



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:37 AM UTC

PDB ID : 2HPC / pdb_00002hpc
Title : Crystal structure of fragment D from Human Fibrinogen Complexed with Gly-Pro-Arg-Pro-amide.
Authors : Doolittle, R.F.; Kollman, J.M.; Chen, A.; Pandi, L.
Deposited on : 2006-07-17
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

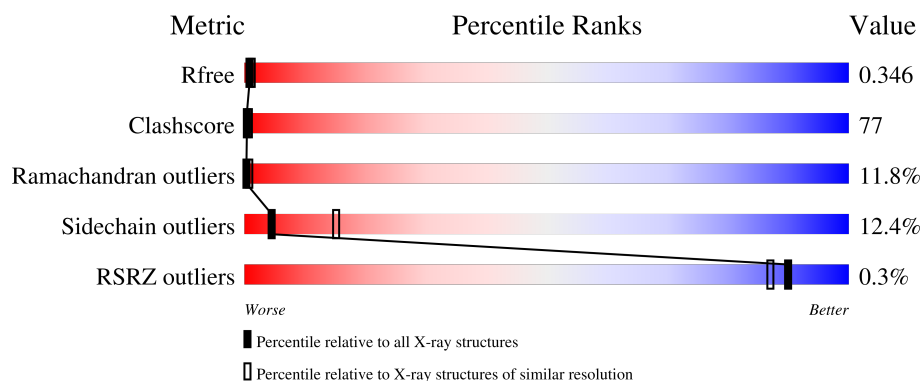
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



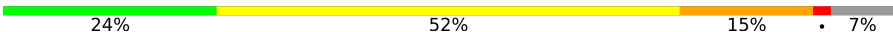
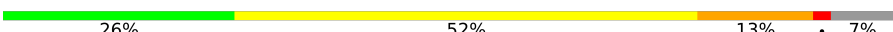
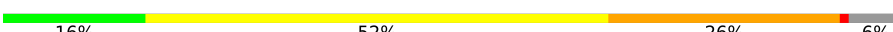
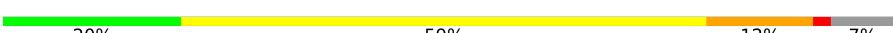
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	87	
1	D	87	
1	G	87	
1	J	87	
2	B	328	

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Mol	Chain	Length	Quality of chain
2	E	328	
2	H	328	
2	K	328	
3	C	323	
3	F	323	
3	I	323	
3	L	323	
4	M	5	
4	N	5	
4	O	5	
4	P	5	
4	Q	5	
4	R	5	
4	S	5	
4	T	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	470	X	-	-	-
5	NAG	E	470	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22270 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			
1	D	71	Total	C	N	O	S	0	0	0
			584	361	112	108	3			
1	G	74	Total	C	N	O	S	0	0	0
			608	377	115	113	3			
1	J	79	Total	C	N	O	S	0	0	0
			652	402	126	121	3			

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	307	Total	C	N	O	S	0	0	0
			2462	1535	433	472	22			
2	E	304	Total	C	N	O	S	0	0	0
			2434	1514	430	468	22			
2	H	307	Total	C	N	O	S	0	0	0
			2462	1535	433	472	22			
2	K	305	Total	C	N	O	S	0	0	0
			2442	1520	431	469	22			

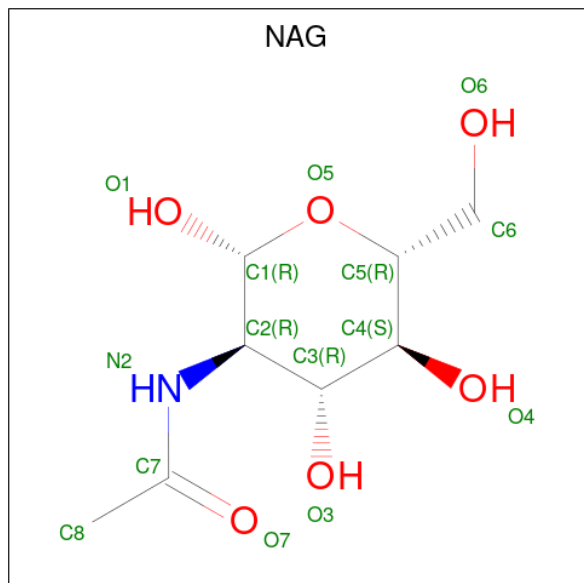
- Molecule 3 is a protein called Fibrinogen, gamma polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	305	Total	C	N	O	S	0	0	0
			2446	1552	410	472	12			
3	F	300	Total	C	N	O	S	0	0	0
			2410	1529	405	464	12			
3	I	305	Total	C	N	O	S	0	0	0
			2446	1552	410	472	12			
3	L	300	Total	C	N	O	S	0	0	0
			2410	1529	405	464	12			

- Molecule 4 is a protein called Gly-Pro-Arg-Pro-amide peptide ligand.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	5	Total	C	N	O	0	0	1
			30	18	8	4			
4	N	5	Total	C	N	O	0	0	1
			30	18	8	4			
4	O	5	Total	C	N	O	0	0	1
			30	18	8	4			
4	P	5	Total	C	N	O	0	0	1
			30	18	8	4			
4	Q	5	Total	C	N	O	0	0	1
			30	18	8	4			
4	R	5	Total	C	N	O	0	0	1
			30	18	8	4			
4	S	5	Total	C	N	O	0	0	1
			30	18	8	4			
4	T	5	Total	C	N	O	0	0	1
			30	18	8	4			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

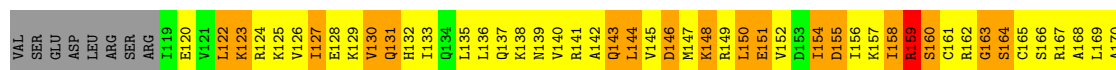
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		
6	E	2	Total	Ca	0	0
			2	2		
6	F	1	Total	Ca	0	0
			1	1		
6	H	1	Total	Ca	0	0
			1	1		
6	I	1	Total	Ca	0	0
			1	1		
6	K	2	Total	Ca	0	0
			2	2		
6	L	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

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

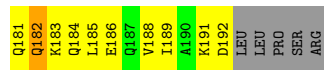
• Molecule 1: Fibrinogen alpha chain

Chain A: 



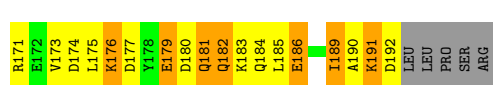
• Molecule 1: Fibrinogen alpha chain

Chain D: 

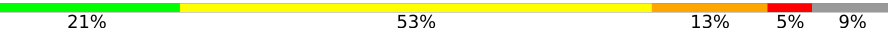


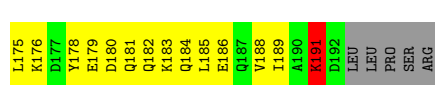
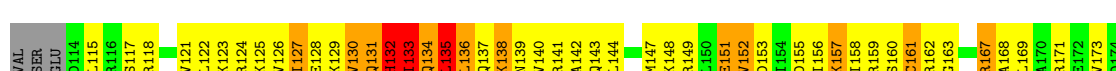
• Molecule 1: Fibrinogen alpha chain

Chain G: 



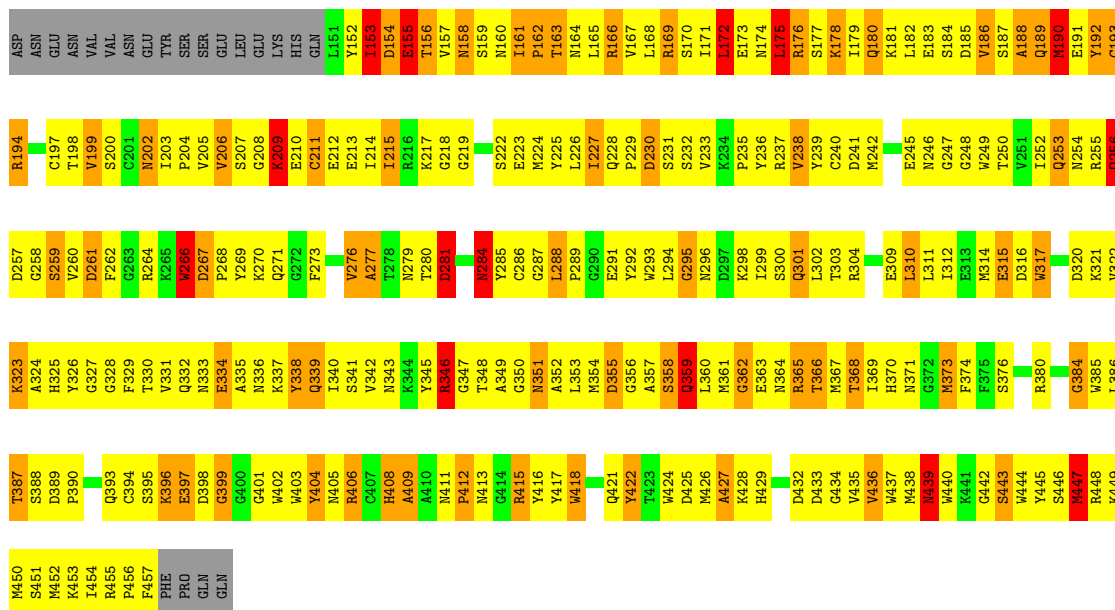
• Molecule 1: Fibrinogen alpha chain

Chain J: 

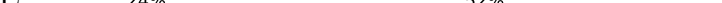


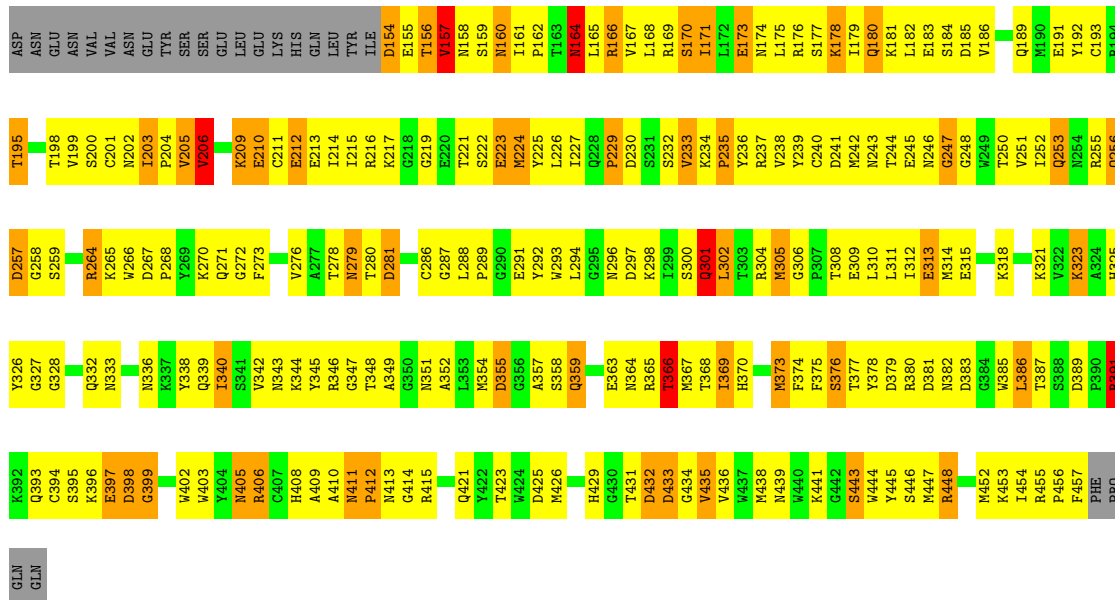
- Molecule 2: Fibrinogen beta chain

Chain B:  15% 55% 20% 6%

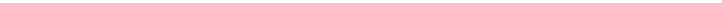


- Molecule 2: Fibrinogen beta chain

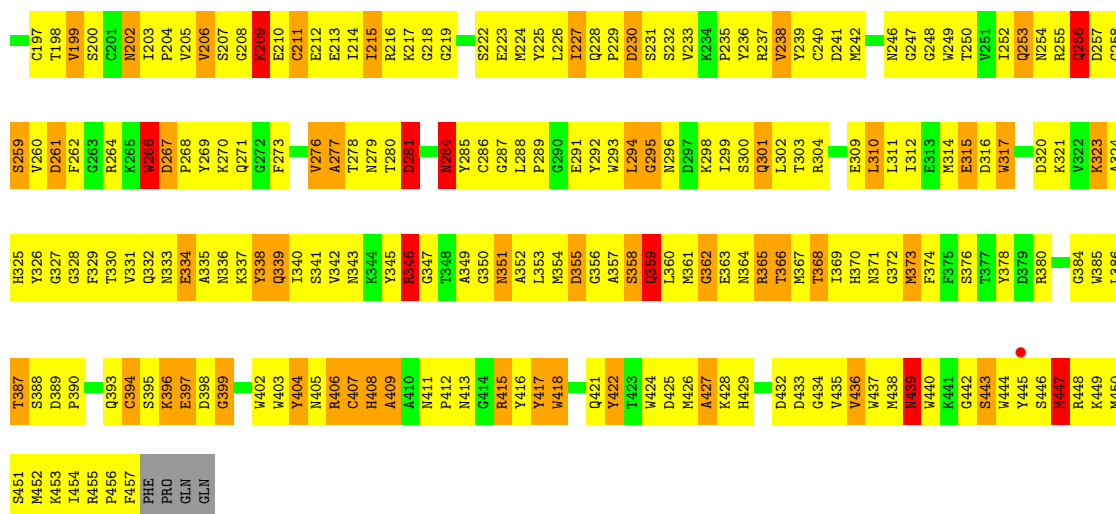
Chain E:  24% 52% 15% • 7%



- Molecule 2: Fibrinogen beta chain

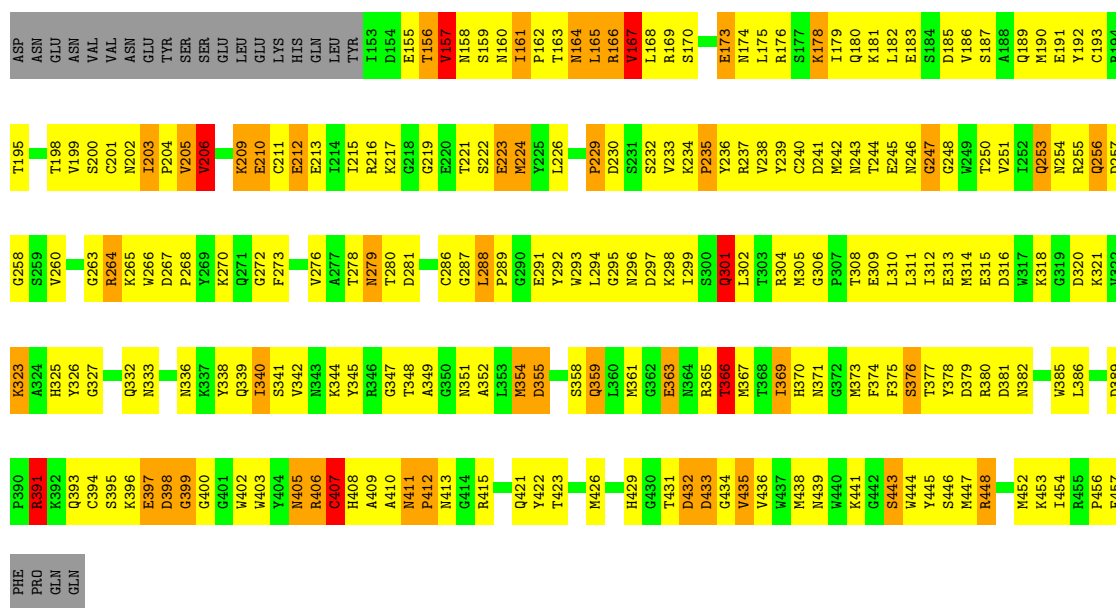
Chain H:  16% 55% 19% 6%





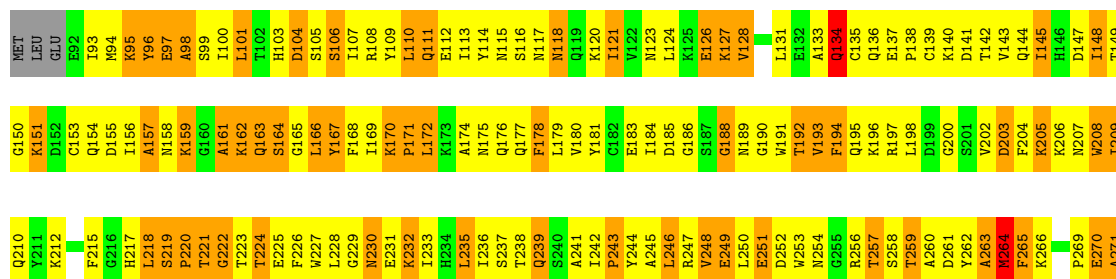
• Molecule 2: Fibrinogen beta chain

Chain K: 26% 52% 13% 7%



• Molecule 3: Fibrinogen, gamma polypeptide

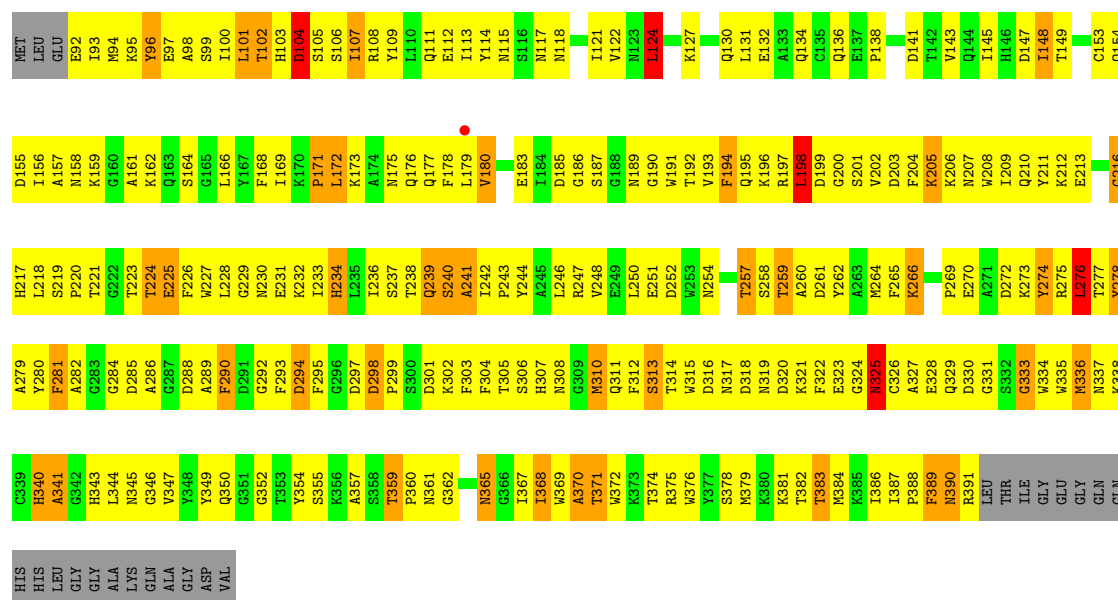
Chain C: 16% 52% 26% 6%





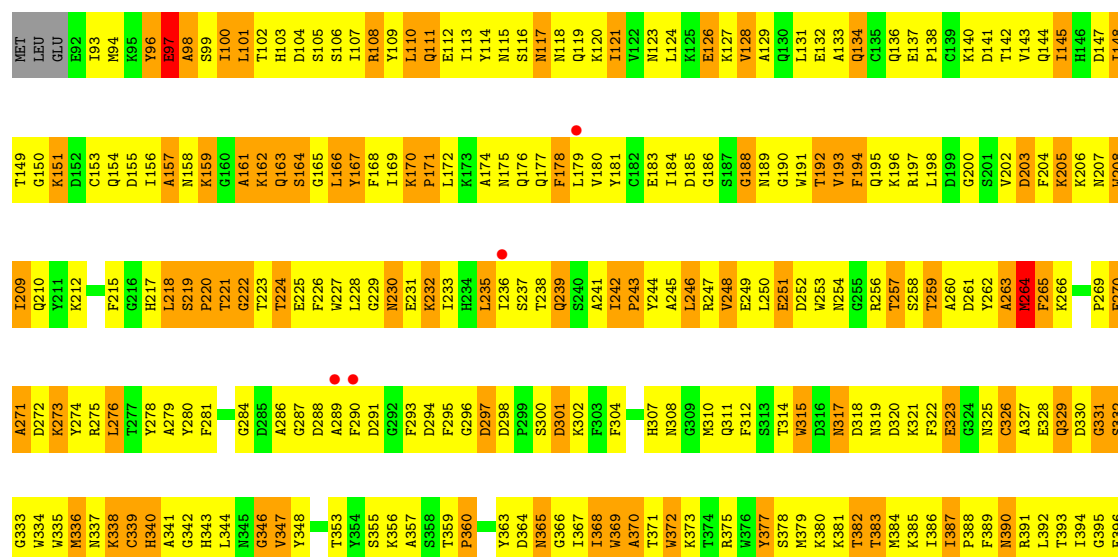
• Molecule 3: Fibrinogen, gamma polypeptide

