2	1:F:141:GLU:O	1.81	0.80
1:O:475:LEU:HD23	1:O:475:LEU:H	1.47	0.80
1:N:353:PRO:CG	1:N:360:LYS:NZ	2.45	0.80
1:E:45:VAL:HG12	1:E:368:VAL:HG22	1.63	0.79
1:A:121:PRO:HG3	1:B:289:CYS:SG	2.23	0.79
1:E:216:THR:O	1:E:217:LYS:HB2	1.82	0.79
1:H:345:CYS:HB3	1:H:363:GLN:NE2	1.97	0.79
1:L:105:VAL:HG12	1:L:106:GLU:N	1.97	0.79
1:N:353:PRO:HD2	1:N:360:LYS:HZ1	1.47	0.79
1:F:121:PRO:HG3	1:G:289:CYS:SG	2.22	0.79
1:E:138:ASN:ND2	1:E:140:SER:HB3	1.98	0.79
1:I:111:GLN:HB3	1:I:112:PRO:HD2	1.63	0.79
1:N:384:LEU:HB3	1:N:389:MET:CE	2.13	0.79
1:L:453:LYS:CG	1:L:453:LYS:CE	2.60	0.79
1:N:384:LEU:HB3	1:N:389:MET:HE1	1.63	0.79
1:A:216:THR:CG2	1:A:218:CYS:HB2	2.12	0.79
1:H:246:MET:O	1:H:246:MET:HG3	1.83	0.79
1:J:111:GLN:HB3	1:J:112:PRO:HD2	1.64	0.78
1:M:111:GLN:HB3	1:M:112:PRO:HD2	1.63	0.78
1:O:345:CYS:HB3	1:O:363:GLN:NE2	1.98	0.78
1:A:313:LEU:HD23	1:A:313:LEU:H	1.49	0.78
1:A:345:CYS:HB3	1:A:363:GLN:NE2	1.97	0.78
1:C:368:VAL:HG12	1:C:369:GLU:N	1.99	0.78
1:C:111:GLN:HB3	1:C:112:PRO:HD2	1.64	0.78
1:F:307:PHE:HE1	1:F:335:ASP:HB2	1.46	0.78
1:C:475:LEU:HD23	1:C:475:LEU:H	1.49	0.78
1:E:273:GLN:NE2	1:E:278:LYS:HE2	1.97	0.78
1:I:246:MET:HG3	1:I:246:MET:O	1.83	0.78
1:F:181:SER:HB2	1:M:89:SER:CB	2.09	0.78
1:H:51:ARG:O	1:H:53:PRO:HD3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:87:ASP:O	1:K:90:ILE:HG12	1.83	0.78
1:F:345:CYS:HB3	1:F:363:GLN:NE2	1.99	0.78
1:G:70:TYR:OH	1:G:232:PRO:HD3	1.84	0.78
1:N:345:CYS:HB3	1:N:363:GLN:NE2	1.98	0.78
1:G:300:VAL:CG1	1:H:255:LEU:HD13	2.14	0.77
1:G:121:PRO:HG3	1:H:289:CYS:SG	2.24	0.77
1:D:151:TYR:CG	1:D:203:THR:HB	2.19	0.77
1:K:105:VAL:HG21	1:K:159:LEU:HD11	1.65	0.77
1:N:353:PRO:CD	1:N:360:LYS:HZ1	1.97	0.77
1:E:126:LEU:HB3	1:E:262:ASN:HB3	1.67	0.76
1:G:214:GLN:OE1	1:G:219:GLU:HB2	1.86	0.76
1:A:111:GLN:HB3	1:A:112:PRO:HD2	1.67	0.76
1:A:353:PRO:CD	1:A:360:LYS:NZ	2.46	0.76
1:G:78:PRO:HD3	1:G:453:LYS:HA	1.67	0.76
1:H:353:PRO:CD	1:H:360:LYS:NZ	2.42	0.76
1:G:140:SER:O	1:G:141:GLU:HB2	1.85	0.75
1:G:368:VAL:HG11	1:H:169:TRP:HZ2	1.51	0.75
1:I:324:CYS:HB3	1:I:328:GLN:O	1.87	0.75
1:J:273:GLN:NE2	1:J:278:LYS:HE2	2.00	0.75
1:N:99:VAL:HG21	1:N:382:ILE:HD11	1.68	0.75
1:B:45:VAL:HG12	1:B:368:VAL:HG22	1.67	0.75
1:B:126:LEU:HB3	1:B:262:ASN:HB3	1.67	0.75
1:B:247:PHE:CE2	1:B:322:GLY:HA2	2.20	0.75
1:D:313:LEU:HD23	1:D:313:LEU:H	1.51	0.75
1:I:105:VAL:HG21	1:I:159:LEU:HD11	1.67	0.75
1:E:247:PHE:CE2	1:E:322:GLY:HA2	2.21	0.75
1:I:273:GLN:NE2	1:I:278:LYS:HE2	2.02	0.75
1:O:353:PRO:CD	1:O:360:LYS:HZ1	1.99	0.75
1:N:111:GLN:HB3	1:N:112:PRO:CD	2.15	0.75
1:O:85:LEU:HB3	1:O:86:PRO:HD2	1.69	0.75
1:H:54:ALA:HB2	1:H:61:ASP:HB2	1.67	0.74
1:O:109:ARG:H	1:O:308:ASN:HD21	1.34	0.74
1:B:105:VAL:HG21	1:B:159:LEU:HD11	1.69	0.74
1:C:45:VAL:HG12	1:C:368:VAL:HG22	1.67	0.74
1:B:105:VAL:HG12	1:B:106:GLU:N	2.00	0.74
1:C:126:LEU:HB3	1:C:262:ASN:HB3	1.69	0.74
1:N:273:GLN:NE2	1:N:278:LYS:HE2	1.99	0.74
1:A:475:LEU:HD23	1:A:475:LEU:H	1.52	0.74
1:K:368:VAL:HG11	1:L:169:TRP:CZ2	2.23	0.74
1:O:126:LEU:HB3	1:O:262:ASN:HB3	1.69	0.74
1:E:105:VAL:HG12	1:E:106:GLU:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:THR:HG22	1:I:218:CYS:HB2	1.69	0.73
1:J:138:ASN:ND2	1:J:140:SER:HB3	2.01	0.73
1:N:353:PRO:HD2	1:N:360:LYS:NZ	2.02	0.73
1:C:246:MET:HG3	1:C:246:MET:O	1.87	0.73
1:L:453:LYS:CD	1:L:453:LYS:CB	2.65	0.73
1:O:138:ASN:ND2	1:O:140:SER:HB3	2.03	0.73
1:B:368:VAL:HG12	1:B:369:GLU:N	2.03	0.73
1:L:396:ASN:ND2	1:L:398:SER:OG	2.21	0.73
1:M:92:ASN:O	1:M:94:GLU:N	2.20	0.73
1:G:64:LYS:CE	1:G:64:LYS:CG	2.66	0.73
1:N:353:PRO:CD	1:N:360:LYS:NZ	2.51	0.73
1:H:368:VAL:HG11	1:I:169:TRP:CZ2	2.24	0.73
1:L:87:ASP:O	1:L:90:ILE:HG12	1.89	0.73
1:N:105:VAL:HG12	1:N:106:GLU:N	2.04	0.73
1:O:314:HIS:O	1:O:315:LYS:HG3	1.89	0.73
1:I:105:VAL:HG12	1:I:106:GLU:N	2.02	0.73
1:A:105:VAL:HG21	1:A:159:LEU:HD11	1.71	0.73
1:L:250:LEU:HB3	1:L:306:LEU:HD21	1.71	0.73
1:N:350:SER:HB3	1:N:351:PRO:HD3	1.69	0.73
1:D:273:GLN:NE2	1:D:278:LYS:HE2	2.04	0.72
1:H:46:GLY:HA3	1:H:65:VAL:HG23	1.69	0.72
1:I:475:LEU:HD23	1:I:475:LEU:H	1.54	0.72
1:J:126:LEU:HB3	1:J:262:ASN:HB3	1.71	0.72
1:G:64:LYS:CD	1:G:64:LYS:NZ	2.52	0.72
1:A:353:PRO:CG	1:A:360:LYS:HZ3	2.01	0.72
1:F:353:PRO:HG2	1:F:360:LYS:NZ	2.02	0.72
1:K:369:GLU:HG3	1:K:371:TYR:HE1	1.54	0.72
1:B:216:THR:O	1:B:217:LYS:HB2	1.89	0.72
1:D:368:VAL:HG11	1:E:169:TRP:CZ2	2.23	0.72
1:J:125:LYS:NZ	1:J:125:LYS:CD	2.51	0.72
1:N:114:GLY:HA3	1:N:340:THR:HG23	1.70	0.72
1:D:126:LEU:HB3	1:D:262:ASN:HB3	1.71	0.72
1:F:273:GLN:NE2	1:F:278:LYS:HE2	2.01	0.72
1:H:307:PHE:CE1	1:H:335:ASP:HB2	2.23	0.72
1:L:307:PHE:HA	1:L:311:TYR:OH	1.90	0.72
1:A:273:GLN:NE2	1:A:278:LYS:HE2	2.02	0.72
1:F:114:GLY:HA3	1:F:340:THR:HG23	1.71	0.72
1:A:368:VAL:HG11	1:B:169:TRP:CZ2	2.25	0.72
1:C:143:VAL:O	1:C:143:VAL:HG12	1.90	0.72
1:F:159:LEU:CD2	1:F:331:VAL:HG22	2.20	0.72
1:N:121:PRO:HG3	1:O:289:CYS:SG	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:247:PHE:CE2	1:N:322:GLY:HA2	2.24	0.72
1:C:70:TYR:OH	1:C:232:PRO:HD3	1.89	0.72
1:E:151:TYR:CG	1:E:203:THR:HB	2.24	0.72
1:G:24:THR:CG2	1:G:320:ASN:HA	2.20	0.72
1:H:138:ASN:HD22	1:H:140:SER:HB3	1.54	0.72
1:A:59:LYS:HD3	1:B:178:ARG:HG3	1.71	0.72
1:I:353:PRO:HG2	1:I:360:LYS:HZ3	1.54	0.71
1:A:293:PRO:HB3	1:E:117:LEU:HD11	1.71	0.71
1:G:353:PRO:HG2	1:G:360:LYS:HZ3	1.53	0.71
1:K:289:CYS:SG	1:O:121:PRO:HG3	2.30	0.71
1:N:344:ILE:HD11	1:O:188:LEU:HD11	1.73	0.71
1:H:313:LEU:HD23	1:H:313:LEU:H	1.55	0.71
1:H:111:GLN:HB3	1:H:112:PRO:HD2	1.72	0.71
1:H:138:ASN:ND2	1:H:140:SER:HB3	2.06	0.71
1:L:453:LYS:CD	1:L:453:LYS:NZ	2.54	0.71
1:D:72:VAL:HG23	1:D:197:ASP:HA	1.71	0.71
1:I:126:LEU:HB3	1:I:262:ASN:HB3	1.73	0.71
1:M:360:LYS:HE2	1:M:361:PHE:CE1	2.25	0.70
1:D:315:LYS:CD	1:D:315:LYS:CB	2.68	0.70
1:F:307:PHE:CE1	1:F:335:ASP:HB2	2.26	0.70
1:I:70:TYR:OH	1:I:232:PRO:HD3	1.91	0.70
1:J:385:THR:OG1	1:J:388:VAL:HG23	1.91	0.70
1:B:246:MET:HG3	1:B:246:MET:O	1.91	0.70
1:I:141:GLU:HG2	1:I:142:ASP:N	2.05	0.70
1:K:111:GLN:HB3	1:K:112:PRO:HD2	1.74	0.70
1:A:85:LEU:HB3	1:A:86:PRO:HD2	1.73	0.70
1:F:247:PHE:CE2	1:F:322:GLY:HA2	2.26	0.70
1:J:45:VAL:HG12	1:J:368:VAL:HG22	1.72	0.70
1:B:138:ASN:ND2	1:B:140:SER:CB	2.24	0.70
1:G:300:VAL:HG13	1:H:255:LEU:HD13	1.74	0.70
1:K:273:GLN:NE2	1:K:278:LYS:HE2	2.06	0.70
1:L:92:ASN:HD21	1:L:95:THR:HG23	1.57	0.70
1:L:114:GLY:HA3	1:L:340:THR:HG23	1.71	0.70
1:M:325:TRP:O	1:M:326:HIS:HB2	1.90	0.70
1:A:281:GLY:HA3	1:G:89:SER:O	1.92	0.70
1:H:96:GLN:HB3	1:H:383:THR:HA	1.72	0.70
1:K:353:PRO:CD	1:K:360:LYS:NZ	2.54	0.70
1:F:151:TYR:CG	1:F:203:THR:HB	2.27	0.70
1:H:141:GLU:HG2	1:H:142:ASP:CB	2.21	0.70
1:K:105:VAL:HG12	1:K:106:GLU:N	2.06	0.70
1:D:92:ASN:O	1:D:94:GLU:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:156:LEU:HG	1:H:334:VAL:HB	1.74	0.69
1:J:475:LEU:HD23	1:J:475:LEU:H	1.55	0.69
1:B:107:ILE:O	1:B:107:ILE:HG22	1.92	0.69
1:D:105:VAL:HG12	1:D:106:GLU:N	2.06	0.69
1:D:249:CYS:O	1:D:250:LEU:HD12	1.92	0.69
1:G:151:TYR:CG	1:G:203:THR:HB	2.27	0.69
1:H:87:ASP:O	1:H:90:ILE:HG12	1.92	0.69
1:I:353:PRO:CD	1:I:360:LYS:NZ	2.55	0.69
1:L:126:LEU:HB3	1:L:262:ASN:CB	2.22	0.69
1:O:87:ASP:O	1:O:90:ILE:HG12	1.93	0.69
1:B:350:SER:HB3	1:B:351:PRO:HD3	1.73	0.69
1:J:384:LEU:HB3	1:J:389:MET:CE	2.22	0.69
1:F:369:GLU:HG3	1:F:371:TYR:HE1	1.57	0.69
1:H:24:THR:CG2	1:H:320:ASN:HA	2.22	0.69
1:F:214:GLN:OE1	1:F:219:GLU:HB2	1.92	0.69
1:I:368:VAL:HG12	1:I:369:GLU:N	2.07	0.69
1:O:273:GLN:HE22	1:O:278:LYS:HE2	1.57	0.69
1:A:282:MET:CG	1:G:89:SER:HB2	2.17	0.69
1:I:151:TYR:CG	1:I:203:THR:HB	2.28	0.69
1:I:307:PHE:HE1	1:I:335:ASP:HB2	1.57	0.69
1:M:368:VAL:HG11	1:N:169:TRP:CZ2	2.27	0.69
1:M:475:LEU:HD23	1:M:475:LEU:H	1.58	0.69
1:B:111:GLN:HB3	1:B:112:PRO:HD2	1.75	0.69
1:B:151:TYR:CG	1:B:203:THR:HB	2.27	0.69
1:B:329:LEU:HD23	1:B:329:LEU:C	2.13	0.69
1:F:233:ASP:OD2	1:J:41:ARG:NH2	2.25	0.69
1:F:253:GLU:HG3	1:J:113:LEU:HD22	1.73	0.69
1:I:121:PRO:HG3	1:J:289:CYS:SG	2.33	0.69
1:A:72:VAL:HG23	1:A:197:ASP:HA	1.75	0.69
1:D:99:VAL:HG21	1:D:382:ILE:HD11	1.74	0.69
1:F:36:HIS:ND1	1:F:37:ALA:N	2.40	0.69
1:L:273:GLN:HE22	1:L:278:LYS:CE	1.96	0.69
1:M:151:TYR:CG	1:M:203:THR:HB	2.28	0.69
1:N:156:LEU:HA	1:N:250:LEU:O	1.92	0.69
1:B:99:VAL:HG21	1:B:382:ILE:HD11	1.75	0.68
1:J:85:LEU:HD12	1:J:88:THR:HA	1.73	0.68
1:A:59:LYS:O	1:A:59:LYS:HG2	1.91	0.68
1:G:141:GLU:O	1:G:141:GLU:HG2	1.93	0.68
1:M:126:LEU:HB3	1:M:262:ASN:CB	2.22	0.68
1:M:126:LEU:CB	1:M:262:ASN:HB3	2.21	0.68
1:O:388:VAL:O	1:O:392:ILE:HG13	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:349:GLN:HG2	1:I:360:LYS:HD2	1.74	0.68
1:G:126:LEU:HB3	1:G:262:ASN:HB3	1.75	0.68
1:L:345:CYS:HB3	1:L:363:GLN:NE2	2.08	0.68
1:N:306:LEU:O	1:N:311:TYR:OH	2.06	0.68
1:H:159:LEU:HD22	1:H:331:VAL:HG22	1.74	0.68
1:J:114:GLY:HA3	1:J:340:THR:HG23	1.75	0.68
1:E:87:ASP:HB3	1:E:90:ILE:HD11	1.75	0.68
1:F:122:PHE:O	1:F:218:CYS:HB3	1.94	0.68
1:D:42:LEU:HB3	1:D:448:TRP:CZ2	2.27	0.68
1:L:353:PRO:CG	1:L:360:LYS:NZ	2.56	0.68
1:N:151:TYR:CG	1:N:203:THR:HB	2.28	0.68
1:G:196:GLU:N	1:G:199:ASP:OD2	2.23	0.68
1:H:475:LEU:HD23	1:H:475:LEU:H	1.58	0.68
1:E:159:LEU:HD22	1:E:331:VAL:HG22	1.77	0.67
1:H:258:ARG:NH1	1:I:130:GLU:OE1	2.26	0.67
1:G:315:LYS:CD	1:G:315:LYS:NZ	2.56	0.67
1:K:353:PRO:CD	1:K:360:LYS:HZ1	2.07	0.67
1:O:91:TYR:HB2	1:O:96:GLN:HG3	1.76	0.67
1:H:109:ARG:H	1:H:308:ASN:ND2	1.91	0.67
1:M:159:LEU:HD22	1:M:331:VAL:HG22	1.76	0.67
1:C:258:ARG:NH1	1:D:130:GLU:OE1	2.27	0.67
1:N:126:LEU:HB3	1:N:262:ASN:HB3	1.77	0.67
1:J:141:GLU:HG3	1:J:142:ASP:N	2.09	0.67
1:C:138:ASN:HD22	1:C:140:SER:HB3	1.60	0.67
1:L:36:HIS:ND1	1:L:37:ALA:N	2.43	0.67
1:B:345:CYS:HB3	1:B:363:GLN:NE2	2.10	0.67
1:C:105:VAL:HG12	1:C:106:GLU:N	2.10	0.67
1:D:159:LEU:CD2	1:D:331:VAL:HG22	2.25	0.67
1:F:233:ASP:CG	1:F:236:GLN:HB3	2.14	0.67
1:H:22:VAL:HG12	1:H:23:ASN:N	2.10	0.67
1:H:24:THR:HG23	1:H:320:ASN:HA	1.75	0.67
1:K:310:PRO:HG2	1:K:310:PRO:O	1.93	0.67
1:M:313:LEU:HD23	1:M:313:LEU:N	2.09	0.67
1:E:87:ASP:O	1:E:90:ILE:HG12	1.95	0.66
1:G:220:VAL:HB	1:G:221:PRO:CD	2.25	0.66
1:C:329:LEU:HD23	1:C:329:LEU:C	2.15	0.66
1:J:122:PHE:O	1:J:218:CYS:HB3	1.96	0.66
1:K:344:ILE:HD11	1:L:188:LEU:HD11	1.77	0.66
1:H:353:PRO:CG	1:H:360:LYS:HZ3	2.08	0.66
1:N:475:LEU:HD23	1:N:475:LEU:N	2.01	0.66
1:E:143:VAL:HG12	1:E:143:VAL:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:THR:O	1:A:217:LYS:HB2	1.94	0.66
1:D:356:TYR:HE2	1:E:142:ASP:HA	1.60	0.66
1:L:85:LEU:HB3	1:L:86:PRO:HD2	1.76	0.66
1:L:105:VAL:HG21	1:L:159:LEU:HD11	1.78	0.66
1:M:345:CYS:HB3	1:M:363:GLN:NE2	2.09	0.66
1:N:369:GLU:HG3	1:N:371:TYR:HE1	1.59	0.66
1:G:249:CYS:O	1:G:250:LEU:HD12	1.96	0.66
1:G:247:PHE:CE2	1:G:322:GLY:HA2	2.30	0.65
1:H:59:LYS:HD3	1:I:178:ARG:HG3	1.76	0.65
1:G:353:PRO:HG2	1:G:360:LYS:NZ	2.11	0.65
1:N:475:LEU:H	1:N:475:LEU:CD2	1.94	0.65
1:H:384:LEU:HB3	1:H:389:MET:CE	2.26	0.65
1:A:151:TYR:CG	1:A:203:THR:HB	2.32	0.65
1:F:117:LEU:HD11	1:G:293:PRO:HB3	1.77	0.65
1:L:307:PHE:HE1	1:L:335:ASP:HB2	1.62	0.65
1:M:121:PRO:HG3	1:N:289:CYS:SG	2.37	0.65
1:F:68:TYR:CE2	1:F:151:TYR:HB2	2.32	0.65
1:G:22:VAL:HG12	1:G:23:ASN:N	2.09	0.65
1:G:353:PRO:CG	1:G:360:LYS:NZ	2.60	0.65
1:O:475:LEU:H	1:O:475:LEU:CD2	2.09	0.65
1:A:307:PHE:HA	1:A:311:TYR:OH	1.95	0.65
1:C:355:GLN:HE22	1:H:386:ALA:HB2	1.59	0.65
1:D:233:ASP:CG	1:D:236:GLN:HB3	2.16	0.65
1:E:45:VAL:CG1	1:E:368:VAL:HG22	2.25	0.65
1:G:324:CYS:HB3	1:G:328:GLN:O	1.96	0.65
1:J:307:PHE:HA	1:J:311:TYR:OH	1.96	0.65
1:A:353:PRO:HG2	1:A:360:LYS:NZ	2.07	0.65
1:A:364:TYR:CD2	1:B:185:CYS:HB2	2.32	0.65
1:C:85:LEU:HB3	1:C:86:PRO:HD2	1.77	0.65
1:F:384:LEU:HB3	1:F:389:MET:HE2	1.77	0.65
1:J:109:ARG:H	1:J:308:ASN:ND2	1.93	0.65
1:L:66:SER:HB3	1:L:69:GLN:HG2	1.77	0.65
1:B:188:LEU:HD22	1:B:188:LEU:N	2.12	0.65
1:B:307:PHE:HE1	1:B:335:ASP:HB2	1.62	0.65
1:B:353:PRO:HD2	1:B:360:LYS:HZ1	1.62	0.65
1:J:151:TYR:CG	1:J:203:THR:HB	2.31	0.65
1:K:185:CYS:HB2	1:O:364:TYR:CD2	2.32	0.65
1:K:475:LEU:H	1:K:475:LEU:CD2	2.10	0.65
1:M:113:LEU:HD22	1:N:253:GLU:HG3	1.77	0.65
1:I:258:ARG:NH1	1:J:130:GLU:OE1	2.29	0.65
1:O:159:LEU:CD2	1:O:331:VAL:HG22	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ILE:HD11	1:B:188:LEU:HD11	1.78	0.64
1:G:345:CYS:HB3	1:G:363:GLN:NE2	2.11	0.64
1:I:216:THR:CG2	1:I:218:CYS:HB2	2.28	0.64
1:E:46:GLY:HA3	1:E:65:VAL:HG23	1.77	0.64
1:I:313:LEU:HD23	1:I:313:LEU:H	1.62	0.64
1:L:246:MET:HG3	1:L:246:MET:O	1.95	0.64
1:E:114:GLY:HA3	1:E:340:THR:HG23	1.80	0.64
1:H:307:PHE:HA	1:H:311:TYR:OH	1.97	0.64
1:M:138:ASN:HD22	1:M:140:SER:HB3	1.62	0.64
1:F:105:VAL:HG12	1:F:106:GLU:N	2.12	0.64
1:N:87:ASP:O	1:N:90:ILE:HG12	1.97	0.64
1:H:72:VAL:HG23	1:H:197:ASP:HA	1.79	0.64
1:K:126:LEU:HB3	1:K:262:ASN:HB3	1.80	0.64
1:N:214:GLN:OE1	1:N:219:GLU:HB2	1.97	0.64
1:B:141:GLU:CB	1:B:141:GLU:CD	2.63	0.64
1:G:143:VAL:O	1:G:143:VAL:HG12	1.98	0.64
1:K:114:GLY:HA3	1:K:340:THR:HG23	1.80	0.64
1:L:233:ASP:CG	1:L:236:GLN:HB3	2.17	0.64
1:M:159:LEU:CD2	1:M:331:VAL:HG22	2.28	0.64
1:N:313:LEU:HD23	1:N:313:LEU:H	1.62	0.64
1:J:141:GLU:HG3	1:J:142:ASP:H	1.63	0.64
1:L:98:LEU:CD2	1:L:381:THR:HG22	2.27	0.64
1:J:109:ARG:H	1:J:308:ASN:HD21	1.44	0.64
1:K:364:TYR:CD2	1:L:185:CYS:HB2	2.33	0.64
1:A:368:VAL:HG12	1:A:369:GLU:N	2.12	0.63
1:B:324:CYS:HB3	1:B:328:GLN:O	1.98	0.63
1:C:24:THR:HG23	1:C:320:ASN:HA	1.80	0.63
1:F:24:THR:CG2	1:F:320:ASN:HA	2.27	0.63
1:J:233:ASP:CG	1:J:236:GLN:HB3	2.17	0.63
1:K:369:GLU:HG3	1:K:371:TYR:CE1	2.32	0.63
1:B:126:LEU:HB3	1:B:262:ASN:CB	2.28	0.63
1:H:233:ASP:CG	1:H:236:GLN:HB3	2.19	0.63
1:F:111:GLN:HB3	1:F:112:PRO:CD	2.29	0.63
1:N:22:VAL:HG12	1:N:23:ASN:N	2.13	0.63
1:O:22:VAL:HG12	1:O:23:ASN:N	2.12	0.63
1:O:193:THR:CG2	1:O:230:LYS:HD3	2.29	0.63
1:B:364:TYR:CG	1:C:185:CYS:HB2	2.34	0.63
1:C:368:VAL:CG1	1:C:369:GLU:N	2.62	0.63
1:G:114:GLY:HA3	1:G:340:THR:HG23	1.80	0.63
1:G:233:ASP:CG	1:G:236:GLN:HB3	2.18	0.63
1:G:390:SER:O	1:G:393:GLN:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:ASP:OD2	1:I:136:THR:OG1	2.13	0.63
1:K:293:PRO:HD3	1:O:117:LEU:HG	1.81	0.63
1:L:353:PRO:HD2	1:L:360:LYS:CE	2.28	0.63
1:M:22:VAL:HG12	1:M:23:ASN:N	2.13	0.63
1:J:307:PHE:HE1	1:J:335:ASP:HB2	1.63	0.63
1:K:188:LEU:N	1:K:188:LEU:HD22	2.13	0.63
1:B:353:PRO:CD	1:B:360:LYS:HZ1	2.12	0.63
1:E:353:PRO:CG	1:E:360:LYS:NZ	2.62	0.63
1:F:364:TYR:CD2	1:G:185:CYS:HB2	2.33	0.63
1:K:24:THR:CG2	1:K:320:ASN:HA	2.27	0.63
1:A:87:ASP:HB3	1:A:90:ILE:HD11	1.81	0.63
1:E:105:VAL:HG21	1:E:159:LEU:HD11	1.80	0.63
1:G:92:ASN:HD21	1:G:95:THR:HG23	1.63	0.63
1:L:99:VAL:HG21	1:L:382:ILE:HD11	1.79	0.63
1:O:109:ARG:H	1:O:308:ASN:ND2	1.96	0.63
1:O:353:PRO:CD	1:O:360:LYS:NZ	2.60	0.63
1:K:151:TYR:CG	1:K:203:THR:HB	2.33	0.63
1:K:353:PRO:CG	1:K:360:LYS:HZ2	2.11	0.63
1:C:71:ARG:HA	1:C:197:ASP:OD1	1.99	0.62
1:D:92:ASN:C	1:D:94:GLU:H	2.01	0.62
1:E:353:PRO:CG	1:E:360:LYS:HZ3	2.11	0.62
1:I:244:ASP:OD1	1:I:320:ASN:ND2	2.28	0.62
1:L:109:ARG:H	1:L:308:ASN:ND2	1.97	0.62
1:L:71:ARG:HA	1:L:197:ASP:OD1	1.99	0.62
1:N:122:PHE:O	1:N:218:CYS:HB3	1.99	0.62
1:C:300:VAL:HG13	1:C:300:VAL:O	1.99	0.62
1:J:247:PHE:CD2	1:J:322:GLY:HA2	2.34	0.62
1:M:376:ILE:HG12	1:M:465:LEU:HD13	1.81	0.62
1:N:368:VAL:HG12	1:N:369:GLU:N	2.12	0.62
1:C:45:VAL:CG1	1:C:368:VAL:HG22	2.28	0.62
1:F:151:TYR:OH	1:F:221:PRO:HB2	1.99	0.62
1:H:390:SER:O	1:H:393:GLN:HB3	1.99	0.62
1:J:388:VAL:O	1:J:392:ILE:HG13	1.99	0.62
1:D:311:TYR:N	1:D:311:TYR:CD1	2.66	0.62
1:G:232:PRO:HB2	1:G:234:TYR:CE1	2.34	0.62
1:K:307:PHE:HA	1:K:311:TYR:OH	1.99	0.62
1:G:105:VAL:HG12	1:G:106:GLU:N	2.14	0.62
1:D:87:ASP:O	1:D:90:ILE:HG12	2.00	0.62
1:F:465:LEU:CD1	1:F:465:LEU:HG	2.16	0.62
1:G:325:TRP:O	1:G:326:HIS:HB2	1.99	0.62
1:L:188:LEU:HD22	1:L:188:LEU:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:191:LYS:CE	1:M:191:LYS:CG	2.76	0.62
1:B:353:PRO:CG	1:B:360:LYS:HZ2	2.07	0.62
1:C:24:THR:CG2	1:C:320:ASN:HA	2.29	0.62
1:H:69:GLN:NE2	1:H:71:ARG:HH22	1.97	0.62
1:B:24:THR:HG23	1:B:319:HIS:O	2.00	0.62
1:C:70:TYR:CE1	1:C:201:VAL:HG12	2.35	0.62
1:D:475:LEU:H	1:D:475:LEU:CD2	2.00	0.62
1:E:74:ARG:HG3	1:E:330:PHE:CE2	2.34	0.62
1:F:98:LEU:CD2	1:F:381:THR:HG22	2.29	0.62
1:H:368:VAL:HG12	1:H:369:GLU:N	2.13	0.62
1:J:324:CYS:HB3	1:J:328:GLN:O	2.00	0.62
1:K:233:ASP:CG	1:K:236:GLN:HB3	2.20	0.61
1:L:151:TYR:CG	1:L:203:THR:HB	2.34	0.61
1:L:390:SER:O	1:L:393:GLN:HB3	2.00	0.61
1:L:351:PRO:O	1:L:352:VAL:HB	2.00	0.61
1:E:233:ASP:CG	1:E:236:GLN:HB3	2.20	0.61
1:F:246:MET:HG3	1:F:246:MET:O	2.00	0.61
1:G:444:LYS:HA	1:G:444:LYS:HE2	1.83	0.61
1:N:353:PRO:HD2	1:N:360:LYS:CE	2.30	0.61
1:C:273:GLN:HE22	1:C:278:LYS:CE	2.02	0.61
1:M:307:PHE:HE1	1:M:335:ASP:HB2	1.64	0.61
1:A:123:TYR:HD2	1:A:125:LYS:HB2	1.64	0.61
1:E:353:PRO:HG2	1:E:360:LYS:NZ	2.13	0.61
1:C:70:TYR:CZ	1:C:201:VAL:HG12	2.35	0.61
1:F:293:PRO:HB3	1:J:117:LEU:HD11	1.82	0.61
1:F:307:PHE:HA	1:F:311:TYR:OH	2.01	0.61
1:F:350:SER:HB3	1:F:351:PRO:HD3	1.82	0.61
1:H:92:ASN:HD21	1:H:95:THR:HG23	1.65	0.61
1:J:316:ALA:HB3	1:J:321:ASN:HA	1.81	0.61
1:L:364:TYR:CD2	1:M:185:CYS:HB2	2.36	0.61
1:O:390:SER:O	1:O:393:GLN:HB3	1.99	0.61
1:A:353:PRO:CG	1:A:360:LYS:NZ	2.63	0.61
1:B:364:TYR:CE2	1:C:185:CYS:HB2	2.36	0.61
1:C:453:LYS:NZ	1:C:453:LYS:CD	2.61	0.61
1:I:113:LEU:HD22	1:J:253:GLU:HG3	1.83	0.61
1:C:368:VAL:HG11	1:D:169:TRP:CZ2	2.36	0.61
1:F:369:GLU:HG3	1:F:371:TYR:CE1	2.36	0.61
1:B:214:GLN:OE1	1:B:219:GLU:HB2	2.01	0.60
1:C:36:HIS:ND1	1:C:37:ALA:N	2.49	0.60
1:D:117:LEU:HD11	1:E:293:PRO:HB3	1.83	0.60
1:E:369:GLU:HG3	1:E:371:TYR:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:VAL:HG12	1:F:369:GLU:N	2.13	0.60
1:G:315:LYS:CE	1:G:315:LYS:CG	2.75	0.60
1:H:151:TYR:CG	1:H:203:THR:HB	2.36	0.60
1:N:216:THR:O	1:N:217:LYS:HB2	2.01	0.60
1:N:307:PHE:HA	1:N:311:TYR:OH	2.01	0.60
1:O:143:VAL:O	1:O:143:VAL:CG1	2.45	0.60
1:H:193:THR:HG21	1:H:230:LYS:HE2	1.84	0.60
1:J:88:THR:O	1:J:88:THR:HG22	2.00	0.60
1:D:138:ASN:HD22	1:D:140:SER:HB3	1.66	0.60
1:F:188:LEU:HD22	1:F:188:LEU:N	2.16	0.60
1:G:300:VAL:HG12	1:H:255:LEU:O	2.01	0.60
1:I:459:ASP:OD2	1:I:459:ASP:N	2.33	0.60
1:K:258:ARG:NH1	1:L:130:GLU:OE1	2.34	0.60
1:L:105:VAL:HG12	1:L:106:GLU:H	1.66	0.60
1:N:21:VAL:HG12	1:N:22:VAL:N	2.15	0.60
1:N:42:LEU:HB3	1:N:448:TRP:CZ2	2.37	0.60
1:C:91:TYR:HB2	1:C:96:GLN:HG3	1.84	0.60
1:D:216:THR:O	1:D:217:LYS:HB2	2.01	0.60
1:H:45:VAL:CG1	1:H:368:VAL:HG22	2.31	0.60
1:H:122:PHE:O	1:H:218:CYS:HB3	2.00	0.60
1:E:246:MET:O	1:E:246:MET:HG3	2.01	0.60
1:F:169:TRP:CZ2	1:J:368:VAL:HG11	2.36	0.60
1:L:109:ARG:H	1:L:308:ASN:HD21	1.49	0.60
1:M:109:ARG:H	1:M:308:ASN:HD21	1.49	0.60
1:B:122:PHE:O	1:B:218:CYS:HB3	2.01	0.60
1:D:315:LYS:CG	1:D:315:LYS:CE	2.78	0.60
1:O:151:TYR:CG	1:O:203:THR:HB	2.35	0.60
1:B:344:ILE:CD1	1:C:188:LEU:HD11	2.29	0.60
1:D:313:LEU:HD23	1:D:313:LEU:N	2.17	0.60
1:F:123:TYR:CB	1:F:147:VAL:HG22	2.31	0.60
1:G:92:ASN:ND2	1:G:95:THR:H	1.98	0.60
1:J:345:CYS:HB3	1:J:363:GLN:NE2	2.16	0.60
1:D:376:ILE:HG12	1:D:465:LEU:HD13	1.84	0.60
1:E:111:GLN:HB3	1:E:112:PRO:CD	2.31	0.60
1:F:313:LEU:HD23	1:F:313:LEU:N	2.15	0.60
1:G:369:GLU:HG3	1:G:371:TYR:HE1	1.66	0.60
1:M:114:GLY:HA3	1:M:340:THR:HG23	1.83	0.60
1:N:88:THR:HG22	1:N:88:THR:O	2.01	0.60
1:A:151:TYR:OH	1:A:221:PRO:HB2	2.02	0.60
1:A:247:PHE:CE2	1:A:322:GLY:HA2	2.36	0.60
1:A:385:THR:OG1	1:A:388:VAL:HG23	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:114:GLY:HA3	1:H:340:THR:HG23	1.84	0.60
1:F:465:LEU:CD1	1:F:465:LEU:CD2	2.74	0.60
1:G:87:ASP:O	1:G:90:ILE:HG12	2.00	0.60
1:K:246:MET:HG3	1:K:246:MET:O	2.02	0.60
1:L:45:VAL:HG12	1:L:368:VAL:HG22	1.83	0.60
1:O:111:GLN:HB3	1:O:112:PRO:HD2	1.82	0.60
1:C:344:ILE:HD11	1:D:188:LEU:HD11	1.83	0.59
1:K:76:GLN:HG3	1:K:453:LYS:HE3	1.84	0.59
1:K:384:LEU:HB3	1:K:389:MET:CE	2.32	0.59
1:A:87:ASP:O	1:A:90:ILE:HG12	2.01	0.59
1:F:34:PHE:CE2	1:F:378:GLN:HB2	2.36	0.59
1:K:69:GLN:NE2	1:K:71:ARG:HH22	1.99	0.59
1:B:293:PRO:O	1:B:293:PRO:HG2	2.01	0.59
1:L:344:ILE:HD11	1:M:188:LEU:HD11	1.83	0.59
1:A:216:THR:HG22	1:A:218:CYS:CB	2.27	0.59
1:D:444:LYS:HA	1:D:444:LYS:HE2	1.83	0.59
1:J:141:GLU:CG	1:J:142:ASP:N	2.65	0.59
1:M:342:LEU:HD22	1:N:208:MET:SD	2.43	0.59
1:O:98:LEU:HD21	1:O:381:THR:HG22	1.83	0.59
1:C:191:LYS:CE	1:C:191:LYS:CG	2.79	0.59
1:G:463:TYR:O	1:G:467:ARG:HG3	2.02	0.59
1:B:307:PHE:HA	1:B:311:TYR:OH	2.02	0.59
1:L:193:THR:HG21	1:L:230:LYS:HE2	1.85	0.59
1:M:368:VAL:HG12	1:M:369:GLU:N	2.16	0.59
1:O:105:VAL:HG21	1:O:159:LEU:HD11	1.83	0.59
1:O:156:LEU:HG	1:O:334:VAL:HB	1.84	0.59
1:E:307:PHE:HA	1:E:311:TYR:OH	2.03	0.59
1:H:109:ARG:H	1:H:308:ASN:HD21	1.49	0.59
1:M:98:LEU:CD2	1:M:381:THR:HG22	2.32	0.59
1:N:313:LEU:HD23	1:N:313:LEU:N	2.17	0.59
1:F:36:HIS:ND1	1:F:36:HIS:C	2.56	0.59
1:H:314:HIS:O	1:H:315:LYS:HG3	2.03	0.59
1:J:384:LEU:HB3	1:J:389:MET:HE1	1.85	0.59
1:A:300:VAL:HG13	1:A:300:VAL:O	2.03	0.59
1:G:24:THR:HG23	1:G:320:ASN:HA	1.84	0.59
1:I:307:PHE:CE1	1:I:335:ASP:HB2	2.37	0.59
1:K:231:TYR:CD1	1:O:112:PRO:HB3	2.38	0.59
1:K:345:CYS:HB3	1:K:363:GLN:NE2	2.18	0.59
1:N:81:ASN:OD1	1:N:98:LEU:HB2	2.03	0.59
1:A:165:ILE:HD12	1:A:165:ILE:N	2.17	0.59
1:D:439:LYS:NZ	1:D:439:LYS:CD	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:TYR:CB	1:I:147:VAL:HG22	2.33	0.59
1:D:111:GLN:HB3	1:D:112:PRO:HD2	1.85	0.58
1:E:360:LYS:HE2	1:E:361:PHE:CE1	2.38	0.58
1:G:475:LEU:HD23	1:G:475:LEU:H	1.67	0.58
1:M:138:ASN:ND2	1:M:140:SER:HB3	2.17	0.58
1:M:390:SER:O	1:M:393:GLN:HB3	2.03	0.58
1:O:307:PHE:HA	1:O:311:TYR:OH	2.02	0.58
1:A:390:SER:O	1:A:393:GLN:HB3	2.03	0.58
1:B:24:THR:CG2	1:B:320:ASN:HA	2.33	0.58
1:B:109:ARG:H	1:B:308:ASN:HD21	1.51	0.58
1:D:475:LEU:HD23	1:D:475:LEU:N	2.05	0.58
1:H:344:ILE:HD11	1:I:188:LEU:HD11	1.85	0.58
1:I:350:SER:HB3	1:I:351:PRO:HD3	1.85	0.58
1:B:226:GLN:OE1	1:B:226:GLN:HA	2.01	0.58
1:G:98:LEU:CD2	1:G:381:THR:HG22	2.33	0.58
1:C:392:ILE:O	1:C:392:ILE:HG22	2.02	0.58
1:J:350:SER:HB3	1:J:351:PRO:HD3	1.84	0.58
1:M:350:SER:HB3	1:M:351:PRO:HD3	1.86	0.58
1:N:233:ASP:CG	1:N:236:GLN:HB3	2.23	0.58
1:D:138:ASN:ND2	1:D:140:SER:HB3	2.18	0.58
1:F:98:LEU:HD13	1:F:379:LEU:HD11	1.85	0.58
1:F:324:CYS:HB3	1:F:328:GLN:O	2.02	0.58
1:J:246:MET:HG3	1:J:246:MET:O	2.04	0.58
1:L:325:TRP:O	1:L:326:HIS:HB2	2.03	0.58
1:M:24:THR:HG23	1:M:319:HIS:O	2.03	0.58
1:C:307:PHE:HE1	1:C:335:ASP:HB2	1.68	0.58
1:D:307:PHE:HE1	1:D:335:ASP:HB2	1.68	0.58
1:F:368:VAL:CG1	1:F:369:GLU:N	2.65	0.58
1:G:99:VAL:HG21	1:G:382:ILE:HD11	1.86	0.58
1:I:369:GLU:HG3	1:I:371:TYR:HE1	1.69	0.58
1:I:369:GLU:HG3	1:I:371:TYR:CE1	2.38	0.58
1:L:138:ASN:ND2	1:L:140:SER:HB3	2.19	0.58
1:M:368:VAL:HG11	1:N:169:TRP:HZ2	1.69	0.58
1:A:105:VAL:HG12	1:A:106:GLU:N	2.19	0.58
1:B:353:PRO:CG	1:B:360:LYS:NZ	2.64	0.58
1:F:254:GLN:HG3	1:F:254:GLN:O	2.03	0.58
1:F:368:VAL:HG11	1:G:169:TRP:CZ2	2.38	0.58
1:G:313:LEU:HD23	1:G:313:LEU:H	1.68	0.58
1:H:74:ARG:NE	1:H:328:GLN:OE1	2.34	0.58
1:H:360:LYS:HE2	1:H:361:PHE:CE1	2.38	0.58
1:C:87:ASP:O	1:C:90:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:PRO:HG3	1:D:289:CYS:SG	2.44	0.58
1:D:45:VAL:CG1	1:D:368:VAL:HG22	2.28	0.58
1:A:389:MET:HG2	1:A:400:LEU:HD21	1.84	0.58
1:B:247:PHE:CD2	1:B:322:GLY:HA2	2.39	0.58
1:C:396:ASN:HB3	1:C:399:ILE:HG13	1.86	0.58
1:D:350:SER:HB3	1:D:351:PRO:HD3	1.86	0.58
1:G:85:LEU:HB3	1:G:86:PRO:HD2	1.85	0.58
1:K:117:LEU:CD1	1:L:260:PHE:HB3	2.34	0.58
1:M:201:VAL:HG11	1:M:334:VAL:HG11	1.84	0.58
1:G:364:TYR:CD2	1:H:185:CYS:HB2	2.39	0.58
1:J:446:LYS:CG	1:J:446:LYS:CE	2.81	0.58
1:L:121:PRO:HG3	1:M:289:CYS:HG	1.63	0.58
1:M:35:TYR:CE2	1:M:458:LEU:HG	2.39	0.58
1:A:214:GLN:OE1	1:A:219:GLU:HB2	2.03	0.57
1:B:131:SER:O	1:B:132:SER:C	2.40	0.57
1:F:71:ARG:HA	1:F:197:ASP:OD1	2.04	0.57
1:F:258:ARG:HG3	1:F:259:HIS:ND1	2.19	0.57
1:G:109:ARG:H	1:G:308:ASN:ND2	2.01	0.57
1:G:307:PHE:O	1:G:308:ASN:HB2	2.03	0.57
1:I:261:TRP:CZ3	1:I:294:SER:HB3	2.38	0.57
1:K:185:CYS:HB2	1:O:364:TYR:CE2	2.39	0.57
1:M:85:LEU:HB3	1:M:86:PRO:HD2	1.86	0.57
1:A:232:PRO:HB2	1:A:234:TYR:CE1	2.39	0.57
1:A:180:LEU:HD21	1:A:186:PRO:HA	1.84	0.57
1:E:390:SER:O	1:E:393:GLN:HB3	2.05	0.57
1:F:475:LEU:H	1:F:475:LEU:CD2	2.12	0.57
1:G:68:TYR:O	1:G:201:VAL:HG22	2.05	0.57
1:L:117:LEU:HD11	1:M:293:PRO:HB3	1.87	0.57
1:C:151:TYR:OH	1:C:221:PRO:HB2	2.04	0.57
1:I:353:PRO:CD	1:I:360:LYS:HZ2	2.12	0.57
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.87	0.57
1:D:244:ASP:OD1	1:D:320:ASN:ND2	2.37	0.57
1:E:446:LYS:CD	1:E:446:LYS:NZ	2.67	0.57
1:H:85:LEU:HB3	1:H:86:PRO:HD2	1.85	0.57
1:M:344:ILE:HD11	1:N:188:LEU:HD11	1.86	0.57
1:N:364:TYR:CE2	1:O:185:CYS:HB2	2.40	0.57
1:E:109:ARG:H	1:E:308:ASN:HD21	1.53	0.57
1:H:36:HIS:ND1	1:H:37:ALA:N	2.51	0.57
1:I:233:ASP:CG	1:I:236:GLN:HB3	2.24	0.57
1:J:46:GLY:HA3	1:J:65:VAL:HG23	1.87	0.57
1:M:191:LYS:CD	1:M:191:LYS:NZ	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:350:SER:HB3	1:O:351:PRO:HD3	1.87	0.57
1:O:376:ILE:HG12	1:O:465:LEU:HD13	1.87	0.57
1:D:390:SER:O	1:D:393:GLN:HB3	2.05	0.57
1:F:384:LEU:HB3	1:F:389:MET:HE1	1.84	0.57
1:G:110:GLY:HA3	1:G:370:GLU:HB3	1.86	0.57
1:K:113:LEU:HD22	1:L:253:GLU:HG3	1.86	0.57
1:D:307:PHE:HA	1:D:311:TYR:OH	2.04	0.57
1:I:72:VAL:HG23	1:I:197:ASP:HA	1.87	0.57
1:N:45:VAL:HG12	1:N:368:VAL:HG22	1.86	0.57
1:N:246:MET:HG3	1:N:246:MET:O	2.05	0.57
1:O:261:TRP:CZ3	1:O:294:SER:HB3	2.39	0.57
1:A:246:MET:HG3	1:A:246:MET:O	2.04	0.57
1:B:85:LEU:HB3	1:B:86:PRO:HD2	1.87	0.57
1:E:85:LEU:HB3	1:E:86:PRO:HD2	1.87	0.57
1:G:113:LEU:HD22	1:H:253:GLU:HG3	1.86	0.57
1:K:42:LEU:HB3	1:K:448:TRP:CZ2	2.39	0.57
1:L:367:HIS:CE1	1:L:369:GLU:OE2	2.58	0.57
1:L:368:VAL:HG11	1:M:169:TRP:CZ2	2.40	0.57
1:M:117:LEU:HG	1:N:293:PRO:HD3	1.85	0.57
1:I:345:CYS:HB3	1:I:363:GLN:NE2	2.20	0.57
1:K:258:ARG:HG3	1:K:259:HIS:ND1	2.19	0.57
1:H:351:PRO:O	1:H:352:VAL:HB	2.05	0.56
1:I:107:ILE:HG22	1:I:107:ILE:O	2.05	0.56
1:I:313:LEU:HD23	1:I:313:LEU:N	2.20	0.56
1:O:159:LEU:HD22	1:O:331:VAL:HG22	1.87	0.56
1:O:193:THR:HG23	1:O:230:LYS:HD3	1.87	0.56
1:G:24:THR:HG21	1:G:320:ASN:HA	1.86	0.56
1:G:140:SER:O	1:G:141:GLU:CB	2.32	0.56
1:L:365:SER:HB2	1:M:290:VAL:HG13	1.86	0.56
1:B:353:PRO:CD	1:B:360:LYS:NZ	2.69	0.56
1:C:384:LEU:HB3	1:C:389:MET:CE	2.35	0.56
1:D:85:LEU:HB3	1:D:86:PRO:HD2	1.87	0.56
1:D:105:VAL:CG2	1:D:159:LEU:HD11	2.34	0.56
1:E:92:ASN:C	1:E:94:GLU:H	2.08	0.56
1:E:105:VAL:HG12	1:E:106:GLU:H	1.69	0.56
1:G:45:VAL:HG12	1:G:368:VAL:HG22	1.87	0.56
1:G:300:VAL:HG13	1:G:300:VAL:O	2.04	0.56
1:I:92:ASN:HD21	1:I:95:THR:HG23	1.70	0.56
1:L:68:TYR:O	1:L:201:VAL:HG22	2.05	0.56
1:L:344:ILE:CD1	1:M:188:LEU:HD11	2.35	0.56
1:D:307:PHE:CE1	1:D:335:ASP:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:GLN:HB3	1:G:112:PRO:CD	2.35	0.56
1:I:159:LEU:CD2	1:I:331:VAL:HG22	2.35	0.56
1:N:71:ARG:HA	1:N:197:ASP:OD1	2.05	0.56
1:N:258:ARG:NH1	1:O:130:GLU:OE1	2.38	0.56
1:C:69:GLN:NE2	1:C:71:ARG:HH22	2.03	0.56
1:G:261:TRP:CZ3	1:G:294:SER:HB3	2.41	0.56
1:G:273:GLN:HE22	1:G:278:LYS:HE2	1.69	0.56
1:J:324:CYS:SG	1:J:329:LEU:HD12	2.45	0.56
1:A:60:GLN:O	1:A:61:ASP:O	2.24	0.56
1:B:368:VAL:CG1	1:B:369:GLU:N	2.68	0.56
1:D:67:ALA:HB2	1:D:367:HIS:CE1	2.41	0.56
1:D:345:CYS:HB3	1:D:363:GLN:NE2	2.21	0.56
1:E:247:PHE:CD2	1:E:322:GLY:HA2	2.40	0.56
1:F:465:LEU:O	1:F:465:LEU:HD22	2.06	0.56
1:H:368:VAL:CG1	1:H:369:GLU:N	2.69	0.56
1:L:117:LEU:HD13	1:M:260:PHE:HB3	1.87	0.56
1:N:148:SER:HB3	1:O:291:TYR:CD2	2.41	0.56
1:B:68:TYR:O	1:B:201:VAL:HG22	2.06	0.56
1:B:396:ASN:HB3	1:B:399:ILE:HG13	1.88	0.56
1:D:92:ASN:HD21	1:D:95:THR:HG23	1.69	0.56
1:E:69:GLN:HE21	1:E:71:ARG:HH12	1.54	0.56
1:M:24:THR:CG2	1:M:320:ASN:HA	2.35	0.56
1:M:92:ASN:C	1:M:94:GLU:H	2.08	0.56
1:N:72:VAL:HG23	1:N:197:ASP:HA	1.87	0.56
1:N:138:ASN:ND2	1:N:140:SER:HB3	2.21	0.56
1:N:316:ALA:CB	1:N:321:ASN:HA	2.36	0.56
1:O:233:ASP:CG	1:O:236:GLN:HB3	2.26	0.56
1:B:140:SER:OG	1:B:141:GLU:N	2.38	0.56
1:D:385:THR:OG1	1:D:388:VAL:HG23	2.05	0.56
1:G:444:LYS:HA	1:G:444:LYS:CE	2.35	0.56
1:L:141:GLU:HG2	1:L:142:ASP:N	2.20	0.56
1:E:52:VAL:HB	1:E:62:ILE:HB	1.88	0.56
1:J:99:VAL:CG2	1:J:382:ILE:HD11	2.33	0.56
1:M:105:VAL:CG2	1:M:159:LEU:HD11	2.31	0.56
1:N:392:ILE:O	1:N:392:ILE:HG22	2.05	0.56
1:A:167:GLU:OE1	1:E:111:GLN:NE2	2.39	0.56
1:C:151:TYR:CG	1:C:203:THR:HB	2.41	0.56
1:E:188:LEU:HD22	1:E:188:LEU:N	2.21	0.56
1:F:24:THR:HG23	1:F:320:ASN:HA	1.88	0.56
1:H:368:VAL:HG11	1:I:169:TRP:HZ2	1.71	0.56
1:M:87:ASP:O	1:M:90:ILE:HG12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:112:PRO:HB3	1:N:231:TYR:CD1	2.41	0.56
1:N:120:HIS:ND1	1:N:121:PRO:HD2	2.21	0.56
1:B:141:GLU:CG	1:B:141:GLU:C	2.75	0.55
1:B:233:ASP:CG	1:B:236:GLN:HB3	2.26	0.55
1:F:464:PRO:HA	1:F:467:ARG:NH1	2.20	0.55
1:G:50:PHE:HA	1:G:64:LYS:HG3	1.86	0.55
1:J:138:ASN:C	1:J:140:SER:H	2.10	0.55
1:K:122:PHE:O	1:K:218:CYS:HB3	2.06	0.55
1:K:200:MET:HE2	1:K:223:ASP:O	2.07	0.55
1:L:475:LEU:HD23	1:L:475:LEU:H	1.71	0.55
1:C:358:ALA:HB2	1:D:141:GLU:O	2.07	0.55
1:D:111:GLN:NE2	1:D:370:GLU:OE1	2.39	0.55
1:E:388:VAL:O	1:E:392:ILE:HG13	2.06	0.55
1:I:368:VAL:HG11	1:J:169:TRP:CZ2	2.41	0.55
1:A:150:ASP:O	1:A:296:SER:HA	2.05	0.55
1:A:258:ARG:HG3	1:A:259:HIS:ND1	2.22	0.55
1:B:258:ARG:NH1	1:C:130:GLU:OE1	2.39	0.55
1:C:307:PHE:HA	1:C:311:TYR:OH	2.06	0.55
1:D:159:LEU:HD22	1:D:331:VAL:HG22	1.88	0.55
1:H:176:LYS:HG3	1:H:177:SER:H	1.69	0.55
1:I:31:THR:HG23	1:I:379:LEU:O	2.06	0.55
1:B:369:GLU:HG3	1:B:371:TYR:HE1	1.70	0.55
1:C:22:VAL:HG12	1:C:23:ASN:N	2.21	0.55
1:C:113:LEU:HD22	1:D:253:GLU:HG3	1.89	0.55
1:F:107:ILE:HG22	1:F:107:ILE:O	2.05	0.55
1:G:109:ARG:H	1:G:308:ASN:HD21	1.55	0.55
1:G:389:MET:O	1:G:393:GLN:HB2	2.06	0.55
1:I:151:TYR:OH	1:I:221:PRO:HB2	2.06	0.55
1:K:293:PRO:O	1:K:293:PRO:HG2	2.04	0.55
1:M:454:GLU:C	1:M:455:LYS:HG2	2.26	0.55
1:C:70:TYR:CE1	1:C:201:VAL:CG1	2.88	0.55
1:D:247:PHE:CE2	1:D:322:GLY:HA2	2.42	0.55
1:H:141:GLU:HG2	1:H:142:ASP:CA	2.34	0.55
1:I:123:TYR:HB2	1:I:147:VAL:HG22	1.89	0.55
1:J:307:PHE:CE1	1:J:335:ASP:HB2	2.41	0.55
1:M:232:PRO:HB2	1:M:234:TYR:CE1	2.41	0.55
1:M:307:PHE:HA	1:M:311:TYR:OH	2.06	0.55
1:N:109:ARG:H	1:N:308:ASN:HD21	1.55	0.55
1:N:364:TYR:CD2	1:O:185:CYS:HB2	2.42	0.55
1:A:24:THR:CG2	1:A:320:ASN:HA	2.37	0.55
1:A:43:LEU:HD13	1:A:370:GLU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:325:TRP:O	1:E:326:HIS:HB2	2.06	0.55
1:G:70:TYR:CE1	1:G:201:VAL:HG12	2.42	0.55
1:G:81:ASN:C	1:G:83:PHE:H	2.10	0.55
1:G:311:TYR:N	1:G:311:TYR:CD1	2.75	0.55
1:A:76:GLN:HG3	1:A:453:LYS:HE3	1.88	0.55
1:B:109:ARG:H	1:B:308:ASN:ND2	2.05	0.55
1:E:309:LYS:NZ	1:E:309:LYS:CD	2.66	0.55
1:G:156:LEU:HG	1:G:334:VAL:HB	1.88	0.55
1:J:123:TYR:HD2	1:J:125:LYS:HB2	1.71	0.55
1:L:372:ASP:OD2	1:L:372:ASP:C	2.44	0.55
1:M:70:TYR:OH	1:M:232:PRO:HD3	2.05	0.55
1:N:33:ILE:HD13	1:N:33:ILE:N	2.22	0.55
1:N:159:LEU:CD2	1:N:331:VAL:HG22	2.37	0.55
1:C:122:PHE:O	1:C:218:CYS:HB3	2.06	0.55
1:H:36:HIS:ND1	1:H:36:HIS:C	2.60	0.55
1:H:108:GLY:HA2	1:H:308:ASN:ND2	2.21	0.55
1:N:85:LEU:HB3	1:N:86:PRO:HD2	1.89	0.55
1:C:307:PHE:CE1	1:C:335:ASP:HB2	2.42	0.55
1:K:169:TRP:CZ2	1:O:368:VAL:HG11	2.42	0.55
1:M:249:CYS:O	1:M:250:LEU:HD12	2.07	0.55
1:O:244:ASP:OD1	1:O:320:ASN:ND2	2.35	0.55
1:O:353:PRO:HG2	1:O:360:LYS:HZ2	1.72	0.55
1:A:112:PRO:HB3	1:B:231:TYR:CD1	2.42	0.54
1:F:112:PRO:HB3	1:G:231:TYR:CD1	2.42	0.54
1:G:159:LEU:CD2	1:G:331:VAL:HG22	2.38	0.54
1:I:156:LEU:HG	1:I:334:VAL:HB	1.88	0.54
1:K:117:LEU:HD13	1:L:260:PHE:HB3	1.90	0.54
1:L:92:ASN:ND2	1:L:95:THR:HG23	2.22	0.54
1:L:111:GLN:HB3	1:L:112:PRO:CD	2.29	0.54
1:F:98:LEU:HD21	1:F:381:THR:HG22	1.89	0.54
1:F:154:THR:HG23	1:F:253:GLU:HB3	1.89	0.54
1:A:24:THR:HG23	1:A:319:HIS:O	2.07	0.54
1:B:69:GLN:NE2	1:B:71:ARG:HH22	2.06	0.54
1:D:384:LEU:HB3	1:D:389:MET:CE	2.37	0.54
