Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 AM GMT

PDB ID	:	2R5J
Title	:	Pentamer Structure of Major Capsid protein L1 of Human Papilloma Virus Type 35
Authors	:	Bishop, B.; Dasgupta, J.; Chen, X.S.
Deposited on	:	2007-09-03
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

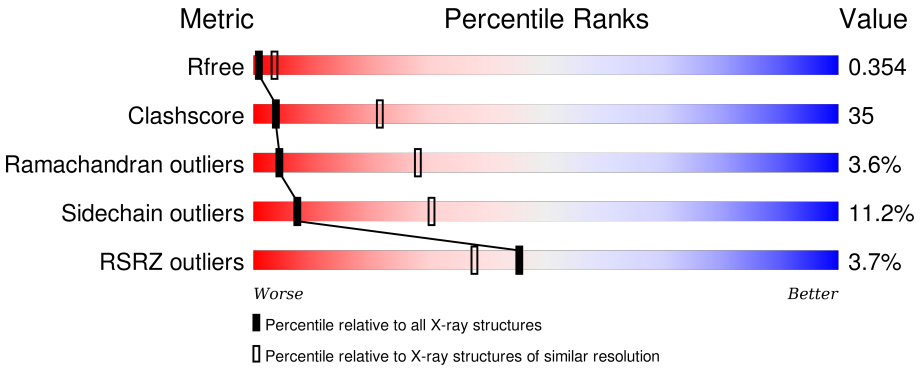
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	423	2% 36% 39% 22%
1	B	423	2% 34% 40% 20%
1	C	423	3% 30% 41% 23% 5%
1	D	423	4% 35% 40% 21%
1	E	423	3% 30% 44% 22%

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Mol	Chain	Length	Quality of chain
1	F	423	5% 34% 39% 22%
1	G	423	2% 33% 44% 20%
1	H	423	4% 34% 44% 17%
1	I	423	3% 30% 41% 24%
1	J	423	3% 33% 40% 23%
1	K	423	5% 28% 45% 23%
1	L	423	3% 34% 41% 22%
1	M	423	5% 29% 45% 22%
1	N	423	3% 33% 44% 19%
1	O	423	6% 30% 44% 20%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 49350 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	B	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	C	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	D	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	E	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	F	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	G	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	H	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	I	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	J	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	K	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	L	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	M	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	N	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			
1	O	417	Total	C	N	O	S	0	0	0
			3290	2089	551	630	20			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ALA	-	EXPRESSION TAG	UNP P27232
A	175	SER	CYS	ENGINEERED	UNP P27232
A	402	GLY	-	LINKER	UNP P27232
A	403	GLY	-	LINKER	UNP P27232
A	404	SER	-	LINKER	UNP P27232
A	405	GLY	-	LINKER	UNP P27232
A	406	GLY	-	LINKER	UNP P27232
B	20	ALA	-	EXPRESSION TAG	UNP P27232
B	175	SER	CYS	ENGINEERED	UNP P27232
B	402	GLY	-	LINKER	UNP P27232
B	403	GLY	-	LINKER	UNP P27232
B	404	SER	-	LINKER	UNP P27232
B	405	GLY	-	LINKER	UNP P27232
B	406	GLY	-	LINKER	UNP P27232
C	20	ALA	-	EXPRESSION TAG	UNP P27232
C	175	SER	CYS	ENGINEERED	UNP P27232
C	402	GLY	-	LINKER	UNP P27232
C	403	GLY	-	LINKER	UNP P27232
C	404	SER	-	LINKER	UNP P27232
C	405	GLY	-	LINKER	UNP P27232
C	406	GLY	-	LINKER	UNP P27232
D	20	ALA	-	EXPRESSION TAG	UNP P27232
D	175	SER	CYS	ENGINEERED	UNP P27232
D	402	GLY	-	LINKER	UNP P27232
D	403	GLY	-	LINKER	UNP P27232
D	404	SER	-	LINKER	UNP P27232
D	405	GLY	-	LINKER	UNP P27232
D	406	GLY	-	LINKER	UNP P27232
E	20	ALA	-	EXPRESSION TAG	UNP P27232
E	175	SER	CYS	ENGINEERED	UNP P27232
E	402	GLY	-	LINKER	UNP P27232
E	403	GLY	-	LINKER	UNP P27232
E	404	SER	-	LINKER	UNP P27232
E	405	GLY	-	LINKER	UNP P27232
E	406	GLY	-	LINKER	UNP P27232
F	20	ALA	-	EXPRESSION TAG	UNP P27232
F	175	SER	CYS	ENGINEERED	UNP P27232
F	402	GLY	-	LINKER	UNP P27232
F	403	GLY	-	LINKER	UNP P27232
F	404	SER	-	LINKER	UNP P27232
F	405	GLY	-	LINKER	UNP P27232
F	406	GLY	-	LINKER	UNP P27232
G	20	ALA	-	EXPRESSION TAG	UNP P27232

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Chain	Residue	Modelled	Actual	Comment	Reference
G	175	SER	CYS	ENGINEERED	UNP P27232
G	402	GLY	-	LINKER	UNP P27232
G	403	GLY	-	LINKER	UNP P27232
G	404	SER	-	LINKER	UNP P27232
G	405	GLY	-	LINKER	UNP P27232
G	406	GLY	-	LINKER	UNP P27232
H	20	ALA	-	EXPRESSION TAG	UNP P27232
H	175	SER	CYS	ENGINEERED	UNP P27232
H	402	GLY	-	LINKER	UNP P27232
H	403	GLY	-	LINKER	UNP P27232
H	404	SER	-	LINKER	UNP P27232
H	405	GLY	-	LINKER	UNP P27232
H	406	GLY	-	LINKER	UNP P27232
I	20	ALA	-	EXPRESSION TAG	UNP P27232
I	175	SER	CYS	ENGINEERED	UNP P27232
I	402	GLY	-	LINKER	UNP P27232
I	403	GLY	-	LINKER	UNP P27232
I	404	SER	-	LINKER	UNP P27232
I	405	GLY	-	LINKER	UNP P27232
I	406	GLY	-	LINKER	UNP P27232
J	20	ALA	-	EXPRESSION TAG	UNP P27232
J	175	SER	CYS	ENGINEERED	UNP P27232
J	402	GLY	-	LINKER	UNP P27232
J	403	GLY	-	LINKER	UNP P27232
J	404	SER	-	LINKER	UNP P27232
J	405	GLY	-	LINKER	UNP P27232
J	406	GLY	-	LINKER	UNP P27232
K	20	ALA	-	EXPRESSION TAG	UNP P27232
K	175	SER	CYS	ENGINEERED	UNP P27232
K	402	GLY	-	LINKER	UNP P27232
K	403	GLY	-	LINKER	UNP P27232
K	404	SER	-	LINKER	UNP P27232
K	405	GLY	-	LINKER	UNP P27232
K	406	GLY	-	LINKER	UNP P27232
L	20	ALA	-	EXPRESSION TAG	UNP P27232
L	175	SER	CYS	ENGINEERED	UNP P27232
L	402	GLY	-	LINKER	UNP P27232
L	403	GLY	-	LINKER	UNP P27232
L	404	SER	-	LINKER	UNP P27232
L	405	GLY	-	LINKER	UNP P27232
L	406	GLY	-	LINKER	UNP P27232
M	20	ALA	-	EXPRESSION TAG	UNP P27232

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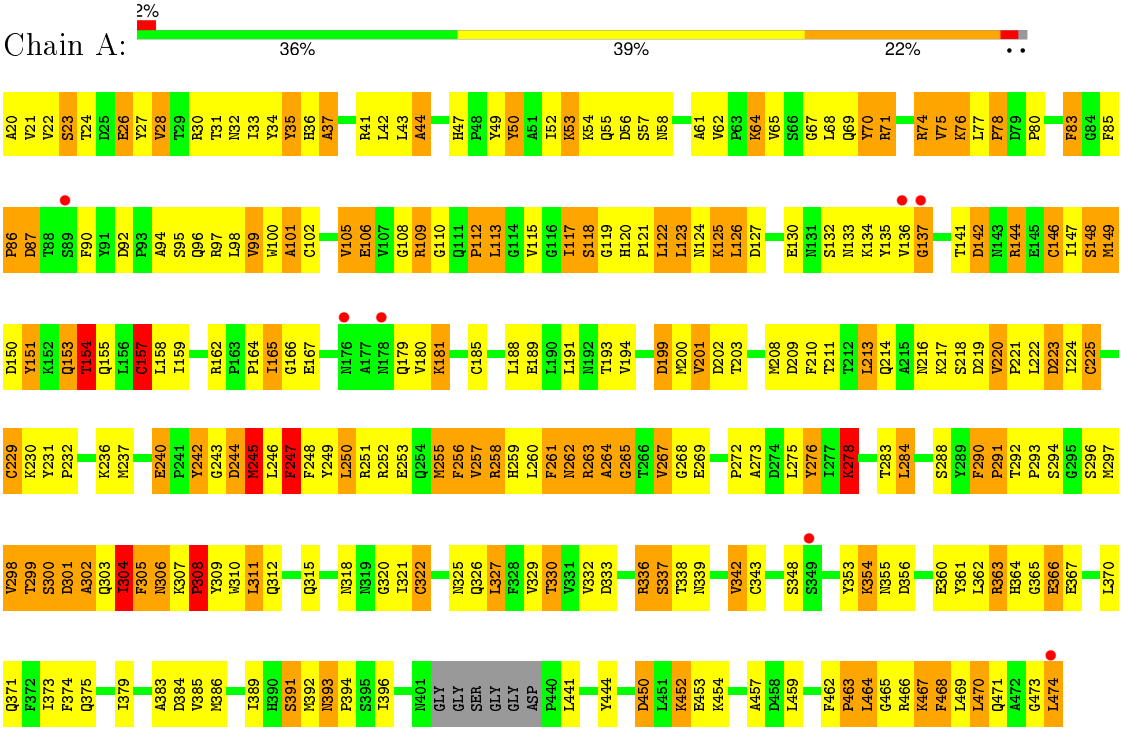
Chain	Residue	Modelled	Actual	Comment	Reference
M	175	SER	CYS	ENGINEERED	UNP P27232
M	402	GLY	-	LINKER	UNP P27232
M	403	GLY	-	LINKER	UNP P27232
M	404	SER	-	LINKER	UNP P27232
M	405	GLY	-	LINKER	UNP P27232
M	406	GLY	-	LINKER	UNP P27232
N	20	ALA	-	EXPRESSION TAG	UNP P27232
N	175	SER	CYS	ENGINEERED	UNP P27232
N	402	GLY	-	LINKER	UNP P27232
N	403	GLY	-	LINKER	UNP P27232
N	404	SER	-	LINKER	UNP P27232
N	405	GLY	-	LINKER	UNP P27232
N	406	GLY	-	LINKER	UNP P27232
O	20	ALA	-	EXPRESSION TAG	UNP P27232
O	175	SER	CYS	ENGINEERED	UNP P27232
O	402	GLY	-	LINKER	UNP P27232
O	403	GLY	-	LINKER	UNP P27232
O	404	SER	-	LINKER	UNP P27232
O	405	GLY	-	LINKER	UNP P27232
O	406	GLY	-	LINKER	UNP P27232

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

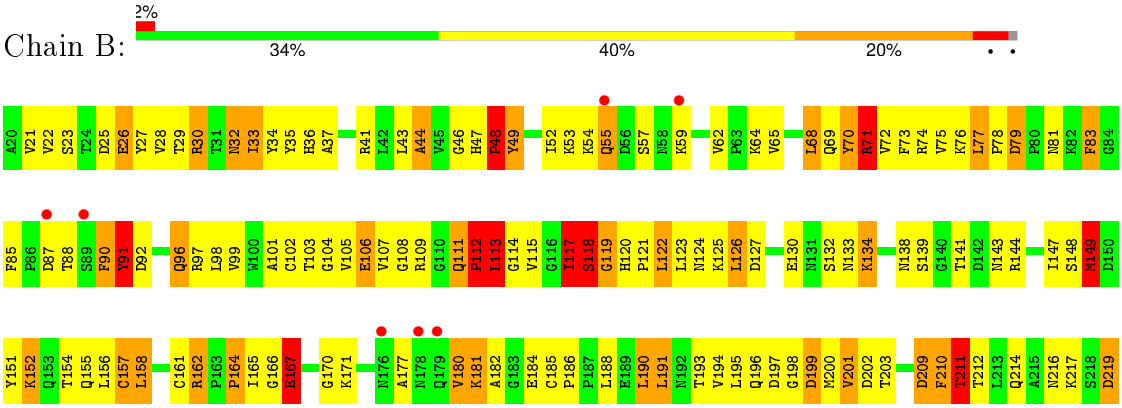
- Molecule 1: Major capsid protein L1

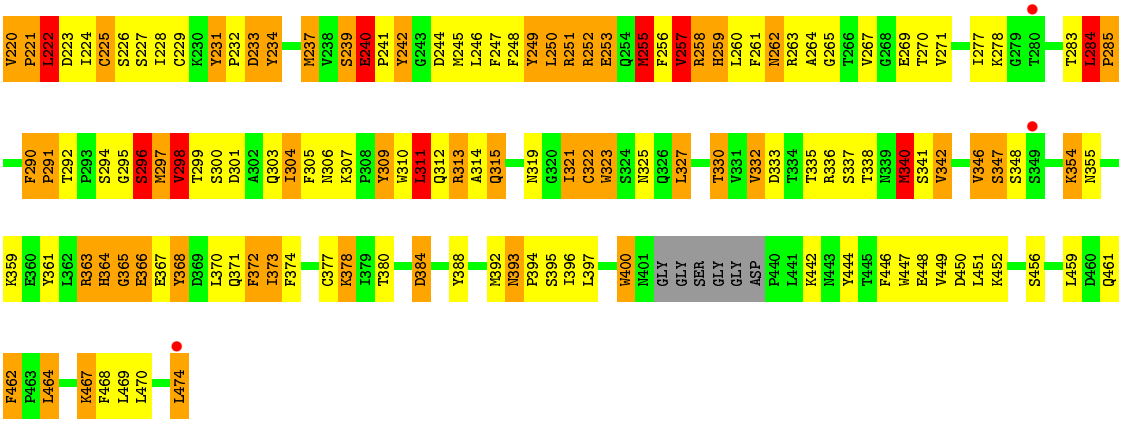
Chain A:



- Molecule 1: Major capsid protein L1

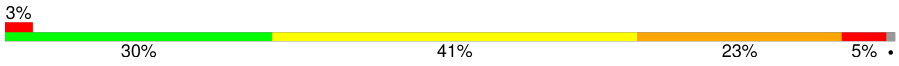
Chain B:

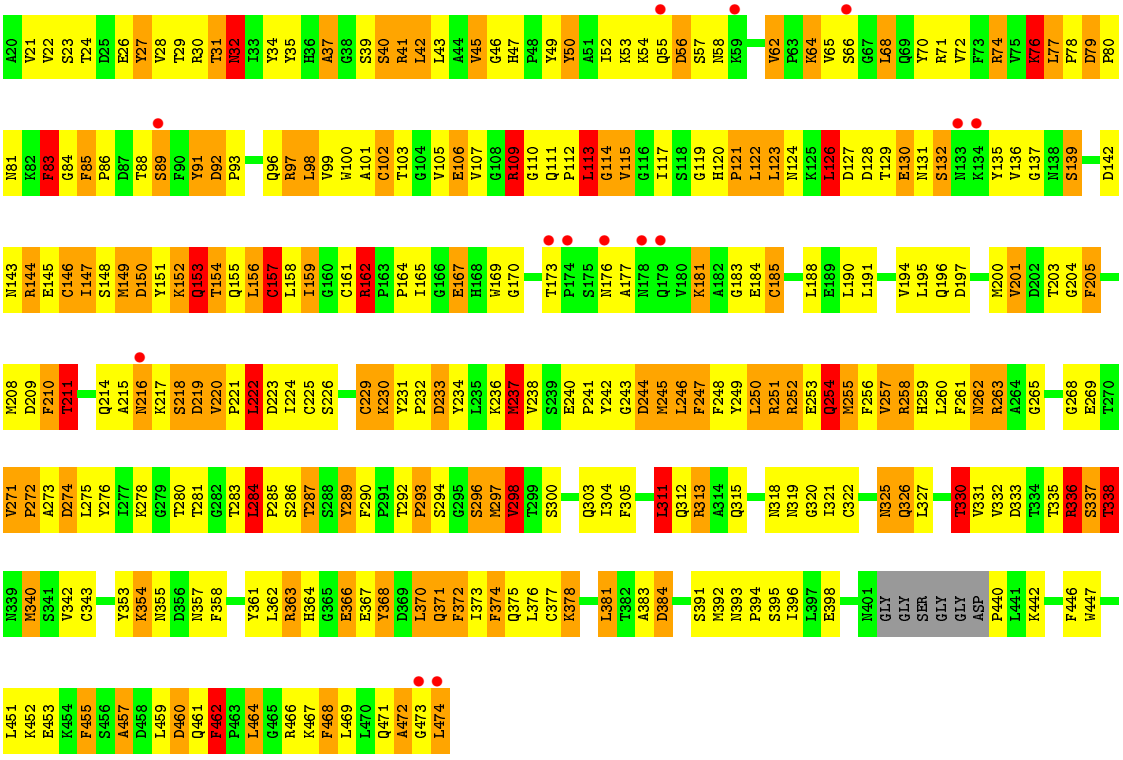




• Molecule 1: Major capsid protein L1

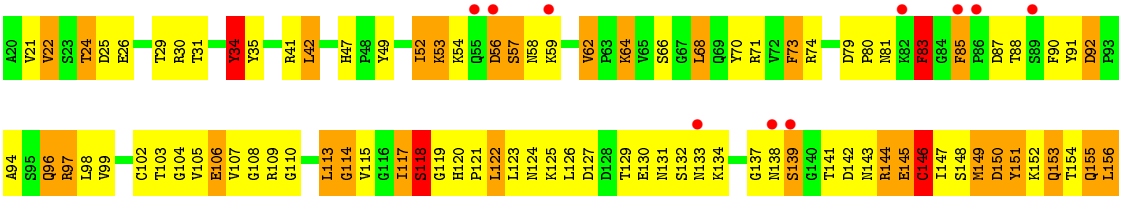
Chain C:

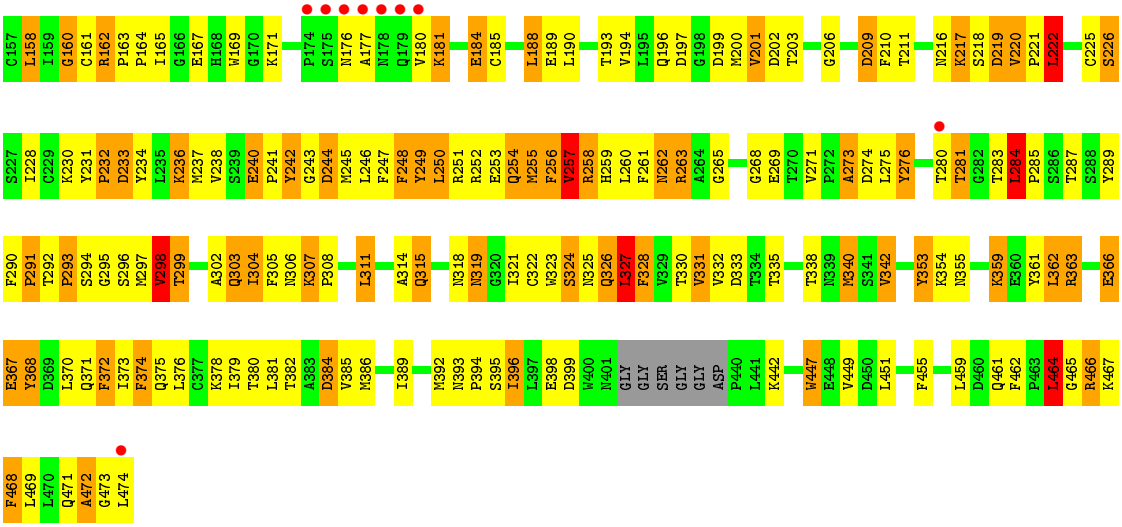




• Molecule 1: Major capsid protein L1

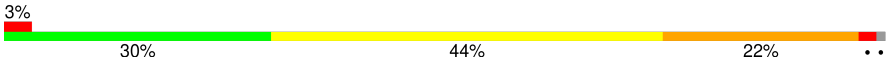
Chain D:

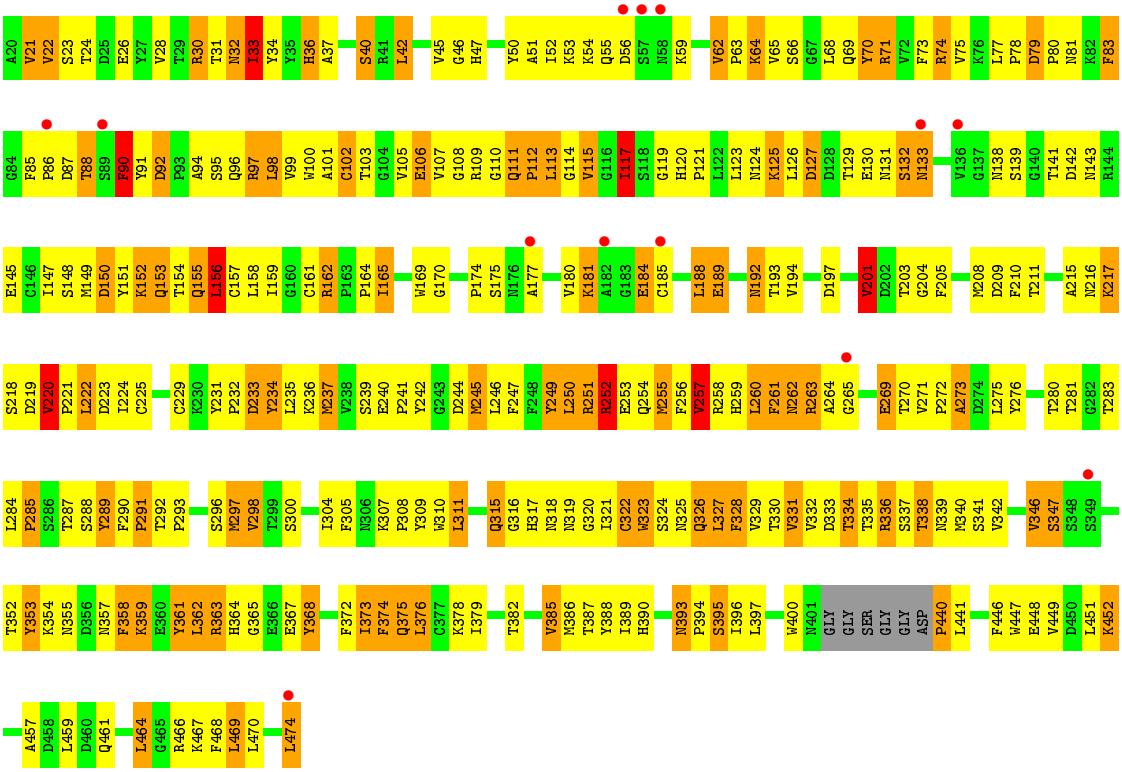




• Molecule 1: Major capsid protein L1

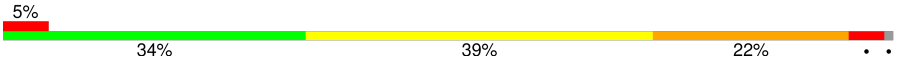
Chain E:

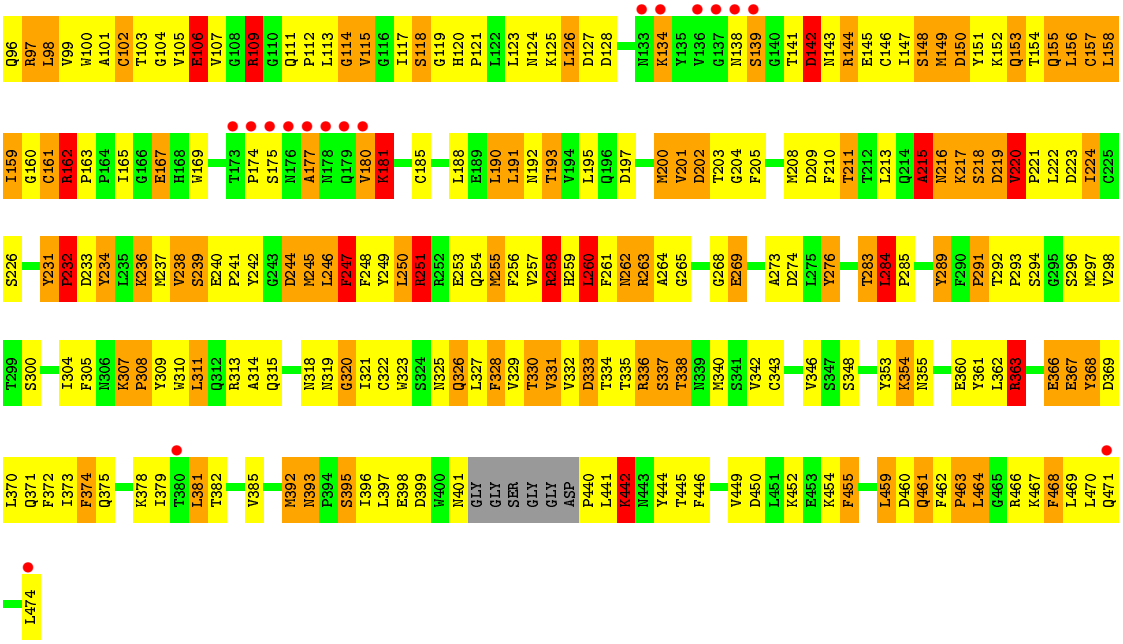




• Molecule 1: Major capsid protein L1

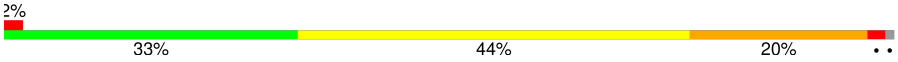
Chain F:

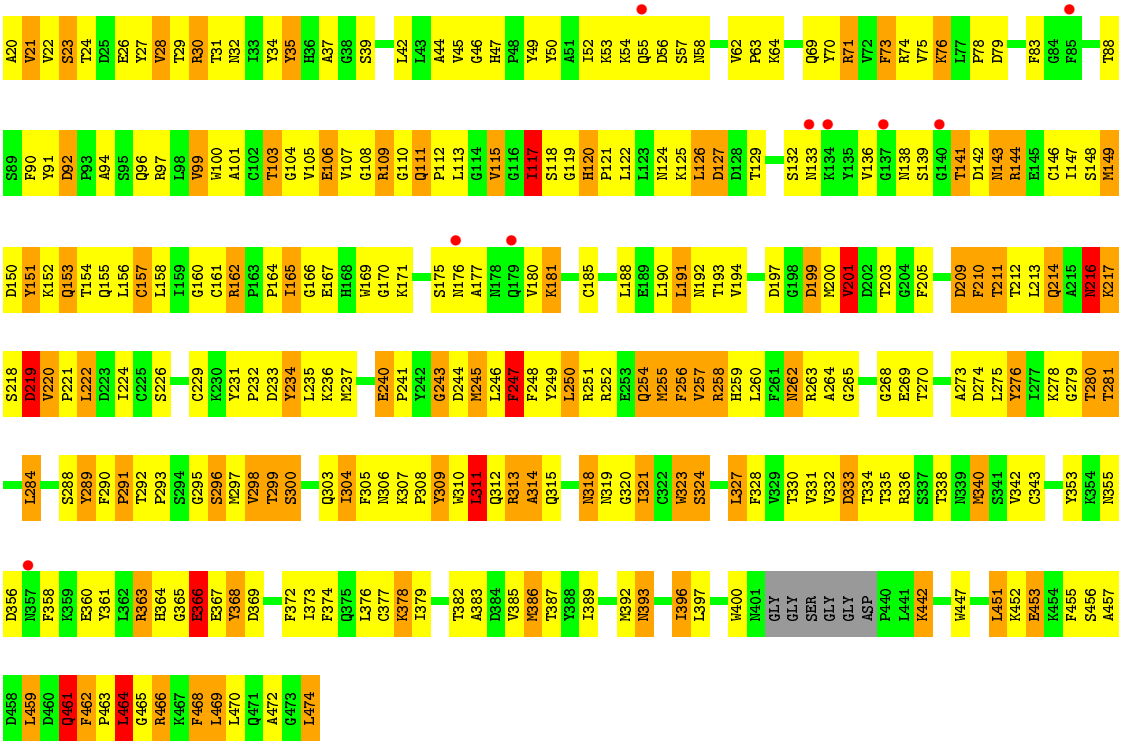




• Molecule 1: Major capsid protein L1

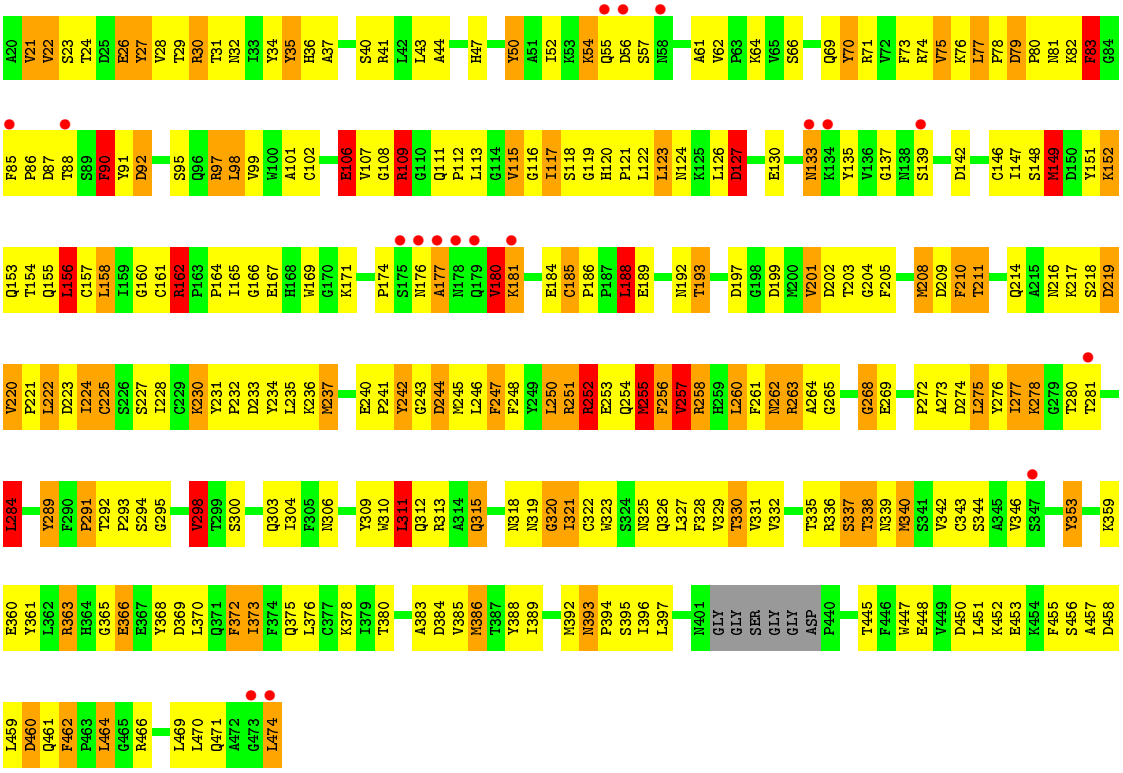
Chain G:





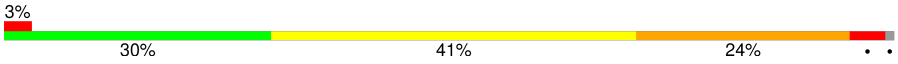
• Molecule 1: Major capsid protein L1

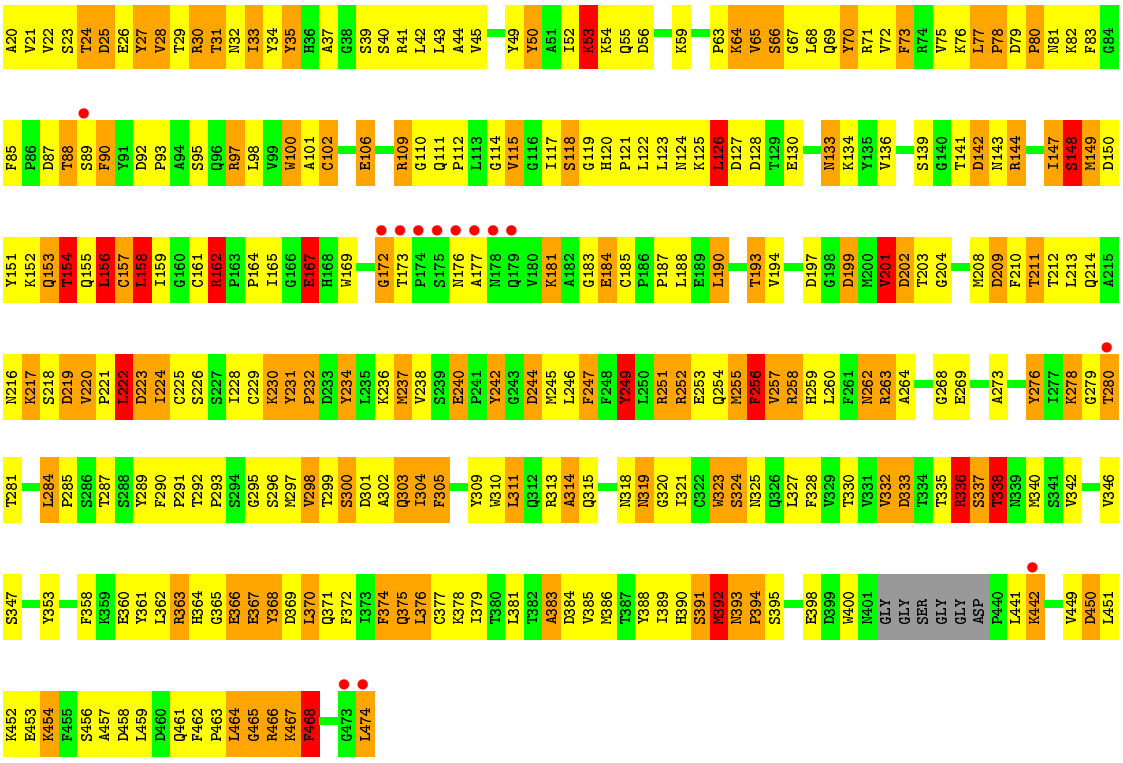
Chain H:



• Molecule 1: Major capsid protein L1

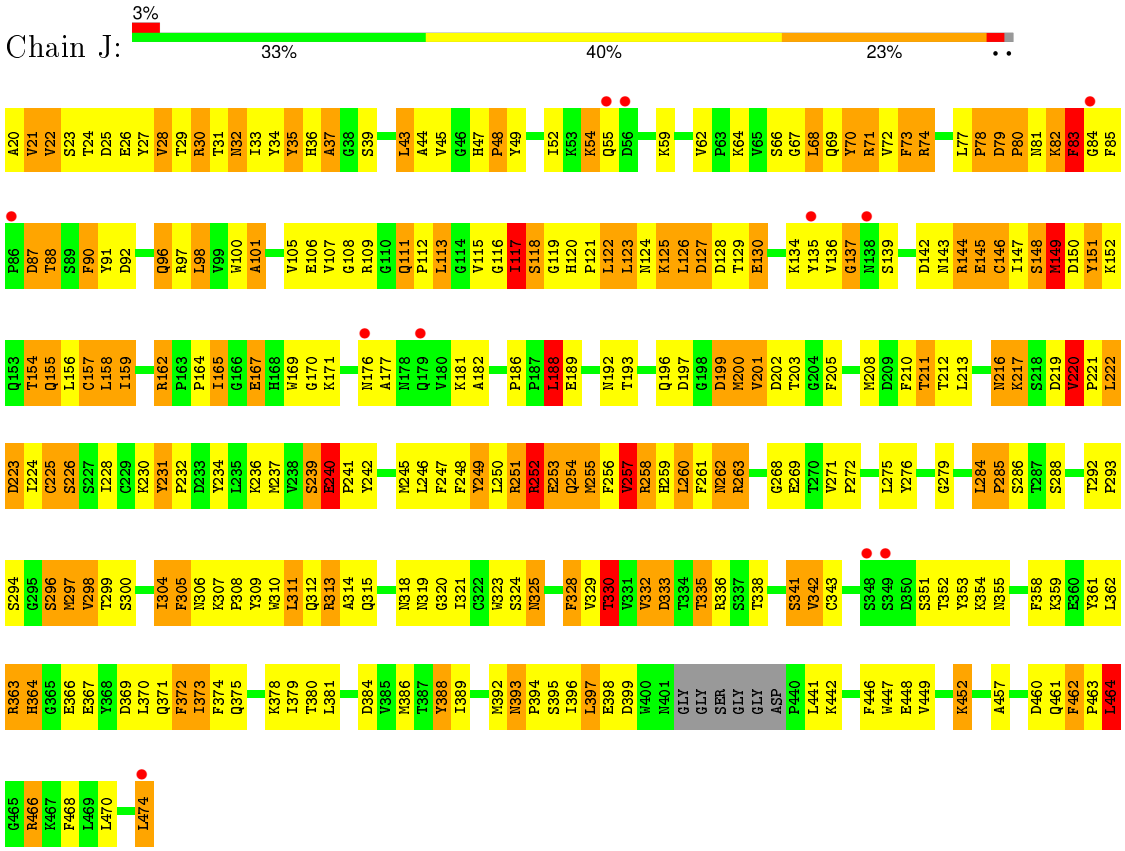
Chain I:





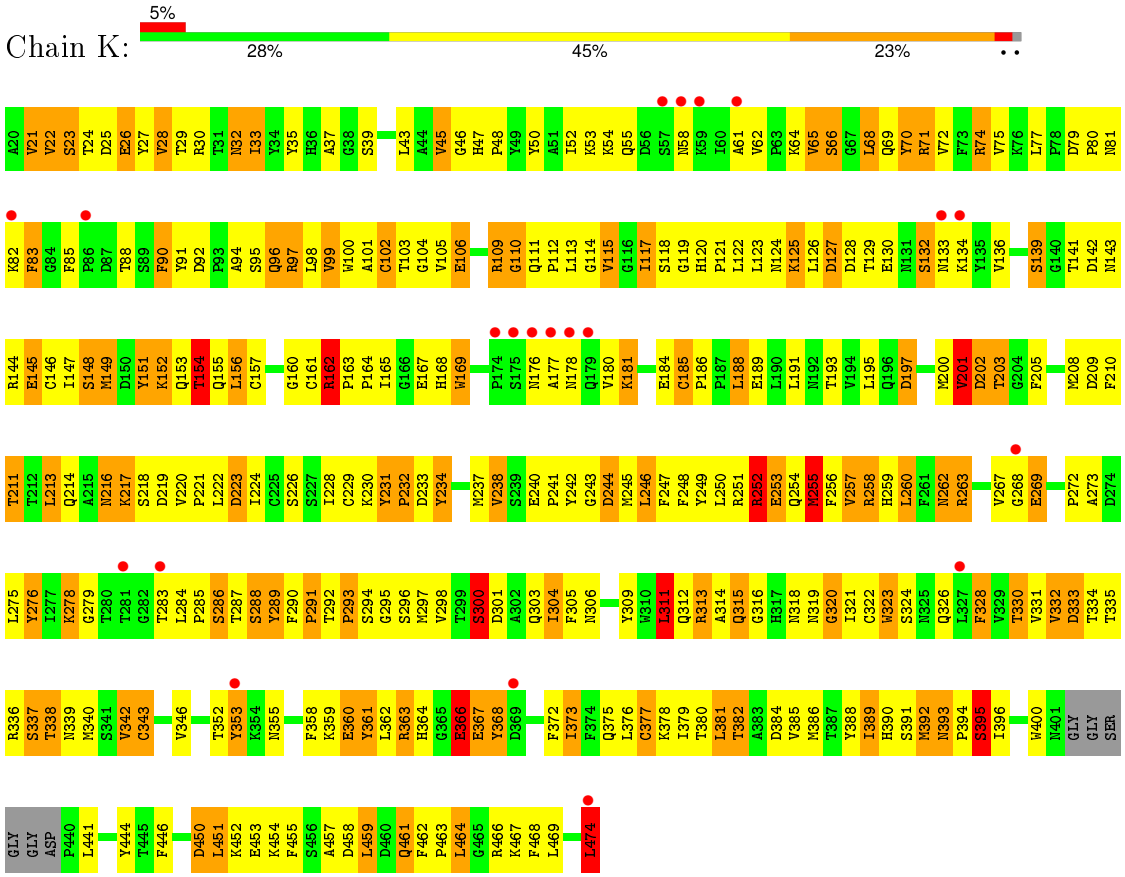
• Molecule 1: Major capsid protein L1

Chain J:



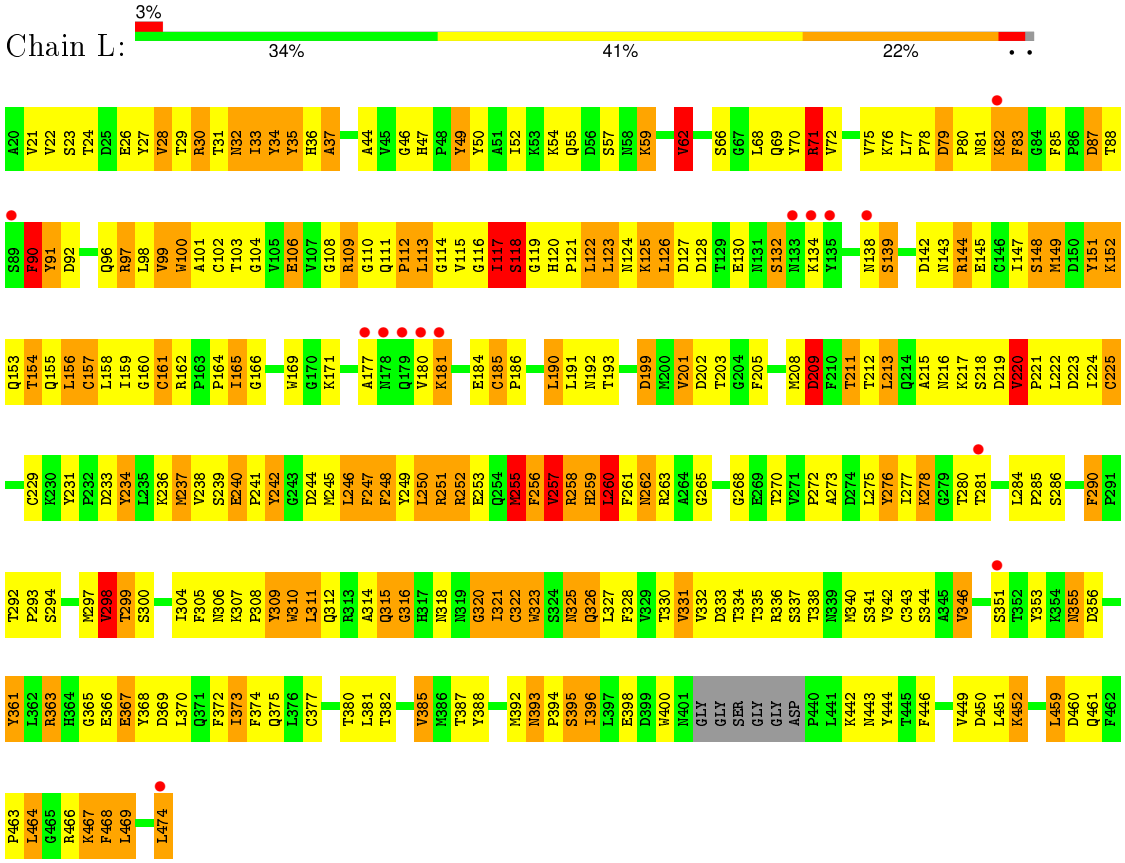
• Molecule 1: Major capsid protein L1

Chain K:



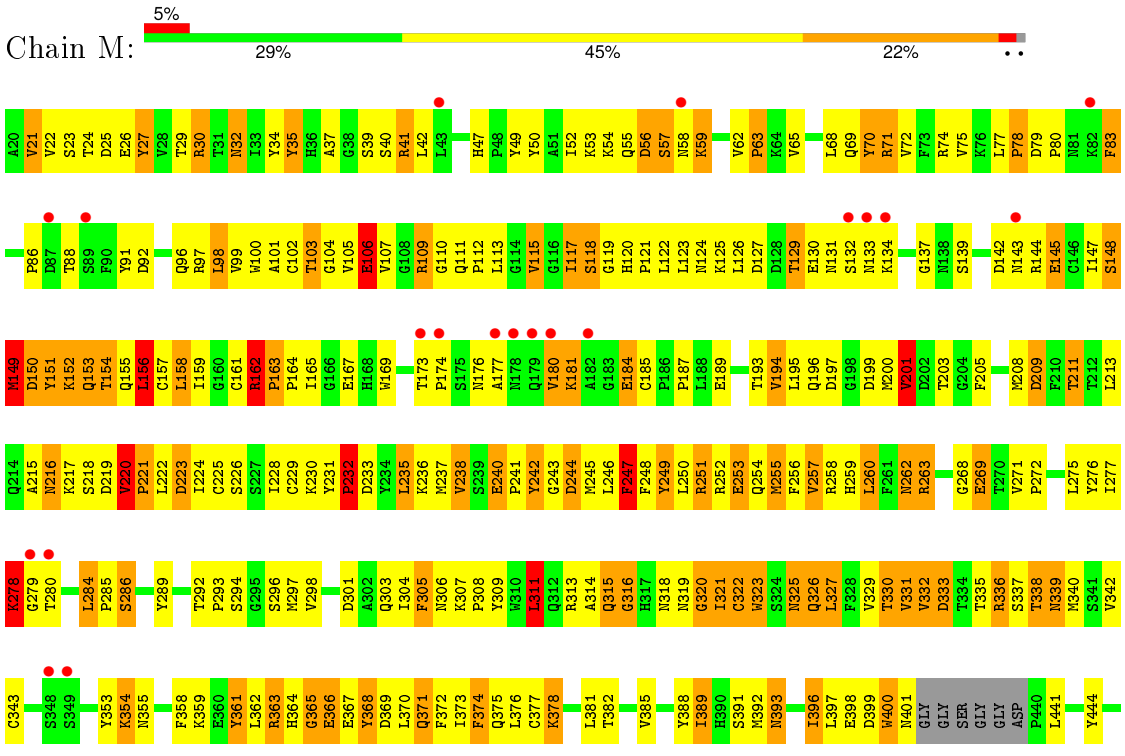
• Molecule 1: Major capsid protein L1

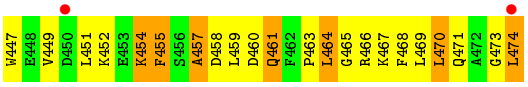
Chain L:



• Molecule 1: Major capsid protein L1

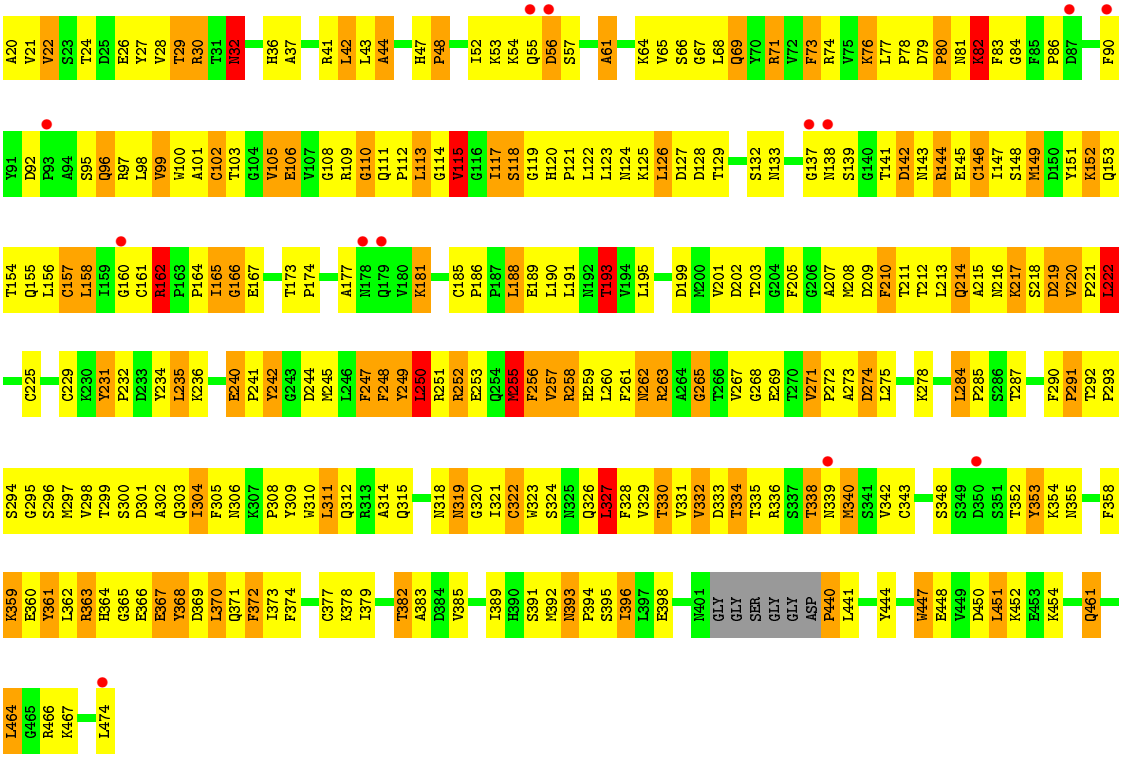
Chain M:





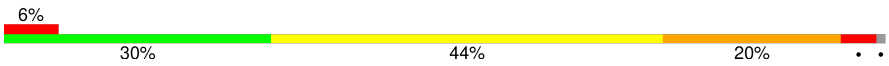
• Molecule 1: Major capsid protein L1

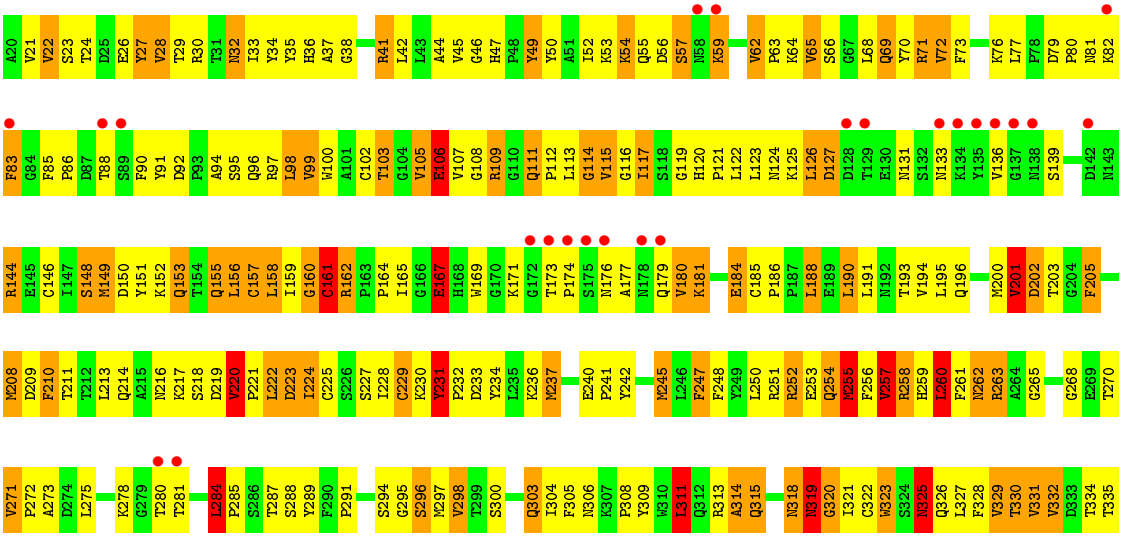
Chain N:

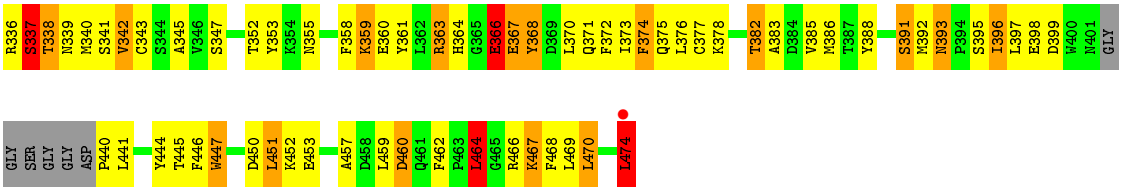


• Molecule 1: Major capsid protein L1

Chain O:






R336
S337
T338
N339
M340
S341
V342
C343
S344
A345
V346
S347
T352
Y353
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N355
F358
K359
E360
Y361
L362
R363
H364
G365
E366
E367
Y368
D369
L370
Q371
F372
I373
F374
Q375
L376
C377
K378
T382
A383
D384
Y385
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E398
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N401
GLY
GLY
SER
GLY
GLY
ASP
P440
L441
Y444
T445
F446
W447
D450
L451
K452
E453
A457
D458
L459
D460
Q461
F462
P463
L464
G465
R466
K467
F468
L469
L470
I474

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	150.41Å 176.61Å 197.07Å 90.00° 92.11° 90.00°	Depositor
Resolution (Å)	15.00 – 3.30 15.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (15.00-3.30) 85.6 (15.00-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	18.90	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.315 , 0.348 0.319 , 0.354	Depositor DCC
R_{free} test set	7364 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 10.3	EDS
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 146166 reflections	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	49350	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	2.22	117/3373 (3.5%)	1.78	69/4580 (1.5%)
1	B	2.19	117/3373 (3.5%)	1.76	66/4580 (1.4%)
1	C	2.23	114/3373 (3.4%)	1.87	83/4580 (1.8%)
1	D	2.20	100/3373 (3.0%)	1.77	70/4580 (1.5%)
1	E	2.14	110/3373 (3.3%)	1.69	59/4580 (1.3%)
1	F	2.25	118/3373 (3.5%)	1.87	76/4580 (1.7%)
1	G	2.13	104/3373 (3.1%)	1.71	59/4580 (1.3%)
1	H	2.13	97/3373 (2.9%)	1.80	79/4580 (1.7%)
1	I	2.20	114/3373 (3.4%)	1.80	81/4580 (1.8%)
1	J	2.24	135/3373 (4.0%)	1.79	77/4580 (1.7%)
1	K	2.16	106/3373 (3.1%)	1.72	63/4580 (1.4%)
1	L	2.19	105/3373 (3.1%)	1.68	57/4580 (1.2%)
1	M	2.24	134/3373 (4.0%)	1.70	57/4580 (1.2%)
1	N	2.15	106/3373 (3.1%)	1.70	56/4580 (1.2%)
1	O	2.20	104/3373 (3.1%)	1.70	62/4580 (1.4%)
All	All	2.19	1681/50595 (3.3%)	1.75	1014/68700 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	D	0	1
1	F	0	1
1	I	0	3
1	J	0	1
1	O	0	1
All	All	0	12