Chain F: 20% 59% 12% 7%



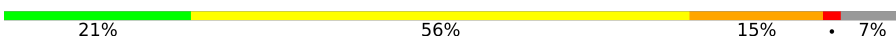
• Molecule 3: Fibrinogen, gamma polypeptide

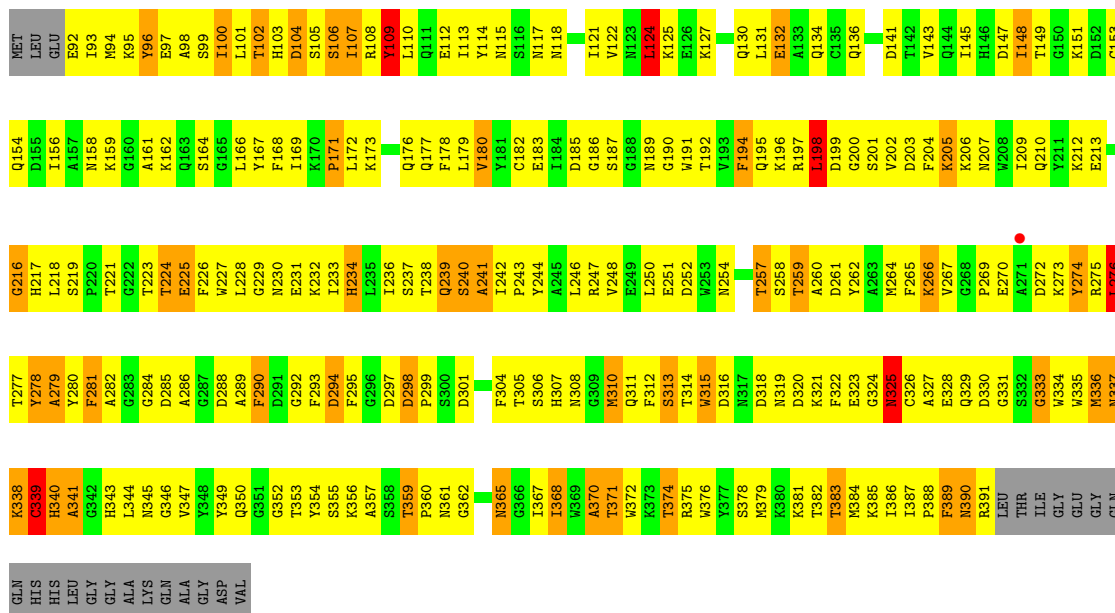
Chain I: 15% 53% 26% 6%



GLY
GLN
GLN
HIS
HIS
LEU
GLY
GLY
GLN
GLN
ALA
ASP
VAL

• Molecule 3: Fibrinogen, gamma polypeptide

Chain L:  21% 56% 15% 7%

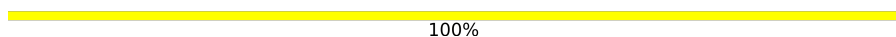


• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain M:  80% 20%

G1
P2
R3
P4
NH25

• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain N:  100%

G1
P2
R3
P4
NH25

• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain O:  60% 40%

G1
P2
R3
P4
NH25

• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain P:  40% 40% 20%



- Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand



- Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand



- Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand



- Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.68Å 46.07Å 429.90Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-2.90) 99.0 (30.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.275 , 0.360 0.265 , 0.346	Depositor DCC
R_{free} test set	3644 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	71.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 95.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22270	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, NAG, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.48	0/609	1.29	13/811 (1.6%)
1	D	0.59	0/585	1.16	5/778 (0.6%)
1	G	0.47	0/609	1.26	12/811 (1.5%)
1	J	0.56	0/653	1.16	7/869 (0.8%)
2	B	0.49	0/2523	1.18	32/3409 (0.9%)
2	E	0.64	1/2494 (0.0%)	1.15	18/3369 (0.5%)
2	H	0.49	0/2523	1.18	30/3409 (0.9%)
2	K	0.65	0/2502	1.16	25/3380 (0.7%)
3	C	0.44	0/2512	1.04	23/3396 (0.7%)
3	F	0.52	0/2476	1.09	28/3347 (0.8%)
3	I	0.44	0/2512	1.06	20/3396 (0.6%)
3	L	0.52	0/2476	1.10	27/3347 (0.8%)
4	M	0.57	0/30	0.94	0/40
4	N	0.74	0/30	0.90	0/40
4	O	0.60	0/30	0.88	0/40
4	P	0.62	0/30	1.11	0/40
4	Q	0.68	0/30	1.36	0/40
4	R	0.66	0/30	0.89	0/40
4	S	0.58	0/30	0.90	0/40
4	T	0.62	0/30	1.12	0/40
All	All	0.53	1/22714 (0.0%)	1.13	240/30642 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	373	MET	SD-CE	5.44	1.93	1.79

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	101	LEU	N-CA-C	-12.58	98.03	113.50
3	L	102	THR	N-CA-C	-12.54	97.69	111.36
1	J	135	LEU	N-CA-C	-12.17	99.10	114.56
2	B	347	GLY	N-CA-C	10.83	122.24	111.95
2	E	409	ALA	N-CA-C	-10.55	101.17	114.56
2	E	178	LYS	N-CA-C	-10.29	100.46	113.43
2	H	347	GLY	N-CA-C	10.02	121.47	111.95
2	K	409	ALA	N-CA-C	-9.82	101.64	114.31
2	H	409	ALA	N-CA-C	-9.76	102.16	114.56
2	H	183	GLU	N-CA-C	-9.73	103.53	114.62
1	G	134	GLN	N-CA-C	-9.71	101.35	113.01
2	H	408	HIS	N-CA-C	9.70	124.15	109.41
3	L	338	LYS	N-CA-C	-9.56	98.46	111.55
2	B	358	SER	N-CA-C	9.55	121.64	111.03
2	K	412	PRO	N-CA-C	-9.46	97.22	111.41
2	E	412	PRO	N-CA-C	-9.43	97.26	111.41
2	H	156	THR	N-CA-C	-9.36	101.12	112.54
2	K	166	ARG	N-CA-C	-9.29	101.51	113.12
2	H	358	SER	N-CA-C	9.27	121.31	111.03
3	I	340	HIS	N-CA-C	9.19	120.38	108.24
2	B	409	ALA	N-CA-C	-8.87	102.87	114.31
3	L	272	ASP	N-CA-C	-8.84	102.58	112.57
2	H	346	ARG	N-CA-C	-8.79	96.08	109.96
1	A	187	GLN	N-CA-C	-8.78	101.51	113.18
3	C	106	SER	N-CA-C	-8.70	102.84	113.19
2	B	175	LEU	N-CA-C	-8.56	103.02	113.97
2	B	172	LEU	N-CA-C	-8.38	102.96	113.01
2	B	178	LYS	N-CA-C	-8.35	102.08	113.18
2	B	346	ARG	N-CA-C	-8.31	96.84	109.96
3	I	96	TYR	N-CA-C	-8.18	102.56	112.54
2	B	156	THR	N-CA-C	-8.09	103.30	113.01
2	B	190	MET	N-CA-C	-8.09	102.30	112.90
1	A	148	LYS	N-CA-C	-8.05	103.17	113.16
2	H	177	SER	N-CA-C	-8.05	102.46	111.07
2	B	408	HIS	N-CA-C	7.88	121.39	109.41
1	G	138	LYS	N-CA-C	-7.83	103.52	113.23
1	G	148	LYS	N-CA-C	-7.81	102.83	113.30
2	K	406	ARG	CA-C-N	7.72	136.28	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	406	ARG	C-N-CA	7.72	136.28	121.54
1	G	181	GLN	N-CA-C	-7.64	102.92	111.71
3	L	359	THR	CA-C-N	7.64	126.91	118.97
3	L	359	THR	C-N-CA	7.64	126.91	118.97
3	C	340	HIS	N-CA-C	7.63	118.32	108.24
2	H	155	GLU	N-CA-C	-7.61	105.16	114.75
3	I	159	LYS	N-CA-C	-7.40	103.83	114.12
1	A	131	GLN	N-CA-C	-7.40	104.23	113.18
3	I	338	LYS	N-CA-C	-7.39	101.17	111.81
2	K	178	LYS	N-CA-C	-7.38	104.89	114.04
3	I	147	ASP	N-CA-C	7.36	119.09	111.14
3	F	274	TYR	N-CA-C	-7.36	101.73	110.41
2	B	193	CYS	N-CA-C	-7.28	104.91	114.31
1	A	123	LYS	N-CA-C	-7.21	104.37	113.02
1	A	138	LYS	N-CA-C	-7.20	102.44	112.45
3	F	359	THR	CA-C-N	7.16	126.42	118.97
3	F	359	THR	C-N-CA	7.16	126.42	118.97
1	G	150	LEU	N-CA-C	-7.14	103.53	111.82
3	C	147	ASP	N-CA-C	7.11	118.82	111.14
3	L	274	TYR	N-CA-C	-7.09	101.75	110.61
3	C	159	LYS	N-CA-C	-7.06	104.31	114.12
2	H	187	SER	N-CA-C	-7.05	104.17	114.39
1	G	131	GLN	N-CA-C	-7.03	103.54	111.07
1	A	176	LYS	N-CA-C	-7.03	104.74	113.38
2	B	209	LYS	N-CA-C	-7.00	104.55	113.23
2	K	433	ASP	N-CA-C	-6.98	101.82	110.41
2	H	209	LYS	N-CA-C	-6.97	104.59	113.23
3	C	110	LEU	N-CA-C	-6.96	104.66	113.43
3	I	338	LYS	CA-C-N	6.96	134.83	121.54
3	I	338	LYS	C-N-CA	6.96	134.83	121.54
2	H	396	LYS	N-CA-C	-6.94	103.73	111.71
1	A	159	ARG	N-CA-C	-6.91	103.95	112.38
3	L	338	LYS	CA-C-N	6.90	134.71	121.54
3	L	338	LYS	C-N-CA	6.90	134.71	121.54
2	E	433	ASP	N-CA-C	-6.81	101.53	110.53
3	F	97	GLU	N-CA-C	-6.80	103.95	113.20
2	E	297	ASP	N-CA-C	-6.80	103.56	110.97
1	A	181	GLN	N-CA-C	-6.75	103.95	111.71
2	B	169	ARG	N-CA-C	-6.71	104.00	111.71
2	H	397	GLU	N-CA-C	-6.70	100.30	109.95
2	B	396	LYS	N-CA-C	-6.69	104.02	111.71
2	H	193	CYS	N-CA-C	-6.68	105.70	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	346	GLY	N-CA-C	6.67	122.86	111.98
2	B	206	VAL	N-CA-C	6.67	117.64	108.84
2	E	347	GLY	N-CA-C	6.66	118.90	110.38
1	G	143	GLN	N-CA-C	-6.65	105.05	113.43
3	C	336	MET	N-CA-C	6.64	119.13	110.43
1	A	164	SER	N-CA-C	-6.54	104.90	114.39
2	K	448	ARG	N-CA-C	-6.50	105.50	113.50
2	H	206	VAL	N-CA-C	6.47	117.39	108.84
3	F	281	PHE	N-CA-C	-6.47	101.29	110.35
2	K	167	VAL	N-CA-C	-6.47	104.02	110.62
2	B	163	THR	N-CA-C	-6.45	104.18	113.21
3	I	101	LEU	N-CA-C	-6.44	105.49	113.15
2	K	347	GLY	N-CA-C	6.42	118.80	110.45
2	K	432	ASP	N-CA-C	6.41	119.58	109.39
2	B	404	TYR	N-CA-C	6.41	119.15	108.96
3	L	281	PHE	N-CA-C	-6.40	101.07	110.42
2	B	397	GLU	N-CA-C	-6.40	100.51	110.17
3	C	346	GLY	N-CA-C	6.39	122.41	111.98
3	F	341	ALA	N-CA-C	-6.39	103.92	112.94
3	C	95	LYS	N-CA-C	-6.36	105.62	113.19
3	I	336	MET	N-CA-C	6.34	118.74	110.43
2	B	427	ALA	N-CA-C	6.33	119.41	110.23
2	H	418	TRP	N-CA-C	6.32	118.92	109.25
3	L	340	HIS	N-CA-C	6.32	118.11	108.07
3	C	242	ILE	CA-C-N	6.30	127.71	119.84
3	C	242	ILE	C-N-CA	6.30	127.71	119.84
3	F	105	SER	N-CA-C	-6.30	104.11	110.97
1	G	144	LEU	N-CA-C	-6.29	105.70	113.19
2	K	443	SER	N-CA-C	6.25	117.89	111.14
1	A	150	LEU	N-CA-C	-6.24	104.54	111.71
2	E	448	ARG	N-CA-C	-6.18	105.90	113.50
2	E	355	ASP	N-CA-C	6.15	120.67	112.30
2	H	436	VAL	N-CA-C	6.15	117.45	108.53
2	H	404	TYR	N-CA-C	6.15	118.74	108.96
2	E	391	ARG	N-CA-C	-6.14	104.51	111.14
1	D	123	LYS	N-CA-C	-6.12	104.53	111.07
3	F	124	LEU	N-CA-C	-6.11	104.54	111.07
2	E	411	ASN	CA-C-N	-6.08	114.01	120.03
2	E	411	ASN	C-N-CA	-6.08	114.01	120.03
3	L	341	ALA	N-CA-C	-6.08	104.37	112.94
2	E	165	LEU	N-CA-C	-6.08	104.29	113.89
2	H	427	ALA	N-CA-C	6.04	118.99	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	216	GLY	N-CA-C	-6.01	104.29	112.52
2	K	407	CYS	N-CA-C	6.00	123.57	110.80
2	E	432	ASP	N-CA-C	5.99	118.92	109.39
3	F	104	ASP	N-CA-C	-5.98	98.07	110.80
2	K	297	ASP	N-CA-C	-5.93	104.51	110.97
2	K	391	ARG	N-CA-C	-5.87	104.78	111.07
3	C	290	PHE	N-CA-C	-5.87	106.12	113.28
2	B	415	ARG	N-CA-C	-5.86	102.80	110.53
3	I	170	LYS	CA-C-N	5.85	127.16	119.84
3	I	170	LYS	C-N-CA	5.85	127.16	119.84
3	I	301	ASP	N-CA-C	-5.85	104.98	111.71
2	B	188	ALA	N-CA-C	-5.84	106.20	113.15
2	E	443	SER	N-CA-C	5.84	117.45	111.14
1	A	122	LEU	N-CA-C	5.84	118.18	109.25
1	G	159	ARG	N-CA-C	-5.82	105.07	111.82
3	C	301	ASP	N-CA-C	-5.81	105.03	111.71
2	H	406	ARG	CA-C-N	5.81	132.63	121.54
2	H	406	ARG	C-N-CA	5.81	132.63	121.54
3	F	257	THR	N-CA-C	5.80	115.94	108.34
1	D	183	LYS	N-CA-C	-5.80	104.96	111.28
3	F	272	ASP	N-CA-C	-5.79	102.89	111.81
2	K	411	ASN	CA-C-N	-5.79	114.30	120.03
2	K	411	ASN	C-N-CA	-5.79	114.30	120.03
3	C	139	CYS	N-CA-C	-5.78	102.34	110.50
2	K	173	GLU	N-CA-C	-5.78	106.07	113.23
3	F	368	ILE	N-CA-C	5.77	118.05	109.17
2	B	418	TRP	N-CA-C	5.75	118.05	109.25
3	C	337	ASN	N-CA-C	-5.67	98.72	110.80
2	B	436	VAL	N-CA-C	5.66	116.74	108.53
1	J	155	ASP	N-CA-C	-5.65	105.03	111.07
3	L	336	MET	N-CA-C	5.64	118.92	109.95
3	F	345	ASN	N-CA-C	-5.62	104.06	112.54
1	G	121	VAL	N-CA-C	5.61	121.02	109.34
2	H	406	ARG	N-CA-C	-5.61	103.67	111.30
3	I	242	ILE	CA-C-N	5.59	126.83	119.84
3	I	242	ILE	C-N-CA	5.59	126.83	119.84
3	F	375	ARG	N-CA-C	-5.58	106.47	113.28
1	J	130	VAL	N-CA-C	5.58	116.22	110.36
2	B	215	ILE	N-CA-C	-5.57	105.76	113.00
3	C	126	GLU	N-CA-C	-5.57	98.94	110.80
2	H	215	ILE	N-CA-C	-5.55	105.78	113.00
3	I	290	PHE	N-CA-C	-5.55	106.51	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	CYS	N-CA-C	-5.54	106.51	113.72
2	K	288	LEU	CA-C-N	-5.53	114.90	120.21
2	K	288	LEU	C-N-CA	-5.53	114.90	120.21
2	B	373	MET	N-CA-C	5.53	119.11	110.32
3	F	276	LEU	N-CA-C	-5.50	102.74	110.50
3	L	276	LEU	N-CA-C	-5.50	102.74	110.50
2	E	166	ARG	N-CA-C	-5.50	104.12	112.04
3	F	368	ILE	CB-CA-C	-5.50	103.69	111.38
2	H	415	ARG	N-CA-C	-5.50	103.28	110.53
3	F	102	THR	N-CA-C	-5.49	104.32	111.02
3	F	310	MET	N-CA-C	5.48	117.64	109.59
1	A	146	ASP	N-CA-C	-5.46	105.36	112.23
3	L	333	GLY	N-CA-C	-5.44	100.28	113.18
2	H	384	GLY	N-CA-C	-5.42	108.22	115.32
2	B	176	ARG	N-CA-C	-5.40	105.29	111.07
3	L	345	ASN	N-CA-C	-5.40	104.65	113.19
1	J	183	LYS	N-CA-C	-5.40	105.39	111.28
3	L	370	ALA	N-CA-C	5.40	120.28	111.37
3	L	368	ILE	N-CA-C	5.40	117.48	109.17
3	L	375	ARG	N-CA-C	-5.40	106.47	113.16
2	H	373	MET	N-CA-C	5.40	118.90	110.32
1	J	136	LEU	N-CA-C	-5.39	105.32	111.14
3	L	109	TYR	N-CA-C	-5.38	105.45	112.23
2	B	384	GLY	N-CA-C	-5.37	108.28	115.32
3	F	333	GLY	N-CA-C	-5.37	100.45	113.18
3	F	99	SER	N-CA-C	-5.36	106.77	113.15
2	E	397	GLU	N-CA-C	-5.33	102.99	110.35
3	L	310	MET	N-CA-C	5.33	117.42	109.59
1	J	191	LYS	N-CA-C	5.32	122.14	110.80
3	I	326	CYS	N-CA-C	-5.32	105.48	111.28
2	H	172	LEU	N-CA-C	-5.32	106.75	113.18
1	J	132	HIS	N-CA-C	-5.31	105.49	111.28
2	B	368	THR	N-CA-C	-5.30	104.24	111.56
3	C	338	LYS	CA-C-N	5.30	131.24	121.70
3	C	338	LYS	C-N-CA	5.30	131.24	121.70
2	K	366	THR	N-CA-C	5.28	117.94	111.82
1	G	149	ARG	N-CA-C	-5.26	107.52	114.04
3	C	170	LYS	CA-C-N	5.26	126.41	119.84
3	C	170	LYS	C-N-CA	5.26	126.41	119.84
2	B	406	ARG	CA-C-N	5.25	131.15	121.70
2	B	406	ARG	C-N-CA	5.25	131.15	121.70
1	D	144	LEU	N-CA-C	-5.24	105.48	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	263	ALA	N-CA-C	5.23	118.34	109.76
2	K	260	VAL	N-CA-C	5.22	116.00	108.48
3	F	370	ALA	N-CA-C	5.22	119.99	111.37
3	C	249	GLU	N-CA-C	-5.22	102.76	110.48
2	K	355	ASP	N-CA-C	5.20	120.40	112.54
3	C	134	GLN	N-CA-C	-5.19	106.90	113.18
2	E	173	GLU	N-CA-C	-5.18	106.81	113.23
3	I	263	ALA	N-CA-C	5.17	118.24	109.76
2	E	366	THR	N-CA-C	5.17	117.81	111.82
3	L	216	GLY	N-CA-C	-5.16	104.68	112.84
2	K	354	MET	N-CA-C	5.16	119.29	112.89
3	F	193	VAL	N-CA-C	5.16	116.12	108.23
1	G	176	LYS	N-CA-C	-5.16	106.94	113.18
3	F	157	ALA	N-CA-C	-5.15	105.79	111.71
3	L	337	ASN	CB-CA-C	-5.14	108.98	116.53
3	I	368	ILE	N-CA-C	5.13	116.54	109.46
3	F	340	HIS	N-CA-C	5.11	116.29	108.42
1	D	143	GLN	N-CA-C	5.11	117.51	111.33
3	L	257	THR	N-CA-C	5.11	116.06	108.86
1	A	175	LEU	N-CA-C	-5.10	106.37	112.59
2	H	368	THR	N-CA-C	-5.09	104.54	111.56
3	L	124	LEU	N-CA-C	-5.07	105.64	111.07
3	I	127	LYS	N-CA-C	-5.07	106.84	112.57
3	C	314	THR	N-CA-C	-5.06	102.70	110.14
2	B	412	PRO	N-CA-C	-5.05	102.07	112.47
2	B	155	GLU	N-CA-C	-5.04	107.08	114.39
3	L	339	CYS	N-CA-C	5.04	121.53	110.80
3	F	336	MET	N-CA-C	5.03	117.95	109.95
2	H	417	TYR	N-CA-C	5.03	116.95	108.96
3	L	151	LYS	N-CA-C	-5.02	106.33	112.90
3	L	368	ILE	CB-CA-C	-5.02	104.36	111.38
2	H	182	LEU	N-CA-C	-5.01	100.12	110.80
2	K	397	GLU	N-CA-C	-5.01	103.43	110.35
3	F	369	TRP	N-CA-C	-5.00	99.07	107.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	378	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	608	0	649	151	0
1	D	584	0	623	84	0
1	G	608	0	649	126	0
1	J	652	0	695	101	0
2	B	2462	0	2327	531	0
2	E	2434	0	2295	259	0
2	H	2462	0	2326	461	0
2	K	2442	0	2307	254	0
3	C	2446	0	2294	489	0
3	F	2410	0	2256	311	0
3	I	2446	0	2294	474	0
3	L	2410	0	2256	328	0
4	M	30	0	32	2	0
4	N	30	0	32	7	0
4	O	30	0	32	4	0
4	P	30	0	32	4	0
4	Q	30	0	32	2	0
4	R	30	0	32	8	0
4	S	30	0	32	8	0
4	T	30	0	32	3	0
5	B	14	0	13	1	0
5	E	14	0	13	0	0
5	H	14	0	13	4	0
5	K	14	0	13	3	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	K	2	0	0	0	0
6	L	1	0	0	0	0
All	All	22270	0	21279	3347	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 77.