1:E:35:TYR:CE2	1:E:458:LEU:HG	2.43	0.54
1:I:353:PRO:CG	1:I:360:LYS:HZ3	2.19	0.54
1:J:68:TYR:CE2	1:J:151:TYR:HB2	2.41	0.54
1:M:122:PHE:O	1:M:218:CYS:HB3	2.07	0.54
1:N:70:TYR:OH	1:N:232:PRO:HD3	2.07	0.54
1:A:92:ASN:HD21	1:A:95:THR:HG23	1.71	0.54
1:A:159:LEU:HD22	1:A:331:VAL:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:390:SER:O	1:F:393:GLN:HB3	2.07	0.54
1:G:244:ASP:OD1	1:G:320:ASN:ND2	2.40	0.54
1:H:349:GLN:HG3	1:H:360:LYS:HD2	1.89	0.54
1:J:156:LEU:HA	1:J:250:LEU:O	2.07	0.54
1:J:446:LYS:CD	1:J:446:LYS:CB	2.76	0.54
1:K:109:ARG:NH2	1:K:369:GLU:OE1	2.41	0.54
1:K:350:SER:HB3	1:K:351:PRO:HD3	1.89	0.54
1:L:156:LEU:HA	1:L:250:LEU:O	2.07	0.54
1:M:329:LEU:HD23	1:M:329:LEU:C	2.27	0.54
1:A:117:LEU:HD11	1:B:293:PRO:HB3	1.89	0.54
1:H:384:LEU:HB3	1:H:389:MET:HE2	1.89	0.54
1:D:122:PHE:O	1:D:218:CYS:HB3	2.08	0.54
1:G:367:HIS:CE1	1:G:369:GLU:OE2	2.61	0.54
1:H:247:PHE:CE2	1:H:322:GLY:HA2	2.42	0.54
1:J:357:ASP:O	1:J:358:ALA:C	2.46	0.54
1:A:36:HIS:ND1	1:A:37:ALA:N	2.56	0.54
1:A:98:LEU:CD2	1:A:381:THR:HG22	2.38	0.54
1:B:159:LEU:HD22	1:B:331:VAL:HG22	1.89	0.54
1:G:364:TYR:CE2	1:H:185:CYS:HB2	2.41	0.54
1:G:369:GLU:HG3	1:G:371:TYR:CE1	2.43	0.54
1:K:310:PRO:O	1:K:310:PRO:CG	2.55	0.54
1:K:396:ASN:ND2	1:K:398:SER:OG	2.41	0.54
1:M:169:TRP:CZ2	1:M:190:LEU:HD13	2.43	0.54
1:A:389:MET:HG2	1:A:400:LEU:CD2	2.37	0.54
1:G:123:TYR:HD2	1:G:125:LYS:HB2	1.73	0.54
1:G:246:MET:HG3	1:G:246:MET:O	2.08	0.54
1:H:196:GLU:HB3	1:H:446:LYS:O	2.06	0.54
1:H:353:PRO:CG	1:H:360:LYS:NZ	2.70	0.54
1:L:368:VAL:HG12	1:L:369:GLU:N	2.23	0.54
1:C:138:ASN:ND2	1:C:140:SER:HB3	2.22	0.54
1:F:87:ASP:O	1:F:90:ILE:HG12	2.08	0.54
1:F:123:TYR:CG	1:F:147:VAL:HG22	2.43	0.54
1:I:36:HIS:ND1	1:I:37:ALA:N	2.56	0.54
1:J:216:THR:O	1:J:217:LYS:HB2	2.07	0.54
1:K:87:ASP:O	1:K:90:ILE:CG1	2.55	0.54
1:K:329:LEU:HD23	1:K:329:LEU:C	2.28	0.54
1:M:353:PRO:HG2	1:M:360:LYS:HZ3	1.71	0.54
1:N:329:LEU:HD23	1:N:329:LEU:C	2.29	0.54
1:C:36:HIS:ND1	1:C:36:HIS:C	2.60	0.53
1:D:22:VAL:HG12	1:D:23:ASN:N	2.23	0.53
1:F:345:CYS:HB3	1:F:363:GLN:HE22	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:ASP:O	1:G:83:PHE:HB2	2.08	0.53
1:H:239:ALA:O	1:H:240:ASP:C	2.46	0.53
1:M:109:ARG:H	1:M:308:ASN:ND2	2.04	0.53
1:N:342:LEU:HD22	1:O:208:MET:SD	2.48	0.53
1:N:369:GLU:HG3	1:N:371:TYR:CE1	2.41	0.53
1:C:351:PRO:O	1:C:352:VAL:HB	2.09	0.53
1:N:35:TYR:CE2	1:N:458:LEU:HG	2.43	0.53
1:A:313:LEU:HD23	1:A:313:LEU:N	2.22	0.53
1:C:69:GLN:HE21	1:C:71:ARG:HH12	1.57	0.53
1:F:152:LYS:HE3	1:F:253:GLU:HB2	1.90	0.53
1:G:35:TYR:CE2	1:G:458:LEU:HG	2.43	0.53
1:H:71:ARG:HA	1:H:197:ASP:OD1	2.07	0.53
1:L:138:ASN:HD22	1:L:140:SER:HB3	1.72	0.53
1:B:126:LEU:CB	1:B:262:ASN:HB3	2.37	0.53
1:D:92:ASN:ND2	1:D:95:THR:HG23	2.23	0.53
1:D:164:ALA:C	1:D:165:ILE:HD12	2.28	0.53
1:E:374:GLN:OE1	1:E:464:PRO:HG2	2.09	0.53
1:F:78:PRO:HG2	1:F:100:TRP:HE1	1.72	0.53
1:F:92:ASN:ND2	1:F:95:THR:HG23	2.23	0.53
1:H:92:ASN:OD1	1:H:94:GLU:HB2	2.08	0.53
1:J:258:ARG:HG3	1:J:259:HIS:ND1	2.24	0.53
1:O:140:SER:O	1:O:141:GLU:HB2	2.08	0.53
1:O:273:GLN:NE2	1:O:278:LYS:HE2	2.23	0.53
1:A:91:TYR:HB2	1:A:96:GLN:HG3	1.90	0.53
1:A:368:VAL:CG1	1:A:369:GLU:N	2.71	0.53
1:C:307:PHE:O	1:C:308:ASN:HB2	2.09	0.53
1:H:156:LEU:C	1:H:156:LEU:HD12	2.29	0.53
1:J:368:VAL:HG12	1:J:369:GLU:N	2.22	0.53
1:K:24:THR:HG23	1:K:320:ASN:HA	1.89	0.53
1:M:300:VAL:O	1:M:300:VAL:HG13	2.07	0.53
1:O:325:TRP:O	1:O:326:HIS:HB2	2.09	0.53
1:D:114:GLY:HA3	1:D:340:THR:HG23	1.91	0.53
1:F:109:ARG:NH1	1:F:371:TYR:CE1	2.77	0.53
1:F:188:LEU:HD11	1:J:344:ILE:HD11	1.90	0.53
1:H:305:GLN:HA	1:H:305:GLN:NE2	2.23	0.53
1:I:293:PRO:HG2	1:I:293:PRO:O	2.08	0.53
1:O:246:MET:HG3	1:O:246:MET:O	2.08	0.53
1:C:261:TRP:CZ3	1:C:294:SER:HB3	2.43	0.53
1:D:165:ILE:HD12	1:D:165:ILE:N	2.22	0.53
1:G:359:THR:HA	1:H:266:THR:HG23	1.91	0.53
1:J:105:VAL:HG21	1:J:159:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:360:LYS:CE	1:L:360:LYS:CG	2.80	0.53
1:N:368:VAL:HG11	1:O:169:TRP:HZ2	1.69	0.53
1:D:342:LEU:HD22	1:E:208:MET:SD	2.49	0.53
1:D:375:PHE:O	1:D:376:ILE:HD13	2.09	0.53
1:F:367:HIS:CE1	1:F:369:GLU:OE2	2.62	0.53
1:G:120:HIS:ND1	1:G:121:PRO:HD2	2.23	0.53
1:M:42:LEU:HB3	1:M:448:TRP:CZ2	2.42	0.53
1:A:306:LEU:O	1:A:311:TYR:OH	2.12	0.53
1:A:328:GLN:O	1:A:329:LEU:HB2	2.09	0.53
1:K:151:TYR:OH	1:K:221:PRO:HB2	2.09	0.53
1:O:387:ASP:OD1	1:O:388:VAL:N	2.42	0.53
1:H:313:LEU:HD23	1:H:313:LEU:N	2.22	0.53
1:K:255:LEU:HD13	1:O:300:VAL:HG13	1.89	0.53
1:M:364:TYR:CD2	1:N:185:CYS:HB2	2.44	0.53
1:N:368:VAL:CG1	1:N:369:GLU:N	2.72	0.53
1:A:350:SER:HB3	1:A:351:PRO:HD3	1.90	0.52
1:B:31:THR:HG23	1:B:379:LEU:O	2.08	0.52
1:B:141:GLU:C	1:B:141:GLU:HG2	2.30	0.52
1:D:36:HIS:ND1	1:D:37:ALA:N	2.57	0.52
1:D:258:ARG:NH1	1:E:130:GLU:OE1	2.42	0.52
1:E:475:LEU:H	1:E:475:LEU:CD2	2.19	0.52
1:G:70:TYR:CZ	1:G:201:VAL:HG12	2.44	0.52
1:H:117:LEU:HD11	1:I:293:PRO:HB3	1.91	0.52
1:I:300:VAL:HG13	1:J:255:LEU:HD13	1.91	0.52
1:L:247:PHE:CE2	1:L:322:GLY:HA2	2.44	0.52
1:L:385:THR:H	1:L:388:VAL:HB	1.74	0.52
1:M:111:GLN:NE2	1:M:370:GLU:OE1	2.42	0.52
1:F:255:LEU:HD13	1:J:300:VAL:HG13	1.91	0.52
1:I:76:GLN:HG3	1:I:453:LYS:HE3	1.91	0.52
1:I:325:TRP:O	1:I:326:HIS:HB2	2.08	0.52
1:K:231:TYR:CG	1:O:112:PRO:HB3	2.44	0.52
1:L:220:VAL:HB	1:L:224:ILE:HD11	1.91	0.52
1:A:188:LEU:HD11	1:E:344:ILE:HD11	1.92	0.52
1:F:45:VAL:HG12	1:F:368:VAL:HG22	1.91	0.52
1:F:79:ASP:O	1:F:83:PHE:HB2	2.09	0.52
1:G:258:ARG:HG3	1:G:259:HIS:ND1	2.25	0.52
1:I:105:VAL:CG1	1:I:106:GLU:N	2.71	0.52
1:A:140:SER:OG	1:A:141:GLU:N	2.42	0.52
1:B:272:PRO:HD2	1:B:275:LEU:HD12	1.92	0.52
1:D:261:TRP:CZ3	1:D:294:SER:HB3	2.44	0.52
1:E:123:TYR:HD2	1:E:125:LYS:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:PHE:HE1	1:G:335:ASP:HB2	1.74	0.52
1:I:444:LYS:HE2	1:I:444:LYS:HA	1.90	0.52
1:J:169:TRP:CZ2	1:J:190:LEU:HD13	2.44	0.52
1:M:255:LEU:HD22	1:M:256:PHE:N	2.24	0.52
1:N:105:VAL:CG1	1:N:106:GLU:N	2.73	0.52
1:N:151:TYR:OH	1:N:221:PRO:HB2	2.09	0.52
1:O:98:LEU:CD2	1:O:381:THR:HG22	2.40	0.52
1:E:313:LEU:H	1:E:313:LEU:HD23	1.75	0.52
1:H:220:VAL:CG2	1:H:225:CYS:HA	2.40	0.52
1:M:72:VAL:HG23	1:M:197:ASP:HA	1.89	0.52
1:A:92:ASN:ND2	1:A:95:THR:HG23	2.23	0.52
1:A:113:LEU:HD22	1:B:253:GLU:HG3	1.92	0.52
1:C:126:LEU:HB3	1:C:262:ASN:CB	2.38	0.52
1:C:258:ARG:HG3	1:C:259:HIS:ND1	2.23	0.52
1:D:113:LEU:HD22	1:E:253:GLU:HG3	1.92	0.52
1:J:367:HIS:CE1	1:J:369:GLU:OE2	2.62	0.52
1:K:368:VAL:HG11	1:L:169:TRP:HZ2	1.73	0.52
1:L:119:GLY:HA2	1:L:148:SER:HA	1.91	0.52
1:L:300:VAL:HG13	1:L:300:VAL:O	2.09	0.52
1:N:247:PHE:CZ	1:N:322:GLY:HA2	2.43	0.52
1:O:156:LEU:HA	1:O:250:LEU:O	2.09	0.52
1:B:156:LEU:HG	1:B:334:VAL:HB	1.91	0.52
1:D:368:VAL:HG11	1:E:169:TRP:HZ2	1.71	0.52
1:F:310:PRO:HG3	1:F:468:LYS:HD3	1.91	0.52
1:D:344:ILE:HD11	1:E:188:LEU:HD11	1.92	0.52
1:F:389:MET:O	1:F:393:GLN:N	2.42	0.52
1:I:47:ASP:C	1:I:47:ASP:OD1	2.47	0.52
1:I:385:THR:OG1	1:I:388:VAL:HG23	2.09	0.52
1:K:188:LEU:HD11	1:O:344:ILE:HD11	1.92	0.52
1:K:260:PHE:HB3	1:O:117:LEU:HD13	1.92	0.52
1:L:307:PHE:CE1	1:L:335:ASP:HB2	2.42	0.52
1:L:350:SER:HB3	1:L:351:PRO:HD3	1.91	0.52
1:A:111:GLN:HB3	1:A:112:PRO:CD	2.39	0.52
1:A:231:TYR:CD1	1:E:112:PRO:HB3	2.45	0.52
1:E:151:TYR:OH	1:E:221:PRO:HB2	2.10	0.52
1:F:117:LEU:HD13	1:G:260:PHE:HB3	1.91	0.52
1:H:105:VAL:HG21	1:H:159:LEU:HD11	1.92	0.52
1:I:126:LEU:HB3	1:I:262:ASN:CB	2.40	0.52
1:I:249:CYS:O	1:I:250:LEU:HD12	2.10	0.52
1:I:364:TYR:CD2	1:J:185:CYS:HB2	2.44	0.52
1:B:220:VAL:HB	1:B:221:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:VAL:O	1:B:392:ILE:HG13	2.10	0.52
1:C:98:LEU:CD2	1:C:381:THR:HG22	2.40	0.52
1:G:368:VAL:HG12	1:G:369:GLU:N	2.25	0.52
1:J:92:ASN:HD21	1:J:94:GLU:HB2	1.75	0.52
1:K:293:PRO:HB3	1:O:117:LEU:HD11	1.91	0.52
1:M:156:LEU:HA	1:M:250:LEU:O	2.09	0.52
1:B:42:LEU:HB3	1:B:448:TRP:CZ2	2.44	0.51
1:B:159:LEU:CD2	1:B:331:VAL:HG22	2.40	0.51
1:B:307:PHE:CE1	1:B:335:ASP:HB2	2.43	0.51
1:C:159:LEU:CD2	1:C:331:VAL:HG22	2.40	0.51
1:F:46:GLY:HA3	1:F:65:VAL:HG23	1.91	0.51
1:F:70:TYR:OH	1:F:232:PRO:HD3	2.10	0.51
1:F:113:LEU:HD22	1:G:253:GLU:HG3	1.92	0.51
1:F:369:GLU:CG	1:F:371:TYR:HE1	2.22	0.51
1:G:313:LEU:HD23	1:G:313:LEU:N	2.24	0.51
1:J:24:THR:HG23	1:J:320:ASN:HA	1.91	0.51
1:J:152:LYS:HE3	1:J:253:GLU:HB2	1.91	0.51
1:J:316:ALA:CB	1:J:321:ASN:HA	2.40	0.51
1:L:112:PRO:HB3	1:M:231:TYR:CD1	2.46	0.51
1:D:368:VAL:HG12	1:D:369:GLU:N	2.24	0.51
1:F:42:LEU:HB3	1:F:448:TRP:CZ2	2.45	0.51
1:H:159:LEU:HD21	1:H:331:VAL:HG22	1.92	0.51
1:M:382:ILE:HD12	1:M:403:TRP:CH2	2.45	0.51
1:O:91:TYR:H	1:O:91:TYR:HD2	1.59	0.51
1:H:43:LEU:CD1	1:H:370:GLU:HB2	2.40	0.51
1:O:258:ARG:HG3	1:O:259:HIS:ND1	2.25	0.51
1:F:353:PRO:HD2	1:F:360:LYS:HZ1	1.76	0.51
1:O:87:ASP:HB3	1:O:90:ILE:HD11	1.92	0.51
1:B:353:PRO:HD2	1:B:360:LYS:NZ	2.26	0.51
1:B:463:TYR:O	1:B:467:ARG:HG3	2.11	0.51
1:I:114:GLY:HA3	1:I:340:THR:HG23	1.92	0.51
1:I:392:ILE:O	1:I:392:ILE:HG22	2.10	0.51
1:M:311:TYR:N	1:M:311:TYR:CD1	2.78	0.51
1:N:159:LEU:HD21	1:N:331:VAL:HG22	1.93	0.51
1:J:69:GLN:NE2	1:J:71:ARG:HH22	2.09	0.51
1:N:87:ASP:HB3	1:N:90:ILE:HD11	1.93	0.51
1:O:42:LEU:HB3	1:O:448:TRP:CZ2	2.46	0.51
1:E:156:LEU:HA	1:E:250:LEU:O	2.11	0.51
1:E:307:PHE:HE1	1:E:335:ASP:HB2	1.75	0.51
1:F:185:CYS:HB2	1:J:364:TYR:CD2	2.46	0.51
1:K:99:VAL:HG21	1:K:382:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:130:GLU:OE1	1:O:258:ARG:NH1	2.44	0.51
1:K:232:PRO:HB2	1:K:234:TYR:CE1	2.45	0.51
1:L:98:LEU:HD13	1:L:379:LEU:HD11	1.93	0.51
1:N:367:HIS:CE1	1:N:369:GLU:OE2	2.64	0.51
1:B:109:ARG:NH2	1:B:369:GLU:OE1	2.44	0.51
1:D:69:GLN:NE2	1:D:71:ARG:HH22	2.09	0.51
1:N:159:LEU:HB2	1:N:248:PHE:HB3	1.93	0.51
1:O:108:GLY:HA2	1:O:308:ASN:ND2	2.25	0.51
1:A:188:LEU:HD22	1:A:188:LEU:N	2.25	0.51
1:A:352:VAL:O	1:A:352:VAL:HG12	2.10	0.51
1:D:155:GLN:OE1	1:D:306:LEU:HB2	2.10	0.51
1:F:50:PHE:HA	1:F:64:LYS:HG3	1.93	0.51
1:I:155:GLN:OE1	1:I:306:LEU:HB2	2.10	0.51
1:M:226:GLN:OE1	1:M:226:GLN:HA	2.11	0.51
1:O:372:ASP:C	1:O:372:ASP:OD2	2.49	0.51
1:G:307:PHE:HA	1:G:311:TYR:OH	2.11	0.51
1:G:368:VAL:CG1	1:G:369:GLU:N	2.73	0.51
1:I:24:THR:HG23	1:I:320:ASN:HA	1.92	0.51
1:K:307:PHE:HA	1:K:311:TYR:HH	1.76	0.51
1:J:251:ARG:HH11	1:J:251:ARG:CG	2.24	0.50
1:K:311:TYR:CD1	1:K:311:TYR:N	2.78	0.50
1:L:71:ARG:HG3	1:L:371:TYR:CZ	2.46	0.50
1:M:314:HIS:O	1:M:315:LYS:HG3	2.11	0.50
1:A:43:LEU:CD1	1:A:370:GLU:HB2	2.41	0.50
1:B:35:TYR:CE2	1:B:458:LEU:HG	2.46	0.50
1:F:364:TYR:CE2	1:G:185:CYS:HB2	2.46	0.50
1:I:42:LEU:HB3	1:I:448:TRP:CZ2	2.46	0.50
1:K:85:LEU:HB3	1:K:86:PRO:HD2	1.93	0.50
1:N:157:CYS:HA	1:N:332:THR:O	2.11	0.50
1:A:99:VAL:O	1:A:380:CYS:HB2	2.11	0.50
1:A:281:GLY:HA3	1:G:89:SER:C	2.30	0.50
1:B:365:SER:O	1:B:366:ARG:HD3	2.11	0.50
1:C:239:ALA:O	1:C:240:ASP:C	2.49	0.50
1:C:369:GLU:HG3	1:C:371:TYR:HE1	1.75	0.50
1:E:369:GLU:HG3	1:E:371:TYR:CE1	2.46	0.50
1:H:141:GLU:HG3	1:H:142:ASP:N	2.21	0.50
1:J:307:PHE:O	1:J:308:ASN:HB2	2.11	0.50
1:M:157:CYS:HA	1:M:332:THR:O	2.11	0.50
1:M:307:PHE:O	1:M:308:ASN:HB2	2.10	0.50
1:O:232:PRO:HB2	1:O:234:TYR:CE1	2.46	0.50
1:E:42:LEU:HB3	1:E:448:TRP:CZ2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:LEU:HA	1:I:250:LEU:O	2.10	0.50
1:L:36:HIS:ND1	1:L:36:HIS:C	2.65	0.50
1:N:353:PRO:HD2	1:N:360:LYS:HE3	1.93	0.50
1:A:396:ASN:HD22	1:A:396:ASN:C	2.15	0.50
1:C:188:LEU:HD12	1:C:213:LEU:HD21	1.91	0.50
1:C:369:GLU:HG3	1:C:371:TYR:CE1	2.47	0.50
1:D:138:ASN:C	1:D:140:SER:H	2.15	0.50
1:E:372:ASP:C	1:E:372:ASP:OD2	2.49	0.50
1:F:396:ASN:HB3	1:F:399:ILE:HG13	1.94	0.50
1:G:58:ASN:HB2	1:H:178:ARG:HH12	0.68	0.50
1:K:344:ILE:CD1	1:L:188:LEU:HD11	2.40	0.50
1:N:196:GLU:HG2	1:N:445:LEU:HB3	1.93	0.50
1:O:59:LYS:O	1:O:60:GLN:HB3	2.12	0.50
1:E:444:LYS:HE2	1:E:444:LYS:HA	1.92	0.50
1:I:136:THR:O	1:I:137:SER:C	2.49	0.50
1:I:463:TYR:O	1:I:467:ARG:HG3	2.11	0.50
1:M:307:PHE:CE1	1:M:335:ASP:HB2	2.46	0.50
1:A:307:PHE:HE1	1:A:335:ASP:HB2	1.77	0.50
1:I:475:LEU:H	1:I:475:LEU:CD2	2.21	0.50
1:M:24:THR:HG21	1:M:320:ASN:HA	1.92	0.50
1:B:142:ASP:CG	1:C:283:ARG:HD2	2.32	0.50
1:B:258:ARG:HG3	1:B:259:HIS:ND1	2.27	0.50
1:B:305:GLN:HA	1:B:305:GLN:NE2	2.27	0.50
1:C:110:GLY:HA3	1:C:370:GLU:CG	2.42	0.50
1:C:156:LEU:HG	1:C:334:VAL:HB	1.94	0.50
1:C:226:GLN:HA	1:C:226:GLN:OE1	2.11	0.50
1:E:109:ARG:H	1:E:308:ASN:ND2	2.10	0.50
1:F:123:TYR:HD2	1:F:125:LYS:HB2	1.76	0.50
1:G:41:ARG:NH2	1:H:233:ASP:OD2	2.44	0.50
1:K:156:LEU:HG	1:K:334:VAL:HB	1.93	0.50
1:K:196:GLU:N	1:K:199:ASP:OD2	2.39	0.50
1:M:216:THR:CG2	1:M:218:CYS:HB2	2.42	0.50
1:M:446:LYS:CD	1:M:446:LYS:CB	2.80	0.50
1:F:325:TRP:O	1:F:326:HIS:HB2	2.12	0.50
1:G:72:VAL:HG21	1:G:195:LEU:O	2.12	0.50
1:I:70:TYR:CZ	1:I:201:VAL:HG12	2.47	0.50
1:J:36:HIS:ND1	1:J:37:ALA:N	2.60	0.50
1:J:325:TRP:O	1:J:326:HIS:HB2	2.12	0.50
1:K:109:ARG:H	1:K:308:ASN:ND2	2.09	0.50
1:L:45:VAL:CG1	1:L:368:VAL:HG22	2.42	0.50
1:L:261:TRP:CZ3	1:L:294:SER:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:HIS:ND1	1:A:36:HIS:C	2.65	0.49
1:B:24:THR:HG23	1:B:320:ASN:HA	1.94	0.49
1:C:233:ASP:CG	1:C:236:GLN:HB3	2.33	0.49
1:C:267:MET:SD	1:C:290:VAL:HG23	2.52	0.49
1:E:392:ILE:HG22	1:E:392:ILE:O	2.12	0.49
1:F:45:VAL:CG1	1:F:368:VAL:HG22	2.42	0.49
1:I:92:ASN:ND2	1:I:95:THR:H	2.10	0.49
1:I:260:PHE:CD2	1:I:260:PHE:N	2.78	0.49
1:M:66:SER:H	1:M:69:GLN:NE2	2.10	0.49
1:M:273:GLN:HE22	1:M:278:LYS:CE	1.98	0.49
1:N:126:LEU:HB3	1:N:262:ASN:CB	2.41	0.49
1:N:142:ASP:CG	1:O:283:ARG:HD2	2.32	0.49
1:O:74:ARG:NH2	1:O:328:GLN:OE1	2.42	0.49
1:A:72:VAL:HG23	1:A:197:ASP:CA	2.41	0.49
1:A:165:ILE:CG2	1:A:166:GLY:N	2.72	0.49
1:A:253:GLU:HG3	1:E:113:LEU:HD22	1.94	0.49
1:C:114:GLY:HA3	1:C:340:THR:HG23	1.94	0.49
1:G:462:GLN:HE22	1:H:21:VAL:HB	1.77	0.49
1:K:120:HIS:CD2	1:K:222:LEU:CD1	2.94	0.49
1:L:122:PHE:O	1:L:218:CYS:HB3	2.12	0.49
1:L:216:THR:O	1:L:217:LYS:HB2	2.12	0.49
1:M:105:VAL:HG12	1:M:106:GLU:N	2.27	0.49
1:O:45:VAL:HG12	1:O:368:VAL:HG22	1.94	0.49
1:A:123:TYR:CD2	1:A:125:LYS:HB2	2.47	0.49
1:D:96:GLN:HB3	1:D:383:THR:HA	1.94	0.49
1:D:99:VAL:HG21	1:D:382:ILE:CD1	2.40	0.49
1:E:71:ARG:HA	1:E:197:ASP:OD1	2.12	0.49
1:E:74:ARG:NE	1:E:328:GLN:OE1	2.45	0.49
1:E:307:PHE:CE1	1:E:335:ASP:HB2	2.47	0.49
1:F:307:PHE:O	1:F:308:ASN:HB2	2.12	0.49
1:H:92:ASN:C	1:H:94:GLU:H	2.14	0.49
1:I:111:GLN:HB3	1:I:112:PRO:CD	2.39	0.49
1:K:68:TYR:O	1:K:201:VAL:HG22	2.12	0.49
1:M:233:ASP:CG	1:M:236:GLN:HB3	2.33	0.49
1:N:92:ASN:C	1:N:94:GLU:H	2.15	0.49
1:N:376:ILE:HG12	1:N:465:LEU:HD13	1.94	0.49
1:O:389:MET:O	1:O:393:GLN:HB2	2.12	0.49
1:C:475:LEU:H	1:C:475:LEU:CD2	2.21	0.49
1:D:70:TYR:CZ	1:D:201:VAL:HG12	2.47	0.49
1:D:329:LEU:C	1:D:329:LEU:HD23	2.32	0.49
1:H:126:LEU:HB3	1:H:262:ASN:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:326:HIS:CD2	1:H:402:ASP:OD1	2.65	0.49
1:J:52:VAL:HB	1:J:62:ILE:HB	1.92	0.49
1:N:328:GLN:O	1:N:329:LEU:HB2	2.12	0.49
1:O:122:PHE:O	1:O:218:CYS:HB3	2.12	0.49
1:A:349:GLN:HG3	1:A:360:LYS:HD2	1.93	0.49
1:H:369:GLU:HG3	1:H:371:TYR:HE1	1.77	0.49
1:K:36:HIS:C	1:K:36:HIS:ND1	2.66	0.49
1:N:24:THR:HG23	1:N:320:ASN:HA	1.94	0.49
1:N:105:VAL:HG21	1:N:159:LEU:HD11	1.95	0.49
1:A:24:THR:HG23	1:A:320:ASN:HA	1.94	0.49
1:C:131:SER:O	1:C:132:SER:C	2.50	0.49
1:M:246:MET:O	1:M:246:MET:HG3	2.12	0.49
1:N:21:VAL:CG1	1:N:22:VAL:N	2.75	0.49
1:N:41:ARG:NH2	1:O:233:ASP:OD2	2.46	0.49
1:N:156:LEU:HG	1:N:334:VAL:HB	1.95	0.49
1:B:87:ASP:O	1:B:90:ILE:HG12	2.13	0.49
1:D:232:PRO:HB2	1:D:234:TYR:CE1	2.47	0.49
1:E:107:ILE:O	1:E:107:ILE:HG22	2.13	0.49
1:G:368:VAL:HG21	1:H:169:TRP:CE2	2.48	0.49
1:H:138:ASN:C	1:H:140:SER:H	2.16	0.49
1:I:123:TYR:HD2	1:I:125:LYS:HB2	1.77	0.49
1:J:368:VAL:CG1	1:J:369:GLU:N	2.75	0.49
1:L:105:VAL:CG1	1:L:106:GLU:N	2.72	0.49
1:M:366:ARG:HA	1:M:366:ARG:HD3	1.66	0.49
1:F:120:HIS:ND1	1:F:121:PRO:HD2	2.28	0.49
1:F:353:PRO:CG	1:F:360:LYS:NZ	2.71	0.49
1:K:35:TYR:CE2	1:K:458:LEU:HG	2.48	0.49
1:B:46:GLY:HA3	1:B:65:VAL:HG23	1.94	0.49
1:D:151:TYR:OH	1:D:221:PRO:HB2	2.13	0.49
1:F:247:PHE:CD2	1:F:322:GLY:HA2	2.47	0.49
1:G:117:LEU:HD11	1:H:293:PRO:HB3	1.94	0.49
1:J:81:ASN:C	1:J:83:PHE:H	2.16	0.49
1:K:317:GLN:NE2	1:K:317:GLN:C	2.67	0.49
1:K:324:CYS:SG	1:K:329:LEU:HD12	2.53	0.49
1:N:464:PRO:HA	1:N:467:ARG:NH1	2.27	0.49
1:A:111:GLN:NE2	1:A:370:GLU:OE1	2.44	0.49
1:B:70:TYR:OH	1:B:232:PRO:HD3	2.12	0.49
1:C:67:ALA:HB2	1:C:367:HIS:CE1	2.48	0.49
1:C:459:ASP:OD2	1:C:459:ASP:N	2.44	0.49
1:E:384:LEU:HB3	1:E:389:MET:CE	2.43	0.49
1:H:70:TYR:OH	1:H:232:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:242:TYR:CE2	1:J:395:MET:HG3	2.47	0.49
1:L:119:GLY:HA3	1:M:291:TYR:CE1	2.48	0.49
1:L:142:ASP:CG	1:M:283:ARG:HD2	2.33	0.49
1:L:196:GLU:HG2	1:L:445:LEU:HB3	1.95	0.49
1:N:92:ASN:O	1:N:94:GLU:N	2.46	0.49
1:A:233:ASP:CG	1:A:236:GLN:HB3	2.32	0.48
1:B:72:VAL:HG23	1:B:197:ASP:HA	1.95	0.48
1:B:313:LEU:H	1:B:313:LEU:HD23	1.78	0.48
1:F:69:GLN:NE2	1:F:71:ARG:HH22	2.11	0.48
1:F:92:ASN:HD21	1:F:95:THR:HG23	1.78	0.48
1:F:99:VAL:HG21	1:F:382:ILE:HD11	1.93	0.48
1:F:123:TYR:HB2	1:F:147:VAL:HG22	1.95	0.48
1:G:92:ASN:OD1	1:G:94:GLU:HB2	2.13	0.48
1:H:141:GLU:CG	1:H:142:ASP:HB2	2.36	0.48
1:I:85:LEU:HB3	1:I:86:PRO:HD2	1.95	0.48
1:J:87:ASP:O	1:J:90:ILE:HG12	2.13	0.48
1:K:22:VAL:HG12	1:K:23:ASN:N	2.28	0.48
1:L:156:LEU:HG	1:L:334:VAL:HB	1.95	0.48
1:O:47:ASP:OD1	1:O:49:TYR:N	2.37	0.48
1:O:120:HIS:ND1	1:O:121:PRO:HD2	2.28	0.48
1:A:109:ARG:H	1:A:308:ASN:ND2	2.11	0.48
1:A:169:TRP:CE2	1:E:368:VAL:HG21	2.48	0.48
1:D:112:PRO:HB3	1:E:231:TYR:CD1	2.48	0.48
1:G:92:ASN:ND2	1:G:95:THR:HG23	2.27	0.48
1:G:92:ASN:C	1:G:94:GLU:H	2.16	0.48
1:H:349:GLN:CG	1:H:360:LYS:HD2	2.43	0.48
1:J:70:TYR:OH	1:J:232:PRO:HD3	2.13	0.48
1:K:110:GLY:HA3	1:K:370:GLU:CD	2.33	0.48
1:L:353:PRO:HG2	1:L:360:LYS:NZ	2.16	0.48
1:L:353:PRO:CG	1:L:360:LYS:HZ3	2.10	0.48
1:M:388:VAL:O	1:M:392:ILE:HG13	2.13	0.48
1:A:138:ASN:C	1:A:140:SER:H	2.16	0.48
1:B:196:GLU:N	1:B:199:ASP:OD2	2.42	0.48
1:C:92:ASN:O	1:C:94:GLU:N	2.45	0.48
1:C:188:LEU:CD1	1:C:213:LEU:HD21	2.44	0.48
1:F:444:LYS:HE2	1:F:444:LYS:HA	1.95	0.48
1:G:307:PHE:CE1	1:G:335:ASP:HB2	2.48	0.48
1:H:92:ASN:ND2	1:H:95:THR:HG23	2.28	0.48
1:I:141:GLU:HG2	1:I:142:ASP:H	1.75	0.48
1:J:110:GLY:HA3	1:J:370:GLU:HB3	1.95	0.48
1:A:216:THR:O	1:A:217:LYS:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:LEU:HB3	1:C:389:MET:HE1	1.96	0.48
1:E:24:THR:HG23	1:E:320:ASN:HA	1.96	0.48
1:F:159:LEU:HD21	1:F:331:VAL:HG22	1.93	0.48
1:J:96:GLN:HB3	1:J:383:THR:HA	1.93	0.48
1:J:247:PHE:HB2	1:J:316:ALA:HB1	1.95	0.48
1:N:91:TYR:HB2	1:N:96:GLN:HG3	1.95	0.48
1:O:142:ASP:OD2	1:O:144:ARG:NE	2.42	0.48
1:A:156:LEU:HG	1:A:334:VAL:HB	1.95	0.48
1:A:349:GLN:CG	1:A:360:LYS:HD2	2.43	0.48
1:G:247:PHE:CD2	1:G:322:GLY:HA2	2.48	0.48
1:H:68:TYR:O	1:H:201:VAL:HG22	2.13	0.48
1:K:96:GLN:HB3	1:K:383:THR:HA	1.96	0.48
1:K:254:GLN:HE21	1:K:298:SER:H	1.62	0.48
1:M:67:ALA:HB2	1:M:367:HIS:CE1	2.48	0.48
1:B:364:TYR:CD2	1:C:185:CYS:CB	2.93	0.48
1:D:72:VAL:HG23	1:D:197:ASP:CA	2.42	0.48
1:D:310:PRO:O	1:D:310:PRO:HG2	2.14	0.48
1:G:109:ARG:NH2	1:G:369:GLU:OE1	2.45	0.48
1:H:364:TYR:CG	1:I:185:CYS:HB2	2.48	0.48
1:L:140:SER:O	1:L:141:GLU:HB2	2.14	0.48
1:L:342:LEU:HD22	1:M:208:MET:SD	2.54	0.48
1:M:367:HIS:CE1	1:M:369:GLU:OE2	2.66	0.48
1:A:300:VAL:CG1	1:B:255:LEU:HD13	2.43	0.48
1:G:122:PHE:O	1:G:218:CYS:HB3	2.14	0.48
1:G:342:LEU:HD22	1:H:208:MET:SD	2.54	0.48
1:H:96:GLN:NE2	1:H:383:THR:OG1	2.47	0.48
1:L:111:GLN:CB	1:L:112:PRO:CD	2.91	0.48
1:A:384:LEU:HD22	1:A:389:MET:HG3	1.95	0.48
1:C:232:PRO:HB2	1:C:234:TYR:CE1	2.49	0.48
1:D:109:ARG:H	1:D:308:ASN:ND2	2.12	0.48
1:F:231:TYR:CD1	1:J:112:PRO:HB3	2.48	0.48
1:F:267:MET:SD	1:F:290:VAL:HG23	2.53	0.48
1:F:365:SER:O	1:F:366:ARG:HD3	2.14	0.48
1:K:316:ALA:CB	1:K:321:ASN:HA	2.44	0.48
1:O:151:TYR:CE2	1:O:221:PRO:HG2	2.49	0.48
1:O:368:VAL:HG12	1:O:369:GLU:N	2.27	0.48
1:B:41:ARG:HG2	1:B:41:ARG:O	2.13	0.48
1:F:261:TRP:CZ3	1:F:294:SER:HB3	2.48	0.48
1:G:45:VAL:CG1	1:G:368:VAL:HG22	2.44	0.48
1:I:77:LEU:HB3	1:I:78:PRO:HD2	1.96	0.48
1:I:368:VAL:CG1	1:I:369:GLU:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:MET:HG3	1:D:246:MET:O	2.13	0.48
1:E:92:ASN:O	1:E:94:GLU:N	2.46	0.48
1:E:260:PHE:N	1:E:260:PHE:CD2	2.81	0.48
1:F:66:SER:H	1:F:69:GLN:NE2	2.12	0.48
1:F:385:THR:H	1:F:388:VAL:HB	1.79	0.48
1:L:131:SER:O	1:L:132:SER:C	2.52	0.48
1:B:311:TYR:N	1:B:311:TYR:CD1	2.82	0.47
1:C:367:HIS:CE1	1:C:369:GLU:OE2	2.67	0.47
1:J:127:ASP:OD1	1:J:127:ASP:N	2.45	0.47
1:L:125:LYS:HG3	1:L:261:TRP:CG	2.49	0.47
1:L:462:GLN:HE22	1:M:21:VAL:H	1.61	0.47
1:M:344:ILE:CD1	1:N:188:LEU:HD11	2.43	0.47
1:M:353:PRO:HD2	1:M:360:LYS:HZ2	1.79	0.47
1:N:300:VAL:HG13	1:O:255:LEU:HD13	1.95	0.47
1:C:332:THR:O	1:C:333:VAL:HG23	2.14	0.47
1:E:59:LYS:O	1:E:60:GLN:HB3	2.13	0.47
1:F:72:VAL:HG23	1:F:197:ASP:HA	1.96	0.47
1:F:159:LEU:HD22	1:F:331:VAL:HG22	1.95	0.47
1:G:375:PHE:CD1	1:G:375:PHE:N	2.82	0.47
1:M:120:HIS:ND1	1:M:121:PRO:HD2	2.30	0.47
1:O:105:VAL:HG12	1:O:106:GLU:N	2.29	0.47
1:B:59:LYS:O	1:B:60:GLN:HB3	2.15	0.47
1:C:85:LEU:HD12	1:C:88:THR:HG23	1.96	0.47
1:C:98:LEU:HD21	1:C:381:THR:HG22	1.97	0.47
1:D:156:LEU:HA	1:D:250:LEU:O	2.14	0.47
1:D:300:VAL:HG13	1:E:255:LEU:HD13	1.96	0.47
1:E:151:TYR:CD2	1:E:203:THR:HB	2.48	0.47
1:E:353:PRO:HG3	1:E:360:LYS:HD2	1.95	0.47
1:K:364:TYR:CE2	1:L:185:CYS:HB2	2.48	0.47
1:M:369:GLU:HG3	1:M:371:TYR:HE1	1.78	0.47
1:B:105:VAL:CG1	1:B:106:GLU:N	2.75	0.47
1:B:300:VAL:HG13	1:C:255:LEU:HD13	1.97	0.47
1:C:123:TYR:HD2	1:C:125:LYS:HB2	1.80	0.47
1:C:188:LEU:N	1:C:188:LEU:HD22	2.29	0.47
1:G:24:THR:HG23	1:G:319:HIS:O	2.14	0.47
1:H:31:THR:HG23	1:H:379:LEU:O	2.15	0.47
1:H:125:LYS:HD2	1:H:261:TRP:NE1	2.30	0.47
1:I:99:VAL:HG12	1:I:100:TRP:N	2.29	0.47
1:L:159:LEU:CD2	1:L:331:VAL:HG22	2.45	0.47
1:N:138:ASN:HD22	1:N:140:SER:HB3	1.78	0.47
1:A:164:ALA:C	1:A:165:ILE:HD12	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:CYS:O	1:A:250:LEU:HD12	2.15	0.47
1:C:59:LYS:O	1:C:60:GLN:HB3	2.14	0.47
1:G:22:VAL:CG1	1:G:23:ASN:N	2.77	0.47
1:H:51:ARG:CZ	1:H:61:ASP:OD2	2.60	0.47
1:I:99:VAL:HG21	1:I:382:ILE:HD11	1.96	0.47
1:L:46:GLY:HA3	1:L:65:VAL:HG23	1.97	0.47
1:L:376:ILE:HG12	1:L:465:LEU:HD13	1.95	0.47
1:M:200:MET:HE2	1:M:223:ASP:O	2.15	0.47
1:A:74:ARG:NH2	1:A:328:GLN:OE1	2.46	0.47
1:A:185:CYS:HB2	1:E:364:TYR:CG	2.49	0.47
1:G:98:LEU:HD21	1:G:381:THR:HG22	1.96	0.47
1:H:155:GLN:OE1	1:H:306:LEU:HB2	2.14	0.47
1:J:105:VAL:HG12	1:J:106:GLU:N	2.29	0.47
1:J:384:LEU:HB3	1:J:389:MET:HE2	1.95	0.47
1:L:351:PRO:O	1:L:352:VAL:CB	2.63	0.47
1:M:446:LYS:HD3	1:M:446:LYS:HA	1.97	0.47
1:N:261:TRP:CZ3	1:N:294:SER:HB3	2.49	0.47
1:B:368:VAL:HG11	1:C:169:TRP:CZ2	2.50	0.47
1:D:92:ASN:C	1:D:94:GLU:N	2.64	0.47
1:F:329:LEU:HD23	1:F:329:LEU:C	2.35	0.47
1:F:387:ASP:O	1:F:388:VAL:C	2.53	0.47
1:H:52:VAL:HB	1:H:62:ILE:HB	1.96	0.47
1:H:66:SER:HB3	1:H:69:GLN:HG2	1.97	0.47
1:H:113:LEU:HD22	1:I:253:GLU:HG3	1.96	0.47
1:J:231:TYR:O	1:J:232:PRO:C	2.50	0.47
1:K:49:TYR:O	1:K:50:PHE:HB3	2.15	0.47
1:K:143:VAL:O	1:K:143:VAL:HG12	2.14	0.47
1:L:220:VAL:CG2	1:L:224:ILE:HG13	2.44	0.47
1:M:368:VAL:CG1	1:M:369:GLU:N	2.77	0.47
1:N:36:HIS:C	1:N:36:HIS:ND1	2.67	0.47
1:N:68:TYR:CE2	1:N:151:TYR:HB2	2.49	0.47
1:N:126:LEU:HG	1:N:127:ASP:OD2	2.15	0.47
1:O:111:GLN:NE2	1:O:370:GLU:OE1	2.48	0.47
1:O:125:LYS:HD2	1:O:261:TRP:CE2	2.50	0.47
1:O:140:SER:OG	1:O:141:GLU:N	2.47	0.47
1:O:196:GLU:HB3	1:O:446:LYS:O	2.15	0.47
1:A:130:GLU:OE1	1:E:258:ARG:NH1	2.48	0.47
1:B:131:SER:O	1:B:132:SER:O	2.33	0.47
1:C:159:LEU:HD22	1:C:331:VAL:HG22	1.96	0.47
1:I:88:THR:HG22	1:I:88:THR:O	2.15	0.47
1:L:121:PRO:CG	1:M:289:CYS:SG	2.84	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:22:VAL:CG1	1:M:23:ASN:N	2.77	0.47
1:M:262:ASN:HD22	1:M:262:ASN:HA	1.28	0.47
1:M:300:VAL:HG13	1:N:255:LEU:HD13	1.96	0.47
1:N:109:ARG:H	1:N:308:ASN:ND2	2.12	0.47
1:D:385:THR:H	1:D:388:VAL:HB	1.79	0.47
1:F:22:VAL:HG12	1:F:23:ASN:N	2.30	0.47
1:F:373:LEU:N	1:F:373:LEU:HD23	2.29	0.47
1:H:273:GLN:HE22	1:H:278:LYS:CE	1.95	0.47
1:I:24:THR:CG2	1:I:320:ASN:HA	2.45	0.47
1:I:232:PRO:HB2	1:I:234:TYR:CE1	2.50	0.47
1:K:120:HIS:CD2	1:K:222:LEU:HD13	2.50	0.47
1:K:369:GLU:CG	1:K:371:TYR:HE1	2.27	0.47
1:M:261:TRP:CZ3	1:M:294:SER:HB3	2.50	0.47
1:A:126:LEU:HB3	1:A:262:ASN:CB	2.45	0.47
1:A:159:LEU:CD2	1:A:331:VAL:HG22	2.44	0.47
1:A:165:ILE:N	1:A:165:ILE:CD1	2.79	0.47
1:B:390:SER:O	1:B:393:GLN:HB3	2.14	0.47
1:E:216:THR:O	1:E:217:LYS:CB	2.56	0.47
1:G:159:LEU:HD22	1:G:331:VAL:HG22	1.96	0.47
1:J:214:GLN:OE1	1:J:219:GLU:HB2	2.15	0.47
1:K:45:VAL:HG12	1:K:368:VAL:HG22	1.97	0.47
1:L:96:GLN:HB3	1:L:383:THR:HA	1.96	0.47
1:L:196:GLU:N	1:L:199:ASP:OD2	2.48	0.47
1:N:140:SER:O	1:N:141:GLU:HB2	2.14	0.47
1:N:316:ALA:HB2	1:N:321:ASN:HA	1.97	0.47
1:O:108:GLY:HA2	1:O:308:ASN:HD22	1.80	0.47
1:B:135:ALA:O	1:B:136:THR:HG23	2.15	0.46
1:C:254:GLN:O	1:C:255:LEU:HB3	2.15	0.46
1:D:50:PHE:C	1:D:50:PHE:CD1	2.89	0.46
1:D:369:GLU:HG3	1:D:371:TYR:CE1	2.50	0.46
1:G:366:ARG:HA	1:G:366:ARG:HD3	1.81	0.46
1:H:109:ARG:NH2	1:H:369:GLU:OE1	2.47	0.46
1:L:68:TYR:CZ	1:L:151:TYR:HB2	2.49	0.46
1:L:108:GLY:HA2	1:L:308:ASN:ND2	2.31	0.46
1:O:316:ALA:CB	1:O:321:ASN:HA	2.45	0.46
1:B:138:ASN:C	1:B:140:SER:H	2.18	0.46
1:D:36:HIS:ND1	1:D:36:HIS:C	2.68	0.46
1:D:324:CYS:HB3	1:D:328:GLN:O	2.15	0.46
1:G:357:ASP:O	1:G:358:ALA:C	2.53	0.46
1:K:188:LEU:N	1:K:188:LEU:CD2	2.78	0.46
1:M:125:LYS:HD2	1:M:261:TRP:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:113:LEU:HD22	1:O:253:GLU:HG3	1.98	0.46
1:A:467:ARG:O	1:A:471:VAL:HG23	2.15	0.46
1:A:475:LEU:H	1:A:475:LEU:CD2	2.24	0.46
1:B:141:GLU:HG2	1:B:141:GLU:O	2.15	0.46
1:C:125:LYS:HG3	1:C:261:TRP:CG	2.50	0.46
1:C:366:ARG:HA	1:C:366:ARG:HD3	1.77	0.46
1:E:196:GLU:N	1:E:199:ASP:OD2	2.40	0.46
1:F:185:CYS:HB2	1:J:364:TYR:CE2	2.50	0.46
1:G:300:VAL:HG13	1:H:255:LEU:CD1	2.43	0.46
1:I:369:GLU:CG	1:I:371:TYR:HE1	2.28	0.46
1:J:86:PRO:HB3	1:J:458:LEU:HD11	1.98	0.46
1:M:216:THR:O	1:M:217:LYS:HB2	2.15	0.46
1:O:34:PHE:CE2	1:O:378:GLN:HB2	2.49	0.46
1:A:169:TRP:CZ2	1:E:368:VAL:HG11	2.50	0.46
1:A:180:LEU:O	1:A:181:SER:C	2.50	0.46
1:B:367:HIS:CE1	1:B:369:GLU:OE2	2.68	0.46
1:C:364:TYR:CD2	1:D:185:CYS:HB2	2.51	0.46
1:H:143:VAL:O	1:H:143:VAL:HG12	2.15	0.46
1:H:325:TRP:O	1:H:326:HIS:HB2	2.15	0.46
1:J:99:VAL:CG2	1:J:382:ILE:CD1	2.94	0.46
1:K:92:ASN:C	1:K:94:GLU:H	2.17	0.46
1:K:366:ARG:HD3	1:K:366:ARG:HA	1.75	0.46
1:N:69:GLN:NE2	1:N:71:ARG:HH22	2.14	0.46
1:E:70:TYR:OH	1:E:232:PRO:HD3	2.16	0.46
1:G:123:TYR:CB	1:G:147:VAL:HG22	2.46	0.46
1:H:109:ARG:N	1:H:308:ASN:HD21	2.11	0.46
1:J:22:VAL:HG12	1:J:23:ASN:N	2.31	0.46
1:K:138:ASN:ND2	1:K:140:SER:HB3	2.31	0.46
1:L:22:VAL:HG12	1:L:23:ASN:N	2.30	0.46
1:M:349:GLN:CG	1:M:360:LYS:HD2	2.45	0.46
1:N:356:TYR:CD2	1:O:142:ASP:OD2	2.69	0.46
1:N:384:LEU:HB3	1:N:389:MET:HE2	1.92	0.46
1:A:109:ARG:H	1:A:308:ASN:HD21	1.62	0.46
1:A:367:HIS:CE1	1:A:369:GLU:OE2	2.69	0.46
1:B:369:GLU:HG3	1:B:371:TYR:CE1	2.48	0.46
1:C:156:LEU:HA	1:C:250:LEU:O	2.15	0.46
1:E:79:ASP:C	1:E:79:ASP:OD1	2.53	0.46
1:E:92:ASN:C	1:E:94:GLU:N	2.69	0.46
1:G:211:SER:HA	1:G:226:GLN:OE1	2.15	0.46
1:J:140:SER:OG	1:J:141:GLU:N	2.43	0.46
1:N:216:THR:HG22	1:N:218:CYS:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:262:ASN:HD22	1:N:262:ASN:HA	1.33	0.46
1:D:92:ASN:HD21	1:D:94:GLU:HB2	1.81	0.46
1:E:368:VAL:HG12	1:E:369:GLU:N	2.27	0.46
1:E:459:ASP:OD2	1:E:459:ASP:N	2.48	0.46
1:F:109:ARG:H	1:F:308:ASN:ND2	2.14	0.46
1:G:138:ASN:ND2	1:G:140:SER:HB3	2.30	0.46
1:H:45:VAL:C	1:H:65:VAL:HG21	2.36	0.46
1:H:267:MET:SD	1:H:290:VAL:HG23	2.55	0.46
1:I:50:PHE:CD1	1:I:50:PHE:C	2.89	0.46
1:J:367:HIS:HE1	1:J:369:GLU:OE2	1.99	0.46
1:K:156:LEU:HA	1:K:250:LEU:O	2.16	0.46
1:L:267:MET:SD	1:L:290:VAL:HG23	2.56	0.46
1:O:36:HIS:ND1	1:O:37:ALA:N	2.64	0.46
1:O:71:ARG:HG3	1:O:371:TYR:OH	2.16	0.46
1:A:255:LEU:HD13	1:E:300:VAL:HG13	1.98	0.46
1:A:311:TYR:CD1	1:A:311:TYR:N	2.84	0.46
1:C:216:THR:HG22	1:C:218:CYS:HB2	1.96	0.46
1:D:143:VAL:O	1:D:143:VAL:HG12	2.16	0.46
1:E:159:LEU:CD2	1:E:331:VAL:HG22	2.44	0.46
1:F:24:THR:HG21	1:F:320:ASN:HA	1.96	0.46
1:F:130:GLU:OE1	1:J:259:HIS:HE1	1.98	0.46
1:H:369:GLU:HG3	1:H:371:TYR:CE1	2.51	0.46
1:J:107:ILE:N	1:J:107:ILE:HD12	2.31	0.46
1:K:71:ARG:HA	1:K:197:ASP:OD1	2.16	0.46
1:L:71:ARG:HG3	1:L:371:TYR:OH	2.16	0.46
1:L:244:ASP:OD1	1:L:320:ASN:ND2	2.46	0.46
1:L:258:ARG:HG3	1:L:259:HIS:ND1	2.31	0.46
1:M:43:LEU:HD12	1:M:369:GLU:O	2.16	0.46
1:M:382:ILE:HD12	1:M:403:TRP:HH2	1.80	0.46
1:A:117:LEU:HG	1:B:293:PRO:HD3	1.98	0.46
1:A:185:CYS:HB2	1:E:364:TYR:CD2	2.50	0.46
1:B:237:MET:HB3	1:B:246:MET:HG2	1.97	0.46
1:D:369:GLU:CG	1:D:371:TYR:HE1	2.29	0.46
1:E:96:GLN:HB3	1:E:383:THR:HA	1.97	0.46
1:F:42:LEU:H	1:F:42:LEU:HG	1.47	0.46
1:F:97:ARG:O	1:F:98:LEU:HD23	2.15	0.46
1:G:58:ASN:CA	1:H:178:ARG:NH1	2.77	0.46
1:G:372:ASP:C	1:G:372:ASP:OD2	2.54	0.46
1:H:385:THR:H	1:H:388:VAL:HB	1.81	0.46
1:I:79:ASP:O	1:I:83:PHE:HB2	2.16	0.46
1:I:92:ASN:ND2	1:I:95:THR:HG23	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:329:LEU:HD23	1:J:329:LEU:C	2.35	0.46
1:K:36:HIS:ND1	1:K:37:ALA:N	2.64	0.46
1:K:475:LEU:HD23	1:K:475:LEU:N	2.19	0.46
1:L:220:VAL:HG21	1:L:224:ILE:HG13	1.98	0.46
1:L:260:PHE:N	1:L:260:PHE:CD2	2.83	0.46
1:M:258:ARG:HG3	1:M:259:HIS:ND1	2.30	0.46
1:B:475:LEU:HD23	1:B:475:LEU:H	1.81	0.46
1:D:24:THR:HG23	1:D:320:ASN:HA	1.98	0.46
1:F:232:PRO:HB2	1:F:234:TYR:CE1	2.51	0.46
1:K:256:PHE:CD1	1:K:256:PHE:C	2.88	0.46
1:O:66:SER:H	1:O:69:GLN:NE2	2.14	0.46
1:A:360:LYS:HE2	1:A:361:PHE:CE1	2.51	0.45
1:A:368:VAL:CG1	1:B:169:TRP:CZ2	2.99	0.45
1:E:308:ASN:HD22	1:E:308:ASN:HA	1.51	0.45
1:F:47:ASP:OD1	1:F:49:TYR:N	2.36	0.45
1:F:112:PRO:HB3	1:G:231:TYR:CG	2.51	0.45
1:F:165:ILE:N	1:F:165:ILE:HD12	2.31	0.45
1:F:389:MET:HG2	1:F:400:LEU:HD21	1.98	0.45
1:F:396:ASN:O	1:F:399:ILE:HG13	2.15	0.45
1:G:148:SER:HB3	1:H:291:TYR:CD2	2.51	0.45
1:J:99:VAL:HG11	1:J:323:VAL:CG1	2.47	0.45
1:M:52:VAL:HB	1:M:62:ILE:HB	1.98	0.45
1:N:368:VAL:CG1	1:O:169:TRP:CZ2	2.95	0.45
1:O:375:PHE:O	1:O:376:ILE:HD13	2.16	0.45
1:A:185:CYS:HB2	1:E:364:TYR:CD1	2.51	0.45
1:A:314:HIS:ND1	1:A:314:HIS:N	2.63	0.45
1:B:163:PRO:HD3	1:B:330:PHE:CZ	2.51	0.45
1:D:262:ASN:HD22	1:D:262:ASN:HA	1.37	0.45
1:H:72:VAL:HG23	1:H:197:ASP:CA	2.43	0.45
1:I:74:ARG:HH22	1:I:440:ASP:CG	2.20	0.45
1:I:159:LEU:HB2	1:I:248:PHE:HB3	1.98	0.45
1:J:141:GLU:O	1:J:142:ASP:C	2.54	0.45
1:J:333:VAL:HG11	1:J:371:TYR:HE2	1.81	0.45
1:N:47:ASP:C	1:N:47:ASP:OD1	2.54	0.45
1:N:111:GLN:CB	1:N:112:PRO:CD	2.90	0.45
1:N:120:HIS:CD2	1:N:222:LEU:HD13	2.51	0.45
1:O:99:VAL:HG21	1:O:382:ILE:HD11	1.98	0.45
1:A:382:ILE:HD12	1:A:403:TRP:CH2	2.51	0.45
1:D:323:VAL:HG11	1:D:325:TRP:CZ2	2.51	0.45
1:F:384:LEU:C	1:F:389:MET:HE2	2.37	0.45
1:I:69:GLN:HE21	1:I:71:ARG:HH12	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:210:PHE:HE1	1:K:229:CYS:HG	1.64	0.45
1:K:353:PRO:CG	1:K:360:LYS:NZ	2.77	0.45
1:L:111:GLN:CB	1:L:112:PRO:HD2	2.33	0.45
1:M:90:ILE:HD12	1:M:90:ILE:HG23	1.75	0.45
1:A:114:GLY:HA3	1:A:340:THR:HG23	1.99	0.45
1:B:464:PRO:HA	1:B:467:ARG:NH1	2.32	0.45
1:H:125:LYS:HG3	1:H:261:TRP:CD2	2.51	0.45
1:I:349:GLN:CG	1:I:360:LYS:HD2	2.45	0.45
1:J:293:PRO:HG2	1:J:293:PRO:O	2.16	0.45
1:A:74:ARG:NE	1:A:328:GLN:OE1	2.45	0.45
1:A:188:LEU:HD11	1:E:344:ILE:CD1	2.46	0.45
1:A:364:TYR:CE2	1:B:185:CYS:HB2	2.51	0.45
1:C:109:ARG:H	1:C:308:ASN:ND2	2.15	0.45
1:D:308:ASN:HD22	1:D:308:ASN:HA	1.56	0.45
1:D:465:LEU:O	1:D:465:LEU:HD22	2.17	0.45
1:E:24:THR:CG2	1:E:320:ASN:HA	2.46	0.45
1:E:105:VAL:CG1	1:E:106:GLU:N	2.74	0.45
1:F:117:LEU:CD1	1:G:293:PRO:HB3	2.45	0.45
1:H:22:VAL:CG1	1:H:23:ASN:N	2.79	0.45
1:H:126:LEU:HB3	1:H:262:ASN:HB3	1.99	0.45