All (1681) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	467	LYS	CD-CE	15.78	1.90	1.51
1	N	152	LYS	CE-NZ	15.76	1.88	1.49
1	M	152	LYS	CE-NZ	15.45	1.87	1.49
1	A	26	GLU	CD-OE1	14.40	1.41	1.25
1	A	391	SER	CB-OG	14.30	1.60	1.42
1	D	359	LYS	CD-CE	14.04	1.86	1.51
1	F	354	LYS	CE-NZ	13.63	1.83	1.49
1	C	254	GLN	CB-CG	-13.60	1.15	1.52
1	B	467	LYS	CD-CE	12.91	1.83	1.51
1	L	467	LYS	CE-NZ	12.58	1.80	1.49
1	D	374	PHE	CE2-CZ	12.54	1.61	1.37
1	F	83	PHE	CE1-CZ	12.10	1.60	1.37
1	F	336	ARG	CZ-NH1	12.00	1.48	1.33
1	E	359	LYS	CE-NZ	11.98	1.78	1.49
1	A	125	LYS	CD-CE	11.91	1.81	1.51
1	M	240	GLU	CD-OE1	11.84	1.38	1.25
1	J	239	SER	CB-OG	11.80	1.57	1.42
1	J	309	TYR	CE2-CZ	11.70	1.53	1.38
1	F	73	PHE	CD2-CE2	11.66	1.62	1.39
1	F	309	TYR	CE2-CZ	11.63	1.53	1.38
1	N	152	LYS	CD-CE	11.60	1.80	1.51
1	I	53	LYS	CE-NZ	11.59	1.78	1.49
1	A	267	VAL	CB-CG2	11.47	1.76	1.52
1	C	466	ARG	CZ-NH2	11.41	1.47	1.33
1	B	134	LYS	CE-NZ	11.32	1.77	1.49
1	A	276	TYR	CG-CD2	11.31	1.53	1.39
1	I	367	GLU	CG-CD	11.16	1.68	1.51
1	M	322	CYS	CB-SG	-11.08	1.63	1.82
1	F	83	PHE	CG-CD2	11.07	1.55	1.38
1	N	447	TRP	CE3-CZ3	10.99	1.57	1.38
1	N	249	TYR	CD2-CE2	-10.98	1.22	1.39
1	O	337	SER	CB-OG	10.91	1.56	1.42
1	F	366	GLU	CD-OE2	10.90	1.37	1.25
1	L	467	LYS	CG-CD	10.87	1.89	1.52
1	D	217	LYS	CE-NZ	10.85	1.76	1.49
1	M	184	GLU	CG-CD	10.77	1.68	1.51
1	B	366	GLU	CD-OE1	10.76	1.37	1.25
1	B	336	ARG	CZ-NH1	10.75	1.47	1.33
1	O	59	LYS	CE-NZ	10.73	1.75	1.49
1	K	242	TYR	CE2-CZ	10.58	1.52	1.38
1	J	257	VAL	CB-CG1	-10.56	1.30	1.52
1	D	276	TYR	CD2-CE2	10.49	1.55	1.39
1	L	452	LYS	CG-CD	10.43	1.88	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	444	TYR	CD2-CE2	-10.38	1.23	1.39
1	L	256	PHE	CD2-CE2	10.31	1.59	1.39
1	K	248	PHE	CE1-CZ	10.28	1.56	1.37
1	I	28	VAL	CB-CG2	-10.27	1.31	1.52
1	O	367	GLU	CD-OE2	10.25	1.36	1.25
1	B	70	TYR	CD1-CE1	10.24	1.54	1.39
1	G	383	ALA	CA-CB	-10.22	1.30	1.52
1	L	185	CYS	CB-SG	-10.20	1.65	1.82
1	N	359	LYS	CG-CD	10.18	1.87	1.52
1	G	360	GLU	CD-OE2	10.17	1.36	1.25
1	K	377	CYS	CB-SG	10.16	1.99	1.82
1	I	332	VAL	CB-CG2	-10.16	1.31	1.52
1	J	343	CYS	CB-SG	-10.13	1.65	1.82
1	L	59	LYS	CE-NZ	10.13	1.74	1.49
1	D	130	GLU	CD-OE2	10.12	1.36	1.25
1	A	342	VAL	CB-CG2	-10.02	1.31	1.52
1	O	161	CYS	CB-SG	9.99	1.99	1.82
1	A	310	TRP	CG-CD1	9.91	1.50	1.36
1	J	44	ALA	CA-CB	9.91	1.73	1.52
1	L	249	TYR	CB-CG	9.91	1.66	1.51
1	L	328	PHE	CE1-CZ	9.87	1.56	1.37
1	N	146	CYS	CB-SG	9.81	1.99	1.82
1	J	39	SER	CB-OG	9.80	1.54	1.42
1	M	115	VAL	CB-CG2	9.76	1.73	1.52
1	M	336	ARG	CZ-NH2	9.75	1.45	1.33
1	D	161	CYS	CB-SG	-9.72	1.65	1.82
1	M	354	LYS	CE-NZ	9.72	1.73	1.49
1	M	59	LYS	CD-CE	9.72	1.75	1.51
1	I	35	TYR	CD2-CE2	9.71	1.53	1.39
1	O	444	TYR	CD2-CE2	-9.70	1.24	1.39
1	L	256	PHE	CE1-CZ	9.70	1.55	1.37
1	A	367	GLU	CG-CD	9.69	1.66	1.51
1	A	298	VAL	CB-CG1	-9.67	1.32	1.52
1	J	130	GLU	CD-OE2	9.67	1.36	1.25
1	C	109	ARG	CZ-NH1	9.66	1.45	1.33
1	E	242	TYR	CE2-CZ	9.58	1.50	1.38
1	F	258	ARG	CG-CD	-9.56	1.28	1.51
1	B	336	ARG	CZ-NH2	9.56	1.45	1.33
1	G	455	PHE	CE2-CZ	9.56	1.55	1.37
1	D	144	ARG	CZ-NH1	9.55	1.45	1.33
1	F	309	TYR	CD2-CE2	9.53	1.53	1.39
1	G	205	PHE	CE2-CZ	9.51	1.55	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	249	TYR	CD1-CE1	-9.49	1.25	1.39
1	I	64	LYS	CE-NZ	9.48	1.72	1.49
1	O	273	ALA	CA-CB	9.48	1.72	1.52
1	I	276	TYR	CD2-CE2	9.43	1.53	1.39
1	B	91	TYR	CD2-CE2	9.41	1.53	1.39
1	C	336	ARG	CZ-NH1	9.37	1.45	1.33
1	G	256	PHE	CB-CG	9.35	1.67	1.51
1	O	38	GLY	C-O	-9.34	1.08	1.23
1	L	444	TYR	CD2-CE2	9.31	1.53	1.39
1	H	248	PHE	CE2-CZ	9.28	1.54	1.37
1	B	30	ARG	CZ-NH2	9.27	1.45	1.33
1	B	134	LYS	CD-CE	9.27	1.74	1.51
1	B	234	TYR	CD2-CE2	9.26	1.53	1.39
1	C	31	THR	CA-CB	9.24	1.77	1.53
1	K	289	TYR	CG-CD2	-9.21	1.27	1.39
1	A	265	GLY	C-O	-9.19	1.08	1.23
1	I	64	LYS	CD-CE	9.16	1.74	1.51
1	E	260	LEU	CG-CD1	-9.13	1.18	1.51
1	A	360	GLU	CB-CG	9.12	1.69	1.52
1	C	378	LYS	N-CA	-9.10	1.28	1.46
1	D	137	GLY	C-O	9.07	1.38	1.23
1	J	336	ARG	CZ-NH1	9.04	1.44	1.33
1	F	336	ARG	CZ-NH2	9.02	1.44	1.33
1	I	247	PHE	CE2-CZ	-9.00	1.20	1.37
1	L	336	ARG	CZ-NH2	9.00	1.44	1.33
1	D	467	LYS	CD-CE	8.99	1.73	1.51
1	L	248	PHE	CD1-CE1	8.99	1.57	1.39
1	F	157	CYS	N-CA	-8.98	1.28	1.46
1	G	234	TYR	CG-CD2	-8.95	1.27	1.39
1	M	336	ARG	CZ-NH1	8.95	1.44	1.33
1	J	83	PHE	CE1-CZ	8.95	1.54	1.37
1	J	210	PHE	CE1-CZ	-8.94	1.20	1.37
1	O	114	GLY	C-O	8.94	1.38	1.23
1	J	70	TYR	CB-CG	-8.93	1.38	1.51
1	K	169	TRP	CG-CD1	8.93	1.49	1.36
1	L	444	TYR	CD1-CE1	8.90	1.52	1.39
1	A	125	LYS	CE-NZ	8.90	1.71	1.49
1	N	76	LYS	CD-CE	8.89	1.73	1.51
1	M	400	TRP	CB-CG	8.89	1.66	1.50
1	H	448	GLU	CG-CD	8.87	1.65	1.51
1	M	247	PHE	CE1-CZ	8.84	1.54	1.37
1	A	366	GLU	CB-CG	8.84	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	242	TYR	CD1-CE1	8.83	1.52	1.39
1	C	297	MET	CB-CG	8.82	1.79	1.51
1	D	374	PHE	CG-CD2	8.81	1.51	1.38
1	D	298	VAL	CB-CG1	-8.79	1.34	1.52
1	B	234	TYR	CE1-CZ	8.77	1.50	1.38
1	C	367	GLU	CD-OE1	8.76	1.35	1.25
1	I	76	LYS	CD-CE	8.75	1.73	1.51
1	A	83	PHE	CG-CD2	8.72	1.51	1.38
1	C	290	PHE	CE2-CZ	8.72	1.53	1.37
1	F	444	TYR	CD1-CE1	-8.71	1.26	1.39
1	D	83	PHE	CE1-CZ	8.70	1.53	1.37
1	H	366	GLU	CB-CG	8.70	1.68	1.52
1	O	103	THR	C-O	8.69	1.39	1.23
1	B	388	TYR	CE2-CZ	-8.68	1.27	1.38
1	L	130	GLU	CG-CD	8.67	1.65	1.51
1	I	95	SER	C-O	8.66	1.39	1.23
1	H	157	CYS	CB-SG	8.63	1.97	1.82
1	A	454	LYS	CD-CE	8.61	1.72	1.51
1	H	448	GLU	CD-OE2	8.60	1.35	1.25
1	I	53	LYS	CD-CE	8.59	1.72	1.51
1	E	271	VAL	CB-CG2	-8.55	1.34	1.52
1	L	100	TRP	CD2-CE2	-8.54	1.31	1.41
1	H	130	GLU	CD-OE2	8.53	1.35	1.25
1	G	254	GLN	CB-CG	8.51	1.75	1.52
1	M	247	PHE	CG-CD2	8.51	1.51	1.38
1	E	448	GLU	CD-OE2	8.51	1.35	1.25
1	C	218	SER	CB-OG	8.50	1.53	1.42
1	G	167	GLU	CB-CG	-8.48	1.36	1.52
1	O	398	GLU	CD-OE2	8.44	1.34	1.25
1	L	257	VAL	CB-CG1	-8.41	1.35	1.52
1	O	59	LYS	CD-CE	8.39	1.72	1.51
1	F	106	GLU	CG-CD	8.38	1.64	1.51
1	C	286	SER	CA-CB	8.37	1.65	1.52
1	L	336	ARG	CZ-NH1	8.34	1.43	1.33
1	F	99	VAL	CB-CG2	-8.32	1.35	1.52
1	N	448	GLU	CG-CD	8.32	1.64	1.51
1	J	125	LYS	CE-NZ	8.31	1.69	1.49
1	D	374	PHE	CG-CD1	8.31	1.51	1.38
1	F	134	LYS	CE-NZ	8.30	1.69	1.49
1	N	353	TYR	CE1-CZ	8.30	1.49	1.38
1	F	161	CYS	C-O	-8.29	1.07	1.23
1	N	210	PHE	CE1-CZ	8.29	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	279	GLY	N-CA	-8.28	1.33	1.46
1	B	112	PRO	CA-C	8.28	1.69	1.52
1	J	117	ILE	CA-CB	-8.27	1.35	1.54
1	C	34	TYR	CA-CB	8.24	1.72	1.53
1	F	247	PHE	CG-CD2	8.24	1.51	1.38
1	M	189	GLU	CG-CD	8.24	1.64	1.51
1	K	332	VAL	CB-CG2	-8.24	1.35	1.52
1	L	249	TYR	CD1-CE1	-8.23	1.27	1.39
1	O	248	PHE	CE2-CZ	8.23	1.52	1.37
1	A	322	CYS	CB-SG	8.21	1.96	1.82
1	B	91	TYR	CD1-CE1	8.21	1.51	1.39
1	F	346	VAL	CB-CG1	-8.21	1.35	1.52
1	D	353	TYR	CD1-CE1	8.21	1.51	1.39
1	A	64	LYS	CG-CD	8.19	1.80	1.52
1	M	366	GLU	CB-CG	8.19	1.67	1.52
1	M	152	LYS	CD-CE	8.19	1.71	1.51
1	G	39	SER	CB-OG	8.19	1.52	1.42
1	D	134	LYS	CD-CE	8.18	1.71	1.51
1	D	258	ARG	CG-CD	8.17	1.72	1.51
1	A	264	ALA	CA-CB	-8.17	1.35	1.52
1	A	28	VAL	CB-CG2	-8.14	1.35	1.52
1	D	367	GLU	CD-OE2	8.13	1.34	1.25
1	J	83	PHE	CG-CD2	8.12	1.50	1.38
1	C	64	LYS	CD-CE	8.12	1.71	1.51
1	I	224	ILE	C-O	8.11	1.38	1.23
1	D	281	THR	CA-CB	8.10	1.74	1.53
1	G	35	TYR	C-O	8.10	1.38	1.23
1	A	194	VAL	CB-CG2	-8.10	1.35	1.52
1	H	257	VAL	CB-CG1	-8.10	1.35	1.52
1	J	373	ILE	C-O	8.10	1.38	1.23
1	D	466	ARG	CB-CG	8.08	1.74	1.52
1	L	148	SER	CB-OG	8.08	1.52	1.42
1	G	201	VAL	CB-CG2	8.08	1.69	1.52
1	C	249	TYR	CD1-CE1	-8.07	1.27	1.39
1	I	66	SER	CB-OG	8.06	1.52	1.42
1	G	368	TYR	CE1-CZ	8.05	1.49	1.38
1	M	375	GLN	CG-CD	8.05	1.69	1.51
1	C	298	VAL	CB-CG1	-8.04	1.35	1.52
1	F	239	SER	CB-OG	8.03	1.52	1.42
1	A	302	ALA	CA-CB	8.03	1.69	1.52
1	I	320	GLY	C-O	8.03	1.36	1.23
1	H	70	TYR	CE1-CZ	8.01	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	70	TYR	CD2-CE2	8.01	1.51	1.39
1	C	368	TYR	CZ-OH	8.00	1.51	1.37
1	J	310	TRP	CB-CG	-8.00	1.35	1.50
1	N	100	TRP	CE3-CZ3	8.00	1.52	1.38
1	K	366	GLU	CD-OE2	7.99	1.34	1.25
1	O	261	PHE	CE2-CZ	7.98	1.52	1.37
1	A	301	ASP	C-O	-7.98	1.08	1.23
1	M	367	GLU	CD-OE2	7.98	1.34	1.25
1	H	83	PHE	CE1-CZ	7.98	1.52	1.37
1	F	461	GLN	CB-CG	-7.97	1.31	1.52
1	C	377	CYS	CB-SG	-7.97	1.68	1.82
1	C	296	SER	CB-OG	7.95	1.52	1.42
1	L	162	ARG	CG-CD	7.93	1.71	1.51
1	B	467	LYS	CE-NZ	7.92	1.68	1.49
1	J	231	TYR	CD1-CE1	-7.92	1.27	1.39
1	K	328	PHE	CE1-CZ	7.91	1.52	1.37
1	G	366	GLU	CD-OE1	7.91	1.34	1.25
1	K	278	LYS	C-O	7.89	1.38	1.23
1	M	50	TYR	CD1-CE1	7.89	1.51	1.39
1	E	102	CYS	CB-SG	-7.88	1.68	1.82
1	J	363	ARG	CZ-NH1	7.88	1.43	1.33
1	K	253	GLU	CB-CG	7.88	1.67	1.52
1	E	130	GLU	CD-OE2	7.88	1.34	1.25
1	F	218	SER	CB-OG	7.87	1.52	1.42
1	H	225	CYS	CB-SG	-7.87	1.68	1.82
1	K	151	TYR	CD1-CE1	7.87	1.51	1.39
1	L	468	PHE	CE2-CZ	7.87	1.52	1.37
1	N	242	TYR	CZ-OH	7.86	1.51	1.37
1	O	359	LYS	CD-CE	7.85	1.70	1.51
1	M	251	ARG	CG-CD	7.84	1.71	1.51
1	G	99	VAL	CB-CG2	-7.81	1.36	1.52
1	G	298	VAL	CB-CG2	-7.80	1.36	1.52
1	N	363	ARG	CZ-NH1	7.80	1.43	1.33
1	K	444	TYR	CE1-CZ	7.79	1.48	1.38
1	G	374	PHE	CG-CD2	7.79	1.50	1.38
1	J	234	TYR	CE1-CZ	7.78	1.48	1.38
1	G	366	GLU	CG-CD	7.78	1.63	1.51
1	L	336	ARG	CG-CD	-7.78	1.32	1.51
1	L	320	GLY	N-CA	7.78	1.57	1.46
1	I	338	THR	CA-CB	7.77	1.73	1.53
1	N	354	LYS	CD-CE	7.74	1.70	1.51
1	N	366	GLU	CB-CG	7.74	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	271	VAL	CB-CG2	-7.73	1.36	1.52
1	B	368	TYR	CE1-CZ	7.72	1.48	1.38
1	D	366	GLU	CD-OE1	7.72	1.34	1.25
1	I	367	GLU	CB-CG	7.72	1.66	1.52
1	H	277	ILE	CA-CB	7.70	1.72	1.54
1	F	374	PHE	CE1-CZ	7.70	1.51	1.37
1	E	62	VAL	CB-CG1	-7.70	1.36	1.52
1	G	240	GLU	CB-CG	7.70	1.66	1.52
1	A	247	PHE	CE2-CZ	-7.69	1.22	1.37
1	B	72	VAL	CA-CB	7.69	1.71	1.54
1	O	359	LYS	CE-NZ	7.69	1.68	1.49
1	O	329	VAL	CB-CG1	7.68	1.69	1.52
1	I	234	TYR	CD1-CE1	7.68	1.50	1.39
1	M	276	TYR	CE1-CZ	7.67	1.48	1.38
1	N	359	LYS	CD-CE	7.67	1.70	1.51
1	O	65	VAL	CB-CG2	-7.67	1.36	1.52
1	C	204	GLY	N-CA	-7.66	1.34	1.46
1	K	320	GLY	N-CA	7.66	1.57	1.46
1	K	102	CYS	CB-SG	7.63	1.95	1.82
1	J	466	ARG	CZ-NH2	7.63	1.43	1.33
1	D	307	LYS	CB-CG	7.63	1.73	1.52
1	J	372	PHE	CD1-CE1	7.63	1.54	1.39
1	M	242	TYR	CE2-CZ	7.62	1.48	1.38
1	B	368	TYR	CB-CG	-7.62	1.40	1.51
1	A	288	SER	CA-CB	7.62	1.64	1.52
1	N	271	VAL	CB-CG2	7.61	1.68	1.52
1	J	307	LYS	CD-CE	7.61	1.70	1.51
1	O	309	TYR	CE1-CZ	-7.61	1.28	1.38
1	E	53	LYS	CD-CE	7.59	1.70	1.51
1	O	260	LEU	CG-CD1	-7.59	1.23	1.51
1	I	167	GLU	CG-CD	7.59	1.63	1.51
1	I	73	PHE	CE1-CZ	-7.57	1.23	1.37
1	A	367	GLU	CD-OE1	7.56	1.33	1.25
1	O	157	CYS	CB-SG	7.56	1.95	1.82
1	F	73	PHE	N-CA	-7.54	1.31	1.46
1	J	91	TYR	CG-CD1	-7.53	1.29	1.39
1	O	146	CYS	CB-SG	7.52	1.95	1.82
1	E	242	TYR	CG-CD2	7.52	1.49	1.39
1	B	119	GLY	C-O	7.51	1.35	1.23
1	I	449	VAL	CA-CB	7.51	1.70	1.54
1	B	240	GLU	CD-OE2	7.50	1.33	1.25
1	D	177	ALA	CA-CB	7.50	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	298	VAL	N-CA	7.50	1.61	1.46
1	O	467	LYS	CD-CE	7.50	1.70	1.51
1	J	231	TYR	CD2-CE2	-7.50	1.28	1.39
1	J	372	PHE	CE1-CZ	-7.49	1.23	1.37
1	J	468	PHE	C-O	-7.49	1.09	1.23
1	B	70	TYR	CD2-CE2	7.47	1.50	1.39
1	J	447	TRP	CZ3-CH2	-7.46	1.28	1.40
1	C	372	PHE	CD1-CE1	7.46	1.54	1.39
1	J	332	VAL	CB-CG1	7.46	1.68	1.52
1	J	309	TYR	N-CA	7.46	1.61	1.46
1	G	157	CYS	CB-SG	7.46	1.95	1.82
1	N	348	SER	CB-OG	7.46	1.51	1.42
1	F	354	LYS	CD-CE	7.45	1.69	1.51
1	N	383	ALA	CA-CB	-7.45	1.36	1.52
1	K	367	GLU	CG-CD	7.45	1.63	1.51
1	H	79	ASP	C-O	-7.45	1.09	1.23
1	I	465	GLY	C-O	7.45	1.35	1.23
1	J	100	TRP	CG-CD1	-7.44	1.26	1.36
1	A	467	LYS	CE-NZ	7.44	1.67	1.49
1	H	204	GLY	N-CA	-7.43	1.34	1.46
1	A	130	GLU	CD-OE2	7.42	1.33	1.25
1	K	323	TRP	CZ3-CH2	7.41	1.51	1.40
1	G	256	PHE	CD2-CE2	-7.41	1.24	1.39
1	D	302	ALA	CA-CB	7.39	1.68	1.52
1	F	331	VAL	CA-CB	-7.38	1.39	1.54
1	J	447	TRP	CE3-CZ3	7.38	1.51	1.38
1	C	462	PHE	CD1-CE1	7.37	1.53	1.39
1	F	367	GLU	CG-CD	7.37	1.63	1.51
1	I	234	TYR	CD2-CE2	7.37	1.50	1.39
1	B	346	VAL	CB-CG2	-7.36	1.37	1.52
1	H	83	PHE	CG-CD2	7.36	1.49	1.38
1	E	269	GLU	CD-OE2	7.36	1.33	1.25
1	I	336	ARG	CZ-NH2	7.36	1.42	1.33
1	K	267	VAL	CB-CG2	7.35	1.68	1.52
1	C	343	CYS	CB-SG	7.35	1.94	1.82
1	K	286	SER	CB-OG	7.35	1.51	1.42
1	C	40	SER	CB-OG	7.34	1.51	1.42
1	A	166	GLY	C-O	-7.32	1.11	1.23
1	B	267	VAL	CB-CG2	-7.32	1.37	1.52
1	F	454	LYS	CD-CE	7.32	1.69	1.51
1	J	354	LYS	CE-NZ	7.32	1.67	1.49
1	K	328	PHE	CD2-CE2	7.31	1.53	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	138	ASN	CG-ND2	7.31	1.51	1.32
1	M	70	TYR	CD2-CE2	-7.30	1.28	1.39
1	E	322	CYS	C-O	-7.30	1.09	1.23
1	N	157	CYS	CB-SG	7.29	1.94	1.82
1	A	64	LYS	CD-CE	7.29	1.69	1.51
1	H	90	PHE	N-CA	7.29	1.60	1.46
1	I	65	VAL	CB-CG2	-7.29	1.37	1.52
1	K	359	LYS	CE-NZ	7.28	1.67	1.49
1	N	358	PHE	CE1-CZ	7.28	1.51	1.37
1	F	242	TYR	CD2-CE2	-7.27	1.28	1.39
1	J	100	TRP	CD2-CE2	-7.27	1.32	1.41
1	F	104	GLY	N-CA	-7.27	1.35	1.46
1	I	90	PHE	CB-CG	7.27	1.63	1.51
1	A	151	TYR	CG-CD2	-7.26	1.29	1.39
1	H	366	GLU	C-O	-7.26	1.09	1.23
1	F	84	GLY	C-O	7.26	1.35	1.23
1	E	161	CYS	C-O	7.25	1.37	1.23
1	F	454	LYS	CE-NZ	7.25	1.67	1.49
1	D	59	LYS	CE-NZ	7.25	1.67	1.49
1	N	309	TYR	CG-CD1	7.24	1.48	1.39
1	F	91	TYR	CD2-CE2	-7.24	1.28	1.39
1	I	454	LYS	CD-CE	7.24	1.69	1.51
1	N	214	GLN	N-CA	7.23	1.60	1.46
1	A	354	LYS	CE-NZ	7.23	1.67	1.49
1	F	320	GLY	C-O	7.23	1.35	1.23
1	M	103	THR	CB-CG2	7.23	1.76	1.52
1	D	145	GLU	CB-CG	7.22	1.65	1.52
1	I	144	ARG	CB-CG	7.22	1.72	1.52
1	B	269	GLU	CD-OE2	7.21	1.33	1.25
1	A	44	ALA	CA-CB	-7.21	1.37	1.52
1	F	181	LYS	CE-NZ	7.21	1.67	1.49
1	N	105	VAL	CA-CB	-7.21	1.39	1.54
1	F	28	VAL	CA-CB	-7.20	1.39	1.54
1	I	313	ARG	CZ-NH1	7.20	1.42	1.33
1	N	444	TYR	CD1-CE1	-7.20	1.28	1.39
1	O	332	VAL	CB-CG2	7.20	1.68	1.52
1	K	395	SER	CB-OG	7.20	1.51	1.42
1	B	309	TYR	CE2-CZ	7.19	1.47	1.38
1	H	242	TYR	CD1-CE1	-7.19	1.28	1.39
1	B	75	VAL	CB-CG1	-7.18	1.37	1.52
1	G	219	ASP	CB-CG	7.18	1.66	1.51
1	I	280	THR	CB-CG2	7.18	1.76	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	289	TYR	CG-CD2	-7.18	1.29	1.39
1	C	242	TYR	CG-CD2	7.17	1.48	1.39
1	K	83	PHE	CG-CD2	7.17	1.49	1.38
1	C	98	LEU	N-CA	-7.17	1.32	1.46
1	D	254	GLN	CB-CG	7.17	1.72	1.52
1	M	238	VAL	CB-CG1	7.16	1.67	1.52
1	H	336	ARG	CG-CD	-7.16	1.34	1.51
1	M	184	GLU	CD-OE1	7.16	1.33	1.25
1	B	259	HIS	N-CA	7.16	1.60	1.46
1	D	328	PHE	CE1-CZ	7.16	1.50	1.37
1	F	238	VAL	CB-CG1	7.16	1.67	1.52
1	G	162	ARG	CZ-NH1	7.15	1.42	1.33
1	K	91	TYR	CD1-CE1	-7.15	1.28	1.39
1	D	167	GLU	CB-CG	-7.15	1.38	1.52
1	D	353	TYR	CE1-CZ	7.15	1.47	1.38
1	G	456	SER	CA-CB	7.14	1.63	1.52
1	J	321	ILE	CA-CB	-7.14	1.38	1.54
1	A	35	TYR	CD2-CE2	7.14	1.50	1.39
1	K	230	LYS	CB-CG	7.14	1.71	1.52
1	J	271	VAL	CB-CG2	-7.14	1.37	1.52
1	O	388	TYR	CE2-CZ	7.14	1.47	1.38
1	C	248	PHE	CE1-CZ	7.13	1.50	1.37
1	G	21	VAL	C-O	-7.13	1.09	1.23
1	L	152	LYS	CB-CG	7.13	1.71	1.52
1	G	310	TRP	CG-CD1	-7.13	1.26	1.36
1	G	360	GLU	CG-CD	7.13	1.62	1.51
1	M	320	GLY	C-O	7.13	1.35	1.23
1	J	49	TYR	CZ-OH	7.12	1.50	1.37
1	N	368	TYR	CE1-CZ	7.12	1.47	1.38
1	J	358	PHE	CB-CG	-7.12	1.39	1.51
1	B	378	LYS	CD-CE	7.11	1.69	1.51
1	L	331	VAL	CB-CG1	7.11	1.67	1.52
1	A	76	LYS	CG-CD	7.10	1.76	1.52
1	I	360	GLU	CB-CG	7.10	1.65	1.52
1	M	454	LYS	CD-CE	7.10	1.69	1.51
1	J	217	LYS	CE-NZ	7.10	1.66	1.49
1	J	226	SER	CB-OG	7.10	1.51	1.42
1	M	34	TYR	CZ-OH	7.08	1.49	1.37
1	D	242	TYR	CE2-CZ	7.08	1.47	1.38
1	J	276	TYR	CE2-CZ	7.07	1.47	1.38
1	E	251	ARG	CG-CD	7.07	1.69	1.51
1	A	240	GLU	CD-OE2	7.07	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	336	ARG	N-CA	7.06	1.60	1.46
1	K	26	GLU	CB-CG	7.05	1.65	1.52
1	N	145	GLU	CG-CD	7.05	1.62	1.51
1	H	70	TYR	CZ-OH	7.05	1.49	1.37
1	E	249	TYR	CD1-CE1	-7.03	1.28	1.39
1	B	27	TYR	CD2-CE2	7.03	1.49	1.39
1	E	328	PHE	CE1-CZ	7.03	1.50	1.37
1	C	83	PHE	CG-CD2	7.03	1.49	1.38
1	A	247	PHE	CE1-CZ	7.01	1.50	1.37
1	K	75	VAL	CB-CG1	7.00	1.67	1.52
1	A	261	PHE	CD1-CE1	6.99	1.53	1.39
1	E	252	ARG	CG-CD	6.99	1.69	1.51
1	G	205	PHE	CE1-CZ	-6.98	1.24	1.37
1	H	320	GLY	CA-C	6.98	1.63	1.51
1	E	365	GLY	N-CA	-6.97	1.35	1.46
1	A	242	TYR	CD2-CE2	-6.95	1.28	1.39
1	A	105	VAL	CB-CG1	-6.95	1.38	1.52
1	N	205	PHE	CD1-CE1	6.94	1.53	1.39
1	C	254	GLN	N-CA	-6.93	1.32	1.46
1	K	309	TYR	CG-CD2	6.92	1.48	1.39
1	M	303	GLN	C-O	6.92	1.36	1.23
1	H	337	SER	CA-CB	6.92	1.63	1.52
1	D	467	LYS	CE-NZ	6.92	1.66	1.49
1	G	243	GLY	C-O	6.91	1.34	1.23
1	D	398	GLU	CD-OE2	6.91	1.33	1.25
1	N	309	TYR	CE2-CZ	6.90	1.47	1.38
1	O	148	SER	CA-C	6.90	1.71	1.52
1	H	234	TYR	CE1-CZ	6.90	1.47	1.38
1	O	202	ASP	CG-OD1	6.90	1.41	1.25
1	M	107	VAL	CB-CG2	-6.90	1.38	1.52
1	A	225	CYS	CB-SG	6.89	1.94	1.82
1	C	194	VAL	CB-CG2	-6.89	1.38	1.52
1	J	135	TYR	CD1-CE1	6.89	1.49	1.39
1	A	109	ARG	C-O	-6.88	1.10	1.23
1	B	30	ARG	CB-CG	-6.88	1.33	1.52
1	O	234	TYR	CE1-CZ	6.88	1.47	1.38
1	J	249	TYR	CD1-CE1	-6.88	1.29	1.39
1	N	302	ALA	CA-CB	6.88	1.66	1.52
1	G	368	TYR	CD1-CE1	-6.88	1.29	1.39
1	G	367	GLU	CD-OE1	6.88	1.33	1.25
1	M	276	TYR	CD2-CE2	6.87	1.49	1.39
1	H	242	TYR	CD2-CE2	-6.87	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	446	PHE	CE2-CZ	6.86	1.50	1.37
1	L	34	TYR	CG-CD2	6.86	1.48	1.39
1	D	184	GLU	CD-OE1	6.85	1.33	1.25
1	J	37	ALA	CA-CB	-6.85	1.38	1.52
1	L	239	SER	CB-OG	6.85	1.51	1.42
1	G	466	ARG	CB-CG	6.85	1.71	1.52
1	K	466	ARG	CZ-NH1	6.84	1.42	1.33
1	O	383	ALA	CA-CB	-6.84	1.38	1.52
1	D	134	LYS	CE-NZ	6.84	1.66	1.49
1	K	151	TYR	CE2-CZ	6.83	1.47	1.38
1	L	90	PHE	CE2-CZ	6.83	1.50	1.37
1	G	324	SER	CB-OG	6.83	1.51	1.42
1	M	305	PHE	N-CA	6.83	1.60	1.46
1	O	28	VAL	C-O	-6.83	1.10	1.23
1	A	242	TYR	CZ-OH	6.82	1.49	1.37
1	L	76	LYS	CE-NZ	6.81	1.66	1.49
1	I	230	LYS	CD-CE	6.81	1.68	1.51
1	C	453	GLU	CD-OE1	6.81	1.33	1.25
1	E	388	TYR	CE2-CZ	6.81	1.47	1.38
1	N	398	GLU	CD-OE1	6.81	1.33	1.25
1	H	353	TYR	CE1-CZ	-6.80	1.29	1.38
1	K	95	SER	CB-OG	-6.80	1.33	1.42
1	N	32	ASN	CB-CG	6.79	1.66	1.51
1	B	297	MET	N-CA	-6.79	1.32	1.46
1	C	146	CYS	CB-SG	6.79	1.93	1.82
1	L	249	TYR	CG-CD1	6.79	1.48	1.39
1	L	110	GLY	C-O	-6.78	1.12	1.23
1	D	324	SER	CB-OG	6.78	1.51	1.42
1	N	73	PHE	CE2-CZ	6.78	1.50	1.37
1	D	256	PHE	CB-CG	6.77	1.62	1.51
1	N	113	LEU	C-O	-6.77	1.10	1.23
1	M	34	TYR	C-O	6.77	1.36	1.23
1	M	367	GLU	CG-CD	6.77	1.62	1.51
1	O	167	GLU	CD-OE2	6.77	1.33	1.25
1	H	95	SER	N-CA	6.77	1.59	1.46
1	E	448	GLU	CG-CD	6.76	1.62	1.51
1	H	383	ALA	CA-CB	-6.76	1.38	1.52
1	N	235	LEU	N-CA	6.76	1.59	1.46
1	J	333	ASP	C-O	-6.76	1.10	1.23
1	M	83	PHE	CD1-CE1	6.76	1.52	1.39
1	N	249	TYR	CG-CD1	6.76	1.48	1.39
1	C	89	SER	C-O	6.75	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	298	VAL	N-CA	6.75	1.59	1.46
1	H	185	CYS	CB-SG	-6.74	1.70	1.82
1	J	67	GLY	C-O	6.74	1.34	1.23
1	G	220	VAL	CB-CG1	6.74	1.67	1.52
1	L	310	TRP	CE2-CZ2	6.74	1.51	1.39
1	A	53	LYS	CE-NZ	6.73	1.65	1.49
1	J	328	PHE	CE1-CZ	6.73	1.50	1.37
1	O	27	TYR	CE1-CZ	6.73	1.47	1.38
1	E	309	TYR	CD2-CE2	6.72	1.49	1.39
1	H	27	TYR	CD2-CE2	6.71	1.49	1.39
1	L	37	ALA	CA-CB	6.71	1.66	1.52
1	A	117	ILE	C-O	6.71	1.36	1.23
1	J	452	LYS	CE-NZ	6.71	1.65	1.49
1	K	451	LEU	N-CA	6.71	1.59	1.46
1	F	309	TYR	CG-CD1	6.70	1.47	1.39
1	K	130	GLU	CB-CG	6.70	1.64	1.52
1	N	76	LYS	CG-CD	6.70	1.75	1.52
1	G	194	VAL	CB-CG1	-6.70	1.38	1.52
1	D	447	TRP	CB-CG	6.69	1.62	1.50
1	I	240	GLU	CD-OE1	6.69	1.33	1.25
1	C	233	ASP	C-O	6.69	1.36	1.23
1	O	383	ALA	N-CA	-6.68	1.32	1.46
1	J	298	VAL	CA-CB	-6.68	1.40	1.54
1	C	152	LYS	CD-CE	6.68	1.68	1.51
1	G	136	VAL	CB-CG2	6.68	1.66	1.52
1	I	375	GLN	CA-C	6.67	1.70	1.52
1	N	255	MET	CG-SD	6.67	1.98	1.81
1	C	368	TYR	CE1-CZ	6.67	1.47	1.38
1	I	77	LEU	C-O	6.66	1.36	1.23
1	I	258	ARG	C-O	-6.66	1.10	1.23
1	M	65	VAL	CB-CG2	-6.66	1.38	1.52
1	D	90	PHE	N-CA	6.66	1.59	1.46
1	G	103	THR	C-O	6.65	1.35	1.23
1	O	69	GLN	N-CA	6.65	1.59	1.46
1	A	444	TYR	CD1-CE1	6.65	1.49	1.39
1	G	224	ILE	CB-CG2	-6.64	1.32	1.52
1	O	388	TYR	CG-CD1	6.64	1.47	1.39
1	B	194	VAL	CB-CG1	6.64	1.66	1.52
1	K	90	PHE	CE1-CZ	6.64	1.50	1.37
1	M	301	ASP	CB-CG	6.64	1.65	1.51
1	M	249	TYR	CD2-CE2	6.63	1.49	1.39
1	H	231	TYR	CD2-CE2	-6.63	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	368	TYR	CD1-CE1	6.63	1.49	1.39
1	I	388	TYR	CD1-CE1	-6.63	1.29	1.39
1	G	234	TYR	CE1-CZ	-6.63	1.29	1.38
1	B	309	TYR	CG-CD1	6.62	1.47	1.39
1	N	240	GLU	CD-OE2	6.62	1.32	1.25
1	G	169	TRP	CB-CG	6.61	1.62	1.50
1	L	344	SER	CB-OG	-6.61	1.33	1.42
1	C	313	ARG	CG-CD	6.61	1.68	1.51
1	D	122	LEU	C-O	-6.61	1.10	1.23
1	E	152	LYS	CD-CE	6.61	1.67	1.51
1	F	445	THR	CB-CG2	6.61	1.74	1.52
1	E	125	LYS	CD-CE	6.61	1.67	1.51
1	D	468	PHE	CE1-CZ	6.61	1.49	1.37
1	F	30	ARG	CG-CD	6.61	1.68	1.51
1	D	22	VAL	CB-CG2	-6.60	1.39	1.52
1	M	100	TRP	CG-CD1	-6.60	1.27	1.36
1	O	338	THR	C-O	6.60	1.35	1.23
1	A	95	SER	CB-OG	-6.60	1.33	1.42
1	N	467	LYS	CE-NZ	6.60	1.65	1.49
1	E	204	GLY	C-O	6.60	1.34	1.23
1	M	148	SER	CB-OG	6.60	1.50	1.42
1	H	257	VAL	CA-CB	-6.59	1.41	1.54
1	H	372	PHE	CD1-CE1	6.59	1.52	1.39
1	E	390	HIS	C-O	6.59	1.35	1.23
1	E	155	GLN	CD-NE2	6.59	1.49	1.32
1	E	358	PHE	CE1-CZ	-6.59	1.24	1.37
1	J	388	TYR	CB-CG	6.59	1.61	1.51
1	H	209	ASP	CB-CG	6.58	1.65	1.51
1	O	115	VAL	CB-CG1	6.58	1.66	1.52
1	K	224	ILE	C-O	6.58	1.35	1.23
1	C	455	PHE	CD1-CE1	6.57	1.52	1.39
1	L	28	VAL	CB-CG1	6.57	1.66	1.52
1	M	184	GLU	CB-CG	6.57	1.64	1.52
1	F	232	PRO	CA-C	-6.56	1.39	1.52
1	F	204	GLY	N-CA	-6.56	1.36	1.46
1	A	87	ASP	CB-CG	-6.56	1.38	1.51
1	B	448	GLU	CD-OE2	6.56	1.32	1.25
1	G	468	PHE	CE2-CZ	6.55	1.49	1.37
1	A	110	GLY	N-CA	-6.55	1.36	1.46
1	D	90	PHE	CE2-CZ	6.55	1.49	1.37
1	G	146	CYS	CB-SG	6.55	1.93	1.82
1	J	22	VAL	CB-CG1	-6.55	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	113	LEU	C-O	6.55	1.35	1.23
1	A	290	PHE	CD2-CE2	-6.55	1.26	1.39
1	J	155	GLN	CB-CG	-6.55	1.34	1.52
1	N	165	ILE	CA-CB	6.55	1.70	1.54
1	L	151	TYR	CE1-CZ	6.54	1.47	1.38
1	J	148	SER	CB-OG	6.54	1.50	1.42
1	D	96	GLN	CB-CG	6.53	1.70	1.52
1	F	234	TYR	CD1-CE1	-6.53	1.29	1.39
1	K	201	VAL	CB-CG2	6.53	1.66	1.52
1	N	354	LYS	CE-NZ	6.52	1.65	1.49
1	M	35	TYR	CZ-OH	-6.52	1.26	1.37
1	J	359	LYS	CE-NZ	6.52	1.65	1.49
1	B	34	TYR	CB-CG	6.51	1.61	1.51
1	B	101	ALA	CA-CB	6.51	1.66	1.52
1	E	97	ARG	CG-CD	6.51	1.68	1.51
1	J	144	ARG	CB-CG	-6.51	1.34	1.52
1	L	249	TYR	CD2-CE2	-6.50	1.29	1.39
1	E	358	PHE	CG-CD2	-6.50	1.28	1.38
1	L	255	MET	CB-CG	6.50	1.72	1.51
1	G	231	TYR	CD2-CE2	6.50	1.49	1.39
1	I	366	GLU	CD-OE2	6.50	1.32	1.25
1	G	466	ARG	CZ-NH1	6.49	1.41	1.33
1	L	130	GLU	CD-OE2	6.49	1.32	1.25
1	E	73	PHE	CE1-CZ	6.49	1.49	1.37
1	A	304	ILE	CG1-CD1	6.49	1.95	1.50
1	H	50	TYR	CG-CD2	6.49	1.47	1.39
1	J	83	PHE	CD1-CE1	6.48	1.52	1.39
1	L	240	GLU	CG-CD	6.48	1.61	1.51
1	N	115	VAL	C-O	6.48	1.35	1.23
1	N	166	GLY	C-O	-6.47	1.13	1.23
1	D	354	LYS	CE-NZ	6.46	1.65	1.49
1	G	105	VAL	CB-CG2	6.46	1.66	1.52
1	I	214	GLN	CG-CD	-6.46	1.36	1.51
1	D	90	PHE	CG-CD1	6.46	1.48	1.38
1	E	264	ALA	CA-CB	-6.46	1.38	1.52
1	E	353	TYR	CD1-CE1	6.46	1.49	1.39
1	H	166	GLY	C-O	6.45	1.33	1.23
1	I	391	SER	CB-OG	6.44	1.50	1.42
1	M	316	GLY	N-CA	6.44	1.55	1.46
1	J	398	GLU	CD-OE2	6.43	1.32	1.25
1	O	167	GLU	CB-CG	6.43	1.64	1.52
1	B	255	MET	CG-SD	6.43	1.97	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	230	LYS	CB-CG	6.43	1.70	1.52
1	C	298	VAL	C-O	6.43	1.35	1.23
1	M	331	VAL	CB-CG2	6.43	1.66	1.52
1	O	331	VAL	CA-CB	-6.43	1.41	1.54
1	B	257	VAL	CB-CG1	-6.42	1.39	1.52
1	N	145	GLU	CD-OE1	6.42	1.32	1.25
1	H	338	THR	C-O	6.42	1.35	1.23
1	M	367	GLU	CD-OE1	6.41	1.32	1.25
1	D	73	PHE	CD1-CE1	6.41	1.52	1.39
1	D	299	THR	C-O	-6.41	1.11	1.23
1	F	251	ARG	CZ-NH2	6.41	1.41	1.33
1	G	231	TYR	CE2-CZ	6.40	1.46	1.38
1	M	339	ASN	C-O	-6.40	1.11	1.23
1	I	50	TYR	CE1-CZ	6.39	1.46	1.38
1	N	374	PHE	CG-CD2	6.39	1.48	1.38
1	I	372	PHE	CG-CD2	6.38	1.48	1.38
1	A	444	TYR	CE2-CZ	6.38	1.46	1.38
1	I	442	LYS	CE-NZ	6.38	1.65	1.49
1	D	83	PHE	CG-CD2	6.38	1.48	1.38
1	F	328	PHE	CB-CG	-6.38	1.40	1.51
1	N	153	GLN	CB-CG	6.38	1.69	1.52
1	A	306	ASN	CA-CB	-6.37	1.36	1.53
1	K	269	GLU	CD-OE2	6.37	1.32	1.25
1	L	307	LYS	C-O	6.37	1.35	1.23
1	N	24	THR	CB-CG2	-6.37	1.31	1.52
1	K	390	HIS	C-O	6.36	1.35	1.23
1	N	474	LEU	C-OXT	6.36	1.35	1.23
1	I	392	MET	CB-CG	6.36	1.71	1.51
1	A	452	LYS	CE-NZ	6.36	1.65	1.49
1	C	367	GLU	CD-OE2	6.36	1.32	1.25
1	F	162	ARG	CZ-NH1	6.35	1.41	1.33
1	N	248	PHE	CD1-CE1	6.35	1.51	1.39
1	H	135	TYR	CD2-CE2	6.34	1.48	1.39
1	E	261	PHE	CD1-CE1	-6.34	1.26	1.39
1	J	309	TYR	CG-CD1	6.34	1.47	1.39
1	M	220	VAL	CB-CG2	6.34	1.66	1.52
1	A	385	VAL	CB-CG2	6.34	1.66	1.52
1	O	320	GLY	N-CA	6.34	1.55	1.46
1	A	157	CYS	CA-CB	-6.34	1.40	1.53
1	A	307	LYS	CD-CE	6.34	1.67	1.51
1	H	255	MET	C-O	6.34	1.35	1.23
1	E	257	VAL	CB-CG1	-6.33	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	232	PRO	CA-C	-6.33	1.40	1.52
1	O	254	GLN	C-O	-6.33	1.11	1.23
1	K	216	ASN	CG-ND2	6.32	1.48	1.32
1	N	284	LEU	C-O	6.32	1.35	1.23
1	L	366	GLU	CD-OE1	6.32	1.32	1.25
1	F	238	VAL	CB-CG2	-6.32	1.39	1.52
1	J	125	LYS	CD-CE	6.32	1.67	1.51
1	B	374	PHE	C-O	6.32	1.35	1.23
1	C	91	TYR	CE1-CZ	6.32	1.46	1.38
1	L	286	SER	C-O	6.32	1.35	1.23
1	B	271	VAL	CB-CG2	-6.32	1.39	1.52
1	G	248	PHE	CE1-CZ	6.32	1.49	1.37
1	B	332	VAL	CA-CB	-6.31	1.41	1.54
1	E	40	SER	C-O	6.31	1.35	1.23
1	M	50	TYR	CD2-CE2	6.31	1.48	1.39
1	O	160	GLY	C-O	6.31	1.33	1.23
1	I	368	TYR	CD1-CE1	6.30	1.48	1.39
1	D	468	PHE	CB-CG	6.30	1.62	1.51
1	A	310	TRP	CD2-CE2	6.30	1.49	1.41
1	H	64	LYS	CD-CE	6.30	1.67	1.51
1	K	342	VAL	CB-CG2	-6.29	1.39	1.52
1	O	99	VAL	CB-CG1	6.29	1.66	1.52
1	K	189	GLU	CD-OE1	6.29	1.32	1.25
1	N	372	PHE	CE2-CZ	6.29	1.49	1.37
1	A	27	TYR	C-O	6.29	1.35	1.23
1	D	209	ASP	C-O	-6.28	1.11	1.23
1	N	450	ASP	C-O	6.28	1.35	1.23
1	J	43	LEU	CG-CD1	6.28	1.75	1.51
1	E	215	ALA	CA-CB	-6.28	1.39	1.52
1	L	446	PHE	CE2-CZ	6.27	1.49	1.37
1	L	34	TYR	CD2-CE2	-6.27	1.29	1.39
1	N	368	TYR	CB-CG	-6.27	1.42	1.51
1	M	309	TYR	CD1-CE1	6.26	1.48	1.39
1	C	368	TYR	CE2-CZ	6.26	1.46	1.38
1	B	296	SER	CB-OG	-6.26	1.34	1.42
1	J	286	SER	CB-OG	6.26	1.50	1.42
1	N	366	GLU	CD-OE2	6.26	1.32	1.25
1	A	283	THR	C-O	6.26	1.35	1.23
1	B	157	CYS	CB-SG	6.26	1.92	1.82
1	H	35	TYR	CZ-OH	6.26	1.48	1.37
1	A	23	SER	CB-OG	6.25	1.50	1.42
1	H	224	ILE	C-O	6.25	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	371	GLN	C-O	6.25	1.35	1.23
1	M	117	ILE	CB-CG2	6.25	1.72	1.52
1	I	276	TYR	CD1-CE1	6.24	1.48	1.39
1	N	212	THR	C-O	-6.24	1.11	1.23
1	E	189	GLU	CD-OE1	6.24	1.32	1.25
1	K	338	THR	C-O	6.24	1.35	1.23
1	L	355	ASN	CB-CG	6.24	1.65	1.51
1	M	253	GLU	CD-OE2	6.24	1.32	1.25
1	G	457	ALA	CA-CB	-6.23	1.39	1.52
1	O	38	GLY	N-CA	6.23	1.55	1.46
1	E	33	ILE	CB-CG2	-6.23	1.33	1.52
1	M	260	LEU	C-O	6.22	1.35	1.23
1	D	68	LEU	C-O	-6.21	1.11	1.23
1	G	256	PHE	CE1-CZ	-6.21	1.25	1.37
1	K	254	GLN	CG-CD	-6.21	1.36	1.51
1	B	222	LEU	N-CA	6.21	1.58	1.46
1	G	300	SER	CA-CB	6.20	1.62	1.52
1	O	106	GLU	CD-OE1	6.20	1.32	1.25
1	B	55	GLN	CG-CD	6.20	1.65	1.51
1	D	449	VAL	CA-CB	6.20	1.67	1.54
1	D	291	PRO	N-CA	-6.20	1.36	1.47
1	N	240	GLU	CD-OE1	6.19	1.32	1.25
1	H	336	ARG	CZ-NH1	6.19	1.41	1.33
1	A	309	TYR	CE2-CZ	6.19	1.46	1.38
1	I	20	ALA	N-CA	6.18	1.58	1.46
1	A	37	ALA	CA-CB	6.18	1.65	1.52
1	C	41	ARG	CB-CG	6.18	1.69	1.52
1	L	130	GLU	CD-OE1	6.18	1.32	1.25
1	F	247	PHE	CE1-CZ	6.18	1.49	1.37
1	K	70	TYR	CE2-CZ	6.18	1.46	1.38
1	L	145	GLU	CD-OE1	-6.18	1.18	1.25
1	F	70	TYR	CG-CD1	6.17	1.47	1.39
1	G	231	TYR	CG-CD2	6.17	1.47	1.39
1	I	252	ARG	C-O	6.17	1.35	1.23
1	D	167	GLU	C-O	-6.17	1.11	1.23
1	F	74	ARG	CZ-NH2	6.17	1.41	1.33
1	H	73	PHE	CE1-CZ	6.16	1.49	1.37
1	C	457	ALA	CA-CB	6.16	1.65	1.52
1	L	100	TRP	CG-CD1	-6.16	1.28	1.36
1	D	64	LYS	CD-CE	6.15	1.66	1.51
1	M	115	VAL	C-O	6.15	1.35	1.23
1	O	49	TYR	CD1-CE1	6.15	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	99	VAL	CB-CG2	-6.15	1.40	1.52
1	B	365	GLY	C-O	6.15	1.33	1.23
1	F	398	GLU	CD-OE2	6.15	1.32	1.25
1	M	49	TYR	CZ-OH	-6.14	1.27	1.37
1	E	209	ASP	CB-CG	6.14	1.64	1.51
1	K	453	GLU	CD-OE2	6.14	1.32	1.25
1	C	391	SER	CB-OG	6.13	1.50	1.42
1	C	64	LYS	CE-NZ	6.13	1.64	1.49
1	F	217	LYS	CE-NZ	-6.13	1.33	1.49
1	L	35	TYR	C-O	6.13	1.34	1.23
1	B	248	PHE	CD1-CE1	6.13	1.51	1.39
1	F	102	CYS	C-O	6.13	1.34	1.23
1	K	64	LYS	CE-NZ	6.13	1.64	1.49
1	C	440	PRO	N-CD	6.12	1.56	1.47
1	M	377	CYS	CB-SG	-6.12	1.71	1.82
1	M	393	ASN	C-O	6.12	1.34	1.23
1	G	453	GLU	CD-OE2	6.12	1.32	1.25
1	K	444	TYR	CG-CD1	6.12	1.47	1.39
1	L	82	LYS	CB-CG	6.12	1.69	1.52
1	H	328	PHE	CB-CG	6.12	1.61	1.51
1	J	363	ARG	CB-CG	-6.12	1.36	1.52
1	L	70	TYR	CZ-OH	-6.12	1.27	1.37
1	F	70	TYR	CE1-CZ	6.12	1.46	1.38
1	G	90	PHE	N-CA	6.12	1.58	1.46
1	D	257	VAL	CB-CG1	-6.11	1.40	1.52
1	K	65	VAL	CB-CG1	-6.11	1.40	1.52
1	E	165	ILE	CA-CB	-6.11	1.40	1.54
1	L	452	LYS	CE-NZ	6.10	1.64	1.49
1	O	366	GLU	CB-CG	6.10	1.63	1.52
1	C	210	PHE	CD1-CE1	6.10	1.51	1.39
1	E	234	TYR	CE1-CZ	6.10	1.46	1.38
1	L	70	TYR	CD1-CE1	6.10	1.48	1.39
1	D	155	GLN	CG-CD	-6.10	1.37	1.51
1	K	99	VAL	CA-CB	-6.10	1.42	1.54
1	D	155	GLN	CD-NE2	6.10	1.48	1.32
1	G	456	SER	CB-OG	6.10	1.50	1.42
1	J	145	GLU	CD-OE1	6.10	1.32	1.25
1	G	323	TRP	CZ3-CH2	6.09	1.49	1.40
1	H	291	PRO	CA-CB	-6.09	1.41	1.53
1	C	229	CYS	CB-SG	6.09	1.92	1.82
1	F	369	ASP	C-O	-6.09	1.11	1.23
1	H	258	ARG	CZ-NH2	6.08	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	59	LYS	CE-NZ	6.08	1.64	1.49
1	B	70	TYR	CZ-OH	-6.08	1.27	1.37
1	H	298	VAL	CB-CG1	6.08	1.65	1.52
1	C	167	GLU	CG-CD	6.08	1.61	1.51
1	F	224	ILE	CA-CB	6.08	1.68	1.54
1	C	371	GLN	C-O	6.07	1.34	1.23
1	F	468	PHE	CB-CG	6.07	1.61	1.51
1	C	354	LYS	CE-NZ	6.06	1.64	1.49
1	C	374	PHE	CG-CD2	6.06	1.47	1.38
1	D	146	CYS	N-CA	6.05	1.58	1.46
1	C	272	PRO	C-O	-6.05	1.11	1.23
1	H	34	TYR	CE1-CZ	-6.05	1.30	1.38
1	L	442	LYS	CE-NZ	6.05	1.64	1.49
1	M	21	VAL	CB-CG1	6.05	1.65	1.52
1	N	236	LYS	CE-NZ	6.05	1.64	1.49
1	K	205	PHE	CD2-CE2	6.04	1.51	1.39
1	L	325	ASN	C-O	6.04	1.34	1.23
1	C	115	VAL	CB-CG1	6.04	1.65	1.52
1	G	472	ALA	CA-CB	-6.04	1.39	1.52
1	C	98	LEU	CG-CD1	6.03	1.74	1.51
1	E	233	ASP	C-O	6.03	1.34	1.23
1	D	389	ILE	CB-CG2	-6.03	1.34	1.52
1	A	148	SER	CB-OG	-6.03	1.34	1.42
1	G	71	ARG	CA-CB	6.02	1.67	1.53
1	E	331	VAL	CB-CG1	6.02	1.65	1.52
1	G	291	PRO	N-CA	-6.01	1.37	1.47
1	C	93	PRO	CG-CD	-6.01	1.30	1.50
1	E	374	PHE	CE2-CZ	6.01	1.48	1.37
1	G	289	TYR	CE2-CZ	-6.01	1.30	1.38
1	L	99	VAL	CB-CG1	6.01	1.65	1.52
1	M	466	ARG	C-O	6.01	1.34	1.23
1	L	309	TYR	CE2-CZ	6.00	1.46	1.38
1	F	70	TYR	C-O	6.00	1.34	1.23
1	L	161	CYS	CB-SG	-6.00	1.72	1.82
1	L	255	MET	C-O	6.00	1.34	1.23
1	M	162	ARG	CG-CD	6.00	1.67	1.51
1	D	91	TYR	CG-CD1	6.00	1.47	1.39
1	J	87	ASP	C-O	5.99	1.34	1.23
1	A	151	TYR	CB-CG	-5.99	1.42	1.51
1	A	276	TYR	CE1-CZ	5.99	1.46	1.38
1	C	135	TYR	CD1-CE1	5.99	1.48	1.39
1	M	323	TRP	CE3-CZ3	5.99	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	378	LYS	CE-NZ	5.99	1.64	1.49
1	N	368	TYR	CD2-CE2	5.99	1.48	1.39
1	F	45	VAL	CA-CB	-5.99	1.42	1.54
1	K	444	TYR	CE2-CZ	5.99	1.46	1.38
1	I	153	GLN	CB-CG	5.98	1.68	1.52
1	B	307	LYS	CB-CG	5.98	1.68	1.52
1	F	455	PHE	CE2-CZ	5.98	1.48	1.37
1	K	389	ILE	C-O	5.98	1.34	1.23
1	C	157	CYS	N-CA	-5.98	1.34	1.46
1	F	401	ASN	C-O	5.98	1.34	1.23
1	F	247	PHE	CE2-CZ	-5.98	1.25	1.37
1	K	185	CYS	CB-SG	-5.97	1.72	1.81
1	J	240	GLU	CB-CG	5.97	1.63	1.52
1	L	310	TRP	CZ3-CH2	5.97	1.49	1.40
1	O	347	SER	CB-OG	5.97	1.50	1.42
1	G	210	PHE	CE1-CZ	5.96	1.48	1.37
1	J	308	PRO	CA-C	-5.96	1.41	1.52
1	L	331	VAL	CA-CB	5.96	1.67	1.54
1	N	20	ALA	C-O	5.96	1.34	1.23
1	H	21	VAL	CB-CG1	-5.96	1.40	1.52
1	D	85	PHE	CD2-CE2	5.95	1.51	1.39
1	A	337	SER	CB-OG	-5.95	1.34	1.42
1	I	376	LEU	CB-CG	5.95	1.69	1.52
1	K	359	LYS	CD-CE	5.95	1.66	1.51
1	I	467	LYS	CE-NZ	5.95	1.64	1.49
1	I	173	THR	CA-CB	5.95	1.68	1.53
1	D	206	GLY	N-CA	-5.94	1.37	1.46
1	M	455	PHE	CD1-CE1	5.94	1.51	1.39
1	M	388	TYR	CD1-CE1	-5.94	1.30	1.39
1	G	171	LYS	CB-CG	-5.94	1.36	1.52
1	K	276	TYR	CE1-CZ	5.94	1.46	1.38
1	F	236	LYS	CG-CD	5.94	1.72	1.52
1	I	240	GLU	CD-OE2	5.94	1.32	1.25
1	N	82	LYS	CB-CG	5.93	1.68	1.52
1	G	453	GLU	CG-CD	5.93	1.60	1.51
1	O	27	TYR	CG-CD1	5.93	1.46	1.39
1	D	35	TYR	CE2-CZ	5.93	1.46	1.38
1	D	53	LYS	CE-NZ	5.93	1.63	1.49
1	H	320	GLY	N-CA	5.93	1.54	1.46
1	C	37	ALA	C-O	5.93	1.34	1.23
1	B	105	VAL	CB-CG2	-5.93	1.40	1.52
1	I	100	TRP	CB-CG	5.93	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	210	PHE	CG-CD1	5.93	1.47	1.38
1	J	261	PHE	CG-CD2	-5.92	1.29	1.38
1	K	290	PHE	CE2-CZ	5.92	1.48	1.37
1	I	468	PHE	CD2-CE2	-5.92	1.27	1.39
1	F	232	PRO	N-CD	-5.92	1.39	1.47
1	K	248	PHE	CD2-CE2	5.92	1.51	1.39
1	N	309	TYR	CD2-CE2	-5.91	1.30	1.39
1	E	359	LYS	C-O	5.91	1.34	1.23
1	I	101	ALA	CA-CB	-5.91	1.40	1.52
1	B	198	GLY	C-O	5.91	1.33	1.23
1	E	289	TYR	CE2-CZ	5.91	1.46	1.38
1	J	188	LEU	C-O	-5.91	1.12	1.23
1	O	27	TYR	CD1-CE1	5.91	1.48	1.39
1	B	70	TYR	CB-CG	-5.91	1.42	1.51
1	A	154	THR	CA-CB	5.90	1.68	1.53
1	C	261	PHE	CD1-CE1	5.90	1.51	1.39
1	O	98	LEU	C-O	5.90	1.34	1.23
1	M	389	ILE	C-O	5.90	1.34	1.23
1	D	149	MET	CB-CG	5.89	1.70	1.51
1	N	466	ARG	CZ-NH2	5.89	1.40	1.33
1	K	444	TYR	CD1-CE1	5.89	1.48	1.39
1	O	323	TRP	CZ3-CH2	5.89	1.49	1.40
1	H	230	LYS	CE-NZ	5.89	1.63	1.49
1	C	153	GLN	CG-CD	5.89	1.64	1.51
1	E	269	GLU	CD-OE1	5.89	1.32	1.25
1	F	215	ALA	CA-CB	-5.89	1.40	1.52
1	G	314	ALA	CA-C	-5.89	1.37	1.52
1	N	29	THR	N-CA	-5.89	1.34	1.46
1	D	30	ARG	CZ-NH1	-5.88	1.25	1.33
1	I	456	SER	CB-OG	5.88	1.49	1.42
1	J	48	PRO	N-CA	-5.88	1.37	1.47
1	C	91	TYR	CE2-CZ	5.88	1.46	1.38
1	C	245	MET	N-CA	-5.88	1.34	1.46
1	C	249	TYR	CG-CD2	-5.88	1.31	1.39
1	J	202	ASP	C-O	5.87	1.34	1.23
1	N	398	GLU	CD-OE2	5.87	1.32	1.25
1	J	248	PHE	CE2-CZ	5.87	1.48	1.37
1	F	283	THR	CA-CB	5.87	1.68	1.53
1	J	21	VAL	CB-CG2	5.87	1.65	1.52
1	J	366	GLU	CD-OE1	5.87	1.32	1.25
1	B	372	PHE	CD1-CE1	5.86	1.50	1.39
1	C	263	ARG	CZ-NH1	5.86	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	345	ALA	CA-CB	5.86	1.64	1.52
1	E	21	VAL	CB-CG2	5.86	1.65	1.52
1	N	336	ARG	CZ-NH1	5.85	1.40	1.33
1	H	336	ARG	CZ-NH2	5.85	1.40	1.33
1	G	309	TYR	CE2-CZ	5.85	1.46	1.38
1	I	231	TYR	CG-CD1	5.85	1.46	1.39
1	N	219	ASP	N-CA	5.85	1.58	1.46
1	A	108	GLY	N-CA	-5.85	1.37	1.46
1	L	49	TYR	CD1-CE1	-5.85	1.30	1.39
1	F	308	PRO	N-CA	-5.84	1.37	1.47
1	F	336	ARG	NE-CZ	5.84	1.40	1.33
1	H	261	PHE	CE2-CZ	5.84	1.48	1.37
1	M	374	PHE	CE1-CZ	5.84	1.48	1.37
1	O	171	LYS	CE-NZ	5.84	1.63	1.49
1	J	364	HIS	C-O	5.84	1.34	1.23
1	K	336	ARG	CZ-NH2	5.84	1.40	1.33
1	A	105	VAL	CA-CB	-5.83	1.42	1.54
1	F	331	VAL	N-CA	-5.83	1.34	1.46
1	I	249	TYR	CD2-CE2	5.83	1.48	1.39
1	E	368	TYR	CG-CD2	-5.83	1.31	1.39
1	H	130	GLU	CD-OE1	5.83	1.32	1.25
1	E	250	LEU	C-O	5.82	1.34	1.23
1	F	111	GLN	CB-CG	-5.82	1.36	1.52
1	M	276	TYR	CE2-CZ	5.82	1.46	1.38
1	I	305	PHE	CB-CG	5.82	1.61	1.51
1	C	144	ARG	CZ-NH2	-5.82	1.25	1.33
1	C	272	PRO	CA-C	-5.82	1.41	1.52
1	F	38	GLY	N-CA	5.82	1.54	1.46
1	F	360	GLU	CD-OE1	5.82	1.32	1.25
1	J	296	SER	CB-OG	-5.82	1.34	1.42
1	J	34	TYR	CD1-CE1	5.81	1.48	1.39
1	D	194	VAL	CB-CG2	5.81	1.65	1.52
1	L	156	LEU	C-O	5.81	1.34	1.23
1	M	215	ALA	CA-CB	-5.81	1.40	1.52
1	K	368	TYR	CE1-CZ	5.81	1.46	1.38
1	M	169	TRP	CD2-CE3	-5.81	1.31	1.40
1	N	242	TYR	CE1-CZ	5.81	1.46	1.38
1	J	374	PHE	CE1-CZ	5.81	1.48	1.37
1	M	59	LYS	CE-NZ	5.81	1.63	1.49
1	K	113	LEU	CG-CD1	5.80	1.73	1.51
1	K	231	TYR	CD1-CE1	-5.80	1.30	1.39
1	E	261	PHE	CA-CB	5.80	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	309	TYR	CE2-CZ	5.80	1.46	1.38
1	H	309	TYR	CD2-CE2	5.80	1.48	1.39
1	C	130	GLU	CD-OE1	5.80	1.32	1.25
1	E	114	GLY	C-O	5.79	1.32	1.23
1	J	170	GLY	C-O	-5.79	1.14	1.23
1	L	211	THR	CB-CG2	-5.79	1.33	1.52
1	I	27	TYR	C-O	5.79	1.34	1.23
1	I	324	SER	CA-CB	5.79	1.61	1.52
1	H	26	GLU	CD-OE1	5.79	1.32	1.25
1	O	358	PHE	CE2-CZ	5.79	1.48	1.37
1	G	463	PRO	N-CA	-5.79	1.37	1.47
1	N	90	PHE	N-CA	5.78	1.57	1.46
1	E	361	TYR	CD2-CE2	5.78	1.48	1.39
1	K	70	TYR	CA-CB	-5.78	1.41	1.53
1	O	72	VAL	CB-CG2	5.78	1.65	1.52
1	K	368	TYR	CD1-CE1	5.78	1.48	1.39
1	K	27	TYR	CE1-CZ	5.77	1.46	1.38
1	B	284	LEU	C-O	-5.77	1.12	1.23
1	F	444	TYR	CD2-CE2	-5.77	1.30	1.39
1	M	153	GLN	CD-OE1	5.77	1.36	1.24
1	B	377	CYS	CB-SG	-5.77	1.72	1.81
1	E	291	PRO	CA-CB	-5.77	1.42	1.53
1	J	367	GLU	CD-OE2	5.77	1.31	1.25
1	J	372	PHE	CG-CD2	5.77	1.47	1.38
1	C	66	SER	CB-OG	5.76	1.49	1.42
1	G	107	VAL	C-O	5.76	1.34	1.23
1	K	353	TYR	CE1-CZ	5.76	1.46	1.38
1	N	231	TYR	C-O	-5.76	1.12	1.23
1	B	253	GLU	CD-OE2	5.76	1.31	1.25
1	M	220	VAL	CB-CG1	5.76	1.65	1.52
1	L	205	PHE	CG-CD1	5.76	1.47	1.38
1	D	217	LYS	CD-CE	5.76	1.65	1.51
1	E	309	TYR	CD1-CE1	5.76	1.48	1.39
1	H	75	VAL	CA-CB	-5.76	1.42	1.54
1	G	217	LYS	CE-NZ	5.75	1.63	1.49
1	L	398	GLU	CB-CG	5.75	1.63	1.52
1	O	230	LYS	C-O	5.75	1.34	1.23
1	F	175	SER	CB-OG	5.75	1.49	1.42
1	K	309	TYR	CE2-CZ	5.75	1.46	1.38
1	M	145	GLU	CG-CD	5.75	1.60	1.51
1	I	148	SER	CA-CB	5.75	1.61	1.52
1	M	444	TYR	CD2-CE2	-5.75	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	342	VAL	CB-CG2	5.75	1.65	1.52
1	A	83	PHE	CE1-CZ	5.75	1.48	1.37
1	B	166	GLY	N-CA	-5.75	1.37	1.46
1	E	261	PHE	CD2-CE2	-5.74	1.27	1.39
1	M	368	TYR	CA-CB	-5.74	1.41	1.53
1	D	328	PHE	CB-CG	-5.74	1.41	1.51
1	A	135	TYR	CG-CD1	5.74	1.46	1.39
1	B	271	VAL	CB-CG1	-5.74	1.40	1.52
1	E	53	LYS	CE-NZ	5.74	1.63	1.49
1	M	70	TYR	CD1-CE1	-5.74	1.30	1.39
1	G	75	VAL	CB-CG1	-5.74	1.40	1.52
1	J	279	GLY	C-O	5.74	1.32	1.23
1	A	130	GLU	CB-CG	-5.74	1.41	1.52
1	A	202	ASP	C-O	5.74	1.34	1.23
1	E	40	SER	CA-C	5.73	1.67	1.52
1	F	107	VAL	C-O	-5.73	1.12	1.23
1	G	378	LYS	CE-NZ	5.73	1.63	1.49
1	J	328	PHE	CD2-CE2	5.73	1.50	1.39
1	M	354	LYS	CD-CE	5.73	1.65	1.51
1	A	76	LYS	CD-CE	5.73	1.65	1.51
1	E	353	TYR	CD2-CE2	5.73	1.48	1.39
1	E	327	LEU	N-CA	-5.73	1.34	1.46
1	F	289	TYR	CE1-CZ	5.72	1.46	1.38
1	L	467	LYS	CB-CG	5.72	1.68	1.52
1	F	366	GLU	CG-CD	5.72	1.60	1.51
1	O	257	VAL	C-O	5.72	1.34	1.23
1	B	400	TRP	CE3-CZ3	-5.72	1.28	1.38
1	G	23	SER	CB-OG	-5.72	1.34	1.42
1	F	177	ALA	CA-CB	5.72	1.64	1.52
1	B	130	GLU	CD-OE1	-5.71	1.19	1.25
1	C	39	SER	CA-CB	-5.71	1.44	1.52
1	G	310	TRP	CA-CB	-5.71	1.41	1.53
1	K	66	SER	CB-OG	5.71	1.49	1.42
1	N	265	GLY	C-O	5.71	1.32	1.23
1	K	28	VAL	CB-CG2	-5.71	1.40	1.52
1	N	340	MET	CB-CG	-5.71	1.33	1.51
1	K	300	SER	CB-OG	5.71	1.49	1.42
1	E	50	TYR	CB-CG	-5.70	1.43	1.51
1	I	305	PHE	CG-CD1	5.70	1.47	1.38
1	E	346	VAL	CB-CG2	-5.70	1.40	1.52
1	I	231	TYR	CD1-CE1	5.70	1.47	1.39
1	J	135	TYR	CD2-CE2	5.70	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	367	GLU	CG-CD	5.70	1.60	1.51
1	A	308	PRO	N-CA	-5.70	1.37	1.47
1	A	151	TYR	CD1-CE1	5.70	1.47	1.39
1	L	460	ASP	CB-CG	5.70	1.63	1.51
1	O	185	CYS	CB-SG	5.70	1.92	1.82
1	G	149	MET	CB-CG	5.69	1.69	1.51
1	B	305	PHE	CD1-CE1	5.69	1.50	1.39
1	H	274	ASP	CB-CG	5.69	1.63	1.51
1	H	329	VAL	CB-CG1	5.69	1.64	1.52
1	F	45	VAL	CB-CG2	-5.69	1.41	1.52
1	E	201	VAL	CB-CG2	5.68	1.64	1.52
1	H	70	TYR	CD2-CE2	-5.68	1.30	1.39
1	M	106	GLU	CD-OE2	5.68	1.31	1.25
1	K	91	TYR	CD2-CE2	-5.68	1.30	1.39
1	K	363	ARG	CG-CD	5.68	1.66	1.51
1	F	307	LYS	CE-NZ	5.68	1.63	1.49
1	L	361	TYR	CE1-CZ	5.68	1.46	1.38
1	J	91	TYR	CZ-OH	5.67	1.47	1.37
1	F	77	LEU	CG-CD1	-5.67	1.30	1.51
1	O	82	LYS	CD-CE	5.67	1.65	1.51
1	O	336	ARG	CZ-NH1	5.67	1.40	1.33
1	A	308	PRO	CB-CG	-5.67	1.21	1.50
1	B	363	ARG	CA-CB	5.67	1.66	1.53
1	J	307	LYS	CB-CG	5.67	1.67	1.52
1	K	152	LYS	CD-CE	5.67	1.65	1.51
1	G	210	PHE	CG-CD2	5.66	1.47	1.38
1	I	157	CYS	CA-CB	-5.66	1.41	1.53
1	I	242	TYR	CB-CG	5.66	1.60	1.51
1	M	361	TYR	CD2-CE2	5.66	1.47	1.39
1	B	44	ALA	CA-CB	5.66	1.64	1.52
1	I	30	ARG	CZ-NH1	-5.66	1.25	1.33
1	H	115	VAL	C-O	5.66	1.34	1.23
1	K	388	TYR	CE2-CZ	5.66	1.46	1.38
1	A	144	ARG	CZ-NH1	5.65	1.40	1.33
1	D	160	GLY	C-O	5.65	1.32	1.23
1	G	73	PHE	CE2-CZ	5.65	1.48	1.37
1	G	205	PHE	CD1-CE1	5.65	1.50	1.39
1	A	151	TYR	CD2-CE2	5.65	1.47	1.39
1	A	307	LYS	CE-NZ	5.65	1.63	1.49
1	B	285	PRO	C-O	5.65	1.34	1.23
1	K	468	PHE	CD1-CE1	-5.65	1.27	1.39
1	M	173	THR	CA-CB	5.65	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	113	LEU	CG-CD2	5.64	1.72	1.51
1	E	231	TYR	CE1-CZ	-5.64	1.31	1.38
1	H	373	ILE	CA-CB	-5.63	1.41	1.54
1	B	211	THR	CB-CG2	5.63	1.71	1.52
1	C	222	LEU	N-CA	5.63	1.57	1.46
1	M	365	GLY	C-O	5.63	1.32	1.23
1	E	22	VAL	CB-CG1	-5.62	1.41	1.52
1	H	205	PHE	CE1-CZ	5.62	1.48	1.37
1	G	249	TYR	CZ-OH	5.62	1.47	1.37
1	N	44	ALA	CA-CB	5.62	1.64	1.52
1	L	298	VAL	CB-CG2	-5.62	1.41	1.52
1	F	353	TYR	CG-CD1	5.62	1.46	1.39
1	K	457	ALA	CA-CB	-5.62	1.40	1.52
1	L	91	TYR	CD2-CE2	5.62	1.47	1.39
1	B	74	ARG	CG-CD	5.61	1.66	1.51
1	J	374	PHE	CG-CD1	5.61	1.47	1.38
1	A	65	VAL	CB-CG2	-5.61	1.41	1.52
1	L	90	PHE	CD1-CE1	5.61	1.50	1.39
1	E	51	ALA	CA-CB	-5.61	1.40	1.52
1	B	194	VAL	CB-CG2	-5.61	1.41	1.52
1	C	76	LYS	CG-CD	5.61	1.71	1.52
1	C	114	GLY	C-O	5.61	1.32	1.23
1	C	183	GLY	C-O	-5.61	1.14	1.23
1	C	398	GLU	CB-CG	5.61	1.62	1.52
1	E	220	VAL	CB-CG2	5.61	1.64	1.52
1	G	115	VAL	C-O	5.61	1.34	1.23
1	K	252	ARG	CB-CG	5.60	1.67	1.52
1	E	83	PHE	CG-CD2	5.60	1.47	1.38
1	G	367	GLU	CD-OE2	5.60	1.31	1.25
1	L	68	LEU	CG-CD1	5.60	1.72	1.51
1	O	444	TYR	CD1-CE1	-5.60	1.30	1.39
1	G	240	GLU	CG-CD	5.60	1.60	1.51
1	A	101	ALA	CA-CB	-5.59	1.40	1.52
1	A	112	PRO	C-O	-5.59	1.12	1.23
1	A	309	TYR	C-O	-5.59	1.12	1.23
1	I	358	PHE	CG-CD2	5.59	1.47	1.38
1	M	321	ILE	CB-CG2	5.59	1.70	1.52
1	C	99	VAL	CB-CG1	5.59	1.64	1.52
1	C	374	PHE	CE1-CZ	5.58	1.48	1.37
1	I	374	PHE	CG-CD2	5.58	1.47	1.38
1	K	90	PHE	CE2-CZ	5.58	1.48	1.37
1	A	348	SER	C-O	5.58	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	146	CYS	CB-SG	5.58	1.91	1.82
1	H	368	TYR	C-O	-5.58	1.12	1.23
1	I	63	PRO	C-O	-5.58	1.12	1.23
1	I	372	PHE	CE1-CZ	5.58	1.48	1.37
1	L	276	TYR	CE1-CZ	5.58	1.45	1.38
1	O	173	THR	CA-CB	5.57	1.67	1.53
1	L	290	PHE	CD2-CE2	5.57	1.50	1.39
1	M	173	THR	C-N	5.57	1.44	1.34
1	A	304	ILE	CA-CB	-5.57	1.42	1.54
1	L	62	VAL	CB-CG1	5.57	1.64	1.52
1	J	35	TYR	CB-CG	-5.57	1.43	1.51
1	L	240	GLU	CB-CG	5.57	1.62	1.52
1	C	121	PRO	CB-CG	5.56	1.77	1.50
1	D	103	THR	C-O	5.56	1.33	1.23
1	G	396	ILE	CB-CG2	-5.56	1.35	1.52
1	K	132	SER	CA-CB	5.56	1.61	1.52
1	E	115	VAL	CA-CB	5.56	1.66	1.54
1	G	175	SER	CB-OG	5.56	1.49	1.42
1	H	360	GLU	CG-CD	5.56	1.60	1.51
1	J	116	GLY	C-O	-5.56	1.14	1.23
1	K	276	TYR	CG-CD2	5.56	1.46	1.39
1	C	261	PHE	CA-CB	-5.56	1.41	1.53
1	A	278	LYS	CD-CE	5.55	1.65	1.51
1	H	157	CYS	N-CA	-5.55	1.35	1.46
1	J	20	ALA	N-CA	5.55	1.57	1.46
1	L	387	THR	CB-CG2	5.55	1.70	1.52
1	B	106	GLU	CB-CG	5.55	1.62	1.52
1	B	333	ASP	CG-OD2	5.55	1.38	1.25
1	F	258	ARG	C-O	5.55	1.33	1.23
1	L	334	THR	CA-CB	5.54	1.67	1.53
1	H	135	TYR	CD1-CE1	5.54	1.47	1.39
1	K	145	GLU	CG-CD	5.54	1.60	1.51
1	J	248	PHE	CG-CD1	5.54	1.47	1.38
1	I	474	LEU	CG-CD2	5.54	1.72	1.51
1	K	202	ASP	CB-CG	5.53	1.63	1.51
1	A	70	TYR	CG-CD2	-5.53	1.31	1.39
1	F	466	ARG	CZ-NH2	5.53	1.40	1.33
1	F	90	PHE	N-CA	5.53	1.57	1.46
1	F	102	CYS	N-CA	-5.53	1.35	1.46
1	M	129	THR	C-O	5.53	1.33	1.23
1	H	91	TYR	CD2-CE2	5.52	1.47	1.39
1	L	281	THR	CA-CB	5.52	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	395	SER	CB-OG	-5.52	1.35	1.42
1	E	452	LYS	CD-CE	5.52	1.65	1.51
1	L	76	LYS	CD-CE	5.52	1.65	1.51
1	G	314	ALA	CA-CB	-5.52	1.40	1.52
1	F	276	TYR	CE2-CZ	5.52	1.45	1.38
1	G	151	TYR	CD1-CE1	5.52	1.47	1.39
1	I	130	GLU	CD-OE2	5.52	1.31	1.25
1	A	305	PHE	CD2-CE2	-5.52	1.28	1.39
1	J	217	LYS	CD-CE	5.52	1.65	1.51
1	N	162	ARG	CZ-NH1	5.51	1.40	1.33
1	A	457	ALA	CA-CB	-5.51	1.40	1.52
1	J	398	GLU	CD-OE1	5.51	1.31	1.25
1	B	400	TRP	CD2-CE3	5.51	1.48	1.40
1	J	62	VAL	CA-CB	-5.51	1.43	1.54
1	F	300	SER	CB-OG	-5.51	1.35	1.42
1	G	154	THR	C-O	5.51	1.33	1.23
1	K	232	PRO	CG-CD	5.51	1.68	1.50
1	M	21	VAL	C-O	-5.51	1.12	1.23
1	M	104	GLY	N-CA	-5.51	1.37	1.46
1	N	322	CYS	CB-SG	5.51	1.91	1.82
1	D	113	LEU	CA-CB	-5.50	1.41	1.53
1	L	169	TRP	CB-CG	-5.50	1.40	1.50
1	C	167	GLU	CD-OE2	5.50	1.31	1.25
1	A	27	TYR	CG-CD2	-5.50	1.31	1.39
1	I	309	TYR	CE2-CZ	5.50	1.45	1.38
1	L	395	SER	CA-CB	-5.50	1.44	1.52
1	O	194	VAL	CB-CG2	5.50	1.64	1.52
1	F	269	GLU	CD-OE2	5.50	1.31	1.25
1	E	64	LYS	CG-CD	5.50	1.71	1.52
1	B	347	SER	CB-OG	5.49	1.49	1.42
1	C	305	PHE	CB-CG	-5.49	1.42	1.51
1	I	453	GLU	CD-OE2	5.49	1.31	1.25
1	C	289	TYR	CB-CG	-5.49	1.43	1.51
1	E	90	PHE	N-CA	5.49	1.57	1.46
1	N	332	VAL	CA-CB	-5.49	1.43	1.54
1	M	467	LYS	CE-NZ	5.49	1.62	1.49
1	B	28	VAL	CA-CB	-5.49	1.43	1.54
1	L	385	VAL	CB-CG1	5.49	1.64	1.52
1	M	455	PHE	CE2-CZ	5.49	1.47	1.37
1	B	366	GLU	CA-CB	5.48	1.66	1.53
1	N	328	PHE	CE1-CZ	5.48	1.47	1.37
1	O	224	ILE	CG1-CD1	5.48	1.88	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	152	LYS	CB-CG	5.48	1.67	1.52
1	H	289	TYR	CZ-OH	5.48	1.47	1.37
1	M	78	PRO	N-CA	-5.48	1.38	1.47
1	A	290	PHE	C-O	5.48	1.33	1.23
1	L	380	THR	C-O	5.48	1.33	1.23
1	M	63	PRO	CB-CG	5.48	1.77	1.50
1	I	375	GLN	C-O	5.48	1.33	1.23
1	B	91	TYR	CE1-CZ	-5.47	1.31	1.38
1	C	50	TYR	CG-CD2	5.47	1.46	1.39
1	B	249	TYR	CZ-OH	5.47	1.47	1.37
1	B	83	PHE	CG-CD2	5.47	1.47	1.38
1	B	447	TRP	CE3-CZ3	5.47	1.47	1.38
1	B	210	PHE	CE1-CZ	-5.47	1.26	1.37
1	B	309	TYR	CG-CD2	5.47	1.46	1.39
1	K	254	GLN	C-O	5.47	1.33	1.23
1	J	182	ALA	CA-CB	-5.47	1.41	1.52
1	N	256	PHE	CE1-CZ	5.47	1.47	1.37
1	A	153	GLN	CG-CD	-5.47	1.38	1.51
1	B	336	ARG	N-CA	-5.46	1.35	1.46
1	I	70	TYR	CG-CD1	5.46	1.46	1.39
1	I	97	ARG	C-O	5.46	1.33	1.23
1	O	169	TRP	CD2-CE2	-5.46	1.34	1.41
1	E	83	PHE	CE1-CZ	5.46	1.47	1.37
1	K	234	TYR	C-O	5.45	1.33	1.23
1	A	258	ARG	N-CA	-5.45	1.35	1.46
1	C	289	TYR	CA-CB	5.45	1.66	1.53
1	O	167	GLU	CD-OE1	5.45	1.31	1.25
1	K	474	LEU	C-OXT	5.45	1.33	1.23
1	M	327	LEU	C-O	5.45	1.33	1.23
1	M	359	LYS	CD-CE	5.45	1.64	1.51
1	E	373	ILE	CA-CB	-5.45	1.42	1.54
1	M	169	TRP	CB-CG	-5.45	1.40	1.50
1	C	65	VAL	CB-CG2	-5.44	1.41	1.52
1	L	70	TYR	CD2-CE2	5.44	1.47	1.39
1	A	132	SER	CB-OG	5.44	1.49	1.42
1	L	323	TRP	CE3-CZ3	5.44	1.47	1.38
1	M	132	SER	CA-CB	5.44	1.61	1.52
1	O	220	VAL	CB-CG1	-5.44	1.41	1.52
1	B	130	GLU	CB-CG	-5.44	1.41	1.52
1	D	240	GLU	CB-CG	5.44	1.62	1.52
1	H	269	GLU	CD-OE2	5.44	1.31	1.25
1	B	191	LEU	C-O	-5.44	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	121	PRO	N-CD	5.43	1.55	1.47
1	B	330	THR	CA-CB	-5.43	1.39	1.53
1	C	135	TYR	CD2-CE2	5.43	1.47	1.39
1	O	323	TRP	C-O	5.43	1.33	1.23
1	A	90	PHE	CD2-CE2	-5.43	1.28	1.39
1	I	158	LEU	CA-CB	-5.43	1.41	1.53
1	M	83	PHE	CD2-CE2	5.43	1.50	1.39
1	O	453	GLU	CD-OE2	5.43	1.31	1.25
1	D	327	LEU	C-O	5.43	1.33	1.23
1	F	246	LEU	N-CA	5.43	1.57	1.46
1	H	336	ARG	C-O	-5.43	1.13	1.23
1	O	95	SER	N-CA	5.43	1.57	1.46
1	C	152	LYS	C-O	5.42	1.33	1.23
1	F	191	LEU	CG-CD2	-5.42	1.31	1.51
1	H	106	GLU	CD-OE2	5.42	1.31	1.25
1	I	197	ASP	N-CA	-5.42	1.35	1.46
1	K	238	VAL	CB-CG1	5.42	1.64	1.52
1	D	240	GLU	CG-CD	5.42	1.60	1.51
1	N	102	CYS	C-O	5.42	1.33	1.23
1	A	50	TYR	CD1-CE1	-5.42	1.31	1.39
1	D	189	GLU	CB-CG	-5.42	1.41	1.52
1	H	336	ARG	CD-NE	5.42	1.55	1.46
1	M	106	GLU	CG-CD	5.42	1.60	1.51
1	E	388	TYR	CE1-CZ	5.42	1.45	1.38
1	K	360	GLU	CG-CD	5.41	1.60	1.51
1	M	75	VAL	CB-CG2	-5.41	1.41	1.52
1	G	372	PHE	CD1-CE1	5.41	1.50	1.39
1	J	149	MET	CA-CB	5.41	1.65	1.53
1	N	372	PHE	CD2-CE2	5.41	1.50	1.39
1	O	160	GLY	N-CA	5.41	1.54	1.46
1	E	296	SER	C-O	5.41	1.33	1.23
1	J	49	TYR	CD2-CE2	5.41	1.47	1.39
1	A	375	GLN	CA-CB	-5.40	1.42	1.53
1	B	444	TYR	CG-CD2	5.40	1.46	1.39
1	E	239	SER	CB-OG	5.40	1.49	1.42
1	F	200	MET	N-CA	-5.40	1.35	1.46
1	J	373	ILE	CA-CB	-5.40	1.42	1.54
1	E	388	TYR	CD1-CE1	5.40	1.47	1.39
1	B	456	SER	C-O	-5.40	1.13	1.23
1	C	338	THR	C-O	5.40	1.33	1.23
1	K	191	LEU	C-O	-5.40	1.13	1.23
1	N	366	GLU	CG-CD	5.40	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	361	TYR	C-O	5.39	1.33	1.23
1	F	99	VAL	CA-CB	-5.39	1.43	1.54
1	M	280	THR	CB-CG2	5.39	1.70	1.52
1	B	239	SER	CB-OG	5.39	1.49	1.42
1	G	299	THR	CB-CG2	5.39	1.70	1.52
1	C	65	VAL	C-O	5.38	1.33	1.23
1	E	222	LEU	CA-CB	-5.38	1.41	1.53
1	I	309	TYR	CG-CD2	5.38	1.46	1.39
1	C	27	TYR	CG-CD2	-5.38	1.32	1.39
1	K	104	GLY	C-O	5.38	1.32	1.23
1	M	368	TYR	CE1-CZ	5.38	1.45	1.38
1	E	466	ARG	CZ-NH2	5.37	1.40	1.33
1	I	256	PHE	CD1-CE1	-5.37	1.28	1.39
1	J	314	ALA	C-O	5.37	1.33	1.23
1	K	136	VAL	CB-CG2	5.37	1.64	1.52
1	B	224	ILE	C-O	-5.37	1.13	1.23
1	D	455	PHE	CD1-CE1	5.37	1.50	1.39
1	E	79	ASP	C-O	-5.37	1.13	1.23
1	J	84	GLY	C-O	5.37	1.32	1.23
1	M	40	SER	CA-CB	5.37	1.61	1.52
1	O	382	THR	CA-CB	5.37	1.67	1.53
1	O	447	TRP	CZ3-CH2	5.37	1.48	1.40
1	H	177	ALA	CA-CB	5.37	1.63	1.52
1	H	95	SER	C-O	-5.37	1.13	1.23
1	K	346	VAL	CB-CG1	-5.37	1.41	1.52
1	L	35	TYR	CE1-CZ	-5.36	1.31	1.38
1	E	194	VAL	CB-CG1	5.36	1.64	1.52
1	B	242	TYR	CB-CG	5.36	1.59	1.51
1	J	216	ASN	C-O	5.36	1.33	1.23
1	L	220	VAL	CB-CG1	5.36	1.64	1.52
1	G	166	GLY	CA-C	5.36	1.60	1.51
1	I	50	TYR	CD1-CE1	-5.36	1.31	1.39
1	M	278	LYS	CE-NZ	5.36	1.62	1.49
1	B	249	TYR	CE2-CZ	5.35	1.45	1.38
1	B	322	CYS	CA-CB	5.35	1.65	1.53
1	E	229	CYS	CB-SG	-5.35	1.73	1.81
1	I	309	TYR	CG-CD1	5.35	1.46	1.39
1	C	79	ASP	C-O	-5.35	1.13	1.23
1	M	151	TYR	CG-CD1	-5.35	1.32	1.39
1	E	362	LEU	CG-CD2	5.35	1.71	1.51
1	I	89	SER	CB-OG	5.35	1.49	1.42
1	L	234	TYR	C-O	5.35	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	190	LEU	C-O	-5.35	1.13	1.23
1	K	154	THR	CA-CB	5.35	1.67	1.53
1	L	153	GLN	CG-CD	5.34	1.63	1.51
1	E	234	TYR	CD2-CE2	5.34	1.47	1.39
1	I	323	TRP	CE3-CZ3	5.34	1.47	1.38
1	B	341	SER	C-O	5.33	1.33	1.23
1	C	205	PHE	CD1-CE1	5.33	1.50	1.39
1	B	33	ILE	N-CA	-5.33	1.35	1.46
1	H	309	TYR	C-O	-5.33	1.13	1.23
1	I	217	LYS	CD-CE	5.33	1.64	1.51
1	M	323	TRP	C-O	5.33	1.33	1.23
1	K	230	LYS	CD-CE	-5.33	1.38	1.51
1	J	189	GLU	CD-OE1	5.33	1.31	1.25
1	K	353	TYR	CB-CG	-5.33	1.43	1.51
1	B	49	TYR	CD1-CE1	-5.32	1.31	1.39
1	H	189	GLU	CD-OE1	5.32	1.31	1.25
1	B	368	TYR	CD1-CE1	5.32	1.47	1.39
1	G	20	ALA	N-CA	5.32	1.56	1.46
1	N	138	ASN	CG-OD1	5.32	1.35	1.24
1	D	56	ASP	CB-CG	5.32	1.62	1.51
1	E	108	GLY	C-O	5.32	1.32	1.23
1	H	309	TYR	CD1-CE1	5.32	1.47	1.39
1	E	150	ASP	CB-CG	5.31	1.62	1.51
1	B	447	TRP	CB-CG	5.31	1.59	1.50
1	E	452	LYS	CB-CG	-5.31	1.38	1.52
1	E	367	GLU	CB-CG	-5.31	1.42	1.52
1	F	367	GLU	CD-OE2	5.30	1.31	1.25
1	F	146	CYS	CB-SG	5.30	1.91	1.82
1	J	151	TYR	CD1-CE1	-5.30	1.31	1.39
1	G	216	ASN	C-O	-5.29	1.13	1.23
1	B	446	PHE	CD2-CE2	5.29	1.49	1.39
1	O	374	PHE	C-O	5.29	1.33	1.23
1	G	99	VAL	CA-CB	-5.29	1.43	1.54
1	O	360	GLU	CG-CD	5.29	1.59	1.51
1	A	468	PHE	CG-CD2	5.29	1.46	1.38
1	H	346	VAL	CB-CG2	-5.29	1.41	1.52
1	O	314	ALA	C-O	5.29	1.33	1.23
1	D	331	VAL	N-CA	5.28	1.56	1.46
1	J	66	SER	CB-OG	-5.28	1.35	1.42
1	A	71	ARG	CZ-NH1	5.28	1.40	1.33
1	F	313	ARG	CG-CD	5.28	1.65	1.51
1	H	253	GLU	CD-OE2	5.28	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	30	ARG	CZ-NH2	5.28	1.40	1.33
1	G	455	PHE	CG-CD1	5.28	1.46	1.38
1	N	220	VAL	CB-CG1	5.28	1.64	1.52
1	J	73	PHE	CE2-CZ	5.28	1.47	1.37
1	M	41	ARG	CG-CD	-5.28	1.38	1.51
1	C	185	CYS	CB-SG	5.27	1.91	1.82
1	M	269	GLU	CD-OE1	5.27	1.31	1.25
1	G	151	TYR	CE2-CZ	5.27	1.45	1.38
1	G	247	PHE	CG-CD1	-5.27	1.30	1.38
1	L	341	SER	CB-OG	5.27	1.49	1.42
1	E	64	LYS	CA-CB	-5.27	1.42	1.53
1	J	359	LYS	CD-CE	5.27	1.64	1.51
1	F	155	GLN	CD-NE2	5.26	1.46	1.32
1	D	91	TYR	CE1-CZ	5.26	1.45	1.38
1	F	274	ASP	CB-CG	5.26	1.62	1.51
1	N	69	GLN	CG-CD	5.26	1.63	1.51
1	O	358	PHE	CB-CG	-5.26	1.42	1.51
1	A	67	GLY	C-O	5.26	1.32	1.23
1	F	95	SER	N-CA	5.26	1.56	1.46
1	I	102	CYS	CB-SG	5.26	1.91	1.82
1	A	336	ARG	CZ-NH2	5.26	1.39	1.33
1	F	40	SER	C-O	5.26	1.33	1.23
1	M	57	SER	CB-OG	5.26	1.49	1.42
1	M	378	LYS	N-CA	-5.26	1.35	1.46
1	F	328	PHE	CD2-CE2	5.25	1.49	1.39
1	L	118	SER	CB-OG	5.25	1.49	1.42
1	H	34	TYR	CG-CD1	5.25	1.46	1.39
1	B	76	LYS	CG-CD	5.24	1.70	1.52
1	B	64	LYS	CE-NZ	5.24	1.62	1.49
1	A	70	TYR	CE1-CZ	5.24	1.45	1.38
1	E	310	TRP	CE3-CZ3	-5.24	1.29	1.38
1	J	288	SER	CB-OG	5.24	1.49	1.42
1	E	323	TRP	CE2-CZ2	5.24	1.48	1.39
1	F	239	SER	C-O	-5.24	1.13	1.23
1	H	448	GLU	CD-OE1	5.24	1.31	1.25
1	I	147	ILE	C-O	-5.24	1.13	1.23
1	C	305	PHE	CG-CD2	-5.24	1.30	1.38
1	D	249	TYR	CE2-CZ	5.24	1.45	1.38
1	L	369	ASP	C-O	5.24	1.33	1.23
1	G	363	ARG	CZ-NH1	5.24	1.39	1.33
1	B	310	TRP	CE3-CZ3	-5.23	1.29	1.38
1	O	65	VAL	C-O	5.23	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	42	LEU	CG-CD2	5.23	1.71	1.51
1	B	118	SER	CB-OG	5.22	1.49	1.42
1	C	173	THR	CB-CG2	5.22	1.69	1.52
1	I	71	ARG	CG-CD	5.22	1.65	1.51
1	J	88	THR	CA-C	5.22	1.66	1.52
1	O	139	SER	CB-OG	5.22	1.49	1.42
1	A	165	ILE	CA-CB	5.22	1.66	1.54
1	A	272	PRO	CG-CD	5.22	1.67	1.50
1	C	383	ALA	CA-CB	-5.22	1.41	1.52
1	I	290	PHE	CG-CD2	5.22	1.46	1.38
1	I	320	GLY	CA-C	5.22	1.60	1.51
1	D	194	VAL	CB-CG1	-5.22	1.41	1.52
1	F	231	TYR	C-O	5.22	1.33	1.23
1	N	86	PRO	C-O	5.21	1.33	1.23
1	E	50	TYR	CG-CD1	-5.21	1.32	1.39
1	F	442	LYS	CD-CE	5.21	1.64	1.51
1	M	263	ARG	CZ-NH1	5.21	1.39	1.33
1	A	452	LYS	CD-CE	5.21	1.64	1.51
1	M	151	TYR	CE2-CZ	-5.21	1.31	1.38
1	F	115	VAL	CB-CG2	5.21	1.63	1.52
1	G	150	ASP	CA-CB	5.21	1.65	1.53
1	J	220	VAL	CB-CG1	-5.21	1.42	1.52
1	J	64	LYS	CD-CE	5.21	1.64	1.51
1	J	460	ASP	CG-OD2	5.21	1.37	1.25
1	B	48	PRO	N-CA	-5.20	1.38	1.47
1	G	442	LYS	CG-CD	5.20	1.70	1.52
1	O	136	VAL	CB-CG2	5.20	1.63	1.52
1	A	189	GLU	CB-CG	-5.20	1.42	1.52
1	D	248	PHE	CD1-CE1	5.20	1.49	1.39
1	I	136	VAL	CB-CG2	5.20	1.63	1.52
1	L	205	PHE	CE1-CZ	5.20	1.47	1.37
1	M	100	TRP	CZ3-CH2	5.20	1.48	1.40
1	N	361	TYR	CD1-CE1	5.20	1.47	1.39
1	O	309	TYR	CD1-CE1	-5.20	1.31	1.39
1	B	182	ALA	CA-CB	-5.20	1.41	1.52
1	F	289	TYR	CZ-OH	5.20	1.46	1.37
1	G	276	TYR	CG-CD2	5.20	1.46	1.39
1	O	388	TYR	CD1-CE1	-5.20	1.31	1.39
1	M	187	PRO	CA-C	5.19	1.63	1.52
1	O	322	CYS	CB-SG	5.19	1.91	1.82
1	K	148	SER	CB-OG	5.19	1.49	1.42
1	L	321	ILE	N-CA	-5.19	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	352	THR	CB-CG2	5.19	1.69	1.52
1	B	354	LYS	CD-CE	5.19	1.64	1.51
1	C	358	PHE	CE2-CZ	5.19	1.47	1.37
1	D	466	ARG	CZ-NH1	5.19	1.39	1.33
1	E	296	SER	CA-C	5.19	1.66	1.52
1	K	178	ASN	CA-C	5.18	1.66	1.52
1	N	377	CYS	CB-SG	5.18	1.91	1.82
1	C	173	THR	CA-CB	5.18	1.66	1.53
1	K	288	SER	CA-CB	5.18	1.60	1.52
1	O	155	GLN	CD-NE2	5.18	1.45	1.32
1	M	391	SER	CB-OG	-5.18	1.35	1.42
1	O	391	SER	N-CA	5.18	1.56	1.46
1	K	117	ILE	CB-CG2	5.17	1.68	1.52
1	M	242	TYR	CD1-CE1	5.17	1.47	1.39
1	F	307	LYS	CB-CG	5.17	1.66	1.52
1	N	367	GLU	CD-OE2	5.17	1.31	1.25
1	A	356	ASP	CB-CG	5.17	1.62	1.51
1	D	24	THR	C-O	5.17	1.33	1.23
1	H	98	LEU	C-O	5.17	1.33	1.23
1	I	136	VAL	CB-CG1	5.17	1.63	1.52
1	E	91	TYR	CD2-CE2	5.17	1.47	1.39
1	O	220	VAL	C-O	5.17	1.33	1.23
1	B	342	VAL	CA-CB	-5.17	1.43	1.54
1	C	107	VAL	CB-CG1	5.17	1.63	1.52
1	H	373	ILE	C-O	-5.17	1.13	1.23
1	E	88	THR	CA-C	5.17	1.66	1.52
1	E	375	GLN	CB-CG	-5.17	1.38	1.52
1	I	371	GLN	C-O	5.17	1.33	1.23
1	J	111	GLN	CA-C	-5.16	1.39	1.52
1	E	376	LEU	C-O	-5.16	1.13	1.23
1	N	327	LEU	CG-CD2	5.16	1.71	1.51
1	O	367	GLU	CG-CD	5.16	1.59	1.51
1	L	322	CYS	CB-SG	5.16	1.91	1.82
1	M	125	LYS	CE-NZ	5.16	1.61	1.49
1	D	169	TRP	N-CA	-5.16	1.36	1.46
1	I	150	ASP	CA-CB	5.16	1.65	1.53
1	J	49	TYR	CE2-CZ	5.16	1.45	1.38
1	A	261	PHE	CD2-CE2	5.15	1.49	1.39
1	B	71	ARG	CB-CG	5.15	1.66	1.52
1	F	162	ARG	NE-CZ	5.15	1.39	1.33
1	F	264	ALA	CA-CB	-5.15	1.41	1.52
1	E	65	VAL	CB-CG2	-5.15	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	27	TYR	CG-CD1	5.15	1.45	1.39
1	H	311	LEU	N-CA	5.15	1.56	1.46
1	M	286	SER	CB-OG	5.15	1.49	1.42
1	N	250	LEU	N-CA	5.15	1.56	1.46
1	D	258	ARG	CB-CG	-5.15	1.38	1.52
1	G	120	HIS	C-N	-5.15	1.24	1.34
1	I	157	CYS	C-O	5.15	1.33	1.23
1	B	26	GLU	CD-OE2	-5.14	1.20	1.25
1	N	27	TYR	CE1-CZ	5.14	1.45	1.38
1	I	276	TYR	CG-CD2	5.14	1.45	1.39
1	N	374	PHE	CG-CD1	5.14	1.46	1.38
1	O	296	SER	CA-CB	5.14	1.60	1.52
1	C	74	ARG	CZ-NH1	5.14	1.39	1.33
1	I	37	ALA	CA-CB	-5.14	1.41	1.52
1	I	219	ASP	CG-OD1	5.14	1.37	1.25
1	N	367	GLU	CB-CG	5.14	1.61	1.52
1	E	368	TYR	C-O	-5.13	1.13	1.23
1	G	457	ALA	N-CA	-5.13	1.36	1.46
1	A	35	TYR	CD1-CE1	-5.13	1.31	1.39
1	H	309	TYR	CE2-CZ	5.13	1.45	1.38
1	J	101	ALA	CA-CB	5.13	1.63	1.52
1	H	99	VAL	CA-CB	-5.13	1.44	1.54
1	A	50	TYR	CE2-CZ	-5.13	1.31	1.38
1	A	276	TYR	CD2-CE2	5.13	1.47	1.39
1	I	106	GLU	CB-CG	5.13	1.61	1.52
1	M	400	TRP	CE3-CZ3	-5.13	1.29	1.38
1	N	193	THR	C-O	5.12	1.33	1.23
1	N	258	ARG	CZ-NH1	5.12	1.39	1.33
1	M	240	GLU	CB-CG	5.12	1.61	1.52
1	J	253	GLU	CB-CG	5.12	1.61	1.52
1	M	441	LEU	C-O	5.12	1.33	1.23
1	J	231	TYR	CG-CD1	5.12	1.45	1.39
1	M	92	ASP	CB-CG	5.12	1.62	1.51
1	J	297	MET	C-O	5.12	1.33	1.23
1	F	159	ILE	N-CA	-5.12	1.36	1.46
1	C	191	LEU	N-CA	5.11	1.56	1.46
1	F	245	MET	C-O	5.11	1.33	1.23
1	K	110	GLY	N-CA	-5.11	1.38	1.46
1	B	209	ASP	CB-CG	5.11	1.62	1.51
1	H	22	VAL	CB-CG2	-5.11	1.42	1.52
1	H	321	ILE	CB-CG2	5.11	1.68	1.52
1	L	162	ARG	CD-NE	5.11	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	250	LEU	CG-CD1	-5.11	1.32	1.51
1	N	309	TYR	CE1-CZ	5.11	1.45	1.38
1	C	194	VAL	CB-CG1	5.11	1.63	1.52
1	N	374	PHE	CE2-CZ	5.11	1.47	1.37
1	J	230	LYS	CB-CG	5.11	1.66	1.52
1	M	396	ILE	CA-CB	5.11	1.66	1.54
1	A	336	ARG	N-CA	5.10	1.56	1.46
1	O	27	TYR	CD2-CE2	5.10	1.47	1.39
1	C	113	LEU	CG-CD2	5.10	1.70	1.51
1	I	172	GLY	C-O	5.10	1.31	1.23
1	L	201	VAL	C-O	5.10	1.33	1.23
1	O	318	ASN	CB-CG	5.10	1.62	1.51
1	J	448	GLU	CD-OE1	5.09	1.31	1.25
1	J	74	ARG	CB-CG	-5.09	1.38	1.52
1	J	372	PHE	CE2-CZ	5.09	1.47	1.37
1	A	20	ALA	N-CA	5.09	1.56	1.46
1	I	453	GLU	CB-CG	5.09	1.61	1.52
1	E	192	ASN	CB-CG	5.09	1.62	1.51
1	J	83	PHE	CA-C	5.09	1.66	1.52
1	A	50	TYR	CE1-CZ	-5.08	1.31	1.38
1	J	342	VAL	CA-CB	-5.08	1.44	1.54
1	E	217	LYS	CB-CG	-5.08	1.38	1.52
1	F	112	PRO	N-CA	-5.08	1.38	1.47
1	C	290	PHE	CD1-CE1	5.08	1.49	1.39
1	J	341	SER	CB-OG	5.08	1.48	1.42
1	C	209	ASP	CB-CG	5.08	1.62	1.51
1	D	118	SER	C-O	5.08	1.33	1.23
1	J	70	TYR	CG-CD1	5.08	1.45	1.39
1	N	153	GLN	CA-CB	5.08	1.65	1.53
1	B	35	TYR	N-CA	-5.08	1.36	1.46
1	B	79	ASP	C-O	-5.08	1.13	1.23
1	D	372	PHE	CD1-CE1	5.08	1.49	1.39
1	G	340	MET	C-O	5.08	1.33	1.23
1	I	34	TYR	CE2-CZ	5.08	1.45	1.38
1	I	394	PRO	CG-CD	-5.08	1.33	1.50
1	D	271	VAL	CB-CG1	-5.08	1.42	1.52
1	F	101	ALA	N-CA	5.08	1.56	1.46
1	I	125	LYS	CD-CE	5.07	1.64	1.51
1	J	224	ILE	C-O	-5.07	1.13	1.23
1	M	309	TYR	CG-CD1	5.07	1.45	1.39
1	A	453	GLU	CD-OE1	5.07	1.31	1.25
1	G	264	ALA	CA-CB	-5.07	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	21	VAL	C-O	-5.07	1.13	1.23
1	M	374	PHE	CD2-CE2	5.07	1.49	1.39
1	N	84	GLY	N-CA	5.07	1.53	1.46
1	C	374	PHE	CB-CG	-5.07	1.42	1.51
1	G	214	GLN	C-O	5.07	1.32	1.23
1	M	201	VAL	CB-CG1	5.07	1.63	1.52
1	I	89	SER	CA-CB	5.06	1.60	1.52
1	A	229	CYS	C-O	5.06	1.32	1.23
1	B	363	ARG	CG-CD	-5.06	1.39	1.51
1	G	374	PHE	CD2-CE2	5.06	1.49	1.39
1	J	261	PHE	CE1-CZ	-5.06	1.27	1.37
1	E	361	TYR	CZ-OH	-5.06	1.29	1.37
1	J	151	TYR	CE1-CZ	5.06	1.45	1.38
1	N	61	ALA	N-CA	5.06	1.56	1.46
1	O	338	THR	CA-C	5.06	1.66	1.52
1	E	145	GLU	CB-CG	-5.06	1.42	1.52
1	H	458	ASP	CB-CG	5.06	1.62	1.51
1	J	366	GLU	CA-CB	5.06	1.65	1.53
1	K	39	SER	C-O	-5.06	1.13	1.23
1	L	367	GLU	CB-CG	5.06	1.61	1.52
1	B	152	LYS	CD-CE	5.05	1.63	1.51
1	E	34	TYR	CG-CD1	5.05	1.45	1.39
1	B	447	TRP	CZ3-CH2	-5.05	1.31	1.40
1	I	49	TYR	CE2-CZ	5.05	1.45	1.38
1	C	170	GLY	N-CA	-5.05	1.38	1.46
1	F	231	TYR	CZ-OH	-5.05	1.29	1.37
1	M	130	GLU	CB-CG	-5.05	1.42	1.52
1	O	341	SER	CA-CB	5.05	1.60	1.52
1	G	49	TYR	CD2-CE2	-5.04	1.31	1.39
1	O	83	PHE	CE2-CZ	5.04	1.47	1.37
1	E	36	HIS	C-O	-5.04	1.13	1.23
1	H	115	VAL	CB-CG2	5.04	1.63	1.52
1	I	65	VAL	C-O	-5.04	1.13	1.23
1	M	34	TYR	CD1-CE1	-5.04	1.31	1.39
1	D	466	ARG	CZ-NH2	5.04	1.39	1.33
1	J	169	TRP	C-O	-5.04	1.13	1.23
1	M	169	TRP	CZ2-CH2	-5.04	1.27	1.37
1	N	334	THR	C-O	5.04	1.32	1.23
1	M	99	VAL	CB-CG2	5.04	1.63	1.52
1	M	221	PRO	C-O	5.04	1.33	1.23
1	J	330	THR	CB-CG2	5.04	1.69	1.52
1	B	290	PHE	CE2-CZ	5.04	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	226	SER	CB-OG	-5.03	1.35	1.42
1	F	34	TYR	C-O	5.03	1.32	1.23
1	M	332	VAL	CB-CG2	5.03	1.63	1.52
1	E	70	TYR	CD1-CE1	5.03	1.46	1.39
1	H	91	TYR	CD1-CE1	5.03	1.46	1.39
1	F	167	GLU	CD-OE2	5.03	1.31	1.25
1	F	449	VAL	CA-CB	5.03	1.65	1.54
1	C	363	ARG	CB-CG	-5.03	1.39	1.52
1	D	153	GLN	CB-CG	5.03	1.66	1.52
1	C	92	ASP	C-O	5.03	1.32	1.23
1	K	115	VAL	CB-CG2	5.03	1.63	1.52
1	H	91	TYR	CE2-CZ	5.02	1.45	1.38
1	H	251	ARG	CZ-NH2	5.02	1.39	1.33
1	K	450	ASP	C-O	5.02	1.32	1.23
1	C	85	PHE	CE2-CZ	5.02	1.46	1.37
1	K	149	MET	CB-CG	5.02	1.67	1.51
1	M	248	PHE	N-CA	-5.02	1.36	1.46
1	O	319	ASN	C-O	5.02	1.32	1.23
1	J	254	GLN	CD-OE1	5.02	1.34	1.24
1	M	308	PRO	N-CA	-5.02	1.38	1.47
1	O	208	MET	C-O	5.02	1.32	1.23
1	O	111	GLN	C-O	5.02	1.32	1.23
1	D	180	VAL	CB-CG1	5.01	1.63	1.52
1	I	441	LEU	N-CA	5.01	1.56	1.46
1	J	335	THR	CA-C	5.01	1.66	1.52
1	M	398	GLU	CD-OE1	5.01	1.31	1.25
1	O	205	PHE	CE2-CZ	-5.01	1.27	1.37
1	O	352	THR	C-O	5.01	1.32	1.23
1	D	375	GLN	CB-CG	-5.01	1.39	1.52
1	H	291	PRO	CA-C	5.01	1.62	1.52
1	M	39	SER	CB-OG	5.01	1.48	1.42
1	D	150	ASP	C-O	5.01	1.32	1.23
1	D	199	ASP	C-O	-5.01	1.13	1.23
1	O	360	GLU	CD-OE1	5.01	1.31	1.25
1	D	114	GLY	CA-C	5.01	1.59	1.51
1	F	99	VAL	CB-CG1	5.01	1.63	1.52
1	J	111	GLN	CG-CD	5.01	1.62	1.51
1	K	149	MET	CA-CB	-5.01	1.43	1.53
1	B	59	LYS	CE-NZ	5.00	1.61	1.49
1	B	310	TRP	CE2-CZ2	-5.00	1.31	1.39
1	L	215	ALA	CA-CB	5.00	1.62	1.52
1	N	309	TYR	CD1-CE1	-5.00	1.31	1.39