All (3347) 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)
2:B:165:LEU:H	2:B:166:ARG:NH2	1.45	1.15
3:C:197:ARG:HA	3:C:225:GLU:HG2	1.27	1.14
1:G:147:MET:HE2	2:H:179:ILE:HG12	1.28	1.12
3:I:197:ARG:HA	3:I:225:GLU:HG2	1.30	1.12
3:I:171:PRO:HB2	3:I:174:ALA:HB2	1.33	1.06
3:C:171:PRO:HB2	3:C:174:ALA:HB2	1.33	1.05
2:B:165:LEU:N	2:B:166:ARG:HH21	1.56	1.03
3:C:154:GLN:HE22	3:C:189:ASN:HA	1.25	1.01
3:C:212:LYS:HG2	3:C:231:GLU:HB2	1.42	1.01
3:I:169:ILE:HD12	3:I:171:PRO:HD3	1.41	1.01
3:I:212:LYS:HG2	3:I:231:GLU:HB2	1.43	1.01
1:D:147:MET:HG3	2:E:175:LEU:HD22	1.41	1.00
3:F:148:ILE:HD12	3:F:148:ILE:H	1.24	1.00
2:B:176:ARG:HA	2:B:179:ILE:HD12	1.40	0.99
3:C:169:ILE:HD12	3:C:171:PRO:HD3	1.43	0.99
2:B:249:TRP:HH2	2:B:325:HIS:HE2	1.11	0.98
2:H:249:TRP:HH2	2:H:325:HIS:HE2	1.12	0.98
3:I:154:GLN:HE22	3:I:189:ASN:HA	1.29	0.98
3:L:96:TYR:H	3:L:96:TYR:HD2	1.09	0.97
2:K:367:MET:HB2	2:K:406:ARG:HB3	1.48	0.96
3:I:189:ASN:ND2	3:I:391:ARG:HB3	1.79	0.96
2:B:193:CYS:HB3	3:C:134:GLN:HE22	1.32	0.95
2:K:367:MET:SD	2:K:406:ARG:HG2	2.07	0.95
2:H:210:GLU:HA	2:H:227:ILE:HB	1.49	0.94
2:E:212:GLU:O	2:E:215:ILE:HG22	1.70	0.92
2:K:212:GLU:O	2:K:215:ILE:HG22	1.70	0.92
2:B:204:PRO:HA	3:C:217:HIS:HA	1.52	0.92
3:I:154:GLN:HE21	3:I:158:ASN:ND2	1.68	0.92
3:C:209:ILE:H	3:C:209:ILE:HD12	1.35	0.92
3:I:193:VAL:HG12	3:I:194:PHE:N	1.85	0.91
2:H:357:ALA:HA	2:H:439:ASN:HD21	1.34	0.91
3:C:193:VAL:HG12	3:C:194:PHE:H	1.32	0.91
2:K:187:SER:HA	2:K:190:MET:HE3	1.51	0.91
2:H:204:PRO:HA	3:I:217:HIS:HA	1.53	0.91
2:H:359:GLN:O	2:H:360:LEU:HD23	1.70	0.91
3:I:209:ILE:H	3:I:209:ILE:HD12	1.35	0.91
3:C:189:ASN:ND2	3:C:391:ARG:HB3	1.85	0.90
3:C:154:GLN:HE21	3:C:158:ASN:ND2	1.69	0.90
2:B:210:GLU:HA	2:B:227:ILE:HB	1.53	0.90
3:I:193:VAL:HG12	3:I:194:PHE:H	1.34	0.90
3:C:249:GLU:HB3	3:C:383:THR:HG23	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:249:GLU:HB3	3:I:383:THR:HG23	1.54	0.90
3:L:148:ILE:H	3:L:148:ILE:HD12	1.33	0.90
2:B:180:GLN:O	2:B:183:GLU:HB3	1.71	0.89
3:I:103:HIS:O	3:I:107:ILE:HG12	1.73	0.89
1:A:143:GLN:HA	1:A:143:GLN:HE21	1.35	0.89
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.20	0.89
3:L:230:ASN:HA	3:L:233:ILE:HD12	1.54	0.89
1:A:167:ARG:HH12	1:A:169:LEU:HD23	1.35	0.89
3:L:258:SER:HB2	3:L:286:ALA:HB2	1.55	0.89
3:C:287:GLY:HA3	3:C:371:THR:O	1.72	0.88
1:A:148:LYS:NZ	2:B:425:ASP:HB2	1.89	0.88
2:B:357:ALA:HA	2:B:439:ASN:HD21	1.39	0.88
2:E:373:MET:HG3	2:E:405:ASN:HB2	1.56	0.88
2:H:373:MET:SD	2:H:405:ASN:HB2	2.13	0.88
3:C:196:LYS:HG2	3:C:198:LEU:HD11	1.56	0.88
2:B:310:LEU:HD11	2:B:312:ILE:HG13	1.56	0.88
3:L:227:TRP:HZ2	3:L:230:ASN:HD21	1.17	0.88
3:I:107:ILE:HG13	3:I:108:ARG:H	1.38	0.88
2:B:256:GLN:HE21	2:B:449:LYS:HE2	1.36	0.87
3:I:196:LYS:HG2	3:I:198:LEU:HD11	1.57	0.87
3:C:193:VAL:HG12	3:C:194:PHE:N	1.83	0.87
2:H:310:LEU:HD11	2:H:312:ILE:HG13	1.56	0.87
1:J:167:ARG:HA	1:J:167:ARG:CZ	2.03	0.87
2:B:165:LEU:HD23	2:B:166:ARG:NH2	1.90	0.87
3:F:258:SER:HB2	3:F:286:ALA:HB2	1.57	0.87
1:G:148:LYS:HD3	1:G:182:GLN:HE22	1.38	0.87
3:F:172:LEU:HD13	3:F:240:SER:HB3	1.56	0.87
2:K:373:MET:HG3	2:K:405:ASN:HB2	1.55	0.87
1:A:144:LEU:HD21	1:A:182:GLN:HG2	1.54	0.87
3:I:196:LYS:HE3	3:I:198:LEU:HD21	1.56	0.87
2:H:357:ALA:HA	2:H:439:ASN:ND2	1.90	0.86
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.54	0.86
2:K:412:PRO:O	2:K:413:ASN:HB2	1.76	0.86
2:B:256:GLN:HB3	2:B:449:LYS:HE2	1.57	0.86
3:C:196:LYS:HE3	3:C:198:LEU:HD21	1.57	0.86
3:I:109:TYR:O	3:I:112:GLU:HB3	1.76	0.85
3:L:172:LEU:HD13	3:L:240:SER:HB3	1.58	0.85
2:H:292:TYR:HE2	2:H:294:LEU:HB2	1.42	0.85
2:H:237:ARG:HH11	2:H:237:ARG:HG3	1.41	0.85
2:B:193:CYS:HB3	3:C:134:GLN:NE2	1.91	0.85
2:B:398:ASP:HA	2:B:433:ASP:CB	2.07	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLN:HE22	3:F:117:ASN:HB2	1.39	0.85
1:A:128:GLU:O	1:A:131:GLN:HG2	1.76	0.84
3:C:118:ASN:HD22	3:C:118:ASN:H	1.20	0.84
3:I:154:GLN:HE21	3:I:158:ASN:HD21	1.23	0.84
1:A:169:LEU:HD13	1:A:170:ALA:N	1.91	0.84
3:C:340:HIS:O	4:O:1:GLY:HA2	1.77	0.84
2:K:175:LEU:O	2:K:179:ILE:HG13	1.78	0.84
2:H:256:GLN:HE21	2:H:449:LYS:HE2	1.43	0.84
3:C:230:ASN:HD22	3:C:230:ASN:N	1.72	0.84
2:H:168:LEU:HD23	3:I:110:LEU:HD12	1.60	0.84
1:G:160:SER:OG	2:H:261:ASP:HB3	1.78	0.84
3:C:154:GLN:HE21	3:C:158:ASN:HD21	1.22	0.84
2:H:166:ARG:HH12	2:H:169:ARG:HD2	1.41	0.84
2:H:238:VAL:HG21	2:H:250:THR:HG23	1.59	0.84
2:B:357:ALA:HA	2:B:439:ASN:ND2	1.94	0.83
2:B:237:ARG:HG3	2:B:237:ARG:HH11	1.42	0.83
3:I:287:GLY:HA3	3:I:371:THR:O	1.77	0.83
3:C:193:VAL:CG1	3:C:194:PHE:H	1.91	0.83
3:C:230:ASN:HD22	3:C:230:ASN:H	1.23	0.83
3:I:250:LEU:HD12	3:I:382:THR:HA	1.61	0.83
2:H:215:ILE:HD12	2:H:219:GLY:O	1.79	0.83
3:C:110:LEU:C	3:C:112:GLU:H	1.85	0.82
3:F:230:ASN:HA	3:F:233:ILE:HD12	1.60	0.82
2:B:237:ARG:HH21	3:C:143:VAL:HG23	1.43	0.82
3:I:325:ASN:HD21	3:I:327:ALA:HB3	1.42	0.82
3:L:194:PHE:HD1	3:L:233:ILE:HG12	1.41	0.82
2:H:161:ILE:HG21	3:I:103:HIS:CE1	2.13	0.82
2:H:309:GLU:HB3	2:H:325:HIS:HE1	1.42	0.82
3:F:149:THR:O	3:F:156:ILE:HG12	1.78	0.82
1:J:129:LYS:O	1:J:133:ILE:HG22	1.79	0.82
3:F:166:LEU:HB3	3:F:179:LEU:HD11	1.60	0.82
2:H:256:GLN:HB3	2:H:449:LYS:HE2	1.60	0.82
3:I:227:TRP:HZ2	3:I:230:ASN:HD21	1.25	0.82
2:B:215:ILE:HB	2:B:242:MET:HE3	1.62	0.82
3:F:278:TYR:CZ	3:F:308:ASN:HB2	2.14	0.82
2:H:398:ASP:HA	2:H:433:ASP:CB	2.10	0.82
3:I:107:ILE:HG13	3:I:108:ARG:N	1.94	0.82
2:B:162:PRO:C	2:B:166:ARG:HD2	2.05	0.82
2:B:238:VAL:HG21	2:B:250:THR:HG23	1.61	0.81
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.44	0.81
3:C:230:ASN:H	3:C:230:ASN:ND2	1.76	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:230:ASN:HD22	3:I:230:ASN:N	1.76	0.81
3:L:251:GLU:HB3	3:L:381:LYS:HB2	1.60	0.81
2:H:215:ILE:HD13	2:H:242:MET:HB3	1.62	0.81
2:B:164:ASN:H	2:B:166:ARG:NE	1.77	0.81
2:B:309:GLU:HB3	2:B:325:HIS:HE1	1.44	0.81
3:I:246:LEU:HD12	3:I:247:ARG:N	1.96	0.81
2:B:359:GLN:O	2:B:360:LEU:HD23	1.80	0.81
2:H:237:ARG:HH21	3:I:143:VAL:HG23	1.44	0.81
1:A:160:SER:OG	2:B:261:ASP:HB3	1.80	0.81
2:B:166:ARG:NE	2:B:166:ARG:H	1.78	0.81
2:E:175:LEU:O	2:E:179:ILE:HG13	1.80	0.80
3:C:246:LEU:HD12	3:C:247:ARG:N	1.96	0.80
3:C:250:LEU:HD12	3:C:382:THR:HA	1.62	0.80
3:F:194:PHE:HD1	3:F:233:ILE:HG12	1.44	0.80
2:B:267:ASP:HB2	2:B:268:PRO:HD3	1.62	0.80
3:C:143:VAL:HG12	3:C:220:PRO:HD3	1.63	0.80
2:E:265:LYS:O	2:E:268:PRO:HD2	1.80	0.80
2:K:179:ILE:O	2:K:183:GLU:HG3	1.81	0.80
3:I:273:LYS:HE3	3:I:319:ASN:ND2	1.96	0.80
1:D:132:HIS:HB3	3:F:107:ILE:HD11	1.63	0.80
3:I:230:ASN:HD22	3:I:230:ASN:H	1.29	0.80
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.63	0.80
1:D:132:HIS:HB3	3:F:107:ILE:CD1	2.12	0.79
3:F:117:ASN:O	3:F:121:ILE:HG13	1.80	0.79
3:I:193:VAL:CG1	3:I:194:PHE:H	1.95	0.79
2:B:373:MET:SD	2:B:405:ASN:HB2	2.22	0.79
3:L:149:THR:O	3:L:156:ILE:HG12	1.82	0.79
3:L:338:LYS:HG3	4:T:3:ARG:HB2	1.63	0.79
3:C:278:TYR:OH	3:C:308:ASN:HB2	1.82	0.79
3:C:264:MET:HE2	3:F:279:ALA:HA	1.64	0.79
2:K:393:GLN:HB2	2:K:396:LYS:HG2	1.62	0.79
1:A:128:GLU:HG2	1:A:129:LYS:HD2	1.64	0.79
2:E:412:PRO:O	2:E:413:ASN:HB2	1.83	0.79
1:G:181:GLN:O	1:G:184:GLN:HG3	1.82	0.79
3:I:367:ILE:HG22	3:I:379:MET:HG2	1.64	0.79
3:L:278:TYR:CZ	3:L:308:ASN:HB2	2.17	0.79
2:B:176:ARG:HA	2:B:179:ILE:CD1	2.13	0.78
2:B:373:MET:HE2	2:B:404:TYR:O	1.82	0.78
2:B:399:GLY:HA3	2:B:415:ARG:HD3	1.63	0.78
3:C:325:ASN:HD21	3:C:327:ALA:HB3	1.46	0.78
1:G:169:LEU:HD22	1:G:170:ALA:H	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:330:ASP:HB3	3:I:365:ASN:HB3	1.64	0.78
3:I:163:GLN:HA	3:I:163:GLN:HE21	1.47	0.78
2:B:292:TYR:HE2	2:B:294:LEU:HB2	1.48	0.78
3:C:273:LYS:HE3	3:C:319:ASN:ND2	1.98	0.78
3:I:340:HIS:O	4:S:1:GLY:HA2	1.84	0.78
3:L:322:PHE:HB2	3:L:338:LYS:HD2	1.66	0.78
2:B:215:ILE:HD13	2:B:242:MET:HB3	1.66	0.78
2:B:455:ARG:HG3	2:B:456:PRO:HD2	1.66	0.78
2:E:205:VAL:HG12	2:E:206:VAL:N	1.97	0.78
1:A:155:ASP:HA	1:A:171:ARG:NH2	1.99	0.78
1:D:185:LEU:HB2	2:E:171:ILE:CD1	2.13	0.77
2:H:267:ASP:HB2	2:H:268:PRO:HD3	1.64	0.77
2:H:270:LYS:HA	2:H:296:ASN:HB2	1.66	0.77
3:I:230:ASN:H	3:I:230:ASN:ND2	1.80	0.77
3:L:195:GLN:HG3	3:L:227:TRP:CE3	2.18	0.77
2:H:223:GLU:HB2	2:H:287:GLY:HA2	1.66	0.77
3:I:256:ARG:HG3	3:I:256:ARG:HH11	1.46	0.77
2:K:373:MET:HA	2:K:373:MET:HE3	1.67	0.77
3:C:367:ILE:HG22	3:C:379:MET:HG2	1.65	0.77
3:I:193:VAL:HG12	3:I:195:GLN:H	1.48	0.77
3:L:262:TYR:OH	3:L:290:PHE:HB2	1.84	0.77
1:A:122:LEU:HD23	1:A:122:LEU:H	1.49	0.77
3:C:228:LEU:HD12	3:C:228:LEU:O	1.84	0.77
3:C:256:ARG:HH11	3:C:256:ARG:HG3	1.47	0.77
2:H:186:VAL:HG11	3:I:128:VAL:HG22	1.67	0.77
2:K:351:ASN:HD21	2:K:354:MET:H	1.32	0.77
3:L:166:LEU:HB3	3:L:179:LEU:HD11	1.66	0.77
2:B:284:ASN:H	2:B:284:ASN:HD22	1.30	0.77
3:C:154:GLN:NE2	3:C:189:ASN:HA	1.99	0.77
3:L:117:ASN:O	3:L:121:ILE:HG13	1.85	0.77
2:B:187:SER:HA	2:B:190:MET:HB3	1.66	0.77
2:H:373:MET:HE2	2:H:404:TYR:O	1.84	0.77
1:J:161:CYS:C	1:J:163:GLY:H	1.91	0.77
3:F:195:GLN:HG3	3:F:227:TRP:CE3	2.20	0.77
2:H:411:ASN:HB3	2:H:436:VAL:HG22	1.66	0.77
2:B:223:GLU:HB2	2:B:287:GLY:HA2	1.66	0.76
4:R:3:ARG:HB3	4:R:4:PRO:CD	2.15	0.76
2:B:165:LEU:N	2:B:166:ARG:NH2	2.23	0.76
2:B:165:LEU:HD11	3:C:107:ILE:HA	1.67	0.76
2:B:177:SER:HA	2:B:180:GLN:CG	2.16	0.76
2:K:352:ALA:HB2	2:K:439:ASN:ND2	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.67	0.76
3:C:330:ASP:HB3	3:C:365:ASN:HB3	1.65	0.76
2:H:317:TRP:CD1	2:H:317:TRP:H	2.01	0.76
3:I:170:LYS:HE3	3:I:177:GLN:HB3	1.67	0.76
3:I:337:ASN:C	3:I:339:CYS:H	1.93	0.76
1:G:144:LEU:HD21	1:G:182:GLN:HG3	1.67	0.76
3:I:110:LEU:C	3:I:112:GLU:H	1.92	0.76
1:G:186:GLU:HA	1:G:189:ILE:HG22	1.68	0.76
2:H:159:SER:C	2:H:162:PRO:HD2	2.10	0.76
3:I:278:TYR:OH	3:I:308:ASN:HB2	1.86	0.76
2:K:205:VAL:HG12	2:K:206:VAL:N	2.00	0.76