1:J:43:LEU:HA	1:J:43:LEU:HD12	1.77	0.45
1:L:74:ARG:NE	1:L:328:GLN:OE1	2.46	0.45
1:N:22:VAL:CG1	1:N:23:ASN:N	2.79	0.45
1:O:74:ARG:HG3	1:O:330:PHE:CE2	2.52	0.45
1:A:126:LEU:HD13	1:A:264:ALA:HB2	1.99	0.45
1:B:79:ASP:C	1:B:79:ASP:OD1	2.54	0.45
1:B:151:TYR:OH	1:B:221:PRO:HB2	2.16	0.45
1:E:43:LEU:CD1	1:E:370:GLU:HB2	2.47	0.45
1:I:239:ALA:O	1:I:240:ASP:C	2.55	0.45
1:N:62:ILE:HG23	1:N:62:ILE:HD12	1.67	0.45
1:N:152:LYS:HE3	1:N:253:GLU:HB2	1.99	0.45
1:C:52:VAL:HB	1:C:62:ILE:HB	1.98	0.45
1:D:366:ARG:HD3	1:D:366:ARG:HA	1.71	0.45
1:F:21:VAL:HB	1:J:462:GLN:HE22	1.82	0.45
1:H:307:PHE:HE1	1:H:335:ASP:CB	2.25	0.45
1:J:247:PHE:CZ	1:J:322:GLY:HA2	2.51	0.45
1:J:249:CYS:O	1:J:250:LEU:HD12	2.17	0.45
1:J:451:ASP:OD2	1:J:453:LYS:HD2	2.16	0.45
1:M:308:ASN:HD22	1:M:308:ASN:HA	1.58	0.45
1:N:68:TYR:CZ	1:N:151:TYR:HB2	2.51	0.45
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ARG:O	1:C:41:ARG:HG2	2.17	0.45
1:C:213:LEU:HA	1:C:213:LEU:HD12	1.73	0.45
1:D:68:TYR:CE2	1:D:151:TYR:HB2	2.52	0.45
1:D:70:TYR:OH	1:D:232:PRO:HD3	2.17	0.45
1:D:306:LEU:O	1:D:311:TYR:OH	2.30	0.45
1:G:220:VAL:HG23	1:G:225:CYS:HA	1.98	0.45
1:G:300:VAL:CG1	1:H:255:LEU:CD1	2.92	0.45
1:G:464:PRO:HA	1:G:467:ARG:NH1	2.32	0.45
1:H:35:TYR:CE2	1:H:458:LEU:HG	2.52	0.45
1:I:78:PRO:HG2	1:I:100:TRP:HE1	1.81	0.45
1:I:349:GLN:HG2	1:I:360:LYS:CD	2.45	0.45
1:J:111:GLN:CB	1:J:112:PRO:HD2	2.41	0.45
1:J:165:ILE:HD12	1:J:165:ILE:N	2.32	0.45
1:K:123:TYR:HD2	1:K:125:LYS:HB2	1.82	0.45
1:L:113:LEU:HD22	1:M:253:GLU:HG3	1.98	0.45
1:L:126:LEU:CB	1:L:262:ASN:HB3	2.33	0.45
1:N:109:ARG:NH1	1:N:371:TYR:CE1	2.85	0.45
1:E:262:ASN:HD22	1:E:262:ASN:HA	1.38	0.45
1:E:267:MET:SD	1:E:290:VAL:HG23	2.57	0.45
1:F:77:LEU:HB3	1:F:78:PRO:HD2	1.99	0.45
1:F:216:THR:HG22	1:F:218:CYS:N	2.32	0.45
1:H:344:ILE:CD1	1:I:188:LEU:HD11	2.46	0.45
1:K:131:SER:O	1:K:132:SER:C	2.54	0.45
1:K:353:PRO:HD2	1:K:360:LYS:CE	2.47	0.45
1:B:151:TYR:CD2	1:B:203:THR:HB	2.52	0.45
1:D:216:THR:O	1:D:217:LYS:CB	2.65	0.45
1:D:364:TYR:CZ	1:E:268:GLY:HA3	2.51	0.45
1:G:150:ASP:O	1:G:296:SER:HA	2.16	0.45
1:J:71:ARG:HA	1:J:197:ASP:OD1	2.17	0.45
1:J:108:GLY:HA2	1:J:308:ASN:ND2	2.32	0.45
1:L:300:VAL:HG13	1:M:255:LEU:HD13	1.99	0.45
1:O:92:ASN:HA	1:O:93:PRO:HD2	1.63	0.45
1:O:96:GLN:HB3	1:O:383:THR:HA	1.99	0.45
1:B:148:SER:HB3	1:C:291:TYR:CD2	2.53	0.44
1:C:79:ASP:C	1:C:79:ASP:OD1	2.56	0.44
1:C:111:GLN:HB3	1:C:112:PRO:CD	2.43	0.44
1:F:226:GLN:HG3	1:G:275:LEU:HD23	1.99	0.44
1:F:235:LEU:HD12	1:J:370:GLU:OE2	2.16	0.44
1:H:262:ASN:HD22	1:H:262:ASN:HA	1.34	0.44
1:H:475:LEU:H	1:H:475:LEU:CD2	2.28	0.44
1:I:316:ALA:CB	1:I:321:ASN:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:314:HIS:ND1	1:K:314:HIS:N	2.63	0.44
1:M:96:GLN:HB3	1:M:383:THR:HA	1.99	0.44
1:N:52:VAL:HB	1:N:62:ILE:HB	1.99	0.44
1:O:71:ARG:HA	1:O:197:ASP:OD1	2.17	0.44
1:A:122:PHE:HB3	1:A:144:ARG:HD2	2.00	0.44
1:A:317:GLN:CG	1:A:318:GLY:N	2.80	0.44
1:B:391:TYR:C	1:B:393:GLN:N	2.70	0.44
1:D:135:ALA:O	1:D:136:THR:CG2	2.65	0.44
1:F:244:ASP:OD1	1:F:320:ASN:ND2	2.48	0.44
1:F:353:PRO:CD	1:F:360:LYS:HZ1	2.30	0.44
1:G:376:ILE:HG12	1:G:465:LEU:HD13	1.97	0.44
1:I:109:ARG:H	1:I:308:ASN:HD21	1.65	0.44
1:I:353:PRO:CD	1:I:360:LYS:HZ3	2.29	0.44
1:J:119:GLY:HA2	1:J:148:SER:HA	1.98	0.44
1:M:255:LEU:HA	1:M:297:GLY:HA2	2.00	0.44
1:O:22:VAL:CG1	1:O:23:ASN:N	2.80	0.44
1:O:193:THR:HG21	1:O:230:LYS:HD3	2.00	0.44
1:O:329:LEU:HD23	1:O:329:LEU:O	2.17	0.44
1:A:255:LEU:HD13	1:E:300:VAL:CG1	2.48	0.44
1:C:111:GLN:NE2	1:C:370:GLU:OE1	2.50	0.44
1:C:150:ASP:O	1:C:296:SER:HA	2.17	0.44
1:F:59:LYS:HD3	1:G:178:ARG:HG3	2.00	0.44
1:G:42:LEU:HB3	1:G:448:TRP:CZ2	2.52	0.44
1:G:66:SER:O	1:G:69:GLN:HG2	2.17	0.44
1:G:368:VAL:CG1	1:H:169:TRP:CZ2	2.95	0.44
1:H:163:PRO:HD3	1:H:330:PHE:CZ	2.52	0.44
1:H:300:VAL:CG1	1:I:255:LEU:HD13	2.47	0.44
1:I:341:ASN:HD22	1:I:341:ASN:HA	1.59	0.44
1:J:267:MET:SD	1:J:290:VAL:HG23	2.57	0.44
1:K:349:GLN:HG3	1:K:360:LYS:HD2	2.00	0.44
1:M:205:TYR:CD2	1:M:220:VAL:HG12	2.53	0.44
1:A:376:ILE:HG12	1:A:465:LEU:HD13	1.99	0.44
1:C:313:LEU:N	1:C:313:LEU:HD23	2.33	0.44
1:D:307:PHE:O	1:D:309:LYS:HG3	2.18	0.44
1:E:98:LEU:HD13	1:E:379:LEU:HD11	1.99	0.44
1:E:368:VAL:CG1	1:E:369:GLU:N	2.78	0.44
1:F:216:THR:HG22	1:F:218:CYS:H	1.81	0.44
1:I:262:ASN:HD22	1:I:262:ASN:HA	1.45	0.44
1:J:314:HIS:O	1:J:315:LYS:HG3	2.17	0.44
1:K:385:THR:OG1	1:K:388:VAL:HG23	2.17	0.44
1:L:31:THR:HG23	1:L:379:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:71:ARG:HA	1:M:197:ASP:OD1	2.17	0.44
1:M:349:GLN:HG3	1:M:360:LYS:HD2	2.00	0.44
1:D:151:TYR:CD2	1:D:203:THR:HB	2.53	0.44
1:D:316:ALA:CB	1:D:321:ASN:HA	2.47	0.44
1:F:68:TYR:CZ	1:F:151:TYR:HB2	2.52	0.44
1:H:108:GLY:HA2	1:H:308:ASN:HD22	1.83	0.44
1:H:172:GLY:C	1:H:173:THR:O	2.54	0.44
1:I:70:TYR:CE1	1:I:201:VAL:HG12	2.51	0.44
1:I:148:SER:HB3	1:J:291:TYR:CD2	2.52	0.44
1:I:460:LEU:HB2	1:I:470:LEU:HD11	2.00	0.44
1:J:150:ASP:O	1:J:296:SER:HA	2.17	0.44
1:C:24:THR:HG23	1:C:319:HIS:O	2.17	0.44
1:C:96:GLN:HB3	1:C:383:THR:HA	1.99	0.44
1:C:375:PHE:O	1:C:376:ILE:HD13	2.17	0.44
1:D:66:SER:HB3	1:D:69:GLN:HG2	1.99	0.44
1:D:126:LEU:HB3	1:D:262:ASN:CB	2.43	0.44
1:F:92:ASN:C	1:F:92:ASN:OD1	2.55	0.44
1:F:178:ARG:HG3	1:J:59:LYS:HD2	1.99	0.44
1:I:115:VAL:HG13	1:J:255:LEU:HD21	1.99	0.44
1:J:353:PRO:C	1:J:355:GLN:H	2.21	0.44
1:K:87:ASP:HB3	1:K:90:ILE:HD11	1.99	0.44
1:L:68:TYR:CE2	1:L:151:TYR:HB2	2.52	0.44
1:O:68:TYR:CE2	1:O:151:TYR:HB2	2.53	0.44
1:O:72:VAL:H	1:O:197:ASP:HB2	1.82	0.44
1:O:214:GLN:OE1	1:O:219:GLU:HB2	2.17	0.44
1:O:279:GLY:O	1:O:284:ALA:HA	2.18	0.44
1:O:365:SER:O	1:O:366:ARG:HD3	2.18	0.44
1:C:68:TYR:CZ	1:C:151:TYR:HB2	2.52	0.44
1:E:366:ARG:HD3	1:E:366:ARG:HA	1.64	0.44
1:F:311:TYR:CD1	1:F:311:TYR:N	2.86	0.44
1:G:112:PRO:HB3	1:H:231:TYR:CD1	2.52	0.44
1:G:131:SER:O	1:G:132:SER:C	2.56	0.44
1:L:306:LEU:O	1:L:311:TYR:OH	2.36	0.44
1:M:124:ASN:N	1:M:218:CYS:O	2.42	0.44
1:M:235:LEU:HA	1:M:235:LEU:HD23	1.81	0.44
1:M:384:LEU:HB3	1:M:389:MET:CE	2.48	0.44
1:N:60:GLN:HG3	1:N:61:ASP:N	2.33	0.44
1:O:399:ILE:HG21	1:O:399:ILE:HD13	1.67	0.44
1:B:62:ILE:HA	1:B:63:PRO:HD3	1.80	0.44
1:D:120:HIS:CD2	1:D:222:LEU:CD1	3.01	0.44
1:E:138:ASN:C	1:E:140:SER:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:ASN:O	1:G:83:PHE:N	2.49	0.44
1:G:92:ASN:HA	1:G:93:PRO:HD2	1.75	0.44
1:K:244:ASP:OD1	1:K:320:ASN:ND2	2.34	0.44
1:M:43:LEU:HD12	1:M:43:LEU:HA	1.80	0.44
1:M:353:PRO:HG2	1:M:360:LYS:NZ	2.32	0.44
1:M:471:VAL:C	1:M:473:ALA:N	2.71	0.44
1:N:105:VAL:HG12	1:N:106:GLU:H	1.80	0.44
1:N:220:VAL:HG23	1:N:225:CYS:HA	1.99	0.44
1:N:367:HIS:HE1	1:N:369:GLU:OE2	2.00	0.44
1:A:77:LEU:N	1:A:77:LEU:HD23	2.32	0.44
1:A:300:VAL:HG13	1:B:255:LEU:HD13	2.00	0.44
1:B:151:TYR:CE2	1:B:221:PRO:HG2	2.52	0.44
1:B:317:GLN:CD	1:B:318:GLY:N	2.71	0.44
1:C:43:LEU:CD1	1:C:370:GLU:HB2	2.47	0.44
1:C:72:VAL:HG23	1:C:197:ASP:HA	2.00	0.44
1:C:117:LEU:HD11	1:D:293:PRO:HB3	2.00	0.44
1:D:214:GLN:OE1	1:D:219:GLU:HB2	2.18	0.44
1:D:258:ARG:HG3	1:D:259:HIS:ND1	2.33	0.44
1:F:157:CYS:HA	1:F:332:THR:O	2.18	0.44
1:F:260:PHE:HB3	1:J:117:LEU:HD13	2.00	0.44
1:H:51:ARG:NH2	1:H:61:ASP:OD1	2.51	0.44
1:H:374:GLN:OE1	1:H:464:PRO:HG2	2.18	0.44
1:I:397:SER:O	1:I:398:SER:C	2.56	0.44
1:K:96:GLN:HB3	1:K:96:GLN:HE21	1.45	0.44
1:K:272:PRO:HB2	1:K:275:LEU:HG	1.98	0.44
1:L:92:ASN:HA	1:L:93:PRO:HD2	1.60	0.44
1:N:316:ALA:HB3	1:N:321:ASN:HA	1.98	0.44
1:O:48:PRO:HG2	1:O:49:TYR:CD2	2.53	0.44
1:O:316:ALA:HB3	1:O:321:ASN:HA	1.99	0.44
1:O:324:CYS:HB3	1:O:328:GLN:O	2.18	0.44
1:A:351:PRO:O	1:A:352:VAL:HB	2.18	0.43
1:A:382:ILE:HG21	1:A:382:ILE:HD13	1.70	0.43
1:D:344:ILE:CD1	1:E:188:LEU:HD11	2.48	0.43
1:F:213:LEU:HA	1:F:213:LEU:HD12	1.79	0.43
1:J:310:PRO:O	1:J:310:PRO:HG2	2.17	0.43
1:L:316:ALA:HB3	1:L:321:ASN:HA	2.00	0.43
1:O:347:SER:HA	1:O:361:PHE:HA	2.00	0.43
1:A:385:THR:H	1:A:388:VAL:HB	1.83	0.43
1:B:96:GLN:HE21	1:B:96:GLN:HB3	1.49	0.43
1:B:123:TYR:HD2	1:B:125:LYS:HB2	1.83	0.43
1:B:385:THR:H	1:B:388:VAL:HB	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:GLU:HG3	1:D:371:TYR:HE1	1.83	0.43
1:G:467:ARG:HD2	1:H:317:GLN:O	2.18	0.43
1:I:47:ASP:OD1	1:I:48:PRO:N	2.51	0.43
1:I:49:TYR:O	1:I:50:PHE:HB3	2.19	0.43
1:I:67:ALA:HB2	1:I:367:HIS:CE1	2.52	0.43
1:I:351:PRO:C	1:I:352:VAL:HG23	2.38	0.43
1:J:254:GLN:HE21	1:J:298:SER:H	1.65	0.43
1:J:311:TYR:N	1:J:311:TYR:CD1	2.85	0.43
1:K:112:PRO:HB3	1:L:231:TYR:CD1	2.52	0.43
1:K:144:ARG:O	1:L:283:ARG:NH1	2.51	0.43
1:O:372:ASP:OD2	1:O:372:ASP:O	2.35	0.43
1:B:465:LEU:HA	1:B:465:LEU:HD23	1.70	0.43
1:F:372:ASP:OD2	1:F:372:ASP:C	2.57	0.43
1:G:117:LEU:HD13	1:H:260:PHE:HB3	1.99	0.43
1:H:300:VAL:HG13	1:H:300:VAL:O	2.19	0.43
1:H:384:LEU:HB3	1:H:389:MET:HE1	1.99	0.43
1:K:249:CYS:O	1:K:250:LEU:HD12	2.19	0.43
1:K:255:LEU:HD13	1:O:300:VAL:CG1	2.48	0.43
1:L:237:MET:HB3	1:L:246:MET:HG2	2.00	0.43
1:M:36:HIS:ND1	1:M:37:ALA:N	2.67	0.43
1:M:216:THR:HG22	1:M:218:CYS:HB2	2.01	0.43
1:A:261:TRP:CZ3	1:A:294:SER:HB3	2.53	0.43
1:A:310:PRO:O	1:A:310:PRO:HG2	2.18	0.43
1:B:111:GLN:HB3	1:B:112:PRO:CD	2.48	0.43
1:B:143:VAL:O	1:B:143:VAL:HG12	2.17	0.43
1:D:98:LEU:CD2	1:D:381:THR:HG22	2.48	0.43
1:E:92:ASN:OD1	1:E:94:GLU:HB2	2.18	0.43
1:E:350:SER:HB3	1:E:351:PRO:HD3	1.99	0.43
1:F:24:THR:HG23	1:F:319:HIS:O	2.18	0.43
1:F:169:TRP:HZ2	1:J:368:VAL:HG11	1.83	0.43
1:F:306:LEU:HA	1:F:306:LEU:HD12	1.58	0.43
1:G:176:LYS:HB2	1:G:176:LYS:NZ	2.33	0.43
1:I:224:ILE:HD13	1:I:224:ILE:HG21	1.82	0.43
1:I:360:LYS:HE2	1:I:361:PHE:CE1	2.54	0.43
1:J:110:GLY:O	1:J:111:GLN:O	2.37	0.43
1:J:325:TRP:CD2	1:J:399:ILE:HD13	2.53	0.43
1:K:68:TYR:CE2	1:K:151:TYR:HB2	2.52	0.43
1:K:126:LEU:HB3	1:K:262:ASN:CB	2.45	0.43
1:K:219:GLU:C	1:K:220:VAL:HG13	2.38	0.43
1:L:24:THR:HG23	1:L:320:ASN:HA	2.01	0.43
1:N:83:PHE:CG	1:N:84:GLY:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:324:CYS:SG	1:N:329:LEU:HD12	2.58	0.43
1:A:71:ARG:HA	1:A:197:ASP:OD1	2.17	0.43
1:C:262:ASN:HD22	1:C:262:ASN:HA	1.47	0.43
1:D:107:ILE:HD12	1:D:107:ILE:N	2.33	0.43
1:D:224:ILE:O	1:D:225:CYS:C	2.56	0.43
1:E:376:ILE:HG12	1:E:465:LEU:HD13	2.00	0.43
1:H:244:ASP:OD1	1:H:320:ASN:ND2	2.51	0.43
1:I:123:TYR:CG	1:I:147:VAL:CG2	3.01	0.43
1:I:311:TYR:CD1	1:I:311:TYR:N	2.86	0.43
1:I:316:ALA:HB3	1:I:321:ASN:HA	2.00	0.43
1:I:366:ARG:HD3	1:I:366:ARG:HA	1.55	0.43
1:J:261:TRP:CZ3	1:J:294:SER:HB3	2.54	0.43
1:K:351:PRO:O	1:K:352:VAL:HB	2.19	0.43
1:L:110:GLY:O	1:L:111:GLN:O	2.36	0.43
1:L:453:LYS:CD	1:L:453:LYS:HB2	2.44	0.43
1:M:92:ASN:HD21	1:M:95:THR:HG23	1.83	0.43
1:A:247:PHE:CD2	1:A:322:GLY:HA2	2.54	0.43
1:A:344:ILE:CD1	1:B:188:LEU:HD11	2.48	0.43
1:B:114:GLY:HA3	1:B:340:THR:HG23	2.00	0.43
1:C:48:PRO:HG2	1:C:49:TYR:CD2	2.53	0.43
1:C:220:VAL:HG23	1:C:225:CYS:HA	2.00	0.43
1:D:46:GLY:HA3	1:D:65:VAL:HG23	2.00	0.43
1:D:79:ASP:O	1:D:83:PHE:HB2	2.18	0.43
1:F:126:LEU:HB3	1:F:262:ASN:CB	2.39	0.43
1:F:379:LEU:HG	1:F:380:CYS:N	2.33	0.43
1:G:154:THR:HG23	1:G:253:GLU:HB3	2.00	0.43
1:J:213:LEU:HD12	1:J:213:LEU:HA	1.68	0.43
1:K:92:ASN:O	1:K:94:GLU:N	2.51	0.43
1:M:125:LYS:HD2	1:M:261:TRP:NE1	2.33	0.43
1:C:75:VAL:CG1	1:C:452:LEU:HD12	2.48	0.43
1:C:92:ASN:C	1:C:94:GLU:H	2.22	0.43
1:C:110:GLY:HA3	1:C:370:GLU:CD	2.39	0.43
1:C:324:CYS:HB3	1:C:328:GLN:O	2.18	0.43
1:D:224:ILE:HD13	1:D:224:ILE:HG21	1.71	0.43
1:E:216:THR:HG22	1:E:218:CYS:HB2	2.01	0.43
1:E:249:CYS:O	1:E:250:LEU:HD12	2.18	0.43
1:G:353:PRO:HG3	1:G:360:LYS:HD2	2.00	0.43
1:H:364:TYR:CD2	1:I:185:CYS:HB2	2.54	0.43
1:K:24:THR:HG23	1:K:319:HIS:O	2.19	0.43
1:K:261:TRP:CZ3	1:K:294:SER:HB3	2.53	0.43
1:M:81:ASN:C	1:M:83:PHE:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:196:GLU:N	1:N:199:ASP:OD2	2.48	0.43
1:N:324:CYS:HB3	1:N:328:GLN:O	2.19	0.43
1:O:188:LEU:HD22	1:O:188:LEU:N	2.33	0.43
1:A:78:PRO:HD2	1:A:456:PHE:CE1	2.53	0.43
1:A:396:ASN:C	1:A:396:ASN:ND2	2.72	0.43
1:F:231:TYR:CD1	1:F:232:PRO:HD2	2.54	0.43
1:G:167:GLU:HB3	1:G:233:ASP:HB2	2.01	0.43
1:I:36:HIS:ND1	1:I:36:HIS:C	2.71	0.43
1:I:135:ALA:O	1:I:136:THR:CG2	2.67	0.43
1:I:267:MET:HE2	1:I:267:MET:HA	2.01	0.43
1:K:316:ALA:HB2	1:K:321:ASN:HA	2.01	0.43
1:M:385:THR:OG1	1:M:388:VAL:HG23	2.19	0.43
1:N:49:TYR:O	1:N:64:LYS:HE3	2.19	0.43
1:N:96:GLN:HE21	1:N:96:GLN:HB3	1.57	0.43
1:N:115:VAL:HG21	1:O:257:ALA:HB2	2.01	0.43
1:O:216:THR:HG21	1:O:219:GLU:OE2	2.18	0.43
1:O:384:LEU:HD22	1:O:389:MET:HG3	2.01	0.43
1:A:70:TYR:OH	1:A:232:PRO:HD3	2.19	0.43
1:B:349:GLN:HG2	1:B:360:LYS:CG	2.49	0.43
1:E:150:ASP:O	1:E:296:SER:HA	2.18	0.43
1:E:367:HIS:CE1	1:E:369:GLU:OE2	2.72	0.43
1:F:50:PHE:CA	1:F:64:LYS:HG3	2.48	0.43
1:G:50:PHE:CA	1:G:64:LYS:HG3	2.48	0.43
1:I:92:ASN:C	1:I:94:GLU:H	2.22	0.43
1:I:117:LEU:HG	1:J:293:PRO:HD3	2.00	0.43
1:I:151:TYR:CD2	1:I:203:THR:HB	2.52	0.43
1:J:369:GLU:HG3	1:J:371:TYR:CE1	2.54	0.43
1:K:105:VAL:CG1	1:K:106:GLU:N	2.78	0.43
1:M:98:LEU:HD23	1:M:381:THR:HG22	2.01	0.43
1:M:369:GLU:HG3	1:M:371:TYR:CE1	2.54	0.43
1:N:117:LEU:HD13	1:O:260:PHE:HB3	2.01	0.43
1:N:373:LEU:N	1:N:373:LEU:HD23	2.30	0.43
1:B:235:LEU:HD23	1:B:235:LEU:HA	1.75	0.43
1:D:34:PHE:CE2	1:D:378:GLN:HB2	2.53	0.43
1:E:464:PRO:HA	1:E:467:ARG:NH1	2.34	0.43
1:F:240:ASP:HA	1:F:241:PRO:HD2	1.75	0.43
1:F:349:GLN:HG3	1:F:360:LYS:HD2	2.01	0.43
1:G:201:VAL:HG11	1:G:334:VAL:HG21	2.01	0.43
1:I:123:TYR:CG	1:I:147:VAL:HG22	2.54	0.43
1:I:171:LYS:HB2	1:I:213:LEU:CD1	2.49	0.43
1:J:156:LEU:HG	1:J:334:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:69:GLN:HE21	1:L:71:ARG:HH12	1.67	0.43
1:L:69:GLN:NE2	1:L:71:ARG:HH22	2.17	0.43
1:L:109:ARG:HD3	1:L:335:ASP:OD2	2.18	0.43
1:N:46:GLY:HA3	1:N:65:VAL:HG23	2.01	0.43
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.77	0.42
1:A:257:ALA:HB2	1:E:115:VAL:HG21	2.01	0.42
1:D:315:LYS:CD	1:D:315:LYS:HB2	2.49	0.42
1:F:216:THR:CG2	1:F:218:CYS:HB2	2.48	0.42
1:F:366:ARG:HG3	1:F:366:ARG:HH11	1.84	0.42
1:G:119:GLY:HA2	1:G:148:SER:HA	2.01	0.42
1:H:464:PRO:HG2	1:H:465:LEU:H	1.84	0.42
1:I:108:GLY:HA2	1:I:308:ASN:ND2	2.34	0.42
1:K:85:LEU:HD12	1:K:88:THR:HA	2.01	0.42
1:K:226:GLN:OE1	1:K:226:GLN:HA	2.18	0.42
1:K:384:LEU:HB3	1:K:389:MET:HE2	1.99	0.42
1:A:369:GLU:HG3	1:A:371:TYR:CE1	2.54	0.42
1:C:300:VAL:CG1	1:D:255:LEU:HD13	2.49	0.42
1:E:69:GLN:NE2	1:E:71:ARG:HH22	2.16	0.42
1:G:36:HIS:ND1	1:G:37:ALA:N	2.67	0.42
1:G:138:ASN:C	1:G:140:SER:H	2.23	0.42
1:G:151:TYR:CD2	1:G:203:THR:HB	2.53	0.42
1:G:237:MET:HB3	1:G:246:MET:HG2	2.01	0.42
1:J:210:PHE:HE1	1:J:229:CYS:HG	1.67	0.42
1:K:247:PHE:CE2	1:K:322:GLY:HA2	2.54	0.42
1:L:216:THR:O	1:L:217:LYS:CB	2.66	0.42
1:N:392:ILE:O	1:N:392:ILE:CG2	2.67	0.42
1:O:22:VAL:HG12	1:O:23:ASN:H	1.84	0.42
1:O:475:LEU:HD23	1:O:475:LEU:N	2.24	0.42
1:A:256:PHE:CD1	1:A:256:PHE:C	2.93	0.42
1:F:396:ASN:C	1:F:396:ASN:HD22	2.22	0.42
1:F:465:LEU:CD2	1:F:465:LEU:O	2.68	0.42
1:G:126:LEU:HB3	1:G:262:ASN:CB	2.48	0.42
1:G:262:ASN:HD22	1:G:262:ASN:HA	1.30	0.42
1:G:333:VAL:HG11	1:G:371:TYR:HE2	1.84	0.42
1:I:50:PHE:CD1	1:I:50:PHE:O	2.72	0.42
1:I:117:LEU:HD11	1:J:293:PRO:HB3	2.01	0.42
1:I:126:LEU:CB	1:I:262:ASN:HB3	2.44	0.42
1:K:76:GLN:CG	1:K:453:LYS:HE3	2.48	0.42
1:K:349:GLN:CG	1:K:360:LYS:HD2	2.49	0.42
1:K:353:PRO:HG2	1:K:360:LYS:NZ	2.24	0.42
1:L:42:LEU:HB3	1:L:448:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:300:VAL:HG13	1:O:300:VAL:O	2.18	0.42
1:A:389:MET:O	1:A:393:GLN:HB2	2.20	0.42
1:B:105:VAL:HG21	1:B:159:LEU:CD1	2.45	0.42
1:B:366:ARG:HD3	1:B:366:ARG:HA	1.64	0.42
1:C:196:GLU:N	1:C:199:ASP:OD2	2.41	0.42
1:C:372:ASP:OD2	1:C:372:ASP:C	2.57	0.42
1:D:71:ARG:HA	1:D:197:ASP:OD1	2.20	0.42
1:D:117:LEU:HD13	1:E:260:PHE:HB3	2.00	0.42
1:E:22:VAL:HG12	1:E:23:ASN:N	2.33	0.42
1:H:150:ASP:O	1:H:296:SER:HA	2.20	0.42
1:I:92:ASN:O	1:I:94:GLU:N	2.52	0.42
1:I:307:PHE:HA	1:I:311:TYR:OH	2.19	0.42
1:K:460:LEU:H	1:K:460:LEU:HG	1.57	0.42
1:L:278:LYS:NZ	1:L:278:LYS:HG2	2.35	0.42
1:M:392:ILE:O	1:M:392:ILE:HG22	2.20	0.42
1:O:126:LEU:HB3	1:O:262:ASN:CB	2.43	0.42
1:O:216:THR:O	1:O:217:LYS:HB2	2.19	0.42
1:A:110:GLY:HA3	1:A:370:GLU:CG	2.49	0.42
1:B:314:HIS:O	1:B:315:LYS:HG3	2.20	0.42
1:E:146:ASN:C	1:E:146:ASN:OD1	2.57	0.42
1:G:374:GLN:OE1	1:G:464:PRO:HG2	2.20	0.42
1:I:92:ASN:HA	1:I:93:PRO:HD2	1.82	0.42
1:K:159:LEU:CD2	1:K:331:VAL:HG22	2.50	0.42
1:O:104:GLY:C	1:O:105:VAL:HG23	2.39	0.42
1:A:91:TYR:H	1:A:91:TYR:HD2	1.67	0.42
1:A:143:VAL:O	1:A:143:VAL:HG12	2.20	0.42
1:B:22:VAL:HG12	1:B:23:ASN:N	2.34	0.42
1:C:385:THR:H	1:C:388:VAL:HB	1.84	0.42
1:E:396:ASN:C	1:E:396:ASN:HD22	2.21	0.42
1:G:98:LEU:CD2	1:G:380:CYS:O	2.67	0.42
1:I:72:VAL:HG23	1:I:197:ASP:CA	2.49	0.42
1:I:149:VAL:HG22	1:I:150:ASP:N	2.35	0.42
1:K:308:ASN:HD22	1:K:308:ASN:HA	1.64	0.42
1:L:67:ALA:HB2	1:L:367:HIS:CE1	2.55	0.42
1:M:324:CYS:HB3	1:M:328:GLN:O	2.19	0.42
1:N:131:SER:O	1:N:132:SER:C	2.56	0.42
1:N:353:PRO:HG3	1:N:360:LYS:HD2	2.00	0.42
1:O:308:ASN:HD22	1:O:308:ASN:HA	1.56	0.42
1:A:119:GLY:HA2	1:A:148:SER:HA	2.00	0.42
1:B:317:GLN:CG	1:B:318:GLY:N	2.83	0.42
1:C:260:PHE:CD2	1:C:260:PHE:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:VAL:C	1:E:65:VAL:HG21	2.40	0.42
1:F:220:VAL:CG2	1:F:225:CYS:HA	2.49	0.42
1:F:366:ARG:HD3	1:F:366:ARG:HA	1.64	0.42
1:H:351:PRO:O	1:H:352:VAL:CB	2.68	0.42
1:I:123:TYR:CD2	1:I:125:LYS:HB2	2.54	0.42
1:K:31:THR:HG23	1:K:379:LEU:O	2.19	0.42
1:K:209:ASP:O	1:K:213:LEU:HB2	2.19	0.42
1:O:124:ASN:OD1	1:O:264:ALA:HB3	2.20	0.42
1:O:454:GLU:C	1:O:455:LYS:HG2	2.40	0.42
1:A:283:ARG:HD2	1:E:142:ASP:CG	2.40	0.42
1:A:369:GLU:HG3	1:A:371:TYR:HE1	1.85	0.42
1:E:78:PRO:HD2	1:E:456:PHE:CZ	2.55	0.42
1:F:316:ALA:CB	1:F:321:ASN:HA	2.50	0.42
1:G:98:LEU:HA	1:G:98:LEU:HD23	1.84	0.42
1:G:217:LYS:HE3	1:G:226:GLN:NE2	2.35	0.42
1:H:366:ARG:HD3	1:H:366:ARG:HA	1.74	0.42
1:K:108:GLY:HA2	1:K:308:ASN:ND2	2.35	0.42
1:K:117:LEU:CD1	1:L:260:PHE:CB	2.97	0.42
1:M:92:ASN:ND2	1:M:95:THR:H	2.17	0.42
1:N:74:ARG:HH22	1:N:440:ASP:CG	2.23	0.42
1:N:98:LEU:CD2	1:N:381:THR:HG22	2.50	0.42
1:B:92:ASN:HD21	1:B:94:GLU:HB2	1.84	0.42
1:D:201:VAL:H	1:D:201:VAL:HG22	1.60	0.42
1:E:99:VAL:HG21	1:E:382:ILE:HD11	2.01	0.42
1:E:151:TYR:CE2	1:E:221:PRO:HG2	2.54	0.42
1:G:235:LEU:HA	1:G:235:LEU:HD23	1.80	0.42
1:H:98:LEU:CD2	1:H:381:THR:HG22	2.50	0.42
1:H:160:GLY:HA2	1:H:247:PHE:CZ	2.55	0.42
1:H:258:ARG:HG3	1:H:259:HIS:ND1	2.34	0.42
1:I:216:THR:HG22	1:I:218:CYS:CB	2.46	0.42
1:K:98:LEU:CD2	1:K:381:THR:HG22	2.50	0.42
1:L:66:SER:H	1:L:69:GLN:NE2	2.18	0.42
1:A:271:VAL:HA	1:A:272:PRO:HD3	1.87	0.42
1:B:36:HIS:ND1	1:B:37:ALA:N	2.68	0.42
1:F:283:ARG:HD2	1:J:142:ASP:CG	2.40	0.42
1:F:306:LEU:O	1:F:311:TYR:OH	2.30	0.42
1:G:306:LEU:HA	1:G:306:LEU:HD12	1.77	0.42
1:H:260:PHE:CD2	1:H:260:PHE:N	2.87	0.42
1:K:42:LEU:H	1:K:42:LEU:HG	1.57	0.42
1:K:325:TRP:O	1:K:326:HIS:HB2	2.20	0.42
1:A:35:TYR:CE2	1:A:458:LEU:HG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ASP:OD2	1:A:459:ASP:N	2.51	0.41
1:B:325:TRP:O	1:B:326:HIS:HB2	2.19	0.41
1:C:143:VAL:O	1:C:143:VAL:CG1	2.63	0.41
1:D:372:ASP:OD2	1:D:372:ASP:C	2.58	0.41
1:F:385:THR:OG1	1:F:388:VAL:HG23	2.21	0.41
1:G:98:LEU:HD22	1:G:380:CYS:O	2.19	0.41
1:G:232:PRO:HB2	1:G:234:TYR:CZ	2.54	0.41
1:J:99:VAL:HG12	1:J:100:TRP:N	2.34	0.41
1:L:92:ASN:OD1	1:L:94:GLU:HB2	2.20	0.41
1:L:364:TYR:CE2	1:M:185:CYS:HB2	2.55	0.41
1:N:366:ARG:HD3	1:N:366:ARG:HA	1.72	0.41
1:B:71:ARG:HA	1:B:197:ASP:OD1	2.20	0.41
1:B:92:ASN:C	1:B:94:GLU:H	2.22	0.41
1:B:271:VAL:HA	1:B:272:PRO:HD3	1.86	0.41
1:C:105:VAL:CG1	1:C:106:GLU:N	2.81	0.41
1:H:42:LEU:HB3	1:H:448:TRP:CZ2	2.55	0.41
1:H:317:GLN:HG3	1:H:318:GLY:H	1.85	0.41
1:I:45:VAL:HG12	1:I:368:VAL:HG13	2.03	0.41
1:J:369:GLU:HG3	1:J:371:TYR:HE1	1.85	0.41
1:L:115:VAL:HG13	1:M:255:LEU:HD21	2.00	0.41
1:M:180:LEU:HD12	1:M:180:LEU:HA	1.89	0.41
1:M:216:THR:HG22	1:M:218:CYS:N	2.35	0.41
1:N:459:ASP:OD2	1:N:459:ASP:N	2.53	0.41
1:O:33:ILE:HD12	1:O:33:ILE:HG23	1.87	0.41
1:O:155:GLN:HA	1:O:334:VAL:O	2.21	0.41
1:O:201:VAL:HG11	1:O:334:VAL:HG11	2.02	0.41
1:B:90:ILE:O	1:B:90:ILE:HG22	2.20	0.41
1:C:33:ILE:HB	1:C:379:LEU:HB3	2.03	0.41
1:C:66:SER:O	1:C:69:GLN:HG2	2.20	0.41
1:C:138:ASN:C	1:C:140:SER:H	2.24	0.41
1:C:160:GLY:HA2	1:C:247:PHE:CZ	2.56	0.41
1:C:467:ARG:O	1:C:471:VAL:HG23	2.20	0.41
1:D:464:PRO:HA	1:D:467:ARG:NH1	2.35	0.41
1:H:105:VAL:HG12	1:H:106:GLU:N	2.35	0.41
1:H:214:GLN:OE1	1:H:219:GLU:HB2	2.20	0.41
1:H:320:ASN:C	1:H:320:ASN:OD1	2.58	0.41
1:H:353:PRO:HD2	1:H:360:LYS:CE	2.49	0.41
1:K:364:TYR:CE2	1:L:268:GLY:HA3	2.55	0.41
1:L:119:GLY:HA3	1:M:291:TYR:CZ	2.55	0.41
1:L:313:LEU:HD23	1:L:313:LEU:H	1.85	0.41
1:L:460:LEU:H	1:L:460:LEU:HG	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:347:SER:HA	1:M:361:PHE:HA	2.02	0.41
1:N:36:HIS:ND1	1:N:37:ALA:N	2.68	0.41
1:N:123:TYR:CG	1:N:147:VAL:HG22	2.56	0.41
1:A:65:VAL:O	1:A:367:HIS:HB3	2.21	0.41
1:A:260:PHE:HB3	1:E:117:LEU:HD13	2.02	0.41
1:A:324:CYS:SG	1:A:329:LEU:HD12	2.60	0.41
1:B:35:TYR:CZ	1:B:458:LEU:HD21	2.56	0.41
1:B:213:LEU:HA	1:B:213:LEU:HD12	1.81	0.41
1:C:460:LEU:H	1:C:460:LEU:HG	1.68	0.41
1:D:141:GLU:HG2	1:D:142:ASP:N	2.35	0.41
1:D:347:SER:HA	1:D:361:PHE:HA	2.02	0.41
1:E:36:HIS:ND1	1:E:36:HIS:C	2.74	0.41
1:E:258:ARG:HG3	1:E:259:HIS:ND1	2.36	0.41
1:F:138:ASN:ND2	1:F:140:SER:HB3	2.36	0.41
1:F:255:LEU:HD13	1:J:300:VAL:CG1	2.49	0.41
1:F:291:TYR:CD2	1:J:148:SER:HB3	2.55	0.41
1:F:374:GLN:OE1	1:F:465:LEU:HB2	2.20	0.41
1:G:316:ALA:CB	1:G:321:ASN:HA	2.50	0.41
1:G:351:PRO:O	1:G:352:VAL:HB	2.20	0.41
1:H:24:THR:HG21	1:H:320:ASN:HA	2.00	0.41
1:H:67:ALA:HB2	1:H:367:HIS:CE1	2.55	0.41
1:H:332:THR:O	1:H:333:VAL:HG23	2.20	0.41
1:H:332:THR:C	1:H:333:VAL:HG23	2.40	0.41
1:J:85:LEU:HB3	1:J:86:PRO:HD2	2.01	0.41
1:N:217:LYS:HE3	1:O:274:SER:O	2.21	0.41
1:O:125:LYS:HD2	1:O:261:TRP:NE1	2.36	0.41
1:B:333:VAL:HG11	1:B:371:TYR:HE2	1.85	0.41
1:C:92:ASN:HA	1:C:93:PRO:HD2	1.87	0.41
1:C:247:PHE:CE2	1:C:322:GLY:HA2	2.56	0.41
1:D:332:THR:C	1:D:333:VAL:HG23	2.40	0.41
1:F:140:SER:OG	1:F:141:GLU:N	2.53	0.41
1:G:105:VAL:CG1	1:G:106:GLU:N	2.83	0.41
1:G:384:LEU:HB3	1:G:389:MET:CE	2.51	0.41
1:H:51:ARG:O	1:H:53:PRO:CD	2.62	0.41
1:H:329:LEU:HD23	1:H:329:LEU:C	2.41	0.41
1:H:347:SER:HA	1:H:361:PHE:HA	2.03	0.41
1:J:151:TYR:OH	1:J:221:PRO:HB2	2.20	0.41
1:K:98:LEU:HD23	1:K:98:LEU:HA	1.88	0.41
1:L:249:CYS:O	1:L:250:LEU:HD12	2.21	0.41
1:L:262:ASN:HD22	1:L:262:ASN:HA	1.34	0.41
1:L:308:ASN:HD22	1:L:308:ASN:HA	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:42:LEU:H	1:N:42:LEU:HG	1.54	0.41
1:N:216:THR:CG2	1:N:218:CYS:HB2	2.51	0.41
1:N:247:PHE:CD2	1:N:322:GLY:HA2	2.53	0.41
1:O:42:LEU:HA	1:O:42:LEU:HD23	1.80	0.41
1:O:172:GLY:HA3	1:O:187:PRO:HG2	2.01	0.41
1:A:131:SER:O	1:A:132:SER:C	2.59	0.41
1:A:364:TYR:N	1:A:364:TYR:CD1	2.89	0.41
1:B:52:VAL:HB	1:B:62:ILE:HB	2.02	0.41
1:D:46:GLY:HA3	1:D:65:VAL:CG2	2.50	0.41
1:E:43:LEU:HD12	1:E:43:LEU:HA	1.84	0.41
1:F:141:GLU:O	1:F:141:GLU:CG	2.61	0.41
1:F:255:LEU:CD2	1:J:115:VAL:HG13	2.51	0.41
1:F:316:ALA:HB3	1:F:321:ASN:HA	2.03	0.41
1:H:224:ILE:HG21	1:H:224:ILE:HD13	1.77	0.41
1:I:163:PRO:HB2	1:I:194:VAL:HG13	2.02	0.41
1:I:216:THR:O	1:I:217:LYS:HB2	2.20	0.41
1:I:440:ASP:HB3	1:I:443:ASP:CG	2.41	0.41
1:L:254:GLN:O	1:L:255:LEU:HB3	2.21	0.41
1:L:300:VAL:CG1	1:M:255:LEU:HD13	2.50	0.41
1:M:156:LEU:HG	1:M:334:VAL:HB	2.03	0.41
1:N:464:PRO:HG2	1:N:465:LEU:H	1.86	0.41
1:N:470:LEU:HD23	1:N:470:LEU:HA	1.86	0.41
1:A:454:GLU:C	1:A:455:LYS:HG2	2.41	0.41
1:B:262:ASN:HD22	1:B:262:ASN:HA	1.37	0.41
1:B:275:LEU:HA	1:B:275:LEU:HD23	1.87	0.41
1:C:46:GLY:HA3	1:C:65:VAL:HG23	2.02	0.41
1:E:33:ILE:HG23	1:E:33:ILE:HD12	1.86	0.41
1:F:22:VAL:CG1	1:F:23:ASN:N	2.84	0.41
1:F:42:LEU:HA	1:F:42:LEU:HD23	1.71	0.41
1:F:308:ASN:HD22	1:F:308:ASN:HA	1.61	0.41
1:H:247:PHE:CD2	1:H:322:GLY:HA2	2.56	0.41
1:J:460:LEU:HD12	1:J:470:LEU:HD21	2.02	0.41
1:N:92:ASN:HA	1:N:93:PRO:HD2	1.84	0.41
1:N:109:ARG:NH2	1:N:369:GLU:OE1	2.53	0.41
1:N:260:PHE:CD2	1:N:260:PHE:N	2.86	0.41
1:N:467:ARG:O	1:N:470:LEU:HB2	2.21	0.41
1:O:156:LEU:C	1:O:156:LEU:HD12	2.41	0.41
1:A:201:VAL:O	1:A:203:THR:HG23	2.20	0.41
1:A:233:ASP:OD2	1:E:41:ARG:NH2	2.53	0.41
1:A:260:PHE:CD2	1:A:260:PHE:N	2.84	0.41
1:A:317:GLN:HG3	1:A:318:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:HIS:CG	1:C:37:ALA:N	2.88	0.41
1:D:109:ARG:HA	1:D:109:ARG:HD2	1.71	0.41
1:H:92:ASN:HD21	1:H:94:GLU:HB2	1.86	0.41
1:H:316:ALA:CB	1:H:321:ASN:HA	2.50	0.41
1:I:68:TYR:CZ	1:I:151:TYR:HB2	2.55	0.41
1:I:81:ASN:C	1:I:83:PHE:H	2.24	0.41
1:I:258:ARG:HG3	1:I:259:HIS:ND1	2.35	0.41
1:J:59:LYS:O	1:J:60:GLN:HB3	2.21	0.41
1:J:308:ASN:HD22	1:J:308:ASN:HA	1.63	0.41
1:K:139:VAL:HG12	1:K:139:VAL:O	2.20	0.41
1:L:24:THR:CG2	1:L:320:ASN:HA	2.50	0.41
1:N:150:ASP:O	1:N:296:SER:HA	2.21	0.41
1:N:389:MET:O	1:N:393:GLN:HB2	2.20	0.41
1:O:59:LYS:O	1:O:60:GLN:CB	2.69	0.41
1:O:307:PHE:O	1:O:308:ASN:HB2	2.20	0.41
1:A:463:TYR:O	1:A:467:ARG:HG3	2.20	0.41
1:B:51:ARG:O	1:B:53:PRO:HD3	2.21	0.41
1:B:156:LEU:HA	1:B:250:LEU:O	2.21	0.41
1:C:22:VAL:CG1	1:C:23:ASN:N	2.83	0.41
1:C:35:TYR:CE2	1:C:458:LEU:HG	2.55	0.41
1:C:96:GLN:NE2	1:C:383:THR:OG1	2.54	0.41
1:C:123:TYR:CB	1:C:147:VAL:HG22	2.50	0.41
1:D:76:GLN:HG3	1:D:453:LYS:HE3	2.03	0.41
1:F:46:GLY:HA3	1:F:65:VAL:CG2	2.51	0.41
1:F:52:VAL:HB	1:F:62:ILE:HB	2.03	0.41
1:F:59:LYS:O	1:F:60:GLN:HB3	2.19	0.41
1:F:120:HIS:HA	1:F:121:PRO:HD3	1.95	0.41
1:F:251:ARG:HH11	1:F:251:ARG:CG	2.34	0.41
1:G:62:ILE:HA	1:G:63:PRO:HD3	1.80	0.41
1:G:81:ASN:C	1:G:83:PHE:N	2.75	0.41
1:G:299:ILE:HA	1:H:256:PHE:HB3	2.02	0.41
1:H:125:LYS:HD2	1:H:261:TRP:CE2	2.56	0.41
1:H:126:LEU:HB3	1:H:262:ASN:HB2	2.03	0.41
1:H:163:PRO:HB2	1:H:194:VAL:HG13	2.03	0.41
1:H:311:TYR:CD1	1:H:311:TYR:N	2.89	0.41
1:H:376:ILE:HD12	1:H:376:ILE:HG23	1.66	0.41
1:I:87:ASP:O	1:I:90:ILE:HG12	2.21	0.41
1:I:109:ARG:NH2	1:I:369:GLU:OE1	2.54	0.41
1:J:42:LEU:HB3	1:J:448:TRP:CZ2	2.56	0.41
1:J:156:LEU:HD21	1:J:334:VAL:HG21	2.02	0.41
1:J:392:ILE:HG22	1:J:392:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:454:GLU:C	1:J:455:LYS:HG2	2.41	0.41
1:K:72:VAL:HG23	1:K:197:ASP:HA	2.03	0.41
1:K:79:ASP:O	1:K:83:PHE:HB2	2.20	0.41
1:L:98:LEU:HD21	1:L:381:THR:HG22	2.00	0.41
1:L:324:CYS:HB3	1:L:328:GLN:O	2.21	0.41
1:M:247:PHE:CE2	1:M:322:GLY:HA2	2.56	0.41
1:N:156:LEU:HD21	1:N:334:VAL:HG21	2.02	0.41
1:N:165:ILE:HD12	1:N:165:ILE:N	2.36	0.41
1:N:463:TYR:O	1:N:467:ARG:HG3	2.21	0.41
1:O:71:ARG:HG3	1:O:371:TYR:CZ	2.55	0.41
1:O:157:CYS:HA	1:O:332:THR:O	2.21	0.41
1:O:367:HIS:CE1	1:O:369:GLU:OE2	2.74	0.41
1:O:459:ASP:OD2	1:O:459:ASP:N	2.53	0.41
1:A:112:PRO:HB3	1:B:231:TYR:CG	2.55	0.41
1:A:293:PRO:HB3	1:E:117:LEU:CD1	2.44	0.41
1:B:113:LEU:HD22	1:C:253:GLU:HG3	2.03	0.41
1:D:119:GLY:HA2	1:D:148:SER:HA	2.03	0.41
1:E:128:ASP:O	1:E:132:SER:HB3	2.21	0.41
1:E:254:GLN:HE21	1:E:298:SER:H	1.69	0.41
1:F:130:GLU:OE1	1:J:258:ARG:NH1	2.54	0.41
1:G:127:ASP:HB2	1:G:136:THR:HG21	2.03	0.41
1:H:180:LEU:HD12	1:H:180:LEU:HA	1.90	0.41
1:H:464:PRO:O	1:H:465:LEU:C	2.58	0.41
1:J:99:VAL:HG11	1:J:323:VAL:HG13	2.03	0.41
1:L:151:TYR:OH	1:L:221:PRO:HB2	2.21	0.41
1:L:465:LEU:HA	1:L:465:LEU:HD23	1.91	0.41
1:M:140:SER:O	1:M:141:GLU:HB2	2.21	0.41
1:N:333:VAL:HG11	1:N:371:TYR:HE2	1.86	0.41
1:A:92:ASN:C	1:A:94:GLU:H	2.24	0.40
1:A:96:GLN:O	1:A:97:ARG:NH1	2.52	0.40
1:B:273:GLN:HE22	1:B:278:LYS:CE	2.02	0.40
1:D:159:LEU:HD21	1:D:331:VAL:HG22	2.01	0.40
1:E:43:LEU:HD12	1:E:369:GLU:O	2.21	0.40
1:E:143:VAL:O	1:E:143:VAL:CG1	2.66	0.40
1:F:41:ARG:O	1:F:41:ARG:HG2	2.19	0.40
1:G:67:ALA:HB2	1:G:367:HIS:CE1	2.56	0.40
1:H:77:LEU:HB3	1:H:78:PRO:HD2	2.04	0.40
1:I:92:ASN:O	1:I:92:ASN:CG	2.58	0.40
1:J:36:HIS:ND1	1:J:36:HIS:C	2.74	0.40
1:K:176:LYS:HB2	1:K:176:LYS:NZ	2.37	0.40
1:K:232:PRO:HB2	1:K:234:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:369:GLU:HG3	1:L:371:TYR:CE1	2.56	0.40
1:M:45:VAL:HG12	1:M:368:VAL:HG22	2.03	0.40
1:M:148:SER:HB3	1:N:291:TYR:CD2	2.56	0.40
1:M:357:ASP:O	1:M:358:ALA:C	2.60	0.40
1:O:237:MET:HB3	1:O:246:MET:HG2	2.03	0.40
1:A:196:GLU:N	1:A:199:ASP:OD2	2.32	0.40
1:A:470:LEU:HD23	1:A:470:LEU:HA	1.83	0.40
1:B:259:HIS:HE1	1:C:130:GLU:OE1	2.03	0.40
1:B:261:TRP:CZ3	1:B:294:SER:HB3	2.57	0.40
1:B:317:GLN:HG3	1:B:318:GLY:H	1.86	0.40
1:C:376:ILE:HG12	1:C:465:LEU:HD13	2.02	0.40
1:E:111:GLN:H	1:E:111:GLN:HG2	1.63	0.40
1:F:70:TYR:CE1	1:F:201:VAL:HG12	2.56	0.40
1:F:333:VAL:HG11	1:F:371:TYR:HE2	1.86	0.40
1:G:49:TYR:HA	1:G:223:ASP:HB3	2.04	0.40
1:G:396:ASN:HB3	1:G:399:ILE:HG13	2.02	0.40
1:H:22:VAL:HG12	1:H:23:ASN:H	1.86	0.40
1:I:24:THR:HG23	1:I:319:HIS:O	2.21	0.40
1:I:115:VAL:HG13	1:J:255:LEU:CD2	2.52	0.40
1:K:126:LEU:HG	1:K:127:ASP:OD2	2.22	0.40
1:K:171:LYS:HB2	1:K:213:LEU:CD1	2.51	0.40
1:K:368:VAL:CG1	1:L:169:TRP:CZ2	2.98	0.40
1:L:249:CYS:O	1:L:250:LEU:CD1	2.70	0.40
1:N:35:TYR:OH	1:N:86:PRO:HD3	2.21	0.40
1:N:158:ILE:HG21	1:N:158:ILE:HD13	1.83	0.40
1:N:242:TYR:CE2	1:N:395:MET:HG3	2.57	0.40
1:O:465:LEU:HA	1:O:465:LEU:HD23	1.69	0.40
1:A:156:LEU:HA	1:A:250:LEU:O	2.20	0.40
1:B:444:LYS:HA	1:B:444:LYS:HE2	2.03	0.40
1:D:21:VAL:HG12	1:D:22:VAL:N	2.35	0.40
1:D:384:LEU:HB3	1:D:389:MET:HE2	2.03	0.40
1:E:110:GLY:O	1:E:111:GLN:O	2.40	0.40
1:E:123:TYR:CD2	1:E:125:LYS:HB2	2.56	0.40
1:E:314:HIS:ND1	1:E:314:HIS:N	2.68	0.40
1:F:96:GLN:HB3	1:F:383:THR:HA	2.01	0.40
1:F:353:PRO:CD	1:F:360:LYS:NZ	2.84	0.40
1:G:36:HIS:ND1	1:G:36:HIS:C	2.75	0.40
1:G:396:ASN:O	1:G:399:ILE:HG13	2.22	0.40
1:H:254:GLN:O	1:H:255:LEU:HB3	2.21	0.40
1:H:376:ILE:HA	1:H:376:ILE:HD13	1.78	0.40
1:J:216:THR:O	1:J:217:LYS:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:366:ARG:HA	1:J:366:ARG:HD3	1.78	0.40
1:K:237:MET:HB3	1:K:246:MET:HG2	2.01	0.40
1:K:372:ASP:OD2	1:K:372:ASP:C	2.59	0.40
1:L:34:PHE:CE2	1:L:378:GLN:HB2	2.57	0.40
1:M:99:VAL:HG21	1:M:382:ILE:HD11	2.02	0.40
1:M:111:GLN:HB3	1:M:112:PRO:CD	2.42	0.40
1:N:216:THR:O	1:N:217:LYS:CB	2.69	0.40
1:A:70:TYR:CZ	1:A:201:VAL:HG12	2.56	0.40
1:A:267:MET:HE2	1:E:363:GLN:HB3	2.03	0.40
1:B:42:LEU:H	1:B:42:LEU:HG	1.58	0.40
1:B:157:CYS:HA	1:B:332:THR:O	2.22	0.40
1:E:242:TYR:CE2	1:E:395:MET:HG3	2.57	0.40
1:E:353:PRO:CG	1:E:360:LYS:HD2	2.52	0.40
1:F:118:SER:O	1:F:149:VAL:N	2.54	0.40
1:F:123:TYR:CG	1:F:147:VAL:CG2	3.05	0.40
1:F:220:VAL:HG23	1:F:225:CYS:HA	2.04	0.40
1:F:353:PRO:HG3	1:F:360:LYS:HD2	2.03	0.40
1:G:35:TYR:CZ	1:G:458:LEU:HD21	2.57	0.40
1:H:364:TYR:CD1	1:I:185:CYS:HB2	2.56	0.40
1:J:114:GLY:CA	1:J:340:THR:HG23	2.50	0.40
1:J:444:LYS:HE2	1:J:444:LYS:HA	2.02	0.40
1:L:368:VAL:CG1	1:L:369:GLU:N	2.83	0.40
1:M:31:THR:HG23	1:M:379:LEU:O	2.21	0.40
1:M:92:ASN:C	1:M:94:GLU:N	2.71	0.40
1:M:216:THR:O	1:M:217:LYS:CB	2.69	0.40
1:N:213:LEU:HD12	1:N:213:LEU:HA	1.57	0.40
1:B:163:PRO:HB2	1:B:194:VAL:HG13	2.03	0.40
1:B:349:GLN:HG3	1:B:360:LYS:HD2	2.03	0.40
1:C:159:LEU:HB2	1:C:248:PHE:HB3	2.03	0.40
1:C:275:LEU:HD23	1:C:275:LEU:HA	1.79	0.40
1:D:440:ASP:OD1	1:D:442:TYR:HB2	2.20	0.40
1:E:201:VAL:HG11	1:E:334:VAL:HG11	2.03	0.40
1:F:35:TYR:OH	1:F:86:PRO:HD3	2.22	0.40
1:F:156:LEU:HA	1:F:250:LEU:O	2.21	0.40
1:H:52:VAL:HA	1:H:53:PRO:HD2	1.81	0.40
1:H:171:LYS:HB2	1:H:213:LEU:CD1	2.52	0.40
1:I:143:VAL:HG12	1:I:143:VAL:O	2.20	0.40
1:I:180:LEU:HD12	1:I:180:LEU:HA	1.74	0.40
1:I:370:GLU:OE2	1:J:235:LEU:HD12	2.22	0.40
1:I:400:LEU:HD23	1:I:400:LEU:HA	1.92	0.40
1:J:88:THR:O	1:J:88:THR:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:157:CYS:HA	1:J:332:THR:O	2.21	0.40
1:J:375:PHE:O	1:J:376:ILE:HD13	2.21	0.40
1:L:107:ILE:HD12	1:L:107:ILE:N	2.37	0.40
1:L:300:VAL:H	1:L:300:VAL:HG12	1.63	0.40
1:M:126:LEU:HD12	1:M:126:LEU:HA	1.60	0.40
1:O:72:VAL:HG23	1:O:197:ASP:HA	2.04	0.40
1:O:109:ARG:N	1:O:308:ASN:HD21	2.12	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ASP:OD2	1:C:360:LYS:NZ[1_565]	2.12	0.08