All (1014) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	336	ARG	NE-CZ-NH2	-20.83	109.88	120.30
1	F	336	ARG	NE-CZ-NH2	-17.28	111.66	120.30
1	C	109	ARG	NE-CZ-NH2	-16.56	112.02	120.30
1	C	251	ARG	NE-CZ-NH1	16.29	128.44	120.30
1	L	30	ARG	NE-CZ-NH1	-16.14	112.23	120.30
1	A	71	ARG	NE-CZ-NH2	-15.71	112.44	120.30
1	C	258	ARG	NE-CZ-NH1	-15.57	112.52	120.30
1	F	144	ARG	NE-CZ-NH1	14.40	127.50	120.30
1	C	336	ARG	NE-CZ-NH1	14.20	127.40	120.30
1	A	263	ARG	NE-CZ-NH2	-13.70	113.45	120.30
1	K	97	ARG	NE-CZ-NH1	13.49	127.05	120.30
1	N	244	ASP	CB-CG-OD1	13.40	130.36	118.30
1	C	466	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	H	109	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	C	333	ASP	CB-CG-OD2	13.14	130.12	118.30
1	L	467	LYS	CD-CE-NZ	-13.09	81.60	111.70
1	J	466	ARG	NE-CZ-NH2	13.05	126.83	120.30
1	B	79	ASP	CB-CG-OD1	13.02	130.01	118.30
1	H	363	ARG	NE-CZ-NH2	-12.99	113.81	120.30
1	A	223	ASP	CB-CG-OD1	12.86	129.88	118.30
1	A	144	ARG	NE-CZ-NH1	12.71	126.66	120.30
1	F	109	ARG	NE-CZ-NH1	12.41	126.50	120.30
1	F	30	ARG	NE-CZ-NH1	-12.38	114.11	120.30
1	F	77	LEU	CB-CG-CD1	-12.36	89.98	111.00
1	F	336	ARG	NE-CZ-NH1	12.31	126.46	120.30
1	E	109	ARG	NE-CZ-NH1	12.22	126.41	120.30
1	B	134	LYS	CD-CE-NZ	-12.20	83.64	111.70
1	D	30	ARG	NE-CZ-NH2	12.19	126.39	120.30
1	N	162	ARG	NE-CZ-NH2	-12.16	114.22	120.30
1	I	30	ARG	NE-CZ-NH2	12.01	126.30	120.30
1	F	333	ASP	CB-CG-OD2	11.95	129.06	118.30
1	B	336	ARG	NE-CZ-NH1	-11.81	114.39	120.30
1	B	30	ARG	NE-CZ-NH1	-11.80	114.40	120.30
1	J	363	ARG	NE-CZ-NH2	-11.78	114.41	120.30
1	I	313	ARG	NE-CZ-NH2	-11.77	114.41	120.30
1	O	263	ARG	NE-CZ-NH2	-11.72	114.44	120.30
1	O	284	LEU	CB-CG-CD1	-11.67	91.16	111.00
1	H	109	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	J	30	ARG	NE-CZ-NH2	11.58	126.09	120.30
1	K	109	ARG	NE-CZ-NH1	-11.58	114.51	120.30
1	A	30	ARG	NE-CZ-NH1	-11.58	114.51	120.30
1	C	109	ARG	NE-CZ-NH1	11.51	126.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	252	ARG	NE-CZ-NH1	-11.29	114.65	120.30
1	E	30	ARG	NE-CZ-NH1	-11.27	114.66	120.30
1	M	251	ARG	NE-CZ-NH1	11.23	125.92	120.30
1	B	30	ARG	NE-CZ-NH2	11.21	125.91	120.30
1	H	97	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	N	263	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	C	263	ARG	NE-CZ-NH2	-11.05	114.77	120.30
1	F	71	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	L	30	ARG	NE-CZ-NH2	11.03	125.81	120.30
1	N	263	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	F	263	ARG	NE-CZ-NH2	-10.99	114.80	120.30
1	D	30	ARG	NE-CZ-NH1	-10.94	114.83	120.30
1	B	258	ARG	NE-CZ-NH1	-10.78	114.91	120.30
1	A	30	ARG	NE-CZ-NH2	10.73	125.66	120.30
1	G	144	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	N	162	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	D	233	ASP	CB-CG-OD1	10.54	127.79	118.30
1	C	223	ASP	CB-CG-OD2	-10.53	108.82	118.30
1	H	41	ARG	NE-CZ-NH2	10.46	125.53	120.30
1	O	363	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	L	336	ARG	NE-CZ-NH1	-10.39	115.11	120.30
1	J	74	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	F	258	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	M	162	ARG	NE-CZ-NH2	-10.29	115.15	120.30
1	M	152	LYS	CD-CE-NZ	-10.28	88.05	111.70
1	C	144	ARG	NE-CZ-NH1	10.21	125.40	120.30
1	D	97	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	N	144	ARG	NE-CZ-NH1	-10.17	115.22	120.30
1	K	450	ASP	CB-CG-OD2	-10.15	109.16	118.30
1	I	363	ARG	NE-CZ-NH1	-10.15	115.22	120.30
1	H	208	MET	CG-SD-CE	10.15	116.44	100.20
1	D	363	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	J	128	ASP	CB-CG-OD1	10.04	127.34	118.30
1	F	150	ASP	CB-CG-OD2	-10.04	109.27	118.30
1	H	197	ASP	CB-CG-OD1	10.03	127.32	118.30
1	J	71	ARG	NE-CZ-NH1	-10.00	115.30	120.30
1	C	97	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	O	263	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	O	363	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	B	219	ASP	CB-CG-OD2	-9.96	109.33	118.30
1	N	329	VAL	CA-CB-CG1	-9.96	95.96	110.90
1	E	363	ARG	NE-CZ-NH2	-9.94	115.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	258	ARG	NE-CZ-NH1	-9.91	115.34	120.30
1	O	113	LEU	CB-CG-CD2	-9.91	94.15	111.00
1	G	336	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	A	336	ARG	NE-CZ-NH1	-9.87	115.36	120.30
1	M	251	ARG	NE-CZ-NH2	-9.86	115.37	120.30
1	C	251	ARG	NE-CZ-NH2	-9.85	115.38	120.30
1	F	74	ARG	NE-CZ-NH1	-9.83	115.39	120.30
1	N	340	MET	CG-SD-CE	-9.75	84.59	100.20
1	H	41	ARG	NE-CZ-NH1	-9.72	115.44	120.30
1	E	235	LEU	CB-CG-CD1	-9.70	94.50	111.00
1	C	370	LEU	CB-CG-CD1	9.70	127.48	111.00
1	I	263	ARG	NE-CZ-NH1	-9.68	115.46	120.30
1	B	77	LEU	CB-CG-CD1	-9.61	94.66	111.00
1	D	399	ASP	CB-CG-OD2	9.59	126.93	118.30
1	H	336	ARG	NE-CZ-NH1	-9.56	115.52	120.30
1	G	97	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	O	71	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	D	92	ASP	CB-CG-OD1	-9.51	109.74	118.30
1	G	79	ASP	CB-CG-OD2	-9.43	109.81	118.30
1	J	199	ASP	CB-CG-OD2	9.43	126.79	118.30
1	J	134	LYS	CD-CE-NZ	-9.39	90.10	111.70
1	F	144	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	B	251	ARG	NE-CZ-NH2	9.30	124.95	120.30
1	B	313	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	M	71	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	E	105	VAL	CG1-CB-CG2	-9.24	96.11	110.90
1	N	244	ASP	CB-CG-OD2	-9.21	110.01	118.30
1	F	219	ASP	CB-CG-OD1	-9.20	110.02	118.30
1	F	202	ASP	CB-CG-OD2	9.18	126.56	118.30
1	D	41	ARG	NE-CZ-NH1	-9.17	115.72	120.30
1	O	64	LYS	CD-CE-NZ	-9.15	90.66	111.70
1	I	258	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	A	336	ARG	NE-CZ-NH2	9.08	124.84	120.30
1	H	162	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	J	188	LEU	CB-CG-CD2	-9.07	95.57	111.00
1	H	74	ARG	NE-CZ-NH1	-9.06	115.77	120.30
1	C	244	ASP	CB-CG-OD1	9.05	126.45	118.30
1	O	464	LEU	CB-CG-CD1	-9.03	95.65	111.00
1	J	158	LEU	CB-CG-CD2	-8.95	95.79	111.00
1	J	359	LYS	CD-CE-NZ	-8.94	91.13	111.70
1	D	156	LEU	CB-CG-CD2	-8.93	95.82	111.00
1	E	336	ARG	CG-CD-NE	8.91	130.51	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	258	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	B	199	ASP	CB-CG-OD1	-8.87	110.31	118.30
1	I	128	ASP	CB-CG-OD1	8.87	126.28	118.30
1	N	152	LYS	CD-CE-NZ	-8.86	91.32	111.70
1	D	87	ASP	CB-CG-OD2	8.86	126.27	118.30
1	F	156	LEU	CB-CG-CD1	-8.85	95.95	111.00
1	G	97	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	M	458	ASP	CB-CG-OD2	-8.83	110.35	118.30
1	F	158	LEU	CB-CG-CD2	-8.82	96.00	111.00
1	O	109	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	K	450	ASP	CB-CG-OD1	8.79	126.21	118.30
1	B	333	ASP	CB-CG-OD1	-8.79	110.39	118.30
1	C	466	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	D	217	LYS	CD-CE-NZ	-8.78	91.50	111.70
1	K	71	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	H	338	THR	CA-CB-CG2	-8.77	100.12	112.40
1	B	149	MET	CG-SD-CE	-8.76	86.19	100.20
1	J	113	LEU	CB-CG-CD2	-8.74	96.14	111.00
1	I	76	LYS	CD-CE-NZ	-8.73	91.61	111.70
1	L	363	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	K	68	LEU	CB-CG-CD2	-8.71	96.19	111.00
1	B	71	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	463	PRO	N-CD-CG	-8.69	90.16	103.20
1	G	99	VAL	CB-CA-C	-8.66	94.94	111.40
1	H	233	ASP	CB-CG-OD2	8.63	126.06	118.30
1	K	65	VAL	CG1-CB-CG2	-8.62	97.10	110.90
1	I	459	LEU	CB-CG-CD2	-8.61	96.37	111.00
1	D	92	ASP	CB-CG-OD2	8.57	126.02	118.30
1	D	199	ASP	CB-CG-OD1	-8.57	110.58	118.30
1	G	201	VAL	CG1-CB-CG2	8.57	124.61	110.90
1	M	333	ASP	CB-CG-OD2	8.54	125.99	118.30
1	O	336	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	F	74	ARG	NE-CZ-NH2	8.50	124.55	120.30
1	H	336	ARG	CG-CD-NE	8.49	129.62	111.80
1	E	209	ASP	CB-CG-OD2	8.48	125.94	118.30
1	E	77	LEU	CB-CG-CD1	-8.47	96.59	111.00
1	H	369	ASP	CB-CG-OD2	8.46	125.91	118.30
1	A	356	ASP	CB-CG-OD1	8.43	125.89	118.30
1	M	30	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	G	209	ASP	CB-CG-OD1	-8.42	110.72	118.30
1	N	30	ARG	NE-CZ-NH1	-8.41	116.09	120.30
1	E	125	LYS	CD-CE-NZ	-8.39	92.41	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	113	LEU	CB-CG-CD1	8.37	125.24	111.00
1	K	336	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	G	71	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	J	369	ASP	CB-CG-OD2	-8.33	110.81	118.30
1	I	126	LEU	CB-CG-CD1	8.32	125.15	111.00
1	E	336	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	C	258	ARG	NH1-CZ-NH2	8.27	128.50	119.40
1	H	43	LEU	CB-CG-CD2	-8.27	96.94	111.00
1	O	460	ASP	CB-CG-OD2	8.26	125.74	118.30
1	N	195	LEU	CB-CG-CD2	8.23	125.00	111.00
1	J	74	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	M	263	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	I	30	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	F	162	ARG	NE-CZ-NH1	8.15	124.37	120.30
1	H	311	LEU	CA-CB-CG	-8.13	96.61	115.30
1	H	149	MET	CG-SD-CE	-8.11	87.22	100.20
1	I	219	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	F	258	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	H	258	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	H	469	LEU	CB-CG-CD1	-8.05	97.31	111.00
1	L	122	LEU	CB-CG-CD2	8.04	124.67	111.00
1	K	258	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	G	245	MET	CG-SD-CE	8.03	113.04	100.20
1	J	252	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	G	469	LEU	CB-CG-CD1	-8.02	97.37	111.00
1	K	384	ASP	CB-CG-OD2	8.01	125.51	118.30
1	B	384	ASP	CB-CG-OD1	8.01	125.51	118.30
1	H	223	ASP	CB-CG-OD2	-8.01	111.10	118.30
1	D	144	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	M	25	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	I	52	ILE	CG1-CB-CG2	-7.97	93.87	111.40
1	C	74	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	L	87	ASP	CB-CG-OD1	-7.95	111.14	118.30
1	A	77	LEU	CB-CG-CD1	-7.95	97.48	111.00
1	A	68	LEU	CB-CG-CD1	7.94	124.49	111.00
1	G	246	LEU	CB-CG-CD1	7.93	124.49	111.00
1	N	202	ASP	CB-CG-OD2	7.91	125.42	118.30
1	K	381	LEU	CB-CG-CD2	-7.91	97.56	111.00
1	C	77	LEU	CB-CG-CD1	-7.90	97.56	111.00
1	J	144	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	I	337	SER	N-CA-C	7.89	132.30	111.00
1	M	244	ASP	CB-CG-OD1	7.89	125.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	464	LEU	CA-CB-CG	7.88	133.43	115.30
1	H	223	ASP	CB-CG-OD1	7.86	125.37	118.30
1	A	64	LYS	CG-CD-CE	-7.83	88.42	111.90
1	B	43	LEU	CB-CG-CD1	-7.82	97.70	111.00
1	J	165	ILE	CG1-CB-CG2	-7.82	94.19	111.40
1	I	244	ASP	CB-CG-OD1	7.81	125.33	118.30
1	C	466	ARG	CD-NE-CZ	7.81	134.53	123.60
1	N	199	ASP	CB-CG-OD2	7.81	125.33	118.30
1	F	25	ASP	CB-CG-OD1	-7.79	111.28	118.30
1	E	363	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	M	449	VAL	CG1-CB-CG2	-7.75	98.50	110.90
1	D	171	LYS	CD-CE-NZ	-7.74	93.89	111.70
1	K	263	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	C	126	LEU	CB-CG-CD1	7.71	124.10	111.00
1	F	244	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	299	THR	CA-CB-CG2	-7.70	101.62	112.40
1	G	363	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	F	98	LEU	CB-CG-CD2	7.69	124.07	111.00
1	L	208	MET	CB-CG-SD	7.69	135.46	112.40
1	C	113	LEU	CB-CG-CD2	-7.67	97.95	111.00
1	I	451	LEU	CB-CG-CD1	-7.66	97.98	111.00
1	N	363	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	F	68	LEU	CA-CB-CG	-7.64	97.73	115.30
1	E	260	LEU	CB-CG-CD1	-7.62	98.04	111.00
1	F	113	LEU	CB-CG-CD2	-7.62	98.04	111.00
1	O	202	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	F	309	TYR	CG-CD2-CE2	-7.60	115.22	121.30
1	C	110	GLY	N-CA-C	-7.60	94.11	113.10
1	D	52	ILE	CG1-CB-CG2	-7.59	94.70	111.40
1	J	220	VAL	CG1-CB-CG2	-7.56	98.80	110.90
1	F	363	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	D	327	LEU	CB-CG-CD2	-7.54	98.18	111.00
1	K	197	ASP	CB-CG-OD1	7.54	125.08	118.30
1	A	244	ASP	CB-CG-OD1	7.52	125.07	118.30
1	K	128	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	D	209	ASP	CB-CG-OD1	-7.50	111.55	118.30
1	L	257	VAL	CA-CB-CG1	-7.49	99.67	110.90
1	J	354	LYS	CD-CE-NZ	-7.48	94.50	111.70
1	O	59	LYS	CD-CE-NZ	-7.45	94.58	111.70
1	D	233	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	E	449	VAL	CG1-CB-CG2	-7.44	98.99	110.90
1	F	244	ASP	CB-CG-OD2	-7.44	111.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	464	LEU	CB-CG-CD2	7.43	123.64	111.00
1	H	30	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	F	142	ASP	CB-CG-OD2	7.42	124.98	118.30
1	E	237	MET	CG-SD-CE	7.41	112.05	100.20
1	H	158	LEU	CB-CG-CD1	-7.41	98.41	111.00
1	N	330	THR	CA-CB-CG2	-7.40	102.04	112.40
1	D	42	LEU	CB-CG-CD2	-7.40	98.42	111.00
1	J	381	LEU	CB-CG-CD2	-7.38	98.46	111.00
1	H	237	MET	CG-SD-CE	7.38	112.00	100.20
1	E	127	ASP	CB-CG-OD1	7.37	124.94	118.30
1	G	356	ASP	CB-CG-OD2	-7.36	111.67	118.30
1	J	260	LEU	CB-CG-CD1	-7.35	98.50	111.00
1	M	333	ASP	CB-CG-OD1	-7.35	111.69	118.30
1	A	87	ASP	CB-CG-OD1	-7.35	111.69	118.30
1	D	459	LEU	CB-CG-CD2	-7.34	98.52	111.00
1	A	284	LEU	CB-CG-CD1	-7.34	98.53	111.00
1	K	459	LEU	CB-CG-CD2	-7.33	98.53	111.00
1	H	156	LEU	CB-CG-CD1	-7.33	98.54	111.00
1	D	222	LEU	CB-CG-CD1	7.32	123.45	111.00
1	E	71	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	J	162	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	L	190	LEU	CB-CG-CD2	7.31	123.43	111.00
1	K	162	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	J	397	LEU	CB-CG-CD1	-7.25	98.67	111.00
1	M	189	GLU	OE1-CD-OE2	-7.25	114.61	123.30
1	N	98	LEU	CB-CG-CD1	-7.23	98.71	111.00
1	C	194	VAL	CA-CB-CG2	-7.23	100.06	110.90
1	H	365	GLY	N-CA-C	7.22	131.15	113.10
1	N	274	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	D	142	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	386	MET	CG-SD-CE	7.19	111.70	100.20
1	K	197	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	I	251	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	J	466	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	K	188	LEU	CB-CG-CD2	-7.16	98.83	111.00
1	N	74	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	B	190	LEU	CB-CG-CD1	-7.14	98.85	111.00
1	J	162	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	A	202	ASP	CB-CG-OD2	7.14	124.72	118.30
1	C	209	ASP	CB-CG-OD2	7.12	124.71	118.30
1	E	297	MET	CG-SD-CE	-7.12	88.81	100.20
1	N	113	LEU	CB-CG-CD1	7.11	123.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	333	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	C	144	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	C	156	LEU	CB-CG-CD2	-7.09	98.94	111.00
1	K	134	LYS	CD-CE-NZ	-7.09	95.40	111.70
1	I	128	ASP	CB-CG-OD2	-7.08	111.92	118.30
1	A	68	LEU	CA-CB-CG	-7.08	99.01	115.30
1	E	252	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	E	464	LEU	CA-CB-CG	7.07	131.56	115.30
1	E	109	ARG	CD-NE-CZ	7.07	133.49	123.60
1	C	222	LEU	CB-CG-CD2	7.05	122.99	111.00
1	J	98	LEU	CA-CB-CG	-7.05	99.08	115.30
1	O	474	LEU	CB-CG-CD2	7.05	122.98	111.00
1	E	64	LYS	CD-CE-NZ	-7.04	95.50	111.70
1	I	150	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	L	467	LYS	CG-CD-CE	-7.03	90.80	111.90
1	J	257	VAL	CA-CB-CG1	-7.02	100.37	110.90
1	M	79	ASP	CB-CG-OD2	-7.02	111.99	118.30
1	I	202	ASP	CB-CG-OD2	7.01	124.61	118.30
1	B	74	ARG	NE-CZ-NH1	-7.01	116.80	120.30
1	B	68	LEU	CA-CB-CG	-7.01	99.18	115.30
1	D	162	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	B	79	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	I	25	ASP	CB-CG-OD2	7.00	124.60	118.30
1	L	363	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	H	386	MET	CG-SD-CE	6.99	111.38	100.20
1	K	244	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	H	263	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	A	263	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	E	223	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	K	162	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	M	134	LYS	CD-CE-NZ	-6.95	95.72	111.70
1	N	235	LEU	CB-CG-CD1	6.93	122.78	111.00
1	N	222	LEU	CA-CB-CG	6.92	131.21	115.30
1	G	147	ILE	CG1-CB-CG2	-6.91	96.20	111.40
1	F	470	LEU	CB-CG-CD1	-6.91	99.25	111.00
1	B	309	TYR	CD1-CE1-CZ	-6.90	113.59	119.80
1	B	98	LEU	CB-CG-CD1	-6.88	99.31	111.00
1	F	309	TYR	CG-CD1-CE1	6.87	126.80	121.30
1	H	209	ASP	CB-CG-OD2	6.87	124.48	118.30
1	J	464	LEU	CB-CG-CD2	-6.87	99.33	111.00
1	A	356	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	C	27	TYR	CB-CG-CD1	6.86	125.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	84	GLY	N-CA-C	-6.85	95.98	113.10
1	L	251	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	C	97	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	E	74	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	J	71	ARG	CG-CD-NE	-6.82	97.47	111.80
1	B	313	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	L	460	ASP	CB-CG-OD1	6.82	124.44	118.30
1	K	125	LYS	CD-CE-NZ	-6.82	96.02	111.70
1	L	199	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	C	211	THR	CA-CB-CG2	-6.81	102.86	112.40
1	L	128	ASP	CB-CG-OD1	6.81	124.43	118.30
1	L	165	ILE	CG1-CB-CG2	-6.81	96.42	111.40
1	F	97	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	H	98	LEU	CB-CG-CD1	-6.80	99.43	111.00
1	N	145	GLU	OE1-CD-OE2	-6.80	115.14	123.30
1	O	313	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	275	LEU	CA-CB-CG	6.79	130.93	115.30
1	D	162	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	M	470	LEU	CB-CG-CD2	-6.79	99.45	111.00
1	H	30	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	C	298	VAL	CA-CB-CG1	-6.74	100.78	110.90
1	N	249	TYR	CD1-CE1-CZ	-6.74	113.73	119.80
1	C	122	LEU	CA-CB-CG	6.74	130.80	115.30
1	C	142	ASP	CB-CG-OD2	6.74	124.36	118.30
1	I	53	LYS	CD-CE-NZ	-6.74	96.21	111.70
1	H	43	LEU	CA-CB-CG	-6.73	99.81	115.30
1	J	105	VAL	CG1-CB-CG2	-6.73	100.13	110.90
1	A	123	LEU	CB-CG-CD2	-6.73	99.56	111.00
1	B	211	THR	CA-CB-CG2	-6.72	103.00	112.40
1	A	276	TYR	CZ-CE2-CD2	-6.70	113.77	119.80
1	G	92	ASP	CB-CG-OD1	-6.70	112.27	118.30
1	N	217	LYS	CD-CE-NZ	-6.70	96.30	111.70
1	F	71	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	A	327	LEU	CB-CG-CD1	6.68	122.35	111.00
1	F	128	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	H	250	LEU	CB-CG-CD2	6.67	122.34	111.00
1	G	74	ARG	NE-CZ-NH2	6.66	123.63	120.30
1	B	363	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	O	258	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	C	362	LEU	CB-CG-CD2	-6.66	99.69	111.00
1	O	209	ASP	CB-CG-OD1	-6.66	112.31	118.30
1	H	79	ASP	CB-CG-OD1	6.65	124.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	201	VAL	CB-CA-C	-6.64	98.78	111.40
1	M	71	ARG	NH1-CZ-NH2	6.64	126.71	119.40
1	B	298	VAL	CA-CB-CG2	-6.64	100.94	110.90
1	E	113	LEU	CB-CG-CD2	-6.64	99.71	111.00
1	H	209	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	A	275	LEU	CB-CG-CD2	6.61	122.23	111.00
1	B	25	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	D	219	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	D	144	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	I	370	LEU	CB-CG-CD2	6.59	122.21	111.00
1	G	141	THR	CA-CB-CG2	-6.59	103.17	112.40
1	M	56	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	C	142	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	F	190	LEU	CB-CG-CD1	-6.58	99.82	111.00
1	N	267	VAL	CG1-CB-CG2	-6.57	100.39	110.90
1	C	336	ARG	CG-CD-NE	6.56	125.58	111.80
1	K	45	VAL	CA-CB-CG1	-6.56	101.06	110.90
1	J	470	LEU	CA-CB-CG	6.55	130.37	115.30
1	D	244	ASP	CB-CG-OD1	6.55	124.19	118.30
1	M	311	LEU	CA-CB-CG	-6.54	100.26	115.30
1	D	374	PHE	CG-CD2-CE2	-6.53	113.61	120.80
1	O	459	LEU	CB-CG-CD2	6.53	122.10	111.00
1	G	466	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	F	274	ASP	CB-CG-OD1	6.52	124.17	118.30
1	M	235	LEU	CB-CG-CD2	-6.52	99.91	111.00
1	F	128	ASP	CB-CG-OD1	6.52	124.17	118.30
1	K	99	VAL	CB-CA-C	-6.51	99.03	111.40
1	B	330	THR	CA-CB-CG2	-6.51	103.29	112.40
1	D	368	TYR	CZ-CE2-CD2	-6.51	113.94	119.80
1	L	369	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	451	LEU	CB-CG-CD2	-6.50	99.95	111.00
1	F	134	LYS	CD-CE-NZ	-6.50	96.76	111.70
1	H	230	LYS	CB-CG-CD	-6.49	94.73	111.60
1	B	98	LEU	CB-CG-CD2	6.48	122.02	111.00
1	F	459	LEU	CB-CG-CD2	-6.48	99.98	111.00
1	J	263	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	D	451	LEU	CB-CG-CD1	-6.46	100.01	111.00
1	I	167	GLU	OE1-CD-OE2	-6.46	115.55	123.30
1	H	142	ASP	CB-CG-OD2	6.46	124.11	118.30
1	J	125	LYS	CD-CE-NZ	-6.46	96.85	111.70
1	O	30	ARG	NE-CZ-NH1	-6.45	117.07	120.30
1	F	41	ARG	NE-CZ-NH1	-6.45	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	397	LEU	CA-CB-CG	-6.45	100.47	115.30
1	B	327	LEU	CB-CG-CD1	6.45	121.96	111.00
1	J	82	LYS	CD-CE-NZ	6.44	126.51	111.70
1	H	34	TYR	CD1-CE1-CZ	-6.43	114.01	119.80
1	J	298	VAL	CA-CB-CG2	-6.43	101.25	110.90
1	K	384	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	L	87	ASP	CB-CG-OD2	6.42	124.08	118.30
1	H	284	LEU	CB-CG-CD1	-6.41	100.10	111.00
1	A	87	ASP	OD1-CG-OD2	6.41	135.48	123.30
1	M	75	VAL	CA-CB-CG2	-6.41	101.28	110.90
1	I	156	LEU	CB-CG-CD1	-6.41	100.10	111.00
1	K	202	ASP	CB-CG-OD2	6.40	124.06	118.30
1	L	237	MET	CG-SD-CE	6.40	110.44	100.20
1	M	150	ASP	CB-CG-OD1	-6.40	112.54	118.30
1	I	333	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	L	71	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	N	271	VAL	CG1-CB-CG2	6.39	121.13	110.90
1	K	333	ASP	N-CA-C	6.39	128.26	111.00
1	C	250	LEU	CB-CG-CD2	6.39	121.86	111.00
1	D	113	LEU	CB-CG-CD1	6.38	121.84	111.00
1	H	295	GLY	N-CA-C	-6.37	97.17	113.10
1	L	452	LYS	CB-CG-CD	-6.37	95.03	111.60
1	M	149	MET	CG-SD-CE	6.37	110.40	100.20
1	C	42	LEU	CB-CG-CD2	-6.37	100.17	111.00
1	H	157	CYS	CA-CB-SG	-6.36	102.55	114.00
1	N	466	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	M	98	LEU	CB-CG-CD2	6.35	121.80	111.00
1	M	451	LEU	CB-CG-CD2	-6.35	100.20	111.00
1	A	122	LEU	CB-CG-CD2	-6.33	100.24	111.00
1	O	220	VAL	CB-CA-C	-6.33	99.38	111.40
1	K	311	LEU	CB-CG-CD2	-6.32	100.25	111.00
1	N	99	VAL	CB-CA-C	-6.32	99.38	111.40
1	B	373	ILE	CA-CB-CG1	-6.32	99.00	111.00
1	H	211	THR	N-CA-C	-6.32	93.95	111.00
1	M	117	ILE	CG1-CB-CG2	6.32	125.29	111.40
1	O	188	LEU	CB-CG-CD1	6.32	121.74	111.00
1	J	149	MET	CG-SD-CE	-6.31	90.10	100.20
1	D	222	LEU	CB-CG-CD2	-6.30	100.29	111.00
1	E	156	LEU	CB-CG-CD1	-6.30	100.30	111.00
1	I	68	LEU	CA-CB-CG	-6.29	100.83	115.30
1	O	144	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	G	333	ASP	CB-CG-OD1	6.28	123.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	464	LEU	CB-CG-CD2	6.28	121.67	111.00
1	I	450	ASP	CB-CG-OD1	6.27	123.94	118.30
1	K	258	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	F	29	THR	CA-CB-CG2	6.26	121.17	112.40
1	G	144	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	N	74	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	N	301	ASP	CB-CG-OD1	6.25	123.93	118.30
1	O	245	MET	CG-SD-CE	6.25	110.20	100.20
1	O	450	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	134	LYS	CD-CE-NZ	-6.25	97.33	111.70
1	O	71	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	199	ASP	CB-CG-OD2	6.24	123.92	118.30
1	H	62	VAL	CB-CA-C	-6.24	99.55	111.40
1	G	275	LEU	CB-CG-CD1	-6.23	100.41	111.00
1	I	199	ASP	CB-CG-OD2	6.23	123.90	118.30
1	L	346	VAL	CG1-CB-CG2	-6.22	100.95	110.90
1	A	321	ILE	CA-CB-CG2	-6.22	98.47	110.90
1	K	382	THR	CA-CB-CG2	-6.21	103.70	112.40
1	M	369	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	L	209	ASP	CB-CG-OD2	6.21	123.89	118.30
1	F	251	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	C	102	CYS	CA-CB-SG	-6.21	102.82	114.00
1	E	223	ASP	CB-CG-OD1	6.21	123.89	118.30
1	D	25	ASP	CB-CG-OD2	6.19	123.87	118.30
1	H	263	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	H	233	ASP	CB-CG-OD1	-6.18	112.73	118.30
1	M	74	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	G	466	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	87	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	K	74	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	L	260	LEU	CB-CG-CD2	6.17	121.49	111.00
1	A	98	LEU	CB-CG-CD2	6.16	121.48	111.00
1	K	97	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	K	115	VAL	CG1-CB-CG2	6.16	120.76	110.90
1	F	250	LEU	CB-CG-CD2	6.16	121.48	111.00
1	I	237	MET	CG-SD-CE	-6.16	90.34	100.20
1	N	363	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	56	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	N	448	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	F	41	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	J	313	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	I	64	LYS	CD-CE-NZ	-6.14	97.57	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	242	TYR	CZ-CE2-CD2	-6.14	114.27	119.80
1	J	309	TYR	CD1-CE1-CZ	-6.14	114.28	119.80
1	I	150	ASP	CB-CG-OD1	6.14	123.82	118.30
1	F	30	ARG	NH1-CZ-NH2	6.13	126.15	119.40
1	J	151	TYR	CZ-CE2-CD2	-6.13	114.29	119.80
1	H	222	LEU	CA-CB-CG	6.12	129.39	115.30
1	I	52	ILE	CB-CG1-CD1	-6.12	96.77	113.90
1	J	222	LEU	CA-CB-CG	6.11	129.36	115.30
1	E	157	CYS	CA-CB-SG	-6.11	103.00	114.00
1	M	327	LEU	CB-CG-CD2	-6.11	100.61	111.00
1	G	105	VAL	CG1-CB-CG2	6.11	120.68	110.90
1	D	125	LYS	CD-CE-NZ	-6.11	97.65	111.70
1	J	43	LEU	CB-CG-CD2	-6.11	100.62	111.00
1	M	246	LEU	CB-CG-CD1	6.11	121.38	111.00
1	C	337	SER	N-CA-C	6.10	127.48	111.00
1	D	284	LEU	CB-CG-CD1	6.10	121.37	111.00
1	I	41	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	O	114	GLY	N-CA-C	-6.10	97.86	113.10
1	F	127	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	H	92	ASP	CB-CG-OD2	6.09	123.78	118.30
1	K	25	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	O	217	LYS	CD-CE-NZ	-6.09	97.69	111.70
1	C	275	LEU	CB-CG-CD2	6.09	121.34	111.00
1	I	376	LEU	CB-CG-CD1	6.08	121.33	111.00
1	A	337	SER	N-CA-C	6.08	127.40	111.00
1	E	386	MET	CA-CB-CG	-6.07	102.98	113.30
1	A	343	CYS	CA-CB-SG	-6.07	103.07	114.00
1	N	249	TYR	CE1-CZ-CE2	6.07	129.51	119.80
1	A	199	ASP	CB-CG-OD2	6.06	123.76	118.30
1	K	275	LEU	CB-CG-CD1	-6.06	100.70	111.00
1	L	321	ILE	CB-CG1-CD1	6.06	130.87	113.90
1	J	474	LEU	CA-CB-CG	6.06	129.23	115.30
1	F	263	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	H	255	MET	CA-CB-CG	6.05	123.58	113.30
1	H	217	LYS	CD-CE-NZ	-6.04	97.80	111.70
1	L	117	ILE	CG1-CB-CG2	-6.04	98.11	111.40
1	L	123	LEU	CB-CG-CD2	-6.04	100.72	111.00
1	B	239	SER	N-CA-CB	-6.04	101.44	110.50
1	C	219	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	E	201	VAL	CB-CA-C	-6.03	99.94	111.40
1	J	329	VAL	CA-CB-CG1	-6.02	101.86	110.90
1	L	68	LEU	CB-CG-CD1	6.02	121.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	64	LYS	CB-CG-CD	-6.01	95.97	111.60
1	A	208	MET	CG-SD-CE	6.00	109.80	100.20
1	L	299	THR	CA-CB-CG2	-6.00	104.00	112.40
1	I	77	LEU	CB-CG-CD1	-6.00	100.80	111.00
1	D	359	LYS	CG-CD-CE	-5.99	93.93	111.90
1	A	258	ARG	CG-CD-NE	5.99	124.37	111.80
1	L	109	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	O	313	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	D	399	ASP	CB-CG-OD1	-5.97	112.92	118.30
1	I	212	THR	N-CA-C	5.97	127.12	111.00
1	A	42	LEU	CB-CG-CD2	-5.97	100.86	111.00
1	E	361	TYR	CB-CG-CD1	5.96	124.58	121.00
1	I	65	VAL	CG1-CB-CG2	-5.96	101.37	110.90
1	F	284	LEU	CB-CG-CD1	-5.95	100.88	111.00
1	H	98	LEU	CB-CG-CD2	5.95	121.12	111.00
1	F	353	TYR	CD1-CE1-CZ	-5.95	114.44	119.80
1	B	114	GLY	N-CA-C	-5.95	98.23	113.10
1	B	92	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	G	464	LEU	C-N-CA	-5.94	109.82	122.30
1	F	197	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	70	TYR	CZ-CE2-CD2	-5.94	114.46	119.80
1	N	152	LYS	CG-CD-CE	-5.93	94.10	111.90
1	H	77	LEU	CA-CB-CG	5.93	128.95	115.30
1	C	68	LEU	CA-CB-CG	-5.93	101.66	115.30
1	B	258	ARG	CA-CB-CG	5.92	126.44	113.40
1	D	379	ILE	CG1-CB-CG2	5.92	124.42	111.40
1	E	233	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	65	VAL	CB-CA-C	-5.91	100.16	111.40
1	B	202	ASP	CB-CG-OD2	5.90	123.61	118.30
1	K	103	THR	CA-CB-CG2	-5.90	104.14	112.40
1	M	250	LEU	CA-CB-CG	5.90	128.87	115.30
1	B	237	MET	CG-SD-CE	5.90	109.64	100.20
1	G	197	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	D	22	VAL	CA-CB-CG1	5.89	119.74	110.90
1	D	298	VAL	CG1-CB-CG2	-5.89	101.48	110.90
1	E	387	THR	CA-CB-CG2	-5.88	104.16	112.40
1	B	92	ASP	CB-CG-OD2	5.88	123.59	118.30
1	F	251	ARG	CG-CD-NE	5.88	124.14	111.80
1	B	397	LEU	CB-CG-CD1	-5.88	101.01	111.00
1	M	301	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	125	LYS	CD-CE-NZ	-5.87	98.19	111.70
1	O	113	LEU	CB-CG-CD1	5.87	120.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	298	VAL	CA-CB-CG2	-5.87	102.10	110.90
1	I	313	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	O	127	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	E	469	LEU	CA-CB-CG	-5.86	101.81	115.30
1	H	156	LEU	CB-CG-CD2	-5.86	101.03	111.00
1	B	30	ARG	CB-CG-CD	5.86	126.83	111.60
1	H	75	VAL	CA-CB-CG2	-5.86	102.11	110.90
1	I	194	VAL	CA-CB-CG2	-5.86	102.11	110.90
1	K	74	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	M	220	VAL	CG1-CB-CG2	5.85	120.25	110.90
1	G	165	ILE	CG1-CB-CG2	-5.84	98.56	111.40
1	F	109	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	I	73	PHE	CG-CD2-CE2	-5.83	114.39	120.80
1	D	22	VAL	CG1-CB-CG2	-5.83	101.58	110.90
1	I	122	LEU	CB-CG-CD2	-5.82	101.11	111.00
1	E	378	LYS	CD-CE-NZ	-5.81	98.33	111.70
1	E	95	SER	N-CA-CB	-5.81	101.79	110.50
1	J	59	LYS	CD-CE-NZ	-5.80	98.36	111.70
1	O	231	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	D	362	LEU	CA-CB-CG	-5.80	101.97	115.30
1	E	257	VAL	CA-CB-CG1	-5.80	102.21	110.90
1	K	156	LEU	CB-CG-CD1	-5.80	101.14	111.00
1	B	239	SER	CA-CB-OG	-5.79	95.56	111.20
1	F	106	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	I	246	LEU	CB-CG-CD1	5.79	120.84	111.00
1	G	113	LEU	CB-CG-CD1	5.79	120.84	111.00
1	A	247	PHE	CG-CD1-CE1	-5.79	114.44	120.80
1	G	79	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	43	LEU	CB-CG-CD2	-5.78	101.17	111.00
1	D	274	ASP	CB-CG-OD2	5.78	123.50	118.30
1	M	209	ASP	CB-CG-OD2	5.78	123.50	118.30
1	O	234	TYR	CZ-CE2-CD2	-5.78	114.60	119.80
1	L	256	PHE	CZ-CE2-CD2	-5.77	113.17	120.10
1	H	235	LEU	CB-CG-CD1	-5.77	101.19	111.00
1	I	88	THR	CA-CB-CG2	-5.77	104.32	112.40
1	D	158	LEU	CB-CG-CD1	-5.77	101.20	111.00
1	I	162	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	C	242	TYR	CZ-CE2-CD2	-5.76	114.61	119.80
1	F	369	ASP	O-C-N	-5.76	113.48	122.70
1	K	255	MET	CB-CG-SD	5.76	129.69	112.40
1	C	123	LEU	CB-CG-CD1	-5.76	101.22	111.00
1	A	304	ILE	CG1-CB-CG2	5.75	124.06	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	258	ARG	CA-CB-CG	5.75	126.06	113.40
1	G	149	MET	CG-SD-CE	-5.75	90.99	100.20
1	D	303	GLN	CB-CA-C	-5.75	98.90	110.40
1	E	263	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	N	110	GLY	N-CA-C	-5.74	98.74	113.10
1	F	114	GLY	N-CA-C	-5.74	98.75	113.10
1	B	364	HIS	C-N-CA	-5.74	110.25	122.30
1	G	313	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	162	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	271	VAL	CB-CA-C	-5.74	100.50	111.40
1	I	338	THR	N-CA-CB	5.74	121.20	110.30
1	N	370	LEU	CB-CG-CD1	5.74	120.75	111.00
1	F	247	PHE	CG-CD1-CE1	-5.73	114.50	120.80
1	G	474	LEU	CA-CB-CG	5.72	128.46	115.30
1	L	144	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	O	470	LEU	CB-CG-CD1	-5.71	101.29	111.00
1	I	109	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	J	150	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	K	363	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	K	313	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	L	31	THR	CA-CB-CG2	-5.69	104.43	112.40
1	H	453	GLU	OE1-CD-OE2	5.69	130.13	123.30
1	G	105	VAL	CB-CA-C	-5.69	100.59	111.40
1	E	323	TRP	O-C-N	5.69	131.80	122.70
1	B	327	LEU	CB-CG-CD2	-5.68	101.34	111.00
1	C	62	VAL	CA-CB-CG1	-5.68	102.38	110.90
1	C	157	CYS	CB-CA-C	5.68	121.76	110.40
1	I	383	ALA	N-CA-CB	-5.67	102.16	110.10
1	M	56	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	122	LEU	CB-CG-CD1	5.67	120.63	111.00
1	B	384	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	A	99	VAL	CB-CA-C	-5.65	100.66	111.40
1	G	30	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	F	263	ARG	CA-CB-CG	5.65	125.83	113.40
1	H	31	THR	CA-CB-CG2	-5.64	104.50	112.40
1	O	451	LEU	CA-CB-CG	5.64	128.28	115.30
1	L	242	TYR	CZ-CE2-CD2	-5.64	114.72	119.80
1	K	246	LEU	CB-CG-CD2	5.64	120.58	111.00
1	M	98	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	G	191	LEU	CB-CG-CD2	-5.63	101.43	111.00
1	J	77	LEU	CB-CG-CD1	-5.62	101.44	111.00
1	F	463	PRO	N-CD-CG	-5.62	94.77	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	374	PHE	CB-CG-CD1	-5.62	116.87	120.80
1	A	362	LEU	CB-CG-CD1	5.62	120.55	111.00
1	J	123	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	O	41	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	O	459	LEU	CA-CB-CG	-5.61	102.40	115.30
1	H	219	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	J	167	GLU	OE1-CD-OE2	5.60	130.02	123.30
1	I	247	PHE	CG-CD1-CE1	-5.60	114.64	120.80
1	B	321	ILE	N-CA-C	-5.59	95.90	111.00
1	N	144	ARG	NH1-CZ-NH2	5.59	125.55	119.40
1	J	91	TYR	CD1-CE1-CZ	5.58	124.83	119.80
1	I	222	LEU	CA-CB-CG	5.58	128.14	115.30
1	M	474	LEU	CB-CG-CD1	-5.58	101.51	111.00
1	G	45	VAL	CG1-CB-CG2	-5.58	101.97	110.90
1	M	399	ASP	CB-CG-OD1	-5.58	113.28	118.30
1	K	466	ARG	CG-CD-NE	5.58	123.51	111.80
1	D	303	GLN	N-CA-C	5.57	126.05	111.00
1	I	197	ASP	CB-CG-OD1	-5.57	113.28	118.30
1	I	232	PRO	CA-CB-CG	-5.57	93.41	104.00
1	N	158	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	A	470	LEU	CB-CG-CD1	-5.57	101.53	111.00
1	J	258	ARG	CG-CD-NE	-5.57	100.10	111.80
1	A	450	ASP	CB-CG-OD1	5.56	123.31	118.30
1	E	233	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	C	384	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	J	144	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	122	LEU	CB-CG-CD1	5.55	120.44	111.00
1	K	260	LEU	CA-CB-CG	5.55	128.07	115.30
1	C	45	VAL	C-N-CA	-5.55	110.64	122.30
1	O	309	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	C	128	ASP	CB-CG-OD1	5.54	123.29	118.30
1	J	336	ARG	CG-CD-NE	-5.54	100.16	111.80
1	C	62	VAL	CG1-CB-CG2	-5.54	102.03	110.90
1	I	122	LEU	CA-CB-CG	-5.54	102.56	115.30
1	M	303	GLN	O-C-N	5.54	131.56	122.70
1	O	237	MET	CG-SD-CE	5.54	109.07	100.20
1	O	467	LYS	CD-CE-NZ	-5.54	98.96	111.70
1	L	125	LYS	CD-CE-NZ	-5.53	98.98	111.70
1	N	126	LEU	CB-CG-CD1	5.53	120.40	111.00
1	C	468	PHE	CG-CD2-CE2	-5.53	114.72	120.80
1	I	333	ASP	OD1-CG-OD2	5.52	133.79	123.30
1	H	34	TYR	CG-CD2-CE2	-5.52	116.88	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	75	VAL	CA-CB-CG2	-5.52	102.62	110.90
1	B	298	VAL	O-C-N	5.52	131.53	122.70
1	E	215	ALA	N-CA-CB	5.52	117.83	110.10
1	H	466	ARG	CG-CD-NE	-5.52	100.21	111.80
1	O	22	VAL	CG1-CB-CG2	5.52	119.73	110.90
1	L	191	LEU	CB-CG-CD1	-5.52	101.62	111.00
1	K	77	LEU	CB-CG-CD2	-5.52	101.62	111.00
1	O	62	VAL	CA-CB-CG1	-5.51	102.63	110.90
1	G	369	ASP	CB-CG-OD2	5.51	123.26	118.30
1	O	167	GLU	OE1-CD-OE2	5.51	129.91	123.30
1	F	251	ARG	CB-CG-CD	-5.51	97.28	111.60
1	H	123	LEU	CA-CB-CG	-5.51	102.63	115.30
1	A	70	TYR	CG-CD2-CE2	5.51	125.71	121.30
1	C	251	ARG	CA-CB-CG	5.51	125.52	113.40
1	G	451	LEU	CA-CB-CG	5.50	127.96	115.30
1	J	248	PHE	CD1-CE1-CZ	-5.50	113.50	120.10
1	C	246	LEU	CA-CB-CG	5.50	127.94	115.30
1	G	199	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	N	56	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	C	330	THR	CA-CB-CG2	-5.50	104.71	112.40
1	G	459	LEU	CB-CG-CD1	-5.50	101.66	111.00
1	A	71	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	I	369	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	L	109	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	J	213	LEU	CB-CG-CD1	5.49	120.33	111.00
1	C	41	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	G	461	GLN	N-CA-C	5.48	125.81	111.00
1	J	68	LEU	CA-CB-CG	-5.48	102.69	115.30
1	O	105	VAL	CB-CA-C	-5.48	100.98	111.40
1	G	363	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	474	LEU	CA-CB-CG	5.48	127.91	115.30
1	C	210	PHE	CZ-CE2-CD2	5.48	126.68	120.10
1	K	213	LEU	CB-CG-CD2	-5.48	101.68	111.00
1	A	250	LEU	CB-CG-CD2	5.48	120.31	111.00
1	L	68	LEU	CA-CB-CG	-5.48	102.70	115.30
1	I	158	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	B	64	LYS	CD-CE-NZ	-5.46	99.13	111.70
1	C	41	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	E	397	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	D	236	LYS	CD-CE-NZ	-5.45	99.16	111.70
1	K	203	THR	CA-CB-CG2	-5.45	104.77	112.40
1	O	255	MET	CG-SD-CE	5.45	108.93	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	202	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	C	284	LEU	CB-CG-CD1	-5.45	101.73	111.00
1	C	150	ASP	CB-CG-OD1	5.45	123.20	118.30
1	M	194	VAL	CA-CB-CG2	-5.45	102.73	110.90
1	I	71	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	L	258	ARG	CG-CD-NE	-5.44	100.38	111.80
1	M	109	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	150	ASP	CB-CG-OD1	5.43	123.19	118.30
1	K	389	ILE	O-C-N	5.43	131.39	122.70
1	F	190	LEU	CB-CG-CD2	-5.43	101.78	111.00
1	M	233	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	M	92	ASP	CB-CG-OD1	5.42	123.18	118.30
1	K	279	GLY	N-CA-C	-5.41	99.56	113.10
1	B	260	LEU	CB-CG-CD1	5.41	120.20	111.00
1	A	70	TYR	CD1-CE1-CZ	-5.41	114.93	119.80
1	K	22	VAL	CB-CA-C	-5.40	101.13	111.40
1	O	388	TYR	CG-CD2-CE2	-5.40	116.98	121.30
1	C	381	LEU	CB-CG-CD1	5.39	120.17	111.00
1	F	370	LEU	CA-CB-CG	-5.39	102.89	115.30
1	O	311	LEU	CA-CB-CG	-5.39	102.89	115.30
1	A	245	MET	N-CA-C	-5.39	96.44	111.00
1	F	379	ILE	CG1-CB-CG2	5.39	123.27	111.40
1	C	333	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	J	157	CYS	CA-CB-SG	-5.39	104.30	114.00
1	H	79	ASP	CB-CA-C	5.38	121.17	110.40
1	L	246	LEU	CB-CG-CD2	5.38	120.15	111.00
1	H	252	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	E	457	ALA	N-CA-CB	5.38	117.63	110.10
1	A	41	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	J	159	ILE	CG1-CB-CG2	-5.38	99.57	111.40
1	I	278	LYS	C-N-CA	-5.38	111.01	122.30
1	I	466	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	C	311	LEU	CA-CB-CG	-5.37	102.96	115.30
1	E	231	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	H	26	GLU	OE1-CD-OE2	5.37	129.74	123.30
1	L	388	TYR	CB-CG-CD1	5.37	124.22	121.00
1	I	34	TYR	CB-CG-CD1	-5.36	117.78	121.00
1	M	71	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	I	64	LYS	CG-CD-CE	-5.36	95.82	111.90
1	K	217	LYS	CD-CE-NZ	-5.36	99.38	111.70
1	A	37	ALA	C-N-CA	-5.36	111.05	122.30
1	K	115	VAL	CA-CB-CG1	-5.36	102.86	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	384	ASP	CB-CG-OD2	5.36	123.12	118.30
1	I	162	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	L	97	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	L	298	VAL	N-CA-C	-5.35	96.55	111.00
1	I	232	PRO	N-CD-CG	-5.35	95.18	103.20
1	M	242	TYR	CZ-CE2-CD2	5.35	124.61	119.80
1	F	399	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	M	363	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	444	TYR	CG-CD1-CE1	-5.34	117.03	121.30
1	M	313	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	H	188	LEU	CB-CG-CD1	5.33	120.07	111.00
1	A	194	VAL	CA-CB-CG2	-5.33	102.90	110.90
1	D	202	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	L	252	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	O	65	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	G	470	LEU	CB-CG-CD2	-5.32	101.96	111.00
1	O	156	LEU	CB-CG-CD1	-5.31	101.97	111.00
1	D	202	ASP	CB-CG-OD2	5.31	123.08	118.30
1	E	65	VAL	CB-CA-C	-5.31	101.31	111.40
1	I	336	ARG	CB-CG-CD	-5.31	97.80	111.60
1	H	210	PHE	N-CA-C	5.30	125.32	111.00
1	L	328	PHE	CG-CD2-CE2	5.30	126.64	120.80
1	A	31	THR	CA-CB-CG2	-5.30	104.98	112.40
1	A	165	ILE	CG1-CB-CG2	-5.30	99.74	111.40
1	D	244	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	E	338	THR	CA-CB-CG2	-5.29	104.99	112.40
1	G	311	LEU	CB-CG-CD2	5.29	120.00	111.00
1	M	336	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	I	209	ASP	N-CA-C	-5.29	96.72	111.00
1	N	74	ARG	CB-CG-CD	-5.28	97.87	111.60
1	M	378	LYS	CD-CE-NZ	-5.28	99.57	111.70
1	C	37	ALA	N-CA-C	-5.27	96.76	111.00
1	C	159	ILE	CB-CA-C	-5.27	101.05	111.60
1	O	190	LEU	CA-CB-CG	-5.27	103.18	115.30
1	A	105	VAL	CB-CA-C	-5.27	101.39	111.40
1	E	385	VAL	CB-CA-C	-5.27	101.39	111.40
1	D	467	LYS	CD-CE-NZ	-5.27	99.59	111.70
1	D	34	TYR	CZ-CE2-CD2	-5.26	115.06	119.80
1	E	92	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	146	CYS	CA-CB-SG	-5.26	104.53	114.00
1	J	364	HIS	C-N-CA	-5.26	111.25	122.30
1	H	360	GLU	OE1-CD-OE2	-5.26	116.99	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	313	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	122	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	E	252	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	I	134	LYS	CD-CE-NZ	-5.25	99.63	111.70
1	A	223	ASP	OD1-CG-OD2	-5.25	113.33	123.30
1	C	65	VAL	CG1-CB-CG2	-5.25	102.50	110.90
1	J	212	THR	CA-CB-CG2	-5.25	105.06	112.40
1	F	220	VAL	CB-CA-C	-5.24	101.44	111.40
1	B	388	TYR	CB-CG-CD1	5.24	124.14	121.00
1	C	56	ASP	CB-CG-OD1	5.24	123.01	118.30
1	E	42	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	H	202	ASP	CB-CG-OD2	5.24	123.01	118.30
1	I	102	CYS	CA-CB-SG	-5.24	104.57	114.00
1	L	369	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	D	222	LEU	CA-CB-CG	5.24	127.34	115.30
1	B	191	LEU	CB-CG-CD1	5.23	119.89	111.00
1	L	449	VAL	CA-CB-CG2	-5.23	103.06	110.90
1	D	103	THR	C-N-CA	-5.23	111.32	122.30
1	H	322	CYS	CA-CB-SG	5.23	123.41	114.00
1	N	22	VAL	CG1-CB-CG2	5.23	119.27	110.90
1	O	150	ASP	CB-CG-OD2	5.23	123.00	118.30
1	J	78	PRO	CA-CB-CG	-5.22	94.07	104.00
1	B	336	ARG	CG-CD-NE	-5.22	100.83	111.80
1	C	152	LYS	CD-CE-NZ	-5.22	99.69	111.70
1	N	382	THR	OG1-CB-CG2	5.22	122.01	110.00
1	G	28	VAL	CG1-CB-CG2	5.22	119.25	110.90
1	E	251	ARG	CB-CA-C	5.22	120.84	110.40
1	B	340	MET	CB-CG-SD	-5.22	96.75	112.40
1	J	305	PHE	N-CA-C	5.22	125.08	111.00
1	L	79	ASP	CB-CG-OD2	5.22	123.00	118.30
1	L	469	LEU	CB-CG-CD1	-5.22	102.13	111.00
1	K	72	VAL	CA-CB-CG1	-5.21	103.08	110.90
1	A	75	VAL	CA-CB-CG2	-5.21	103.08	110.90
1	E	98	LEU	CB-CG-CD2	5.21	119.86	111.00
1	L	356	ASP	CB-CG-OD2	5.21	122.98	118.30
1	M	30	ARG	NH1-CZ-NH2	5.21	125.13	119.40
1	O	295	GLY	N-CA-C	-5.21	100.09	113.10
1	I	201	VAL	N-CA-C	-5.20	96.95	111.00
1	D	155	GLN	CB-CA-C	-5.20	100.00	110.40
1	N	263	ARG	CD-NE-CZ	5.20	130.88	123.60
1	I	230	LYS	CD-CE-NZ	-5.20	99.74	111.70
1	K	128	ASP	CB-CG-OD1	5.20	122.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	34	TYR	CG-CD1-CE1	-5.20	117.14	121.30
1	A	202	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	F	238	VAL	CA-CB-CG2	-5.20	103.11	110.90
1	C	237	MET	CG-SD-CE	-5.19	91.89	100.20
1	H	244	ASP	N-CA-C	-5.19	96.99	111.00
1	H	152	LYS	CD-CE-NZ	-5.19	99.77	111.70
1	H	370	LEU	CB-CG-CD1	5.19	119.82	111.00
1	O	258	ARG	NH1-CZ-NH2	5.19	125.11	119.40
1	G	289	TYR	CB-CG-CD2	5.18	124.11	121.00
1	I	295	GLY	N-CA-C	-5.18	100.14	113.10
1	L	259	HIS	N-CA-C	5.18	125.00	111.00
1	K	334	THR	CA-CB-CG2	-5.18	105.15	112.40
1	N	36	HIS	N-CA-C	-5.18	97.02	111.00
1	G	368	TYR	CZ-CE2-CD2	-5.18	115.14	119.80
1	A	42	LEU	CB-CG-CD1	5.17	119.80	111.00
1	J	399	ASP	CB-CG-OD1	5.17	122.96	118.30
1	D	151	TYR	CD1-CE1-CZ	-5.17	115.15	119.80
1	I	251	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	L	98	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	B	167	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	C	191	LEU	CD1-CG-CD2	5.16	125.99	110.50
1	G	258	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	E	53	LYS	CD-CE-NZ	-5.16	99.83	111.70
1	C	327	LEU	CB-CG-CD1	5.16	119.78	111.00
1	D	467	LYS	CG-CD-CE	-5.16	96.42	111.90
1	K	71	ARG	N-CA-C	-5.16	97.07	111.00
1	H	353	TYR	CB-CG-CD2	5.15	124.09	121.00
1	F	126	LEU	CB-CG-CD1	5.15	119.76	111.00
1	I	333	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	F	381	LEU	CB-CG-CD2	5.15	119.75	111.00
1	O	201	VAL	CA-C-O	-5.15	109.28	120.10
1	G	76	LYS	CD-CE-NZ	-5.15	99.86	111.70
1	K	246	LEU	CA-CB-CG	5.14	127.13	115.30
1	C	74	ARG	CD-NE-CZ	-5.14	116.40	123.60
1	I	50	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	I	474	LEU	CB-CG-CD2	5.14	119.74	111.00
1	J	70	TYR	CG-CD2-CE2	-5.14	117.19	121.30
1	N	95	SER	N-CA-CB	-5.14	102.79	110.50
1	K	45	VAL	CG1-CB-CG2	5.14	119.12	110.90
1	O	230	LYS	CD-CE-NZ	-5.14	99.88	111.70
1	J	325	ASN	O-C-N	-5.13	114.49	122.70
1	L	316	GLY	N-CA-C	5.13	125.93	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	248	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	O	338	THR	N-CA-C	5.13	124.86	111.00
1	B	117	ILE	CG1-CB-CG2	-5.13	100.12	111.40
1	M	109	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	E	452	LYS	CD-CE-NZ	5.12	123.48	111.70
1	B	258	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	D	342	VAL	CA-CB-CG2	-5.12	103.22	110.90
1	M	156	LEU	CA-CB-CG	-5.12	103.53	115.30
1	G	103	THR	CA-CB-CG2	-5.12	105.24	112.40
1	F	30	ARG	CG-CD-NE	-5.12	101.06	111.80
1	G	222	LEU	CB-CG-CD1	5.12	119.70	111.00
1	M	126	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	D	31	THR	CA-CB-CG2	-5.11	105.24	112.40
1	H	460	ASP	CB-CG-OD2	5.11	122.90	118.30
1	I	33	ILE	CB-CA-C	-5.11	101.38	111.60
1	K	21	VAL	CG1-CB-CG2	-5.11	102.72	110.90
1	G	374	PHE	O-C-N	-5.11	114.52	122.70
1	K	244	ASP	N-CA-C	-5.11	97.20	111.00
1	N	42	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	G	162	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	F	102	CYS	CA-CB-SG	-5.10	104.81	114.00
1	D	87	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	G	109	ARG	CB-CG-CD	-5.10	98.34	111.60
1	J	321	ILE	N-CA-C	-5.10	97.23	111.00
1	J	122	LEU	CB-CG-CD1	5.09	119.66	111.00
1	H	127	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	J	28	VAL	CA-CB-CG1	-5.09	103.27	110.90
1	J	79	ASP	CB-CG-OD1	5.08	122.88	118.30
1	I	314	ALA	N-CA-CB	-5.08	102.99	110.10
1	J	251	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	G	453	GLU	N-CA-C	5.08	124.71	111.00
1	H	319	ASN	C-N-CA	-5.08	111.64	122.30
1	M	25	ASP	CB-CG-OD1	5.08	122.87	118.30
1	I	31	THR	CA-CB-CG2	-5.07	105.30	112.40
1	J	449	VAL	CA-CB-CG1	5.07	118.50	110.90
1	I	42	LEU	CB-CG-CD2	-5.07	102.39	111.00
1	F	247	PHE	CD1-CE1-CZ	5.06	126.18	120.10
1	G	334	THR	CA-CB-CG2	-5.06	105.31	112.40
1	N	370	LEU	CB-CG-CD2	-5.06	102.39	111.00
1	O	229	CYS	N-CA-C	-5.06	97.33	111.00
1	J	372	PHE	CB-CG-CD2	5.06	124.34	120.80
1	O	224	ILE	CG1-CB-CG2	-5.06	100.27	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	62	VAL	CG1-CB-CG2	-5.05	102.81	110.90
1	E	74	ARG	CB-CG-CD	-5.05	98.46	111.60
1	G	318	ASN	CB-CA-C	-5.05	100.30	110.40
1	B	470	LEU	CB-CG-CD2	5.05	119.59	111.00
1	I	237	MET	CB-CG-SD	5.05	127.56	112.40
1	N	77	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	B	113	LEU	CA-CB-CG	5.05	126.91	115.30
1	N	53	LYS	CD-CE-NZ	-5.05	100.09	111.70
1	B	75	VAL	CG1-CB-CG2	-5.05	102.83	110.90
1	F	83	PHE	C-N-CA	-5.05	111.70	122.30
1	O	271	VAL	CB-CA-C	-5.05	101.81	111.40
1	N	128	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	O	242	TYR	CD1-CE1-CZ	-5.04	115.26	119.80
1	J	156	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	A	97	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	G	386	MET	CG-SD-CE	5.04	108.27	100.20
1	I	115	VAL	N-CA-CB	5.04	122.59	111.50
1	K	333	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	J	261	PHE	CG-CD2-CE2	-5.04	115.26	120.80
1	C	152	LYS	CB-CG-CD	-5.04	98.50	111.60
1	E	22	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	D	220	VAL	CA-CB-CG2	-5.04	103.35	110.90
1	H	346	VAL	CG1-CB-CG2	-5.03	102.85	110.90
1	N	165	ILE	CG1-CB-CG2	-5.03	100.32	111.40
1	C	147	ILE	CB-CG1-CD1	-5.03	99.81	113.90
1	C	274	ASP	CB-CG-OD1	5.03	122.83	118.30
1	E	307	LYS	N-CA-C	-5.03	97.42	111.00
1	H	275	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	M	457	ALA	N-CA-C	-5.03	97.42	111.00
1	I	154	THR	CA-CB-CG2	-5.03	105.36	112.40
1	D	396	ILE	CG1-CB-CG2	5.03	122.46	111.40
1	J	22	VAL	CB-CA-C	-5.03	101.85	111.40
1	A	74	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	F	147	ILE	CG1-CB-CG2	-5.02	100.35	111.40
1	C	162	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	K	33	ILE	CG1-CB-CG2	-5.02	100.36	111.40
1	B	242	TYR	CB-CG-CD2	5.01	124.01	121.00
1	D	200	MET	CB-CA-C	-5.01	100.37	110.40
1	O	127	ASP	CB-CG-OD1	5.01	122.81	118.30
1	F	260	LEU	CB-CG-CD2	-5.01	102.48	111.00
1	B	372	PHE	CG-CD1-CE1	-5.01	115.29	120.80
1	C	275	LEU	CA-CB-CG	5.01	126.82	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	166	GLY	CA-C-O	-5.01	111.59	120.60
1	O	469	LEU	CA-CB-CG	-5.01	103.78	115.30
1	D	276	TYR	CD1-CE1-CZ	5.00	124.30	119.80
1	E	244	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	F	337	SER	N-CA-C	5.00	124.51	111.00
1	N	271	VAL	CB-CA-C	-5.00	101.90	111.40