3:L:281:PHE:HB2	3:L:288:ASP:OD2	1.85	0.76
2:B:161:ILE:HG21	3:C:103:HIS:CD2	2.20	0.76
2:H:399:GLY:HA3	2:H:415:ARG:HD3	1.67	0.76
2:B:411:ASN:HB3	2:B:436:VAL:HG22	1.68	0.76
3:F:212:LYS:HG3	3:F:231:GLU:HB2	1.67	0.76
2:K:216:ARG:HB2	2:K:216:ARG:NH1	2.00	0.76
3:L:204:PHE:C	3:L:206:LYS:H	1.94	0.76
3:F:262:TYR:OH	3:F:290:PHE:HB2	1.84	0.75
2:H:455:ARG:HG3	2:H:456:PRO:HD2	1.68	0.75
2:K:216:ARG:CB	2:K:216:ARG:HH11	1.99	0.75
1:A:143:GLN:HE22	3:C:118:ASN:ND2	1.85	0.75
3:C:197:ARG:C	3:C:198:LEU:HD12	2.11	0.75
2:H:309:GLU:HB3	2:H:325:HIS:CE1	2.22	0.75
2:H:346:ARG:HH11	2:H:346:ARG:HB2	1.50	0.75
2:H:333:ASN:OD1	2:H:335:ALA:HB3	1.86	0.75
2:H:315:GLU:HB2	2:H:321:LYS:HB3	1.68	0.75
1:J:143:GLN:HE22	3:L:117:ASN:HB2	1.50	0.75
3:C:154:GLN:NE2	3:C:158:ASN:HD21	1.84	0.75
3:F:94:MET:HB3	3:F:96:TYR:CE1	2.21	0.75
2:B:178:LYS:C	2:B:180:GLN:H	1.95	0.75
1:D:124:ARG:HD3	1:D:124:ARG:H	1.50	0.75
3:L:337:ASN:C	3:L:339:CYS:H	1.93	0.75
3:C:342:GLY:H	3:C:368:ILE:HG13	1.52	0.75
3:F:251:GLU:HA	3:F:257:THR:HG22	1.68	0.75
2:H:187:SER:O	2:H:191:GLU:HB2	1.86	0.75
3:I:304:PHE:HB3	3:I:338:LYS:HB3	1.69	0.75
1:J:158:ILE:HG23	2:K:189:GLN:HE21	1.51	0.75
1:A:184:GLN:C	1:A:186:GLU:H	1.95	0.74
2:H:398:ASP:HA	2:H:433:ASP:HB3	1.69	0.74
3:L:326:CYS:HB3	3:L:336:MET:HE3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.68	0.74
2:B:309:GLU:HB3	2:B:325:HIS:CE1	2.23	0.74
3:C:193:VAL:HG12	3:C:195:GLN:H	1.51	0.74
2:E:352:ALA:HB2	2:E:439:ASN:ND2	2.02	0.74
2:E:393:GLN:HB2	2:E:396:LYS:HG2	1.68	0.74
3:I:143:VAL:HG12	3:I:220:PRO:HD3	1.68	0.74
3:F:281:PHE:HB2	3:F:288:ASP:OD2	1.86	0.74
2:H:369:ILE:H	2:H:405:ASN:HD22	1.36	0.74
3:I:154:GLN:NE2	3:I:158:ASN:HD21	1.84	0.74
3:F:204:PHE:C	3:F:206:LYS:H	1.95	0.74
3:F:229:GLY:O	3:F:233:ILE:HG13	1.88	0.74
3:I:97:GLU:C	3:I:99:SER:H	1.93	0.74
3:I:203:ASP:O	3:I:206:LYS:HE3	1.87	0.74
3:I:264:MET:N	3:I:264:MET:SD	2.60	0.74
3:C:170:LYS:HE3	3:C:177:GLN:HB3	1.69	0.74
2:E:216:ARG:CB	2:E:216:ARG:HH11	2.00	0.74
3:I:197:ARG:C	3:I:198:LEU:HD12	2.12	0.74
2:B:164:ASN:C	2:B:166:ARG:HE	1.96	0.74
3:F:297:ASP:O	3:F:298:ASP:HB3	1.88	0.74
3:C:172:LEU:HB2	3:C:239:GLN:HB3	1.70	0.74
3:L:292:GLY:N	3:L:306:SER:HA	2.02	0.74
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.34	0.74
2:H:199:VAL:O	3:I:142:THR:HG23	1.88	0.74
3:I:250:LEU:O	3:I:257:THR:HB	1.87	0.74
3:L:212:LYS:HG3	3:L:231:GLU:HB2	1.69	0.74
2:H:215:ILE:HB	2:H:242:MET:HE3	1.69	0.74
2:H:284:ASN:HD22	2:H:284:ASN:H	1.34	0.74
2:H:301:GLN:HE21	2:H:301:GLN:C	1.95	0.74
1:J:175:LEU:HD21	2:K:426:MET:HE2	1.70	0.74
3:F:96:TYR:H	3:F:96:TYR:HD1	1.35	0.73
3:I:154:GLN:NE2	3:I:189:ASN:HA	2.02	0.73
2:K:312:ILE:HG12	2:K:452:MET:HG2	1.68	0.73
3:C:172:LEU:HD13	3:C:239:GLN:CB	2.19	0.73
3:C:382:THR:HG22	3:C:382:THR:O	1.88	0.73
1:D:136:LEU:HD23	2:E:168:LEU:HD13	1.70	0.73
2:H:385:TRP:HB2	2:H:406:ARG:HA	1.71	0.73
2:H:438:MET:HE3	2:H:443:SER:HB2	1.70	0.73
1:J:144:LEU:HD23	2:K:175:LEU:HD21	1.70	0.73
2:B:317:TRP:CZ3	2:B:448:ARG:HD3	2.23	0.73
3:F:278:TYR:OH	3:F:308:ASN:HB2	1.87	0.73
2:B:185:ASP:HA	2:B:188:ALA:HB3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:180:GLN:HG3	2:E:181:LYS:N	2.03	0.73
2:E:216:ARG:NH1	2:E:216:ARG:HB2	2.03	0.73
2:E:373:MET:HA	2:E:373:MET:HE3	1.70	0.73
2:B:215:ILE:HD12	2:B:219:GLY:O	1.88	0.73
2:B:310:LEU:HD11	2:B:312:ILE:CG1	2.18	0.73
3:C:281:PHE:CE2	3:C:288:ASP:HB2	2.23	0.73
3:I:117:ASN:N	3:I:117:ASN:HD22	1.86	0.73
3:L:229:GLY:O	3:L:233:ILE:HG13	1.89	0.73
3:F:96:TYR:C	3:F:98:ALA:H	1.95	0.73
2:H:176:ARG:HA	2:H:179:ILE:CD1	2.18	0.73
2:B:317:TRP:CD1	2:B:317:TRP:H	2.05	0.73
2:H:162:PRO:C	2:H:164:ASN:H	1.96	0.73
3:L:183:GLU:HB3	3:L:191:TRP:HB2	1.70	0.73
1:G:169:LEU:HD13	1:G:171:ARG:N	2.04	0.73
3:I:218:LEU:O	3:I:219:SER:HB3	1.87	0.73
1:A:133:ILE:O	1:A:137:GLN:HB2	1.88	0.73
1:A:156:ILE:HD11	2:B:416:TYR:N	2.04	0.73
2:E:229:PRO:HG3	2:E:301:GLN:HE22	1.52	0.73
2:E:438:MET:HE3	2:E:443:SER:OG	1.88	0.73
2:H:310:LEU:HD11	2:H:312:ILE:CG1	2.19	0.73
1:A:123:LYS:H	1:A:124:ARG:HH11	1.36	0.72
2:H:211:CYS:O	2:H:242:MET:HE1	1.89	0.72
2:B:169:ARG:O	2:B:173:GLU:HB2	1.89	0.72
3:F:325:ASN:C	3:F:325:ASN:HD22	1.96	0.72
2:H:161:ILE:HG22	2:H:162:PRO:HD3	1.70	0.72
3:I:172:LEU:HB2	3:I:239:GLN:HB3	1.71	0.72
3:C:222:GLY:O	3:C:224:THR:HG22	1.89	0.72
3:F:240:SER:O	3:F:242:ILE:HG13	1.89	0.72
3:L:251:GLU:HA	3:L:257:THR:HG22	1.71	0.72
3:C:172:LEU:H	3:C:172:LEU:HD12	1.54	0.72
3:L:297:ASP:O	3:L:298:ASP:HB3	1.89	0.72
2:B:315:GLU:HB2	2:B:321:LYS:HB3	1.70	0.72
3:C:203:ASP:O	3:C:206:LYS:HE3	1.90	0.72
3:F:238:THR:HG22	3:F:266:LYS:HE2	1.70	0.72
2:H:176:ARG:HA	2:H:179:ILE:HD12	1.69	0.72
2:B:300:SER:O	2:B:304:ARG:HG2	1.89	0.72
1:D:140:VAL:HG13	1:D:141:ARG:N	2.04	0.72
2:E:155:GLU:HG3	2:E:156:THR:N	2.05	0.72
2:E:230:ASP:OD2	2:E:232:SER:HB2	1.89	0.72
3:I:222:GLY:O	3:I:224:THR:HG22	1.90	0.72
2:B:211:CYS:O	2:B:242:MET:HE1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:218:LEU:O	3:C:219:SER:HB3	1.88	0.72
2:H:223:GLU:CB	2:H:287:GLY:HA2	2.19	0.72
3:I:342:GLY:H	3:I:368:ILE:HG13	1.54	0.72
3:I:364:ASP:OD2	3:I:368:ILE:HD13	1.89	0.72
3:L:325:ASN:C	3:L:325:ASN:HD22	1.97	0.72
2:B:432:ASP:OD2	2:B:443:SER:OG	2.07	0.72
3:I:228:LEU:HD12	3:I:228:LEU:O	1.89	0.72
2:H:241:ASP:HB3	2:H:249:TRP:HB2	1.71	0.72
3:I:264:MET:HE2	3:L:279:ALA:HA	1.71	0.72
1:A:144:LEU:HD23	1:A:145:VAL:HG23	1.72	0.71
1:A:133:ILE:HG21	2:B:164:ASN:ND2	2.05	0.71
3:I:120:LYS:HA	3:I:123:ASN:HD22	1.55	0.71
2:B:199:VAL:O	3:C:142:THR:HG23	1.90	0.71
1:G:164:SER:HB3	3:I:137:GLU:O	1.89	0.71
2:H:346:ARG:HH11	2:H:346:ARG:CB	2.03	0.71
3:L:325:ASN:HD21	3:L:327:ALA:HB3	1.55	0.71
1:A:158:ILE:HD11	2:B:189:GLN:HB3	1.72	0.71
3:C:97:GLU:C	3:C:99:SER:H	1.96	0.71
2:E:351:ASN:C	2:E:351:ASN:HD22	1.98	0.71
3:F:246:LEU:HD22	3:F:265:PHE:CD1	2.25	0.71
3:I:103:HIS:HA	3:I:106:SER:HB3	1.72	0.71
2:B:346:ARG:HB2	2:B:346:ARG:HH11	1.55	0.71
2:B:412:PRO:HA	2:B:450:MET:HE1	1.72	0.71
1:G:159:ARG:HB3	2:H:258:GLY:HA3	1.72	0.71
2:H:292:TYR:CE2	2:H:294:LEU:HB2	2.25	0.71
2:H:300:SER:O	2:H:304:ARG:HG2	1.90	0.71
1:G:132:HIS:C	1:G:133:ILE:HD12	2.16	0.71
3:I:171:PRO:CB	3:I:174:ALA:HB2	2.18	0.71
3:I:189:ASN:HD21	3:I:391:ARG:HB3	1.54	0.71
2:B:256:GLN:HA	2:B:449:LYS:HG2	1.72	0.71
2:B:346:ARG:HH11	2:B:346:ARG:CB	2.04	0.71
2:B:369:ILE:H	2:B:405:ASN:HD22	1.38	0.71
2:E:179:ILE:O	2:E:183:GLU:HG3	1.89	0.71
2:H:172:LEU:HD23	2:H:172:LEU:O	1.90	0.71
2:B:191:GLU:C	2:B:193:CYS:H	1.99	0.71
3:L:105:SER:HA	3:L:108:ARG:HG2	1.71	0.71
3:L:145:ILE:HG21	3:L:168:PHE:CE2	2.26	0.71
2:B:165:LEU:HD23	2:B:166:ARG:HH22	1.56	0.70
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.72	0.70
3:C:171:PRO:CB	3:C:174:ALA:HB2	2.19	0.70
2:B:333:ASN:OD1	2:B:335:ALA:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:325:ASN:ND2	3:I:327:ALA:HB3	2.06	0.70
2:H:242:MET:SD	2:H:248:GLY:HA2	2.31	0.70
2:H:317:TRP:CZ3	2:H:448:ARG:HD3	2.26	0.70
1:J:151:GLU:HG3	1:J:178:TYR:CE2	2.25	0.70
3:L:320:ASP:HB2	3:L:337:ASN:O	1.91	0.70
2:B:210:GLU:OE2	2:B:212:GLU:HB3	1.91	0.70
3:C:250:LEU:O	3:C:257:THR:HB	1.91	0.70
3:F:270:GLU:HB2	3:F:274:TYR:OH	1.92	0.70
1:G:157:LYS:O	1:G:160:SER:HB3	1.91	0.70
3:I:382:THR:HG22	3:I:382:THR:O	1.90	0.70
3:L:292:GLY:HA2	3:L:305:THR:C	2.17	0.70
2:B:157:VAL:O	2:B:158:ASN:HB2	1.90	0.70
2:E:200:SER:H	2:E:279:ASN:ND2	1.89	0.70
3:F:101:LEU:O	3:F:104:ASP:HB3	1.91	0.70
3:F:251:GLU:CB	3:F:381:LYS:HB2	2.21	0.70
1:A:176:LYS:O	1:A:180:ASP:HB2	1.92	0.70
1:D:161:CYS:C	1:D:163:GLY:H	1.98	0.70
3:C:118:ASN:HD22	3:C:118:ASN:N	1.90	0.70
3:C:264:MET:N	3:C:264:MET:SD	2.64	0.70
2:H:256:GLN:HA	2:H:449:LYS:HG2	1.73	0.70
2:B:183:GLU:O	2:B:186:VAL:HG12	1.91	0.70
2:B:223:GLU:CB	2:B:287:GLY:HA2	2.21	0.70
3:L:194:PHE:CD1	3:L:233:ILE:HG12	2.25	0.70
2:B:242:MET:SD	2:B:248:GLY:HA2	2.32	0.70
2:B:253:GLN:HB2	2:B:293:TRP:CE3	2.26	0.70
2:B:439:ASN:HD22	2:B:439:ASN:H	1.40	0.70
3:C:365:ASN:HD22	3:C:365:ASN:H	1.38	0.70
1:A:184:GLN:HE21	1:A:185:LEU:HB2	1.57	0.70
3:F:292:GLY:N	3:F:306:SER:HA	2.06	0.70
3:I:263:ALA:HB3	3:I:279:ALA:HB3	1.73	0.70
3:I:365:ASN:HD22	3:I:365:ASN:H	1.38	0.70
3:L:278:TYR:HD1	3:L:279:ALA:N	1.88	0.70
3:F:243:PRO:O	3:F:389:PHE:N	2.25	0.69
3:C:170:LYS:HG3	3:C:175:ASN:O	1.92	0.69
1:D:185:LEU:HB2	2:E:171:ILE:HD13	1.74	0.69
2:E:215:ILE:HA	2:E:219:GLY:O	1.92	0.69
2:E:406:ARG:HH21	4:N:5:NH2:N	1.90	0.69
3:I:367:ILE:HB	3:I:379:MET:H	1.56	0.69
2:B:345:TYR:CE2	2:B:351:ASN:HB2	2.28	0.69
3:F:391:ARG:NH1	3:F:391:ARG:HB2	2.07	0.69
1:D:175:LEU:HD21	2:E:426:MET:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:235:PRO:HG2	3:F:168:PHE:HE1	1.56	0.69
3:F:278:TYR:HD1	3:F:279:ALA:N	1.89	0.69
3:F:365:ASN:HD22	3:F:365:ASN:H	1.36	0.69
3:I:318:ASP:HB2	3:I:320:ASP:OD1	1.92	0.69
2:K:373:MET:SD	2:K:405:ASN:ND2	2.65	0.69
3:L:243:PRO:O	3:L:389:PHE:N	2.26	0.69
3:L:246:LEU:HD22	3:L:265:PHE:CD1	2.27	0.69
3:L:391:ARG:NH1	3:L:391:ARG:HB2	2.07	0.69
2:H:434:GLY:O	2:H:436:VAL:N	2.26	0.69
3:I:343:HIS:O	3:I:367:ILE:HA	1.91	0.69
1:D:143:GLN:NE2	3:F:117:ASN:HB2	2.08	0.69
3:C:322:PHE:HD1	3:C:338:LYS:HG3	1.56	0.69
3:F:320:ASP:HB2	3:F:337:ASN:O	1.93	0.69
2:H:316:ASP:HB2	2:H:445:TYR:HE2	1.57	0.69
2:H:351:ASN:ND2	2:H:354:MET:H	1.90	0.69
3:I:325:ASN:HD21	3:I:327:ALA:CB	2.06	0.69
2:K:406:ARG:HE	4:R:3:ARG:HB2	1.58	0.69
3:C:364:ASP:OD2	3:C:368:ILE:HD13	1.93	0.69
2:E:351:ASN:HD21	2:E:354:MET:H	1.40	0.69
2:E:373:MET:SD	2:E:405:ASN:ND2	2.66	0.69
2:H:310:LEU:HA	2:H:454:ILE:HG22	1.74	0.69
3:I:172:LEU:H	3:I:172:LEU:HD12	1.57	0.69
1:J:126:VAL:HG13	1:J:127:ILE:N	2.06	0.69
3:L:238:THR:HG22	3:L:266:LYS:HE2	1.75	0.69
2:B:193:CYS:CB	3:C:134:GLN:HE22	2.06	0.69
3:C:194:PHE:CZ	3:C:384:MET:HE2	2.27	0.69
3:C:343:HIS:O	3:C:367:ILE:HA	1.92	0.69
2:B:173:GLU:HA	2:B:176:ARG:HB2	1.75	0.68