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	419/428 (98%)	372 (89%)	34 (8%)	13 (3%)	4 23
1	B	419/428 (98%)	370 (88%)	34 (8%)	15 (4%)	3 21
1	C	419/428 (98%)	372 (89%)	36 (9%)	11 (3%)	5 26
1	D	419/428 (98%)	373 (89%)	38 (9%)	8 (2%)	8 31
1	E	419/428 (98%)	373 (89%)	34 (8%)	12 (3%)	4 24
1	F	419/428 (98%)	367 (88%)	43 (10%)	9 (2%)	7 30
1	G	419/428 (98%)	366 (87%)	42 (10%)	11 (3%)	5 26
1	H	419/428 (98%)	362 (86%)	46 (11%)	11 (3%)	5 26
1	I	419/428 (98%)	373 (89%)	32 (8%)	14 (3%)	4 22
1	J	419/428 (98%)	369 (88%)	39 (9%)	11 (3%)	5 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	419/428 (98%)	370 (88%)	39 (9%)	10 (2%)	6	28
1	L	419/428 (98%)	369 (88%)	36 (9%)	14 (3%)	4	22
1	M	419/428 (98%)	367 (88%)	37 (9%)	15 (4%)	3	21
1	N	419/428 (98%)	376 (90%)	30 (7%)	13 (3%)	4	23
1	O	419/428 (98%)	372 (89%)	38 (9%)	9 (2%)	7	30
All	All	6285/6420 (98%)	5551 (88%)	558 (9%)	176 (3%)	5	24