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	PHE	Sidechain
1	A	35	TYR	Sidechain
1	A	468	PHE	Sidechain
1	B	231	TYR	Sidechain
1	B	462	PHE	Sidechain
1	D	34	TYR	Sidechain
1	F	258	ARG	Sidechain
1	I	256	PHE	Sidechain
1	I	27	TYR	Sidechain
1	I	468	PHE	Sidechain
1	J	70	TYR	Sidechain
1	O	231	TYR	Sidechain

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	3290	0	3191	235	0
1	B	3290	0	3191	243	0
1	C	3290	0	3191	282	0
1	D	3290	0	3191	251	0
1	E	3290	0	3191	251	0
1	F	3290	0	3191	283	0
1	G	3290	0	3191	222	0
1	H	3290	0	3191	219	0
1	I	3290	0	3191	252	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	3290	0	3191	221	0
1	K	3290	0	3191	249	0
1	L	3290	0	3191	286	0
1	M	3290	0	3191	279	0
1	N	3290	0	3191	245	0
1	O	3290	0	3191	260	0
All	All	49350	0	47865	3403	0

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 35.

All (3403) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:379:ILE:CG1	1:K:379:ILE:CD1	1.74	1.65
1:F:117:ILE:CD1	1:F:117:ILE:CG1	1.75	1.65
1:G:254:GLN:CB	1:G:254:GLN:CG	1.75	1.63
1:O:228:ILE:CD1	1:O:228:ILE:CG1	1.76	1.62
1:N:76:LYS:CG	1:N:76:LYS:CD	1.75	1.62
1:A:64:LYS:CG	1:A:64:LYS:CD	1.80	1.60
1:E:224:ILE:CD1	1:E:224:ILE:CG1	1.74	1.60
1:A:267:VAL:CG2	1:A:267:VAL:CB	1.76	1.58
1:M:59:LYS:CD	1:M:59:LYS:CE	1.75	1.58
1:I:304:ILE:CD1	1:I:304:ILE:CG1	1.76	1.58
1:N:152:LYS:CD	1:N:152:LYS:CE	1.80	1.58
1:A:76:LYS:CD	1:A:76:LYS:CG	1.76	1.58
1:I:280:THR:CG2	1:I:280:THR:CB	1.76	1.58
1:C:297:MET:CG	1:C:297:MET:CB	1.79	1.58
1:A:125:LYS:CD	1:A:125:LYS:CE	1.81	1.57
1:J:43:LEU:CD1	1:J:43:LEU:CG	1.75	1.56
1:O:359:LYS:CE	1:O:359:LYS:NZ	1.68	1.56
1:M:103:THR:CG2	1:M:103:THR:CB	1.76	1.55
1:C:31:THR:CB	1:C:31:THR:CA	1.77	1.55
1:B:467:LYS:CE	1:B:467:LYS:CD	1.83	1.55
1:N:389:ILE:CD1	1:N:389:ILE:CG1	1.79	1.53
1:M:396:ILE:CD1	1:M:396:ILE:CG1	1.81	1.53
1:F:134:LYS:NZ	1:F:134:LYS:CE	1.69	1.52
1:D:359:LYS:CE	1:D:359:LYS:CD	1.86	1.52
1:M:354:LYS:NZ	1:M:354:LYS:CE	1.73	1.52
1:A:125:LYS:NZ	1:A:125:LYS:CE	1.71	1.51
1:N:359:LYS:CG	1:N:359:LYS:CD	1.87	1.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:64:LYS:NZ	1:I:64:LYS:CE	1.72	1.51
1:A:467:LYS:NZ	1:A:467:LYS:CE	1.67	1.51
1:B:467:LYS:CE	1:B:467:LYS:NZ	1.68	1.50
1:J:125:LYS:NZ	1:J:125:LYS:CE	1.69	1.49
1:L:59:LYS:CE	1:L:59:LYS:NZ	1.74	1.49
1:L:452:LYS:CG	1:L:452:LYS:CD	1.87	1.49
1:O:224:ILE:CG1	1:O:224:ILE:CD1	1.88	1.49
1:L:467:LYS:CD	1:L:467:LYS:CE	1.90	1.48
1:L:392:MET:SD	1:L:392:MET:CE	2.02	1.48
1:O:59:LYS:NZ	1:O:59:LYS:CE	1.75	1.48
1:D:217:LYS:CE	1:D:217:LYS:NZ	1.76	1.48
1:I:392:MET:CE	1:I:392:MET:SD	2.01	1.47
1:L:467:LYS:CD	1:L:467:LYS:CG	1.89	1.46
1:B:134:LYS:CE	1:B:134:LYS:NZ	1.77	1.46
1:E:359:LYS:CE	1:E:359:LYS:NZ	1.79	1.45
1:L:467:LYS:NZ	1:L:467:LYS:CE	1.80	1.45
1:I:53:LYS:NZ	1:I:53:LYS:CE	1.78	1.44
1:C:392:MET:CE	1:C:392:MET:SD	2.05	1.43
1:A:304:ILE:CG1	1:A:304:ILE:CD1	1.95	1.43
1:C:121:PRO:CB	1:C:121:PRO:CG	1.77	1.41
1:F:354:LYS:NZ	1:F:354:LYS:CE	1.83	1.39
1:M:152:LYS:CE	1:M:152:LYS:NZ	1.87	1.38
1:N:152:LYS:NZ	1:N:152:LYS:CE	1.88	1.34
1:M:63:PRO:CG	1:M:63:PRO:CB	1.77	1.26
1:N:255:MET:HG2	1:N:256:PHE:N	1.57	1.19
1:O:219:ASP:HB2	1:O:263:ARG:NH1	1.59	1.14
1:M:311:LEU:N	1:M:311:LEU:HD23	1.58	1.14
1:B:311:LEU:H	1:B:311:LEU:HD23	1.16	1.10
1:H:386:MET:HG2	1:H:397:LEU:HD21	1.32	1.09
1:M:219:ASP:HB2	1:M:263:ARG:NH1	1.70	1.06
1:M:311:LEU:CD2	1:M:311:LEU:H	1.70	1.05
1:A:257:VAL:HG22	1:E:115:VAL:HG21	1.34	1.03
1:M:311:LEU:H	1:M:311:LEU:HD23	0.85	1.02
1:C:311:LEU:H	1:C:311:LEU:HD23	1.23	1.02
1:J:78:PRO:HD3	1:J:452:LYS:HA	1.39	1.01
1:C:211:THR:HG23	1:C:226:SER:HA	1.38	1.00
1:J:250:LEU:HB2	1:J:304:ILE:HD11	1.43	1.00
1:I:304:ILE:CD1	1:I:304:ILE:CG2	2.40	0.99
1:I:115:VAL:HG21	1:J:257:VAL:HG22	1.46	0.98
1:M:373:ILE:HD12	1:M:464:LEU:HD22	1.45	0.98
1:G:393:ASN:HB3	1:G:396:ILE:HD12	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ARG:HB3	1:F:109:ARG:NH1	1.80	0.97
1:M:154:THR:HG23	1:M:253:GLU:HB3	1.43	0.97
1:C:219:ASP:HB2	1:C:263:ARG:NH1	1.80	0.97
1:L:297:MET:HE2	1:M:296:SER:HB2	1.45	0.96
1:G:124:ASN:HB3	1:G:219:ASP:HB3	1.47	0.96
1:A:64:LYS:CE	1:A:64:LYS:CG	2.43	0.96
1:I:242:TYR:CE2	1:I:392:MET:HG3	2.01	0.96
1:I:201:VAL:HG11	1:I:332:VAL:HG11	1.43	0.96
1:K:52:ILE:HD12	1:K:62:VAL:HB	1.44	0.95
1:C:109:ARG:HB3	1:C:109:ARG:HH11	1.32	0.94
1:F:78:PRO:HD3	1:F:452:LYS:HA	1.47	0.94
1:D:188:LEU:HD22	1:D:188:LEU:N	1.80	0.94
1:B:115:VAL:HG21	1:C:257:VAL:HG22	1.50	0.94
1:N:242:TYR:CD2	1:N:392:MET:HG3	2.03	0.94
1:F:174:PRO:HG3	1:F:180:VAL:CG2	1.98	0.94
1:O:97:ARG:O	1:O:98:LEU:HD23	1.66	0.93
1:O:165:ILE:HG13	1:O:165:ILE:O	1.66	0.93
1:C:78:PRO:HD3	1:C:452:LYS:HA	1.50	0.93
1:B:255:MET:HG2	1:B:256:PHE:N	1.84	0.93
1:O:255:MET:HG2	1:O:256:PHE:N	1.84	0.93
1:K:201:VAL:HG11	1:K:332:VAL:HG11	1.50	0.93
1:N:373:ILE:HD12	1:N:464:LEU:HD22	1.50	0.92
1:K:333:ASP:OD1	1:K:335:THR:HG23	1.70	0.92
1:E:263:ARG:HB2	1:E:288:SER:OG	1.68	0.92
1:J:255:MET:HG2	1:J:256:PHE:N	1.82	0.91
1:O:181:LYS:HD3	1:O:181:LYS:H	1.34	0.91
1:B:149:MET:HE3	1:B:292:THR:HG23	1.53	0.91
1:F:121:PRO:HD3	1:F:222:LEU:HD21	1.53	0.91
1:F:149:MET:CE	1:F:293:PRO:HD2	2.01	0.90
1:N:219:ASP:O	1:N:220:VAL:HG13	1.71	0.90
1:C:109:ARG:HB3	1:C:109:ARG:NH1	1.85	0.90
1:F:149:MET:HE3	1:F:293:PRO:HD2	1.54	0.90
1:E:79:ASP:OD1	1:E:81:ASN:HB2	1.72	0.90
1:E:255:MET:HG2	1:E:256:PHE:N	1.86	0.90
1:K:146:CYS:O	1:K:147:ILE:HG13	1.71	0.89
1:B:134:LYS:CD	1:B:134:LYS:NZ	2.34	0.89
1:F:188:LEU:N	1:F:188:LEU:HD22	1.86	0.89
1:M:461:GLN:HE22	1:N:21:VAL:HB	1.33	0.89
1:I:242:TYR:CD2	1:I:392:MET:HG3	2.07	0.88
1:M:393:ASN:HB3	1:M:396:ILE:HD12	1.55	0.88
1:F:174:PRO:HG3	1:F:180:VAL:HG21	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:201:VAL:HG11	1:J:332:VAL:HG11	1.53	0.88
1:N:162:ARG:HB3	1:N:162:ARG:HH11	1.39	0.88
1:K:43:LEU:CD2	1:K:367:GLU:HG3	2.04	0.88
1:O:124:ASN:HB3	1:O:219:ASP:HB3	1.55	0.88
1:M:98:LEU:HD13	1:M:376:LEU:HD11	1.55	0.88
1:C:156:LEU:HG	1:C:332:VAL:HB	1.54	0.88
1:L:54:LYS:HD2	1:L:55:GLN:H	1.39	0.87
1:F:318:ASN:OD1	1:F:321:ILE:HB	1.73	0.87
1:A:105:VAL:HG12	1:A:106:GLU:N	1.87	0.87
1:J:154:THR:HG23	1:J:253:GLU:HB3	1.55	0.87
1:E:272:PRO:HD2	1:E:275:LEU:HD12	1.56	0.87
1:I:219:ASP:HB2	1:I:263:ARG:NH1	1.89	0.87
1:A:64:LYS:CB	1:A:64:LYS:CD	2.52	0.87
1:C:297:MET:HE2	1:D:256:PHE:HD2	1.38	0.87
1:L:115:VAL:HG21	1:M:257:VAL:HG22	1.56	0.87
1:K:167:GLU:HG3	1:K:167:GLU:O	1.75	0.87
1:G:117:ILE:HG21	1:H:291:PRO:HD3	1.55	0.87
1:L:452:LYS:CB	1:L:452:LYS:CD	2.54	0.86
1:L:393:ASN:HB3	1:L:396:ILE:HG13	1.57	0.86
1:C:311:LEU:N	1:C:311:LEU:HD23	1.90	0.86
1:N:92:ASP:O	1:N:96:GLN:HG3	1.76	0.86
1:D:52:ILE:HD12	1:D:62:VAL:HB	1.57	0.86
1:F:124:ASN:HB3	1:F:219:ASP:HB3	1.56	0.86
1:M:139:SER:HB2	1:M:143:ASN:HD21	1.41	0.86
1:F:393:ASN:HB3	1:F:396:ILE:HG13	1.58	0.86
1:C:254:GLN:O	1:C:254:GLN:HG3	1.74	0.86
1:E:219:ASP:HB2	1:E:263:ARG:NH1	1.90	0.85
1:A:311:LEU:H	1:A:311:LEU:HD23	1.39	0.85
1:F:165:ILE:CD1	1:F:236:LYS:HD3	2.06	0.85
1:K:474:LEU:HD23	1:K:474:LEU:H	1.40	0.85
1:G:305:PHE:HE1	1:G:333:ASP:HB2	1.42	0.85
1:M:284:LEU:HD12	1:M:285:PRO:HD2	1.56	0.85
1:N:152:LYS:CG	1:N:152:LYS:CE	2.54	0.85
1:J:305:PHE:HE1	1:J:333:ASP:HB2	1.42	0.85
1:L:121:PRO:HD3	1:L:222:LEU:HD21	1.59	0.85
1:E:311:LEU:HD23	1:E:311:LEU:H	1.42	0.85
1:C:297:MET:HE3	1:C:297:MET:HB2	1.56	0.85
1:F:109:ARG:HB3	1:F:109:ARG:HH11	1.42	0.85
1:J:311:LEU:HD23	1:J:311:LEU:H	1.40	0.85
1:I:304:ILE:CD1	1:I:304:ILE:HG21	2.07	0.85
1:C:284:LEU:HD12	1:C:285:PRO:HD2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:THR:HG23	1:F:226:SER:HA	1.57	0.84
1:L:52:ILE:HD13	1:M:269:GLU:CD	1.97	0.84
1:L:151:TYR:CE1	1:L:203:THR:HG21	2.12	0.84
1:B:77:LEU:HB2	1:B:325:ASN:O	1.77	0.84
1:I:304:ILE:CD1	1:I:304:ILE:CB	2.55	0.84
1:O:247:PHE:CE2	1:O:320:GLY:HA2	2.13	0.84
1:N:258:ARG:HB3	1:N:292:THR:HG22	1.58	0.84
1:D:242:TYR:CE2	1:D:392:MET:HG3	2.12	0.84
1:O:155:GLN:HB3	1:O:304:ILE:HG21	1.58	0.84
1:I:364:HIS:HD2	1:I:365:GLY:H	1.22	0.84
1:E:126:LEU:HB3	1:E:262:ASN:HB3	1.58	0.84
1:E:149:MET:CE	1:E:293:PRO:HD2	2.07	0.83
1:H:35:TYR:CE2	1:H:457:ALA:HB2	2.13	0.83
1:J:43:LEU:HG	1:J:43:LEU:CD1	2.03	0.83
1:A:126:LEU:HB3	1:A:262:ASN:HB3	1.59	0.83
1:B:109:ARG:H	1:B:306:ASN:HD21	1.24	0.82
1:D:121:PRO:HB3	1:E:285:PRO:HG2	1.60	0.82
1:G:115:VAL:HG21	1:H:257:VAL:HG22	1.61	0.82
1:C:30:ARG:HB3	1:C:375:GLN:HE22	1.41	0.82
1:L:467:LYS:CD	1:L:467:LYS:NZ	2.42	0.82
1:A:371:GLN:HB3	1:A:464:LEU:HD12	1.61	0.82
1:K:121:PRO:HB3	1:L:285:PRO:HG2	1.62	0.82
1:K:219:ASP:HB2	1:K:263:ARG:NH1	1.93	0.82
1:G:78:PRO:HD3	1:G:452:LYS:HA	1.59	0.82
1:D:359:LYS:CG	1:D:359:LYS:CE	2.58	0.82
1:K:181:LYS:HD3	1:K:181:LYS:H	1.42	0.82
1:O:111:GLN:NE2	1:O:367:GLU:OE1	2.12	0.82
1:O:159:ILE:HD12	1:O:329:VAL:HG22	1.59	0.82
1:D:155:GLN:OE1	1:D:304:ILE:HG22	1.79	0.82
1:C:246:LEU:O	1:C:246:LEU:HD12	1.79	0.82
1:N:250:LEU:HB2	1:N:304:ILE:HD11	1.62	0.82
1:F:134:LYS:CD	1:F:134:LYS:NZ	2.43	0.81
1:O:34:TYR:CE2	1:O:375:GLN:HG3	2.15	0.81
1:F:291:PRO:HD3	1:J:117:ILE:HG21	1.61	0.81
1:J:85:PHE:HB2	1:J:88:THR:OG1	1.80	0.81
1:K:343:CYS:HB2	1:K:360:GLU:OE2	1.80	0.81
1:M:77:LEU:HD22	1:M:455:PHE:HZ	1.46	0.81
1:N:115:VAL:HG21	1:O:257:VAL:HG22	1.62	0.81
1:M:258:ARG:HG3	1:M:259:HIS:ND1	1.95	0.81
1:E:54:LYS:HZ3	1:E:55:GLN:HB3	1.45	0.81
1:H:111:GLN:HB3	1:H:112:PRO:HD2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ILE:HG13	1:D:260:LEU:HD22	1.61	0.81
1:I:112:PRO:HB3	1:J:231:TYR:CD1	2.15	0.81
1:O:42:LEU:HD22	1:O:447:TRP:NE1	1.94	0.81
1:L:373:ILE:CD1	1:L:464:LEU:HD22	2.11	0.81
1:K:43:LEU:HD23	1:K:367:GLU:HG3	1.62	0.80
1:I:133:ASN:HD22	1:I:133:ASN:N	1.78	0.80
1:K:74:ARG:NH2	1:K:441:LEU:HD12	1.96	0.80
1:J:83:PHE:HD2	1:J:85:PHE:CZ	1.99	0.80
1:N:47:HIS:HB2	1:N:52:ILE:HD11	1.62	0.80
1:H:115:VAL:HG21	1:I:257:VAL:HG22	1.62	0.80
1:L:382:THR:OG1	1:L:385:VAL:HG23	1.81	0.80
1:L:154:THR:HG23	1:L:253:GLU:HB3	1.64	0.80
1:G:393:ASN:HB3	1:G:396:ILE:CD1	2.10	0.80
1:I:201:VAL:CG1	1:I:332:VAL:HG11	2.11	0.80
1:E:246:LEU:HD12	1:E:246:LEU:O	1.80	0.80
1:C:29:THR:HB	1:C:378:LYS:HG2	1.62	0.80
1:A:70:TYR:OH	1:A:232:PRO:HD3	1.82	0.80
1:J:393:ASN:HD22	1:J:394:PRO:HD2	1.46	0.80
1:N:68:LEU:HD23	1:N:334:THR:HG21	1.64	0.80
1:H:124:ASN:HB3	1:H:219:ASP:HB3	1.64	0.80
1:O:22:VAL:CG1	1:O:26:GLU:HG3	2.13	0.80
1:L:246:LEU:O	1:L:246:LEU:HD12	1.82	0.80
1:O:24:THR:HG23	1:O:318:ASN:HA	1.61	0.79
1:D:217:LYS:CD	1:D:217:LYS:NZ	2.44	0.79
1:B:121:PRO:HB3	1:C:285:PRO:HG2	1.63	0.79
1:M:77:LEU:HD22	1:M:455:PHE:CZ	2.16	0.79
1:H:372:PHE:O	1:H:373:ILE:HG13	1.82	0.79
1:N:373:ILE:CD1	1:N:464:LEU:HD22	2.12	0.79
1:G:161:CYS:SG	1:G:244:ASP:HB3	2.22	0.79
1:N:141:THR:HG22	1:N:142:ASP:N	1.98	0.79
1:H:386:MET:HG2	1:H:397:LEU:CD2	2.12	0.79
1:I:156:LEU:HG	1:I:332:VAL:HB	1.64	0.79
1:H:108:GLY:HA2	1:H:306:ASN:ND2	1.98	0.78
1:N:232:PRO:HB2	1:N:234:TYR:CE1	2.18	0.78
1:H:98:LEU:HD13	1:H:376:LEU:HD11	1.65	0.78
1:B:258:ARG:HG3	1:B:259:HIS:ND1	1.98	0.78
1:N:359:LYS:HD3	1:O:268:GLY:HA2	1.65	0.78
1:O:42:LEU:HD22	1:O:447:TRP:HE1	1.47	0.78
1:G:99:VAL:HG11	1:G:321:ILE:HG22	1.66	0.78
1:I:237:MET:HG2	1:I:245:MET:HG2	1.65	0.78
1:B:355:ASN:HB3	1:C:265:GLY:HA2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:234:TYR:O	1:K:238:VAL:HG23	1.84	0.78
1:C:149:MET:CE	1:C:293:PRO:HD2	2.13	0.78
1:C:22:VAL:HG12	1:C:23:SER:N	1.97	0.78
1:K:161:CYS:SG	1:K:244:ASP:HB3	2.23	0.78
1:B:372:PHE:O	1:B:373:ILE:HG13	1.83	0.78
1:F:156:LEU:HG	1:F:332:VAL:HB	1.65	0.78
1:M:24:THR:HG21	1:M:321:ILE:HG13	1.65	0.77
1:F:155:GLN:OE1	1:F:304:ILE:HG22	1.84	0.77
1:J:216:ASN:O	1:J:217:LYS:HG2	1.83	0.77
1:D:373:ILE:HD12	1:D:464:LEU:HD22	1.67	0.77
1:I:193:THR:CG2	1:I:230:LYS:HE2	2.15	0.77
1:I:304:ILE:HD13	1:I:304:ILE:CG2	2.15	0.77
1:O:162:ARG:HH11	1:O:162:ARG:HB3	1.48	0.77
1:H:54:LYS:NZ	1:H:55:GLN:HB3	1.99	0.77
1:L:82:LYS:O	1:L:83:PHE:O	2.03	0.77
1:D:151:TYR:CG	1:D:203:THR:HB	2.20	0.77
1:I:193:THR:HG21	1:I:230:LYS:HE2	1.65	0.77
1:G:96:GLN:NE2	1:G:378:LYS:HD3	1.98	0.77
1:O:158:LEU:O	1:O:159:ILE:HD13	1.85	0.77
1:K:459:LEU:HD12	1:K:469:LEU:HD21	1.66	0.77
1:K:162:ARG:HB3	1:K:162:ARG:NH1	2.00	0.77
1:L:234:TYR:O	1:L:238:VAL:HG23	1.84	0.76
1:D:188:LEU:HD22	1:D:188:LEU:H	1.49	0.76
1:N:242:TYR:CE2	1:N:392:MET:HG3	2.20	0.76
1:M:70:TYR:OH	1:M:232:PRO:HD3	1.85	0.76
1:A:463:PRO:O	1:A:467:LYS:HG3	1.85	0.76
1:K:300:SER:OG	1:L:253:GLU:HG2	1.85	0.76
1:D:373:ILE:CD1	1:D:464:LEU:HD22	2.15	0.76
1:B:121:PRO:HG3	1:C:287:THR:HG23	1.66	0.76
1:A:393:ASN:HD22	1:A:394:PRO:HD2	1.50	0.76
1:G:99:VAL:HG11	1:G:321:ILE:CG2	2.16	0.76
1:F:154:THR:HG22	1:F:155:GLN:N	1.99	0.76
1:K:162:ARG:HB3	1:K:162:ARG:HH11	1.50	0.76
1:K:394:PRO:HG2	1:K:395:SER:H	1.51	0.76
1:C:311:LEU:CD2	1:C:311:LEU:H	1.93	0.76
1:M:97:ARG:O	1:M:98:LEU:HD23	1.86	0.76
1:C:156:LEU:HD12	1:C:156:LEU:C	2.05	0.76
1:D:49:TYR:O	1:D:64:LYS:HE3	1.85	0.76
1:O:156:LEU:HD12	1:O:157:CYS:N	2.00	0.76
1:K:323:TRP:O	1:K:324:SER:HB2	1.86	0.76
1:L:373:ILE:HG13	1:L:464:LEU:HD13	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:54:LYS:HZ2	1:K:55:GLN:N	1.83	0.76
1:K:85:PHE:HB2	1:K:88:THR:OG1	1.85	0.76
1:F:231:TYR:CD1	1:J:112:PRO:HB3	2.21	0.75
1:K:258:ARG:HG3	1:K:259:HIS:ND1	2.01	0.75
1:I:121:PRO:HD3	1:I:222:LEU:HD21	1.67	0.75
1:L:331:VAL:HG11	1:L:368:TYR:HE2	1.51	0.75
1:A:155:GLN:HB3	1:A:304:ILE:HG21	1.68	0.75
1:L:297:MET:HE2	1:M:296:SER:CB	2.15	0.75
1:L:250:LEU:HB2	1:L:304:ILE:HD11	1.68	0.75
1:H:312:GLN:HG3	1:H:313:ARG:H	1.51	0.75
1:M:69:GLN:HA	1:M:199:ASP:O	1.86	0.75
1:C:255:MET:HG2	1:C:256:PHE:N	2.00	0.75
1:M:59:LYS:CG	1:M:59:LYS:CE	2.64	0.75
1:O:219:ASP:HB2	1:O:263:ARG:HH11	1.51	0.75
1:M:333:ASP:OD1	1:M:335:THR:HG23	1.86	0.75
1:K:97:ARG:O	1:K:98:LEU:HD23	1.87	0.75
1:B:237:MET:HG2	1:B:245:MET:HG2	1.68	0.75
1:I:255:MET:HG2	1:I:256:PHE:N	2.01	0.75
1:J:305:PHE:CE1	1:J:333:ASP:HB2	2.22	0.75
1:J:124:ASN:HB3	1:J:219:ASP:HB3	1.68	0.75
1:M:152:LYS:NZ	1:M:152:LYS:CD	2.49	0.75
1:H:109:ARG:H	1:H:306:ASN:HD21	1.34	0.75
1:K:451:LEU:HB3	1:K:454:LYS:HB2	1.69	0.75
1:E:124:ASN:HB3	1:E:219:ASP:HB3	1.69	0.74
1:A:158:LEU:O	1:A:159:ILE:HD13	1.87	0.74
1:M:159:ILE:HG22	1:M:247:PHE:HE1	1.52	0.74
1:L:33:ILE:HD13	1:L:33:ILE:N	2.01	0.74
1:G:240:GLU:HG2	1:G:243:GLY:H	1.52	0.74
1:N:54:LYS:HB3	1:N:57:SER:HB3	1.68	0.74
1:D:232:PRO:HB2	1:D:234:TYR:CE1	2.22	0.74
1:E:164:PRO:HA	1:E:245:MET:HG3	1.70	0.74
1:I:154:THR:HG23	1:I:253:GLU:HB3	1.68	0.74
1:M:149:MET:HE3	1:M:293:PRO:HD2	1.69	0.74
1:E:78:PRO:HD3	1:E:452:LYS:HA	1.69	0.74
1:K:151:TYR:CG	1:K:203:THR:HB	2.23	0.74
1:N:22:VAL:CG1	1:N:26:GLU:HG3	2.18	0.74
1:O:155:GLN:OE1	1:O:304:ILE:HG22	1.88	0.74
1:M:393:ASN:HB3	1:M:396:ILE:CD1	2.18	0.74
1:M:272:PRO:O	1:M:275:LEU:HB2	1.86	0.74
1:O:107:VAL:O	1:O:107:VAL:HG12	1.86	0.74
1:I:304:ILE:HD12	1:I:304:ILE:HG21	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:124:ASN:HB3	1:I:219:ASP:HB3	1.67	0.74
1:F:257:VAL:HG22	1:J:115:VAL:HG21	1.67	0.74
1:B:158:LEU:HD12	1:B:164:PRO:HG3	1.70	0.74
1:F:139:SER:HB2	1:F:143:ASN:HD21	1.52	0.74
1:C:297:MET:HE2	1:D:256:PHE:CD2	2.22	0.73
1:O:181:LYS:HD3	1:O:181:LYS:N	2.02	0.73
1:F:211:THR:HG23	1:F:226:SER:CA	2.17	0.73
1:F:154:THR:HG22	1:F:155:GLN:H	1.52	0.73
1:J:125:LYS:NZ	1:J:125:LYS:CD	2.51	0.73
1:G:305:PHE:CE1	1:G:333:ASP:HB2	2.22	0.73
1:C:297:MET:HE3	1:C:297:MET:CB	2.18	0.73
1:I:162:ARG:HB3	1:I:162:ARG:NH1	2.02	0.73
1:D:240:GLU:HG2	1:D:243:GLY:H	1.53	0.73
1:I:364:HIS:CD2	1:I:365:GLY:H	2.06	0.73
1:O:201:VAL:HG11	1:O:332:VAL:HG11	1.69	0.73
1:I:23:SER:O	1:I:25:ASP:N	2.22	0.73
1:D:201:VAL:HG11	1:D:332:VAL:HG11	1.71	0.73
1:G:314:ALA:HB2	1:G:319:ASN:HA	1.70	0.73
1:B:219:ASP:O	1:B:220:VAL:HG13	1.88	0.73
1:A:121:PRO:HB3	1:B:285:PRO:HG2	1.71	0.73
1:B:41:ARG:HH11	1:C:190:LEU:HD23	1.53	0.73
1:L:452:LYS:CG	1:L:452:LYS:CE	2.67	0.73
1:M:78:PRO:HD3	1:M:452:LYS:HA	1.70	0.73
1:H:237:MET:HB2	1:H:246:LEU:HD21	1.71	0.73
1:G:119:GLY:HA3	1:H:289:TYR:CE1	2.24	0.73
1:D:85:PHE:HB2	1:D:88:THR:OG1	1.89	0.73
1:E:54:LYS:HZ3	1:E:55:GLN:CB	2.02	0.73
1:I:78:PRO:HG2	1:I:100:TRP:HE1	1.51	0.73
1:K:389:ILE:O	1:K:392:MET:HB3	1.89	0.73
1:C:297:MET:CE	1:C:297:MET:HB2	2.18	0.73
1:L:373:ILE:HD12	1:L:464:LEU:HD22	1.71	0.73
1:N:68:LEU:HD13	1:N:151:TYR:HD1	1.53	0.73
1:F:322:CYS:HB3	1:F:326:GLN:O	1.89	0.73
1:J:109:ARG:H	1:J:306:ASN:HD21	1.37	0.73
1:H:66:SER:HB3	1:H:69:GLN:HG3	1.70	0.73
1:C:297:MET:CE	1:D:256:PHE:HD2	2.00	0.72
1:D:242:TYR:CD2	1:D:392:MET:HG3	2.24	0.72
1:A:124:ASN:HB3	1:A:219:ASP:HB3	1.70	0.72
1:N:355:ASN:HB3	1:O:265:GLY:HA2	1.71	0.72
1:H:363:ARG:HG3	1:I:188:LEU:HD21	1.71	0.72
1:F:260:LEU:HD22	1:J:117:ILE:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:VAL:HB	1:J:461:GLN:HE22	1.55	0.72
1:C:91:TYR:HD1	1:C:96:GLN:NE2	1.87	0.72
1:C:232:PRO:HB2	1:C:234:TYR:CE1	2.23	0.72
1:E:339:ASN:ND2	1:E:364:HIS:HB2	2.03	0.72
1:G:254:GLN:CG	1:G:254:GLN:CA	2.63	0.72
1:F:174:PRO:HG3	1:F:180:VAL:HG23	1.70	0.72
1:F:257:VAL:HG11	1:F:260:LEU:HD21	1.71	0.72
1:C:258:ARG:HG3	1:C:259:HIS:ND1	2.04	0.72
1:K:98:LEU:HD13	1:K:376:LEU:HD11	1.70	0.72
1:O:149:MET:HE1	1:O:205:PHE:CZ	2.24	0.72
1:A:164:PRO:HG3	1:A:330:THR:OG1	1.88	0.72
1:E:98:LEU:HD13	1:E:376:LEU:HD11	1.70	0.72
1:A:76:LYS:CD	1:A:76:LYS:CB	2.66	0.72
1:E:339:ASN:HD22	1:E:364:HIS:HB2	1.53	0.72
1:M:35:TYR:CE2	1:M:457:ALA:HB2	2.23	0.72
1:H:22:VAL:HG12	1:H:23:SER:N	2.03	0.72
1:I:121:PRO:CD	1:I:222:LEU:HD21	2.19	0.72
1:O:120:HIS:CD2	1:O:222:LEU:HD13	2.24	0.72
1:C:210:PHE:O	1:C:214:GLN:HB2	1.89	0.72
1:A:112:PRO:HB3	1:B:231:TYR:CD1	2.24	0.72
1:L:255:MET:HG2	1:L:256:PHE:N	2.05	0.72
1:E:54:LYS:HZ2	1:E:55:GLN:N	1.87	0.72
1:N:440:PRO:HG2	1:N:441:LEU:N	2.04	0.72
1:D:99:VAL:HG11	1:D:321:ILE:HG22	1.72	0.72
1:O:373:ILE:HD12	1:O:464:LEU:HD22	1.72	0.72
1:M:149:MET:CE	1:M:293:PRO:HD2	2.20	0.72
1:E:133:ASN:HD22	1:E:133:ASN:N	1.87	0.72
1:N:108:GLY:HA2	1:N:306:ASN:ND2	2.05	0.72
1:N:359:LYS:CB	1:N:359:LYS:CD	2.67	0.72
1:B:311:LEU:H	1:B:311:LEU:CD2	1.91	0.72
1:D:70:TYR:OH	1:D:232:PRO:HD3	1.90	0.72
1:D:117:ILE:HG13	1:E:260:LEU:CD2	2.20	0.72
1:M:52:ILE:HD12	1:M:62:VAL:HB	1.70	0.72
1:C:115:VAL:H	1:C:338:THR:HG23	1.54	0.71
1:F:254:GLN:O	1:F:254:GLN:HG3	1.90	0.71
1:L:342:VAL:HG22	1:L:361:TYR:HB2	1.72	0.71
1:B:170:GLY:HA3	1:B:191:LEU:HD12	1.72	0.71
1:G:117:ILE:HD12	1:H:260:LEU:HD23	1.71	0.71
1:I:112:PRO:HB3	1:J:231:TYR:HD1	1.54	0.71
1:D:240:GLU:OE2	1:D:245:MET:HB2	1.89	0.71
1:M:201:VAL:HG11	1:M:332:VAL:HG11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:76:LYS:CD	1:N:76:LYS:CB	2.67	0.71
1:D:155:GLN:HB3	1:D:304:ILE:HG21	1.71	0.71
1:O:311:LEU:HD23	1:O:311:LEU:H	1.55	0.71
1:M:162:ARG:HH11	1:M:162:ARG:HB3	1.54	0.71
1:H:298:VAL:HG11	1:H:335:THR:HA	1.73	0.71
1:F:371:GLN:HB3	1:F:464:LEU:HD12	1.71	0.71
1:C:121:PRO:HD3	1:C:222:LEU:HD21	1.71	0.71
1:B:148:SER:HB3	1:C:289:TYR:CD2	2.24	0.71
1:F:258:ARG:HG3	1:F:259:HIS:ND1	2.06	0.71
1:D:188:LEU:N	1:D:188:LEU:CD2	2.53	0.71
1:E:107:VAL:O	1:E:107:VAL:HG12	1.90	0.71
1:C:322:CYS:HB3	1:C:326:GLN:O	1.91	0.71
1:L:322:CYS:HB3	1:L:326:GLN:O	1.91	0.71
1:E:162:ARG:HB3	1:E:162:ARG:HH11	1.56	0.71
1:E:393:ASN:HB3	1:E:396:ILE:HD12	1.72	0.71
1:J:149:MET:HE2	1:J:293:PRO:HD2	1.71	0.71
1:E:149:MET:HE3	1:E:293:PRO:HD2	1.71	0.71
1:L:52:ILE:HD13	1:M:269:GLU:OE1	1.91	0.71
1:I:44:ALA:O	1:I:365:GLY:HA2	1.90	0.71
1:D:181:LYS:H	1:D:181:LYS:HD3	1.55	0.71
1:C:298:VAL:HG11	1:C:335:THR:HA	1.72	0.71
1:M:21:VAL:HG21	1:M:241:PRO:HB2	1.72	0.71
1:D:380:THR:HG21	1:H:380:THR:HG21	1.71	0.71
1:O:79:ASP:OD1	1:O:81:ASN:HB2	1.91	0.71
1:L:124:ASN:HB3	1:L:219:ASP:HB3	1.72	0.71
1:M:113:LEU:O	1:N:152:LYS:NZ	2.24	0.71
1:C:297:MET:CE	1:D:256:PHE:CD2	2.74	0.71
1:A:106:GLU:HG2	1:A:308:PRO:HA	1.73	0.71
1:F:260:LEU:HB3	1:J:117:ILE:HD12	1.71	0.71
1:H:30:ARG:HB3	1:H:375:GLN:NE2	2.06	0.71
1:O:272:PRO:HD2	1:O:275:LEU:HD12	1.73	0.71
1:H:126:LEU:HB3	1:H:262:ASN:HB3	1.73	0.70
1:G:52:ILE:HD12	1:G:62:VAL:HB	1.73	0.70
1:G:96:GLN:HE22	1:G:378:LYS:HD3	1.54	0.70
1:N:79:ASP:HB3	1:N:82:LYS:HG3	1.73	0.70
1:H:361:TYR:CG	1:I:185:CYS:HB2	2.26	0.70
1:A:219:ASP:HB2	1:A:263:ARG:NH1	2.06	0.70
1:I:155:GLN:HB3	1:I:304:ILE:HG21	1.73	0.70
1:M:139:SER:HB2	1:M:143:ASN:ND2	2.05	0.70
1:K:372:PHE:O	1:K:373:ILE:HG13	1.91	0.70
1:G:355:ASN:HB3	1:H:265:GLY:HA2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:467:LYS:CG	1:L:467:LYS:CE	2.70	0.70
1:O:158:LEU:C	1:O:159:ILE:HD13	2.12	0.70
1:F:156:LEU:HA	1:F:250:LEU:O	1.91	0.70
1:L:79:ASP:OD1	1:L:81:ASN:HB2	1.90	0.70
1:E:155:GLN:OE1	1:E:304:ILE:HG22	1.91	0.70
1:B:467:LYS:CE	1:B:467:LYS:CG	2.69	0.70
1:O:42:LEU:CD2	1:O:447:TRP:HE1	2.04	0.70
1:G:151:TYR:CG	1:G:203:THR:HB	2.27	0.70
1:O:393:ASN:HB3	1:O:396:ILE:CD1	2.21	0.70
1:C:123:LEU:HD23	1:C:147:ILE:HB	1.74	0.70
1:F:251:ARG:HH11	1:F:251:ARG:HG3	1.55	0.70
1:A:120:HIS:HA	1:A:222:LEU:CD2	2.22	0.70
1:N:440:PRO:HG2	1:N:441:LEU:H	1.57	0.70
1:F:119:GLY:HA3	1:G:289:TYR:CE1	2.27	0.70
1:F:77:LEU:HD22	1:F:455:PHE:HZ	1.56	0.70
1:O:59:LYS:NZ	1:O:59:LYS:CD	2.55	0.70
1:B:154:THR:HG23	1:B:253:GLU:HB3	1.74	0.70
1:O:80:PRO:HD2	1:O:325:ASN:OD1	1.91	0.70
1:K:37:ALA:HA	1:K:454:LYS:O	1.92	0.69
1:H:342:VAL:O	1:H:342:VAL:HG23	1.91	0.69
1:E:151:TYR:CG	1:E:203:THR:HB	2.27	0.69
1:J:188:LEU:HD22	1:J:188:LEU:H	1.57	0.69
1:B:117:ILE:O	1:B:117:ILE:HG23	1.91	0.69
1:G:53:LYS:HD3	1:G:58:ASN:HA	1.75	0.69
1:O:340:MET:HG2	1:O:363:ARG:O	1.92	0.69
1:I:181:LYS:H	1:I:181:LYS:HD3	1.57	0.69
1:E:165:ILE:HG23	1:E:245:MET:SD	2.32	0.69
1:E:162:ARG:HB3	1:E:162:ARG:NH1	2.07	0.69
1:N:299:THR:HG22	1:O:254:GLN:HB2	1.74	0.69
1:H:161:CYS:SG	1:H:244:ASP:HB3	2.32	0.69
1:D:123:LEU:HG	1:D:124:ASN:N	2.07	0.69
1:E:165:ILE:HD11	1:E:233:ASP:HB3	1.73	0.69
1:D:97:ARG:O	1:D:98:LEU:HD23	1.92	0.69
1:J:126:LEU:HG	1:J:127:ASP:OD1	1.92	0.69
1:A:155:GLN:OE1	1:A:304:ILE:HG22	1.93	0.69
1:G:219:ASP:HB2	1:G:263:ARG:NH1	2.07	0.69
1:G:117:ILE:CD1	1:H:260:LEU:HB3	2.22	0.69
1:M:363:ARG:HG3	1:N:188:LEU:HD21	1.74	0.69
1:N:121:PRO:HD3	1:N:222:LEU:HD21	1.73	0.69
1:N:124:ASN:HB3	1:N:219:ASP:HB3	1.73	0.69
1:K:43:LEU:HD21	1:K:367:GLU:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:LEU:HB2	1:D:304:ILE:HD11	1.74	0.69
1:J:79:ASP:OD1	1:J:81:ASN:HB2	1.93	0.69
1:E:54:LYS:NZ	1:E:55:GLN:HB3	2.07	0.69
1:M:211:THR:HG23	1:M:226:SER:HA	1.75	0.69
1:L:85:PHE:O	1:L:88:THR:OG1	2.09	0.69
1:G:162:ARG:HH11	1:G:162:ARG:HB3	1.58	0.69
1:A:105:VAL:HG12	1:A:106:GLU:H	1.57	0.69
1:G:117:ILE:HD11	1:H:260:LEU:HB3	1.75	0.69
1:B:211:THR:HG23	1:B:226:SER:HA	1.73	0.69
1:L:123:LEU:CD2	1:L:147:ILE:HB	2.22	0.69
1:F:149:MET:HE2	1:F:205:PHE:CE1	2.28	0.69
1:F:156:LEU:HD12	1:F:156:LEU:C	2.12	0.69
1:E:156:LEU:CD2	1:E:332:VAL:HB	2.22	0.68
1:I:110:GLY:O	1:I:111:GLN:HB2	1.92	0.68
1:I:323:TRP:O	1:I:324:SER:HB2	1.91	0.68
1:B:125:LYS:O	1:B:125:LYS:HD3	1.93	0.68
1:K:283:THR:O	1:K:283:THR:HG22	1.93	0.68
1:A:92:ASP:OD1	1:A:94:ALA:HB3	1.92	0.68
1:I:216:ASN:O	1:I:217:LYS:HG2	1.93	0.68
1:D:154:THR:HG23	1:D:253:GLU:HB3	1.75	0.68
1:N:123:LEU:HA	1:N:218:SER:O	1.92	0.68
1:C:91:TYR:CE1	1:C:96:GLN:HB2	2.29	0.68
1:B:36:HIS:ND1	1:B:37:ALA:N	2.41	0.68
1:F:117:ILE:HG23	1:F:117:ILE:O	1.93	0.68
1:C:121:PRO:HB3	1:D:285:PRO:HG2	1.75	0.68
1:N:26:GLU:HA	1:N:26:GLU:OE2	1.93	0.68
1:J:123:LEU:HD23	1:J:147:ILE:HD12	1.74	0.68
1:K:117:ILE:HG13	1:L:260:LEU:HD22	1.76	0.68
1:K:168:HIS:NE2	1:K:228:ILE:HD13	2.07	0.68
1:N:385:VAL:HG12	1:N:389:ILE:HD12	1.75	0.68
1:O:65:VAL:O	1:O:364:HIS:HB3	1.92	0.68
1:A:52:ILE:HD12	1:A:62:VAL:HB	1.74	0.68
1:F:85:PHE:HB2	1:F:88:THR:OG1	1.94	0.68
1:F:149:MET:HE2	1:F:205:PHE:HE1	1.59	0.68
1:L:78:PRO:HD3	1:L:452:LYS:HA	1.76	0.68
1:I:102:CYS:O	1:I:311:LEU:HD11	1.94	0.68
1:L:99:VAL:HG11	1:L:321:ILE:CG2	2.23	0.68
1:G:211:THR:HG23	1:G:226:SER:HA	1.75	0.68
1:G:106:GLU:HG2	1:G:308:PRO:HA	1.76	0.68
1:M:272:PRO:HD2	1:M:275:LEU:HD12	1.76	0.68
1:M:162:ARG:NH1	1:M:162:ARG:HB3	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:311:LEU:H	1:L:311:LEU:HD23	1.58	0.68
1:L:258:ARG:HB2	1:L:294:SER:HB2	1.76	0.68
1:E:110:GLY:O	1:E:111:GLN:HB2	1.92	0.68
1:D:323:TRP:O	1:D:324:SER:HB2	1.92	0.68
1:M:396:ILE:CD1	1:M:396:ILE:CB	2.72	0.68
1:F:69:GLN:NE2	1:F:71:ARG:HH22	1.91	0.68
1:B:162:ARG:HB3	1:B:162:ARG:HH11	1.59	0.68
1:F:463:PRO:O	1:F:467:LYS:HG3	1.94	0.68
1:B:54:LYS:HB3	1:B:57:SER:HB3	1.74	0.68
1:A:76:LYS:CG	1:A:76:LYS:CE	2.71	0.67
1:L:372:PHE:O	1:L:373:ILE:HG13	1.94	0.67
1:F:53:LYS:HD3	1:F:58:ASN:HA	1.75	0.67
1:I:304:ILE:HG23	1:I:304:ILE:HD13	1.77	0.67
1:C:37:ALA:HB1	1:C:451:LEU:HD13	1.75	0.67
1:L:113:LEU:HD22	1:M:253:GLU:HG3	1.76	0.67
1:O:159:ILE:HG22	1:O:247:PHE:HE1	1.59	0.67
1:K:219:ASP:O	1:K:220:VAL:HG13	1.95	0.67
1:L:155:GLN:HB2	1:L:252:ARG:HB3	1.75	0.67
1:E:123:LEU:HA	1:E:218:SER:O	1.92	0.67
1:D:117:ILE:HG13	1:E:260:LEU:HD22	1.76	0.67
1:M:120:HIS:HB2	1:M:221:PRO:HA	1.75	0.67
1:C:297:MET:CB	1:C:297:MET:CE	2.72	0.67
1:L:114:GLY:HA2	1:M:255:MET:SD	2.34	0.67
1:N:78:PRO:HD3	1:N:452:LYS:HA	1.77	0.67
1:M:165:ILE:HG23	1:M:245:MET:SD	2.33	0.67
1:N:240:GLU:OE2	1:N:245:MET:HB2	1.93	0.67
1:F:169:TRP:CZ3	1:F:190:LEU:HB2	2.29	0.67
1:O:54:LYS:HZ2	1:O:55:GLN:N	1.92	0.67
1:O:108:GLY:HA2	1:O:306:ASN:ND2	2.10	0.67
1:C:21:VAL:HG21	1:C:241:PRO:HB2	1.76	0.67
1:G:117:ILE:CG2	1:H:291:PRO:HD3	2.24	0.67
1:C:155:GLN:HB3	1:C:304:ILE:HG21	1.77	0.67
1:N:165:ILE:HG23	1:N:245:MET:SD	2.34	0.67
1:D:462:PHE:O	1:D:466:ARG:HB2	1.94	0.67
1:G:120:HIS:ND1	1:G:122:LEU:N	2.43	0.67
1:D:99:VAL:HG11	1:D:321:ILE:CG2	2.23	0.67
1:D:181:LYS:HE2	1:D:184:GLU:HG2	1.77	0.67
1:L:123:LEU:HD23	1:L:147:ILE:HB	1.74	0.67
1:I:254:GLN:HG3	1:I:254:GLN:O	1.93	0.67
1:F:188:LEU:HD22	1:F:188:LEU:H	1.57	0.67
1:L:54:LYS:HD2	1:L:55:GLN:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:LEU:HB3	1:D:372:PHE:CZ	2.30	0.67
1:H:385:VAL:O	1:H:389:ILE:HG13	1.95	0.67
1:K:156:LEU:HG	1:K:332:VAL:HB	1.75	0.67
1:B:121:PRO:HD3	1:B:222:LEU:HD21	1.77	0.67
1:D:98:LEU:HD13	1:D:376:LEU:HD11	1.75	0.67
1:M:342:VAL:HG21	1:N:185:CYS:SG	2.35	0.67
1:H:149:MET:CE	1:H:293:PRO:HD2	2.25	0.67
1:J:211:THR:HG23	1:J:226:SER:HA	1.77	0.67
1:B:22:VAL:CG1	1:B:26:GLU:HG3	2.25	0.67
1:K:126:LEU:HB3	1:K:262:ASN:HB3	1.77	0.66
1:D:181:LYS:H	1:D:181:LYS:CD	2.07	0.66
1:F:209:ASP:O	1:F:213:LEU:HB2	1.94	0.66
1:J:124:ASN:HD22	1:J:263:ARG:HD2	1.60	0.66
1:C:149:MET:HE3	1:C:293:PRO:HD2	1.75	0.66
1:I:121:PRO:HB3	1:J:285:PRO:HG2	1.77	0.66
1:O:148:SER:O	1:O:149:MET:HB3	1.95	0.66
1:E:30:ARG:HB3	1:E:375:GLN:NE2	2.09	0.66
1:O:164:PRO:HA	1:O:245:MET:HG3	1.77	0.66
1:L:151:TYR:CD1	1:L:203:THR:CG2	2.77	0.66
1:B:342:VAL:O	1:B:342:VAL:HG23	1.95	0.66
1:L:467:LYS:CD	1:L:467:LYS:CB	2.74	0.66
1:J:109:ARG:H	1:J:306:ASN:ND2	1.93	0.66
1:C:24:THR:CG2	1:C:318:ASN:HA	2.25	0.66
1:M:311:LEU:CD2	1:M:311:LEU:N	2.38	0.66
1:A:149:MET:HE2	1:A:293:PRO:HD2	1.77	0.66
1:B:222:LEU:HD22	1:B:222:LEU:H	1.60	0.66
1:K:259:HIS:H	1:K:292:THR:HB	1.60	0.66
1:K:273:ALA:HA	1:K:276:TYR:CE2	2.31	0.66
1:F:77:LEU:HD22	1:F:455:PHE:CZ	2.30	0.66
1:H:155:GLN:OE1	1:H:304:ILE:HG22	1.96	0.66
1:L:297:MET:HG3	1:M:256:PHE:HB3	1.77	0.66
1:M:149:MET:HA	1:N:260:LEU:HD13	1.76	0.66
1:L:44:ALA:O	1:L:365:GLY:HA2	1.95	0.66
1:G:125:LYS:O	1:G:125:LYS:HD3	1.95	0.66
1:J:154:THR:HG23	1:J:253:GLU:CB	2.26	0.66
1:I:162:ARG:HB3	1:I:162:ARG:HH11	1.60	0.66
1:O:149:MET:HE1	1:O:205:PHE:HZ	1.61	0.66
1:N:152:LYS:HE3	1:N:253:GLU:HB2	1.76	0.65
1:L:52:ILE:CD1	1:M:269:GLU:CD	2.64	0.65
1:I:258:ARG:HG3	1:I:259:HIS:ND1	2.11	0.65
1:C:54:LYS:HB3	1:C:57:SER:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:HIS:NE2	1:B:366:GLU:OE1	2.29	0.65
1:E:22:VAL:CG1	1:E:26:GLU:HG3	2.26	0.65
1:M:105:VAL:HG12	1:M:106:GLU:N	2.11	0.65
1:A:267:VAL:CA	1:A:267:VAL:CG2	2.71	0.65
1:M:124:ASN:HB3	1:M:219:ASP:HB3	1.78	0.65
1:N:372:PHE:O	1:N:373:ILE:HG13	1.96	0.65
1:F:165:ILE:HD11	1:F:236:LYS:HD3	1.79	0.65
1:E:164:PRO:HA	1:E:245:MET:CG	2.27	0.65
1:H:228:ILE:HG22	1:H:230:LYS:HG2	1.77	0.65
1:E:474:LEU:HD23	1:E:474:LEU:H	1.62	0.65
1:D:150:ASP:OD1	1:D:294:SER:HA	1.96	0.65
1:B:111:GLN:HB3	1:B:112:PRO:HD2	1.76	0.65
1:I:45:VAL:N	1:I:65:VAL:HG21	2.12	0.65
1:F:103:THR:HG21	1:F:468:PHE:CE1	2.31	0.65
1:C:115:VAL:HG21	1:D:257:VAL:HG22	1.77	0.65
1:B:124:ASN:HB3	1:B:219:ASP:HB3	1.79	0.65
1:I:149:MET:HE3	1:I:292:THR:HG23	1.77	0.65
1:H:149:MET:HE3	1:H:293:PRO:HD2	1.77	0.65
1:F:474:LEU:HD23	1:F:474:LEU:H	1.61	0.65
1:M:322:CYS:HB3	1:M:326:GLN:O	1.96	0.65
1:I:463:PRO:O	1:I:467:LYS:HG3	1.96	0.65
1:E:331:VAL:HG11	1:E:368:TYR:HE2	1.60	0.65
1:A:267:VAL:CG2	1:A:267:VAL:CG1	2.71	0.65
1:C:31:THR:CG2	1:C:31:THR:CA	2.72	0.65
1:K:459:LEU:HB2	1:K:469:LEU:HD11	1.77	0.65
1:H:342:VAL:CG2	1:H:361:TYR:HB2	2.26	0.65
1:N:29:THR:HG22	1:N:30:ARG:N	2.11	0.65
1:A:125:LYS:CG	1:A:125:LYS:CE	2.73	0.65
1:J:393:ASN:HD22	1:J:394:PRO:CD	2.09	0.65
1:O:162:ARG:NH1	1:O:162:ARG:HB3	2.11	0.65
1:G:121:PRO:HD3	1:G:222:LEU:HD21	1.77	0.65
1:F:21:VAL:HG21	1:F:241:PRO:HB2	1.78	0.65
1:B:54:LYS:HD2	1:B:55:GLN:H	1.62	0.65
1:F:103:THR:HG21	1:F:468:PHE:HE1	1.62	0.65
1:K:246:LEU:HD12	1:K:246:LEU:O	1.96	0.65
1:M:21:VAL:HG12	1:M:22:VAL:N	2.09	0.65
1:H:30:ARG:HB3	1:H:375:GLN:HE22	1.62	0.65
1:I:117:ILE:HG13	1:J:260:LEU:HD22	1.77	0.65
1:I:53:LYS:NZ	1:I:53:LYS:CD	2.60	0.65
1:K:314:ALA:HB2	1:K:319:ASN:HA	1.79	0.65
1:L:82:LYS:O	1:L:83:PHE:C	2.35	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:CYS:O	1:A:147:ILE:HG13	1.97	0.64
1:A:148:SER:O	1:A:149:MET:HB3	1.96	0.64
1:L:151:TYR:CG	1:L:203:THR:HB	2.32	0.64
1:I:162:ARG:HG3	1:I:244:ASP:HB3	1.79	0.64
1:E:32:ASN:C	1:E:33:ILE:HD13	2.17	0.64
1:D:188:LEU:H	1:D:188:LEU:CD2	2.11	0.64
1:C:246:LEU:C	1:C:246:LEU:HD12	2.17	0.64
1:B:122:LEU:O	1:B:144:ARG:HD2	1.97	0.64
1:O:359:LYS:CD	1:O:359:LYS:NZ	2.60	0.64
1:G:233:ASP:O	1:G:237:MET:HG3	1.98	0.64
1:C:394:PRO:HG2	1:C:395:SER:H	1.61	0.64
1:O:474:LEU:HD23	1:O:474:LEU:H	1.62	0.64
1:I:64:LYS:NZ	1:I:64:LYS:CD	2.60	0.64
1:M:121:PRO:HD3	1:M:222:LEU:HD21	1.79	0.64
1:H:208:MET:HE2	1:H:214:GLN:NE2	2.12	0.64
1:F:342:VAL:CG2	1:F:361:TYR:HB2	2.27	0.64
1:M:151:TYR:CG	1:M:203:THR:HB	2.33	0.64
1:K:53:LYS:HD3	1:K:58:ASN:HA	1.78	0.64
1:E:346:VAL:HG23	1:E:357:ASN:O	1.98	0.64
1:J:85:PHE:HB2	1:J:88:THR:CG2	2.27	0.64
1:M:77:LEU:HB2	1:M:325:ASN:O	1.97	0.64
1:L:373:ILE:HD11	1:L:464:LEU:HD22	1.79	0.64
1:O:123:LEU:HA	1:O:218:SER:O	1.98	0.64
1:O:393:ASN:HB3	1:O:396:ILE:HD12	1.79	0.64
1:K:188:LEU:HD22	1:K:188:LEU:N	2.12	0.64
1:M:209:ASP:O	1:M:213:LEU:HB2	1.97	0.64
1:I:141:THR:HG22	1:I:142:ASP:N	2.13	0.64
1:C:273:ALA:HA	1:C:276:TYR:CE2	2.32	0.64
1:G:255:MET:HG2	1:G:256:PHE:N	2.13	0.64
1:J:188:LEU:N	1:J:188:LEU:HD22	2.13	0.64
1:H:300:SER:O	1:H:303:GLN:HB2	1.98	0.64
1:D:149:MET:HE2	1:D:292:THR:HG23	1.80	0.64
1:M:258:ARG:HB3	1:M:292:THR:HG22	1.80	0.64
1:I:119:GLY:CA	1:I:148:SER:HA	2.28	0.64
1:A:75:VAL:HB	1:A:327:LEU:HB2	1.80	0.64
1:E:372:PHE:O	1:E:373:ILE:HG13	1.98	0.64
1:N:155:GLN:HB2	1:N:252:ARG:HB3	1.80	0.64
1:G:200:MET:O	1:G:229:CYS:HA	1.97	0.64
1:I:392:MET:CE	1:I:392:MET:CG	2.76	0.64
1:B:109:ARG:H	1:B:306:ASN:ND2	1.95	0.64
1:B:242:TYR:CE2	1:B:392:MET:HG3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:151:TYR:CG	1:F:203:THR:HB	2.32	0.64
1:K:200:MET:HE2	1:K:223:ASP:O	1.97	0.64
1:C:30:ARG:HB3	1:C:375:GLN:NE2	2.11	0.64
1:J:393:ASN:HB3	1:J:396:ILE:HD12	1.78	0.64
1:F:71:ARG:O	1:F:330:THR:HA	1.98	0.64
1:F:255:MET:HG2	1:F:256:PHE:N	2.12	0.64
1:L:331:VAL:HG11	1:L:368:TYR:CE2	2.31	0.64
1:E:165:ILE:CD1	1:E:233:ASP:HB3	2.28	0.64
1:L:157:CYS:HA	1:L:330:THR:O	1.98	0.63
1:C:79:ASP:OD1	1:C:81:ASN:HB2	1.98	0.63
1:L:151:TYR:CD1	1:L:203:THR:HG21	2.32	0.63
1:K:68:LEU:HD13	1:K:151:TYR:HD1	1.63	0.63
1:H:162:ARG:HB3	1:H:162:ARG:NH1	2.12	0.63
1:C:49:TYR:O	1:C:64:LYS:HE3	1.97	0.63
1:B:118:SER:HB3	1:B:223:ASP:OD2	1.98	0.63
1:A:118:SER:HB3	1:A:223:ASP:OD2	1.98	0.63
1:N:122:LEU:HD13	1:N:144:ARG:NH2	2.13	0.63
1:O:156:LEU:HA	1:O:250:LEU:O	1.98	0.63
1:M:298:VAL:HG11	1:M:335:THR:HA	1.80	0.63
1:O:62:VAL:HG12	1:O:63:PRO:HD2	1.81	0.63
1:K:118:SER:HB3	1:K:223:ASP:OD2	1.98	0.63
1:M:336:ARG:O	1:M:338:THR:N	2.29	0.63
1:K:155:GLN:HB3	1:K:304:ILE:HG21	1.78	0.63
1:N:451:LEU:HB3	1:N:454:LYS:HB2	1.78	0.63
1:F:83:PHE:HD2	1:F:85:PHE:CZ	2.16	0.63
1:M:342:VAL:HG23	1:M:342:VAL:O	1.97	0.63
1:E:33:ILE:N	1:E:33:ILE:HD13	2.13	0.63
1:E:440:PRO:O	1:E:441:LEU:HD23	1.99	0.63
1:G:22:VAL:CG1	1:G:26:GLU:HG3	2.29	0.63
1:L:216:ASN:O	1:M:277:ILE:HD12	1.99	0.63
1:D:120:HIS:CD2	1:D:222:LEU:HD13	2.34	0.63
1:H:54:LYS:HB3	1:H:57:SER:HB3	1.80	0.63
1:O:35:TYR:CE2	1:O:457:ALA:HB2	2.34	0.63
1:A:259:HIS:H	1:A:292:THR:HB	1.64	0.63
1:B:151:TYR:CG	1:B:203:THR:HB	2.34	0.63
1:I:148:SER:O	1:I:149:MET:HB3	1.98	0.63
1:M:159:ILE:HG22	1:M:247:PHE:CE1	2.31	0.63
1:J:108:GLY:HA2	1:J:306:ASN:ND2	2.13	0.63
1:H:21:VAL:HG21	1:H:241:PRO:HB2	1.80	0.63
1:C:162:ARG:HB3	1:C:162:ARG:HH11	1.62	0.63
1:D:298:VAL:HG11	1:D:335:THR:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:GLN:OE1	1:C:304:ILE:HG22	1.98	0.63
1:N:353:TYR:HE1	1:O:216:ASN:HB2	1.63	0.63
1:L:99:VAL:HG11	1:L:321:ILE:HG23	1.80	0.63
1:M:118:SER:HB3	1:M:223:ASP:OD2	1.99	0.63
1:L:126:LEU:HB3	1:L:262:ASN:HB3	1.80	0.63
1:K:263:ARG:HB2	1:K:288:SER:OG	1.99	0.63
1:F:289:TYR:CD2	1:J:148:SER:HB3	2.34	0.63
1:N:54:LYS:HD2	1:N:55:GLN:H	1.63	0.63
1:I:22:VAL:HG12	1:I:23:SER:N	2.14	0.63
1:A:305:PHE:HE1	1:A:333:ASP:HB2	1.64	0.63
1:L:121:PRO:HB3	1:M:285:PRO:HG2	1.79	0.63
1:C:97:ARG:HG2	1:C:381:LEU:HD11	1.80	0.63
1:H:162:ARG:HH11	1:H:162:ARG:HB3	1.63	0.63
1:K:123:LEU:HG	1:K:124:ASN:N	2.13	0.62
1:I:120:HIS:HA	1:I:222:LEU:CD2	2.29	0.62
1:E:393:ASN:HB3	1:E:396:ILE:CD1	2.28	0.62
1:O:72:VAL:HG21	1:O:195:LEU:O	1.98	0.62
1:M:354:LYS:NZ	1:M:354:LYS:CD	2.62	0.62
1:I:133:ASN:ND2	1:I:133:ASN:N	2.47	0.62
1:H:123:LEU:HD23	1:H:147:ILE:HD12	1.81	0.62
1:O:123:LEU:HD12	1:O:218:SER:O	1.99	0.62
1:L:461:GLN:HE22	1:M:21:VAL:HB	1.64	0.62
1:L:237:MET:HG2	1:L:245:MET:HG2	1.81	0.62
1:K:257:VAL:HG22	1:O:115:VAL:HG21	1.81	0.62
1:G:342:VAL:CG2	1:G:361:TYR:HB2	2.28	0.62
1:N:44:ALA:O	1:N:365:GLY:HA2	1.99	0.62
1:C:211:THR:HG23	1:C:226:SER:CA	2.21	0.62
1:D:109:ARG:H	1:D:306:ASN:HD21	1.47	0.62
1:A:322:CYS:HB3	1:A:326:GLN:O	1.99	0.62
1:L:34:TYR:CE2	1:L:375:GLN:HB2	2.34	0.62
1:C:152:LYS:HE3	1:C:253:GLU:HB2	1.81	0.62
1:N:151:TYR:CG	1:N:203:THR:HB	2.34	0.62
1:J:118:SER:HB3	1:J:223:ASP:OD2	1.99	0.62
1:K:285:PRO:HG2	1:O:121:PRO:HB3	1.80	0.62
1:G:373:ILE:HG13	1:G:464:LEU:HD13	1.80	0.62
1:E:101:ALA:HA	1:E:320:GLY:O	2.00	0.62
1:N:68:LEU:HD23	1:N:334:THR:CG2	2.29	0.62
1:A:121:PRO:CD	1:A:222:LEU:HD21	2.28	0.62
1:N:164:PRO:HG3	1:N:330:THR:OG1	1.99	0.62
1:C:162:ARG:NH1	1:C:162:ARG:HB3	2.14	0.62
1:A:64:LYS:HE2	1:A:64:LYS:CG	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:123:LEU:HA	1:H:218:SER:O	2.00	0.62
1:E:237:MET:HG2	1:E:245:MET:HG2	1.80	0.62
1:N:364:HIS:HD2	1:N:365:GLY:H	1.47	0.62
1:H:82:LYS:O	1:H:83:PHE:O	2.17	0.62
1:C:43:LEU:HD21	1:D:190:LEU:HD22	1.80	0.62
1:G:110:GLY:C	1:G:111:GLN:HG2	2.20	0.62
1:F:220:VAL:HG12	1:F:224:ILE:HD11	1.82	0.62
1:N:21:VAL:HG21	1:N:241:PRO:HB2	1.80	0.62
1:E:246:LEU:HD12	1:E:246:LEU:C	2.18	0.62
1:E:328:PHE:HE2	1:E:446:PHE:CE1	2.17	0.62
1:O:188:LEU:H	1:O:188:LEU:HD22	1.65	0.62
1:D:237:MET:SD	1:D:246:LEU:HD23	2.38	0.62
1:N:152:LYS:CD	1:N:152:LYS:NZ	2.63	0.62
1:O:181:LYS:HE2	1:O:184:GLU:HG2	1.82	0.62
1:C:155:GLN:HB2	1:C:252:ARG:HB3	1.80	0.62
1:O:34:TYR:CZ	1:O:375:GLN:HG3	2.33	0.62
1:E:155:GLN:HB3	1:E:304:ILE:HG21	1.81	0.62
1:N:112:PRO:HB3	1:O:231:TYR:CD1	2.35	0.62
1:L:112:PRO:HB3	1:M:231:TYR:CD1	2.35	0.62
1:J:246:LEU:C	1:J:246:LEU:HD12	2.20	0.62
1:J:36:HIS:ND1	1:J:37:ALA:N	2.47	0.62
1:H:361:TYR:CD1	1:I:185:CYS:HB2	2.35	0.62
1:H:164:PRO:HA	1:H:245:MET:HG3	1.81	0.62
1:K:211:THR:HG23	1:K:226:SER:HA	1.82	0.62
1:N:389:ILE:CB	1:N:389:ILE:CD1	2.77	0.61
1:N:68:LEU:HD13	1:N:151:TYR:CD1	2.34	0.61
1:K:22:VAL:CG1	1:K:26:GLU:HG3	2.30	0.61
1:F:253:GLU:HG3	1:J:113:LEU:HD22	1.82	0.61
1:L:156:LEU:HG	1:L:332:VAL:HB	1.82	0.61
1:M:331:VAL:HG11	1:M:368:TYR:HE2	1.64	0.61
1:N:117:ILE:HG23	1:N:117:ILE:O	1.98	0.61
1:F:159:ILE:HD12	1:F:329:VAL:HG22	1.79	0.61
1:K:296:SER:OG	1:K:297:MET:N	2.27	0.61
1:E:250:LEU:HB2	1:E:304:ILE:HD11	1.81	0.61
1:N:364:HIS:HD2	1:N:365:GLY:N	1.97	0.61
1:C:92:ASP:HB2	1:I:383:ALA:HB3	1.81	0.61
1:M:254:GLN:O	1:M:254:GLN:HG3	2.00	0.61
1:B:32:ASN:C	1:B:33:ILE:HD13	2.20	0.61
1:I:161:CYS:SG	1:I:244:ASP:HB3	2.40	0.61
1:H:22:VAL:CG1	1:H:26:GLU:HG3	2.30	0.61
1:E:174:PRO:HG3	1:E:180:VAL:HG23	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:247:PHE:CE2	1:N:320:GLY:HA2	2.35	0.61
1:A:450:ASP:OD1	1:A:452:LYS:HG3	2.00	0.61
1:I:305:PHE:HE1	1:I:333:ASP:HB2	1.65	0.61
1:J:79:ASP:HB3	1:J:82:LYS:HG3	1.81	0.61
1:F:181:LYS:H	1:F:181:LYS:HD3	1.65	0.61
1:J:96:GLN:NE2	1:J:378:LYS:HD3	2.15	0.61
1:J:258:ARG:HB2	1:J:294:SER:HB2	1.82	0.61
1:K:124:ASN:HB3	1:K:219:ASP:HB3	1.81	0.61
1:A:141:THR:HG23	1:E:354:LYS:HA	1.82	0.61
1:C:240:GLU:CG	1:C:241:PRO:HD2	2.30	0.61
1:B:97:ARG:HE	1:B:400:TRP:HB3	1.65	0.61
1:G:155:GLN:HB3	1:G:304:ILE:HG21	1.82	0.61
1:F:97:ARG:O	1:F:98:LEU:HD23	1.99	0.61
1:B:73:PHE:CD1	1:B:370:LEU:HD11	2.36	0.61
1:O:263:ARG:HB2	1:O:288:SER:OG	2.00	0.61
1:O:102:CYS:O	1:O:311:LEU:HD11	2.01	0.61
1:M:161:CYS:SG	1:M:244:ASP:HB3	2.41	0.61
1:F:331:VAL:HG11	1:F:368:TYR:HE2	1.64	0.61
1:O:29:THR:O	1:O:377:CYS:HB3	2.00	0.61
1:C:31:THR:HA	1:C:31:THR:CB	2.18	0.61
1:A:260:LEU:HD13	1:E:149:MET:HA	1.81	0.61
1:E:54:LYS:HD2	1:E:55:GLN:H	1.66	0.61
1:K:255:MET:HG2	1:K:256:PHE:N	2.15	0.61
1:D:322:CYS:HB3	1:D:326:GLN:O	2.01	0.61
1:F:260:LEU:HB3	1:J:117:ILE:CD1	2.30	0.61
1:G:54:LYS:HZ3	1:G:56:ASP:H	1.48	0.61
1:A:256:PHE:HD2	1:E:297:MET:HE2	1.64	0.61
1:K:201:VAL:CG1	1:K:332:VAL:HG11	2.28	0.61
1:E:120:HIS:HB2	1:E:221:PRO:HA	1.82	0.61
1:N:219:ASP:HB2	1:N:263:ARG:NH1	2.16	0.61
1:F:461:GLN:HE22	1:G:21:VAL:HB	1.65	0.61
1:J:69:GLN:HE21	1:J:71:ARG:NH2	1.99	0.61
1:O:36:HIS:ND1	1:O:37:ALA:N	2.49	0.61
1:M:59:LYS:NZ	1:M:59:LYS:CD	2.63	0.61
1:M:152:LYS:HE3	1:M:253:GLU:HB2	1.82	0.61
1:N:255:MET:HG2	1:N:256:PHE:H	1.60	0.61
1:L:115:VAL:CG2	1:M:257:VAL:HG22	2.30	0.61
1:L:241:PRO:HG2	1:L:242:TYR:H	1.66	0.61
1:N:99:VAL:HG11	1:N:321:ILE:CG2	2.30	0.61
1:C:361:TYR:CE2	1:D:268:GLY:HA3	2.35	0.61
1:E:24:THR:CG2	1:E:318:ASN:HA	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:333:ASP:OD1	1:G:335:THR:HG23	2.00	0.60
1:H:123:LEU:HD23	1:H:147:ILE:HB	1.83	0.60
1:L:299:THR:HG22	1:M:254:GLN:HB2	1.83	0.60
1:G:181:LYS:HD3	1:G:181:LYS:H	1.65	0.60
1:K:382:THR:OG1	1:K:385:VAL:HG23	2.00	0.60
1:I:223:ASP:OD1	1:I:224:ILE:HG23	2.01	0.60
1:O:174:PRO:HG3	1:O:180:VAL:HG23	1.83	0.60
1:M:103:THR:CA	1:M:103:THR:CG2	2.72	0.60
1:C:124:ASN:HB3	1:C:219:ASP:HB3	1.82	0.60
1:I:162:ARG:HG3	1:I:244:ASP:CB	2.30	0.60
1:N:22:VAL:HG11	1:N:26:GLU:HG3	1.83	0.60
1:H:155:GLN:HB2	1:H:252:ARG:HB3	1.83	0.60
1:J:107:VAL:HG12	1:J:107:VAL:O	2.01	0.60
1:D:24:THR:HG23	1:D:318:ASN:HA	1.82	0.60
1:A:298:VAL:O	1:A:298:VAL:HG23	2.00	0.60
1:F:157:CYS:O	1:F:249:TYR:HA	2.01	0.60
1:B:164:PRO:HG2	1:B:195:LEU:HD12	1.82	0.60
1:A:159:ILE:HG22	1:A:247:PHE:HE1	1.66	0.60
1:M:156:LEU:HG	1:M:332:VAL:HB	1.82	0.60
1:I:361:TYR:CE2	1:J:268:GLY:HA3	2.37	0.60
1:F:117:ILE:HG12	1:F:148:SER:HB2	1.82	0.60
1:F:257:VAL:CG1	1:F:260:LEU:HD21	2.30	0.60
1:I:353:TYR:HE1	1:J:216:ASN:HB2	1.66	0.60
1:C:97:ARG:C	1:C:98:LEU:HD23	2.22	0.60
1:H:461:GLN:HE22	1:I:21:VAL:HB	1.65	0.60
1:B:107:VAL:HG12	1:B:107:VAL:O	2.01	0.60
1:G:21:VAL:HG21	1:G:241:PRO:HB2	1.82	0.60
1:C:165:ILE:CD1	1:C:236:LYS:HD3	2.31	0.60
1:M:110:GLY:O	1:M:111:GLN:HB2	2.01	0.60
1:H:151:TYR:CG	1:H:203:THR:HB	2.37	0.60
1:L:452:LYS:CD	1:L:452:LYS:HB2	2.31	0.60
1:C:154:THR:HG22	1:C:155:GLN:H	1.67	0.60
1:O:156:LEU:C	1:O:156:LEU:HD12	2.21	0.60
1:L:24:THR:HG21	1:L:321:ILE:HG13	1.82	0.60
1:G:181:LYS:HD3	1:G:181:LYS:N	2.16	0.60
1:D:355:ASN:HB3	1:E:265:GLY:HA2	1.83	0.60
1:C:461:GLN:HE22	1:D:21:VAL:HB	1.65	0.60
1:C:126:LEU:HB3	1:C:262:ASN:HB3	1.84	0.60
1:L:340:MET:HB2	1:M:208:MET:SD	2.41	0.60
1:C:372:PHE:HB2	1:C:374:PHE:CE1	2.37	0.60
1:K:201:VAL:CG1	1:K:332:VAL:HG21	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:311:LEU:CD2	1:J:311:LEU:H	2.11	0.60
1:L:32:ASN:C	1:L:33:ILE:HD13	2.22	0.60
1:F:361:TYR:CG	1:G:185:CYS:HB2	2.37	0.60
1:N:248:PHE:O	1:N:249:TYR:HB3	2.01	0.60
1:C:200:MET:O	1:C:229:CYS:HA	2.02	0.60
1:E:298:VAL:HG11	1:E:335:THR:HA	1.83	0.60
1:B:21:VAL:HG21	1:B:241:PRO:HB2	1.83	0.60
1:D:148:SER:HB3	1:E:289:TYR:CD2	2.36	0.60
1:L:111:GLN:HB3	1:L:112:PRO:HD2	1.82	0.60
1:K:120:HIS:CD2	1:K:222:LEU:HD13	2.37	0.60
1:H:250:LEU:HB3	1:H:304:ILE:HD11	1.84	0.60
1:K:133:ASN:N	1:K:133:ASN:HD22	2.00	0.60
1:A:33:ILE:HD11	1:A:87:ASP:OD2	2.01	0.60
1:N:123:LEU:HD22	1:N:147:ILE:HB	1.84	0.60
1:B:222:LEU:CD2	1:B:222:LEU:H	2.13	0.60
1:F:152:LYS:NZ	1:J:113:LEU:O	2.33	0.60
1:F:336:ARG:O	1:F:338:THR:N	2.31	0.60
1:C:459:LEU:HD12	1:C:469:LEU:HD21	1.84	0.60
1:L:97:ARG:HG2	1:L:381:LEU:HD11	1.84	0.60
1:M:373:ILE:CD1	1:M:464:LEU:HD22	2.26	0.60
1:H:54:LYS:HZ3	1:H:55:GLN:CB	2.14	0.60
1:L:259:HIS:H	1:L:292:THR:HB	1.67	0.60
1:J:22:VAL:CG1	1:J:26:GLU:HG3	2.32	0.60
1:M:155:GLN:OE1	1:M:304:ILE:HG22	2.02	0.60
1:C:130:GLU:HB2	1:C:260:LEU:HD12	1.84	0.59
1:G:259:HIS:H	1:G:292:THR:HB	1.67	0.59
1:F:106:GLU:HG2	1:F:308:PRO:HA	1.83	0.59
1:I:118:SER:HB3	1:I:223:ASP:OD2	2.02	0.59
1:A:188:LEU:HD22	1:A:188:LEU:N	2.17	0.59
1:N:173:THR:HG22	1:N:174:PRO:HD2	1.84	0.59
1:D:219:ASP:HB2	1:D:263:ARG:NH1	2.16	0.59
1:L:69:GLN:HE21	1:L:71:ARG:NH2	1.99	0.59
1:C:188:LEU:HD22	1:C:188:LEU:N	2.17	0.59
1:B:216:ASN:O	1:B:217:LYS:C	2.40	0.59
1:K:342:VAL:HG23	1:K:342:VAL:O	2.01	0.59
1:A:167:GLU:HG2	1:A:231:TYR:O	2.02	0.59
1:B:155:GLN:HB2	1:B:252:ARG:HB3	1.83	0.59
1:A:125:LYS:NZ	1:A:125:LYS:CD	2.66	0.59
1:A:102:CYS:HB3	1:A:311:LEU:HD11	1.83	0.59
1:L:37:ALA:HB1	1:L:451:LEU:HD13	1.83	0.59
1:M:162:ARG:HG3	1:M:244:ASP:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:21:VAL:HG21	1:L:241:PRO:HB2	1.83	0.59
1:A:220:VAL:HB	1:A:224:ILE:HD11	1.84	0.59
1:J:47:HIS:ND1	1:J:48:PRO:HD2	2.17	0.59
1:E:322:CYS:HB3	1:E:326:GLN:O	2.02	0.59
1:I:237:MET:CG	1:I:245:MET:HG2	2.31	0.59
1:G:250:LEU:HB2	1:G:304:ILE:HD11	1.84	0.59
1:E:42:LEU:HB3	1:E:447:TRP:CZ2	2.37	0.59
1:G:42:LEU:HB3	1:G:447:TRP:CZ2	2.37	0.59
1:E:80:PRO:HD2	1:E:325:ASN:OD1	2.03	0.59
1:A:216:ASN:HB2	1:E:353:TYR:HE1	1.68	0.59
1:N:54:LYS:CB	1:N:57:SER:HB3	2.32	0.59
1:K:68:LEU:HD13	1:K:151:TYR:CD1	2.37	0.59
1:M:123:LEU:HA	1:M:218:SER:O	2.03	0.59
1:O:382:THR:OG1	1:O:385:VAL:HG23	2.02	0.59
1:O:280:THR:O	1:O:281:THR:HB	2.03	0.59
1:N:371:GLN:HB3	1:N:464:LEU:HD12	1.84	0.59
1:F:69:GLN:HE21	1:F:71:ARG:NH2	1.99	0.59
1:I:255:MET:HE3	1:I:293:PRO:HB3	1.84	0.59
1:O:237:MET:HG2	1:O:245:MET:HG2	1.85	0.59
1:H:133:ASN:N	1:H:133:ASN:HD22	2.01	0.59
1:H:37:ALA:HB1	1:H:451:LEU:HD13	1.84	0.59
1:C:280:THR:O	1:C:281:THR:HB	2.02	0.59
1:H:258:ARG:HB2	1:H:294:SER:HB2	1.83	0.59
1:H:44:ALA:HB2	1:H:447:TRP:CH2	2.38	0.59
1:A:462:PHE:O	1:A:466:ARG:HB2	2.02	0.59
1:D:121:PRO:HG3	1:E:287:THR:OG1	2.03	0.59
1:L:220:VAL:HG23	1:L:225:CYS:HB2	1.85	0.59
1:B:44:ALA:O	1:B:365:GLY:HA2	2.03	0.59
1:I:142:ASP:OD2	1:I:144:ARG:NE	2.35	0.59
1:G:373:ILE:HD12	1:G:464:LEU:HD22	1.84	0.59
1:N:117:ILE:HG13	1:O:260:LEU:HD22	1.85	0.59
1:M:382:THR:OG1	1:M:385:VAL:HG23	2.02	0.59
1:B:47:HIS:HB2	1:B:52:ILE:HD11	1.84	0.59
1:I:280:THR:CG2	1:I:280:THR:HB	2.18	0.59
1:L:52:ILE:HD13	1:M:269:GLU:CG	2.32	0.59
1:O:47:HIS:HB3	1:O:50:TYR:O	2.03	0.59
1:B:99:VAL:HG11	1:B:321:ILE:CG2	2.33	0.59
1:B:322:CYS:O	1:B:323:TRP:C	2.40	0.59
1:C:89:SER:O	1:I:384:ASP:OD1	2.20	0.59
1:A:151:TYR:CG	1:A:203:THR:HB	2.37	0.59
1:A:304:ILE:CB	1:A:304:ILE:CD1	2.79	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:MET:HE2	1:G:292:THR:HG23	1.84	0.59
1:L:85:PHE:HB2	1:L:88:THR:OG1	2.03	0.59
1:N:162:ARG:HB3	1:N:162:ARG:NH1	2.15	0.58
1:F:155:GLN:HB3	1:F:304:ILE:HG21	1.85	0.58
1:I:204:GLY:HA3	1:I:293:PRO:HG3	1.84	0.58
1:E:133:ASN:ND2	1:E:133:ASN:N	2.51	0.58
1:E:156:LEU:HA	1:E:250:LEU:O	2.03	0.58
1:G:181:LYS:H	1:G:181:LYS:CD	2.16	0.58
1:B:47:HIS:ND1	1:B:48:PRO:HD2	2.18	0.58
1:O:181:LYS:CD	1:O:181:LYS:H	2.12	0.58
1:N:220:VAL:HG23	1:N:225:CYS:CB	2.33	0.58
1:K:231:TYR:CD1	1:O:112:PRO:HB3	2.37	0.58
1:M:122:LEU:HD13	1:M:144:ARG:NH2	2.18	0.58
1:J:372:PHE:O	1:J:373:ILE:HG12	2.02	0.58
1:J:72:VAL:HG23	1:J:197:ASP:N	2.18	0.58
1:A:125:LYS:CD	1:A:125:LYS:O	2.52	0.58
1:K:54:LYS:NZ	1:K:55:GLN:HB3	2.19	0.58
1:B:79:ASP:OD1	1:B:81:ASN:HB2	2.03	0.58
1:E:192:ASN:ND2	1:E:236:LYS:HE2	2.18	0.58
1:B:222:LEU:N	1:B:222:LEU:HD22	2.18	0.58
1:J:219:ASP:HB2	1:J:263:ARG:NH1	2.17	0.58
1:E:155:GLN:HB2	1:E:252:ARG:HB3	1.85	0.58
1:B:364:HIS:HD2	1:B:365:GLY:N	2.02	0.58
1:D:233:ASP:CG	1:D:236:LYS:HB2	2.23	0.58
1:B:181:LYS:H	1:B:181:LYS:HD3	1.68	0.58
1:H:474:LEU:HD23	1:H:474:LEU:H	1.68	0.58
1:M:71:ARG:O	1:M:330:THR:HA	2.04	0.58
1:A:21:VAL:HB	1:E:461:GLN:HE22	1.69	0.58
1:N:359:LYS:CG	1:N:359:LYS:CE	2.80	0.58
1:N:141:THR:CG2	1:N:142:ASP:N	2.65	0.58
1:A:265:GLY:HA2	1:E:355:ASN:HB3	1.85	0.58
1:G:54:LYS:NZ	1:G:56:ASP:H	2.00	0.58
1:B:216:ASN:O	1:B:217:LYS:HG2	2.03	0.58
1:I:126:LEU:HB3	1:I:262:ASN:HB3	1.84	0.58
1:D:79:ASP:O	1:D:81:ASN:N	2.36	0.58
1:F:305:PHE:O	1:F:307:LYS:HG3	2.04	0.58
1:F:268:GLY:HA3	1:J:361:TYR:CZ	2.38	0.58
1:L:393:ASN:HD22	1:L:394:PRO:HD2	1.68	0.58
1:F:21:VAL:HG11	1:F:241:PRO:O	2.04	0.58
1:B:170:GLY:HA3	1:B:191:LEU:CD1	2.33	0.58
1:M:162:ARG:HG3	1:M:244:ASP:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:269:GLU:OE1	1:O:363:ARG:NH2	2.36	0.58
1:O:174:PRO:HG3	1:O:180:VAL:CG2	2.34	0.58
1:H:44:ALA:HB2	1:H:447:TRP:HH2	1.69	0.58
1:M:88:THR:HB	1:M:91:TYR:CD2	2.39	0.58
1:G:164:PRO:HG3	1:G:330:THR:HG21	1.86	0.58
1:L:171:LYS:HE3	1:L:212:THR:O	2.02	0.58
1:K:102:CYS:O	1:K:311:LEU:HD11	2.03	0.58
1:G:201:VAL:HG11	1:G:332:VAL:HG11	1.85	0.58
1:F:165:ILE:HD13	1:F:236:LYS:HD3	1.84	0.58
1:G:108:GLY:HA2	1:G:306:ASN:ND2	2.18	0.58
1:K:181:LYS:HE2	1:K:184:GLU:CG	2.34	0.58
1:D:262:ASN:ND2	1:D:289:TYR:CD2	2.72	0.58
1:C:149:MET:HE2	1:C:293:PRO:HD2	1.83	0.58
1:B:237:MET:SD	1:B:246:LEU:HD23	2.43	0.58
1:G:165:ILE:HG23	1:G:245:MET:SD	2.43	0.58
1:K:297:MET:HG3	1:L:256:PHE:HB3	1.85	0.58
1:C:123:LEU:HA	1:C:218:SER:O	2.04	0.58
1:A:162:ARG:HG3	1:A:244:ASP:HB3	1.85	0.58
1:L:202:ASP:HA	1:L:229:CYS:HB3	1.86	0.58
1:N:47:HIS:HB2	1:N:52:ILE:CD1	2.31	0.58
1:H:109:ARG:H	1:H:306:ASN:ND2	2.01	0.58
1:I:24:THR:HG21	1:I:321:ILE:HG13	1.86	0.58
1:A:121:PRO:HD3	1:A:222:LEU:HD21	1.85	0.58
1:F:247:PHE:CE2	1:F:320:GLY:HA2	2.39	0.58
1:K:80:PRO:HD3	1:K:100:TRP:CD1	2.39	0.58
1:N:166:GLY:N	1:N:193:THR:O	2.33	0.58
1:K:149:MET:HE2	1:K:292:THR:HG23	1.85	0.58
1:H:312:GLN:HG3	1:H:313:ARG:N	2.19	0.58
1:I:119:GLY:HA3	1:I:148:SER:HA	1.84	0.58
1:B:79:ASP:OD1	1:B:81:ASN:ND2	2.32	0.58
1:A:253:GLU:HG3	1:E:113:LEU:HD22	1.84	0.58
1:L:298:VAL:HG23	1:M:255:MET:O	2.04	0.58
1:D:113:LEU:HD22	1:E:253:GLU:HG3	1.86	0.58
1:G:258:ARG:O	1:G:259:HIS:ND1	2.36	0.58
1:C:98:LEU:HD13	1:C:376:LEU:HD11	1.86	0.58
1:C:24:THR:HG23	1:C:318:ASN:HA	1.86	0.58
1:N:111:GLN:NE2	1:N:367:GLU:OE1	2.35	0.58
1:K:96:GLN:HE22	1:K:378:LYS:HD3	1.69	0.58
1:I:155:GLN:HB3	1:I:304:ILE:CG2	2.34	0.57
1:N:342:VAL:HG23	1:N:342:VAL:O	2.04	0.57
1:C:119:GLY:HA3	1:D:289:TYR:CE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:372:PHE:C	1:L:373:ILE:HG13	2.24	0.57
1:M:305:PHE:HE1	1:M:333:ASP:HB2	1.69	0.57
1:G:149:MET:CE	1:G:292:THR:HG23	2.33	0.57
1:L:219:ASP:HB2	1:L:263:ARG:NH1	2.19	0.57
1:A:52:ILE:O	1:A:61:ALA:HB3	2.03	0.57
1:M:220:VAL:HG23	1:M:225:CYS:CB	2.33	0.57
1:N:272:PRO:O	1:N:274:ASP:N	2.37	0.57
1:K:202:ASP:HA	1:K:229:CYS:HB3	1.85	0.57
1:A:299:THR:C	1:A:301:ASP:N	2.57	0.57
1:F:115:VAL:HG21	1:G:257:VAL:HG22	1.84	0.57
1:G:386:MET:HG2	1:G:397:LEU:HD21	1.85	0.57
1:F:188:LEU:N	1:F:188:LEU:CD2	2.64	0.57
1:K:260:LEU:CD1	1:O:149:MET:HA	2.34	0.57
1:M:21:VAL:CG1	1:M:22:VAL:N	2.67	0.57
1:K:117:ILE:HD11	1:L:260:LEU:HB3	1.86	0.57
1:L:161:CYS:SG	1:L:244:ASP:HB3	2.44	0.57
1:J:96:GLN:HE22	1:J:378:LYS:HD3	1.67	0.57
1:K:133:ASN:N	1:K:133:ASN:ND2	2.52	0.57
1:A:21:VAL:HG12	1:A:22:VAL:N	2.19	0.57
1:E:280:THR:O	1:E:281:THR:HB	2.05	0.57
1:C:42:LEU:HB3	1:C:447:TRP:CZ2	2.39	0.57
1:G:379:ILE:HD12	1:G:400:TRP:HH2	1.68	0.57
1:N:209:ASP:O	1:N:213:LEU:HB2	2.04	0.57
1:I:43:LEU:HD23	1:I:367:GLU:HG3	1.84	0.57
1:G:31:THR:OG1	1:G:376:LEU:O	2.16	0.57
1:J:192:ASN:ND2	1:J:236:LYS:HE2	2.19	0.57
1:K:298:VAL:HG11	1:K:335:THR:HA	1.87	0.57
1:J:305:PHE:HE1	1:J:333:ASP:CB	2.16	0.57
1:L:35:TYR:O	1:L:373:ILE:HA	2.03	0.57
1:H:54:LYS:HZ3	1:H:55:GLN:HB3	1.70	0.57
1:F:333:ASP:OD2	1:F:336:ARG:NH1	2.37	0.57
1:I:80:PRO:HD2	1:I:325:ASN:OD1	2.04	0.57
1:K:105:VAL:HG12	1:K:106:GLU:N	2.20	0.57
1:M:54:LYS:HG3	1:M:56:ASP:H	1.67	0.57
1:L:109:ARG:NH1	1:L:109:ARG:HB3	2.20	0.57
1:C:35:TYR:CE2	1:C:457:ALA:HB2	2.39	0.57
1:C:474:LEU:HD23	1:C:474:LEU:H	1.68	0.57
1:I:389:ILE:O	1:I:392:MET:HB3	2.04	0.57
1:C:115:VAL:N	1:C:338:THR:HG23	2.17	0.57
1:B:109:ARG:N	1:B:306:ASN:HD21	1.99	0.57
1:B:41:ARG:NH1	1:C:190:LEU:HD23	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:461:GLN:HE22	1:H:21:VAL:HB	1.68	0.57
1:J:72:VAL:HG21	1:J:196:GLN:CA	2.35	0.57
1:N:395:SER:O	1:N:396:ILE:C	2.43	0.57
1:C:233:ASP:O	1:C:233:ASP:OD1	2.22	0.57
1:J:151:TYR:CG	1:J:203:THR:HB	2.39	0.57
1:J:155:GLN:HB2	1:J:252:ARG:HB3	1.87	0.57
1:K:122:LEU:HD13	1:K:144:ARG:NH2	2.18	0.57
1:C:149:MET:HE2	1:C:205:PHE:HE1	1.70	0.57
1:F:69:GLN:NE2	1:F:71:ARG:NH2	2.52	0.57
1:G:165:ILE:HD11	1:G:236:LYS:HD3	1.86	0.57
1:C:97:ARG:O	1:C:98:LEU:HD23	2.04	0.57
1:L:342:VAL:HG23	1:L:342:VAL:O	2.02	0.57
1:I:43:LEU:CD2	1:I:367:GLU:HG3	2.34	0.57
1:G:126:LEU:HB3	1:G:262:ASN:HB3	1.86	0.57
1:F:216:ASN:HB2	1:J:353:TYR:HE1	1.69	0.57
1:F:219:ASP:HB2	1:F:263:ARG:NH1	2.19	0.57
1:K:120:HIS:HB3	1:K:123:LEU:HB2	1.87	0.57
1:F:251:ARG:HH11	1:F:251:ARG:CG	2.14	0.57