3:C:227:TRP:CD1	3:C:229:GLY:HA2	2.28	0.68
2:E:406:ARG:NH2	4:N:5:NH2:N	2.41	0.68
3:L:240:SER:O	3:L:242:ILE:HG13	1.93	0.68
3:F:289:ALA:HB2	3:F:371:THR:OG1	1.93	0.68
2:K:351:ASN:C	2:K:351:ASN:HD22	2.00	0.68
4:N:3:ARG:HB3	4:N:4:PRO:HD2	1.76	0.68
2:H:345:TYR:CE2	2:H:351:ASN:HB2	2.29	0.68
3:I:227:TRP:CD1	3:I:229:GLY:HA2	2.29	0.68
3:I:278:TYR:CZ	3:I:308:ASN:HB2	2.29	0.68
2:K:351:ASN:ND2	2:K:354:MET:H	1.91	0.68
3:C:151:LYS:HB2	3:C:155:ASP:HB2	1.74	0.68
2:H:172:LEU:HD21	3:I:113:ILE:HG22	1.76	0.68
3:I:172:LEU:HD13	3:I:239:GLN:CB	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:229:PRO:HG3	2:K:301:GLN:HE22	1.58	0.68
2:K:265:LYS:O	2:K:268:PRO:HD2	1.93	0.68
3:L:270:GLU:HB2	3:L:274:TYR:OH	1.94	0.68
3:C:179:LEU:HD23	3:C:218:LEU:HD12	1.74	0.68
3:C:278:TYR:CZ	3:C:308:ASN:HB2	2.29	0.68
3:F:94:MET:HB3	3:F:96:TYR:HE1	1.57	0.68
3:I:120:LYS:HA	3:I:123:ASN:ND2	2.08	0.68
3:I:154:GLN:CD	3:I:190:GLY:H	2.02	0.68
3:L:365:ASN:HD22	3:L:365:ASN:H	1.39	0.68
3:I:194:PHE:CZ	3:I:384:MET:HE2	2.29	0.68
2:K:352:ALA:HB2	2:K:439:ASN:HD22	1.56	0.68
3:F:292:GLY:HA2	3:F:305:THR:C	2.19	0.68
3:I:197:ARG:NH2	3:I:346:GLY:O	2.27	0.68
2:B:161:ILE:HG21	3:C:103:HIS:HD2	1.59	0.68
2:B:301:GLN:NE2	2:B:302:LEU:HD23	2.09	0.68
2:B:370:HIS:O	2:B:373:MET:HB2	1.94	0.68
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.76	0.68
3:C:273:LYS:HE3	3:C:319:ASN:HD21	1.58	0.68
2:H:402:TRP:CH2	2:H:412:PRO:HG2	2.29	0.68
2:E:312:ILE:HG12	2:E:452:MET:HG2	1.76	0.67
1:J:133:ILE:CD1	2:K:161:ILE:HG23	2.24	0.67
3:C:126:GLU:C	3:C:128:VAL:H	2.01	0.67
3:I:110:LEU:HD23	3:I:110:LEU:N	2.08	0.67
2:K:180:GLN:HG3	2:K:181:LYS:N	2.08	0.67
2:B:402:TRP:CH2	2:B:412:PRO:HG2	2.29	0.67
3:C:154:GLN:CD	3:C:190:GLY:H	2.02	0.67
2:H:173:GLU:C	2:H:175:LEU:H	2.01	0.67
2:H:210:GLU:OE2	2:H:212:GLU:HB3	1.94	0.67
2:H:373:MET:HE3	2:H:374:PHE:H	1.58	0.67
3:I:365:ASN:HD22	3:I:365:ASN:N	1.89	0.67
2:B:316:ASP:HB2	2:B:445:TYR:HE2	1.58	0.67
2:B:434:GLY:O	2:B:436:VAL:N	2.28	0.67
3:C:221:THR:OG1	3:C:222:GLY:N	2.23	0.67
3:C:263:ALA:HB3	3:C:279:ALA:HB3	1.75	0.67
2:H:193:CYS:HB3	3:I:134:GLN:NE2	2.10	0.67
3:I:221:THR:OG1	3:I:222:GLY:N	2.21	0.67
3:I:281:PHE:CE2	3:I:288:ASP:HB2	2.29	0.67
2:H:299:ILE:O	2:H:303:THR:HG23	1.94	0.67
1:J:117:SER:O	1:J:121:VAL:HG23	1.95	0.67
3:L:278:TYR:OH	3:L:308:ASN:HB2	1.94	0.67
2:E:239:TYR:CZ	2:E:289:PRO:HD3	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:352:ALA:HB2	2:E:439:ASN:HD22	1.59	0.67
3:F:195:GLN:HG3	3:F:227:TRP:CZ3	2.28	0.67
2:H:304:ARG:NH2	2:H:333:ASN:N	2.43	0.67
3:I:310:MET:HE1	3:I:321:LYS:HE3	1.77	0.67
3:C:365:ASN:HD22	3:C:365:ASN:N	1.89	0.67
3:F:194:PHE:CD1	3:F:233:ILE:HG12	2.29	0.67
2:H:287:GLY:O	2:H:288:LEU:HD23	1.95	0.67
2:E:393:GLN:HB2	2:E:396:LYS:CG	2.25	0.67
2:H:364:ASN:ND2	5:H:470:NAG:H62	2.10	0.67
3:I:251:GLU:HB3	3:I:381:LYS:HB2	1.77	0.67
1:A:179:GLU:HG3	1:A:182:GLN:OE1	1.94	0.67
2:B:238:VAL:HG22	2:B:239:TYR:N	2.09	0.67
2:B:438:MET:HE3	2:B:443:SER:HB2	1.77	0.67
1:D:160:SER:HA	2:E:258:GLY:O	1.95	0.67
3:F:100:ILE:HG22	3:F:103:HIS:HB2	1.76	0.67
3:F:305:THR:HB	3:F:341:ALA:HB2	1.77	0.67
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.10	0.66
2:B:204:PRO:HA	3:C:217:HIS:CA	2.22	0.66
3:C:197:ARG:NH2	3:C:346:GLY:O	2.29	0.66
2:E:203:ILE:HD12	2:E:203:ILE:N	2.10	0.66
3:I:111:GLN:HG2	3:I:111:GLN:O	1.93	0.66
3:F:237:SER:HB3	3:F:266:LYS:HA	1.76	0.66
3:I:170:LYS:HG3	3:I:175:ASN:O	1.95	0.66
2:K:230:ASP:OD2	2:K:232:SER:HB2	1.94	0.66
2:K:391:ARG:HG2	2:K:391:ARG:HH11	1.59	0.66
3:C:367:ILE:HB	3:C:379:MET:H	1.59	0.66
1:G:139:ASN:HB3	3:I:114:TYR:CZ	2.30	0.66
2:H:301:GLN:HE21	2:H:302:LEU:N	1.93	0.66
2:H:439:ASN:HD22	2:H:439:ASN:H	1.42	0.66
3:I:133:ALA:HA	3:I:136:GLN:HG2	1.76	0.66
3:I:151:LYS:HB2	3:I:155:ASP:HB2	1.75	0.66
3:I:250:LEU:HD23	3:I:372:TRP:CZ3	2.30	0.66
2:B:165:LEU:N	2:B:166:ARG:HE	1.92	0.66
2:B:236:TYR:OH	2:B:302:LEU:HD21	1.96	0.66
3:F:145:ILE:HD13	3:F:168:PHE:HE2	1.59	0.66
1:G:124:ARG:H	1:G:124:ARG:HD2	1.60	0.66
2:H:270:LYS:HE3	2:H:334:GLU:OE1	1.95	0.66
2:H:432:ASP:OD2	2:H:443:SER:OG	2.14	0.66
1:J:133:ILE:O	1:J:133:ILE:HG12	1.94	0.66
2:K:203:ILE:HD12	2:K:203:ILE:N	2.10	0.66
1:A:167:ARG:HG3	2:B:192:TYR:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:241:ASP:O	2:B:248:GLY:N	2.28	0.66
3:C:389:PHE:C	3:C:391:ARG:H	2.03	0.66
2:H:301:GLN:NE2	2:H:302:LEU:HD23	2.11	0.66
1:J:138:LYS:HB2	1:J:138:LYS:NZ	2.09	0.66
1:J:156:ILE:HG22	1:J:157:LYS:HZ2	1.61	0.66
3:L:305:THR:HB	3:L:341:ALA:HB2	1.76	0.66
2:B:213:GLU:HG2	2:B:217:LYS:HE3	1.78	0.66
2:H:203:ILE:HG21	2:H:226:LEU:HD22	1.77	0.66
2:H:204:PRO:HA	3:I:217:HIS:CA	2.23	0.66
2:K:393:GLN:HB2	2:K:396:LYS:CG	2.26	0.66
2:B:301:GLN:HE21	2:B:301:GLN:C	2.03	0.66
3:C:325:ASN:ND2	3:C:327:ALA:HB3	2.11	0.66
3:F:325:ASN:HD21	3:F:327:ALA:HB3	1.61	0.66
2:H:213:GLU:HG2	2:H:217:LYS:HE3	1.78	0.66
3:I:273:LYS:HE3	3:I:319:ASN:HD21	1.58	0.66
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.29	0.66
2:B:351:ASN:ND2	2:B:354:MET:H	1.92	0.66
3:C:227:TRP:CZ2	3:C:230:ASN:ND2	2.64	0.66
2:H:237:ARG:HG3	2:H:237:ARG:NH1	2.06	0.66
2:H:241:ASP:O	2:H:248:GLY:N	2.28	0.66
3:I:163:GLN:HE21	3:I:163:GLN:CA	2.08	0.66
3:L:227:TRP:CZ2	3:L:230:ASN:ND2	2.61	0.66
2:B:162:PRO:HA	2:B:166:ARG:HD2	1.78	0.66
3:C:167:TYR:CD1	3:C:167:TYR:N	2.64	0.66
3:C:251:GLU:HA	3:C:257:THR:HA	1.75	0.66
3:F:234:HIS:NE2	3:F:269:PRO:HB3	2.11	0.66
2:H:370:HIS:O	2:H:373:MET:HB2	1.96	0.66
3:I:103:HIS:C	3:I:105:SER:H	2.04	0.66
2:K:159:SER:C	2:K:160:ASN:HD22	2.03	0.66
2:K:215:ILE:HA	2:K:219:GLY:O	1.95	0.66
2:K:267:ASP:HB3	2:K:268:PRO:HD3	1.78	0.66
3:L:141:ASP:OD1	3:L:143:VAL:HG22	1.96	0.66
2:B:165:LEU:HD13	3:C:110:LEU:HD22	1.78	0.66
2:B:345:TYR:CD2	2:B:351:ASN:HB2	2.31	0.66
3:C:178:PHE:CE1	3:C:232:LYS:HG2	2.31	0.66
3:F:145:ILE:HG21	3:F:168:PHE:CE2	2.31	0.66
1:G:121:VAL:HG12	1:G:124:ARG:HE	1.60	0.66
3:I:330:ASP:HB3	3:I:365:ASN:CB	2.26	0.66
2:K:406:ARG:NH2	4:R:5:NH2:N	2.43	0.66
3:L:96:TYR:CD2	3:L:96:TYR:N	2.63	0.66
4:R:3:ARG:HB3	4:R:4:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:154:GLN:C	3:F:156:ILE:H	2.04	0.65
3:I:389:PHE:C	3:I:391:ARG:H	2.04	0.65
2:E:391:ARG:HG2	2:E:391:ARG:HH11	1.59	0.65
2:H:214:ILE:HD13	2:H:225:TYR:HD2	1.61	0.65
2:H:412:PRO:HA	2:H:450:MET:HE1	1.79	0.65
3:L:251:GLU:CB	3:L:381:LYS:HB2	2.26	0.65
3:C:141:ASP:OD2	3:C:143:VAL:HG22	1.96	0.65
1:G:132:HIS:O	1:G:133:ILE:HD12	1.97	0.65
2:K:161:ILE:HB	2:K:162:PRO:HD3	1.77	0.65
2:K:167:VAL:HG12	2:K:168:LEU:HD22	1.77	0.65
2:B:294:LEU:O	2:B:295:GLY:O	2.14	0.65
3:C:189:ASN:HD21	3:C:391:ARG:HB3	1.59	0.65
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.77	0.65
3:F:162:LYS:HE3	3:F:186:GLY:HA2	1.78	0.65
1:A:124:ARG:N	1:A:124:ARG:HD2	2.12	0.65
1:A:167:ARG:HD2	1:A:168:ALA:N	2.12	0.65
2:B:203:ILE:HG21	2:B:226:LEU:HD22	1.78	0.65
3:C:103:HIS:HA	3:C:106:SER:HB2	1.78	0.65
3:I:178:PHE:CE1	3:I:232:LYS:HG2	2.32	0.65
2:B:292:TYR:CE2	2:B:294:LEU:HB2	2.31	0.65
2:B:373:MET:HE3	2:B:374:PHE:H	1.60	0.65
3:C:197:ARG:HA	3:C:225:GLU:CG	2.16	0.65
3:C:330:ASP:HB3	3:C:365:ASN:CB	2.27	0.65
3:F:246:LEU:HD13	3:F:265:PHE:CE2	2.30	0.65
3:I:227:TRP:HZ2	3:I:230:ASN:ND2	1.94	0.65
2:B:177:SER:HA	2:B:180:GLN:HG3	1.79	0.65
2:E:166:ARG:O	2:E:169:ARG:HB3	1.97	0.65
2:E:251:VAL:HG22	2:E:453:LYS:HG2	1.78	0.65
2:E:256:GLN:N	2:E:291:GLU:OE2	2.29	0.65
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.79	0.65
3:F:326:CYS:HB3	3:F:336:MET:HE3	1.79	0.65
2:H:294:LEU:O	2:H:295:GLY:O	2.15	0.65
3:I:310:MET:HE2	3:I:310:MET:HA	1.77	0.65
1:A:148:LYS:HE3	2:B:425:ASP:O	1.97	0.65
2:B:270:LYS:HE3	2:B:334:GLU:OE1	1.97	0.65
2:B:328:GLY:O	2:B:342:VAL:HA	1.96	0.65
3:C:193:VAL:CG1	3:C:195:GLN:H	2.10	0.65
2:E:199:VAL:HG23	3:F:141:ASP:HA	1.79	0.65
2:E:359:GLN:OE1	2:E:438:MET:HB3	1.96	0.65
2:H:202:ASN:ND2	2:H:284:ASN:HB2	2.11	0.65
2:K:239:TYR:CZ	2:K:289:PRO:HD3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:302:LEU:HD13	2:K:454:ILE:HD11	1.76	0.65
3:L:154:GLN:C	3:L:156:ILE:H	2.05	0.65
3:L:166:LEU:HD22	3:L:218:LEU:HB3	1.79	0.65
2:B:252:ILE:HD11	2:B:454:ILE:HG12	1.79	0.65
2:H:255:ARG:NH1	2:H:413:ASN:HA	2.12	0.65
2:H:304:ARG:NH2	2:H:333:ASN:H	1.95	0.65
3:I:249:GLU:HB3	3:I:383:THR:CG2	2.24	0.65
2:B:238:VAL:CG2	2:B:239:TYR:N	2.59	0.65
2:B:369:ILE:H	2:B:405:ASN:ND2	1.94	0.65
2:B:412:PRO:CA	2:B:450:MET:HE1	2.27	0.65
2:K:373:MET:HE3	2:K:374:PHE:H	1.61	0.65
2:B:304:ARG:NH2	2:B:333:ASN:N	2.45	0.64
3:C:343:HIS:HB3	3:C:366:GLY:O	1.97	0.64
3:C:367:ILE:O	3:C:378:SER:HA	1.98	0.64
2:H:253:GLN:HB2	2:H:293:TRP:CE3	2.32	0.64
2:H:345:TYR:CD2	2:H:351:ASN:HB2	2.32	0.64
3:I:97:GLU:O	3:I:99:SER:N	2.29	0.64
3:L:145:ILE:HG21	3:L:168:PHE:HE2	1.62	0.64
2:B:158:ASN:HA	2:B:162:PRO:HG2	1.79	0.64
3:C:235:LEU:H	3:C:235:LEU:HD12	1.63	0.64
3:C:318:ASP:HB2	3:C:320:ASP:OD1	1.97	0.64
1:D:123:LYS:C	1:D:125:LYS:H	2.04	0.64
1:G:168:ALA:HA	2:H:189:GLN:NE2	2.12	0.64
3:I:141:ASP:OD2	3:I:143:VAL:HG22	1.97	0.64
3:L:97:GLU:HA	3:L:100:ILE:HG13	1.79	0.64
2:B:159:SER:N	2:B:162:PRO:HD2	2.13	0.64
2:B:162:PRO:HA	2:B:166:ARG:HH11	1.62	0.64
2:B:299:ILE:O	2:B:303:THR:HG23	1.97	0.64
3:C:310:MET:HE1	3:C:321:LYS:HE3	1.79	0.64
3:I:347:VAL:HG23	3:I:365:ASN:O	1.98	0.64
2:E:189:GLN:O	2:E:193:CYS:SG	2.54	0.64
2:H:328:GLY:O	2:H:342:VAL:HA	1.97	0.64
2:K:327:GLY:HA3	2:K:344:LYS:HB2	1.77	0.64
1:A:140:VAL:O	1:A:143:GLN:N	2.30	0.64
2:B:153:ILE:C	2:B:155:GLU:H	2.05	0.64
2:B:237:ARG:HG3	2:B:237:ARG:NH1	2.07	0.64
3:C:100:ILE:O	3:C:100:ILE:HG22	1.98	0.64
3:C:389:PHE:HE1	3:C:392:LEU:HD22	1.61	0.64
2:E:200:SER:H	2:E:279:ASN:HD21	1.44	0.64
2:H:190:MET:O	2:H:193:CYS:HB2	1.97	0.64
2:K:200:SER:H	2:K:279:ASN:ND2	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:3:ARG:HB3	4:N:4:PRO:CD	2.27	0.64