All (176) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	131	SER
1	A	135	ALA
1	B	59	LYS
1	B	131	SER
1	B	135	ALA
1	B	298	SER
1	C	40	SER
1	C	137	SER
1	D	59	LYS
1	D	139	VAL
1	E	55	GLY
1	E	135	ALA
1	F	59	LYS
1	F	131	SER
1	G	59	LYS
1	H	135	ALA
1	H	173	THR
1	I	55	GLY
1	I	59	LYS
1	I	137	SER
1	I	142	ASP
1	J	59	LYS
1	K	40	SER
1	K	131	SER
1	K	137	SER
1	K	139	VAL
1	L	54	ALA
1	L	55	GLY
1	L	59	LYS

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Mol	Chain	Res	Type
1	L	131	SER
1	L	142	ASP
1	M	55	GLY
1	M	59	LYS
1	O	137	SER
1	A	40	SER
1	A	56	GLY
1	A	139	VAL
1	A	296	SER
1	B	40	SER
1	B	132	SER
1	B	137	SER
1	B	461	ASP
1	C	55	GLY
1	C	82	LYS
1	C	139	VAL
1	C	142	ASP
1	D	135	ALA
1	D	137	SER
1	E	131	SER
1	F	55	GLY
1	F	135	ALA
1	F	139	VAL
1	F	140	SER
1	G	40	SER
1	G	55	GLY
1	H	40	SER
1	H	54	ALA
1	H	139	VAL
1	I	93	PRO
1	I	131	SER
1	J	139	VAL
1	J	140	SER
1	J	142	ASP
1	K	54	ALA
1	K	55	GLY
1	K	142	ASP
1	L	137	SER
1	M	54	ALA
1	M	137	SER
1	M	142	ASP
1	M	461	ASP