1:H:342:VAL:O	1:H:342:VAL:CG2	2.52	0.57
1:B:200:MET:HE2	1:B:223:ASP:O	2.05	0.57
1:I:167:GLU:HG3	1:I:231:TYR:O	2.04	0.57
1:N:342:VAL:CG2	1:N:361:TYR:HB2	2.35	0.57
1:C:154:THR:HG22	1:C:155:GLN:N	2.20	0.57
1:O:24:THR:CG2	1:O:318:ASN:HA	2.34	0.57
1:D:373:ILE:CD1	1:D:464:LEU:HD13	2.35	0.57
1:E:201:VAL:HG11	1:E:332:VAL:HG11	1.87	0.57
1:I:311:LEU:H	1:I:311:LEU:HD23	1.69	0.57
1:B:69:GLN:NE2	1:B:71:ARG:HH22	2.03	0.57
1:F:283:THR:O	1:F:284:LEU:HB3	2.05	0.57
1:A:355:ASN:HB3	1:B:265:GLY:HA2	1.86	0.57
1:I:310:TRP:CH2	1:I:464:LEU:CD2	2.88	0.57
1:D:258:ARG:HB2	1:D:294:SER:HB2	1.86	0.57
1:C:297:MET:HE1	1:D:296:SER:HB2	1.86	0.57
1:C:371:GLN:C	1:C:372:PHE:CD1	2.79	0.57
1:O:42:LEU:HB3	1:O:447:TRP:CZ2	2.39	0.57
1:C:22:VAL:CG1	1:C:23:SER:N	2.65	0.57
1:G:35:TYR:O	1:G:373:ILE:HA	2.04	0.57
1:B:155:GLN:OE1	1:B:304:ILE:HG22	2.04	0.57
1:M:150:ASP:OD1	1:M:294:SER:HA	2.03	0.57
1:F:24:THR:HG23	1:F:318:ASN:HA	1.87	0.57
1:L:342:VAL:CG2	1:L:361:TYR:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:PRO:HD2	1:F:325:ASN:OD1	2.04	0.57
1:C:53:LYS:HD3	1:C:58:ASN:HA	1.86	0.57
1:H:311:LEU:H	1:H:311:LEU:HD23	1.69	0.57
1:J:312:GLN:HG3	1:J:313:ARG:H	1.68	0.57
1:I:151:TYR:CG	1:I:203:THR:HB	2.40	0.57
1:K:322:CYS:HB3	1:K:326:GLN:O	2.05	0.57
1:I:115:VAL:H	1:I:338:THR:HG23	1.70	0.56
1:F:160:GLY:HA3	1:F:245:MET:O	2.05	0.56
1:H:219:ASP:HB2	1:H:263:ARG:NH1	2.20	0.56
1:K:260:LEU:HD11	1:O:149:MET:HA	1.87	0.56
1:B:36:HIS:CE1	1:B:37:ALA:O	2.57	0.56
1:M:121:PRO:HB3	1:N:285:PRO:HG2	1.87	0.56
1:O:202:ASP:HA	1:O:229:CYS:HB3	1.86	0.56
1:A:181:LYS:N	1:A:181:LYS:HD3	2.19	0.56
1:E:219:ASP:O	1:E:220:VAL:HG13	2.04	0.56
1:I:219:ASP:O	1:I:220:VAL:HG13	2.05	0.56
1:J:311:LEU:HG	1:J:311:LEU:O	2.04	0.56
1:N:298:VAL:HG23	1:N:298:VAL:O	2.05	0.56
1:L:305:PHE:HE1	1:L:333:ASP:HB2	1.69	0.56
1:E:45:VAL:HG12	1:E:46:GLY:N	2.19	0.56
1:L:119:GLY:HA2	1:L:148:SER:HA	1.87	0.56
1:K:139:SER:HB2	1:K:143:ASN:HD21	1.70	0.56
1:B:393:ASN:HD22	1:B:394:PRO:HD2	1.70	0.56
1:J:152:LYS:HG3	1:J:255:MET:HB3	1.86	0.56
1:O:98:LEU:HD13	1:O:376:LEU:HD11	1.87	0.56
1:N:369:ASP:OD2	1:N:371:GLN:HG3	2.04	0.56
1:F:257:VAL:CG2	1:J:115:VAL:HG21	2.33	0.56
1:C:149:MET:HE2	1:C:205:PHE:CE1	2.39	0.56
1:G:222:LEU:H	1:G:222:LEU:HD22	1.69	0.56
1:H:69:GLN:HA	1:H:199:ASP:O	2.05	0.56
1:F:105:VAL:HG12	1:F:106:GLU:N	2.18	0.56
1:J:149:MET:HE1	1:J:205:PHE:HZ	1.70	0.56
1:C:123:LEU:CD2	1:C:147:ILE:HB	2.34	0.56
1:L:149:MET:HA	1:M:260:LEU:CD1	2.35	0.56
1:N:160:GLY:HA3	1:N:245:MET:O	2.05	0.56
1:B:22:VAL:HG11	1:B:26:GLU:HG3	1.87	0.56
1:M:42:LEU:HD22	1:M:447:TRP:NE1	2.19	0.56
1:H:240:GLU:HG2	1:H:243:GLY:H	1.71	0.56
1:F:382:THR:OG1	1:F:385:VAL:HG23	2.06	0.56
1:F:234:TYR:O	1:F:238:VAL:HG23	2.04	0.56
1:K:233:ASP:O	1:K:237:MET:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:299:THR:O	1:I:301:ASP:N	2.39	0.56
1:K:185:CYS:HB2	1:O:361:TYR:CD1	2.40	0.56
1:H:155:GLN:HB3	1:H:304:ILE:HG21	1.87	0.56
1:A:167:GLU:O	1:A:167:GLU:HG3	2.06	0.56
1:G:92:ASP:OD2	1:G:94:ALA:HB3	2.05	0.56
1:O:366:GLU:HG3	1:O:368:TYR:HE1	1.70	0.56
1:G:459:LEU:HD12	1:G:469:LEU:HD21	1.87	0.56
1:O:224:ILE:CB	1:O:224:ILE:CD1	2.80	0.56
1:L:300:SER:OG	1:M:253:GLU:HG2	2.06	0.56
1:A:255:MET:HG2	1:A:256:PHE:N	2.21	0.56
1:F:109:ARG:HB3	1:F:109:ARG:CZ	2.35	0.56
1:F:121:PRO:HD3	1:F:222:LEU:CD2	2.33	0.56
1:F:156:LEU:HD12	1:F:157:CYS:N	2.20	0.56
1:I:394:PRO:O	1:I:398:GLU:HG3	2.06	0.56
1:D:394:PRO:HG2	1:D:395:SER:H	1.70	0.56
1:M:373:ILE:HD11	1:M:465:GLY:HA2	1.87	0.56
1:M:297:MET:HE2	1:N:256:PHE:HD2	1.71	0.56
1:A:300:SER:OG	1:B:253:GLU:HG2	2.05	0.56
1:C:240:GLU:HG3	1:C:241:PRO:HD2	1.88	0.56
1:L:237:MET:CG	1:L:245:MET:HG2	2.35	0.56
1:N:28:VAL:HG22	1:N:379:ILE:HG12	1.86	0.56
1:B:119:GLY:HA2	1:B:148:SER:HA	1.88	0.56
1:N:259:HIS:H	1:N:292:THR:HB	1.71	0.56
1:D:165:ILE:O	1:D:165:ILE:HG13	2.05	0.56
1:A:231:TYR:CD1	1:E:112:PRO:HB3	2.41	0.56
1:O:256:PHE:CD1	1:O:256:PHE:C	2.79	0.56
1:H:389:ILE:HG22	1:H:389:ILE:O	2.06	0.56
1:J:196:GLN:N	1:J:199:ASP:OD2	2.31	0.56
1:H:181:LYS:H	1:H:181:LYS:HD3	1.71	0.56
1:M:364:HIS:HD2	1:M:365:GLY:H	1.54	0.56
1:A:273:ALA:HA	1:A:276:TYR:CE2	2.41	0.56
1:L:466:ARG:NH1	1:M:315:GLN:O	2.39	0.56
1:B:311:LEU:N	1:B:311:LEU:HD23	2.02	0.56
1:H:386:MET:O	1:H:397:LEU:HD11	2.05	0.56
1:M:219:ASP:HB2	1:M:263:ARG:CZ	2.35	0.56
1:H:312:GLN:CG	1:H:313:ARG:H	2.19	0.56
1:O:298:VAL:HG11	1:O:335:THR:HA	1.88	0.56
1:F:169:TRP:H	1:F:208:MET:HA	1.69	0.56
1:E:315:GLN:NE2	1:E:315:GLN:C	2.59	0.56
1:E:22:VAL:HG12	1:E:23:SER:N	2.19	0.56
1:L:272:PRO:HD2	1:L:275:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLU:OE1	1:D:132:SER:HB3	2.05	0.56
1:O:258:ARG:HB2	1:O:294:SER:HB2	1.86	0.56
1:D:163:PRO:HD3	1:D:328:PHE:CZ	2.41	0.56
1:H:27:TYR:CE2	1:H:388:TYR:HE2	2.23	0.56
1:C:29:THR:CG2	1:C:30:ARG:N	2.69	0.56
1:H:156:LEU:HA	1:H:250:LEU:O	2.06	0.56
1:E:22:VAL:HG11	1:E:26:GLU:HG3	1.88	0.56
1:N:29:THR:CG2	1:N:30:ARG:N	2.69	0.56
1:G:156:LEU:HA	1:G:250:LEU:O	2.04	0.56
1:K:70:TYR:CD2	1:K:195:LEU:HD22	2.41	0.56
1:O:126:LEU:HB3	1:O:262:ASN:HB3	1.87	0.56
1:I:152:LYS:HE3	1:I:253:GLU:HB2	1.86	0.55
1:J:221:PRO:O	1:J:225:CYS:HB3	2.06	0.55
1:I:366:GLU:HG3	1:I:368:TYR:HE1	1.71	0.55
1:A:200:MET:O	1:A:229:CYS:HA	2.06	0.55
1:B:295:GLY:O	1:B:296:SER:HB3	2.05	0.55
1:D:152:LYS:HE2	1:D:253:GLU:HB2	1.88	0.55
1:L:247:PHE:CE2	1:L:320:GLY:HA2	2.41	0.55
1:A:242:TYR:CE2	1:A:392:MET:HG3	2.41	0.55
1:K:152:LYS:HE3	1:K:253:GLU:HB2	1.87	0.55
1:M:223:ASP:OD1	1:M:224:ILE:HG23	2.07	0.55
1:G:361:TYR:CE2	1:H:268:GLY:HA3	2.41	0.55
1:D:342:VAL:O	1:D:342:VAL:HG23	2.06	0.55
1:N:120:HIS:CD2	1:N:222:LEU:HD13	2.40	0.55
1:G:298:VAL:HG11	1:G:335:THR:HA	1.87	0.55
1:O:247:PHE:CZ	1:O:320:GLY:HA2	2.41	0.55
1:J:119:GLY:HA2	1:J:148:SER:HA	1.89	0.55
1:N:364:HIS:CD2	1:N:365:GLY:N	2.75	0.55
1:B:139:SER:HB2	1:B:143:ASN:HD21	1.71	0.55
1:N:41:ARG:HH11	1:O:190:LEU:HD23	1.69	0.55
1:F:259:HIS:H	1:F:292:THR:HB	1.71	0.55
1:O:210:PHE:CZ	1:O:224:ILE:HD12	2.41	0.55
1:N:258:ARG:HB2	1:N:294:SER:HB2	1.88	0.55
1:C:393:ASN:HB3	1:C:396:ILE:CD1	2.35	0.55
1:C:331:VAL:HG11	1:C:368:TYR:HE2	1.72	0.55
1:A:201:VAL:HG13	1:A:332:VAL:HG21	1.87	0.55
1:G:71:ARG:HB3	1:G:73:PHE:CE1	2.41	0.55
1:C:121:PRO:CB	1:D:285:PRO:HG2	2.37	0.55
1:N:219:ASP:HB2	1:N:263:ARG:CZ	2.37	0.55
1:K:68:LEU:CD1	1:K:151:TYR:HD1	2.19	0.55
1:G:120:HIS:HE1	1:G:122:LEU:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:MET:HA	1:I:260:LEU:CD1	2.36	0.55
1:K:461:GLN:HE22	1:L:21:VAL:HB	1.72	0.55
1:I:35:TYR:CE2	1:I:457:ALA:HB2	2.42	0.55
1:F:117:ILE:HG13	1:G:260:LEU:HD22	1.89	0.55
1:E:224:ILE:CB	1:E:224:ILE:CD1	2.76	0.55
1:A:467:LYS:NZ	1:A:467:LYS:CD	2.66	0.55
1:L:393:ASN:HB3	1:L:396:ILE:CG1	2.30	0.55
1:J:119:GLY:CA	1:J:148:SER:HA	2.37	0.55
1:J:393:ASN:HB3	1:J:396:ILE:CD1	2.36	0.55
1:J:109:ARG:N	1:J:306:ASN:HD21	2.05	0.55
1:D:461:GLN:HE22	1:E:21:VAL:HB	1.72	0.55
1:H:156:LEU:HG	1:H:332:VAL:H	1.71	0.55
1:I:346:VAL:HG12	1:I:346:VAL:O	2.06	0.55
1:C:181:LYS:H	1:C:181:LYS:CD	2.19	0.55
1:D:54:LYS:HG3	1:D:56:ASP:H	1.71	0.55
1:O:68:LEU:HD23	1:O:334:THR:HG21	1.88	0.55
1:M:124:ASN:HD21	1:M:263:ARG:HB3	1.72	0.55
1:G:117:ILE:HD12	1:H:260:LEU:CD2	2.37	0.55
1:B:120:HIS:HA	1:B:222:LEU:CD2	2.37	0.55
1:H:54:LYS:HD2	1:H:55:GLN:H	1.72	0.55
1:C:114:GLY:O	1:C:335:THR:O	2.23	0.55
1:H:353:TYR:HE1	1:I:216:ASN:HB2	1.70	0.55
1:E:21:VAL:HG21	1:E:241:PRO:HB2	1.88	0.55
1:K:342:VAL:CG2	1:K:361:TYR:HB2	2.37	0.55
1:L:22:VAL:CG1	1:L:26:GLU:HG3	2.36	0.55
1:J:462:PHE:CD1	1:J:462:PHE:N	2.75	0.55
1:C:297:MET:CG	1:C:297:MET:CA	2.79	0.55
1:K:258:ARG:HB3	1:K:292:THR:HG22	1.89	0.55
1:B:258:ARG:HG3	1:B:259:HIS:CE1	2.41	0.55
1:K:154:THR:HG23	1:K:253:GLU:CB	2.37	0.55
1:C:394:PRO:HG2	1:C:395:SER:N	2.20	0.55
1:M:318:ASN:HD21	1:M:323:TRP:HE1	1.55	0.55
1:I:29:THR:HB	1:I:378:LYS:HG3	1.89	0.55
1:C:139:SER:HB2	1:C:143:ASN:HD21	1.71	0.55
1:C:101:ALA:O	1:C:375:GLN:N	2.35	0.55
1:C:336:ARG:O	1:C:338:THR:N	2.39	0.55
1:B:119:GLY:O	1:B:221:PRO:HA	2.07	0.55
1:M:80:PRO:HD2	1:M:325:ASN:OD1	2.07	0.55
1:H:69:GLN:HE21	1:H:71:ARG:NH2	2.05	0.55
1:L:149:MET:HE2	1:L:293:PRO:HD2	1.89	0.55
1:O:54:LYS:HD2	1:O:55:GLN:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:ARG:HG3	1:E:188:LEU:HD21	1.89	0.55
1:C:312:GLN:HG3	1:C:313:ARG:H	1.72	0.55
1:M:181:LYS:N	1:M:181:LYS:HD3	2.22	0.55
1:A:459:LEU:O	1:A:465:GLY:HA3	2.07	0.55
1:L:103:THR:O	1:L:103:THR:HG22	2.07	0.55
1:C:77:LEU:HD22	1:C:455:PHE:CZ	2.41	0.55
1:O:228:ILE:CB	1:O:228:ILE:CD1	2.77	0.55
1:C:353:TYR:HE1	1:D:216:ASN:HB2	1.72	0.55
1:K:343:CYS:HB2	1:K:360:GLU:CD	2.27	0.55
1:C:91:TYR:HE1	1:C:96:GLN:HB2	1.71	0.55
1:J:126:LEU:HG	1:J:127:ASP:CG	2.26	0.55
1:D:233:ASP:OD1	1:D:236:LYS:HB2	2.07	0.55
1:L:181:LYS:H	1:L:181:LYS:HD3	1.72	0.55
1:H:280:THR:O	1:H:281:THR:HB	2.06	0.55
1:F:260:LEU:CD2	1:J:117:ILE:HD12	2.37	0.54
1:L:77:LEU:HD11	1:L:374:PHE:CE2	2.42	0.54
1:O:117:ILE:HG13	1:O:148:SER:HB2	1.89	0.54
1:E:125:LYS:HE2	1:E:261:PHE:CE2	2.42	0.54
1:D:42:LEU:HB3	1:D:447:TRP:CZ2	2.42	0.54
1:C:136:VAL:HG12	1:C:137:GLY:N	2.21	0.54
1:C:158:LEU:O	1:C:159:ILE:HD13	2.07	0.54
1:G:263:ARG:HB2	1:G:288:SER:OG	2.07	0.54
1:K:45:VAL:C	1:K:65:VAL:HG21	2.26	0.54
1:H:363:ARG:HG3	1:H:363:ARG:HH11	1.72	0.54
1:J:118:SER:O	1:J:149:MET:N	2.35	0.54
1:G:106:GLU:HG2	1:G:308:PRO:CA	2.37	0.54
1:L:209:ASP:C	1:L:209:ASP:OD2	2.44	0.54
1:F:91:TYR:CE1	1:F:96:GLN:HB2	2.42	0.54
1:C:27:TYR:CD1	1:C:28:VAL:HG23	2.43	0.54
1:A:259:HIS:O	1:A:260:LEU:HD23	2.07	0.54
1:C:102:CYS:HB3	1:C:311:LEU:HD11	1.89	0.54
1:K:52:ILE:HD12	1:K:62:VAL:CB	2.29	0.54
1:J:69:GLN:HE21	1:J:71:ARG:HH22	1.56	0.54
1:O:37:ALA:HB1	1:O:451:LEU:HD13	1.88	0.54
1:N:181:LYS:HD3	1:N:181:LYS:N	2.22	0.54
1:D:314:ALA:HB2	1:D:319:ASN:HA	1.89	0.54
1:E:103:THR:HB	1:E:373:ILE:O	2.08	0.54
1:F:216:ASN:O	1:F:217:LYS:HG2	2.07	0.54
1:D:366:GLU:HG3	1:D:368:TYR:HE1	1.72	0.54
1:D:225:CYS:SG	1:D:226:SER:N	2.80	0.54
1:C:296:SER:OG	1:C:297:MET:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:CG1	1:A:106:GLU:N	2.67	0.54
1:B:231:TYR:OH	1:B:253:GLU:OE2	2.23	0.54
1:D:333:ASP:OD1	1:D:335:THR:HG23	2.08	0.54
1:M:385:VAL:O	1:M:389:ILE:HG13	2.07	0.54
1:C:85:PHE:HB2	1:C:88:THR:CG2	2.37	0.54
1:B:157:CYS:HA	1:B:330:THR:O	2.07	0.54
1:F:45:VAL:HG12	1:F:46:GLY:N	2.21	0.54
1:K:79:ASP:OD1	1:K:81:ASN:HB2	2.08	0.54
1:C:151:TYR:CG	1:C:203:THR:HB	2.43	0.54
1:L:59:LYS:CD	1:L:59:LYS:NZ	2.67	0.54
1:F:174:PRO:CG	1:F:180:VAL:CG2	2.79	0.54
1:K:201:VAL:HG13	1:K:332:VAL:HG21	1.88	0.54
1:B:112:PRO:HB3	1:C:231:TYR:CD1	2.43	0.54
1:B:113:LEU:HD22	1:C:253:GLU:HG3	1.90	0.54
1:A:121:PRO:HD2	1:A:222:LEU:HD21	1.90	0.54
1:N:440:PRO:CG	1:N:441:LEU:N	2.71	0.54
1:G:54:LYS:HD2	1:G:55:GLN:H	1.73	0.54
1:I:151:TYR:OH	1:I:221:PRO:HB2	2.08	0.54
1:M:181:LYS:HD3	1:M:181:LYS:H	1.72	0.54
1:M:101:ALA:HA	1:M:320:GLY:O	2.08	0.54
1:H:193:THR:HG21	1:H:230:LYS:HE2	1.89	0.54
1:H:342:VAL:HG22	1:H:361:TYR:HB2	1.90	0.54
1:B:242:TYR:CD2	1:B:392:MET:HG3	2.43	0.54
1:J:69:GLN:NE2	1:J:71:ARG:HH22	2.04	0.54
1:J:342:VAL:HG23	1:J:361:TYR:HB2	1.88	0.54
1:J:157:CYS:HA	1:J:330:THR:O	2.07	0.54
1:F:149:MET:HE2	1:F:293:PRO:HD2	1.85	0.54
1:N:343:CYS:HB3	1:O:214:GLN:HA	1.89	0.54
1:B:134:LYS:NZ	1:B:134:LYS:HD3	2.22	0.54
1:O:179:GLN:O	1:O:181:LYS:N	2.41	0.54
1:D:156:LEU:HG	1:D:332:VAL:HB	1.89	0.54
1:K:151:TYR:OH	1:K:221:PRO:HB2	2.08	0.54
1:L:152:LYS:HG3	1:L:255:MET:HB3	1.90	0.54
1:O:80:PRO:HD3	1:O:100:TRP:NE1	2.23	0.54
1:N:113:LEU:HD22	1:O:253:GLU:HG3	1.89	0.54
1:E:261:PHE:HB2	1:E:290:PHE:CE2	2.42	0.54
1:F:151:TYR:CD2	1:F:203:THR:HB	2.42	0.54
1:D:110:GLY:HA3	1:D:367:GLU:CD	2.28	0.54
1:F:185:CYS:HB2	1:J:361:TYR:CD2	2.43	0.54
1:M:318:ASN:ND2	1:M:323:TRP:HE1	2.06	0.54
1:A:474:LEU:H	1:A:474:LEU:HD23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PHE:HB3	1:A:86:PRO:HD2	1.89	0.54
1:E:36:HIS:ND1	1:E:37:ALA:N	2.55	0.54
1:N:210:PHE:HD2	1:N:214:GLN:OE1	1.90	0.54
1:A:361:TYR:CG	1:B:185:CYS:HB2	2.43	0.54
1:B:384:ASP:OD2	1:J:92:ASP:HB2	2.08	0.54
1:C:219:ASP:HB2	1:C:263:ARG:CZ	2.38	0.54
1:O:155:GLN:HB3	1:O:304:ILE:CG2	2.34	0.54
1:M:159:ILE:HD12	1:M:329:VAL:HG22	1.90	0.54
1:D:104:GLY:O	1:D:372:PHE:HA	2.07	0.54
1:I:85:PHE:HB2	1:I:88:THR:OG1	2.08	0.54
1:C:297:MET:CB	1:C:297:MET:SD	2.93	0.54
1:I:298:VAL:HG11	1:I:335:THR:HA	1.89	0.54
1:F:393:ASN:HB3	1:F:396:ILE:CG1	2.36	0.54
1:I:255:MET:CE	1:I:293:PRO:HB3	2.37	0.54
1:O:311:LEU:HD23	1:O:311:LEU:N	2.23	0.54
1:M:342:VAL:CG2	1:M:361:TYR:HB2	2.38	0.54
1:F:342:VAL:HG22	1:F:361:TYR:HB2	1.90	0.54
1:E:174:PRO:HG3	1:E:180:VAL:CG2	2.38	0.54
1:C:366:GLU:HG3	1:C:368:TYR:HE1	1.72	0.54
1:F:314:ALA:HB2	1:F:319:ASN:HA	1.89	0.54
1:D:124:ASN:HB3	1:D:219:ASP:HB3	1.90	0.53
1:F:174:PRO:CG	1:F:180:VAL:HG21	2.35	0.53
1:I:364:HIS:CD2	1:I:365:GLY:N	2.75	0.53
1:K:54:LYS:HZ2	1:K:55:GLN:H	1.54	0.53
1:N:353:TYR:CD1	1:O:144:ARG:NH1	2.76	0.53
1:I:181:LYS:H	1:I:181:LYS:CD	2.20	0.53
1:B:211:THR:HG23	1:B:226:SER:CA	2.38	0.53
1:F:361:TYR:CE2	1:G:268:GLY:HA3	2.42	0.53
1:M:353:TYR:HE1	1:N:216:ASN:HB2	1.72	0.53
1:I:220:VAL:HG23	1:I:225:CYS:HA	1.89	0.53
1:K:123:LEU:HA	1:K:218:SER:O	2.08	0.53
1:L:372:PHE:O	1:L:373:ILE:CG1	2.56	0.53
1:H:120:HIS:HB3	1:H:123:LEU:HB2	1.90	0.53
1:N:148:SER:O	1:N:149:MET:HB3	2.08	0.53
1:M:88:THR:HB	1:M:91:TYR:HD2	1.73	0.53
1:K:21:VAL:HG21	1:K:241:PRO:HB2	1.89	0.53
1:I:114:GLY:HA3	1:I:338:THR:OG1	2.08	0.53
1:N:106:GLU:HG2	1:N:308:PRO:HA	1.90	0.53
1:H:363:ARG:NH2	1:I:269:GLU:OE1	2.40	0.53
1:O:153:GLN:HG2	1:O:254:GLN:HG2	1.91	0.53
1:I:142:ASP:OD2	1:I:144:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:THR:HG22	1:E:254:GLN:HB2	1.90	0.53
1:D:255:MET:HG2	1:D:256:PHE:N	2.24	0.53
1:H:106:GLU:HG3	1:H:464:LEU:HG	1.91	0.53
1:A:393:ASN:HD22	1:A:394:PRO:CD	2.19	0.53
1:O:372:PHE:O	1:O:373:ILE:HG13	2.09	0.53
1:N:272:PRO:HD2	1:N:275:LEU:HD12	1.90	0.53
1:K:155:GLN:OE1	1:K:304:ILE:HG22	2.09	0.53
1:F:268:GLY:HA3	1:J:361:TYR:CE2	2.44	0.53
1:A:154:THR:HG23	1:A:253:GLU:HB3	1.91	0.53
1:J:68:LEU:HD22	1:J:151:TYR:HD1	1.73	0.53
1:A:268:GLY:HA3	1:E:361:TYR:CE2	2.43	0.53
1:J:27:TYR:CE2	1:J:388:TYR:HE2	2.26	0.53
1:O:233:ASP:OD1	1:O:236:LYS:HB2	2.08	0.53
1:K:115:VAL:HA	1:K:337:SER:OG	2.09	0.53
1:A:53:LYS:HD3	1:A:58:ASN:HA	1.89	0.53
1:B:298:VAL:HG11	1:B:335:THR:HA	1.90	0.53
1:L:52:ILE:HD13	1:M:269:GLU:HG2	1.89	0.53
1:H:54:LYS:HG3	1:H:56:ASP:H	1.73	0.53
1:G:297:MET:HG3	1:H:255:MET:O	2.09	0.53
1:D:109:ARG:H	1:D:306:ASN:ND2	2.06	0.53
1:L:50:TYR:CE2	1:M:271:VAL:HG22	2.44	0.53
1:J:318:ASN:OD1	1:J:319:ASN:N	2.41	0.53
1:E:258:ARG:HG3	1:E:259:HIS:ND1	2.24	0.53
1:N:76:LYS:CG	1:N:76:LYS:CE	2.85	0.53
1:A:149:MET:CE	1:A:293:PRO:HD2	2.38	0.53
1:B:120:HIS:HA	1:B:222:LEU:HD21	1.91	0.53
1:H:109:ARG:N	1:H:306:ASN:HD21	2.04	0.53
1:G:192:ASN:ND2	1:G:236:LYS:HE2	2.23	0.53
1:N:164:PRO:HA	1:N:245:MET:HG3	1.91	0.53
1:G:24:THR:HG23	1:G:318:ASN:HA	1.88	0.53
1:B:33:ILE:N	1:B:33:ILE:HD13	2.23	0.53
1:K:79:ASP:HB3	1:K:82:LYS:HE2	1.91	0.53
1:G:188:LEU:N	1:G:188:LEU:HD22	2.23	0.53
1:O:106:GLU:HG2	1:O:308:PRO:HA	1.90	0.53
1:C:195:LEU:HD23	1:C:230:LYS:HD2	1.90	0.53
1:H:192:ASN:ND2	1:H:236:LYS:HE2	2.23	0.53
1:O:386:MET:HG2	1:O:397:LEU:HD21	1.90	0.53
1:D:259:HIS:H	1:D:292:THR:HB	1.73	0.53
1:J:83:PHE:HD2	1:J:85:PHE:HZ	1.50	0.53
1:I:255:MET:HG2	1:I:256:PHE:H	1.73	0.53
1:B:69:GLN:HE21	1:B:71:ARG:NH2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:305:PHE:CE1	1:E:333:ASP:HB2	2.44	0.53
1:A:49:TYR:O	1:A:64:LYS:HD2	2.08	0.53
1:D:149:MET:HE2	1:D:293:PRO:HD2	1.89	0.53
1:I:50:TYR:O	1:I:50:TYR:CD1	2.62	0.53
1:E:152:LYS:HE2	1:E:253:GLU:HB2	1.91	0.53
1:M:97:ARG:HG2	1:M:381:LEU:HD11	1.91	0.53
1:F:291:PRO:HD3	1:J:117:ILE:CG2	2.35	0.53
1:A:124:ASN:HD22	1:A:263:ARG:HD2	1.73	0.53
1:K:154:THR:HG23	1:K:253:GLU:HB3	1.89	0.53
1:D:24:THR:CG2	1:D:318:ASN:HA	2.39	0.53
1:O:105:VAL:HG12	1:O:106:GLU:N	2.24	0.53
1:E:336:ARG:HG3	1:E:336:ARG:HH11	1.73	0.53
1:C:122:LEU:HD13	1:C:144:ARG:NH2	2.24	0.53
1:H:35:TYR:CZ	1:H:457:ALA:HB2	2.42	0.53
1:B:162:ARG:HB3	1:B:162:ARG:NH1	2.24	0.53
1:G:342:VAL:HG23	1:G:342:VAL:O	2.08	0.53
1:K:96:GLN:NE2	1:K:378:LYS:HD3	2.23	0.53
1:C:77:LEU:HD22	1:C:455:PHE:HZ	1.73	0.53
1:C:471:GLN:O	1:C:473:GLY:N	2.41	0.53
1:D:148:SER:HG	1:E:129:THR:HG1	1.49	0.53
1:L:115:VAL:HG22	1:M:255:MET:CE	2.39	0.53
1:N:222:LEU:HA	1:N:225:CYS:SG	2.48	0.53
1:F:237:MET:CG	1:F:245:MET:HG2	2.39	0.53
1:N:258:ARG:HB3	1:N:292:THR:CG2	2.37	0.53
1:C:117:ILE:HG23	1:C:117:ILE:O	2.07	0.53
1:G:99:VAL:HG12	1:G:100:TRP:N	2.23	0.53
1:F:215:ALA:O	1:F:217:LYS:N	2.42	0.53
1:O:151:TYR:CG	1:O:203:THR:HB	2.43	0.53
1:B:459:LEU:HD12	1:B:469:LEU:HD21	1.90	0.53
1:G:109:ARG:NH2	1:G:333:ASP:OD2	2.39	0.52
1:C:234:TYR:O	1:C:238:VAL:HG23	2.08	0.52
1:H:165:ILE:HG23	1:H:245:MET:SD	2.49	0.52
1:C:462:PHE:N	1:C:462:PHE:CD1	2.76	0.52
1:H:36:HIS:ND1	1:H:37:ALA:N	2.56	0.52
1:N:393:ASN:HB3	1:N:396:ILE:HD12	1.92	0.52
1:M:474:LEU:HD23	1:M:474:LEU:H	1.73	0.52
1:G:160:GLY:HA2	1:G:247:PHE:CE1	2.44	0.52
1:D:164:PRO:HG3	1:D:330:THR:OG1	2.09	0.52
1:F:257:VAL:HG11	1:F:260:LEU:CD2	2.39	0.52
1:O:22:VAL:HG12	1:O:23:SER:N	2.24	0.52
1:A:124:ASN:HD21	1:A:264:ALA:H	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:255:MET:SD	1:O:114:GLY:HA2	2.48	0.52
1:O:80:PRO:HD3	1:O:100:TRP:CD1	2.44	0.52
1:F:460:ASP:OD2	1:F:460:ASP:O	2.28	0.52
1:B:371:GLN:HB3	1:B:464:LEU:HD12	1.91	0.52
1:E:220:VAL:O	1:E:221:PRO:C	2.45	0.52
1:I:124:ASN:OD1	1:I:264:ALA:HB3	2.09	0.52
1:B:108:GLY:HA2	1:B:306:ASN:ND2	2.25	0.52
1:J:149:MET:HE3	1:J:292:THR:HG23	1.91	0.52
1:B:361:TYR:CZ	1:C:268:GLY:HA3	2.44	0.52
1:E:331:VAL:HG11	1:E:368:TYR:CE2	2.42	0.52
1:E:87:ASP:O	1:E:90:PHE:CE1	2.63	0.52
1:E:305:PHE:HE1	1:E:333:ASP:CG	2.13	0.52
1:E:333:ASP:OD1	1:E:335:THR:HG23	2.10	0.52
1:K:99:VAL:HG12	1:K:100:TRP:N	2.24	0.52
1:M:314:ALA:HB2	1:M:319:ASN:HA	1.90	0.52
1:C:216:ASN:O	1:C:217:LYS:C	2.47	0.52
1:H:393:ASN:ND2	1:H:395:SER:H	2.07	0.52
1:J:125:LYS:HD2	1:J:145:GLU:OE2	2.09	0.52
1:L:373:ILE:CG1	1:L:464:LEU:HD13	2.37	0.52
1:M:363:ARG:NH2	1:N:269:GLU:OE1	2.40	0.52
1:L:466:ARG:NH1	1:M:316:GLY:HA2	2.25	0.52
1:I:31:THR:OG1	1:I:376:LEU:HB3	2.08	0.52
1:H:344:SER:HB3	1:I:183:GLY:O	2.09	0.52
1:K:144:ARG:NH1	1:K:218:SER:OG	2.42	0.52
1:D:373:ILE:HD12	1:D:464:LEU:CD2	2.38	0.52
1:I:121:PRO:HD2	1:I:222:LEU:HD21	1.92	0.52
1:C:146:CYS:O	1:C:147:ILE:HG13	2.10	0.52
1:O:342:VAL:HG22	1:O:361:TYR:HB2	1.90	0.52
1:L:28:VAL:HG11	1:L:321:ILE:HD12	1.92	0.52
1:A:220:VAL:HG23	1:A:225:CYS:HB3	1.90	0.52
1:E:37:ALA:HB1	1:E:451:LEU:HD13	1.92	0.52
1:D:261:PHE:HB2	1:D:290:PHE:CE2	2.45	0.52
1:G:232:PRO:HB2	1:G:234:TYR:CE1	2.44	0.52
1:I:73:PHE:O	1:I:328:PHE:HA	2.09	0.52
1:A:339:ASN:ND2	1:A:364:HIS:ND1	2.58	0.52
1:F:102:CYS:HB3	1:F:311:LEU:HD11	1.90	0.52
1:C:45:VAL:HG12	1:C:46:GLY:N	2.23	0.52
1:E:149:MET:HE2	1:E:205:PHE:HE1	1.73	0.52
1:L:298:VAL:HG11	1:L:335:THR:HA	1.91	0.52
1:K:152:LYS:HA	1:K:255:MET:HB2	1.90	0.52
1:B:69:GLN:NE2	1:B:71:ARG:NH2	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:VAL:CG2	1:A:225:CYS:HA	2.39	0.52
1:B:298:VAL:CG1	1:B:335:THR:HA	2.39	0.52
1:C:357:ASN:ND2	1:C:357:ASN:O	2.43	0.52
1:H:75:VAL:HB	1:H:327:LEU:HB2	1.92	0.52
1:G:29:THR:HG22	1:G:30:ARG:O	2.09	0.52
1:L:106:GLU:HG2	1:L:308:PRO:HA	1.91	0.52
1:O:196:GLN:HB3	1:O:445:THR:O	2.10	0.52
1:E:131:ASN:O	1:E:132:SER:O	2.26	0.52
1:O:76:LYS:HB3	1:O:452:LYS:NZ	2.25	0.52
1:A:47:HIS:O	1:A:64:LYS:HA	2.10	0.52
1:D:120:HIS:HB2	1:D:221:PRO:HA	1.92	0.52
1:E:54:LYS:NZ	1:E:55:GLN:N	2.58	0.52
1:H:54:LYS:NZ	1:H:55:GLN:CB	2.68	0.52
1:G:28:VAL:HG22	1:G:379:ILE:HG12	1.91	0.52
1:L:109:ARG:H	1:L:306:ASN:HD21	1.58	0.52
1:J:120:HIS:HB2	1:J:221:PRO:HA	1.92	0.52
1:D:273:ALA:HA	1:D:276:TYR:CE2	2.44	0.52
1:M:72:VAL:HG21	1:M:196:GLN:CA	2.40	0.52
1:A:106:GLU:HB3	1:A:371:GLN:HB2	1.90	0.52
1:A:463:PRO:HG2	1:A:464:LEU:H	1.75	0.52
1:J:79:ASP:OD1	1:J:81:ASN:N	2.42	0.52
1:J:124:ASN:ND2	1:J:263:ARG:HD2	2.23	0.52
1:N:188:LEU:HD22	1:N:188:LEU:N	2.24	0.52
1:D:42:LEU:HB3	1:D:447:TRP:HZ2	1.74	0.52
1:C:340:MET:HG2	1:C:363:ARG:O	2.10	0.52
1:E:382:THR:OG1	1:E:385:VAL:HG23	2.10	0.52
1:K:112:PRO:HB3	1:L:231:TYR:CD1	2.45	0.52
1:F:117:ILE:CD1	1:F:117:ILE:CB	2.80	0.52
1:N:220:VAL:HG23	1:N:225:CYS:HB2	1.92	0.52
1:C:156:LEU:HA	1:C:250:LEU:O	2.10	0.52
1:B:117:ILE:HD11	1:C:260:LEU:HB3	1.91	0.52
1:F:37:ALA:HB3	1:F:372:PHE:HB2	1.90	0.52
1:A:181:LYS:N	1:A:181:LYS:CD	2.73	0.52
1:L:119:GLY:N	1:L:221:PRO:HB3	2.24	0.52
1:H:27:TYR:CE2	1:H:388:TYR:CE2	2.98	0.52
1:B:157:CYS:O	1:B:249:TYR:HA	2.10	0.52
1:K:355:ASN:HB3	1:L:265:GLY:HA2	1.91	0.52
1:L:463:PRO:HG3	1:M:238:VAL:HG12	1.91	0.52
1:G:141:THR:HG22	1:G:142:ASP:N	2.23	0.52
1:A:165:ILE:CD1	1:A:236:LYS:HD3	2.40	0.52
1:O:314:ALA:HB2	1:O:319:ASN:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:471:GLN:C	1:M:473:GLY:H	2.13	0.52
1:B:363:ARG:NH2	1:C:269:GLU:OE1	2.40	0.52
1:D:149:MET:CE	1:D:292:THR:HG23	2.40	0.52
1:N:156:LEU:HA	1:N:250:LEU:O	2.09	0.52
1:H:152:LYS:HB2	1:H:255:MET:HG3	1.92	0.52
1:G:149:MET:HE2	1:G:293:PRO:HD2	1.91	0.52
1:E:24:THR:HG23	1:E:318:ASN:HA	1.92	0.52
1:F:333:ASP:OD1	1:F:335:THR:HG23	2.08	0.52
1:J:24:THR:HG23	1:J:318:ASN:HA	1.92	0.52
1:F:246:LEU:HD12	1:F:246:LEU:O	2.10	0.52
1:F:257:VAL:CG1	1:F:260:LEU:CD2	2.87	0.51
1:E:54:LYS:NZ	1:E:55:GLN:CB	2.67	0.51
1:B:258:ARG:HD2	1:C:130:GLU:OE1	2.11	0.51
1:G:237:MET:SD	1:G:245:MET:HG2	2.51	0.51
1:I:77:LEU:HB3	1:I:78:PRO:HD2	1.91	0.51
1:E:96:GLN:O	1:E:97:ARG:HD3	2.10	0.51
1:A:298:VAL:C	1:A:299:THR:CG2	2.75	0.51
1:K:80:PRO:HD3	1:K:100:TRP:NE1	2.25	0.51
1:J:318:ASN:C	1:J:318:ASN:OD1	2.47	0.51
1:L:474:LEU:HD23	1:L:474:LEU:H	1.75	0.51
1:K:30:ARG:HB3	1:K:375:GLN:NE2	2.25	0.51
1:E:85:PHE:HB2	1:E:88:THR:OG1	2.10	0.51
1:F:149:MET:HA	1:G:260:LEU:CD1	2.40	0.51
1:F:395:SER:O	1:F:396:ILE:C	2.44	0.51
1:F:162:ARG:HG3	1:F:244:ASP:HB3	1.92	0.51
1:A:151:TYR:CD1	1:A:203:THR:HB	2.46	0.51
1:J:72:VAL:HG21	1:J:196:GLN:HA	1.92	0.51
1:J:342:VAL:O	1:J:342:VAL:HG23	2.11	0.51
1:C:105:VAL:HG12	1:C:106:GLU:N	2.25	0.51
1:F:22:VAL:HG12	1:F:23:SER:N	2.25	0.51
1:K:92:ASP:OD1	1:K:94:ALA:HB3	2.10	0.51
1:D:68:LEU:HD22	1:D:203:THR:HG22	1.92	0.51
1:L:370:LEU:HB3	1:L:372:PHE:CE1	2.45	0.51
1:K:101:ALA:HB2	1:K:377:CYS:SG	2.50	0.51
1:I:69:GLN:HA	1:I:199:ASP:O	2.09	0.51
1:M:112:PRO:HB3	1:N:231:TYR:CD1	2.44	0.51
1:N:121:PRO:CD	1:N:222:LEU:HD21	2.41	0.51
1:N:144:ARG:NH1	1:N:218:SER:OG	2.43	0.51
1:L:247:PHE:HA	1:L:315:GLN:HG3	1.93	0.51
1:H:22:VAL:CG1	1:H:23:SER:N	2.73	0.51
1:L:258:ARG:HB3	1:L:292:THR:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:HIS:CD2	1:B:365:GLY:N	2.79	0.51
1:I:117:ILE:HG13	1:J:260:LEU:CD2	2.40	0.51
1:A:113:LEU:HD12	1:A:113:LEU:H	1.75	0.51
1:J:28:VAL:HG22	1:J:379:ILE:HG12	1.93	0.51
1:N:125:LYS:HD3	1:N:125:LYS:O	2.11	0.51
1:A:125:LYS:HE2	1:A:261:PHE:CE2	2.46	0.51
1:C:76:LYS:HD2	1:C:452:LYS:NZ	2.25	0.51
1:I:240:GLU:OE2	1:I:245:MET:HB2	2.09	0.51
1:F:157:CYS:HA	1:F:330:THR:O	2.10	0.51
1:K:459:LEU:HD12	1:K:469:LEU:CD2	2.37	0.51
1:K:394:PRO:HG2	1:K:395:SER:N	2.23	0.51
1:I:123:LEU:HA	1:I:218:SER:O	2.10	0.51
1:A:157:CYS:HA	1:A:330:THR:O	2.11	0.51
1:D:181:LYS:N	1:D:181:LYS:HD3	2.24	0.51
1:O:272:PRO:O	1:O:275:LEU:HB2	2.11	0.51
1:L:149:MET:HA	1:M:260:LEU:HD13	1.93	0.51
1:E:315:GLN:HE21	1:E:315:GLN:C	2.13	0.51
1:B:366:GLU:HG3	1:B:368:TYR:HE1	1.74	0.51
1:E:305:PHE:HE1	1:E:333:ASP:HB2	1.74	0.51
1:A:78:PRO:O	1:A:78:PRO:HG2	2.11	0.51
1:F:273:ALA:HA	1:F:276:TYR:CE2	2.46	0.51
1:M:133:ASN:N	1:M:133:ASN:HD22	2.07	0.51
1:K:28:VAL:HG22	1:K:379:ILE:HG12	1.91	0.51
1:C:153:GLN:O	1:C:253:GLU:HA	2.10	0.51
1:K:258:ARG:HB2	1:K:294:SER:HB2	1.93	0.51
1:A:120:HIS:ND1	1:A:122:LEU:N	2.53	0.51
1:H:363:ARG:HG3	1:I:188:LEU:CD2	2.38	0.51
1:O:120:HIS:HB2	1:O:221:PRO:HA	1.92	0.51
1:L:233:ASP:O	1:L:237:MET:HG3	2.11	0.51
1:L:240:GLU:CG	1:L:241:PRO:HD2	2.40	0.51
1:F:159:ILE:HG22	1:F:247:PHE:HE1	1.75	0.51
1:K:361:TYR:CE2	1:L:268:GLY:HA3	2.45	0.51
1:L:108:GLY:HA2	1:L:306:ASN:ND2	2.26	0.51
1:F:246:LEU:C	1:F:246:LEU:HD12	2.30	0.51
1:H:462:PHE:CD1	1:H:462:PHE:N	2.79	0.51
1:F:95:SER:O	1:F:381:LEU:HB2	2.10	0.51
1:C:300:SER:O	1:C:303:GLN:HB2	2.10	0.51
1:A:125:LYS:O	1:A:125:LYS:HD2	2.10	0.51
1:L:54:LYS:CD	1:L:55:GLN:H	2.19	0.51
1:M:158:LEU:O	1:M:159:ILE:HD13	2.10	0.51
1:E:110:GLY:O	1:E:111:GLN:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:LEU:HD23	1:D:311:LEU:H	1.74	0.51
1:C:164:PRO:HG3	1:C:330:THR:OG1	2.10	0.51
1:A:250:LEU:HB2	1:A:304:ILE:HD11	1.92	0.51
1:F:121:PRO:CD	1:F:222:LEU:HD21	2.35	0.51
1:F:162:ARG:HG3	1:F:244:ASP:CB	2.40	0.51
1:L:85:PHE:HB2	1:L:88:THR:CG2	2.41	0.51
1:K:361:TYR:CZ	1:L:268:GLY:HA3	2.45	0.51
1:A:165:ILE:HG23	1:A:245:MET:SD	2.50	0.51
1:O:45:VAL:HG12	1:O:46:GLY:N	2.25	0.51
1:J:87:ASP:O	1:J:90:PHE:CE1	2.64	0.51
1:F:148:SER:OG	1:G:129:THR:OG1	2.27	0.51
1:D:152:LYS:HA	1:D:255:MET:HB2	1.91	0.51
1:C:29:THR:HG22	1:C:30:ARG:N	2.26	0.51
1:C:219:ASP:HB2	1:C:263:ARG:HH11	1.74	0.51
1:F:120:HIS:HB2	1:F:221:PRO:HA	1.93	0.51
1:M:305:PHE:O	1:M:307:LYS:HG3	2.11	0.51
1:A:247:PHE:CE2	1:A:320:GLY:HA2	2.46	0.51
1:E:164:PRO:HB2	1:E:237:MET:SD	2.51	0.51
1:E:151:TYR:CD2	1:E:203:THR:HB	2.46	0.51
1:M:361:TYR:CE2	1:N:268:GLY:HA3	2.45	0.51
1:G:22:VAL:HG12	1:G:26:GLU:HG3	1.93	0.51
1:N:65:VAL:O	1:N:364:HIS:HB3	2.11	0.51
1:M:54:LYS:HD2	1:M:55:GLN:H	1.75	0.51
1:A:181:LYS:H	1:A:181:LYS:CD	2.24	0.51
1:J:120:HIS:CD2	1:J:222:LEU:HD13	2.46	0.51
1:A:185:CYS:HB2	1:E:361:TYR:CD2	2.46	0.51
1:A:74:ARG:NH2	1:A:441:LEU:HD12	2.26	0.51
1:D:123:LEU:HG	1:D:124:ASN:H	1.75	0.51
1:D:122:LEU:HD13	1:D:144:ARG:NH2	2.26	0.51
1:L:115:VAL:HG21	1:M:257:VAL:CG2	2.36	0.51
1:K:146:CYS:O	1:K:147:ILE:CG1	2.54	0.51
1:M:220:VAL:CG1	1:M:224:ILE:HD11	2.40	0.51
1:M:217:LYS:NZ	1:N:274:ASP:O	2.23	0.51
1:B:96:GLN:O	1:B:97:ARG:HG2	2.11	0.51
1:I:33:ILE:HD11	1:I:87:ASP:HB3	1.91	0.51
1:L:125:LYS:HD3	1:L:125:LYS:O	2.11	0.51
1:C:112:PRO:HB3	1:D:231:TYR:CD1	2.46	0.51
1:A:354:LYS:HA	1:B:141:THR:HG23	1.93	0.51
1:H:101:ALA:HA	1:H:320:GLY:O	2.11	0.51
1:D:209:ASP:C	1:D:209:ASP:OD2	2.47	0.51
1:I:164:PRO:HG3	1:I:330:THR:OG1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:GLY:HA2	1:G:309:TYR:O	2.11	0.51
1:M:102:CYS:O	1:M:311:LEU:HD11	2.11	0.50
1:L:115:VAL:HG22	1:M:255:MET:HE1	1.94	0.50
1:J:117:ILE:HD11	1:J:148:SER:HB2	1.92	0.50
1:I:112:PRO:HA	1:J:231:TYR:CE1	2.46	0.50
1:I:24:THR:CG2	1:I:318:ASN:HA	2.41	0.50
1:A:120:HIS:HA	1:A:222:LEU:HD21	1.93	0.50
1:G:120:HIS:HB2	1:G:221:PRO:HA	1.93	0.50
1:C:96:GLN:O	1:C:97:ARG:HD3	2.11	0.50
1:G:162:ARG:NH1	1:G:162:ARG:HB3	2.23	0.50
1:C:54:LYS:HG3	1:C:56:ASP:H	1.75	0.50
1:L:109:ARG:H	1:L:306:ASN:ND2	2.09	0.50
1:G:323:TRP:O	1:G:324:SER:HB2	2.12	0.50
1:B:340:MET:CE	1:C:169:TRP:CD1	2.94	0.50
1:E:216:ASN:O	1:E:217:LYS:HG2	2.11	0.50
1:B:219:ASP:C	1:B:220:VAL:HG22	2.32	0.50
1:L:52:ILE:HG21	1:M:269:GLU:HG2	1.92	0.50
1:L:36:HIS:ND1	1:L:37:ALA:N	2.59	0.50
1:A:389:ILE:O	1:A:392:MET:HB3	2.10	0.50
1:C:113:LEU:HD23	1:C:298:VAL:HB	1.93	0.50
1:H:149:MET:HA	1:I:260:LEU:HD13	1.93	0.50
1:B:49:TYR:HA	1:B:223:ASP:HB3	1.93	0.50
1:J:22:VAL:HG12	1:J:23:SER:N	2.25	0.50
1:K:115:VAL:HG21	1:L:257:VAL:HG22	1.92	0.50
1:N:333:ASP:OD1	1:N:335:THR:HG23	2.12	0.50
1:I:39:SER:OG	1:I:370:LEU:HB2	2.11	0.50
1:B:151:TYR:OH	1:B:221:PRO:HB2	2.12	0.50
1:J:79:ASP:OD1	1:J:81:ASN:CB	2.57	0.50
1:N:47:HIS:ND1	1:N:48:PRO:HD2	2.26	0.50
1:O:107:VAL:O	1:O:107:VAL:CG1	2.53	0.50
1:B:41:ARG:HH11	1:C:190:LEU:CD2	2.22	0.50
1:G:120:HIS:CE1	1:G:122:LEU:H	2.29	0.50
1:M:22:VAL:HG12	1:M:23:SER:N	2.25	0.50
1:N:79:ASP:O	1:N:81:ASN:N	2.44	0.50
1:L:117:ILE:O	1:L:117:ILE:HG23	2.11	0.50
1:K:358:PHE:CE2	1:L:216:ASN:HA	2.45	0.50
1:F:185:CYS:SG	1:J:363:ARG:NH1	2.84	0.50
1:B:393:ASN:ND2	1:B:395:SER:H	2.09	0.50
1:E:92:ASP:OD1	1:E:94:ALA:HB3	2.11	0.50
1:J:74:ARG:CZ	1:J:441:LEU:HD12	2.41	0.50
1:L:450:ASP:OD2	1:L:452:LYS:HD2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:343:CYS:CB	1:K:360:GLU:OE2	2.56	0.50
1:G:342:VAL:HG22	1:G:361:TYR:HB2	1.94	0.50
1:A:216:ASN:O	1:B:277:ILE:HD12	2.12	0.50
1:M:343:CYS:HB3	1:N:214:GLN:HA	1.93	0.50
1:G:101:ALA:HA	1:G:320:GLY:O	2.11	0.50
1:O:328:PHE:HE2	1:O:446:PHE:CE1	2.30	0.50
1:D:105:VAL:HG12	1:D:106:GLU:N	2.26	0.50
1:I:450:ASP:OD2	1:I:452:LYS:HD2	2.11	0.50
1:O:464:LEU:CD2	1:O:464:LEU:O	2.59	0.50
1:D:382:THR:O	1:D:386:MET:HG3	2.11	0.50
1:I:361:TYR:CZ	1:J:268:GLY:HA3	2.47	0.50
1:D:314:ALA:CB	1:D:319:ASN:HA	2.41	0.50
1:G:29:THR:HG22	1:G:30:ARG:N	2.24	0.50
1:N:305:PHE:HE1	1:N:333:ASP:HB2	1.75	0.50
1:N:71:ARG:HB3	1:N:73:PHE:CE1	2.46	0.50
1:E:273:ALA:HA	1:E:276:TYR:CE2	2.47	0.50
1:G:209:ASP:O	1:G:213:LEU:HB2	2.12	0.50
1:D:115:VAL:HG21	1:E:257:VAL:HG22	1.92	0.50
1:K:208:MET:HE2	1:K:210:PHE:CE2	2.47	0.50
1:J:31:THR:O	1:J:375:GLN:NE2	2.36	0.50
1:J:78:PRO:HG2	1:J:78:PRO:O	2.12	0.50
1:K:54:LYS:NZ	1:K:55:GLN:CB	2.75	0.50
1:M:157:CYS:HA	1:M:330:THR:O	2.12	0.50
1:G:126:LEU:HG	1:G:127:ASP:CG	2.32	0.50
1:B:393:ASN:HD22	1:B:394:PRO:CD	2.24	0.50
1:A:256:PHE:HB3	1:E:297:MET:HG3	1.93	0.50
1:F:244:ASP:O	1:F:245:MET:C	2.50	0.50
1:I:258:ARG:HB3	1:I:292:THR:HG22	1.94	0.50
1:M:47:HIS:HB2	1:M:52:ILE:HD11	1.92	0.50
1:L:80:PRO:HD3	1:L:100:TRP:NE1	2.26	0.50
1:L:299:THR:HG22	1:M:254:GLN:CB	2.41	0.50
1:C:342:VAL:CG2	1:C:361:TYR:HB2	2.41	0.50
1:B:250:LEU:HB2	1:B:304:ILE:HD11	1.93	0.50
1:F:355:ASN:HB3	1:G:265:GLY:HA2	1.94	0.50
1:L:122:LEU:O	1:L:144:ARG:HD2	2.12	0.50
1:F:149:MET:CE	1:F:292:THR:HA	2.42	0.50
1:A:64:LYS:HB2	1:A:64:LYS:CD	2.38	0.50
1:N:114:GLY:C	1:N:115:VAL:CG1	2.80	0.50
1:I:299:THR:C	1:I:301:ASP:N	2.63	0.50
1:J:298:VAL:HG11	1:J:335:THR:HA	1.94	0.50
1:J:126:LEU:HB3	1:J:262:ASN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:117:ILE:HD12	1:M:260:LEU:HD22	1.94	0.50
1:B:54:LYS:HD2	1:B:55:GLN:N	2.25	0.50
1:M:106:GLU:HB3	1:M:371:GLN:HB2	1.92	0.50
1:C:41:ARG:HH11	1:D:190:LEU:HD23	1.75	0.50
1:F:298:VAL:HG11	1:F:335:THR:HA	1.93	0.50
1:H:311:LEU:CD2	1:H:311:LEU:H	2.24	0.50
1:G:462:PHE:O	1:G:466:ARG:HB2	2.11	0.50
1:I:273:ALA:HA	1:I:276:TYR:CE2	2.46	0.50
1:L:139:SER:HB2	1:L:143:ASN:HD21	1.77	0.50
1:I:305:PHE:CE1	1:I:333:ASP:HB2	2.46	0.50
1:D:119:GLY:N	1:D:221:PRO:HB3	2.27	0.50
1:K:393:ASN:HB3	1:K:396:ILE:CD1	2.42	0.50
1:K:24:THR:HG21	1:K:321:ILE:HG13	1.94	0.50
1:F:253:GLU:HG2	1:J:300:SER:OG	2.11	0.50
1:I:22:VAL:CG1	1:I:26:GLU:HG3	2.42	0.50
1:O:122:LEU:O	1:O:218:SER:HB3	2.12	0.50
1:F:254:GLN:HB2	1:J:299:THR:HG22	1.93	0.50
1:C:318:ASN:OD1	1:C:321:ILE:HB	2.12	0.50
1:H:258:ARG:HB3	1:H:292:THR:HG22	1.92	0.50
1:J:68:LEU:HD22	1:J:151:TYR:CD1	2.47	0.50
1:L:343:CYS:SG	1:M:216:ASN:HB3	2.51	0.50
1:G:273:ALA:HA	1:G:276:TYR:CE2	2.47	0.50
1:I:157:CYS:O	1:I:249:TYR:HA	2.12	0.50
1:N:152:LYS:CE	1:N:152:LYS:HG2	2.41	0.49
1:D:258:ARG:HB3	1:D:292:THR:HG22	1.93	0.49
1:O:219:ASP:O	1:O:220:VAL:HG13	2.11	0.49
1:F:24:THR:CG2	1:F:318:ASN:HA	2.41	0.49
1:J:284:LEU:HD12	1:J:285:PRO:HD2	1.94	0.49
1:M:35:TYR:CZ	1:M:457:ALA:HB2	2.46	0.49
1:O:120:HIS:HB3	1:O:123:LEU:HD13	1.94	0.49
1:O:160:GLY:HA3	1:O:245:MET:O	2.12	0.49
1:L:72:VAL:HG22	1:L:330:THR:HG23	1.94	0.49
1:J:72:VAL:HG23	1:J:196:GLN:C	2.32	0.49
1:A:21:VAL:CG1	1:A:22:VAL:N	2.74	0.49
1:L:109:ARG:HH11	1:L:109:ARG:HB3	1.77	0.49
1:G:363:ARG:HG3	1:H:188:LEU:HD21	1.94	0.49
1:C:121:PRO:HG3	1:D:287:THR:OG1	2.12	0.49
1:E:149:MET:HE2	1:E:293:PRO:HD2	1.88	0.49
1:D:117:ILE:HG13	1:E:260:LEU:HD23	1.92	0.49
1:O:54:LYS:HB3	1:O:57:SER:HB3	1.94	0.49
1:A:298:VAL:C	1:A:299:THR:HG23	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:ASN:HD21	1:F:283:THR:CB	2.24	0.49
1:D:73:PHE:O	1:D:328:PHE:HA	2.12	0.49
1:N:41:ARG:NH1	1:O:190:LEU:HD23	2.26	0.49
1:C:27:TYR:CD1	1:C:28:VAL:CG2	2.95	0.49
1:L:248:PHE:CZ	1:L:309:TYR:HB3	2.47	0.49
1:K:340:MET:HG2	1:K:363:ARG:O	2.12	0.49
1:B:147:ILE:HA	1:C:129:THR:O	2.12	0.49
1:O:99:VAL:HG11	1:O:321:ILE:HG23	1.93	0.49
1:I:23:SER:C	1:I:25:ASP:H	2.14	0.49
1:G:120:HIS:CE1	1:G:122:LEU:HB2	2.47	0.49
1:F:373:ILE:HD12	1:F:464:LEU:HD22	1.93	0.49
1:O:79:ASP:OD1	1:O:81:ASN:CB	2.60	0.49
1:E:156:LEU:HD23	1:E:332:VAL:HB	1.92	0.49
1:B:22:VAL:HG12	1:B:26:GLU:HG3	1.94	0.49
1:J:130:GLU:HB2	1:J:260:LEU:HD12	1.94	0.49
1:F:80:PRO:HB2	1:F:98:LEU:HB2	1.93	0.49
1:I:366:GLU:HG3	1:I:368:TYR:CE1	2.47	0.49
1:F:343:CYS:HB3	1:G:214:GLN:HA	1.93	0.49
1:H:171:LYS:HE2	1:H:186:PRO:HG3	1.94	0.49
1:F:144:ARG:NH2	1:G:279:GLY:HA3	2.28	0.49
1:M:53:LYS:HD3	1:M:58:ASN:HA	1.95	0.49
1:F:174:PRO:CG	1:F:180:VAL:HG23	2.40	0.49
1:L:54:LYS:NZ	1:L:55:GLN:HB3	2.27	0.49
1:J:211:THR:HG23	1:J:226:SER:CA	2.42	0.49
1:D:106:GLU:HG2	1:D:308:PRO:HA	1.93	0.49
1:M:27:TYR:CD1	1:M:27:TYR:O	2.65	0.49
1:G:453:GLU:HG3	1:G:453:GLU:O	2.13	0.49
1:G:353:TYR:HE1	1:H:216:ASN:HB2	1.76	0.49
1:I:210:PHE:HE1	1:I:229:CYS:HG	1.58	0.49
1:B:78:PRO:HD3	1:B:452:LYS:HA	1.94	0.49
1:I:304:ILE:HD13	1:I:305:PHE:CE2	2.48	0.49
1:C:222:LEU:HA	1:C:225:CYS:SG	2.53	0.49
1:K:269:GLU:OE1	1:O:52:ILE:HD13	2.12	0.49
1:E:30:ARG:HB3	1:E:375:GLN:HE22	1.76	0.49
1:G:24:THR:HA	1:G:27:TYR:CE2	2.47	0.49
1:E:24:THR:HG21	1:E:319:ASN:H	1.77	0.49
1:G:71:ARG:HG3	1:G:368:TYR:CZ	2.47	0.49
1:H:174:PRO:HG3	1:H:180:VAL:HG23	1.93	0.49
1:J:164:PRO:HA	1:J:245:MET:HG3	1.94	0.49
1:I:462:PHE:O	1:I:466:ARG:HB2	2.12	0.49
1:H:107:VAL:O	1:H:107:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:SER:OG	1:D:253:GLU:HG2	2.12	0.49
1:A:463:PRO:HA	1:A:466:ARG:NH1	2.28	0.49
1:B:237:MET:CG	1:B:245:MET:HG2	2.42	0.49
1:I:152:LYS:HA	1:I:255:MET:HB2	1.95	0.49
1:L:24:THR:HG23	1:L:318:ASN:HA	1.93	0.49
1:D:461:GLN:HB2	1:D:462:PHE:CE1	2.48	0.49
1:D:370:LEU:HB3	1:D:372:PHE:CE1	2.48	0.49
1:N:99:VAL:HG11	1:N:321:ILE:HG22	1.94	0.49
1:M:110:GLY:O	1:M:111:GLN:CB	2.61	0.49
1:A:353:TYR:HE1	1:B:216:ASN:HB2	1.77	0.49
1:M:123:LEU:O	1:M:144:ARG:HB3	2.12	0.49
1:F:269:GLU:OE1	1:J:363:ARG:NH2	2.45	0.49
1:H:24:THR:CG2	1:H:318:ASN:HA	2.43	0.49
1:L:223:ASP:OD1	1:L:224:ILE:HG23	2.13	0.49
1:F:117:ILE:HD11	1:G:260:LEU:HB3	1.95	0.49
1:M:167:GLU:O	1:M:167:GLU:HG3	2.12	0.49
1:K:46:GLY:HA2	1:K:62:VAL:HG12	1.94	0.49
1:M:149:MET:HE2	1:M:205:PHE:CE1	2.47	0.49
1:H:199:ASP:OD2	1:H:230:LYS:NZ	2.43	0.49
1:O:474:LEU:CD2	1:O:474:LEU:H	2.26	0.49
1:L:119:GLY:HA3	1:M:289:TYR:CE1	2.48	0.49
1:A:269:GLU:OE1	1:E:52:ILE:HD13	2.12	0.49
1:O:440:PRO:HG2	1:O:441:LEU:H	1.78	0.49
1:E:139:SER:HB2	1:E:143:ASN:HD21	1.77	0.49
1:F:149:MET:HA	1:G:260:LEU:HD13	1.94	0.49
1:L:467:LYS:O	1:L:468:PHE:C	2.51	0.49
1:H:109:ARG:NH1	1:H:109:ARG:HB3	2.27	0.49
1:M:22:VAL:CG1	1:M:26:GLU:HG3	2.43	0.49
1:D:108:GLY:HA2	1:D:306:ASN:ND2	2.28	0.49
1:H:160:GLY:HA3	1:H:245:MET:O	2.12	0.49
1:F:80:PRO:HD3	1:F:100:TRP:CD1	2.48	0.49
1:I:342:VAL:O	1:I:342:VAL:HG23	2.13	0.49
1:G:69:GLN:NE2	1:G:71:ARG:HH22	2.11	0.49
1:I:54:LYS:HZ3	1:I:55:GLN:N	2.11	0.49
1:A:383:ALA:HB3	1:F:92:ASP:HB2	1.94	0.49
1:A:49:TYR:C	1:A:64:LYS:HD2	2.33	0.49
1:D:149:MET:CE	1:D:293:PRO:HD2	2.42	0.49
1:O:49:TYR:HA	1:O:223:ASP:HB3	1.95	0.49
1:E:152:LYS:CE	1:E:253:GLU:HB2	2.43	0.49
1:L:156:LEU:HA	1:L:250:LEU:O	2.13	0.49
1:H:237:MET:HB2	1:H:246:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:O	1:A:330:THR:HA	2.11	0.49
1:O:233:ASP:OD1	1:O:233:ASP:O	2.31	0.49
1:G:30:ARG:HD3	1:G:377:CYS:SG	2.52	0.49
1:A:240:GLU:HG2	1:A:243:GLY:H	1.78	0.49
1:F:43:LEU:HD23	1:F:367:GLU:HB2	1.95	0.49
1:M:37:ALA:HA	1:M:454:LYS:O	2.13	0.49
1:N:262:ASN:HD22	1:N:262:ASN:HA	1.37	0.49
1:N:297:MET:HE2	1:O:296:SER:HB2	1.95	0.49
1:D:255:MET:HG3	1:D:293:PRO:HB2	1.94	0.49
1:G:109:ARG:H	1:G:306:ASN:HD21	1.60	0.49
1:O:159:ILE:HG22	1:O:247:PHE:CE1	2.44	0.49
1:G:120:HIS:O	1:G:121:PRO:C	2.50	0.49
1:E:68:LEU:HG	1:E:334:THR:HG22	1.95	0.49
1:A:216:ASN:HA	1:E:358:PHE:CE2	2.48	0.49
1:F:70:TYR:OH	1:F:232:PRO:HD3	2.13	0.49
1:C:46:GLY:O	1:C:363:ARG:HD3	2.12	0.49
1:H:70:TYR:OH	1:H:232:PRO:HD3	2.12	0.49
1:D:96:GLN:NE2	1:D:378:LYS:HD3	2.27	0.49
1:H:47:HIS:HB3	1:H:50:TYR:O	2.12	0.49
1:E:141:THR:HG22	1:E:142:ASP:N	2.28	0.49
1:I:172:GLY:O	1:I:187:PRO:HG2	2.12	0.49
1:F:149:MET:HE3	1:F:292:THR:HA	1.95	0.48
1:K:119:GLY:O	1:K:222:LEU:HD22	2.13	0.48
1:L:361:TYR:CZ	1:M:268:GLY:HA3	2.47	0.48
1:L:220:VAL:HG23	1:L:225:CYS:CB	2.42	0.48
1:L:149:MET:HE3	1:L:292:THR:HG23	1.95	0.48
1:H:154:THR:HG22	1:H:155:GLN:N	2.28	0.48
1:F:363:ARG:NH1	1:G:185:CYS:SG	2.86	0.48
1:C:165:ILE:HG23	1:C:245:MET:SD	2.53	0.48
1:A:253:GLU:HG2	1:E:300:SER:OG	2.13	0.48
1:D:393:ASN:HD22	1:D:394:PRO:HD2	1.77	0.48
1:G:69:GLN:NE2	1:G:71:ARG:NH2	2.61	0.48
1:G:88:THR:HB	1:G:91:TYR:CD2	2.47	0.48
1:K:450:ASP:OD1	1:K:452:LYS:HG3	2.13	0.48
1:H:321:ILE:HG21	1:H:323:TRP:CZ2	2.48	0.48
1:F:150:ASP:OD1	1:F:294:SER:HA	2.12	0.48
1:L:104:GLY:HA3	1:L:310:TRP:CE3	2.48	0.48
1:J:272:PRO:O	1:J:275:LEU:HB2	2.13	0.48
1:D:219:ASP:O	1:D:220:VAL:HG13	2.12	0.48
1:N:359:LYS:CD	1:O:268:GLY:HA2	2.40	0.48
1:J:82:LYS:O	1:J:83:PHE:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:47:HIS:CB	1:N:52:ILE:HD11	2.39	0.48
1:H:120:HIS:HB2	1:H:221:PRO:HA	1.94	0.48
1:F:296:SER:HB2	1:J:297:MET:HE2	1.95	0.48
1:B:297:MET:HE2	1:C:256:PHE:HD2	1.77	0.48
1:F:139:SER:HB2	1:F:143:ASN:ND2	2.25	0.48
1:A:120:HIS:CD2	1:A:222:LEU:HD13	2.48	0.48
1:L:123:LEU:HA	1:L:218:SER:O	2.13	0.48
1:L:240:GLU:OE2	1:L:245:MET:HB2	2.12	0.48
1:N:117:ILE:HD11	1:O:260:LEU:HB3	1.95	0.48
1:F:269:GLU:OE1	1:J:52:ILE:HD13	2.13	0.48
1:N:393:ASN:HD22	1:N:394:PRO:HD2	1.77	0.48
1:A:237:MET:SD	1:A:246:LEU:HD23	2.53	0.48
1:D:353:TYR:HE1	1:E:216:ASN:HB2	1.78	0.48
1:B:442:LYS:O	1:B:442:LYS:HG2	2.12	0.48
1:H:119:GLY:CA	1:H:148:SER:HA	2.43	0.48
1:D:283:THR:O	1:D:284:LEU:O	2.32	0.48
1:J:386:MET:HG2	1:J:397:LEU:HD21	1.94	0.48
1:G:254:GLN:CD	1:G:254:GLN:CB	2.70	0.48
1:D:144:ARG:NH1	1:D:218:SER:OG	2.45	0.48
1:D:258:ARG:HD3	1:D:258:ARG:HA	1.65	0.48
1:L:113:LEU:O	1:M:152:LYS:NZ	2.47	0.48
1:K:24:THR:HG23	1:K:318:ASN:HA	1.95	0.48
1:C:43:LEU:CD2	1:D:190:LEU:HD22	2.42	0.48
1:M:195:LEU:HD23	1:M:230:LYS:HD2	1.95	0.48
1:I:450:ASP:OD1	1:I:452:LYS:HD2	2.13	0.48
1:C:370:LEU:HB3	1:C:372:PHE:CE1	2.48	0.48
1:K:303:GLN:HE22	1:K:335:THR:HG21	1.79	0.48
1:K:121:PRO:HD2	1:K:222:LEU:HD21	1.95	0.48
1:A:142:ASP:N	1:E:355:ASN:OD1	2.46	0.48
1:N:29:THR:HB	1:N:378:LYS:HG3	1.96	0.48
1:N:118:SER:O	1:N:149:MET:N	2.45	0.48
1:O:262:ASN:HD22	1:O:262:ASN:HA	1.53	0.48
1:D:54:LYS:HB3	1:D:57:SER:HB3	1.96	0.48
1:M:181:LYS:HE2	1:M:184:GLU:HG2	1.96	0.48
1:A:269:GLU:OE1	1:E:363:ARG:NH2	2.46	0.48
1:F:92:ASP:OD1	1:F:94:ALA:HB3	2.13	0.48
1:D:465:GLY:O	1:D:468:PHE:HB3	2.13	0.48
1:A:210:PHE:HD2	1:A:214:GLN:OE1	1.96	0.48
1:A:47:HIS:HB3	1:A:50:TYR:O	2.14	0.48
1:C:154:THR:HG23	1:C:253:GLU:HB3	1.95	0.48
1:G:305:PHE:HE1	1:G:333:ASP:CB	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:ILE:N	1:L:33:ILE:CD1	2.76	0.48
1:O:70:TYR:CE1	1:O:201:VAL:HA	2.49	0.48
1:O:52:ILE:HD12	1:O:62:VAL:HB	1.96	0.48
1:D:326:GLN:O	1:D:327:LEU:HD23	2.14	0.48
1:H:24:THR:HG23	1:H:318:ASN:HA	1.96	0.48
1:E:52:ILE:HD12	1:E:62:VAL:HB	1.96	0.48
1:D:107:VAL:HG12	1:D:107:VAL:O	2.12	0.48
1:M:327:LEU:HA	1:M:327:LEU:HD23	1.46	0.48
1:K:366:GLU:HG3	1:K:368:TYR:HE1	1.78	0.48
1:K:66:SER:HB3	1:K:69:GLN:HG3	1.94	0.48
1:O:167:GLU:HA	1:O:191:LEU:O	2.13	0.48
1:O:27:TYR:CD1	1:O:28:VAL:HG23	2.49	0.48
1:N:207:ALA:HA	1:N:229:CYS:O	2.12	0.48
1:D:210:PHE:CE2	1:D:220:VAL:HG11	2.48	0.48
1:C:201:VAL:HG11	1:C:332:VAL:HG11	1.95	0.48
1:L:121:PRO:CB	1:M:285:PRO:HG2	2.43	0.48
1:N:440:PRO:CG	1:N:441:LEU:H	2.23	0.48
1:H:162:ARG:HG3	1:H:244:ASP:CB	2.44	0.48
1:B:359:LYS:HB3	1:B:361:TYR:CE1	2.48	0.48
1:E:346:VAL:HG23	1:E:357:ASN:C	2.34	0.48
1:D:34:TYR:HA	1:D:374:PHE:O	2.13	0.48
1:N:323:TRP:O	1:N:324:SER:HB2	2.13	0.48
1:J:139:SER:HB2	1:J:143:ASN:HD21	1.79	0.48
1:J:328:PHE:HE2	1:J:446:PHE:CE1	2.31	0.48
1:A:470:LEU:O	1:A:473:GLY:N	2.45	0.48
1:J:45:VAL:HA	1:J:364:HIS:O	2.14	0.48
1:D:118:SER:O	1:D:148:SER:HA	2.14	0.48
1:O:210:PHE:CE2	1:O:224:ILE:HD12	2.48	0.48
1:G:117:ILE:HD12	1:H:260:LEU:HB3	1.93	0.48
1:K:119:GLY:HA3	1:K:148:SER:HA	1.95	0.48
1:B:117:ILE:CG2	1:B:117:ILE:O	2.60	0.48
1:J:124:ASN:HD21	1:J:263:ARG:HB3	1.78	0.48
1:F:83:PHE:HB3	1:F:85:PHE:CE1	2.48	0.48
1:D:466:ARG:O	1:D:469:LEU:HB2	2.14	0.48
1:L:241:PRO:HG2	1:L:242:TYR:N	2.28	0.48
1:C:280:THR:O	1:C:281:THR:CB	2.62	0.48
1:M:327:LEU:HD12	1:M:374:PHE:CE2	2.49	0.48
1:D:133:ASN:HD22	1:D:133:ASN:N	2.12	0.48
1:L:101:ALA:HB2	1:L:377:CYS:SG	2.54	0.48
1:F:459:LEU:HB2	1:F:469:LEU:HD11	1.96	0.48
1:B:68:LEU:HD22	1:B:203:THR:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:181:LYS:N	1:K:181:LYS:HD3	2.21	0.48
1:A:120:HIS:HA	1:A:222:LEU:HD22	1.93	0.48
1:L:219:ASP:O	1:L:220:VAL:HG13	2.13	0.48
1:M:211:THR:HG23	1:M:226:SER:CA	2.44	0.48
1:B:29:THR:HB	1:B:378:LYS:HG3	1.96	0.48
1:D:471:GLN:O	1:D:473:GLY:N	2.46	0.48
1:D:217:LYS:NZ	1:D:217:LYS:HD3	2.27	0.48
1:E:149:MET:HE2	1:E:205:PHE:CE1	2.48	0.48
1:N:105:VAL:HG13	1:N:372:PHE:CE2	2.49	0.48
1:F:161:CYS:SG	1:F:244:ASP:HB3	2.54	0.48
1:J:298:VAL:O	1:J:299:THR:CG2	2.62	0.48
1:F:363:ARG:NH2	1:G:269:GLU:OE1	2.43	0.48
1:G:70:TYR:OH	1:G:232:PRO:HD3	2.14	0.48
1:O:85:PHE:HB2	1:O:88:THR:CG2	2.43	0.48
1:O:109:ARG:NH1	1:O:109:ARG:HB3	2.29	0.48
1:N:68:LEU:CD2	1:N:334:THR:HG21	2.39	0.48
1:K:33:ILE:HB	1:K:376:LEU:HB3	1.95	0.48
1:D:160:GLY:HA3	1:D:245:MET:O	2.14	0.48
1:L:342:VAL:CG2	1:L:342:VAL:O	2.61	0.48
1:K:373:ILE:HD12	1:K:464:LEU:HD22	1.96	0.48
1:I:141:THR:CG2	1:I:142:ASP:N	2.77	0.48
1:D:233:ASP:O	1:D:237:MET:HG3	2.14	0.48
1:G:54:LYS:HZ3	1:G:55:GLN:N	2.12	0.48
1:F:216:ASN:C	1:F:217:LYS:HG2	2.33	0.48
1:M:145:GLU:OE1	1:N:132:SER:HB3	2.14	0.48
1:E:308:PRO:O	1:E:308:PRO:HG2	2.13	0.48
1:N:261:PHE:HB2	1:N:290:PHE:CE2	2.49	0.48
1:B:184:GLU:HA	1:B:184:GLU:OE1	2.14	0.48
1:I:280:THR:CA	1:I:280:THR:CG2	2.82	0.47
1:N:361:TYR:CE2	1:O:268:GLY:HA3	2.49	0.47
1:A:305:PHE:CE1	1:A:333:ASP:HB2	2.48	0.47
1:F:450:ASP:OD1	1:F:452:LYS:HG3	2.14	0.47
1:C:156:LEU:HG	1:C:332:VAL:CB	2.37	0.47
1:F:165:ILE:N	1:F:237:MET:SD	2.86	0.47
1:H:340:MET:HG2	1:H:363:ARG:O	2.14	0.47
1:H:208:MET:CE	1:H:214:GLN:NE2	2.75	0.47
1:F:114:GLY:N	1:F:335:THR:O	2.42	0.47
1:L:97:ARG:HE	1:L:400:TRP:HB3	1.79	0.47
1:G:29:THR:CG2	1:G:30:ARG:N	2.77	0.47
1:A:136:VAL:O	1:A:137:GLY:O	2.30	0.47
1:D:340:MET:HB2	1:E:208:MET:SD	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LYS:HG3	1:B:255:MET:CB	2.45	0.47
1:F:188:LEU:H	1:F:188:LEU:CD2	2.25	0.47
1:J:85:PHE:CB	1:J:88:THR:OG1	2.58	0.47
1:G:255:MET:HG2	1:G:256:PHE:H	1.78	0.47
1:I:149:MET:HE2	1:I:293:PRO:HD2	1.95	0.47
1:E:237:MET:HG2	1:E:245:MET:CG	2.43	0.47
1:O:79:ASP:OD1	1:O:81:ASN:N	2.44	0.47
1:K:287:THR:HG22	1:K:287:THR:O	2.14	0.47
1:N:363:ARG:HG3	1:O:188:LEU:HD21	1.95	0.47
1:G:54:LYS:HZ3	1:G:56:ASP:N	2.12	0.47
1:K:70:TYR:CE2	1:K:195:LEU:HD22	2.48	0.47
1:M:343:CYS:O	1:N:215:ALA:N	2.47	0.47
1:M:358:PHE:CE2	1:N:216:ASN:HA	2.49	0.47
1:H:277:ILE:O	1:H:278:LYS:C	2.52	0.47
1:O:21:VAL:HG21	1:O:241:PRO:HB2	1.96	0.47
1:N:105:VAL:HG12	1:N:106:GLU:N	2.28	0.47
1:L:219:ASP:HB2	1:L:263:ARG:CZ	2.45	0.47
1:N:79:ASP:OD1	1:N:81:ASN:HB2	2.13	0.47
1:E:240:GLU:CG	1:E:241:PRO:HD2	2.45	0.47
1:C:79:ASP:OD2	1:C:325:ASN:ND2	2.47	0.47
1:J:22:VAL:HG11	1:J:26:GLU:HG3	1.97	0.47
1:D:342:VAL:CG2	1:D:361:TYR:HB2	2.44	0.47
1:I:381:LEU:HB3	1:I:386:MET:CE	2.44	0.47
1:H:85:PHE:HB2	1:H:88:THR:OG1	2.14	0.47
1:I:79:ASP:HB3	1:I:82:LYS:HG3	1.95	0.47
1:M:174:PRO:HG3	1:M:180:VAL:HG23	1.96	0.47
1:N:331:VAL:HG11	1:N:368:TYR:HE2	1.80	0.47
1:J:240:GLU:CG	1:J:241:PRO:HD2	2.44	0.47
1:K:240:GLU:OE2	1:K:245:MET:HB2	2.14	0.47
1:G:133:ASN:N	1:G:133:ASN:HD22	2.12	0.47
1:D:120:HIS:ND1	1:D:122:LEU:C	2.68	0.47
1:B:148:SER:O	1:B:149:MET:HB3	2.15	0.47
1:G:148:SER:O	1:G:149:MET:HB3	2.12	0.47
1:K:185:CYS:HB2	1:O:361:TYR:CG	2.50	0.47
1:G:181:LYS:N	1:G:181:LYS:CD	2.77	0.47
1:D:331:VAL:HG11	1:D:368:TYR:HE2	1.80	0.47
1:I:54:LYS:NZ	1:I:56:ASP:H	2.12	0.47
1:M:29:THR:CG2	1:M:30:ARG:N	2.77	0.47
1:A:256:PHE:CD1	1:A:257:VAL:N	2.83	0.47
1:M:461:GLN:NE2	1:N:21:VAL:HB	2.16	0.47
1:H:123:LEU:HD12	1:H:219:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:LEU:CB	1:F:304:ILE:HD11	2.44	0.47
1:A:123:LEU:HD12	1:A:219:ASP:HA	1.96	0.47
1:H:69:GLN:NE2	1:H:71:ARG:HH22	2.13	0.47
1:L:361:TYR:CD2	1:M:185:CYS:HB2	2.50	0.47
1:J:123:LEU:HD22	1:J:147:ILE:HB	1.96	0.47
1:L:311:LEU:N	1:L:311:LEU:HD23	2.26	0.47
1:H:151:TYR:CD2	1:H:203:THR:HB	2.49	0.47
1:F:102:CYS:O	1:F:311:LEU:HD11	2.14	0.47
1:A:384:ASP:OD2	1:F:92:ASP:HB2	2.14	0.47
1:G:37:ALA:HB1	1:G:451:LEU:HD13	1.96	0.47
1:I:340:MET:HB2	1:J:208:MET:SD	2.54	0.47
1:K:157:CYS:HA	1:K:330:THR:O	2.14	0.47
1:G:278:LYS:HB2	1:J:351:SER:O	2.15	0.47
1:D:148:SER:OG	1:E:129:THR:OG1	2.24	0.47
1:M:311:LEU:HG	1:M:311:LEU:O	2.14	0.47
1:N:114:GLY:HA2	1:O:255:MET:SD	2.55	0.47
1:L:151:TYR:CD1	1:L:203:THR:HB	2.49	0.47
1:M:148:SER:O	1:M:149:MET:HB3	2.15	0.47
1:I:24:THR:HG23	1:I:318:ASN:HA	1.97	0.47
1:B:342:VAL:O	1:B:342:VAL:CG2	2.63	0.47
1:K:257:VAL:CG1	1:K:291:PRO:HB2	2.44	0.47
1:I:342:VAL:HG22	1:I:361:TYR:HB2	1.97	0.47
1:A:220:VAL:HG23	1:A:225:CYS:CB	2.44	0.47
1:C:393:ASN:HB3	1:C:396:ILE:HD12	1.97	0.47
1:A:201:VAL:CG1	1:A:332:VAL:HG21	2.45	0.47
1:G:69:GLN:HA	1:G:199:ASP:O	2.15	0.47
1:K:79:ASP:CB	1:K:82:LYS:HE2	2.44	0.47
1:M:471:GLN:C	1:M:473:GLY:N	2.66	0.47
1:I:381:LEU:HB3	1:I:386:MET:HE1	1.95	0.47
1:C:354:LYS:HA	1:D:141:THR:HG23	1.96	0.47
1:N:190:LEU:HD12	1:N:190:LEU:HA	1.59	0.47
1:D:359:LYS:CE	1:D:359:LYS:HG2	2.40	0.47
1:A:258:ARG:HG3	1:A:259:HIS:ND1	2.30	0.47
1:A:258:ARG:HB2	1:A:294:SER:HB2	1.97	0.47
1:N:370:LEU:HB3	1:N:372:PHE:CZ	2.49	0.47
1:E:220:VAL:HG23	1:E:225:CYS:HA	1.96	0.47
1:E:152:LYS:HB2	1:E:255:MET:HB2	1.96	0.47
1:I:211:THR:HG23	1:I:226:SER:HA	1.97	0.47
1:G:109:ARG:H	1:G:306:ASN:ND2	2.12	0.47
1:H:111:GLN:HB3	1:H:112:PRO:CD	2.40	0.47
1:N:151:TYR:OH	1:N:221:PRO:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:MET:HB2	1:C:292:THR:HG23	1.97	0.47
1:L:71:ARG:HG3	1:L:368:TYR:CZ	2.50	0.47
1:L:156:LEU:HD21	1:L:332:VAL:HG21	1.96	0.47
1:O:298:VAL:CG1	1:O:335:THR:HA	2.44	0.47
1:H:361:TYR:CD2	1:I:185:CYS:HB2	2.49	0.47
1:K:35:TYR:O	1:K:373:ILE:HA	2.14	0.47
1:M:121:PRO:HD3	1:M:222:LEU:CD2	2.44	0.47
1:O:164:PRO:HA	1:O:245:MET:CG	2.44	0.47
1:C:47:HIS:O	1:C:64:LYS:HA	2.15	0.47
1:J:96:GLN:O	1:J:97:ARG:HD3	2.13	0.47
1:G:331:VAL:HG11	1:G:368:TYR:HE2	1.79	0.47
1:O:76:LYS:HB3	1:O:452:LYS:HZ1	1.80	0.47
1:D:311:LEU:CD2	1:D:311:LEU:H	2.27	0.47
1:G:46:GLY:O	1:G:363:ARG:HA	2.15	0.47
1:G:364:HIS:NE2	1:G:366:GLU:OE1	2.48	0.47
1:D:193:THR:HG23	1:D:230:LYS:HD3	1.95	0.47
1:E:117:ILE:HG23	1:E:117:ILE:O	2.15	0.47
1:B:354:LYS:HB2	1:B:354:LYS:HE3	1.65	0.47
1:F:145:GLU:OE1	1:G:132:SER:HB3	2.14	0.47
1:E:181:LYS:HE2	1:E:184:GLU:HG2	1.97	0.47
1:E:467:LYS:O	1:E:470:LEU:HB3	2.14	0.47
1:D:162:ARG:HG3	1:D:244:ASP:HB2	1.95	0.47
1:A:106:GLU:HG3	1:A:464:LEU:HG	1.95	0.47
1:I:385:VAL:O	1:I:389:ILE:HG13	2.15	0.47
1:I:392:MET:HB3	1:I:393:ASN:H	1.54	0.47
1:F:233:ASP:OD1	1:F:236:LYS:HB2	2.14	0.47
1:F:250:LEU:HB2	1:F:304:ILE:HD11	1.96	0.47
1:N:299:THR:O	1:N:300:SER:C	2.53	0.47
1:M:340:MET:HG2	1:M:363:ARG:O	2.15	0.47
1:H:154:THR:HA	1:H:252:ARG:O	2.14	0.47
1:K:287:THR:OG1	1:O:121:PRO:HG3	2.14	0.47
1:C:342:VAL:HG21	1:D:185:CYS:SG	2.55	0.47
1:H:393:ASN:HD22	1:H:394:PRO:HD2	1.80	0.47
1:J:323:TRP:O	1:J:324:SER:HB2	2.14	0.47
1:O:462:PHE:O	1:O:466:ARG:HB2	2.15	0.47
1:O:284:LEU:HD12	1:O:285:PRO:HD2	1.95	0.47
1:J:29:THR:HG22	1:J:30:ARG:N	2.29	0.47
1:C:37:ALA:HB1	1:C:451:LEU:CD1	2.42	0.47
1:A:117:ILE:HA	1:A:149:MET:O	2.15	0.47
1:J:155:GLN:HB3	1:J:304:ILE:HG21	1.97	0.47
1:O:247:PHE:HA	1:O:315:GLN:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:HD12	1:A:329:VAL:HG22	1.97	0.47
1:E:97:ARG:O	1:E:98:LEU:HD23	2.14	0.47
1:O:464:LEU:HD23	1:O:464:LEU:O	2.15	0.47
1:H:29:THR:HG22	1:H:30:ARG:N	2.30	0.47
1:L:118:SER:O	1:L:149:MET:N	2.48	0.47
1:M:194:VAL:O	1:M:196:GLN:HG3	2.14	0.47
1:E:92:ASP:OD1	1:E:94:ALA:CB	2.63	0.47
1:M:27:TYR:HD1	1:M:27:TYR:O	1.98	0.47
1:J:240:GLU:HG3	1:J:241:PRO:HD2	1.96	0.47
1:G:133:ASN:N	1:G:133:ASN:ND2	2.63	0.47
1:I:155:GLN:OE1	1:I:304:ILE:HG22	2.15	0.47
1:N:382:THR:OG1	1:N:385:VAL:HG23	2.15	0.47
1:M:219:ASP:HB2	1:M:263:ARG:HH11	1.70	0.47
1:A:292:THR:HG22	1:A:293:PRO:O	2.14	0.47
1:I:255:MET:CG	1:I:256:PHE:N	2.77	0.47
1:O:149:MET:HE1	1:O:205:PHE:CE1	2.49	0.47
1:O:272:PRO:CD	1:O:275:LEU:HD12	2.43	0.47
1:B:118:SER:CB	1:B:223:ASP:OD2	2.62	0.47
1:A:299:THR:C	1:A:301:ASP:H	2.18	0.47
1:M:96:GLN:HE22	1:M:378:LYS:HD3	1.80	0.47
1:N:129:THR:HG23	1:N:262:ASN:HB2	1.97	0.47
1:L:111:GLN:HB3	1:L:112:PRO:CD	2.45	0.46
1:H:256:PHE:C	1:H:256:PHE:CD1	2.87	0.46
1:K:151:TYR:CD1	1:K:203:THR:HB	2.50	0.46
1:M:68:LEU:O	1:M:201:VAL:HG23	2.15	0.46
1:E:393:ASN:HD22	1:E:394:PRO:N	2.13	0.46
1:H:262:ASN:HA	1:H:262:ASN:HD22	1.28	0.46
1:E:240:GLU:HG3	1:E:241:PRO:HD2	1.97	0.46
1:B:71:ARG:HG3	1:B:368:TYR:CZ	2.50	0.46
1:B:217:LYS:O	1:B:217:LYS:CG	2.64	0.46
1:B:180:VAL:HG12	1:B:184:GLU:HB2	1.97	0.46
1:E:181:LYS:H	1:E:181:LYS:HD3	1.80	0.46
1:J:32:ASN:O	1:J:33:ILE:HD13	2.14	0.46
1:K:458:ASP:O	1:K:462:PHE:HE1	1.98	0.46
1:F:328:PHE:HE2	1:F:446:PHE:CE1	2.33	0.46
1:B:467:LYS:NZ	1:B:467:LYS:CD	2.77	0.46
1:L:111:GLN:NE2	1:M:167:GLU:OE1	2.48	0.46
1:M:154:THR:HG23	1:M:253:GLU:CB	2.29	0.46
1:C:150:ASP:OD1	1:C:294:SER:HA	2.14	0.46
1:B:221:PRO:O	1:B:225:CYS:HB3	2.15	0.46
1:I:298:VAL:C	1:I:299:THR:CG2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:83:PHE:CD2	1:J:85:PHE:CZ	2.90	0.46
1:K:74:ARG:NH2	1:K:441:LEU:CD1	2.74	0.46
1:C:70:TYR:OH	1:C:232:PRO:HD3	2.16	0.46
1:N:29:THR:HG22	1:N:30:ARG:O	2.15	0.46
1:K:304:ILE:HD13	1:K:305:PHE:CE2	2.50	0.46
1:H:82:LYS:C	1:H:83:PHE:O	2.54	0.46
1:A:299:THR:O	1:A:301:ASP:N	2.48	0.46
1:D:21:VAL:HG11	1:D:241:PRO:O	2.15	0.46
1:A:216:ASN:O	1:A:217:LYS:HG2	2.15	0.46
1:B:393:ASN:HB3	1:B:396:ILE:CD1	2.45	0.46
1:K:114:GLY:O	1:K:115:VAL:CG1	2.63	0.46
1:E:340:MET:HG2	1:E:363:ARG:O	2.14	0.46
1:M:41:ARG:HH11	1:N:190:LEU:HD23	1.80	0.46