3:C:325:ASN:HD21	3:C:327:ALA:CB	2.11	0.64
2:H:266:TRP:HA	2:H:266:TRP:CE3	2.31	0.64
2:H:369:ILE:H	2:H:405:ASN:ND2	1.94	0.64
2:K:189:GLN:O	2:K:193:CYS:SG	2.54	0.64
2:E:272:GLY:HA2	2:E:293:TRP:O	1.98	0.64
3:I:251:GLU:HA	3:I:257:THR:HA	1.77	0.64
2:K:315:GLU:HG3	2:K:321:LYS:HG2	1.78	0.64
1:A:128:GLU:HG2	1:A:129:LYS:CD	2.28	0.64
2:B:287:GLY:O	2:B:288:LEU:HD23	1.98	0.64
2:B:310:LEU:HA	2:B:454:ILE:HG22	1.80	0.64
3:F:166:LEU:HD22	3:F:218:LEU:HB3	1.80	0.64
3:F:227:TRP:CZ2	3:F:230:ASN:ND2	2.63	0.64
2:H:191:GLU:C	2:H:193:CYS:H	2.05	0.64
3:I:193:VAL:CG1	3:I:195:GLN:H	2.11	0.64
3:L:237:SER:HB3	3:L:266:LYS:HA	1.78	0.64
2:B:240:CYS:HB3	2:B:242:MET:SD	2.37	0.64
2:E:237:ARG:HH11	2:E:237:ARG:HG3	1.63	0.64
3:I:244:TYR:CD2	3:I:386:ILE:HD12	2.32	0.64
3:I:343:HIS:HB3	3:I:366:GLY:O	1.98	0.64
2:K:270:LYS:HA	2:K:296:ASN:HB2	1.79	0.64
3:L:162:LYS:HE3	3:L:186:GLY:HA2	1.80	0.64
3:L:246:LEU:HD13	3:L:265:PHE:CE2	2.33	0.64
3:I:339:CYS:SG	4:S:3:ARG:CZ	2.86	0.64
2:K:406:ARG:HH21	4:R:5:NH2:N	1.96	0.63
3:L:228:LEU:HD23	3:L:232:LYS:HD2	1.80	0.63
3:C:249:GLU:HB3	3:C:383:THR:CG2	2.26	0.63
3:C:339:CYS:SG	4:O:3:ARG:NH1	2.71	0.63
3:F:194:PHE:CD2	3:F:384:MET:O	2.51	0.63
1:J:171:ARG:HD2	2:K:185:ASP:OD1	1.98	0.63
2:K:406:ARG:NE	4:R:3:ARG:HB2	2.13	0.63
1:A:147:MET:HE1	3:C:121:ILE:HD11	1.81	0.63
2:B:340:ILE:HG22	2:B:373:MET:O	1.98	0.63
3:C:193:VAL:CG1	3:C:194:PHE:N	2.50	0.63
1:D:191:LYS:HG3	1:D:192:ASP:H	1.61	0.63
3:F:228:LEU:HD23	3:F:232:LYS:HD2	1.81	0.63
3:F:312:PHE:HA	3:F:335:TRP:HA	1.81	0.63
3:I:161:ALA:O	3:I:162:LYS:HB2	1.97	0.63
2:B:165:LEU:HB2	2:B:166:ARG:CZ	2.27	0.63
2:B:165:LEU:HD12	3:C:106:SER:O	1.99	0.63
3:C:96:TYR:CD1	3:C:96:TYR:C	2.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:LEU:HD23	3:C:372:TRP:CZ3	2.32	0.63
2:E:367:MET:SD	2:E:406:ARG:HG2	2.38	0.63
3:L:289:ALA:HB2	3:L:371:THR:OG1	1.98	0.63
2:B:301:GLN:HE21	2:B:302:LEU:N	1.97	0.63
2:B:408:HIS:CD2	2:B:411:ASN:HB2	2.33	0.63
3:C:109:TYR:C	3:C:110:LEU:HD12	2.24	0.63
3:C:244:TYR:CD2	3:C:386:ILE:HD12	2.33	0.63
2:H:296:ASN:HB3	2:H:338:TYR:CE1	2.33	0.63
3:L:194:PHE:CZ	3:L:384:MET:HE3	2.33	0.63
2:B:215:ILE:HB	2:B:242:MET:CE	2.29	0.63
3:C:293:PHE:N	3:C:302:LYS:HG3	2.13	0.63
2:B:255:ARG:NH1	2:B:413:ASN:HA	2.13	0.63
2:E:160:ASN:H	2:E:162:PRO:HD2	1.64	0.63
1:G:121:VAL:O	1:G:122:LEU:HD22	1.98	0.63
2:K:389:ASP:OD1	2:K:391:ARG:HB2	1.98	0.63
1:A:143:GLN:CD	3:C:118:ASN:HD21	2.07	0.63
3:C:166:LEU:HD21	3:C:219:SER:O	1.98	0.63
1:D:128:GLU:HA	1:D:131:GLN:HG2	1.81	0.63
2:H:238:VAL:HG22	2:H:239:TYR:N	2.13	0.63
1:A:148:LYS:HZ1	2:B:425:ASP:HB2	1.62	0.63
2:B:214:ILE:HD13	2:B:225:TYR:HD2	1.63	0.63
3:C:161:ALA:O	3:C:162:LYS:HB2	1.98	0.63
3:C:163:GLN:O	3:C:167:TYR:OH	2.17	0.63
2:E:389:ASP:OD1	2:E:391:ARG:HB2	1.97	0.63
1:G:143:GLN:C	1:G:145:VAL:H	2.05	0.63
2:K:359:GLN:OE1	2:K:438:MET:HB3	1.99	0.63
3:L:194:PHE:CD2	3:L:384:MET:O	2.52	0.63
2:B:296:ASN:HB3	2:B:338:TYR:CE1	2.34	0.62
3:C:178:PHE:CD1	3:C:232:LYS:HG2	2.33	0.62
1:G:148:LYS:NZ	2:H:425:ASP:HB2	2.14	0.62
2:H:408:HIS:CD2	2:H:411:ASN:HB2	2.34	0.62
1:J:133:ILE:HD12	2:K:161:ILE:HG23	1.81	0.62
2:K:160:ASN:O	2:K:161:ILE:C	2.42	0.62
3:L:216:GLY:O	3:L:217:HIS:HD2	1.82	0.62
3:I:208:TRP:HA	3:I:314:THR:HG21	1.80	0.62
3:L:96:TYR:O	3:L:100:ILE:HG13	1.99	0.62
3:L:234:HIS:NE2	3:L:269:PRO:HB3	2.15	0.62
3:C:208:TRP:HA	3:C:314:THR:HG21	1.80	0.62
3:C:338:LYS:O	3:C:338:LYS:HG2	1.98	0.62
2:E:210:GLU:OE1	2:E:456:PRO:HG3	1.98	0.62
1:G:144:LEU:HD23	1:G:182:GLN:HE21	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:252:ILE:HD11	2:H:454:ILE:HG12	1.82	0.62
3:I:131:LEU:HD23	3:I:131:LEU:C	2.24	0.62
1:J:185:LEU:O	1:J:185:LEU:HD13	1.99	0.62
3:L:224:THR:O	3:L:226:PHE:HD1	1.80	0.62
1:A:143:GLN:NE2	3:C:118:ASN:ND2	2.48	0.62
3:I:110:LEU:HD23	3:I:110:LEU:H	1.65	0.62
3:I:178:PHE:CE2	3:I:228:LEU:HD11	2.34	0.62
3:I:235:LEU:HD12	3:I:235:LEU:H	1.65	0.62
2:E:308:THR:HA	2:E:456:PRO:HA	1.80	0.62
2:E:355:ASP:HA	2:E:369:ILE:HD13	1.82	0.62
2:H:169:ARG:O	2:H:173:GLU:HG2	1.98	0.62
3:I:197:ARG:HA	3:I:225:GLU:CG	2.19	0.62
1:J:160:SER:HA	2:K:258:GLY:O	1.98	0.62
1:J:167:ARG:HA	1:J:167:ARG:NE	2.14	0.62
1:J:191:LYS:HB2	1:J:191:LYS:NZ	2.14	0.62
2:K:199:VAL:HG23	3:L:141:ASP:HA	1.82	0.62
2:B:175:LEU:O	2:B:178:LYS:HB2	2.00	0.62
2:B:214:ILE:HG21	2:B:225:TYR:CE2	2.34	0.62
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.07	0.62
2:K:165:LEU:HA	2:K:168:LEU:HD23	1.82	0.62
2:B:255:ARG:HA	2:B:291:GLU:OE2	2.00	0.62
3:C:124:LEU:HD12	3:C:127:LYS:HB3	1.80	0.62
3:C:246:LEU:HD12	3:C:247:ARG:H	1.63	0.62
3:F:194:PHE:CZ	3:F:384:MET:HE3	2.34	0.62
2:H:417:TYR:HE1	2:H:433:ASP:O	1.82	0.62
3:I:208:TRP:HZ2	3:I:270:GLU:HG3	1.64	0.62
1:A:144:LEU:CD2	1:A:182:GLN:HG2	2.27	0.62
2:B:163:THR:N	2:B:166:ARG:HD2	2.14	0.62
2:B:177:SER:HA	2:B:180:GLN:HG2	1.81	0.62
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	1.96	0.62
3:F:198:LEU:HB3	3:F:381:LYS:HE2	1.81	0.62
1:G:148:LYS:CD	1:G:182:GLN:HE22	2.11	0.62
2:H:255:ARG:HA	2:H:291:GLU:OE2	2.00	0.62
3:I:167:TYR:N	3:I:167:TYR:CD1	2.68	0.62
3:I:227:TRP:CZ2	3:I:230:ASN:ND2	2.64	0.62
3:L:236:ILE:CG2	3:L:386:ILE:HD11	2.29	0.62
1:A:150:LEU:O	1:A:154:ILE:HB	2.00	0.62
2:B:369:ILE:N	2:B:405:ASN:HD22	1.97	0.62
3:C:344:LEU:HD12	3:C:384:MET:SD	2.40	0.62
2:E:315:GLU:HG3	2:E:321:LYS:HG2	1.81	0.62
2:K:256:GLN:N	2:K:291:GLU:OE2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:C	1:A:126:VAL:H	2.06	0.62
1:A:143:GLN:NE2	3:C:118:ASN:HD21	1.98	0.62
2:B:161:ILE:O	2:B:163:THR:N	2.28	0.62
2:E:198:THR:O	2:E:199:VAL:HG13	1.99	0.62
3:F:153:CYS:SG	3:F:192:THR:HA	2.39	0.62
3:F:280:TYR:O	3:F:281:PHE:C	2.42	0.62
2:H:214:ILE:HG21	2:H:225:TYR:CE2	2.35	0.62
2:H:333:ASN:C	2:H:335:ALA:H	2.07	0.62
3:I:297:ASP:HB2	3:I:301:ASP:OD2	2.00	0.62
3:I:367:ILE:O	3:I:378:SER:HA	2.00	0.62
2:B:373:MET:CG	2:B:405:ASN:HB2	2.29	0.61
1:J:140:VAL:HG13	1:J:141:ARG:N	2.14	0.61
3:L:320:ASP:HA	3:L:336:MET:O	1.99	0.61
1:A:149:ARG:HG2	2:B:426:MET:C	2.25	0.61
2:E:366:THR:HA	2:E:369:ILE:HG13	1.82	0.61
2:H:176:ARG:HA	2:H:179:ILE:CG1	2.30	0.61
2:K:352:ALA:CB	2:K:439:ASN:ND2	2.63	0.61
2:B:271:GLN:O	2:B:295:GLY:HA3	1.99	0.61
3:C:232:LYS:O	3:C:236:ILE:HG12	2.00	0.61
3:F:143:VAL:O	3:F:143:VAL:HG23	2.00	0.61
2:H:416:TYR:OH	2:H:448:ARG:HD2	2.00	0.61
3:I:178:PHE:CD1	3:I:232:LYS:HG2	2.35	0.61
1:J:161:CYS:C	1:J:163:GLY:N	2.59	0.61
3:L:312:PHE:HA	3:L:335:TRP:HA	1.83	0.61
1:D:126:VAL:O	1:D:127:ILE:C	2.43	0.61
2:E:351:ASN:ND2	2:E:354:MET:H	1.98	0.61
3:F:203:ASP:O	3:F:206:LYS:HG2	1.99	0.61
3:L:195:GLN:HG3	3:L:227:TRP:CZ3	2.34	0.61
1:G:129:LYS:O	1:G:130:VAL:HG23	2.01	0.61
2:H:236:TYR:OH	2:H:302:LEU:HD21	2.01	0.61
2:H:238:VAL:CG2	2:H:239:TYR:N	2.63	0.61
3:I:166:LEU:HD21	3:I:219:SER:O	2.00	0.61
3:I:260:ALA:HB2	3:I:286:ALA:HB3	1.82	0.61
3:L:118:ASN:O	3:L:122:VAL:HG23	2.00	0.61
2:B:178:LYS:C	2:B:180:GLN:N	2.56	0.61
2:B:184:SER:O	2:B:187:SER:N	2.33	0.61
3:C:196:LYS:HG2	3:C:198:LEU:CD1	2.30	0.61
2:E:429:HIS:O	2:E:431:THR:HG23	2.00	0.61
1:G:144:LEU:CD2	1:G:182:GLN:HG3	2.29	0.61
2:H:215:ILE:HB	2:H:242:MET:CE	2.30	0.61
3:I:193:VAL:HG12	3:I:195:GLN:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:220:PRO:HG2	3:I:221:THR:H	1.65	0.61
3:I:272:ASP:O	3:I:273:LYS:HB2	1.99	0.61
2:K:198:THR:O	2:K:199:VAL:HG13	2.00	0.61
2:K:235:PRO:HG2	3:L:168:PHE:HE1	1.64	0.61
2:K:361:MET:O	5:K:470:NAG:H82	2.00	0.61
2:K:415:ARG:O	2:K:434:GLY:HA2	2.00	0.61
3:C:368:ILE:HG21	3:C:375:ARG:HA	1.83	0.61
2:E:264:ARG:HG2	3:F:136:GLN:HE22	1.64	0.61
2:H:369:ILE:N	2:H:405:ASN:HD22	1.98	0.61
3:I:117:ASN:C	3:I:119:GLN:H	2.09	0.61
3:I:237:SER:OG	3:I:266:LYS:HA	2.01	0.61
3:I:256:ARG:HG3	3:I:256:ARG:NH1	2.15	0.61
1:J:127:ILE:O	1:J:130:VAL:HB	2.00	0.61
2:K:169:ARG:O	2:K:173:GLU:HG3	2.01	0.61
2:B:304:ARG:NH2	2:B:333:ASN:H	1.99	0.61
3:C:272:ASP:O	3:C:273:LYS:HB2	2.00	0.61
3:F:92:GLU:HG2	3:F:93:ILE:N	2.15	0.61
2:H:298:LYS:O	2:H:302:LEU:HG	2.00	0.61
3:I:383:THR:OG1	3:I:384:MET:N	2.33	0.61
3:L:194:PHE:CE2	3:L:384:MET:HB2	2.36	0.61
2:B:416:TYR:OH	2:B:448:ARG:HD2	2.01	0.61
3:F:246:LEU:HB2	3:F:265:PHE:CG	2.36	0.61
1:G:161:CYS:HB3	1:G:165:CYS:SG	2.40	0.61
2:H:161:ILE:HG22	2:H:162:PRO:CD	2.31	0.61
3:I:196:LYS:HG2	3:I:198:LEU:CD1	2.30	0.61
2:K:332:GLN:HB3	2:K:336:ASN:HB2	1.83	0.61
3:L:153:CYS:SG	3:L:192:THR:HA	2.40	0.61
3:I:179:LEU:HD23	3:I:218:LEU:HD12	1.82	0.60
1:J:157:LYS:HA	1:J:157:LYS:HE3	1.83	0.60
2:K:255:ARG:HA	2:K:291:GLU:OE2	2.01	0.60
2:B:156:THR:HA	2:B:160:ASN:HB2	1.82	0.60
1:D:131:GLN:HG3	1:D:132:HIS:N	2.15	0.60
3:F:194:PHE:CE2	3:F:384:MET:HB2	2.36	0.60
3:F:276:LEU:HD11	3:F:290:PHE:CE2	2.36	0.60
3:I:124:LEU:C	3:I:126:GLU:H	2.08	0.60
1:J:181:GLN:NE2	2:K:174:ASN:ND2	2.49	0.60
3:L:278:TYR:CD1	3:L:279:ALA:N	2.69	0.60
3:C:260:ALA:HB2	3:C:286:ALA:HB3	1.82	0.60
3:F:141:ASP:OD1	3:F:143:VAL:HG22	2.00	0.60
3:C:256:ARG:HG3	3:C:256:ARG:NH1	2.16	0.60
3:F:108:ARG:O	3:F:112:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:359:GLN:HE21	2:H:359:GLN:H	1.48	0.60
2:K:251:VAL:HG22	2:K:453:LYS:HG2	1.82	0.60
2:K:366:THR:HA	2:K:369:ILE:HG13	1.83	0.60
1:A:136:LEU:HD11	3:C:111:GLN:HB2	1.84	0.60
3:C:365:ASN:N	3:C:365:ASN:ND2	2.46	0.60
3:F:278:TYR:CD1	3:F:279:ALA:N	2.69	0.60
3:F:389:PHE:O	3:F:391:ARG:N	2.33	0.60
2:H:271:GLN:O	2:H:295:GLY:HA3	2.01	0.60
3:I:204:PHE:HE1	3:I:225:GLU:HB3	1.67	0.60
3:I:342:GLY:HA2	3:I:368:ILE:O	2.01	0.60
1:G:140:VAL:O	1:G:143:GLN:N	2.29	0.60
2:H:230:ASP:C	2:H:232:SER:H	2.09	0.60
3:I:380:LYS:HD2	3:I:381:LYS:HG2	1.83	0.60
3:L:178:PHE:CZ	3:L:232:LYS:HG2	2.37	0.60
2:B:181:LYS:C	2:B:183:GLU:H	2.10	0.60
3:C:172:LEU:HD13	3:C:239:GLN:HB3	1.84	0.60
3:C:193:VAL:HG12	3:C:195:GLN:N	2.16	0.60