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Mol	Chain	Res	Type
1	N	55	GLY
1	N	137	SER
1	N	142	ASP
1	O	55	GLY
1	O	59	LYS
1	O	139	VAL
1	O	142	ASP
1	O	298	SER
1	A	54	ALA
1	A	60	GLN
1	A	141	GLU
1	C	59	LYS
1	C	93	PRO
1	C	140	SER
1	C	298	SER
1	D	93	PRO
1	E	40	SER
1	E	59	LYS
1	F	222	LEU
1	G	131	SER
1	G	141	GLU
1	G	298	SER
1	H	140	SER
1	H	296	SER
1	H	298	SER
1	I	139	VAL
1	I	298	SER
1	J	40	SER
1	J	131	SER
1	J	464	PRO
1	K	59	LYS
1	K	135	ALA
1	L	40	SER
1	M	40	SER
1	M	93	PRO
1	M	131	SER
1	M	139	VAL
1	N	59	LYS
1	N	93	PRO
1	N	135	ALA
1	N	298	SER
1	A	57	GLY

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Mol	Chain	Res	Type
1	A	82	LYS
1	B	55	GLY
1	C	131	SER
1	D	55	GLY
1	D	298	SER
1	E	111	GLN
1	E	137	SER
1	E	139	VAL
1	E	217	LYS
1	E	298	SER
1	G	82	LYS
1	G	93	PRO
1	I	40	SER
1	I	464	PRO
1	J	134	ALA
1	K	140	SER
1	L	132	SER
1	L	134	ALA
1	M	126	LEU
1	M	141	GLU
1	N	40	SER
1	N	134	ALA
1	B	54	ALA
1	B	82	LYS
1	B	139	VAL
1	B	386	ALA
1	D	131	SER
1	E	54	ALA
1	E	93	PRO
1	G	386	ALA
1	I	54	ALA
1	I	140	SER
1	I	461	ASP
1	J	386	ALA
1	L	139	VAL
1	L	141	GLU
1	L	298	SER
1	M	60	GLN
1	M	135	ALA
1	M	464	PRO
1	N	54	ALA
1	N	139	VAL