1:F:118:SER:HB3	1:F:223:ASP:OD2	2.16	0.46
1:D:442:LYS:HB3	1:D:442:LYS:HE3	1.61	0.46
1:E:149:MET:HE3	1:E:292:THR:HG23	1.98	0.46
1:M:255:MET:HG2	1:M:256:PHE:N	2.29	0.46
1:K:119:GLY:CA	1:K:148:SER:HA	2.45	0.46
1:H:255:MET:HG2	1:H:256:PHE:N	2.29	0.46
1:K:169:TRP:CD1	1:O:340:MET:SD	3.08	0.46
1:M:240:GLU:OE2	1:M:245:MET:HB2	2.16	0.46
1:B:65:VAL:O	1:B:364:HIS:HB3	2.15	0.46
1:D:165:ILE:CD1	1:D:236:LYS:HD3	2.45	0.46
1:N:149:MET:HE2	1:N:293:PRO:HD2	1.97	0.46
1:E:305:PHE:HE1	1:E:333:ASP:CB	2.28	0.46
1:K:361:TYR:CD1	1:L:185:CYS:HB2	2.51	0.46
1:C:471:GLN:C	1:C:473:GLY:H	2.19	0.46
1:I:79:ASP:O	1:I:81:ASN:N	2.49	0.46
1:J:73:PHE:CD1	1:J:370:LEU:HD11	2.51	0.46
1:E:159:ILE:HD12	1:E:329:VAL:HG22	1.96	0.46
1:L:363:ARG:NH2	1:M:269:GLU:OE1	2.47	0.46
1:F:125:LYS:O	1:F:125:LYS:HD3	2.15	0.46
1:O:22:VAL:HG13	1:O:26:GLU:HG3	1.95	0.46
1:A:393:ASN:ND2	1:A:394:PRO:HD2	2.26	0.46
1:F:297:MET:HE2	1:G:256:PHE:CD2	2.51	0.46
1:F:106:GLU:HB3	1:F:371:GLN:HB2	1.96	0.46
1:L:99:VAL:HG11	1:L:321:ILE:HG22	1.96	0.46
1:N:271:VAL:HA	1:N:272:PRO:HD3	1.65	0.46
1:O:188:LEU:HD22	1:O:188:LEU:N	2.29	0.46
1:G:73:PHE:O	1:G:328:PHE:HA	2.15	0.46
1:K:30:ARG:HD3	1:K:377:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:261:PHE:HE2	1:M:131:ASN:OD1	1.97	0.46
1:C:467:LYS:O	1:C:468:PHE:C	2.54	0.46
1:F:327:LEU:HD11	1:F:374:PHE:HE2	1.81	0.46
1:E:138:ASN:HD21	1:E:283:THR:CB	2.29	0.46
1:F:134:LYS:NZ	1:F:134:LYS:HD2	2.28	0.46
1:N:361:TYR:CZ	1:O:268:GLY:HA3	2.51	0.46
1:I:364:HIS:HD2	1:I:365:GLY:N	1.99	0.46
1:C:117:ILE:HG12	1:C:148:SER:HB2	1.97	0.46
1:D:380:THR:HG22	1:D:382:THR:HG23	1.97	0.46
1:E:68:LEU:HD13	1:E:151:TYR:HD1	1.80	0.46
1:L:355:ASN:OD1	1:M:142:ASP:N	2.48	0.46
1:J:72:VAL:CG2	1:J:196:GLN:C	2.83	0.46
1:C:85:PHE:HB2	1:C:88:THR:HG23	1.98	0.46
1:D:102:CYS:O	1:D:311:LEU:HD11	2.16	0.46
1:F:327:LEU:HA	1:F:327:LEU:HD23	1.68	0.46
1:M:262:ASN:HA	1:M:262:ASN:HD22	1.59	0.46
1:A:370:LEU:HA	1:A:370:LEU:HD23	1.72	0.46
1:I:442:LYS:HE3	1:I:442:LYS:HB3	1.71	0.46
1:A:28:VAL:HG22	1:A:379:ILE:HD11	1.96	0.46
1:H:52:ILE:O	1:H:61:ALA:HB3	2.16	0.46
1:B:220:VAL:O	1:B:221:PRO:C	2.52	0.46
1:F:165:ILE:HD11	1:F:236:LYS:CD	2.45	0.46
1:N:54:LYS:HD2	1:N:55:GLN:N	2.31	0.46
1:K:256:PHE:HD2	1:O:297:MET:HE2	1.80	0.46
1:K:295:GLY:O	1:K:296:SER:HB3	2.15	0.46
1:O:337:SER:HA	1:O:364:HIS:CE1	2.50	0.46
1:M:220:VAL:HG23	1:M:225:CYS:HB3	1.96	0.46
1:J:372:PHE:O	1:J:373:ILE:CG1	2.63	0.46
1:O:200:MET:HB3	1:O:229:CYS:SG	2.56	0.46
1:D:56:ASP:O	1:D:57:SER:O	2.34	0.46
1:A:28:VAL:HG22	1:A:379:ILE:CD1	2.46	0.46
1:F:442:LYS:HB3	1:F:442:LYS:HE3	1.61	0.46
1:C:52:ILE:HD13	1:D:269:GLU:OE1	2.16	0.46
1:K:127:ASP:O	1:K:129:THR:HG23	2.16	0.46
1:C:121:PRO:HD3	1:C:222:LEU:CD2	2.42	0.46
1:I:225:CYS:SG	1:I:226:SER:N	2.89	0.46
1:K:54:LYS:HZ3	1:K:55:GLN:HB3	1.79	0.46
1:O:153:GLN:O	1:O:253:GLU:HA	2.16	0.46
1:N:111:GLN:HB3	1:N:112:PRO:HD2	1.97	0.46
1:I:310:TRP:HH2	1:I:464:LEU:CD2	2.29	0.46
1:D:96:GLN:HE22	1:D:378:LYS:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLY:HA2	1:B:309:TYR:O	2.15	0.46
1:B:156:LEU:CD2	1:B:332:VAL:HB	2.46	0.46
1:K:109:ARG:HH11	1:K:109:ARG:HD2	1.41	0.46
1:L:373:ILE:CD1	1:L:464:LEU:HD13	2.46	0.46
1:M:149:MET:HE2	1:M:205:PHE:HE1	1.81	0.46
1:I:28:VAL:HG11	1:I:321:ILE:HD12	1.98	0.46
1:L:123:LEU:HD22	1:L:147:ILE:HB	1.96	0.46
1:M:121:PRO:CD	1:M:222:LEU:HD21	2.45	0.46
1:M:222:LEU:HD12	1:N:275:LEU:HB3	1.98	0.46
1:C:361:TYR:CZ	1:D:268:GLY:HA3	2.51	0.46
1:F:115:VAL:N	1:F:338:THR:HG23	2.31	0.46
1:H:327:LEU:HD23	1:H:327:LEU:HA	1.41	0.46
1:C:103:THR:HB	1:C:373:ILE:O	2.15	0.46
1:M:400:TRP:O	1:M:401:ASN:HB3	2.15	0.46
1:D:296:SER:OG	1:D:297:MET:N	2.48	0.46
1:D:148:SER:HB3	1:E:289:TYR:CE2	2.50	0.46
1:I:110:GLY:O	1:I:111:GLN:CB	2.64	0.46
1:L:24:THR:HA	1:L:27:TYR:CE2	2.51	0.46
1:L:318:ASN:ND2	1:L:323:TRP:HE1	2.14	0.46
1:C:162:ARG:HG3	1:C:244:ASP:HB2	1.98	0.46
1:N:149:MET:HA	1:O:260:LEU:HD13	1.98	0.46
1:B:303:GLN:NE2	1:B:335:THR:HG21	2.31	0.46
1:K:71:ARG:HA	1:K:197:ASP:OD1	2.16	0.46
1:J:200:MET:HB2	1:J:228:ILE:O	2.16	0.46
1:G:382:THR:OG1	1:G:385:VAL:HG23	2.16	0.46
1:D:362:LEU:HA	1:D:362:LEU:HD23	1.72	0.46
1:E:54:LYS:HD2	1:E:55:GLN:N	2.31	0.46
1:L:247:PHE:HB2	1:L:314:ALA:HB1	1.97	0.46
1:K:262:ASN:ND2	1:K:289:TYR:CD2	2.84	0.46
1:I:327:LEU:HA	1:I:327:LEU:HD23	1.53	0.46
1:F:462:PHE:O	1:F:463:PRO:C	2.52	0.46
1:K:188:LEU:H	1:K:188:LEU:HD22	1.81	0.46
1:E:318:ASN:C	1:E:318:ASN:OD1	2.54	0.46
1:M:157:CYS:O	1:M:249:TYR:HA	2.15	0.46
1:K:105:VAL:CG1	1:K:106:GLU:N	2.79	0.46
1:D:361:TYR:CD2	1:E:185:CYS:HB2	2.51	0.46
1:B:468:PHE:O	1:B:469:LEU:C	2.54	0.46
1:M:72:VAL:CG2	1:M:197:ASP:N	2.78	0.46
1:A:99:VAL:HG12	1:A:100:TRP:N	2.31	0.46
1:D:92:ASP:O	1:D:96:GLN:HB2	2.15	0.46
1:B:209:ASP:HB2	1:B:228:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:273:ALA:HA	1:L:276:TYR:CE2	2.50	0.46
1:I:461:GLN:HE22	1:J:21:VAL:HB	1.81	0.46
1:H:78:PRO:HD3	1:H:452:LYS:HA	1.97	0.46
1:M:372:PHE:O	1:M:373:ILE:HG13	2.16	0.45
1:M:373:ILE:HD13	1:M:468:PHE:HB2	1.97	0.45
1:H:97:ARG:O	1:H:98:LEU:HD23	2.16	0.45
1:C:258:ARG:HH11	1:C:258:ARG:HD2	1.46	0.45
1:I:152:LYS:HB2	1:I:255:MET:HG3	1.99	0.45
1:F:372:PHE:O	1:F:373:ILE:HG13	2.16	0.45
1:L:181:LYS:HE2	1:L:184:GLU:HG2	1.97	0.45
1:I:72:VAL:HG22	1:I:330:THR:HG23	1.97	0.45
1:A:54:LYS:HG3	1:A:56:ASP:H	1.80	0.45
1:I:393:ASN:ND2	1:I:395:SER:H	2.14	0.45
1:K:45:VAL:HG12	1:K:46:GLY:N	2.30	0.45
1:N:124:ASN:ND2	1:N:263:ARG:HD3	2.32	0.45
1:O:22:VAL:CG1	1:O:23:SER:N	2.79	0.45
1:F:256:PHE:HD2	1:J:297:MET:HE2	1.81	0.45
1:L:66:SER:HB3	1:L:69:GLN:HG3	1.99	0.45
1:O:54:LYS:HZ3	1:O:55:GLN:HB3	1.81	0.45
1:F:361:TYR:CD1	1:G:185:CYS:HB2	2.51	0.45
1:G:373:ILE:HD13	1:G:373:ILE:HG21	1.70	0.45
1:N:305:PHE:CE1	1:N:333:ASP:HB2	2.51	0.45
1:D:471:GLN:C	1:D:473:GLY:N	2.69	0.45
1:K:209:ASP:O	1:K:213:LEU:HB2	2.16	0.45
1:C:311:LEU:O	1:C:311:LEU:HG	2.16	0.45
1:J:155:GLN:OE1	1:J:304:ILE:HG22	2.16	0.45
1:C:336:ARG:HG3	1:C:336:ARG:HH11	1.81	0.45
1:B:219:ASP:HB2	1:B:263:ARG:NH1	2.32	0.45
1:C:253:GLU:O	1:C:254:GLN:HB3	2.14	0.45
1:D:262:ASN:HA	1:D:262:ASN:HD22	1.49	0.45
1:C:149:MET:HE1	1:C:205:PHE:CZ	2.52	0.45
1:D:234:TYR:O	1:D:238:VAL:HG23	2.16	0.45
1:H:250:LEU:CB	1:H:304:ILE:HD11	2.46	0.45
1:G:24:THR:C	1:G:26:GLU:H	2.19	0.45
1:G:54:LYS:CD	1:G:55:GLN:H	2.29	0.45
1:A:179:GLN:O	1:A:181:LYS:N	2.49	0.45
1:O:258:ARG:O	1:O:259:HIS:ND1	2.50	0.45
1:F:74:ARG:HD2	1:F:446:PHE:HD1	1.82	0.45
1:M:163:PRO:O	1:M:163:PRO:HG2	2.17	0.45
1:G:210:PHE:CE2	1:G:220:VAL:HG11	2.52	0.45
1:F:41:ARG:HH11	1:G:190:LEU:HD23	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:LEU:O	1:J:144:ARG:HD2	2.16	0.45
1:C:355:ASN:HB3	1:D:265:GLY:HA2	1.97	0.45
1:G:254:GLN:NE2	1:G:295:GLY:O	2.47	0.45
1:A:304:ILE:HG23	1:A:305:PHE:N	2.32	0.45
1:I:115:VAL:CG2	1:J:257:VAL:HG22	2.31	0.45
1:L:121:PRO:CD	1:L:222:LEU:HD21	2.38	0.45
1:A:123:LEU:HA	1:A:218:SER:O	2.16	0.45
1:H:169:TRP:H	1:H:208:MET:HA	1.81	0.45
1:O:35:TYR:CZ	1:O:457:ALA:HB2	2.51	0.45
1:C:354:LYS:HA	1:D:141:THR:CG2	2.47	0.45
1:F:25:ASP:OD1	1:F:25:ASP:N	2.47	0.45
1:F:362:LEU:HD23	1:F:362:LEU:HA	1.76	0.45
1:A:34:TYR:HA	1:A:374:PHE:O	2.16	0.45
1:F:117:ILE:CG1	1:F:148:SER:HB2	2.46	0.45
1:I:304:ILE:HG23	1:I:305:PHE:CE2	2.52	0.45
1:O:223:ASP:OD1	1:O:224:ILE:HG23	2.16	0.45
1:F:289:TYR:CE2	1:J:148:SER:HB3	2.50	0.45
1:A:123:LEU:O	1:A:144:ARG:HB3	2.16	0.45
1:F:240:GLU:HG3	1:F:241:PRO:HD2	1.98	0.45
1:E:68:LEU:HD22	1:E:203:THR:HG22	1.98	0.45
1:M:222:LEU:HA	1:M:225:CYS:SG	2.56	0.45
1:M:240:GLU:HG2	1:M:243:GLY:H	1.80	0.45
1:B:361:TYR:CD2	1:C:185:CYS:HB2	2.51	0.45
1:K:155:GLN:HB2	1:K:252:ARG:HB3	1.99	0.45
1:D:114:GLY:O	1:D:335:THR:O	2.34	0.45
1:B:91:TYR:CE1	1:B:96:GLN:HB2	2.51	0.45
1:O:29:THR:HB	1:O:378:LYS:HG2	1.98	0.45
1:I:262:ASN:HA	1:I:262:ASN:HD22	1.57	0.45
1:A:185:CYS:HB2	1:E:361:TYR:CG	2.52	0.45
1:O:233:ASP:C	1:O:233:ASP:OD1	2.54	0.45
1:E:385:VAL:O	1:E:389:ILE:HG13	2.16	0.45
1:B:201:VAL:HG11	1:B:332:VAL:HG11	1.98	0.45
1:B:346:VAL:O	1:B:346:VAL:HG12	2.16	0.45
1:L:367:GLU:OE2	1:M:235:LEU:HD12	2.16	0.45
1:L:165:ILE:CD1	1:L:236:LYS:HD3	2.47	0.45
1:J:101:ALA:HA	1:J:320:GLY:O	2.16	0.45
1:K:163:PRO:HD3	1:K:328:PHE:CZ	2.51	0.45
1:B:373:ILE:HD12	1:B:464:LEU:HD22	1.99	0.45
1:O:304:ILE:HG23	1:O:305:PHE:CD1	2.52	0.45
1:D:371:GLN:HB3	1:D:464:LEU:HD12	1.98	0.45
1:F:296:SER:OG	1:F:297:MET:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:80:PRO:HD2	1:L:325:ASN:OD1	2.17	0.45
1:B:26:GLU:OE2	1:B:26:GLU:HA	2.17	0.45
1:L:216:ASN:O	1:L:217:LYS:HG2	2.16	0.45
1:N:110:GLY:C	1:N:111:GLN:HG2	2.36	0.45
1:M:364:HIS:CD2	1:M:365:GLY:N	2.85	0.45
1:J:27:TYR:CE2	1:J:388:TYR:CE2	3.04	0.45
1:B:340:MET:HE1	1:C:169:TRP:CD1	2.52	0.45
1:L:469:LEU:HA	1:L:469:LEU:HD23	1.82	0.45
1:K:352:THR:HA	1:M:278:LYS:O	2.17	0.45
1:I:208:MET:O	1:I:228:ILE:HA	2.16	0.45
1:M:459:LEU:HD12	1:M:469:LEU:HD21	1.98	0.45
1:J:171:LYS:HE2	1:J:186:PRO:HG3	1.98	0.45
1:I:50:TYR:HA	1:I:64:LYS:HD2	1.99	0.45
1:L:112:PRO:C	1:L:113:LEU:O	2.54	0.45
1:L:54:LYS:HZ3	1:L:55:GLN:HB3	1.81	0.45
1:H:123:LEU:HD12	1:H:218:SER:O	2.17	0.45
1:J:219:ASP:O	1:J:220:VAL:HG13	2.17	0.45
1:L:32:ASN:HA	1:L:32:ASN:HD22	1.24	0.45
1:H:69:GLN:HE21	1:H:71:ARG:HH22	1.64	0.45
1:L:123:LEU:HD23	1:L:147:ILE:HD12	1.97	0.45
1:K:257:VAL:HG13	1:K:291:PRO:HB2	1.97	0.45
1:C:217:LYS:HG3	1:D:276:TYR:HA	1.99	0.45
1:H:393:ASN:HB3	1:H:396:ILE:CD1	2.45	0.45
1:F:75:VAL:HB	1:F:327:LEU:HB2	1.98	0.45
1:B:201:VAL:CG1	1:B:332:VAL:HG21	2.46	0.45
1:B:188:LEU:N	1:B:188:LEU:HD22	2.32	0.45
1:D:280:THR:O	1:D:281:THR:HB	2.17	0.45
1:L:351:SER:O	1:N:278:LYS:HB2	2.16	0.45
1:F:126:LEU:HB3	1:F:262:ASN:HB3	1.98	0.45
1:A:290:PHE:HA	1:A:291:PRO:HD3	1.74	0.45
1:N:295:GLY:O	1:N:296:SER:HB3	2.16	0.45
1:H:221:PRO:O	1:H:225:CYS:HB3	2.17	0.45
1:H:312:GLN:CG	1:H:313:ARG:N	2.79	0.45
1:E:474:LEU:HB3	1:F:474:LEU:HD13	1.98	0.45
1:G:386:MET:HG2	1:G:397:LEU:CD2	2.47	0.45
1:F:314:ALA:CB	1:F:319:ASN:HA	2.46	0.45
1:J:98:LEU:HA	1:J:98:LEU:HD23	1.67	0.45
1:H:272:PRO:HD2	1:H:275:LEU:HD12	1.98	0.45
1:J:83:PHE:HB3	1:J:85:PHE:CE1	2.52	0.45
1:E:246:LEU:CD1	1:E:246:LEU:C	2.85	0.45
1:H:222:LEU:HA	1:H:225:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:219:ASP:HB2	1:J:263:ARG:CZ	2.47	0.45
1:O:77:LEU:HB2	1:O:325:ASN:O	2.16	0.45
1:L:164:PRO:HG3	1:L:330:THR:OG1	2.17	0.45
1:B:97:ARG:O	1:B:378:LYS:HA	2.16	0.45
1:D:79:ASP:CG	1:D:325:ASN:HD21	2.19	0.45
1:F:185:CYS:HB2	1:J:361:TYR:CG	2.51	0.45
1:L:119:GLY:CA	1:L:148:SER:HA	2.46	0.45
1:H:284:LEU:HD12	1:H:284:LEU:HA	1.59	0.45
1:I:232:PRO:HB2	1:I:234:TYR:CE1	2.52	0.45
1:D:53:LYS:HD3	1:D:58:ASN:HA	1.99	0.45
1:I:280:THR:O	1:I:281:THR:HB	2.17	0.45
1:F:291:PRO:O	1:F:291:PRO:HG2	2.16	0.45
1:J:79:ASP:O	1:J:81:ASN:N	2.49	0.45
1:G:119:GLY:O	1:G:221:PRO:HB3	2.17	0.45
1:I:181:LYS:HD3	1:I:181:LYS:N	2.27	0.45
1:I:181:LYS:HE2	1:I:184:GLU:OE2	2.17	0.45
1:O:337:SER:HA	1:O:364:HIS:HE1	1.82	0.45
1:J:107:VAL:CG1	1:J:107:VAL:O	2.61	0.45
1:D:163:PRO:HD3	1:D:328:PHE:CE1	2.52	0.45
1:D:311:LEU:HD23	1:D:311:LEU:N	2.30	0.45
1:E:379:ILE:HD12	1:E:400:TRP:HH2	1.82	0.45
1:B:210:PHE:HD2	1:B:214:GLN:OE1	2.00	0.45
1:B:380:THR:HG21	1:J:380:THR:HG21	1.98	0.45
1:O:300:SER:O	1:O:303:GLN:HB2	2.16	0.45
1:E:327:LEU:HA	1:E:327:LEU:HD23	1.39	0.45
1:K:381:LEU:HD22	1:K:386:MET:HG2	1.98	0.45
1:D:216:ASN:O	1:D:217:LYS:C	2.56	0.44
1:N:122:LEU:O	1:N:144:ARG:HD2	2.17	0.44
1:L:54:LYS:HB3	1:L:57:SER:HB3	1.99	0.44
1:A:222:LEU:HD22	1:A:222:LEU:H	1.82	0.44
1:K:117:ILE:HG13	1:L:260:LEU:CD2	2.45	0.44
1:N:185:CYS:HA	1:N:186:PRO:HD2	1.77	0.44
1:D:109:ARG:NH2	1:D:333:ASP:OD2	2.50	0.44
1:A:151:TYR:CE1	1:A:203:THR:HG21	2.52	0.44
1:F:216:ASN:O	1:F:217:LYS:C	2.55	0.44
1:D:131:ASN:O	1:D:132:SER:C	2.56	0.44
1:F:96:GLN:HE22	1:F:378:LYS:HD3	1.82	0.44
1:M:72:VAL:HG23	1:M:197:ASP:N	2.31	0.44
1:D:209:ASP:HB2	1:D:228:ILE:HG12	1.99	0.44
1:J:165:ILE:HG23	1:J:245:MET:SD	2.57	0.44
1:K:160:GLY:HA3	1:K:245:MET:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:80:PRO:HD2	1:J:325:ASN:OD1	2.17	0.44
1:H:330:THR:O	1:H:331:VAL:HG23	2.17	0.44
1:M:152:LYS:NZ	1:M:152:LYS:HD2	2.31	0.44
1:G:305:PHE:O	1:G:307:LYS:HG3	2.16	0.44
1:L:52:ILE:HB	1:L:62:VAL:HG23	1.98	0.44
1:J:395:SER:O	1:J:396:ILE:C	2.55	0.44
1:A:122:LEU:HD13	1:A:144:ARG:NH2	2.32	0.44
1:O:371:GLN:CB	1:O:464:LEU:HD12	2.48	0.44
1:M:164:PRO:HA	1:M:245:MET:HG3	1.99	0.44
1:B:71:ARG:HA	1:B:71:ARG:HD3	1.72	0.44
1:B:29:THR:HG22	1:B:30:ARG:N	2.30	0.44
1:K:380:THR:O	1:K:382:THR:HG23	2.17	0.44
1:C:368:TYR:CD1	1:C:368:TYR:N	2.85	0.44
1:G:69:GLN:HE21	1:G:71:ARG:NH2	2.15	0.44
1:F:91:TYR:HE1	1:F:96:GLN:HB2	1.81	0.44
1:B:340:MET:HB2	1:C:208:MET:SD	2.58	0.44
1:D:471:GLN:C	1:D:473:GLY:H	2.20	0.44
1:H:220:VAL:HG12	1:H:224:ILE:HD11	1.99	0.44
1:N:257:VAL:HG12	1:N:291:PRO:HB2	1.98	0.44
1:N:66:SER:HB3	1:N:69:GLN:HG3	1.99	0.44
1:I:158:LEU:O	1:I:159:ILE:HD13	2.17	0.44
1:M:103:THR:HB	1:M:373:ILE:HG22	1.99	0.44
1:J:393:ASN:ND2	1:J:394:PRO:HD2	2.23	0.44
1:O:161:CYS:O	1:O:162:ARG:HG2	2.18	0.44
1:O:70:TYR:HE1	1:O:201:VAL:HA	1.82	0.44
1:G:119:GLY:N	1:G:221:PRO:HB3	2.32	0.44
1:E:123:LEU:HD22	1:E:147:ILE:HB	1.99	0.44
1:M:237:MET:HG2	1:M:245:MET:HG2	1.99	0.44
1:M:105:VAL:CG1	1:M:106:GLU:N	2.78	0.44
1:E:372:PHE:C	1:E:373:ILE:HG13	2.37	0.44
1:G:361:TYR:CG	1:H:185:CYS:HB2	2.53	0.44
1:M:364:HIS:CD2	1:M:365:GLY:H	2.35	0.44
1:I:33:ILE:HD11	1:I:87:ASP:CB	2.47	0.44
1:K:331:VAL:HG11	1:K:368:TYR:HE2	1.81	0.44
1:M:32:ASN:HA	1:M:32:ASN:HD22	1.62	0.44
1:G:44:ALA:O	1:G:365:GLY:HA2	2.17	0.44
1:C:101:ALA:O	1:C:374:PHE:HA	2.18	0.44
1:K:45:VAL:CA	1:K:65:VAL:HG21	2.47	0.44
1:N:119:GLY:O	1:N:222:LEU:HD22	2.17	0.44
1:K:148:SER:O	1:K:149:MET:HB3	2.17	0.44
1:J:82:LYS:O	1:J:83:PHE:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:LEU:HD22	1:I:147:ILE:HB	1.99	0.44
1:L:304:ILE:HG21	1:L:304:ILE:HD13	1.59	0.44
1:L:99:VAL:HG12	1:L:100:TRP:O	2.18	0.44
1:B:22:VAL:HG12	1:B:23:SER:N	2.32	0.44
1:N:101:ALA:HA	1:N:320:GLY:O	2.18	0.44
1:E:24:THR:CG2	1:E:319:ASN:H	2.30	0.44
1:I:342:VAL:CG2	1:I:361:TYR:HB2	2.47	0.44
1:L:381:LEU:HD21	1:L:400:TRP:CZ3	2.53	0.44
1:K:165:ILE:HG23	1:K:245:MET:SD	2.57	0.44
1:J:32:ASN:HA	1:J:32:ASN:HD22	1.43	0.44
1:D:120:HIS:HE1	1:D:122:LEU:HB2	1.82	0.44
1:F:109:ARG:CB	1:F:109:ARG:HH11	2.22	0.44
1:N:103:THR:O	1:N:103:THR:HG22	2.17	0.44
1:I:299:THR:C	1:I:301:ASP:H	2.21	0.44
1:I:220:VAL:CG2	1:I:225:CYS:HA	2.47	0.44
1:D:47:HIS:HB2	1:D:52:ILE:HD11	1.99	0.44
1:L:370:LEU:HA	1:L:370:LEU:HD23	1.80	0.44
1:H:54:LYS:CD	1:H:55:GLN:H	2.30	0.44
1:K:22:VAL:HG12	1:K:23:SER:N	2.33	0.44
1:I:120:HIS:HA	1:I:222:LEU:HD22	1.98	0.44
1:E:233:ASP:O	1:E:234:TYR:C	2.55	0.44
1:L:263:ARG:NH1	1:L:290:PHE:CE2	2.85	0.44
1:M:222:LEU:HD12	1:N:275:LEU:HD13	2.00	0.44
1:M:123:LEU:HD12	1:M:218:SER:O	2.18	0.44
1:N:393:ASN:HD22	1:N:394:PRO:CD	2.29	0.44
1:H:181:LYS:HD3	1:H:181:LYS:N	2.32	0.44
1:H:393:ASN:HD22	1:H:394:PRO:CD	2.30	0.44
1:F:311:LEU:H	1:F:311:LEU:HD23	1.83	0.44
1:M:115:VAL:HG21	1:N:257:VAL:HG22	1.99	0.44
1:A:363:ARG:HA	1:A:363:ARG:HD3	1.78	0.44
1:G:47:HIS:O	1:G:64:LYS:HA	2.17	0.44
1:D:156:LEU:HA	1:D:250:LEU:O	2.18	0.44
1:G:144:ARG:NH1	1:G:218:SER:OG	2.50	0.44
1:H:71:ARG:HA	1:H:71:ARG:HD3	1.55	0.44
1:O:311:LEU:CD2	1:O:311:LEU:H	2.23	0.44
1:D:469:LEU:HA	1:D:469:LEU:HD23	1.51	0.44
1:I:117:ILE:HD11	1:J:260:LEU:HB3	1.98	0.44
1:J:362:LEU:C	1:J:363:ARG:HG2	2.38	0.44
1:B:46:GLY:O	1:B:363:ARG:HA	2.18	0.44
1:E:47:HIS:O	1:E:64:LYS:HA	2.17	0.44
1:D:92:ASP:OD1	1:D:94:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:GLU:HG2	1:E:308:PRO:HA	2.00	0.44
1:O:125:LYS:C	1:O:125:LYS:HD3	2.38	0.44
1:H:116:GLY:C	1:H:117:ILE:HG22	2.38	0.44
1:H:242:TYR:CE2	1:H:392:MET:HG3	2.52	0.44
1:A:193:THR:HG21	1:A:230:LYS:HE2	2.00	0.44
1:I:40:SER:HB3	1:I:454:LYS:NZ	2.33	0.44
1:I:363:ARG:NH2	1:J:269:GLU:OE1	2.39	0.44
1:H:373:ILE:HD12	1:H:464:LEU:HD22	1.99	0.44
1:I:120:HIS:HA	1:I:121:PRO:HD3	1.78	0.44
1:B:237:MET:CB	1:B:246:LEU:CD2	2.96	0.44
1:O:373:ILE:CD1	1:O:464:LEU:HD22	2.45	0.44
1:D:466:ARG:NH1	1:E:315:GLN:O	2.50	0.44
1:E:74:ARG:HG3	1:E:328:PHE:CZ	2.52	0.44
1:A:220:VAL:HG21	1:A:225:CYS:HA	1.99	0.44
1:C:233:ASP:O	1:C:237:MET:HG3	2.18	0.44
1:L:209:ASP:O	1:L:209:ASP:OD2	2.36	0.44
1:O:133:ASN:HD22	1:O:133:ASN:N	2.14	0.44
1:J:167:GLU:HG3	1:J:167:GLU:O	2.18	0.44
1:L:92:ASP:C	1:L:92:ASP:OD1	2.55	0.44
1:D:196:GLN:O	1:D:197:ASP:C	2.56	0.44
1:C:74:ARG:HD2	1:C:446:PHE:HD1	1.83	0.44
1:B:327:LEU:HD23	1:B:327:LEU:HA	1.67	0.44
1:A:115:VAL:HG21	1:B:257:VAL:HG22	2.00	0.44
1:B:123:LEU:HD12	1:B:219:ASP:HA	1.99	0.44
1:N:123:LEU:HG	1:N:124:ASN:N	2.32	0.44
1:F:318:ASN:OD1	1:F:321:ILE:CB	2.56	0.44
1:G:299:THR:HG22	1:H:254:GLN:HB2	1.99	0.44
1:D:68:LEU:O	1:D:201:VAL:HG22	2.18	0.44
1:F:257:VAL:HG22	1:J:115:VAL:CG2	2.42	0.44
1:L:69:GLN:NE2	1:L:71:ARG:NH2	2.66	0.44
1:B:167:GLU:HG3	1:B:231:TYR:O	2.17	0.44
1:O:342:VAL:CG2	1:O:361:TYR:HB2	2.48	0.44
1:O:363:ARG:HA	1:O:363:ARG:HD3	1.91	0.44
1:E:103:THR:HG21	1:E:468:PHE:CE1	2.53	0.44
1:K:353:TYR:HE1	1:L:216:ASN:HB2	1.83	0.44
1:H:82:LYS:O	1:H:83:PHE:C	2.56	0.44
1:M:72:VAL:HG21	1:M:196:GLN:HA	2.00	0.44
1:M:278:LYS:HD3	1:M:278:LYS:HA	1.84	0.44
1:B:102:CYS:SG	1:B:103:THR:N	2.91	0.44
1:N:461:GLN:H	1:N:461:GLN:HG2	1.43	0.44
1:C:442:LYS:HB3	1:C:442:LYS:HE3	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:310:TRP:O	1:N:312:GLN:N	2.51	0.44
1:F:440:PRO:HG2	1:F:441:LEU:H	1.81	0.44
1:C:196:GLN:O	1:C:197:ASP:C	2.56	0.44
1:C:102:CYS:O	1:C:311:LEU:HD11	2.18	0.44
1:F:120:HIS:HA	1:F:222:LEU:HD22	1.99	0.44
1:B:299:THR:HG22	1:C:254:GLN:HB2	1.98	0.44
1:K:24:THR:C	1:K:26:GLU:N	2.69	0.44
1:K:200:MET:O	1:K:229:CYS:HA	2.18	0.44
1:N:37:ALA:HA	1:N:454:LYS:O	2.18	0.44
1:G:21:VAL:HG12	1:G:22:VAL:N	2.32	0.44
1:G:363:ARG:HA	1:G:363:ARG:HD3	1.80	0.44
1:L:223:ASP:OD1	1:L:224:ILE:N	2.51	0.44
1:E:47:HIS:HB2	1:E:52:ILE:HD11	1.98	0.44
1:K:157:CYS:O	1:K:249:TYR:HA	2.17	0.44
1:E:75:VAL:HB	1:E:327:LEU:HB2	1.98	0.44
1:N:461:GLN:HE21	1:N:461:GLN:HB3	1.54	0.44
1:K:362:LEU:HA	1:K:362:LEU:HD23	1.79	0.44
1:O:287:THR:HG22	1:O:289:TYR:CE1	2.53	0.44
1:E:66:SER:HB3	1:E:69:GLN:HG3	2.00	0.44
1:C:156:LEU:CD1	1:C:156:LEU:C	2.81	0.43
1:I:300:SER:OG	1:J:253:GLU:HG2	2.18	0.43
1:E:272:PRO:HD2	1:E:275:LEU:CD1	2.39	0.43
1:G:153:GLN:NE2	1:G:298:VAL:HG13	2.33	0.43
1:B:258:ARG:HD2	1:B:258:ARG:HH11	1.57	0.43
1:I:162:ARG:HG3	1:I:244:ASP:HB2	2.00	0.43
1:I:216:ASN:C	1:I:217:LYS:HG2	2.38	0.43
1:O:54:LYS:NZ	1:O:55:GLN:HB3	2.33	0.43
1:D:79:ASP:C	1:D:81:ASN:H	2.21	0.43
1:F:232:PRO:HB2	1:F:234:TYR:CE1	2.53	0.43
1:B:450:ASP:OD1	1:B:452:LYS:HB2	2.18	0.43
1:B:450:ASP:OD1	1:B:452:LYS:HG3	2.18	0.43
1:M:327:LEU:CD1	1:M:374:PHE:HE2	2.31	0.43
1:E:28:VAL:HG22	1:E:379:ILE:HG12	1.98	0.43
1:C:32:ASN:HA	1:C:32:ASN:HD22	1.57	0.43
1:C:297:MET:HB2	1:D:256:PHE:HB3	2.01	0.43
1:O:210:PHE:HD2	1:O:214:GLN:OE1	2.00	0.43
1:O:152:LYS:HA	1:O:255:MET:HB2	1.98	0.43
1:I:299:THR:O	1:I:300:SER:C	2.57	0.43
1:F:125:LYS:HE3	1:F:261:PHE:CE2	2.53	0.43
1:N:52:ILE:O	1:N:61:ALA:HB3	2.18	0.43
1:B:258:ARG:HB2	1:B:294:SER:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:LYS:N	1:D:181:LYS:CD	2.79	0.43
1:D:385:VAL:O	1:D:386:MET:C	2.54	0.43
1:O:44:ALA:O	1:O:65:VAL:HG11	2.19	0.43
1:C:80:PRO:HD2	1:C:325:ASN:OD1	2.18	0.43
1:L:240:GLU:HG3	1:L:241:PRO:HD2	1.99	0.43
1:M:72:VAL:HG11	1:M:195:LEU:O	2.17	0.43
1:E:363:ARG:HA	1:E:363:ARG:HD3	1.84	0.43
1:H:220:VAL:CG1	1:H:224:ILE:HD11	2.48	0.43
1:I:32:ASN:HA	1:I:32:ASN:HD22	1.43	0.43
1:G:312:GLN:HG3	1:G:313:ARG:H	1.83	0.43
1:E:170:GLY:O	1:E:189:GLU:N	2.49	0.43
1:O:66:SER:HB3	1:O:69:GLN:HG3	1.99	0.43
1:B:314:ALA:HB2	1:B:319:ASN:HA	1.99	0.43
1:A:302:ALA:O	1:A:303:GLN:C	2.52	0.43
1:E:220:VAL:CG2	1:E:225:CYS:HA	2.48	0.43
1:K:109:ARG:NH1	1:K:367:GLU:O	2.51	0.43
1:D:52:ILE:HG21	1:E:269:GLU:HG2	2.00	0.43
1:I:244:ASP:O	1:I:245:MET:C	2.56	0.43
1:I:147:ILE:HA	1:J:129:THR:O	2.18	0.43
1:O:117:ILE:CG1	1:O:148:SER:HB2	2.48	0.43
1:D:117:ILE:HG21	1:E:291:PRO:HD3	1.99	0.43
1:K:269:GLU:HG3	1:O:361:TYR:CE2	2.54	0.43
1:C:47:HIS:HB3	1:C:50:TYR:O	2.17	0.43
1:G:111:GLN:HB3	1:G:112:PRO:HD2	1.99	0.43
1:F:283:THR:O	1:F:284:LEU:CB	2.66	0.43
1:A:44:ALA:O	1:A:365:GLY:HA2	2.18	0.43
1:G:212:THR:OG1	1:G:213:LEU:HD13	2.18	0.43
1:F:32:ASN:HD22	1:F:32:ASN:HA	1.35	0.43
1:B:449:VAL:HG12	1:B:449:VAL:O	2.17	0.43
1:B:190:LEU:HD12	1:B:190:LEU:HA	1.61	0.43
1:L:29:THR:HG22	1:L:30:ARG:N	2.32	0.43
1:O:470:LEU:HA	1:O:470:LEU:HD12	1.60	0.43
1:I:297:MET:HG3	1:J:255:MET:O	2.18	0.43
1:E:152:LYS:CB	1:E:255:MET:HB2	2.49	0.43
1:L:120:HIS:HA	1:L:222:LEU:HD22	2.00	0.43
1:O:155:GLN:HB2	1:O:252:ARG:HB3	2.00	0.43
1:K:459:LEU:N	1:K:459:LEU:HD23	2.34	0.43
1:L:368:TYR:N	1:L:368:TYR:CD1	2.86	0.43
1:G:165:ILE:CD1	1:G:236:LYS:HD3	2.49	0.43
1:G:120:HIS:ND1	1:G:122:LEU:C	2.72	0.43
1:M:119:GLY:O	1:M:221:PRO:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:222:LEU:O	1:M:224:ILE:N	2.52	0.43
1:E:346:VAL:O	1:E:347:SER:HB3	2.18	0.43
1:M:91:TYR:CE1	1:M:96:GLN:HB2	2.52	0.43
1:M:42:LEU:HD22	1:M:447:TRP:HE1	1.81	0.43
1:C:312:GLN:HG3	1:C:313:ARG:N	2.32	0.43
1:M:181:LYS:O	1:M:184:GLU:HB2	2.18	0.43
1:O:99:VAL:HG11	1:O:321:ILE:CG2	2.48	0.43
1:G:216:ASN:C	1:G:217:LYS:HG2	2.39	0.43
1:M:29:THR:HG22	1:M:30:ARG:N	2.34	0.43
1:C:52:ILE:HD13	1:D:269:GLU:CD	2.38	0.43
1:F:54:LYS:HD2	1:F:55:GLN:H	1.83	0.43
1:B:171:LYS:HE2	1:B:186:PRO:HG3	2.00	0.43
1:G:143:ASN:OD1	1:G:143:ASN:N	2.50	0.43
1:O:219:ASP:C	1:O:220:VAL:HG22	2.38	0.43
1:E:120:HIS:O	1:E:121:PRO:C	2.56	0.43
1:C:156:LEU:HD12	1:C:157:CYS:N	2.32	0.43
1:I:299:THR:HG22	1:J:254:GLN:HB2	1.99	0.43
1:H:123:LEU:HD23	1:H:147:ILE:CD1	2.48	0.43
1:B:117:ILE:HD12	1:C:260:LEU:CD2	2.49	0.43
1:I:23:SER:O	1:I:24:THR:C	2.56	0.43
1:G:155:GLN:HB3	1:G:304:ILE:CG2	2.49	0.43
1:K:29:THR:HB	1:K:378:LYS:HG2	2.00	0.43
1:C:42:LEU:HB3	1:C:447:TRP:HZ2	1.83	0.43
1:L:49:TYR:HA	1:L:223:ASP:HB3	2.01	0.43
1:D:340:MET:SD	1:E:169:TRP:CD1	3.12	0.43
1:J:324:SER:O	1:J:325:ASN:HB2	2.18	0.43
1:N:167:GLU:O	1:N:167:GLU:HG3	2.19	0.43
1:F:39:SER:OG	1:F:42:LEU:HD11	2.18	0.43
1:B:126:LEU:HB3	1:B:262:ASN:HB3	2.01	0.43
1:L:87:ASP:O	1:L:90:PHE:CE1	2.72	0.43
1:A:117:ILE:HG21	1:B:291:PRO:HD3	2.01	0.43
1:L:46:GLY:O	1:L:363:ARG:HD3	2.19	0.43
1:E:237:MET:CG	1:E:245:MET:HG2	2.47	0.43
1:M:149:MET:HE1	1:M:205:PHE:HZ	1.83	0.43
1:H:361:TYR:CE2	1:I:268:GLY:HA3	2.54	0.43
1:L:180:VAL:HG12	1:L:184:GLU:HB2	2.00	0.43
1:N:181:LYS:H	1:N:181:LYS:HD3	1.83	0.43
1:A:78:PRO:HG2	1:A:100:TRP:HE1	1.84	0.43
1:I:465:GLY:O	1:I:468:PHE:HB3	2.18	0.43
1:N:340:MET:HB2	1:O:208:MET:SD	2.58	0.43
1:O:257:VAL:HG13	1:O:291:PRO:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:PRO:HB2	1:G:284:LEU:HD11	2.01	0.43
1:A:311:LEU:CD2	1:A:311:LEU:H	2.13	0.43
1:B:284:LEU:HA	1:B:285:PRO:HD2	1.80	0.43
1:K:289:TYR:CE1	1:O:119:GLY:HA3	2.53	0.43
1:B:342:VAL:CG2	1:B:361:TYR:HB2	2.49	0.43
1:L:34:TYR:CD1	1:L:34:TYR:N	2.87	0.43
1:K:211:THR:HG23	1:K:226:SER:CA	2.48	0.43
1:N:117:ILE:CG2	1:N:117:ILE:O	2.64	0.43
1:M:155:GLN:HB3	1:M:304:ILE:HG21	2.00	0.43
1:K:361:TYR:CG	1:L:185:CYS:HB2	2.53	0.43
1:K:342:VAL:HG21	1:L:185:CYS:SG	2.58	0.43
1:B:79:ASP:C	1:B:81:ASN:H	2.22	0.43
1:D:74:ARG:HG3	1:D:328:PHE:CZ	2.53	0.43
1:K:114:GLY:C	1:K:115:VAL:HG13	2.38	0.43
1:B:442:LYS:O	1:B:442:LYS:CG	2.67	0.43
1:N:207:ALA:CA	1:N:229:CYS:O	2.67	0.43
1:I:284:LEU:HA	1:I:285:PRO:HD2	1.82	0.43
1:N:42:LEU:HB3	1:N:447:TRP:CZ2	2.53	0.43
1:L:327:LEU:HA	1:L:327:LEU:HD23	1.59	0.43
1:F:117:ILE:CG2	1:F:117:ILE:O	2.65	0.43
1:N:359:LYS:HB3	1:N:359:LYS:CD	2.47	0.43
1:I:336:ARG:O	1:I:338:THR:N	2.51	0.43
1:N:120:HIS:O	1:N:146:CYS:HA	2.18	0.43
1:E:79:ASP:O	1:E:81:ASN:N	2.52	0.43
1:I:67:GLY:H	1:I:364:HIS:CE1	2.37	0.43
1:H:122:LEU:O	1:H:218:SER:HB3	2.18	0.43
1:L:246:LEU:C	1:L:246:LEU:HD12	2.38	0.43
1:C:149:MET:HE1	1:C:205:PHE:HZ	1.84	0.43
1:E:237:MET:HG2	1:E:245:MET:SD	2.59	0.43
1:F:106:GLU:HG2	1:F:308:PRO:CA	2.49	0.43
1:I:327:LEU:HD11	1:I:374:PHE:HE2	1.82	0.43
1:N:43:LEU:HD23	1:N:367:GLU:HG3	2.00	0.43
1:L:185:CYS:HA	1:L:186:PRO:HD2	1.87	0.43
1:G:42:LEU:HB3	1:G:447:TRP:HZ2	1.83	0.43
1:M:343:CYS:H	1:N:214:GLN:HA	1.84	0.43
1:N:216:ASN:O	1:N:217:LYS:HG2	2.19	0.43
1:I:33:ILE:HB	1:I:376:LEU:HB2	2.01	0.43
1:A:165:ILE:HD13	1:A:236:LYS:HD3	1.99	0.43
1:J:35:TYR:CE2	1:J:457:ALA:HB2	2.54	0.43
1:I:278:LYS:HD3	1:I:278:LYS:HA	1.87	0.43
1:H:310:TRP:NE1	1:H:471:GLN:HG3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ASN:O	1:C:132:SER:O	2.36	0.43
1:K:110:GLY:O	1:K:111:GLN:HB2	2.19	0.43
1:B:161:CYS:SG	1:B:244:ASP:HB3	2.59	0.43
1:C:372:PHE:CB	1:C:374:PHE:CE1	3.02	0.43
1:I:53:LYS:HB2	1:I:59:LYS:O	2.19	0.43
1:L:298:VAL:CG1	1:L:335:THR:HA	2.49	0.43
1:C:109:ARG:HB2	1:C:336:ARG:CZ	2.48	0.43
1:N:124:ASN:HD22	1:N:263:ARG:CD	2.32	0.43
1:F:124:ASN:HD21	1:F:263:ARG:HB3	1.83	0.43
1:H:35:TYR:CD2	1:H:456:SER:O	2.72	0.43
1:C:22:VAL:CG1	1:C:26:GLU:HG3	2.49	0.43
1:F:153:GLN:O	1:F:253:GLU:HA	2.18	0.43
1:A:101:ALA:HA	1:A:320:GLY:O	2.18	0.43
1:O:70:TYR:OH	1:O:232:PRO:HD3	2.19	0.43
1:F:220:VAL:CG1	1:F:224:ILE:HD11	2.47	0.43
1:C:262:ASN:HA	1:C:262:ASN:HD22	1.26	0.43
1:N:157:CYS:O	1:N:249:TYR:HA	2.19	0.43
1:E:358:PHE:N	1:E:358:PHE:CD1	2.87	0.43
1:J:342:VAL:CG2	1:J:361:TYR:HB2	2.49	0.43
1:F:284:LEU:HA	1:F:284:LEU:HD12	1.69	0.43
1:C:72:VAL:HG21	1:C:195:LEU:O	2.19	0.43
1:J:139:SER:HB2	1:J:143:ASN:ND2	2.34	0.43
1:J:54:LYS:HZ3	1:J:55:GLN:N	2.16	0.43
1:O:91:TYR:HD1	1:O:96:GLN:NE2	2.17	0.43
1:B:222:LEU:CD2	1:B:222:LEU:N	2.80	0.43
1:N:232:PRO:HB2	1:N:234:TYR:CZ	2.54	0.43
1:L:71:ARG:N	1:L:331:VAL:O	2.52	0.43
1:G:122:LEU:O	1:G:218:SER:HB3	2.19	0.43
1:A:71:ARG:HD3	1:A:71:ARG:HA	1.75	0.43
1:O:114:GLY:N	1:O:335:THR:O	2.44	0.43
1:O:103:THR:HB	1:O:373:ILE:O	2.19	0.43
1:M:220:VAL:O	1:M:221:PRO:C	2.56	0.43
1:B:29:THR:HG22	1:B:30:ARG:O	2.19	0.43
1:F:70:TYR:CE2	1:F:195:LEU:HD22	2.54	0.43
1:F:238:VAL:HG12	1:J:463:PRO:HG3	2.01	0.43
1:O:71:ARG:HG3	1:O:368:TYR:CZ	2.53	0.43
1:A:361:TYR:CD1	1:B:185:CYS:HB2	2.54	0.43
1:B:210:PHE:HE1	1:B:229:CYS:HG	1.66	0.43
1:J:371:GLN:HB2	1:J:464:LEU:HD12	2.01	0.43
1:K:312:GLN:HG3	1:K:313:ARG:H	1.84	0.43
1:G:389:ILE:O	1:G:392:MET:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ASN:N	1:A:133:ASN:HD22	2.17	0.43
1:I:59:LYS:HB3	1:I:59:LYS:HE2	1.77	0.42
1:A:296:SER:HB2	1:E:297:MET:CE	2.49	0.42
1:L:395:SER:O	1:L:396:ILE:C	2.57	0.42
1:A:311:LEU:N	1:A:311:LEU:HD23	2.21	0.42
1:H:120:HIS:HA	1:H:121:PRO:HD3	1.85	0.42
1:K:269:GLU:HG3	1:O:361:TYR:CD2	2.54	0.42
1:H:459:LEU:O	1:H:461:GLN:N	2.52	0.42
1:A:470:LEU:O	1:A:471:GLN:C	2.58	0.42
1:E:469:LEU:HD23	1:E:469:LEU:HA	1.56	0.42
1:E:210:PHE:CD1	1:E:210:PHE:N	2.87	0.42
1:K:145:GLU:OE1	1:L:132:SER:HB3	2.18	0.42
1:A:125:LYS:C	1:A:125:LYS:CD	2.86	0.42
1:G:263:ARG:HG2	1:G:290:PHE:CD2	2.54	0.42
1:C:117:ILE:HD13	1:D:289:TYR:HB3	2.01	0.42
1:B:237:MET:HB2	1:B:246:LEU:HD21	2.01	0.42
1:I:311:LEU:N	1:I:311:LEU:HD23	2.33	0.42
1:A:147:ILE:HD13	1:A:147:ILE:HG21	1.86	0.42
1:L:34:TYR:CD2	1:L:375:GLN:HB2	2.55	0.42
1:F:97:ARG:C	1:F:98:LEU:HG	2.40	0.42
1:C:188:LEU:CD2	1:C:188:LEU:N	2.80	0.42
1:C:181:LYS:CD	1:C:181:LYS:N	2.82	0.42
1:K:79:ASP:OD1	1:K:81:ASN:ND2	2.46	0.42
1:D:29:THR:HB	1:D:378:LYS:HG3	2.01	0.42
1:E:308:PRO:O	1:E:308:PRO:CG	2.67	0.42
1:A:209:ASP:O	1:A:213:LEU:HB2	2.20	0.42
1:M:370:LEU:HB3	1:M:372:PHE:CE1	2.54	0.42
1:A:255:MET:CE	1:A:293:PRO:HB3	2.50	0.42
1:N:103:THR:N	1:N:373:ILE:O	2.49	0.42
1:C:284:LEU:HA	1:C:284:LEU:HD12	1.63	0.42
1:K:142:ASP:OD2	1:K:144:ARG:HG3	2.19	0.42
1:K:85:PHE:CB	1:K:88:THR:OG1	2.60	0.42
1:I:22:VAL:CG1	1:I:23:SER:N	2.81	0.42
1:H:22:VAL:HG12	1:H:23:SER:H	1.78	0.42
1:M:340:MET:HB2	1:N:208:MET:SD	2.59	0.42
1:G:71:ARG:HD3	1:G:71:ARG:HA	1.43	0.42
1:M:181:LYS:CD	1:M:181:LYS:H	2.30	0.42
1:E:342:VAL:CG2	1:E:361:TYR:HB2	2.49	0.42
1:D:92:ASP:HB2	1:H:384:ASP:OD2	2.19	0.42
1:M:235:LEU:HA	1:M:235:LEU:HD23	1.80	0.42
1:B:70:TYR:OH	1:B:232:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:463:PRO:O	1:K:467:LYS:HG3	2.19	0.42
1:N:189:GLU:HG2	1:N:191:LEU:HD23	2.01	0.42
1:M:463:PRO:O	1:M:464:LEU:C	2.57	0.42
1:K:298:VAL:CG1	1:K:335:THR:HA	2.49	0.42
1:E:255:MET:HG2	1:E:256:PHE:H	1.78	0.42
1:G:157:CYS:HB2	1:G:305:PHE:HE2	1.84	0.42
1:O:23:SER:O	1:O:26:GLU:HB2	2.18	0.42
1:N:54:LYS:HZ2	1:N:56:ASP:H	1.68	0.42
1:H:22:VAL:HG11	1:H:26:GLU:HG3	2.01	0.42
1:K:153:GLN:O	1:K:253:GLU:HA	2.19	0.42
1:E:125:LYS:HE3	1:E:147:ILE:HD11	2.01	0.42
1:D:370:LEU:HB3	1:D:372:PHE:HZ	1.83	0.42
1:K:246:LEU:HD12	1:K:246:LEU:C	2.39	0.42
1:M:331:VAL:HG11	1:M:368:TYR:CE2	2.50	0.42
1:F:138:ASN:ND2	1:F:283:THR:OG1	2.35	0.42
1:H:181:LYS:H	1:H:181:LYS:CD	2.31	0.42
1:L:50:TYR:HE2	1:M:271:VAL:HG22	1.83	0.42
1:F:92:ASP:HA	1:F:93:PRO:HD2	1.90	0.42
1:K:458:ASP:O	1:K:462:PHE:CE1	2.72	0.42
1:M:459:LEU:O	1:M:460:ASP:C	2.57	0.42
1:H:242:TYR:CZ	1:H:392:MET:HG3	2.54	0.42
1:L:459:LEU:H	1:L:459:LEU:HG	1.51	0.42
1:I:238:VAL:O	1:I:238:VAL:CG1	2.66	0.42
1:A:373:ILE:O	1:A:373:ILE:HG22	2.17	0.42
1:B:138:ASN:HD21	1:B:283:THR:HB	1.85	0.42
1:F:285:PRO:HG2	1:J:121:PRO:HB3	2.02	0.42
1:N:342:VAL:HG22	1:N:361:TYR:HB2	2.00	0.42
1:A:255:MET:HE3	1:A:293:PRO:HB3	2.01	0.42
1:L:114:GLY:N	1:L:335:THR:O	2.45	0.42
1:C:109:ARG:HB3	1:C:109:ARG:CZ	2.47	0.42
1:N:124:ASN:HD22	1:N:263:ARG:HD3	1.84	0.42
1:J:79:ASP:C	1:J:81:ASN:H	2.23	0.42
1:H:146:CYS:O	1:H:147:ILE:HG13	2.18	0.42
1:H:312:GLN:HG2	1:H:312:GLN:H	1.68	0.42
1:B:165:ILE:HG23	1:B:245:MET:SD	2.59	0.42
1:A:141:THR:HG22	1:A:142:ASP:N	2.33	0.42
1:N:79:ASP:C	1:N:81:ASN:H	2.23	0.42
1:E:156:LEU:HD21	1:E:332:VAL:HB	2.00	0.42
1:H:162:ARG:HG3	1:H:244:ASP:HB3	2.02	0.42
1:B:125:LYS:C	1:B:125:LYS:HD3	2.40	0.42
1:M:165:ILE:HD13	1:M:236:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:GLU:HG2	1:B:242:TYR:H	1.85	0.42
1:D:21:VAL:C	1:D:22:VAL:HG23	2.39	0.42
1:M:71:ARG:HD3	1:M:71:ARG:HA	1.84	0.42
1:F:215:ALA:C	1:F:217:LYS:H	2.23	0.42
1:A:355:ASN:ND2	1:B:264:ALA:HB1	2.35	0.42
1:A:459:LEU:HD12	1:A:469:LEU:HD21	2.01	0.42
1:L:75:VAL:HB	1:L:327:LEU:HB2	2.01	0.42
1:B:232:PRO:O	1:B:234:TYR:N	2.52	0.42
1:F:141:THR:HG22	1:F:142:ASP:N	2.34	0.42
1:E:323:TRP:O	1:E:324:SER:HB2	2.20	0.42
1:N:115:VAL:H	1:N:338:THR:HG23	1.85	0.42
1:F:237:MET:HB3	1:F:245:MET:HG2	2.01	0.42
1:H:54:LYS:CB	1:H:57:SER:HB3	2.49	0.42
1:K:321:ILE:HG21	1:K:323:TRP:CZ2	2.55	0.42
1:K:256:PHE:CD2	1:O:297:MET:HE2	2.54	0.42
1:B:54:LYS:NZ	1:B:55:GLN:HB3	2.34	0.42
1:O:240:GLU:OE2	1:O:245:MET:HB2	2.19	0.42
1:A:327:LEU:HA	1:A:327:LEU:HD23	1.53	0.42
1:C:161:CYS:SG	1:C:244:ASP:HB3	2.60	0.42
1:N:158:LEU:HD23	1:N:249:TYR:HB2	2.01	0.42
1:C:364:HIS:NE2	1:C:366:GLU:OE1	2.52	0.42
1:O:233:ASP:CG	1:O:236:LYS:HB2	2.40	0.42
1:D:384:ASP:OD2	1:H:92:ASP:HB2	2.19	0.42
1:K:214:GLN:HA	1:O:343:CYS:HB3	2.02	0.42
1:L:346:VAL:O	1:L:346:VAL:HG12	2.19	0.42
1:N:343:CYS:SG	1:N:360:GLU:OE2	2.78	0.42
1:L:392:MET:CG	1:L:392:MET:CE	2.94	0.42
1:A:257:VAL:CG2	1:E:115:VAL:HG21	2.26	0.42
1:N:372:PHE:C	1:N:373:ILE:HG13	2.40	0.42
1:D:304:ILE:HG23	1:D:305:PHE:CE2	2.55	0.42
1:H:54:LYS:NZ	1:H:55:GLN:H	2.18	0.42
1:G:255:MET:CG	1:G:256:PHE:N	2.81	0.42
1:A:158:LEU:C	1:A:159:ILE:HD13	2.39	0.42
1:E:339:ASN:ND2	1:E:364:HIS:CB	2.80	0.42
1:O:271:VAL:HA	1:O:272:PRO:HD3	1.77	0.42
1:G:24:THR:C	1:G:26:GLU:N	2.73	0.42
1:L:244:ASP:O	1:L:245:MET:C	2.58	0.42
1:G:342:VAL:HG23	1:G:361:TYR:HB2	1.99	0.42
1:J:258:ARG:HG3	1:J:259:HIS:ND1	2.35	0.42
1:A:224:ILE:HG13	1:A:225:CYS:N	2.34	0.42
1:N:71:ARG:HA	1:N:71:ARG:HD3	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:ASP:OD2	1:J:144:ARG:HG3	2.19	0.42
1:E:327:LEU:HD11	1:E:374:PHE:HE2	1.84	0.42
1:N:327:LEU:HD23	1:N:327:LEU:HA	1.72	0.42
1:O:32:ASN:HA	1:O:32:ASN:HD22	1.48	0.42
1:O:323:TRP:HE1	1:O:392:MET:HE1	1.85	0.42
1:E:175:SER:O	1:E:177:ALA:N	2.52	0.42
1:B:85:PHE:HB2	1:B:88:THR:OG1	2.19	0.42
1:I:314:ALA:HB2	1:I:319:ASN:HA	2.00	0.42
1:I:30:ARG:HB3	1:I:375:GLN:NE2	2.34	0.42
1:F:310:TRP:NE1	1:F:471:GLN:HG3	2.34	0.42
1:O:73:PHE:CD1	1:O:370:LEU:HD11	2.55	0.42
1:O:370:LEU:HD23	1:O:370:LEU:HA	1.71	0.42
1:H:210:PHE:CD1	1:H:210:PHE:N	2.86	0.42
1:C:37:ALA:HB3	1:C:374:PHE:HE1	1.85	0.42
1:I:303:GLN:HE22	1:I:335:THR:HG21	1.84	0.42
1:F:124:ASN:ND2	1:F:263:ARG:HB3	2.35	0.42
1:C:117:ILE:HG13	1:D:260:LEU:CD2	2.41	0.42
1:I:123:LEU:CD2	1:I:147:ILE:HB	2.50	0.42
1:K:33:ILE:HG23	1:K:33:ILE:HD12	1.82	0.42
1:B:164:PRO:HA	1:B:245:MET:HG3	2.00	0.42
1:B:237:MET:HB3	1:B:246:LEU:CD2	2.50	0.42
1:J:298:VAL:H	1:J:298:VAL:HG22	1.35	0.42
1:L:91:TYR:CE1	1:L:96:GLN:HB2	2.54	0.42
1:M:120:HIS:HA	1:M:121:PRO:HD3	1.73	0.42
1:D:71:ARG:HB3	1:D:73:PHE:CE1	2.54	0.42
1:B:228:ILE:HG21	1:B:228:ILE:HD13	1.55	0.42
1:I:159:ILE:HD12	1:I:159:ILE:HG23	1.79	0.42
1:C:460:ASP:O	1:C:460:ASP:OD2	2.37	0.42
1:G:327:LEU:HD23	1:G:327:LEU:HA	1.87	0.42
1:C:150:ASP:HB3	1:D:257:VAL:HG21	2.00	0.42
1:J:117:ILE:HD11	1:J:148:SER:CB	2.49	0.42
1:F:201:VAL:H	1:F:201:VAL:HG22	1.49	0.42
1:G:240:GLU:OE2	1:G:245:MET:HB2	2.19	0.42
1:O:122:LEU:HD13	1:O:144:ARG:NH2	2.35	0.42
1:E:70:TYR:HA	1:E:332:VAL:HG22	2.02	0.42
1:K:185:CYS:HA	1:K:186:PRO:HD2	1.80	0.42
1:H:162:ARG:HG3	1:H:244:ASP:HB2	2.02	0.42
1:K:283:THR:O	1:K:283:THR:CG2	2.63	0.42
1:E:315:GLN:NE2	1:E:316:GLY:N	2.68	0.42
1:C:54:LYS:NZ	1:C:55:GLN:HB3	2.35	0.42
1:B:364:HIS:CD2	1:B:366:GLU:OE1	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:PRO:HD3	1:C:100:TRP:CD1	2.54	0.42
1:C:162:ARG:HG3	1:C:244:ASP:CB	2.50	0.42
1:B:32:ASN:HD22	1:B:32:ASN:HA	1.59	0.42
1:F:80:PRO:HB2	1:F:98:LEU:CB	2.49	0.42
1:D:79:ASP:C	1:D:81:ASN:N	2.73	0.42
1:H:311:LEU:HD23	1:H:311:LEU:N	2.33	0.42
1:L:47:HIS:HB3	1:L:50:TYR:O	2.20	0.42
1:C:71:ARG:O	1:C:330:THR:HA	2.20	0.42
1:I:54:LYS:NZ	1:I:55:GLN:HB3	2.34	0.42
1:M:327:LEU:HD12	1:M:374:PHE:HE2	1.84	0.42
1:B:171:LYS:HE3	1:B:212:THR:O	2.20	0.42
1:I:92:ASP:HA	1:I:93:PRO:HD2	1.78	0.42
1:G:280:THR:OG1	1:G:281:THR:N	2.53	0.42
1:E:99:VAL:HG11	1:E:321:ILE:CG2	2.49	0.42
1:B:151:TYR:CE1	1:B:203:THR:HG21	2.55	0.42
1:N:123:LEU:CD2	1:N:147:ILE:HB	2.50	0.42
1:K:167:GLU:HG2	1:K:231:TYR:O	2.20	0.42
1:L:71:ARG:HA	1:L:71:ARG:HD3	1.67	0.42
1:L:152:LYS:HA	1:L:255:MET:HB2	2.02	0.42
1:K:464:LEU:HA	1:K:464:LEU:HD23	1.73	0.42
1:F:461:GLN:HB3	1:F:461:GLN:HE21	1.62	0.42
1:L:216:ASN:N	1:L:216:ASN:OD1	2.51	0.42
1:M:142:ASP:OD2	1:M:144:ARG:NE	2.53	0.42
1:I:390:HIS:O	1:I:394:PRO:HD3	2.20	0.42
1:D:393:ASN:HB3	1:D:396:ILE:HG13	2.02	0.42
1:L:102:CYS:SG	1:L:103:THR:N	2.93	0.42
1:A:342:VAL:CG2	1:A:361:TYR:HB2	2.50	0.42
1:A:165:ILE:O	1:A:237:MET:CE	2.68	0.42
1:A:383:ALA:HB3	1:F:92:ASP:CG	2.41	0.42
1:O:284:LEU:HA	1:O:284:LEU:HD12	1.72	0.42
1:C:103:THR:HG21	1:C:468:PHE:HE1	1.85	0.42
1:I:70:TYR:OH	1:I:232:PRO:HD3	2.20	0.42
1:J:159:ILE:HG23	1:J:159:ILE:HD12	1.61	0.42
1:I:362:LEU:HA	1:I:362:LEU:HD23	1.90	0.42
1:F:30:ARG:HB3	1:F:375:GLN:HE22	1.84	0.42
1:D:127:ASP:O	1:D:129:THR:HG23	2.20	0.42
1:K:339:ASN:ND2	1:K:364:HIS:HB2	2.34	0.42
1:M:103:THR:HG21	1:M:468:PHE:CE1	2.55	0.41
1:D:68:LEU:HD13	1:D:151:TYR:HD1	1.85	0.41
1:J:284:LEU:HA	1:J:285:PRO:HD2	1.79	0.41
1:I:318:ASN:OD1	1:I:321:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:ASN:ND2	1:E:364:HIS:CG	2.87	0.41
1:I:102:CYS:HA	1:I:374:PHE:CD2	2.55	0.41
1:K:118:SER:CB	1:K:223:ASP:OD2	2.66	0.41
1:D:21:VAL:HG21	1:D:241:PRO:HB2	2.02	0.41
1:N:66:SER:OG	1:N:67:GLY:N	2.52	0.41
1:B:103:THR:HG22	1:B:103:THR:O	2.20	0.41
1:K:32:ASN:HD22	1:K:32:ASN:HA	1.52	0.41
1:O:186:PRO:HG2	1:O:186:PRO:O	2.20	0.41
1:I:379:ILE:HD12	1:I:400:TRP:HH2	1.85	0.41
1:F:323:TRP:HE1	1:F:392:MET:HE1	1.85	0.41
1:M:78:PRO:HD2	1:M:455:PHE:CE1	2.55	0.41
1:H:124:ASN:OD1	1:H:264:ALA:HB3	2.20	0.41
1:I:149:MET:CE	1:I:293:PRO:HD2	2.50	0.41
1:K:262:ASN:ND2	1:K:289:TYR:CE2	2.88	0.41
1:O:371:GLN:OE1	1:O:464:LEU:HB2	2.20	0.41
1:E:31:THR:O	1:E:33:ILE:N	2.51	0.41
1:C:461:GLN:HB2	1:C:462:PHE:CE1	2.55	0.41
1:K:311:LEU:HD23	1:K:311:LEU:H	1.85	0.41
1:A:364:HIS:HD2	1:A:365:GLY:N	2.18	0.41
1:D:471:GLN:O	1:D:472:ALA:C	2.58	0.41
1:C:468:PHE:O	1:C:472:ALA:N	2.38	0.41
1:E:138:ASN:HD21	1:E:283:THR:HB	1.86	0.41
1:F:265:GLY:HA2	1:J:355:ASN:HB3	2.02	0.41
1:G:103:THR:HG21	1:G:468:PHE:HE1	1.84	0.41
1:K:315:GLN:CD	1:K:316:GLY:N	2.74	0.41
1:F:393:ASN:C	1:F:393:ASN:HD22	2.22	0.41
1:O:250:LEU:CB	1:O:304:ILE:HD11	2.49	0.41
1:D:121:PRO:CB	1:E:285:PRO:HG2	2.41	0.41
1:A:393:ASN:HB3	1:A:396:ILE:HD12	2.03	0.41
1:F:240:GLU:CG	1:F:241:PRO:HD2	2.50	0.41
1:L:361:TYR:CE2	1:M:268:GLY:HA3	2.55	0.41
1:G:464:LEU:O	1:G:465:GLY:C	2.59	0.41
1:D:327:LEU:HD23	1:D:327:LEU:HA	1.59	0.41
1:H:76:LYS:O	1:H:451:LEU:HB2	2.20	0.41
1:C:151:TYR:CD2	1:C:203:THR:HB	2.56	0.41
1:I:202:ASP:HA	1:I:229:CYS:HB3	2.01	0.41
1:K:339:ASN:HD22	1:K:364:HIS:HB2	1.84	0.41
1:N:109:ARG:NH1	1:N:109:ARG:HB3	2.35	0.41
1:I:98:LEU:HA	1:I:377:CYS:O	2.20	0.41
1:G:235:LEU:HA	1:G:235:LEU:HD23	1.83	0.41
1:D:119:GLY:HA3	1:E:289:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:LEU:O	1:D:218:SER:HB3	2.20	0.41
1:A:296:SER:HB2	1:E:297:MET:HE2	2.02	0.41
1:I:336:ARG:CG	1:I:336:ARG:HH11	2.33	0.41
1:N:373:ILE:HD11	1:N:464:LEU:HD22	2.01	0.41
1:K:109:ARG:H	1:K:306:ASN:ND2	2.18	0.41
1:I:302:ALA:O	1:I:303:GLN:C	2.58	0.41
1:F:297:MET:HE1	1:G:296:SER:HB2	2.03	0.41
1:E:339:ASN:HD22	1:E:364:HIS:CB	2.27	0.41
1:O:119:GLY:CA	1:O:148:SER:HA	2.51	0.41
1:J:146:CYS:C	1:J:147:ILE:HG13	2.41	0.41
1:M:165:ILE:CD1	1:M:236:LYS:HD3	2.51	0.41
1:N:155:GLN:HA	1:N:332:VAL:O	2.20	0.41
1:E:102:CYS:N	1:E:320:GLY:O	2.51	0.41
1:F:220:VAL:CG1	1:F:224:ILE:CD1	2.98	0.41
1:L:97:ARG:CG	1:L:381:LEU:HD11	2.49	0.41
1:L:22:VAL:HG12	1:L:23:SER:N	2.34	0.41
1:I:458:ASP:O	1:I:462:PHE:HE1	2.02	0.41
1:N:207:ALA:HB1	1:N:229:CYS:O	2.21	0.41
1:E:181:LYS:N	1:E:181:LYS:HD3	2.35	0.41
1:D:315:GLN:HB2	1:D:315:GLN:HE21	1.57	0.41
1:E:249:TYR:N	1:E:249:TYR:CD2	2.88	0.41
1:G:343:CYS:SG	1:G:358:PHE:HB3	2.60	0.41
1:B:196:GLN:O	1:B:199:ASP:OD2	2.39	0.41
1:G:311:LEU:HD23	1:G:311:LEU:H	1.85	0.41
1:I:109:ARG:HH11	1:I:109:ARG:HD2	1.60	0.41
1:A:64:LYS:CG	1:A:64:LYS:O	2.69	0.41
1:D:124:ASN:N	1:D:218:SER:O	2.53	0.41
1:C:31:THR:CB	1:C:31:THR:C	2.76	0.41
1:O:250:LEU:HB2	1:O:304:ILE:HD11	2.01	0.41
1:N:47:HIS:O	1:N:64:LYS:HA	2.21	0.41
1:F:201:VAL:HG11	1:F:332:VAL:HG11	2.02	0.41
1:A:142:ASP:OD2	1:A:144:ARG:NE	2.53	0.41
1:B:54:LYS:HZ3	1:B:55:GLN:CB	2.32	0.41
1:L:103:THR:CG2	1:L:103:THR:O	2.68	0.41
1:N:181:LYS:CD	1:N:181:LYS:N	2.84	0.41
1:M:57:SER:OG	1:M:58:ASN:N	2.53	0.41
1:H:119:GLY:HA3	1:H:148:SER:HA	2.02	0.41
1:A:54:LYS:HD2	1:A:55:GLN:H	1.86	0.41
1:F:262:ASN:HD22	1:F:262:ASN:HA	1.35	0.41
1:I:97:ARG:O	1:I:98:LEU:HD23	2.21	0.41
1:K:47:HIS:ND1	1:K:48:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:92:ASP:OD2	1:O:94:ALA:HB3	2.21	0.41
1:E:71:ARG:HD3	1:E:197:ASP:OD1	2.21	0.41
1:M:242:TYR:CZ	1:M:392:MET:HB2	2.55	0.41
1:C:120:HIS:HA	1:C:121:PRO:HD3	1.96	0.41
1:B:152:LYS:HG3	1:B:255:MET:HB2	2.02	0.41
1:I:298:VAL:C	1:I:299:THR:HG23	2.41	0.41
1:B:111:GLN:NE2	1:B:367:GLU:OE1	2.45	0.41
1:F:261:PHE:O	1:F:289:TYR:HA	2.21	0.41
1:C:22:VAL:HG12	1:C:23:SER:H	1.80	0.41
1:F:251:ARG:NH1	1:F:251:ARG:CG	2.78	0.41
1:F:152:LYS:HA	1:F:255:MET:HB2	2.02	0.41
1:K:97:ARG:HG3	1:K:400:TRP:CD2	2.56	0.41
1:A:124:ASN:OD1	1:A:264:ALA:HB3	2.21	0.41
1:G:149:MET:CE	1:G:293:PRO:HD2	2.49	0.41
1:O:116:GLY:C	1:O:117:ILE:HG22	2.39	0.41
1:A:300:SER:HG	1:B:253:GLU:HG2	1.84	0.41
1:K:296:SER:HB2	1:O:297:MET:CE	2.50	0.41
1:H:298:VAL:CG1	1:H:335:THR:HA	2.47	0.41
1:D:109:ARG:HD2	1:D:109:ARG:HH11	1.68	0.41
1:F:22:VAL:HG12	1:F:23:SER:H	1.85	0.41
1:E:181:LYS:CD	1:E:181:LYS:H	2.34	0.41
1:A:80:PRO:HD2	1:A:325:ASN:OD1	2.20	0.41
1:H:80:PRO:HD2	1:H:325:ASN:OD1	2.21	0.41
1:J:389:ILE:O	1:J:392:MET:HB3	2.21	0.41
1:O:327:LEU:HD12	1:O:374:PHE:HE2	1.86	0.41
1:F:192:ASN:C	1:F:193:THR:HG22	2.40	0.41
1:O:330:THR:O	1:O:331:VAL:HG23	2.21	0.41
1:O:467:LYS:O	1:O:468:PHE:C	2.58	0.41
1:L:159:ILE:HG23	1:L:159:ILE:HD12	1.68	0.41
1:D:120:HIS:CE1	1:D:122:LEU:O	2.74	0.41
1:L:467:LYS:CD	1:L:467:LYS:HB2	2.50	0.41
1:A:126:LEU:HA	1:A:126:LEU:HD12	1.84	0.41
1:C:258:ARG:HB3	1:C:292:THR:HG22	2.02	0.41
1:F:156:LEU:O	1:F:157:CYS:HB2	2.20	0.41
1:F:297:MET:HE2	1:G:256:PHE:HD2	1.86	0.41
1:O:102:CYS:O	1:O:311:LEU:CD1	2.69	0.41
1:M:162:ARG:HG3	1:M:244:ASP:HB3	2.01	0.41
1:H:29:THR:HB	1:H:378:LYS:HG2	2.03	0.41
1:O:395:SER:O	1:O:396:ILE:C	2.58	0.41
1:H:201:VAL:HG11	1:H:332:VAL:HG11	2.02	0.41
1:E:101:ALA:CA	1:E:320:GLY:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:VAL:HG23	1:A:225:CYS:HA	2.01	0.41
1:L:353:TYR:CE2	1:M:144:ARG:HD3	2.55	0.41
1:M:123:LEU:CD2	1:M:147:ILE:HB	2.51	0.41
1:N:298:VAL:H	1:N:298:VAL:HG22	1.43	0.41
1:F:234:TYR:O	1:F:238:VAL:CG2	2.68	0.41
1:C:83:PHE:HD2	1:C:85:PHE:CZ	2.38	0.41
1:C:363:ARG:HA	1:C:363:ARG:HD3	1.73	0.41
1:L:144:ARG:NH2	1:M:279:GLY:HA3	2.34	0.41
1:G:216:ASN:O	1:H:277:ILE:HD12	2.20	0.41
1:H:450:ASP:OD1	1:H:452:LYS:HG3	2.20	0.41
1:E:459:LEU:HD23	1:E:459:LEU:N	2.36	0.41
1:N:32:ASN:HA	1:N:32:ASN:HD22	1.57	0.41
1:L:116:GLY:N	1:L:337:SER:OG	2.50	0.41
1:A:24:THR:HG23	1:A:318:ASN:HA	2.02	0.41
1:A:248:PHE:O	1:A:249:TYR:HB3	2.21	0.41
1:J:136:VAL:O	1:J:137:GLY:O	2.39	0.41
1:H:77:LEU:HD22	1:H:455:PHE:HZ	1.85	0.41
1:F:123:LEU:HA	1:F:218:SER:O	2.20	0.41
1:M:228:ILE:HD13	1:M:228:ILE:HG21	1.67	0.41
1:A:371:GLN:CB	1:A:464:LEU:HD12	2.41	0.41
1:E:153:GLN:O	1:E:253:GLU:HA	2.20	0.41
1:F:162:ARG:O	1:F:163:PRO:C	2.58	0.41
1:G:298:VAL:O	1:H:254:GLN:HA	2.19	0.41
1:J:85:PHE:HB2	1:J:88:THR:HG23	2.02	0.41
1:E:54:LYS:HZ2	1:E:56:ASP:H	1.68	0.41
1:C:149:MET:CE	1:C:205:PHE:CE1	3.04	0.41
1:F:154:THR:O	1:F:155:GLN:HG3	2.20	0.41
1:F:152:LYS:HZ3	1:J:112:PRO:HB2	1.85	0.41
1:I:120:HIS:HB3	1:I:123:LEU:HB2	2.02	0.41
1:O:54:LYS:NZ	1:O:56:ASP:H	2.19	0.41
1:C:240:GLU:HG2	1:C:241:PRO:HD2	2.02	0.41
1:B:364:HIS:HD2	1:B:365:GLY:H	1.68	0.41
1:O:72:VAL:HG21	1:O:195:LEU:C	2.41	0.41
1:M:54:LYS:HD2	1:M:55:GLN:N	2.35	0.41
1:K:139:SER:HB2	1:K:143:ASN:ND2	2.34	0.41
1:G:312:GLN:HG3	1:G:313:ARG:N	2.36	0.41
1:K:312:GLN:HG3	1:K:313:ARG:N	2.36	0.41
1:F:30:ARG:HB3	1:F:375:GLN:NE2	2.36	0.41
1:B:53:LYS:HB3	1:B:53:LYS:HE2	1.72	0.41
1:N:314:ALA:N	1:N:319:ASN:OD1	2.52	0.41
1:B:261:PHE:HB2	1:B:290:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:LEU:HD23	1:D:275:LEU:HA	1.93	0.41
1:H:127:ASP:N	1:H:127:ASP:OD1	2.54	0.41
1:A:155:GLN:HB2	1:A:252:ARG:HB3	2.03	0.41
1:C:150:ASP:CB	1:D:257:VAL:HG21	2.51	0.41
1:B:112:PRO:C	1:B:113:LEU:O	2.55	0.41
1:J:231:TYR:HD2	1:J:232:PRO:O	2.04	0.41
1:H:120:HIS:ND1	1:H:122:LEU:N	2.68	0.41
1:K:234:TYR:O	1:K:238:VAL:CG2	2.61	0.41
1:A:392:MET:HB3	1:A:393:ASN:H	1.74	0.41
1:G:296:SER:OG	1:G:297:MET:N	2.50	0.41
1:I:23:SER:C	1:I:25:ASP:N	2.70	0.41
1:G:258:ARG:C	1:G:259:HIS:ND1	2.73	0.41
1:H:21:VAL:C	1:H:22:VAL:HG23	2.39	0.41
1:H:118:SER:O	1:H:149:MET:N	2.54	0.41
1:B:361:TYR:CE2	1:C:268:GLY:HA3	2.55	0.41
1:E:33:ILE:HD11	1:E:87:ASP:OD2	2.21	0.41
1:G:22:VAL:HG12	1:G:23:SER:N	2.35	0.41
1:O:33:ILE:CG2	1:O:35:TYR:HE1	2.34	0.41
1:D:109:ARG:NH1	1:D:367:GLU:O	2.53	0.41
1:L:126:LEU:CB	1:L:262:ASN:O	2.69	0.41
1:B:52:ILE:HD12	1:B:62:VAL:HB	2.03	0.41
1:L:212:THR:OG1	1:L:213:LEU:HD13	2.21	0.41
1:C:233:ASP:C	1:C:233:ASP:OD1	2.59	0.41
1:H:102:CYS:O	1:H:311:LEU:HD11	2.21	0.41
1:N:28:VAL:HG22	1:N:379:ILE:CD1	2.51	0.41
1:O:258:ARG:HH11	1:O:258:ARG:HD2	1.70	0.41
1:B:295:GLY:O	1:B:296:SER:CB	2.69	0.41
1:C:159:ILE:HD12	1:C:159:ILE:HG23	1.79	0.41
1:F:381:LEU:CD2	1:F:397:LEU:HD21	2.51	0.41
1:O:323:TRP:HE1	1:O:392:MET:CE	2.34	0.41
1:C:384:ASP:OD2	1:I:92:ASP:HB2	2.21	0.41
1:E:71:ARG:O	1:E:330:THR:HA	2.21	0.41
1:A:24:THR:CG2	1:A:318:ASN:HA	2.50	0.41
1:H:77:LEU:HD22	1:H:455:PHE:CZ	2.56	0.41
1:L:190:LEU:HA	1:L:190:LEU:HD12	1.87	0.41
1:N:362:LEU:HA	1:N:362:LEU:HD23	1.52	0.41
1:G:138:ASN:C	1:G:139:SER:O	2.58	0.41
1:I:169:TRP:CZ2	1:I:190:LEU:HD13	2.56	0.41
1:B:87:ASP:O	1:B:90:PHE:CZ	2.74	0.41
1:A:23:SER:O	1:A:26:GLU:HB2	2.21	0.41
1:A:312:GLN:H	1:A:312:GLN:HG2	1.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:133:ASN:HD22	1:N:133:ASN:N	2.18	0.41
1:B:315:GLN:HE21	1:B:315:GLN:HB2	1.49	0.41
1:G:34:TYR:N	1:G:34:TYR:CD1	2.89	0.41
1:G:50:TYR:CD1	1:G:50:TYR:O	2.74	0.41
1:M:355:ASN:HB3	1:N:265:GLY:HA2	2.03	0.41
1:D:146:CYS:O	1:D:147:ILE:HG13	2.21	0.41
1:B:278:LYS:O	1:E:352:THR:HA	2.21	0.41
1:D:248:PHE:O	1:D:249:TYR:HB3	2.21	0.41
1:A:109:ARG:HB3	1:A:336:ARG:CZ	2.50	0.41
1:B:464:LEU:O	1:B:467:LYS:HB2	2.21	0.41
1:A:297:MET:HE2	1:B:256:PHE:CD2	2.55	0.41
1:B:68:LEU:HD13	1:B:151:TYR:HD1	1.86	0.41
1:M:97:ARG:CG	1:M:381:LEU:HD11	2.49	0.41
1:O:158:LEU:H	1:O:158:LEU:HG	1.51	0.41
1:N:250:LEU:HB2	1:N:304:ILE:CD1	2.43	0.41
1:L:246:LEU:O	1:L:315:GLN:OE1	2.39	0.41
1:K:393:ASN:HD22	1:K:394:PRO:HD2	1.86	0.41
1:L:69:GLN:HA	1:L:199:ASP:O	2.19	0.41
1:M:305:PHE:CE1	1:M:333:ASP:HB2	2.51	0.41
1:K:255:MET:HE3	1:K:293:PRO:HB3	2.02	0.41
1:L:147:ILE:HG23	1:M:129:THR:O	2.21	0.41
1:O:53:LYS:O	1:O:54:LYS:C	2.60	0.41
1:C:54:LYS:CB	1:C:57:SER:HB3	2.50	0.41
1:D:22:VAL:HG12	1:D:26:GLU:HG3	2.03	0.41
1:C:151:TYR:OH	1:C:221:PRO:HG2	2.21	0.41
1:D:340:MET:CE	1:E:169:TRP:CD1	3.04	0.41
1:D:53:LYS:HE2	1:D:53:LYS:HB3	1.95	0.41
1:B:102:CYS:HB2	1:B:327:LEU:HD11	2.03	0.41
1:O:91:TYR:CE1	1:O:96:GLN:HB2	2.55	0.41
1:H:247:PHE:HA	1:H:315:GLN:HG3	2.02	0.41
1:K:216:ASN:O	1:K:217:LYS:HG2	2.21	0.41
1:H:273:ALA:HA	1:H:276:TYR:CE2	2.56	0.41
1:M:200:MET:O	1:M:229:CYS:HA	2.20	0.41
1:A:119:GLY:O	1:A:221:PRO:HB3	2.19	0.41
1:D:123:LEU:HB3	1:D:145:GLU:O	2.21	0.40
1:C:31:THR:H	1:C:375:GLN:HE21	1.69	0.40
1:K:52:ILE:O	1:K:61:ALA:HB3	2.21	0.40
1:I:298:VAL:O	1:I:299:THR:HG22	2.20	0.40
1:K:181:LYS:HE2	1:K:184:GLU:HG3	2.01	0.40
1:L:370:LEU:HB3	1:L:372:PHE:HE1	1.86	0.40
1:M:109:ARG:HG3	1:M:305:PHE:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:HD11	1:B:233:ASP:HB3	2.03	0.40
1:A:141:THR:HA	1:E:355:ASN:OD1	2.21	0.40
1:G:119:GLY:HA2	1:G:148:SER:HA	2.03	0.40
1:F:208:MET:HE3	1:F:210:PHE:CD2	2.56	0.40
1:N:318:ASN:OD1	1:N:321:ILE:N	2.39	0.40
1:F:45:VAL:CG1	1:F:46:GLY:N	2.82	0.40
1:C:373:ILE:HG13	1:C:464:LEU:HD13	2.03	0.40
1:A:54:LYS:HB3	1:A:57:SER:HB3	2.03	0.40
1:N:235:LEU:HA	1:N:235:LEU:HD23	1.70	0.40
1:I:165:ILE:O	1:I:165:ILE:HG13	2.21	0.40
1:D:254:GLN:NE2	1:D:295:GLY:O	2.54	0.40
1:N:102:CYS:SG	1:N:311:LEU:HD21	2.61	0.40
1:C:109:ARG:CB	1:C:109:ARG:HH11	2.17	0.40
1:G:299:THR:O	1:G:300:SER:C	2.59	0.40
1:A:262:ASN:HD22	1:A:262:ASN:HA	1.50	0.40
1:L:37:ALA:HB3	1:L:372:PHE:HB2	2.03	0.40
1:O:161:CYS:SG	1:O:161:CYS:O	2.79	0.40
1:E:100:TRP:CZ3	1:E:376:LEU:HB2	2.57	0.40
1:E:393:ASN:ND2	1:E:395:SER:H	2.19	0.40
1:J:149:MET:CE	1:J:292:THR:HG23	2.50	0.40
1:F:119:GLY:CA	1:G:289:TYR:CE1	3.00	0.40
1:B:461:GLN:HE22	1:C:21:VAL:HB	1.86	0.40
1:B:79:ASP:O	1:B:81:ASN:N	2.54	0.40
1:B:469:LEU:HD23	1:B:469:LEU:HA	1.87	0.40
1:K:164:PRO:HA	1:K:245:MET:HG3	2.03	0.40
1:C:247:PHE:CE2	1:C:320:GLY:HA2	2.56	0.40
1:D:139:SER:HB2	1:D:143:ASN:HD21	1.87	0.40
1:A:69:GLN:HA	1:A:199:ASP:O	2.20	0.40
1:L:277:ILE:HG22	1:O:353:TYR:HB2	2.02	0.40
1:C:271:VAL:HA	1:C:272:PRO:HD3	1.92	0.40
1:D:118:SER:O	1:D:149:MET:N	2.53	0.40
1:I:296:SER:HB3	1:I:297:MET:H	1.60	0.40
1:I:115:VAL:HG22	1:J:255:MET:HE1	2.04	0.40
1:B:119:GLY:O	1:B:221:PRO:CA	2.69	0.40
1:K:167:GLU:O	1:K:167:GLU:CG	2.55	0.40
1:H:254:GLN:O	1:H:254:GLN:HG3	2.17	0.40
1:J:311:LEU:CG	1:J:311:LEU:O	2.66	0.40
1:I:112:PRO:CB	1:J:231:TYR:CD1	2.98	0.40
1:L:160:GLY:HA2	1:L:247:PHE:CE1	2.57	0.40
1:L:88:THR:HB	1:L:91:TYR:CD2	2.56	0.40
1:B:71:ARG:NH1	1:B:197:ASP:OD1	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:97:ARG:O	1:N:378:LYS:HA	2.21	0.40
1:J:463:PRO:HA	1:J:466:ARG:NH1	2.36	0.40
1:F:41:ARG:NH1	1:G:190:LEU:HD23	2.36	0.40
1:M:362:LEU:HA	1:M:362:LEU:HD23	1.83	0.40
1:C:220:VAL:CG1	1:C:224:ILE:HD11	2.52	0.40
1:A:36:HIS:ND1	1:A:37:ALA:N	2.69	0.40
1:E:119:GLY:CA	1:E:148:SER:HA	2.50	0.40
1:M:370:LEU:HA	1:M:370:LEU:HD23	1.97	0.40
1:J:249:TYR:C	1:J:250:LEU:HG	2.42	0.40
1:C:76:LYS:HD2	1:C:452:LYS:HZ1	1.86	0.40
1:B:152:LYS:HG3	1:B:255:MET:HB3	2.03	0.40
1:K:156:LEU:HA	1:K:250:LEU:O	2.22	0.40
1:F:321:ILE:HG23	1:F:321:ILE:HD12	1.72	0.40
1:C:283:THR:O	1:C:284:LEU:CB	2.67	0.40
1:L:372:PHE:HB3	1:L:374:PHE:CE1	2.57	0.40
1:J:124:ASN:ND2	1:J:263:ARG:HB3	2.36	0.40
1:O:311:LEU:HG	1:O:311:LEU:O	2.21	0.40
1:K:268:GLY:HA3	1:O:361:TYR:CE2	2.57	0.40
1:L:258:ARG:HB2	1:L:294:SER:CB	2.47	0.40
1:G:110:GLY:O	1:G:111:GLN:CG	2.70	0.40
1:M:123:LEU:HD23	1:M:147:ILE:HB	2.04	0.40
1:C:42:LEU:HD22	1:C:447:TRP:NE1	2.37	0.40
1:J:236:LYS:O	1:J:237:MET:C	2.57	0.40
1:H:27:TYR:CD1	1:H:28:VAL:HG23	2.56	0.40
1:C:312:GLN:H	1:C:312:GLN:HG2	1.55	0.40
1:K:114:GLY:O	1:K:115:VAL:HG12	2.21	0.40
1:K:278:LYS:HA	1:K:278:LYS:HD3	1.85	0.40
1:B:312:GLN:HG3	1:B:313:ARG:N	2.36	0.40
1:H:87:ASP:OD1	1:H:90:PHE:CZ	2.75	0.40
1:L:166:GLY:O	1:L:192:ASN:HA	2.22	0.40
1:H:343:CYS:HA	1:H:359:LYS:O	2.21	0.40
1:E:341:SER:HB3	1:E:362:LEU:HD23	2.03	0.40
1:D:222:LEU:HD22	1:D:222:LEU:H	1.86	0.40
1:D:152:LYS:CE	1:D:253:GLU:HB2	2.51	0.40
1:M:103:THR:HG21	1:M:468:PHE:HE1	1.86	0.40
1:O:220:VAL:O	1:O:225:CYS:HB3	2.21	0.40
1:J:256:PHE:CD1	1:J:257:VAL:N	2.89	0.40
1:E:54:LYS:NZ	1:E:55:GLN:H	2.19	0.40
1:L:315:GLN:CG	1:L:316:GLY:H	2.35	0.40
1:F:249:TYR:HE1	1:F:251:ARG:NH1	2.19	0.40
1:D:83:PHE:HB3	1:D:85:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:TYR:OH	1:E:232:PRO:HD3	2.22	0.40
1:G:155:GLN:OE1	1:G:304:ILE:HG22	2.22	0.40
1:E:24:THR:HG23	1:E:317:HIS:O	2.21	0.40
1:G:42:LEU:HA	1:G:42:LEU:HD23	1.85	0.40
1:E:280:THR:O	1:E:281:THR:CB	2.65	0.40
1:F:459:LEU:HA	1:F:459:LEU:HD23	1.75	0.40
1:B:87:ASP:O	1:B:90:PHE:CE1	2.74	0.40
1:D:147:ILE:HG21	1:D:147:ILE:HD13	1.90	0.40
1:I:165:ILE:HD11	1:I:236:LYS:HB3	2.04	0.40
1:E:150:ASP:CG	1:E:150:ASP:O	2.60	0.40
1:G:76:LYS:HA	1:G:76:LYS:HD3	1.90	0.40
1:H:79:ASP:OD1	1:H:81:ASN:HB2	2.22	0.40
1:G:170:GLY:HA3	1:G:191:LEU:CD1	2.52	0.40
1:K:141:THR:HA	1:O:355:ASN:OD1	2.20	0.40