3:C:204:PHE:HE1	3:C:225:GLU:HB3	1.67	0.60
2:H:412:PRO:HG3	2:H:450:MET:HE1	1.84	0.60
3:I:232:LYS:O	3:I:236:ILE:HG12	2.01	0.60
3:I:322:PHE:HD1	3:I:338:LYS:HG3	1.66	0.60
2:K:210:GLU:OE1	2:K:456:PRO:HG3	2.01	0.60
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.67	0.60
2:B:333:ASN:C	2:B:335:ALA:H	2.08	0.60
3:C:178:PHE:CE2	3:C:228:LEU:HD11	2.36	0.60
1:D:152:VAL:HG21	2:E:426:MET:O	2.01	0.60
1:G:151:GLU:OE2	1:G:173:VAL:HG11	2.00	0.60
1:G:159:ARG:C	1:G:161:CYS:H	2.09	0.60
3:I:246:LEU:HD12	3:I:247:ARG:H	1.66	0.60
3:I:360:PRO:HD2	3:I:365:ASN:OD1	2.02	0.60
3:I:365:ASN:N	3:I:365:ASN:ND2	2.47	0.60
2:K:358:SER:HA	2:K:365:ARG:NH1	2.16	0.60
3:L:389:PHE:O	3:L:391:ARG:N	2.34	0.60
3:F:194:PHE:HA	3:F:228:LEU:HB2	1.84	0.60
2:H:340:ILE:HG22	2:H:373:MET:O	2.01	0.60
2:B:166:ARG:H	2:B:166:ARG:CD	2.14	0.60
3:C:252:ASP:OD2	3:C:254:ASN:HB2	2.02	0.60
2:H:373:MET:CG	2:H:405:ASN:HB2	2.31	0.60
3:I:310:MET:O	3:I:335:TRP:HD1	1.85	0.60
3:L:242:ILE:CG2	3:L:243:PRO:HD2	2.32	0.60
3:C:163:GLN:O	3:C:165:GLY:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:255:ARG:HA	2:E:291:GLU:OE2	2.02	0.59
2:E:352:ALA:CB	2:E:439:ASN:ND2	2.64	0.59
3:F:191:TRP:CZ3	3:F:387:ILE:HB	2.37	0.59
2:H:257:ASP:OD2	2:H:291:GLU:HG3	2.01	0.59
2:H:412:PRO:CA	2:H:450:MET:HE1	2.32	0.59
3:I:193:VAL:CG1	3:I:194:PHE:N	2.53	0.59
3:C:172:LEU:H	3:C:172:LEU:CD1	2.14	0.59
3:C:383:THR:OG1	3:C:384:MET:N	2.34	0.59
3:C:389:PHE:CE1	3:C:392:LEU:HD22	2.37	0.59
2:E:264:ARG:HG2	2:E:264:ARG:HH11	1.67	0.59
2:H:394:CYS:SG	2:H:407:CYS:N	2.75	0.59
3:I:344:LEU:C	3:I:346:GLY:H	2.10	0.59
2:K:215:ILE:HD12	2:K:248:GLY:N	2.17	0.59
3:L:143:VAL:HG23	3:L:143:VAL:O	2.02	0.59
3:L:194:PHE:HA	3:L:228:LEU:HB2	1.84	0.59
1:A:181:GLN:O	1:A:184:GLN:HG3	2.02	0.59
2:E:270:LYS:HA	2:E:296:ASN:HB2	1.83	0.59
3:F:216:GLY:O	3:F:217:HIS:HD2	1.85	0.59
1:G:135:LEU:HD12	1:G:136:LEU:HD22	1.83	0.59
3:I:339:CYS:SG	4:S:3:ARG:NH1	2.76	0.59
3:I:367:ILE:HB	3:I:378:SER:OG	2.02	0.59
3:I:368:ILE:HG21	3:I:375:ARG:HA	1.84	0.59
2:K:308:THR:HA	2:K:456:PRO:HA	1.82	0.59
2:H:178:LYS:C	2:H:180:GLN:H	2.10	0.59
3:I:163:GLN:O	3:I:165:GLY:N	2.35	0.59
3:L:280:TYR:O	3:L:281:PHE:C	2.45	0.59
2:B:266:TRP:HE1	2:B:380:ARG:CZ	2.16	0.59
2:B:402:TRP:CE2	2:B:412:PRO:HD2	2.36	0.59
3:C:191:TRP:CE3	3:C:385:LYS:HE2	2.37	0.59
3:C:194:PHE:CE1	3:C:384:MET:HE2	2.37	0.59
3:C:304:PHE:CD1	3:C:338:LYS:HD3	2.38	0.59
3:C:344:LEU:C	3:C:346:GLY:H	2.10	0.59
3:C:360:PRO:HD2	3:C:365:ASN:OD1	2.03	0.59
1:G:124:ARG:O	1:G:126:VAL:N	2.35	0.59
2:H:239:TYR:CZ	2:H:289:PRO:HD3	2.37	0.59
2:H:175:LEU:O	2:H:179:ILE:HG13	2.02	0.59
3:I:194:PHE:CZ	3:I:384:MET:HB3	2.37	0.59
2:K:438:MET:HE3	2:K:443:SER:OG	2.02	0.59
3:C:369:TRP:CD1	3:C:371:THR:HG1	2.20	0.59
3:F:236:ILE:CG2	3:F:386:ILE:HD11	2.32	0.59
1:G:137:GLN:OE1	1:G:189:ILE:HD12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:162:PRO:O	2:H:164:ASN:N	2.35	0.59
3:I:246:LEU:HD21	3:I:248:VAL:HG23	1.85	0.59
1:A:147:MET:HE2	2:B:179:ILE:HG12	1.84	0.59
1:A:189:ILE:O	1:A:190:ALA:CB	2.51	0.59
2:B:165:LEU:H	2:B:166:ARG:HH21	0.71	0.59
2:E:216:ARG:HH11	2:E:216:ARG:HB2	1.60	0.59
2:E:332:GLN:HB3	2:E:336:ASN:HB2	1.85	0.59
3:F:207:ASN:OD1	3:F:210:GLN:HG3	2.02	0.59
1:G:128:GLU:CD	1:G:129:LYS:HZ2	2.10	0.59
2:H:212:GLU:O	2:H:215:ILE:HG22	2.02	0.59
2:H:351:ASN:HD21	2:H:354:MET:H	1.51	0.59
2:K:423:THR:OG1	2:K:426:MET:HE3	2.03	0.59
3:L:198:LEU:HB3	3:L:381:LYS:HE2	1.84	0.59
3:L:203:ASP:O	3:L:206:LYS:HG2	2.02	0.59
3:C:208:TRP:HZ2	3:C:270:GLU:HG3	1.67	0.59
2:E:223:GLU:HB2	2:E:286:CYS:O	2.03	0.59
2:E:310:LEU:HD21	2:E:312:ILE:HD11	1.85	0.59
2:H:301:GLN:C	2:H:301:GLN:NE2	2.61	0.59
3:I:116:SER:O	3:I:119:GLN:HB3	2.03	0.59
2:K:272:GLY:HA2	2:K:293:TRP:O	2.02	0.59
2:E:397:GLU:C	2:E:399:GLY:H	2.10	0.59
3:F:196:LYS:O	3:F:197:ARG:HD2	2.02	0.59
3:I:200:GLY:N	3:I:225:GLU:OE2	2.20	0.59
3:I:209:ILE:H	3:I:209:ILE:CD1	2.10	0.59
1:J:191:LYS:HB2	1:J:191:LYS:HZ3	1.66	0.59
3:C:105:SER:C	3:C:107:ILE:H	2.09	0.58
3:C:209:ILE:H	3:C:209:ILE:CD1	2.10	0.58
3:C:220:PRO:HG2	3:C:221:THR:H	1.67	0.58
3:F:224:THR:O	3:F:226:PHE:HD1	1.85	0.58
3:F:242:ILE:CG2	3:F:243:PRO:HD2	2.33	0.58
3:F:276:LEU:HD23	3:F:277:THR:N	2.18	0.58
2:H:439:ASN:HD22	2:H:439:ASN:N	2.01	0.58
3:I:273:LYS:HE3	3:I:319:ASN:CG	2.28	0.58
1:A:136:LEU:HD23	1:A:139:ASN:HD22	1.67	0.58
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.67	0.58
2:B:359:GLN:HE21	2:B:359:GLN:H	1.50	0.58
3:I:117:ASN:O	3:I:119:GLN:N	2.36	0.58
3:I:293:PHE:N	3:I:302:LYS:HG3	2.17	0.58
3:I:393:THR:HG22	3:I:393:THR:O	2.02	0.58
1:J:124:ARG:O	1:J:124:ARG:HD3	2.01	0.58
2:B:214:ILE:HG21	2:B:225:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:240:CYS:HB3	2:H:242:MET:SD	2.42	0.58
1:J:152:VAL:HG21	2:K:426:MET:O	2.03	0.58
2:K:355:ASP:HA	2:K:369:ILE:HD13	1.86	0.58
2:B:212:GLU:O	2:B:215:ILE:HG22	2.03	0.58
2:B:230:ASP:C	2:B:232:SER:H	2.10	0.58
3:C:327:ALA:O	3:C:331:GLY:N	2.36	0.58
2:E:215:ILE:HD12	2:E:248:GLY:N	2.18	0.58
3:F:325:ASN:C	3:F:325:ASN:ND2	2.62	0.58
1:G:120:GLU:CD	1:G:121:VAL:N	2.62	0.58
1:G:148:LYS:CE	2:H:425:ASP:HB2	2.33	0.58
2:H:434:GLY:O	2:H:436:VAL:HG13	2.03	0.58
3:I:124:LEU:HD12	3:I:124:LEU:N	2.19	0.58
3:I:389:PHE:O	3:I:391:ARG:N	2.34	0.58
1:J:115:LEU:C	1:J:117:SER:H	2.09	0.58
3:L:325:ASN:C	3:L:325:ASN:ND2	2.62	0.58
1:A:149:ARG:HG2	2:B:426:MET:O	2.02	0.58
3:C:172:LEU:HD13	3:C:239:GLN:HB2	1.85	0.58
3:C:297:ASP:HB2	3:C:301:ASP:OD2	2.02	0.58
3:C:342:GLY:HA2	3:C:368:ILE:O	2.03	0.58
3:C:380:LYS:HD2	3:C:381:LYS:HG2	1.85	0.58
1:D:185:LEU:O	1:D:185:LEU:HD13	2.04	0.58
2:H:254:ASN:OD1	2:H:451:SER:HB3	2.03	0.58
2:K:164:ASN:C	2:K:166:ARG:H	2.11	0.58
3:L:189:ASN:ND2	3:L:391:ARG:HD3	2.18	0.58
3:L:246:LEU:HB2	3:L:265:PHE:CG	2.38	0.58
2:B:417:TYR:HB2	2:B:446:SER:HB3	1.85	0.58
3:C:322:PHE:CD1	3:C:338:LYS:HG3	2.38	0.58
2:E:381:ASP:OD2	2:E:393:GLN:HG2	2.04	0.58
2:K:405:ASN:C	2:K:407:CYS:N	2.53	0.58
1:A:161:CYS:O	1:A:163:GLY:N	2.31	0.58
2:B:310:LEU:C	2:B:310:LEU:HD12	2.29	0.58
3:C:156:ILE:C	3:C:158:ASN:H	2.11	0.58
3:C:237:SER:OG	3:C:266:LYS:HA	2.04	0.58
2:E:397:GLU:O	2:E:399:GLY:N	2.37	0.58
3:F:168:PHE:HD1	3:F:177:GLN:HG3	1.68	0.58
1:G:149:ARG:HG2	2:H:426:MET:C	2.29	0.58
2:H:186:VAL:O	2:H:186:VAL:HG12	2.03	0.58
3:L:276:LEU:HD11	3:L:290:PHE:CE2	2.39	0.58
3:C:286:ALA:O	3:C:372:TRP:HB2	2.03	0.58
3:C:310:MET:HE2	3:C:310:MET:HA	1.86	0.58
1:D:144:LEU:H	1:D:144:LEU:HD12	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:183:GLU:HA	3:F:124:LEU:HD21	1.86	0.58
3:F:178:PHE:CZ	3:F:232:LYS:HG2	2.38	0.58
3:L:196:LYS:O	3:L:197:ARG:HD2	2.04	0.58
2:B:172:LEU:O	2:B:172:LEU:HD13	2.03	0.58
2:B:190:MET:O	2:B:193:CYS:HB2	2.03	0.58
2:B:258:GLY:O	2:B:260:VAL:N	2.36	0.58
3:C:243:PRO:HB3	3:C:264:MET:HE3	1.86	0.58
3:C:317:ASN:HD22	3:C:317:ASN:C	2.12	0.58
3:C:367:ILE:HB	3:C:378:SER:OG	2.04	0.58
1:G:162:ARG:HG2	1:G:168:ALA:HB2	1.85	0.58
2:H:214:ILE:HG21	2:H:225:TYR:CD2	2.39	0.58
2:B:165:LEU:N	2:B:166:ARG:NE	2.51	0.58
2:B:239:TYR:CZ	2:B:289:PRO:HD3	2.39	0.58
2:B:328:GLY:O	2:B:343:ASN:N	2.37	0.58
1:D:140:VAL:CG1	1:D:141:ARG:N	2.67	0.58
2:H:184:SER:O	2:H:187:SER:N	2.35	0.58
3:I:344:LEU:HD12	3:I:384:MET:SD	2.44	0.58
1:J:152:VAL:HG23	1:J:153:ASP:H	1.68	0.58
3:L:304:PHE:CD1	3:L:338:LYS:HB2	2.38	0.58
2:B:298:LYS:O	2:B:302:LEU:HG	2.03	0.57
2:B:412:PRO:HG3	2:B:450:MET:HE1	1.86	0.57
3:C:200:GLY:N	3:C:225:GLU:OE2	2.22	0.57
3:C:347:VAL:HG23	3:C:365:ASN:O	2.04	0.57
1:G:154:ILE:HG22	1:G:171:ARG:HH12	1.68	0.57
3:I:194:PHE:CE2	3:I:384:MET:HB3	2.39	0.57
3:I:383:THR:O	3:I:384:MET:HG3	2.04	0.57
2:K:216:ARG:NH1	2:K:216:ARG:CB	2.64	0.57
2:K:373:MET:HE3	2:K:373:MET:CA	2.34	0.57
3:C:155:ASP:O	3:C:159:LYS:HG3	2.04	0.57
3:F:118:ASN:O	3:F:122:VAL:HG23	2.04	0.57
1:G:176:LYS:O	1:G:176:LYS:HG2	2.03	0.57
3:I:264:MET:O	3:I:265:PHE:C	2.47	0.57
1:J:156:ILE:HG22	1:J:157:LYS:NZ	2.19	0.57
3:L:172:LEU:HD13	3:L:240:SER:CB	2.32	0.57
1:A:147:MET:HG3	2:B:175:LEU:HD21	1.85	0.57
1:A:159:ARG:HB3	2:B:258:GLY:HA3	1.84	0.57
2:B:412:PRO:HA	2:B:450:MET:CE	2.34	0.57
3:C:137:GLU:HB3	3:C:138:PRO:HD2	1.86	0.57
3:F:251:GLU:CD	3:F:381:LYS:HD2	2.29	0.57
2:H:266:TRP:HA	2:H:266:TRP:HE3	1.69	0.57
3:I:156:ILE:C	3:I:158:ASN:H	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:259:THR:O	3:L:286:ALA:HB3	2.04	0.57
1:A:143:GLN:OE1	3:C:118:ASN:ND2	2.37	0.57
2:B:236:TYR:CE2	2:B:298:LYS:HD3	2.40	0.57
2:B:284:ASN:H	2:B:284:ASN:ND2	2.02	0.57
3:C:118:ASN:H	3:C:118:ASN:ND2	1.99	0.57
3:C:310:MET:O	3:C:335:TRP:HD1	1.87	0.57
2:E:183:GLU:HG2	3:F:124:LEU:HG	1.84	0.57
1:G:148:LYS:HZ1	2:H:425:ASP:HB2	1.70	0.57
3:L:328:GLU:C	3:L:330:ASP:H	2.11	0.57
2:E:209:LYS:HG3	2:E:213:GLU:OE1	2.04	0.57
3:F:153:CYS:O	3:F:156:ILE:HB	2.04	0.57
3:F:196:LYS:HA	3:F:382:THR:O	2.04	0.57
1:G:168:ALA:HA	2:H:189:GLN:HE22	1.69	0.57
2:H:166:ARG:O	2:H:167:VAL:HG23	2.04	0.57
2:H:351:ASN:OD1	2:H:354:MET:HE3	2.04	0.57
2:H:402:TRP:CE2	2:H:412:PRO:HD2	2.39	0.57
3:L:154:GLN:OE1	3:L:189:ASN:HA	2.04	0.57
3:L:198:LEU:HA	3:L:381:LYS:HG2	1.87	0.57
1:A:144:LEU:HD11	1:A:182:GLN:HG2	1.85	0.57
1:A:159:ARG:NH2	2:B:418:TRP:CE3	2.73	0.57
3:F:320:ASP:HA	3:F:336:MET:O	2.03	0.57
3:L:273:LYS:HE3	3:L:319:ASN:HD21	1.69	0.57
3:L:322:PHE:CB	3:L:338:LYS:HD2	2.33	0.57
2:B:224:MET:SD	2:B:237:ARG:HB3	2.45	0.57
2:B:367:MET:O	2:B:405:ASN:O	2.23	0.57
2:E:398:ASP:O	2:E:399:GLY:O	2.23	0.57
2:H:176:ARG:HA	2:H:179:ILE:HG13	1.85	0.57
2:H:367:MET:HB2	2:H:406:ARG:HB3	1.85	0.57
3:I:198:LEU:HD22	3:I:223:THR:HA	1.86	0.57
3:L:153:CYS:O	3:L:156:ILE:HB	2.04	0.57
3:L:196:LYS:HA	3:L:382:THR:O	2.05	0.57
3:C:171:PRO:HB3	3:C:239:GLN:HG2	1.87	0.57
3:C:202:VAL:O	3:C:203:ASP:C	2.47	0.57
3:C:246:LEU:HD21	3:C:248:VAL:HG23	1.86	0.57
3:C:295:PHE:HB2	3:C:301:ASP:OD2	2.04	0.57