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Mol	Chain	Res	Type
1	N	386	ALA
1	O	40	SER
1	F	60	GLN
1	F	386	ALA
1	G	139	VAL
1	G	461	ASP
1	H	93	PRO
1	H	179	PRO
1	I	134	ALA
1	J	296	SER
1	L	60	GLN
1	O	82	LYS
1	O	296	SER
1	B	464	PRO
1	J	111	GLN
1	N	464	PRO
1	A	464	PRO
1	B	111	GLN
1	H	464	PRO
1	L	93	PRO

5.3.2 Protein sidechains (i)

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	370/371 (100%)	331 (90%)	39 (10%)	7 25
1	B	370/371 (100%)	339 (92%)	31 (8%)	11 36
1	C	370/371 (100%)	334 (90%)	36 (10%)	8 28
1	D	370/371 (100%)	337 (91%)	33 (9%)	9 33
1	E	370/371 (100%)	337 (91%)	33 (9%)	9 33
1	F	370/371 (100%)	332 (90%)	38 (10%)	7 26
1	G	370/371 (100%)	334 (90%)	36 (10%)	8 28
1	H	370/371 (100%)	335 (90%)	35 (10%)	8 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	370/371 (100%)	337 (91%)	33 (9%)	9	33
1	J	370/371 (100%)	335 (90%)	35 (10%)	8	29
1	K	370/371 (100%)	331 (90%)	39 (10%)	7	25
1	L	370/371 (100%)	330 (89%)	40 (11%)	6	24
1	M	370/371 (100%)	335 (90%)	35 (10%)	8	29
1	N	370/371 (100%)	333 (90%)	37 (10%)	7	27
1	O	370/371 (100%)	338 (91%)	32 (9%)	10	35
All	All	5550/5565 (100%)	5018 (90%)	532 (10%)	8	29

All (532) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	29	THR
1	A	40	SER
1	A	48	PRO
1	A	51	ARG
1	A	60	GLN
1	A	61	ASP
1	A	91	TYR
1	A	96	GLN
1	A	99	VAL
1	A	127	ASP
1	A	157	CYS
1	A	173	THR
1	A	176	LYS
1	A	178	ARG
1	A	188	LEU
1	A	193	THR
1	A	222	LEU
1	A	227	SER
1	A	247	PHE
1	A	249	CYS
1	A	250	LEU
1	A	251	ARG
1	A	255	LEU
1	A	262	ASN
1	A	272	PRO
1	A	293	PRO
1	A	301	THR

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Mol	Chain	Res	Type
1	A	311	TYR
1	A	313	LEU
1	A	317	GLN
1	A	340	THR
1	A	372	ASP
1	A	387	ASP
1	A	396	ASN
1	A	459	ASP
1	A	465	LEU
1	A	472	GLN
1	A	475	LEU
1	B	23	ASN
1	B	29	THR
1	B	48	PRO
1	B	91	TYR
1	B	96	GLN
1	B	127	ASP
1	B	138	ASN
1	B	176	LYS
1	B	178	ARG
1	B	193	THR
1	B	213	LEU
1	B	222	LEU
1	B	227	SER
1	B	247	PHE
1	B	249	CYS
1	B	250	LEU
1	B	251	ARG
1	B	255	LEU
1	B	262	ASN
1	B	293	PRO
1	B	301	THR
1	B	311	TYR
1	B	313	LEU
1	B	317	GLN
1	B	340	THR
1	B	372	ASP
1	B	396	ASN
1	B	459	ASP
1	B	465	LEU
1	B	472	GLN
1	B	475	LEU