There are no symmetry-related clashes.

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	413/423 (98%)	348 (84%)	52 (13%)	13 (3%)	5 32
1	B	413/423 (98%)	343 (83%)	55 (13%)	15 (4%)	4 28
1	C	413/423 (98%)	344 (83%)	47 (11%)	22 (5%)	2 17
1	D	413/423 (98%)	352 (85%)	50 (12%)	11 (3%)	6 35
1	E	413/423 (98%)	336 (81%)	64 (16%)	13 (3%)	5 32
1	F	413/423 (98%)	346 (84%)	55 (13%)	12 (3%)	6 34
1	G	413/423 (98%)	353 (86%)	46 (11%)	14 (3%)	5 29
1	H	413/423 (98%)	347 (84%)	50 (12%)	16 (4%)	4 25
1	I	413/423 (98%)	343 (83%)	53 (13%)	17 (4%)	3 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	413/423 (98%)	351 (85%)	48 (12%)	14 (3%)	5	29
1	K	413/423 (98%)	349 (84%)	49 (12%)	15 (4%)	4	28
1	L	413/423 (98%)	348 (84%)	52 (13%)	13 (3%)	5	32
1	M	413/423 (98%)	338 (82%)	60 (14%)	15 (4%)	4	28
1	N	413/423 (98%)	345 (84%)	56 (14%)	12 (3%)	6	34
1	O	413/423 (98%)	335 (81%)	59 (14%)	19 (5%)	3	21
All	All	6195/6345 (98%)	5178 (84%)	796 (13%)	221 (4%)	4	28