3:C:339:CYS:SG	4:O:3:ARG:CZ	2.93	0.57
3:C:394:ILE:C	3:C:396:GLU:H	2.12	0.57
1:G:147:MET:HE2	2:H:179:ILE:CG1	2.19	0.57
2:H:166:ARG:NH1	2:H:169:ARG:HD2	2.14	0.57
2:H:180:GLN:O	2:H:183:GLU:N	2.38	0.57
3:I:117:ASN:C	3:I:119:GLN:N	2.63	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:131:GLN:NE2	1:J:132:HIS:N	2.53	0.57
1:A:161:CYS:C	1:A:163:GLY:H	2.12	0.57
3:C:96:TYR:C	3:C:96:TYR:HD1	2.11	0.57
3:F:131:LEU:O	3:F:134:GLN:N	2.28	0.57
3:F:172:LEU:HB2	3:F:239:GLN:HB2	1.87	0.57
3:F:328:GLU:C	3:F:330:ASP:H	2.12	0.57
2:H:276:VAL:O	2:H:277:ALA:HB3	2.05	0.57
3:I:355:SER:O	3:I:359:THR:HG23	2.05	0.57
1:J:135:LEU:O	1:J:135:LEU:HD22	2.05	0.57
3:L:276:LEU:HD23	3:L:277:THR:N	2.20	0.57
2:B:175:LEU:HA	2:B:178:LYS:HG3	1.86	0.57
2:B:198:THR:HA	3:C:140:LYS:O	2.05	0.57
2:B:224:MET:SD	2:B:237:ARG:HD3	2.44	0.57
3:C:94:MET:C	3:C:96:TYR:H	2.13	0.57
2:K:264:ARG:HG2	3:L:136:GLN:HE22	1.70	0.57
2:K:315:GLU:OE2	2:K:448:ARG:NH2	2.38	0.57
3:L:180:VAL:HB	3:L:228:LEU:HD11	1.87	0.57
1:A:151:GLU:HG3	1:A:152:VAL:N	2.20	0.56
3:C:133:ALA:HA	3:C:136:GLN:HG2	1.87	0.56
2:E:154:ASP:OD2	2:E:154:ASP:N	2.38	0.56
3:F:145:ILE:HG21	3:F:168:PHE:HE2	1.69	0.56
2:H:230:ASP:O	2:H:232:SER:N	2.34	0.56
3:I:369:TRP:CD1	3:I:371:THR:HG1	2.23	0.56
1:J:175:LEU:HD21	2:K:426:MET:CE	2.35	0.56
1:A:190:ALA:C	1:A:191:LYS:HZ3	2.13	0.56
2:B:165:LEU:HB2	2:B:166:ARG:NH2	2.20	0.56
3:C:264:MET:O	3:C:265:PHE:C	2.48	0.56
3:F:251:GLU:OE1	3:F:381:LYS:HD2	2.05	0.56
1:G:161:CYS:C	1:G:163:GLY:H	2.13	0.56
3:I:246:LEU:HB3	3:I:265:PHE:CD1	2.40	0.56
3:I:327:ALA:O	3:I:331:GLY:N	2.38	0.56
1:J:126:VAL:CG1	1:J:127:ILE:N	2.68	0.56
2:K:367:MET:HB2	2:K:406:ARG:CB	2.31	0.56
2:K:398:ASP:O	2:K:399:GLY:O	2.23	0.56
3:L:168:PHE:HD1	3:L:177:GLN:HG3	1.69	0.56
3:L:207:ASN:OD1	3:L:210:GLN:HG3	2.05	0.56
1:A:159:ARG:O	2:B:259:SER:N	2.37	0.56
1:A:184:GLN:OE1	2:B:167:VAL:HB	2.06	0.56
2:B:164:ASN:N	2:B:166:ARG:NE	2.51	0.56
2:B:304:ARG:HH22	2:B:333:ASN:HB3	1.69	0.56
3:C:232:LYS:HA	3:C:235:LEU:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:240:CYS:HB3	2:E:242:MET:HE2	1.86	0.56
2:H:412:PRO:HA	2:H:450:MET:CE	2.36	0.56
3:I:155:ASP:O	3:I:159:LYS:HG3	2.05	0.56
3:I:181:TYR:CG	3:I:181:TYR:O	2.56	0.56
2:K:264:ARG:HD3	2:K:273:PHE:CD2	2.40	0.56
1:D:169:LEU:H	2:E:189:GLN:HE22	1.52	0.56
3:F:343:HIS:O	3:F:367:ILE:HA	2.04	0.56
1:G:126:VAL:C	1:G:128:GLU:N	2.59	0.56
2:H:417:TYR:HB2	2:H:446:SER:HB3	1.86	0.56
2:H:455:ARG:CG	2:H:456:PRO:HD2	2.34	0.56
2:K:361:MET:HB2	5:K:470:NAG:H81	1.86	0.56
1:A:128:GLU:HA	1:A:131:GLN:HG2	1.86	0.56
1:A:151:GLU:OE2	1:A:173:VAL:HG12	2.06	0.56
2:B:351:ASN:OD1	2:B:354:MET:HE3	2.05	0.56
2:B:385:TRP:N	2:B:406:ARG:HB2	2.20	0.56
2:B:393:GLN:HB2	2:B:396:LYS:HG3	1.86	0.56
3:C:355:SER:O	3:C:359:THR:HG23	2.06	0.56
1:D:162:ARG:O	1:D:162:ARG:HG2	2.06	0.56
1:G:143:GLN:C	1:G:145:VAL:N	2.63	0.56
3:I:172:LEU:H	3:I:172:LEU:CD1	2.18	0.56
3:I:193:VAL:HA	3:I:385:LYS:HB3	1.87	0.56
3:I:219:SER:OG	3:I:224:THR:HG21	2.06	0.56
3:I:330:ASP:CB	3:I:365:ASN:HB3	2.35	0.56
2:B:179:ILE:O	2:B:183:GLU:HB2	2.05	0.56
2:B:237:ARG:HH21	3:C:143:VAL:CG2	2.17	0.56
2:B:310:LEU:HD12	2:B:311:LEU:N	2.20	0.56
2:B:385:TRP:CD1	2:B:387:THR:HG22	2.41	0.56
2:B:439:ASN:HD22	2:B:439:ASN:N	2.04	0.56
3:C:99:SER:C	3:C:101:LEU:H	2.13	0.56
1:D:159:ARG:O	1:D:159:ARG:HG2	2.06	0.56
2:E:169:ARG:O	2:E:173:GLU:HG3	2.05	0.56
2:E:216:ARG:CB	2:E:216:ARG:NH1	2.66	0.56
2:E:406:ARG:O	2:E:406:ARG:CG	2.54	0.56
3:F:259:THR:O	3:F:286:ALA:HB3	2.06	0.56
3:F:293:PHE:CD1	3:F:294:ASP:N	2.74	0.56
1:G:176:LYS:O	1:G:180:ASP:HB2	2.05	0.56
2:H:162:PRO:C	2:H:164:ASN:N	2.61	0.56
2:H:202:ASN:HD22	2:H:284:ASN:HB2	1.68	0.56
2:H:387:THR:C	2:H:389:ASP:H	2.12	0.56
1:J:143:GLN:NE2	3:L:117:ASN:HB2	2.20	0.56
2:K:234:LYS:HD3	2:K:234:LYS:C	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:397:GLU:O	2:K:399:GLY:N	2.38	0.56
3:L:104:ASP:O	3:L:107:ILE:HG22	2.06	0.56
2:B:417:TYR:HE1	2:B:433:ASP:O	1.88	0.56
2:E:327:GLY:HA3	2:E:344:LYS:HB2	1.86	0.56
3:F:185:ASP:OD2	3:F:187:SER:HB3	2.06	0.56
2:H:176:ARG:HH11	2:H:176:ARG:HG2	1.70	0.56
2:H:385:TRP:CD1	2:H:387:THR:HG22	2.41	0.56
3:I:171:PRO:HB3	3:I:239:GLN:HG2	1.88	0.56
3:I:171:PRO:HG2	3:I:236:ILE:HG22	1.88	0.56
2:B:257:ASP:OD2	2:B:291:GLU:HG3	2.04	0.56
1:G:168:ALA:HA	2:H:189:GLN:CD	2.30	0.56
1:G:186:GLU:HA	1:G:189:ILE:CG2	2.34	0.56
2:H:224:MET:SD	2:H:237:ARG:HB3	2.46	0.56
3:I:286:ALA:O	3:I:372:TRP:HB2	2.05	0.56
1:J:126:VAL:O	1:J:127:ILE:C	2.48	0.56
2:B:161:ILE:HG22	2:B:166:ARG:HH12	1.70	0.56
2:B:387:THR:C	2:B:389:ASP:H	2.12	0.56
2:B:398:ASP:CA	2:B:433:ASP:HB3	2.33	0.56
2:H:226:LEU:O	2:H:227:ILE:O	2.24	0.56
3:I:315:TRP:HA	3:I:325:ASN:OD1	2.06	0.56
1:J:148:LYS:O	1:J:152:VAL:HG22	2.06	0.56
2:K:342:VAL:HG23	2:K:354:MET:HG3	1.86	0.56
3:L:195:GLN:HG3	3:L:227:TRP:HE3	1.64	0.56
2:B:254:ASN:OD1	2:B:451:SER:HB3	2.06	0.56
2:B:390:PRO:O	2:B:396:LYS:HE2	2.06	0.56
3:C:194:PHE:CZ	3:C:384:MET:HB3	2.40	0.56
2:E:415:ARG:O	2:E:434:GLY:HA2	2.06	0.56
2:H:365:ARG:O	2:H:367:MET:N	2.39	0.56
3:I:245:ALA:O	3:I:386:ILE:HA	2.06	0.56
3:L:251:GLU:OE1	3:L:381:LYS:HD2	2.06	0.56
2:B:249:TRP:CH2	2:B:325:HIS:NE2	2.71	0.55
3:C:194:PHE:CE2	3:C:384:MET:HB3	2.41	0.55
3:F:180:VAL:HB	3:F:228:LEU:HD11	1.87	0.55
3:I:252:ASP:OD2	3:I:254:ASN:HB2	2.06	0.55
1:J:152:VAL:HG23	1:J:153:ASP:N	2.22	0.55
2:K:240:CYS:HB3	2:K:242:MET:HE2	1.89	0.55
2:K:405:ASN:O	2:K:406:ARG:C	2.49	0.55
3:L:194:PHE:HD1	3:L:233:ILE:CG1	2.16	0.55
3:L:344:LEU:HD22	3:L:382:THR:HG21	1.87	0.55
1:A:156:ILE:HD11	2:B:416:TYR:H	1.71	0.55
2:B:164:ASN:HB2	2:B:166:ARG:NH2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:HD23	3:C:110:LEU:CD2	2.36	0.55
1:D:161:CYS:O	1:D:163:GLY:N	2.39	0.55
3:F:346:GLY:O	3:F:367:ILE:HG12	2.06	0.55
2:H:310:LEU:HB2	2:H:329:PHE:CD2	2.41	0.55
3:I:195:GLN:HA	3:I:226:PHE:O	2.06	0.55
3:L:343:HIS:O	3:L:367:ILE:HA	2.06	0.55
2:B:165:LEU:N	2:B:166:ARG:CZ	2.69	0.55
2:B:202:ASN:ND2	2:B:284:ASN:O	2.40	0.55
3:C:110:LEU:C	3:C:112:GLU:N	2.54	0.55
1:D:144:LEU:HD12	1:D:144:LEU:N	2.21	0.55
3:F:172:LEU:HD13	3:F:240:SER:CB	2.31	0.55
3:F:322:PHE:HB2	3:F:338:LYS:HD2	1.87	0.55
2:H:293:TRP:HE1	2:H:296:ASN:ND2	2.04	0.55
3:I:295:PHE:HB2	3:I:301:ASP:OD2	2.05	0.55
3:C:198:LEU:HD22	3:C:223:THR:HA	1.88	0.55
3:C:205:LYS:O	3:C:205:LYS:HG2	2.06	0.55
3:C:389:PHE:O	3:C:391:ARG:N	2.36	0.55
3:F:154:GLN:OE1	3:F:189:ASN:HA	2.06	0.55
1:G:133:ILE:C	1:G:135:LEU:H	2.14	0.55
3:I:96:TYR:O	3:I:98:ALA:N	2.40	0.55
3:L:355:SER:C	3:L:357:ALA:N	2.64	0.55
2:B:152:TYR:O	2:B:154:ASP:N	2.39	0.55
2:B:162:PRO:HA	2:B:166:ARG:NH1	2.21	0.55
3:C:197:ARG:HH21	3:C:367:ILE:HD11	1.69	0.55
1:D:185:LEU:O	1:D:189:ILE:HG13	2.06	0.55
3:F:148:ILE:H	3:F:148:ILE:CD1	2.00	0.55
3:F:217:HIS:HB2	3:F:224:THR:OG1	2.06	0.55
2:H:180:GLN:C	2:H:182:LEU:H	2.14	0.55
2:H:393:GLN:HB2	2:H:396:LYS:HG3	1.87	0.55
3:I:189:ASN:CG	3:I:391:ARG:HE	2.13	0.55
3:I:209:ILE:HD12	3:I:209:ILE:N	2.14	0.55
3:I:367:ILE:HG22	3:I:379:MET:CG	2.36	0.55
2:K:397:GLU:C	2:K:399:GLY:H	2.14	0.55
2:K:429:HIS:O	2:K:431:THR:HG23	2.06	0.55
3:C:219:SER:HB3	3:C:224:THR:HG21	1.89	0.55
3:C:273:LYS:HE3	3:C:319:ASN:CG	2.32	0.55
3:F:191:TRP:CE3	3:F:387:ILE:HB	2.42	0.55
3:F:246:LEU:HD22	3:F:265:PHE:CE1	2.41	0.55
3:F:293:PHE:CD2	3:F:370:ALA:HB1	2.42	0.55
3:F:389:PHE:O	3:F:390:ASN:C	2.49	0.55
2:H:193:CYS:HB3	3:I:134:GLN:CD	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:117:ASN:ND2	3:I:117:ASN:H	2.05	0.55
3:I:172:LEU:HD13	3:I:239:GLN:HB3	1.89	0.55
3:I:329:GLN:HE22	3:I:363:TYR:HE2	1.55	0.55
1:J:124:ARG:HG2	1:J:124:ARG:HH11	1.71	0.55
2:K:378:TYR:HB2	2:K:396:LYS:HD3	1.88	0.55
3:L:293:PHE:CD2	3:L:370:ALA:HB1	2.42	0.55
1:A:155:ASP:O	1:A:158:ILE:HG22	2.06	0.55
2:B:158:ASN:C	2:B:162:PRO:HG2	2.31	0.55
2:B:359:GLN:O	2:B:359:GLN:HG2	2.07	0.55
3:C:315:TRP:HA	3:C:325:ASN:OD1	2.07	0.55
3:I:202:VAL:O	3:I:203:ASP:C	2.49	0.55
3:I:334:TRP:CH2	3:I:344:LEU:HB2	2.42	0.55
1:J:122:LEU:HD21	3:L:98:ALA:CB	2.36	0.55
3:L:191:TRP:CZ3	3:L:387:ILE:HB	2.42	0.55
2:B:173:GLU:C	2:B:175:LEU:H	2.15	0.55
3:C:166:LEU:HD11	3:C:219:SER:O	2.07	0.55
3:C:279:ALA:HB2	3:F:308:ASN:ND2	2.22	0.55
2:E:373:MET:HE3	2:E:374:PHE:H	1.70	0.55
3:F:276:LEU:HD23	3:F:276:LEU:C	2.31	0.55
2:H:175:LEU:O	2:H:178:LYS:HB2	2.07	0.55
2:H:229:PRO:O	2:H:230:ASP:C	2.49	0.55
2:H:304:ARG:HH22	2:H:333:ASN:HB3	1.71	0.55
2:H:351:ASN:CG	2:H:354:MET:HB2	2.32	0.55
3:L:389:PHE:O	3:L:390:ASN:C	2.49	0.55
2:B:227:ILE:HD13	2:B:238:VAL:HG11	1.88	0.55
2:B:229:PRO:O	2:B:230:ASP:C	2.49	0.55
2:B:360:LEU:O	2:B:361:MET:HG2	2.07	0.55
2:B:384:GLY:C	2:B:406:ARG:HB2	2.32	0.55
3:C:330:ASP:CB	3:C:365:ASN:HB3	2.36	0.55
1:D:186:GLU:OE1	1:D:186:GLU:HA	2.07	0.55
3:F:194:PHE:H	3:F:194:PHE:HD2	1.53	0.55
3:F:195:GLN:NE2	3:F:344:LEU:O	2.40	0.55
3:F:227:TRP:HE1	3:F:230:ASN:ND2	2.05	0.55
1:G:167:ARG:HD2	1:G:167:ARG:C	2.32	0.55
1:G:168:ALA:HA	2:H:189:GLN:OE1	2.07	0.55
1:G:169:LEU:HD13	1:G:170:ALA:N	2.22	0.55
2:H:153:ILE:O	2:H:153:ILE:HG12	2.06	0.55
2:H:249:TRP:CH2	2:H:325:HIS:NE2	2.71	0.55
2:H:351:ASN:OD1	2:H:354:MET:HB2	2.07	0.55
1:J:180:ASP:O	1:J:184:GLN:HG3	2.07	0.55
3:L:293:PHE:CD1	3:L:294:ASP:N	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.42	0.55
1:A:164:SER:HB3	3:C:137:GLU:O	2.05	0.55
2:B:164:ASN:O	2:B:167:VAL:N	2.40	0.55
2:B:255:ARG:HB2	2:B:450:MET:H	1.72	0.55
2:B:421:GLN:HG2	2:B:445:TYR:HD1	1.72	0.55
2:E:358:SER:HA	2:E:365:ARG:NH1	2.21	0.55
3:F:199:ASP:OD1	3:F:201:SER:HB3	2.06	0.55
2:H:390:PRO:O	2:H:396:LYS:HE2	2.07	0.55
2:K:200:SER:H	2:K:279:ASN:HD21	1.55	0.55
2:K:223:GLU:HB2	2:K:286:CYS:O	2.07	0.55
2:K:310:LEU:HD21	2:K:312:ILE:HD11	1.88	0.55
2:K:394:CYS:SG	2:K:407:CYS:N	2.80	0.55
3:L:259:THR:OG1	3:L:260:ALA:N	2.39	0.55
1:A:127:