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Mol	Chain	Res	Type
1	C	23	ASN
1	C	36	HIS
1	C	60	GLN
1	C	91	TYR
1	C	99	VAL
1	C	127	ASP
1	C	133	HIS
1	C	142	ASP
1	C	176	LYS
1	C	178	ARG
1	C	193	THR
1	C	213	LEU
1	C	222	LEU
1	C	225	CYS
1	C	247	PHE
1	C	249	CYS
1	C	250	LEU
1	C	251	ARG
1	C	255	LEU
1	C	256	PHE
1	C	262	ASN
1	C	301	THR
1	C	308	ASN
1	C	310	PRO
1	C	311	TYR
1	C	313	LEU
1	C	317	GLN
1	C	327	ASN
1	C	328	GLN
1	C	340	THR
1	C	372	ASP
1	C	387	ASP
1	C	396	ASN
1	C	459	ASP
1	C	465	LEU
1	C	475	LEU
1	D	23	ASN
1	D	29	THR
1	D	48	PRO
1	D	51	ARG
1	D	91	TYR
1	D	96	GLN

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Mol	Chain	Res	Type
1	D	127	ASP
1	D	173	THR
1	D	176	LYS
1	D	193	THR
1	D	213	LEU
1	D	222	LEU
1	D	227	SER
1	D	247	PHE
1	D	249	CYS
1	D	251	ARG
1	D	255	LEU
1	D	258	ARG
1	D	262	ASN
1	D	300	VAL
1	D	301	THR
1	D	311	TYR
1	D	313	LEU
1	D	317	GLN
1	D	327	ASN
1	D	340	THR
1	D	360	LYS
1	D	372	ASP
1	D	396	ASN
1	D	439	LYS
1	D	459	ASP
1	D	465	LEU
1	D	475	LEU
1	E	23	ASN
1	E	29	THR
1	E	53	PRO
1	E	60	GLN
1	E	91	TYR
1	E	96	GLN
1	E	127	ASP
1	E	133	HIS
1	E	176	LYS
1	E	178	ARG
1	E	187	PRO
1	E	193	THR
1	E	222	LEU
1	E	247	PHE
1	E	249	CYS

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Mol	Chain	Res	Type
1	E	251	ARG
1	E	255	LEU
1	E	258	ARG
1	E	262	ASN
1	E	272	PRO
1	E	301	THR
1	E	311	TYR
1	E	313	LEU
1	E	317	GLN
1	E	327	ASN
1	E	328	GLN
1	E	340	THR
1	E	372	ASP
1	E	387	ASP
1	E	396	ASN
1	E	459	ASP
1	E	465	LEU
1	E	475	LEU
1	F	23	ASN
1	F	29	THR
1	F	36	HIS
1	F	44	THR
1	F	51	ARG
1	F	60	GLN
1	F	91	TYR
1	F	96	GLN
1	F	99	VAL
1	F	112	PRO
1	F	154	THR
1	F	157	CYS
1	F	173	THR
1	F	176	LYS
1	F	178	ARG
1	F	193	THR
1	F	213	LEU
1	F	222	LEU
1	F	227	SER
1	F	246	MET
1	F	247	PHE
1	F	251	ARG
1	F	255	LEU
1	F	262	ASN

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Mol	Chain	Res	Type
1	F	301	THR
1	F	308	ASN
1	F	311	TYR
1	F	313	LEU
1	F	317	GLN
1	F	327	ASN
1	F	328	GLN
1	F	340	THR
1	F	372	ASP
1	F	396	ASN
1	F	459	ASP
1	F	465	LEU
1	F	472	GLN
1	F	475	LEU
1	G	23	ASN
1	G	40	SER
1	G	47	ASP
1	G	88	THR
1	G	91	TYR
1	G	92	ASN
1	G	96	GLN
1	G	118	SER
1	G	127	ASP
1	G	157	CYS
1	G	176	LYS
1	G	178	ARG
1	G	193	THR
1	G	213	LEU
1	G	222	LEU
1	G	227	SER
1	G	232	PRO
1	G	247	PHE
1	G	249	CYS
1	G	251	ARG
1	G	255	LEU
1	G	262	ASN
1	G	295	PRO
1	G	301	THR
1	G	308	ASN
1	G	311	TYR
1	G	313	LEU
1	G	317	GLN

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Mol	Chain	Res	Type
1	G	327	ASN
1	G	340	THR
1	G	372	ASP
1	G	387	ASP
1	G	396	ASN
1	G	459	ASP
1	G	465	LEU
1	G	475	LEU
1	H	23	ASN
1	H	36	HIS
1	H	51	ARG
1	H	53	PRO
1	H	60	GLN
1	H	91	TYR
1	H	127	ASP
1	H	173	THR
1	H	176	LYS
1	H	178	ARG
1	H	193	THR
1	H	222	LEU
1	H	225	CYS
1	H	227	SER
1	H	247	PHE
1	H	249	CYS
1	H	250	LEU
1	H	251	ARG
1	H	255	LEU
1	H	258	ARG
1	H	262	ASN
1	H	301	THR
1	H	311	TYR
1	H	313	LEU
1	H	317	GLN
1	H	340	THR
1	H	365	SER
1	H	366	ARG
1	H	372	ASP
1	H	387	ASP
1	H	396	ASN
1	H	459	ASP
1	H	465	LEU
1	H	472	GLN

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Mol	Chain	Res	Type
1	H	475	LEU
1	I	23	ASN
1	I	51	ARG
1	I	91	TYR
1	I	92	ASN
1	I	96	GLN
1	I	157	CYS
1	I	173	THR
1	I	176	LYS
1	I	178	ARG
1	I	193	THR
1	I	213	LEU
1	I	222	LEU
1	I	227	SER
1	I	232	PRO
1	I	247	PHE
1	I	249	CYS
1	I	251	ARG
1	I	255	LEU
1	I	262	ASN
1	I	272	PRO
1	I	293	PRO
1	I	301	THR
1	I	311	TYR
1	I	313	LEU
1	I	317	GLN
1	I	327	ASN
1	I	340	THR
1	I	372	ASP
1	I	396	ASN
1	I	398	SER
1	I	459	ASP
1	I	465	LEU
1	I	475	LEU
1	J	23	ASN
1	J	51	ARG
1	J	91	TYR
1	J	92	ASN
1	J	96	GLN
1	J	112	PRO
1	J	127	ASP
1	J	157	CYS

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Mol	Chain	Res	Type
1	J	176	LYS
1	J	178	ARG
1	J	187	PRO
1	J	213	LEU
1	J	222	LEU
1	J	225	CYS
1	J	236	GLN
1	J	247	PHE
1	J	249	CYS
1	J	251	ARG
1	J	255	LEU
1	J	258	ARG
1	J	262	ASN
1	J	293	PRO
1	J	301	THR
1	J	311	TYR
1	J	313	LEU
1	J	317	GLN
1	J	340	THR
1	J	372	ASP
1	J	387	ASP
1	J	396	ASN
1	J	401	GLU
1	J	459	ASP
1	J	465	LEU
1	J	472	GLN
1	J	475	LEU
1	K	23	ASN
1	K	29	THR
1	K	36	HIS
1	K	51	ARG
1	K	60	GLN
1	K	91	TYR
1	K	92	ASN
1	K	96	GLN
1	K	112	PRO
1	K	127	ASP
1	K	157	CYS
1	K	176	LYS
1	K	178	ARG
1	K	184	ASP
1	K	193	THR

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Mol	Chain	Res	Type
1	K	222	LEU
1	K	236	GLN
1	K	247	PHE
1	K	249	CYS
1	K	250	LEU
1	K	251	ARG
1	K	255	LEU
1	K	262	ASN
1	K	272	PRO
1	K	293	PRO
1	K	301	THR
1	K	308	ASN
1	K	311	TYR
1	K	313	LEU
1	K	317	GLN
1	K	327	ASN
1	K	328	GLN
1	K	340	THR
1	K	366	ARG
1	K	372	ASP
1	K	396	ASN
1	K	459	ASP
1	K	465	LEU
1	K	475	LEU
1	L	23	ASN
1	L	36	HIS
1	L	60	GLN
1	L	91	TYR
1	L	92	ASN
1	L	96	GLN
1	L	127	ASP
1	L	142	ASP
1	L	173	THR
1	L	176	LYS
1	L	178	ARG
1	L	187	PRO
1	L	193	THR
1	L	201	VAL
1	L	222	LEU
1	L	225	CYS
1	L	227	SER
1	L	247	PHE

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Mol	Chain	Res	Type
1	L	249	CYS
1	L	250	LEU
1	L	251	ARG
1	L	255	LEU
1	L	262	ASN
1	L	270	THR
1	L	272	PRO
1	L	293	PRO
1	L	301	THR
1	L	311	TYR
1	L	313	LEU
1	L	317	GLN
1	L	328	GLN
1	L	340	THR
1	L	372	ASP
1	L	387	ASP
1	L	396	ASN
1	L	398	SER
1	L	459	ASP
1	L	465	LEU
1	L	472	GLN
1	L	475	LEU
1	M	23	ASN
1	M	29	THR
1	M	51	ARG
1	M	60	GLN
1	M	80	PRO
1	M	91	TYR
1	M	92	ASN
1	M	96	GLN
1	M	99	VAL
1	M	127	ASP
1	M	139	VAL
1	M	173	THR
1	M	176	LYS
1	M	178	ARG
1	M	193	THR
1	M	222	LEU
1	M	247	PHE
1	M	249	CYS
1	M	251	ARG
1	M	255	LEU

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Mol	Chain	Res	Type
1	M	262	ASN
1	M	270	THR
1	M	301	THR
1	M	311	TYR
1	M	313	LEU
1	M	317	GLN
1	M	327	ASN
1	M	340	THR
1	M	372	ASP
1	M	387	ASP
1	M	396	ASN
1	M	459	ASP
1	M	465	LEU
1	M	472	GLN
1	M	475	LEU
1	N	23	ASN
1	N	60	GLN
1	N	91	TYR
1	N	96	GLN
1	N	127	ASP
1	N	157	CYS
1	N	159	LEU
1	N	173	THR
1	N	176	LYS
1	N	178	ARG
1	N	201	VAL
1	N	213	LEU
1	N	222	LEU
1	N	225	CYS
1	N	247	PHE
1	N	249	CYS
1	N	250	LEU
1	N	251	ARG
1	N	255	LEU
1	N	262	ASN
1	N	272	PRO
1	N	300	VAL
1	N	301	THR
1	N	311	TYR
1	N	313	LEU
1	N	317	GLN
1	N	327	ASN

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Mol	Chain	Res	Type
1	N	340	THR
1	N	355	GLN
1	N	372	ASP
1	N	387	ASP
1	N	396	ASN
1	N	459	ASP
1	N	461	ASP
1	N	465	LEU
1	N	472	GLN
1	N	475	LEU
1	O	23	ASN
1	O	36	HIS
1	O	47	ASP
1	O	51	ARG
1	O	91	TYR
1	O	127	ASP
1	O	157	CYS
1	O	176	LYS
1	O	178	ARG
1	O	187	PRO
1	O	201	VAL
1	O	213	LEU
1	O	222	LEU
1	O	225	CYS
1	O	247	PHE
1	O	249	CYS
1	O	251	ARG
1	O	255	LEU
1	O	258	ARG
1	O	262	ASN
1	O	293	PRO
1	O	301	THR
1	O	311	TYR
1	O	313	LEU
1	O	317	GLN
1	O	340	THR
1	O	365	SER
1	O	372	ASP
1	O	396	ASN
1	O	459	ASP
1	O	465	LEU
1	O	475	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (221) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	138	ASN
1	A	153	GLN
1	A	182	GLN
1	A	254	GLN
1	A	262	ASN
1	A	273	GLN
1	A	308	ASN
1	A	317	GLN
1	A	341	ASN
1	A	363	GLN
1	A	367	HIS
1	A	396	ASN
1	A	462	GLN
1	B	69	GLN
1	B	96	GLN
1	B	138	ASN
1	B	153	GLN
1	B	182	GLN
1	B	259	HIS
1	B	262	ASN
1	B	273	GLN
1	B	308	ASN
1	B	317	GLN
1	B	341	ASN
1	B	363	GLN
1	B	367	HIS
1	B	396	ASN
1	C	69	GLN
1	C	96	GLN
1	C	138	ASN
1	C	153	GLN
1	C	182	GLN
1	C	262	ASN
1	C	273	GLN
1	C	308	ASN
1	C	317	GLN
1	C	341	ASN
1	C	355	GLN
1	C	363	GLN
1	C	367	HIS

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Mol	Chain	Res	Type
1	C	396	ASN
1	D	69	GLN
1	D	138	ASN
1	D	153	GLN
1	D	182	GLN
1	D	262	ASN
1	D	273	GLN
1	D	308	ASN
1	D	317	GLN
1	D	341	ASN
1	D	363	GLN
1	D	367	HIS
1	D	396	ASN
1	D	462	GLN
1	E	69	GLN
1	E	96	GLN
1	E	138	ASN
1	E	153	GLN
1	E	182	GLN
1	E	254	GLN
1	E	262	ASN
1	E	273	GLN
1	E	308	ASN
1	E	317	GLN
1	E	321	ASN
1	E	341	ASN
1	E	363	GLN
1	E	367	HIS
1	E	396	ASN
1	E	462	GLN
1	F	69	GLN
1	F	96	GLN
1	F	138	ASN
1	F	153	GLN
1	F	182	GLN
1	F	254	GLN
1	F	262	ASN
1	F	273	GLN
1	F	308	ASN
1	F	317	GLN
1	F	326	HIS
1	F	341	ASN

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Mol	Chain	Res	Type
1	F	363	GLN
1	F	367	HIS
1	F	396	ASN
1	G	69	GLN
1	G	138	ASN
1	G	153	GLN
1	G	182	GLN
1	G	254	GLN
1	G	262	ASN
1	G	273	GLN
1	G	308	ASN
1	G	317	GLN
1	G	341	ASN
1	G	363	GLN
1	G	367	HIS
1	G	396	ASN
1	G	462	GLN
1	H	69	GLN
1	H	96	GLN
1	H	138	ASN
1	H	153	GLN
1	H	182	GLN
1	H	254	GLN
1	H	262	ASN
1	H	273	GLN
1	H	308	ASN
1	H	317	GLN
1	H	326	HIS
1	H	341	ASN
1	H	363	GLN
1	H	367	HIS
1	H	396	ASN
1	H	462	GLN
1	I	69	GLN
1	I	92	ASN
1	I	96	GLN
1	I	153	GLN
1	I	182	GLN
1	I	262	ASN
1	I	273	GLN
1	I	308	ASN
1	I	317	GLN

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Mol	Chain	Res	Type
1	I	341	ASN
1	I	363	GLN
1	I	367	HIS
1	I	393	GLN
1	I	396	ASN
1	I	462	GLN
1	J	69	GLN
1	J	96	GLN
1	J	138	ASN
1	J	153	GLN
1	J	182	GLN
1	J	254	GLN
1	J	259	HIS
1	J	262	ASN
1	J	273	GLN
1	J	308	ASN
1	J	317	GLN
1	J	341	ASN
1	J	363	GLN
1	J	367	HIS
1	J	396	ASN
1	J	462	GLN
1	K	69	GLN
1	K	96	GLN
1	K	138	ASN
1	K	153	GLN
1	K	182	GLN
1	K	254	GLN
1	K	262	ASN
1	K	273	GLN
1	K	308	ASN
1	K	317	GLN
1	K	341	ASN
1	K	363	GLN
1	K	367	HIS
1	K	396	ASN
1	L	69	GLN
1	L	96	GLN
1	L	138	ASN
1	L	182	GLN
1	L	254	GLN
1	L	262	ASN

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Mol	Chain	Res	Type
1	L	273	GLN
1	L	308	ASN
1	L	317	GLN
1	L	321	ASN
1	L	341	ASN
1	L	363	GLN
1	L	367	HIS
1	L	396	ASN
1	L	462	GLN
1	M	69	GLN
1	M	96	GLN
1	M	138	ASN
1	M	153	GLN
1	M	182	GLN
1	M	254	GLN
1	M	262	ASN
1	M	273	GLN
1	M	308	ASN
1	M	317	GLN
1	M	326	HIS
1	M	341	ASN
1	M	363	GLN
1	M	367	HIS
1	M	396	ASN
1	M	462	GLN
1	N	69	GLN
1	N	96	GLN
1	N	138	ASN
1	N	153	GLN
1	N	254	GLN
1	N	262	ASN
1	N	273	GLN
1	N	308	ASN
1	N	317	GLN
1	N	341	ASN
1	N	363	GLN
1	N	367	HIS
1	N	396	ASN
1	N	462	GLN
1	O	69	GLN
1	O	96	GLN
1	O	138	ASN

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Mol	Chain	Res	Type
1	O	153	GLN
1	O	182	GLN
1	O	262	ASN
1	O	273	GLN
1	O	308	ASN
1	O	317	GLN
1	O	326	HIS
1	O	341	ASN
1	O	363	GLN
1	O	367	HIS
1	O	396	ASN
1	O	462	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	423/428 (98%)	0.06	21 (4%)	28	29	16, 46, 103, 121	0
1	B	423/428 (98%)	-0.08	19 (4%)	33	33	19, 45, 101, 127	0
1	C	423/428 (98%)	0.08	20 (4%)	31	31	15, 45, 103, 123	0
1	D	423/428 (98%)	-0.15	10 (2%)	59	57	14, 44, 102, 126	0
1	E	423/428 (98%)	-0.19	10 (2%)	59	57	15, 45, 104, 123	0
1	F	423/428 (98%)	0.19	25 (5%)	22	23	19, 50, 105, 123	0
1	G	423/428 (98%)	0.16	22 (5%)	27	27	22, 50, 103, 127	0
1	H	423/428 (98%)	-0.10	14 (3%)	46	45	19, 46, 103, 124	0
1	I	423/428 (98%)	-0.13	13 (3%)	49	48	17, 45, 101, 123	0
1	J	423/428 (98%)	-0.08	17 (4%)	38	37	18, 46, 103, 123	0
1	K	423/428 (98%)	-0.14	11 (2%)	56	54	18, 44, 103, 122	0
1	L	423/428 (98%)	-0.01	20 (4%)	31	31	16, 46, 103, 122	0
1	M	423/428 (98%)	-0.04	20 (4%)	31	31	18, 46, 102, 126	0
1	N	423/428 (98%)	-0.11	18 (4%)	35	35	19, 45, 103, 125	0
1	O	423/428 (98%)	-0.03	17 (4%)	38	37	17, 46, 103, 126	0
All	All	6345/6420 (98%)	-0.04	257 (4%)	37	36	14, 46, 104, 127	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	ALA	7.8
1	D	133	HIS	7.7
1	M	57	GLY	7.5
1	O	134	ALA	7.1
1	N	86	PRO	7.1
1	C	138	ASN	6.9
1	N	135	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
1	J	133	HIS	6.1
1	O	136	THR	6.1
1	A	438	ASN	5.9
1	C	86	PRO	5.9
1	G	86	PRO	5.9
1	H	136	THR	5.8
1	D	135	ALA	5.8
1	E	86	PRO	5.8
1	N	84	GLY	5.8
1	A	138	ASN	5.8
1	O	138	ASN	5.7
1	G	438	ASN	5.6
1	M	138	ASN	5.5
1	K	58	ASN	5.5
1	H	438	ASN	5.5
1	G	136	THR	5.4
1	G	56	GLY	5.4
1	C	90	ILE	5.3
1	M	133	HIS	5.3
1	O	133	HIS	5.3
1	O	137	SER	5.2
1	F	88	THR	5.2
1	I	135	ALA	5.2
1	G	177	SER	5.0
1	F	86	PRO	4.9
1	F	87	ASP	4.9
1	H	134	ALA	4.9
1	L	58	ASN	4.8
1	G	88	THR	4.7
1	A	86	PRO	4.7
1	F	89	SER	4.7
1	G	135	ALA	4.5
1	L	57	GLY	4.4
1	A	85	LEU	4.4
1	C	174	ALA	4.4
1	O	135	ALA	4.3
1	O	139	VAL	4.3
1	A	87	ASP	4.3
1	J	137	SER	4.2
1	L	86	PRO	4.2
1	L	133	HIS	4.2
1	H	135	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	N	134	ALA	4.1
1	M	438	ASN	4.1
1	L	475	LEU	4.1
1	C	58	ASN	4.0
1	K	133	HIS	4.0
1	O	140	SER	4.0
1	O	86	PRO	3.9
1	F	174	ALA	3.9
1	H	89	SER	3.9
1	J	87	ASP	3.8
1	I	133	HIS	3.8
1	L	56	GLY	3.8
1	A	475	LEU	3.8
1	C	88	THR	3.7
1	K	438	ASN	3.7
1	H	140	SER	3.7
1	F	475	LEU	3.6
1	F	136	THR	3.6
1	A	174	ALA	3.6
1	A	439	LYS	3.6
1	D	177	SER	3.6
1	O	475	LEU	3.5
1	F	139	VAL	3.5
1	L	349	GLN	3.5
1	J	134	ALA	3.5
1	D	138	ASN	3.5
1	J	135	ALA	3.5
1	M	58	ASN	3.4
1	J	84	GLY	3.4
1	J	86	PRO	3.4
1	B	438	ASN	3.4
1	E	133	HIS	3.4
1	B	139	VAL	3.4
1	B	136	THR	3.4
1	L	90	ILE	3.4
1	G	475	LEU	3.4
1	I	138	ASN	3.3
1	I	134	ALA	3.3
1	H	141	GLU	3.3
1	C	57	GLY	3.3
1	M	175	SER	3.2
1	I	177	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	178	ARG	3.2
1	C	175	SER	3.2
1	E	90	ILE	3.2
1	F	133	HIS	3.2
1	I	58	ASN	3.2
1	N	88	THR	3.1
1	D	439	LYS	3.1
1	H	88	THR	3.1
1	L	439	LYS	3.1
1	I	350	SER	3.1
1	M	178	ARG	3.1
1	G	57	GLY	3.1
1	N	133	HIS	3.1
1	C	134	ALA	3.1
1	K	86	PRO	3.1
1	D	134	ALA	3.1
1	B	282	MET	3.0
1	A	133	HIS	3.0
1	E	438	ASN	3.0
1	G	141	GLU	3.0
1	M	135	ALA	3.0
1	H	133	HIS	3.0
1	B	179	PRO	3.0
1	L	88	THR	3.0
1	F	132	SER	3.0
1	B	56	GLY	3.0
1	N	180	LEU	3.0
1	B	175	SER	3.0
1	E	172	GLY	2.9
1	K	135	ALA	2.9
1	N	177	SER	2.9
1	L	136	THR	2.9
1	C	133	HIS	2.9
1	A	90	ILE	2.9
1	N	140	SER	2.9
1	E	135	ALA	2.9
1	B	178	ARG	2.9
1	B	57	GLY	2.8
1	F	57	GLY	2.8
1	O	87	ASP	2.8
1	E	88	THR	2.8
1	F	54	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	439	LYS	2.8
1	C	135	ALA	2.7
1	M	56	GLY	2.7
1	C	87	ASP	2.7
1	D	132	SER	2.7
1	C	384	LEU	2.7
1	D	136	THR	2.7
1	G	282	MET	2.7
1	L	176	LYS	2.7
1	C	136	THR	2.7
1	I	351	PRO	2.7
1	G	178	ARG	2.7
1	L	175	SER	2.6
1	A	56	GLY	2.6
1	C	177	SER	2.6
1	G	393	GLN	2.6
1	M	439	LYS	2.6
1	A	140	SER	2.6
1	D	137	SER	2.6
1	N	85	LEU	2.6
1	N	174	ALA	2.6
1	K	57	GLY	2.6
1	N	139	VAL	2.6
1	B	176	LYS	2.6
1	B	401	GLU	2.6
1	C	178	ARG	2.6
1	J	85	LEU	2.6
1	G	318	GLY	2.6
1	N	181	SER	2.6
1	M	314	HIS	2.6
1	B	174	ALA	2.5
1	J	56	GLY	2.5
1	J	438	ASN	2.5
1	J	475	LEU	2.5
1	H	173	THR	2.5
1	H	439	LYS	2.5
1	F	137	SER	2.5
1	L	87	ASP	2.5
1	A	399	ILE	2.5
1	F	176	LYS	2.5
1	O	438	ASN	2.5
1	L	135	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	355	GLN	2.5
1	F	60	GLN	2.5
1	B	133	HIS	2.5
1	O	174	ALA	2.4
1	J	131	SER	2.4
1	G	179	PRO	2.4
1	A	57	GLY	2.4
1	E	55	GLY	2.4
1	C	89	SER	2.4
1	I	84	GLY	2.4
1	B	173	THR	2.4
1	K	87	ASP	2.4
1	C	139	VAL	2.4
1	H	137	SER	2.4
1	M	282	MET	2.4
1	F	175	SER	2.3
1	J	177	SER	2.3
1	M	177	SER	2.3
1	F	59	LYS	2.3
1	D	175	SER	2.3
1	A	55	GLY	2.3
1	C	137	SER	2.3
1	B	350	SER	2.3
1	M	351	PRO	2.3
1	G	85	LEU	2.3
1	M	475	LEU	2.3
1	I	353	PRO	2.3
1	N	175	SER	2.3
1	I	438	ASN	2.3
1	G	58	ASN	2.3
1	O	474	GLY	2.3
1	C	140	SER	2.3
1	F	438	ASN	2.3
1	A	59	LYS	2.3
1	J	175	SER	2.3
1	F	130	GLU	2.2
1	J	57	GLY	2.2
1	M	95	THR	2.2
1	N	179	PRO	2.2
1	A	136	THR	2.2
1	F	179	PRO	2.2
1	I	87	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	134	ALA	2.2
1	K	176	LYS	2.2
1	N	172	GLY	2.2
1	E	394	SER	2.2
1	A	354	GLY	2.2
1	J	58	ASN	2.2
1	G	269	ASP	2.2
1	A	350	SER	2.2
1	H	132	SER	2.2
1	K	88	THR	2.1
1	F	56	GLY	2.1
1	N	58	ASN	2.1
1	G	175	SER	2.1
1	L	474	GLY	2.1
1	B	180	LEU	2.1
1	O	141	GLU	2.1
1	M	188	LEU	2.1
1	G	272	PRO	2.1
1	L	95	THR	2.1
1	L	354	GLY	2.1
1	A	137	SER	2.1
1	O	90	ILE	2.1
1	J	136	THR	2.1
1	H	350	SER	2.1
1	L	132	SER	2.1
1	G	180	LEU	2.1
1	O	176	LYS	2.1
1	M	88	THR	2.1
1	G	139	VAL	2.1
1	K	175	SER	2.1
1	M	136	THR	2.0
1	N	173	THR	2.0
1	B	182	GLN	2.0
1	B	184	ASP	2.0
1	F	100	TRP	2.0
1	F	285	SER	2.0
1	F	344	ILE	2.0
1	K	174	ALA	2.0
1	M	360	LYS	2.0
1	F	348	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.