All (221) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	LEU
1	A	126	LEU
1	A	337	SER
1	B	177	ALA
1	B	323	TRP
1	C	215	ALA
1	C	337	SER
1	D	57	SER
1	D	139	SER
1	D	303	GLN
1	E	132	SER
1	E	337	SER
1	F	216	ASN
1	F	337	SER
1	G	176	ASN
1	G	216	ASN
1	G	284	LEU
1	G	461	GLN
1	H	83	PHE
1	H	176	ASN
1	H	337	SER
1	H	460	ASP
1	I	176	ASN
1	I	184	GLU
1	I	337	SER
1	J	83	PHE
1	J	176	ASN
1	K	139	SER
1	L	83	PHE

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Mol	Chain	Res	Type
1	L	139	SER
1	M	223	ASP
1	M	325	ASN
1	M	337	SER
1	N	461	GLN
1	O	57	SER
1	O	176	ASN
1	O	180	VAL
1	O	184	GLU
1	O	284	LEU
1	O	337	SER
1	A	137	GLY
1	A	180	VAL
1	A	284	LEU
1	A	300	SER
1	B	180	VAL
1	B	348	SER
1	C	176	ASN
1	C	177	ALA
1	C	216	ASN
1	C	278	LYS
1	D	126	LEU
1	E	32	ASN
1	E	117	ILE
1	F	57	SER
1	G	180	VAL
1	G	303	GLN
1	G	442	LYS
1	H	54	LYS
1	H	278	LYS
1	I	24	THR
1	I	126	LEU
1	I	300	SER
1	I	392	MET
1	J	137	GLY
1	L	132	SER
1	L	177	ALA
1	L	396	ILE
1	M	117	ILE
1	M	180	VAL
1	M	278	LYS
1	N	126	LEU

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Mol	Chain	Res	Type
1	N	139	SER
1	N	273	ALA
1	O	126	LEU
1	O	177	ALA
1	A	142	ASP
1	A	278	LYS
1	B	126	LEU
1	B	233	ASP
1	C	32	ASN
1	C	132	SER
1	C	184	GLU
1	C	325	ASN
1	C	460	ASP
1	C	472	ALA
1	D	80	PRO
1	D	138	ASN
1	D	176	ASN
1	D	381	LEU
1	D	472	ALA
1	E	40	SER
1	E	184	GLU
1	E	347	SER
1	F	139	SER
1	F	142	ASP
1	F	284	LEU
1	H	137	GLY
1	H	139	SER
1	H	184	GLU
1	I	139	SER
1	I	177	ALA
1	I	347	SER
1	J	442	LYS
1	K	180	VAL
1	K	311	LEU
1	K	461	GLN
1	L	126	LEU
1	M	177	ALA
1	M	216	ASN
1	M	461	GLN
1	M	470	LEU
1	N	142	ASP
1	N	177	ALA

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Mol	Chain	Res	Type
1	N	322	CYS
1	O	131	ASN
1	O	149	MET
1	O	278	LYS
1	O	303	GLN
1	O	396	ILE
1	B	117	ILE
1	B	133	ASN
1	B	296	SER
1	B	337	SER
1	B	347	SER
1	C	40	SER
1	C	157	CYS
1	C	254	GLN
1	C	284	LEU
1	D	273	ALA
1	D	284	LEU
1	E	284	LEU
1	F	177	ALA
1	F	215	ALA
1	G	281	THR
1	G	296	SER
1	H	40	SER
1	H	177	ALA
1	H	284	LEU
1	H	470	LEU
1	I	284	LEU
1	I	303	GLN
1	J	25	ASP
1	J	54	LYS
1	J	177	ALA
1	J	285	PRO
1	K	176	ASN
1	K	284	LEU
1	K	300	SER
1	K	373	ILE
1	L	134	LYS
1	L	138	ASN
1	L	284	LEU
1	M	176	ASN
1	M	284	LEU
1	N	303	GLN

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Mol	Chain	Res	Type
1	O	54	LYS
1	O	223	ASP
1	O	460	ASP
1	A	291	PRO
1	A	306	ASN
1	B	132	SER
1	B	284	LEU
1	C	139	SER
1	C	237	MET
1	E	273	ALA
1	F	80	PRO
1	F	248	PHE
1	F	392	MET
1	G	57	SER
1	I	142	ASP
1	I	149	MET
1	I	223	ASP
1	J	80	PRO
1	J	126	LEU
1	J	296	SER
1	K	132	SER
1	K	177	ALA
1	K	223	ASP
1	K	392	MET
1	L	117	ILE
1	L	142	ASP
1	M	137	GLY
1	M	306	ASN
1	N	80	PRO
1	N	284	LEU
1	O	325	ASN
1	O	399	ASP
1	A	149	MET
1	B	311	LEU
1	C	126	LEU
1	C	243	GLY
1	G	126	LEU
1	G	177	ALA
1	J	284	LEU
1	K	337	SER
1	L	278	LYS
1	M	86	PRO

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Mol	Chain	Res	Type
1	N	137	GLY
1	F	180	VAL
1	J	111	GLN
1	E	111	GLN
1	E	285	PRO
1	H	86	PRO
1	I	291	PRO
1	J	117	ILE
1	K	243	GLY
1	E	63	PRO
1	G	111	GLN
1	G	117	ILE
1	H	180	VAL
1	I	80	PRO
1	K	320	GLY
1	L	373	ILE
1	N	396	ILE
1	A	86	PRO
1	B	111	GLN
1	C	86	PRO
1	C	111	GLN
1	E	86	PRO
1	H	268	GLY
1	O	86	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	367/369 (100%)	332 (90%)	35 (10%)	11 38
1	B	367/369 (100%)	318 (87%)	49 (13%)	5 21
1	C	367/369 (100%)	324 (88%)	43 (12%)	7 28
1	D	367/369 (100%)	330 (90%)	37 (10%)	9 35
1	E	367/369 (100%)	329 (90%)	38 (10%)	9 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	367/369 (100%)	322 (88%)	45 (12%)	6 25
1	G	367/369 (100%)	328 (89%)	39 (11%)	8 33
1	H	367/369 (100%)	323 (88%)	44 (12%)	6 27
1	I	367/369 (100%)	323 (88%)	44 (12%)	6 27
1	J	367/369 (100%)	326 (89%)	41 (11%)	7 30
1	K	367/369 (100%)	327 (89%)	40 (11%)	8 32
1	L	367/369 (100%)	324 (88%)	43 (12%)	7 28
1	M	367/369 (100%)	334 (91%)	33 (9%)	12 42
1	N	367/369 (100%)	322 (88%)	45 (12%)	6 25
1	O	367/369 (100%)	325 (89%)	42 (11%)	7 29
All	All	5505/5535 (100%)	4887 (89%)	618 (11%)	7 30

All (618) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	78	PRO
1	A	83	PHE
1	A	96	GLN
1	A	106	GLU
1	A	118	SER
1	A	127	ASP
1	A	153	GLN
1	A	154	THR
1	A	157	CYS
1	A	181	LYS
1	A	191	LEU
1	A	201	VAL
1	A	211	THR
1	A	213	LEU
1	A	220	VAL
1	A	245	MET
1	A	247	PHE
1	A	251	ARG
1	A	255	MET
1	A	257	VAL
1	A	262	ASN
1	A	278	LYS

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Mol	Chain	Res	Type
1	A	304	ILE
1	A	308	PRO
1	A	311	LEU
1	A	315	GLN
1	A	330	THR
1	A	338	THR
1	A	363	ARG
1	A	366	GLU
1	A	391	SER
1	A	393	ASN
1	A	464	LEU
1	A	474	LEU
1	B	32	ASN
1	B	48	PRO
1	B	71	ARG
1	B	83	PHE
1	B	90	PHE
1	B	91	TYR
1	B	96	GLN
1	B	106	GLU
1	B	112	PRO
1	B	113	LEU
1	B	118	SER
1	B	127	ASP
1	B	149	MET
1	B	158	LEU
1	B	162	ARG
1	B	164	PRO
1	B	167	GLU
1	B	181	LYS
1	B	193	THR
1	B	201	VAL
1	B	211	THR
1	B	220	VAL
1	B	221	PRO
1	B	222	LEU
1	B	225	CYS
1	B	227	SER
1	B	239	SER
1	B	240	GLU
1	B	247	PHE
1	B	250	LEU

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Mol	Chain	Res	Type
1	B	251	ARG
1	B	252	ARG
1	B	255	MET
1	B	257	VAL
1	B	262	ASN
1	B	270	THR
1	B	291	PRO
1	B	298	VAL
1	B	300	SER
1	B	301	ASP
1	B	304	ILE
1	B	311	LEU
1	B	315	GLN
1	B	338	THR
1	B	340	MET
1	B	393	ASN
1	B	462	PHE
1	B	464	LEU
1	B	474	LEU
1	C	32	ASN
1	C	62	VAL
1	C	68	LEU
1	C	76	LYS
1	C	83	PHE
1	C	106	GLU
1	C	109	ARG
1	C	113	LEU
1	C	127	ASP
1	C	149	MET
1	C	153	GLN
1	C	154	THR
1	C	157	CYS
1	C	162	ARG
1	C	167	GLU
1	C	181	LYS
1	C	201	VAL
1	C	211	THR
1	C	220	VAL
1	C	222	LEU
1	C	247	PHE
1	C	251	ARG
1	C	252	ARG

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Mol	Chain	Res	Type
1	C	254	GLN
1	C	255	MET
1	C	257	VAL
1	C	262	ASN
1	C	274	ASP
1	C	287	THR
1	C	293	PRO
1	C	298	VAL
1	C	311	LEU
1	C	315	GLN
1	C	319	ASN
1	C	326	GLN
1	C	330	THR
1	C	336	ARG
1	C	338	THR
1	C	340	MET
1	C	366	GLU
1	C	462	PHE
1	C	464	LEU
1	C	474	LEU
1	D	62	VAL
1	D	66	SER
1	D	83	PHE
1	D	106	GLU
1	D	117	ILE
1	D	118	SER
1	D	146	CYS
1	D	153	GLN
1	D	158	LEU
1	D	181	LYS
1	D	188	LEU
1	D	201	VAL
1	D	211	THR
1	D	222	LEU
1	D	232	PRO
1	D	247	PHE
1	D	250	LEU
1	D	251	ARG
1	D	252	ARG
1	D	255	MET
1	D	257	VAL
1	D	262	ASN

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Mol	Chain	Res	Type
1	D	263	ARG
1	D	291	PRO
1	D	293	PRO
1	D	298	VAL
1	D	304	ILE
1	D	307	LYS
1	D	311	LEU
1	D	315	GLN
1	D	319	ASN
1	D	326	GLN
1	D	327	LEU
1	D	338	THR
1	D	340	MET
1	D	464	LEU
1	D	474	LEU
1	E	33	ILE
1	E	83	PHE
1	E	90	PHE
1	E	106	GLU
1	E	112	PRO
1	E	117	ILE
1	E	127	ASP
1	E	133	ASN
1	E	153	GLN
1	E	154	THR
1	E	156	LEU
1	E	158	LEU
1	E	162	ARG
1	E	181	LYS
1	E	188	LEU
1	E	193	THR
1	E	201	VAL
1	E	211	THR
1	E	220	VAL
1	E	222	LEU
1	E	245	MET
1	E	247	PHE
1	E	251	ARG
1	E	252	ARG
1	E	255	MET
1	E	257	VAL
1	E	262	ASN

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Mol	Chain	Res	Type
1	E	270	THR
1	E	298	VAL
1	E	311	LEU
1	E	315	GLN
1	E	326	GLN
1	E	334	THR
1	E	338	THR
1	E	393	ASN
1	E	440	PRO
1	E	464	LEU
1	E	474	LEU
1	F	23	SER
1	F	32	ASN
1	F	68	LEU
1	F	83	PHE
1	F	90	PHE
1	F	106	GLU
1	F	109	ARG
1	F	118	SER
1	F	148	SER
1	F	149	MET
1	F	153	GLN
1	F	158	LEU
1	F	162	ARG
1	F	167	GLU
1	F	181	LYS
1	F	191	LEU
1	F	193	THR
1	F	200	MET
1	F	201	VAL
1	F	202	ASP
1	F	211	THR
1	F	220	VAL
1	F	232	PRO
1	F	239	SER
1	F	247	PHE
1	F	251	ARG
1	F	255	MET
1	F	260	LEU
1	F	262	ASN
1	F	291	PRO
1	F	311	LEU

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Mol	Chain	Res	Type
1	F	315	GLN
1	F	326	GLN
1	F	330	THR
1	F	334	THR
1	F	338	THR
1	F	340	MET
1	F	348	SER
1	F	363	ARG
1	F	366	GLU
1	F	368	TYR
1	F	393	ASN
1	F	395	SER
1	F	442	LYS
1	F	464	LEU
1	G	32	ASN
1	G	63	PRO
1	G	83	PHE
1	G	106	GLU
1	G	117	ILE
1	G	118	SER
1	G	127	ASP
1	G	143	ASN
1	G	153	GLN
1	G	158	LEU
1	G	181	LYS
1	G	193	THR
1	G	201	VAL
1	G	211	THR
1	G	219	ASP
1	G	247	PHE
1	G	250	LEU
1	G	251	ARG
1	G	252	ARG
1	G	255	MET
1	G	257	VAL
1	G	262	ASN
1	G	270	THR
1	G	274	ASP
1	G	280	THR
1	G	291	PRO
1	G	304	ILE
1	G	311	LEU

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Mol	Chain	Res	Type
1	G	315	GLN
1	G	321	ILE
1	G	327	LEU
1	G	338	THR
1	G	340	MET
1	G	366	GLU
1	G	387	THR
1	G	393	ASN
1	G	462	PHE
1	G	464	LEU
1	G	474	LEU
1	H	32	ASN
1	H	83	PHE
1	H	90	PHE
1	H	106	GLU
1	H	109	ARG
1	H	117	ILE
1	H	127	ASP
1	H	133	ASN
1	H	149	MET
1	H	153	GLN
1	H	156	LEU
1	H	158	LEU
1	H	162	ARG
1	H	167	GLU
1	H	180	VAL
1	H	181	LYS
1	H	188	LEU
1	H	193	THR
1	H	201	VAL
1	H	211	THR
1	H	220	VAL
1	H	227	SER
1	H	247	PHE
1	H	251	ARG
1	H	252	ARG
1	H	255	MET
1	H	256	PHE
1	H	257	VAL
1	H	260	LEU
1	H	262	ASN
1	H	298	VAL

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Mol	Chain	Res	Type
1	H	311	LEU
1	H	315	GLN
1	H	326	GLN
1	H	330	THR
1	H	338	THR
1	H	339	ASN
1	H	340	MET
1	H	366	GLU
1	H	393	ASN
1	H	445	THR
1	H	462	PHE
1	H	464	LEU
1	H	474	LEU
1	I	53	LYS
1	I	66	SER
1	I	78	PRO
1	I	83	PHE
1	I	90	PHE
1	I	106	GLU
1	I	118	SER
1	I	127	ASP
1	I	133	ASN
1	I	143	ASN
1	I	148	SER
1	I	153	GLN
1	I	154	THR
1	I	156	LEU
1	I	158	LEU
1	I	162	ARG
1	I	167	GLU
1	I	181	LYS
1	I	193	THR
1	I	201	VAL
1	I	209	ASP
1	I	211	THR
1	I	213	LEU
1	I	220	VAL
1	I	222	LEU
1	I	247	PHE
1	I	249	TYR
1	I	251	ARG
1	I	252	ARG

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Mol	Chain	Res	Type
1	I	255	MET
1	I	257	VAL
1	I	262	ASN
1	I	287	THR
1	I	298	VAL
1	I	304	ILE
1	I	311	LEU
1	I	315	GLN
1	I	319	ASN
1	I	336	ARG
1	I	338	THR
1	I	391	SER
1	I	393	ASN
1	I	464	LEU
1	I	474	LEU
1	J	32	ASN
1	J	83	PHE
1	J	90	PHE
1	J	96	GLN
1	J	106	GLU
1	J	117	ILE
1	J	118	SER
1	J	127	ASP
1	J	149	MET
1	J	154	THR
1	J	158	LEU
1	J	162	ARG
1	J	181	LYS
1	J	188	LEU
1	J	193	THR
1	J	200	MET
1	J	201	VAL
1	J	211	THR
1	J	220	VAL
1	J	223	ASP
1	J	225	CYS
1	J	239	SER
1	J	240	GLU
1	J	247	PHE
1	J	251	ARG
1	J	252	ARG
1	J	255	MET

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Mol	Chain	Res	Type
1	J	257	VAL
1	J	262	ASN
1	J	304	ILE
1	J	311	LEU
1	J	315	GLN
1	J	330	THR
1	J	338	THR
1	J	341	SER
1	J	352	THR
1	J	384	ASP
1	J	393	ASN
1	J	462	PHE
1	J	464	LEU
1	J	474	LEU
1	K	23	SER
1	K	32	ASN
1	K	50	TYR
1	K	83	PHE
1	K	90	PHE
1	K	96	GLN
1	K	106	GLU
1	K	125	LYS
1	K	127	ASP
1	K	154	THR
1	K	162	ARG
1	K	181	LYS
1	K	193	THR
1	K	201	VAL
1	K	211	THR
1	K	232	PRO
1	K	247	PHE
1	K	251	ARG
1	K	252	ARG
1	K	255	MET
1	K	257	VAL
1	K	262	ASN
1	K	272	PRO
1	K	286	SER
1	K	291	PRO
1	K	293	PRO
1	K	301	ASP
1	K	304	ILE

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Mol	Chain	Res	Type
1	K	311	LEU
1	K	315	GLN
1	K	330	THR
1	K	338	THR
1	K	343	CYS
1	K	366	GLU
1	K	391	SER
1	K	393	ASN
1	K	395	SER
1	K	455	PHE
1	K	464	LEU
1	K	474	LEU
1	L	32	ASN
1	L	33	ILE
1	L	62	VAL
1	L	71	ARG
1	L	90	PHE
1	L	106	GLU
1	L	112	PRO
1	L	117	ILE
1	L	118	SER
1	L	127	ASP
1	L	149	MET
1	L	154	THR
1	L	157	CYS
1	L	158	LEU
1	L	181	LYS
1	L	193	THR
1	L	201	VAL
1	L	209	ASP
1	L	211	THR
1	L	213	LEU
1	L	220	VAL
1	L	225	CYS
1	L	247	PHE
1	L	250	LEU
1	L	251	ARG
1	L	255	MET
1	L	257	VAL
1	L	260	LEU
1	L	262	ASN
1	L	270	THR

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Mol	Chain	Res	Type
1	L	278	LYS
1	L	280	THR
1	L	298	VAL
1	L	311	LEU
1	L	312	GLN
1	L	315	GLN
1	L	326	GLN
1	L	338	THR
1	L	393	ASN
1	L	443	ASN
1	L	459	LEU
1	L	464	LEU
1	L	474	LEU
1	M	32	ASN
1	M	83	PHE
1	M	106	GLU
1	M	118	SER
1	M	127	ASP
1	M	149	MET
1	M	153	GLN
1	M	154	THR
1	M	156	LEU
1	M	158	LEU
1	M	162	ARG
1	M	163	PRO
1	M	181	LYS
1	M	193	THR
1	M	201	VAL
1	M	211	THR
1	M	220	VAL
1	M	232	PRO
1	M	247	PHE
1	M	251	ARG
1	M	252	ARG
1	M	255	MET
1	M	257	VAL
1	M	262	ASN
1	M	286	SER
1	M	311	LEU
1	M	315	GLN
1	M	326	GLN
1	M	330	THR

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Mol	Chain	Res	Type
1	M	338	THR
1	M	339	ASN
1	M	366	GLU
1	M	464	LEU
1	N	32	ASN
1	N	48	PRO
1	N	71	ARG
1	N	80	PRO
1	N	82	LYS
1	N	83	PHE
1	N	96	GLN
1	N	106	GLU
1	N	115	VAL
1	N	117	ILE
1	N	118	SER
1	N	127	ASP
1	N	143	ASN
1	N	149	MET
1	N	154	THR
1	N	161	CYS
1	N	162	ARG
1	N	181	LYS
1	N	188	LEU
1	N	193	THR
1	N	201	VAL
1	N	211	THR
1	N	222	LEU
1	N	247	PHE
1	N	250	LEU
1	N	251	ARG
1	N	252	ARG
1	N	255	MET
1	N	257	VAL
1	N	262	ASN
1	N	287	THR
1	N	291	PRO
1	N	304	ILE
1	N	311	LEU
1	N	315	GLN
1	N	319	ASN
1	N	326	GLN
1	N	327	LEU

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Mol	Chain	Res	Type
1	N	338	THR
1	N	339	ASN
1	N	352	THR
1	N	391	SER
1	N	393	ASN
1	N	440	PRO
1	N	451	LEU
1	O	32	ASN
1	O	41	ARG
1	O	83	PHE
1	O	90	PHE
1	O	106	GLU
1	O	117	ILE
1	O	127	ASP
1	O	153	GLN
1	O	158	LEU
1	O	161	CYS
1	O	162	ARG
1	O	167	GLU
1	O	181	LYS
1	O	193	THR
1	O	201	VAL
1	O	211	THR
1	O	213	LEU
1	O	220	VAL
1	O	222	LEU
1	O	227	SER
1	O	247	PHE
1	O	251	ARG
1	O	252	ARG
1	O	255	MET
1	O	257	VAL
1	O	260	LEU
1	O	262	ASN
1	O	270	THR
1	O	298	VAL
1	O	311	LEU
1	O	315	GLN
1	O	319	ASN
1	O	325	ASN
1	O	326	GLN
1	O	330	THR

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Mol	Chain	Res	Type
1	O	338	THR
1	O	339	ASN
1	O	366	GLU
1	O	391	SER
1	O	393	ASN
1	O	464	LEU
1	O	474	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (191) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	69	GLN
1	A	124	ASN
1	A	133	ASN
1	A	153	GLN
1	A	262	ASN
1	A	315	GLN
1	A	339	ASN
1	A	393	ASN
1	A	461	GLN
1	B	32	ASN
1	B	69	GLN
1	B	133	ASN
1	B	138	ASN
1	B	143	ASN
1	B	153	GLN
1	B	262	ASN
1	B	303	GLN
1	B	306	ASN
1	B	315	GLN
1	B	339	ASN
1	B	364	HIS
1	B	393	ASN
1	B	461	GLN
1	C	32	ASN
1	C	69	GLN
1	C	96	GLN
1	C	133	ASN
1	C	143	ASN
1	C	153	GLN
1	C	254	GLN

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Mol	Chain	Res	Type
1	C	262	ASN
1	C	326	GLN
1	C	339	ASN
1	C	375	GLN
1	C	393	ASN
1	C	461	GLN
1	D	32	ASN
1	D	69	GLN
1	D	133	ASN
1	D	143	ASN
1	D	153	GLN
1	D	262	ASN
1	D	306	ASN
1	D	315	GLN
1	D	339	ASN
1	D	393	ASN
1	D	461	GLN
1	E	32	ASN
1	E	69	GLN
1	E	96	GLN
1	E	111	GLN
1	E	133	ASN
1	E	143	ASN
1	E	153	GLN
1	E	192	ASN
1	E	262	ASN
1	E	306	ASN
1	E	315	GLN
1	E	339	ASN
1	E	364	HIS
1	E	393	ASN
1	E	461	GLN
1	F	32	ASN
1	F	69	GLN
1	F	96	GLN
1	F	133	ASN
1	F	143	ASN
1	F	153	GLN
1	F	262	ASN
1	F	306	ASN
1	F	315	GLN
1	F	339	ASN

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Mol	Chain	Res	Type
1	F	364	HIS
1	F	393	ASN
1	F	401	ASN
1	F	461	GLN
1	G	32	ASN
1	G	69	GLN
1	G	133	ASN
1	G	153	GLN
1	G	262	ASN
1	G	306	ASN
1	G	339	ASN
1	G	393	ASN
1	G	461	GLN
1	H	32	ASN
1	H	69	GLN
1	H	96	GLN
1	H	133	ASN
1	H	143	ASN
1	H	153	GLN
1	H	192	ASN
1	H	214	GLN
1	H	262	ASN
1	H	306	ASN
1	H	315	GLN
1	H	339	ASN
1	H	364	HIS
1	H	393	ASN
1	H	461	GLN
1	I	32	ASN
1	I	69	GLN
1	I	133	ASN
1	I	143	ASN
1	I	153	GLN
1	I	262	ASN
1	I	312	GLN
1	I	339	ASN
1	I	364	HIS
1	I	393	ASN
1	I	461	GLN
1	J	32	ASN
1	J	69	GLN
1	J	96	GLN

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Mol	Chain	Res	Type
1	J	133	ASN
1	J	138	ASN
1	J	143	ASN
1	J	153	GLN
1	J	192	ASN
1	J	254	GLN
1	J	262	ASN
1	J	306	ASN
1	J	315	GLN
1	J	339	ASN
1	J	393	ASN
1	J	461	GLN
1	K	32	ASN
1	K	69	GLN
1	K	96	GLN
1	K	133	ASN
1	K	143	ASN
1	K	153	GLN
1	K	262	ASN
1	K	303	GLN
1	K	306	ASN
1	K	315	GLN
1	K	339	ASN
1	K	393	ASN
1	K	461	GLN
1	L	32	ASN
1	L	69	GLN
1	L	96	GLN
1	L	133	ASN
1	L	143	ASN
1	L	153	GLN
1	L	262	ASN
1	L	303	GLN
1	L	306	ASN
1	L	315	GLN
1	L	339	ASN
1	L	364	HIS
1	L	393	ASN
1	L	461	GLN
1	M	32	ASN
1	M	69	GLN
1	M	133	ASN

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Mol	Chain	Res	Type
1	M	143	ASN
1	M	153	GLN
1	M	214	GLN
1	M	262	ASN
1	M	315	GLN
1	M	339	ASN
1	M	364	HIS
1	M	393	ASN
1	M	461	GLN
1	N	32	ASN
1	N	69	GLN
1	N	133	ASN
1	N	153	GLN
1	N	262	ASN
1	N	306	ASN
1	N	315	GLN
1	N	339	ASN
1	N	364	HIS
1	N	393	ASN
1	N	461	GLN
1	O	32	ASN
1	O	69	GLN
1	O	96	GLN
1	O	133	ASN
1	O	143	ASN
1	O	153	GLN
1	O	262	ASN
1	O	306	ASN
1	O	315	GLN
1	O	339	ASN
1	O	364	HIS
1	O	393	ASN
1	O	461	GLN
1	O	471	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	417/423 (98%)	-0.00	7 (1%)	73 67	21, 52, 109, 134	0
1	B	417/423 (98%)	0.02	10 (2%)	62 55	25, 51, 110, 139	0
1	C	417/423 (98%)	0.11	14 (3%)	49 42	22, 56, 109, 138	0
1	D	417/423 (98%)	0.11	19 (4%)	36 30	24, 56, 110, 146	0
1	E	417/423 (98%)	0.09	13 (3%)	52 46	24, 54, 112, 139	0
1	F	417/423 (98%)	0.06	23 (5%)	29 23	20, 51, 111, 140	0
1	G	417/423 (98%)	0.01	9 (2%)	65 59	22, 55, 107, 133	0
1	H	417/423 (98%)	0.22	18 (4%)	39 32	21, 57, 112, 140	0
1	I	417/423 (98%)	0.12	13 (3%)	52 46	22, 56, 110, 140	0
1	J	417/423 (98%)	0.05	11 (2%)	59 53	21, 53, 111, 141	0
1	K	417/423 (98%)	0.26	21 (5%)	32 26	25, 66, 112, 140	0
1	L	417/423 (98%)	0.22	14 (3%)	49 42	26, 60, 111, 145	0
1	M	417/423 (98%)	0.26	22 (5%)	30 24	27, 63, 116, 141	0
1	N	417/423 (98%)	0.20	13 (3%)	52 46	22, 62, 113, 144	0
1	O	417/423 (98%)	0.31	25 (5%)	25 20	24, 61, 112, 143	0
All	All	6255/6345 (98%)	0.14	232 (3%)	45 38	20, 57, 111, 146	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	178	ASN	12.7
1	H	176	ASN	11.2
1	O	176	ASN	10.4
1	L	178	ASN	10.0
1	I	178	ASN	9.7
1	M	179	GLN	7.9
1	H	177	ALA	7.3

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Mol	Chain	Res	Type	RSRZ
1	O	175	SER	7.2
1	M	178	ASN	7.1
1	E	474	LEU	7.1
1	D	179	GLN	7.0
1	D	175	SER	6.7
1	L	138	ASN	6.5
1	B	474	LEU	6.4
1	A	136	VAL	6.3
1	N	178	ASN	5.8
1	I	173	THR	5.6
1	L	177	ALA	5.5
1	O	174	PRO	5.5
1	K	58	ASN	5.4
1	F	177	ALA	5.4
1	O	179	GLN	5.4
1	M	173	THR	5.3
1	F	176	ASN	5.3
1	B	179	GLN	5.2
1	C	174	PRO	5.1
1	L	180	VAL	5.0
1	M	174	PRO	4.9
1	L	179	GLN	4.9
1	O	128	ASP	4.9
1	M	349	SER	4.8
1	I	474	LEU	4.8
1	H	133	ASN	4.8
1	H	181	LYS	4.8
1	C	178	ASN	4.7
1	D	176	ASN	4.6
1	E	177	ALA	4.6
1	F	178	ASN	4.5
1	K	176	ASN	4.5
1	B	55	GLN	4.4
1	F	174	PRO	4.4
1	L	134	LYS	4.3
1	H	175	SER	4.3
1	H	134	LYS	4.3
1	E	89	SER	4.3
1	O	136	VAL	4.3
1	L	133	ASN	4.2
1	D	177	ALA	4.2
1	C	134	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	133	ASN	4.2
1	E	58	ASN	4.2
1	G	133	ASN	4.2
1	H	474	LEU	4.1
1	K	175	SER	4.1
1	G	55	GLN	4.1
1	O	173	THR	4.1
1	H	55	GLN	4.1
1	O	59	LYS	4.1
1	M	87	ASP	4.0
1	D	133	ASN	4.0
1	I	89	SER	3.9
1	G	134	LYS	3.9
1	D	139	SER	3.9
1	G	140	GLY	3.9
1	I	175	SER	3.9
1	C	179	GLN	3.8
1	E	56	ASP	3.8
1	C	66	SER	3.8
1	J	86	PRO	3.8
1	K	174	PRO	3.7
1	D	280	THR	3.7
1	D	178	ASN	3.7
1	M	89	SER	3.6
1	K	57	SER	3.6
1	M	177	ALA	3.6
1	F	179	GLN	3.6
1	N	56	ASP	3.5
1	M	133	ASN	3.5
1	H	178	ASN	3.5
1	F	173	THR	3.5
1	F	133	ASN	3.5
1	I	179	GLN	3.4
1	J	56	ASP	3.4
1	H	139	SER	3.4
1	H	281	THR	3.4
1	D	174	PRO	3.4
1	O	133	ASN	3.4
1	N	90	PHE	3.4
1	A	89	SER	3.4
1	G	176	ASN	3.4
1	J	84	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	133	ASN	3.3
1	A	474	LEU	3.3
1	C	474	LEU	3.3
1	M	143	ASN	3.3
1	D	86	PRO	3.2
1	N	87	ASP	3.2
1	J	349	SER	3.2
1	F	55	GLN	3.2
1	O	83	PHE	3.1
1	F	175	SER	3.1
1	O	89	SER	3.1
1	H	179	GLN	3.1
1	F	137	GLY	3.1
1	D	59	LYS	3.1
1	A	137	GLY	3.1
1	L	474	LEU	3.1
1	N	55	GLN	3.1
1	B	89	SER	3.1
1	L	181	LYS	3.1
1	G	357	ASN	3.1
1	L	281	THR	3.0
1	O	134	LYS	3.0
1	G	85	PHE	3.0
1	G	179	GLN	3.0
1	K	281	THR	3.0
1	F	138	ASN	2.9
1	E	182	ALA	2.9
1	I	442	LYS	2.9
1	N	138	ASN	2.9
1	O	178	ASN	2.9
1	D	474	LEU	2.9
1	K	134	LYS	2.9
1	D	56	ASP	2.9
1	O	172	GLY	2.9
1	D	55	GLN	2.8
1	M	180	VAL	2.8
1	N	137	GLY	2.8
1	C	55	GLN	2.8
1	D	180	VAL	2.8
1	H	58	ASN	2.8
1	F	134	LYS	2.8
1	O	82	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	474	LEU	2.8
1	K	59	LYS	2.8
1	I	177	ALA	2.8
1	L	135	TYR	2.7
1	E	349	SER	2.7
1	F	136	VAL	2.7
1	I	280	THR	2.7
1	I	176	ASN	2.7
1	O	281	THR	2.7
1	E	185	CYS	2.6
1	K	177	ALA	2.6
1	F	84	GLY	2.6
1	E	265	GLY	2.6
1	G	137	GLY	2.6
1	K	369	ASP	2.6
1	E	86	PRO	2.6
1	I	174	PRO	2.6
1	B	178	ASN	2.5
1	O	137	GLY	2.5
1	F	86	PRO	2.5
1	F	89	SER	2.5
1	O	142	ASP	2.5
1	M	280	THR	2.5
1	O	129	THR	2.5
1	M	348	SER	2.5
1	B	176	ASN	2.5
1	C	89	SER	2.5
1	K	82	LYS	2.5
1	K	61	ALA	2.5
1	B	280	THR	2.4
1	O	88	THR	2.4
1	O	58	ASN	2.4
1	C	173	THR	2.4
1	F	471	GLN	2.4
1	F	180	VAL	2.4
1	K	327	LEU	2.4
1	E	57	SER	2.4
1	D	82	LYS	2.4
1	O	138	ASN	2.4
1	J	138	ASN	2.4
1	K	86	PRO	2.4
1	O	280	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	59	LYS	2.4
1	J	474	LEU	2.3
1	A	349	SER	2.3
1	N	339	ASN	2.3
1	C	176	ASN	2.3
1	A	176	ASN	2.3
1	K	353	TYR	2.3
1	A	178	ASN	2.3
1	N	160	GLY	2.3
1	I	172	GLY	2.3
1	H	56	ASP	2.3
1	N	179	GLN	2.3
1	H	473	GLY	2.3
1	K	283	THR	2.3
1	F	83	PHE	2.2
1	N	350	ASP	2.2
1	M	474	LEU	2.2
1	D	89	SER	2.2
1	L	351	SER	2.2
1	L	89	SER	2.2
1	M	132	SER	2.2
1	D	138	ASN	2.2
1	H	88	THR	2.2
1	F	474	LEU	2.2
1	M	43	LEU	2.2
1	J	55	GLN	2.2
1	E	136	VAL	2.2
1	F	380	THR	2.2
1	B	59	LYS	2.2
1	D	85	PHE	2.2
1	K	268	GLY	2.2
1	O	135	TYR	2.2
1	F	56	ASP	2.2
1	J	135	TYR	2.1
1	I	473	GLY	2.1
1	J	176	ASN	2.1
1	B	87	ASP	2.1
1	M	58	ASN	2.1
1	O	474	LEU	2.1
1	M	134	LYS	2.1
1	J	348	SER	2.1
1	N	93	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	182	ALA	2.1
1	F	139	SER	2.1
1	J	179	GLN	2.1
1	M	279	GLY	2.1
1	E	133	ASN	2.1
1	C	473	GLY	2.1
1	M	82	LYS	2.1
1	K	179	GLN	2.0
1	H	85	PHE	2.0
1	N	474	LEU	2.0
1	M	450	ASP	2.0
1	L	82	LYS	2.0
1	B	349	SER	2.0
1	H	347	SER	2.0
1	C	216	ASN	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 carbohydrates 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.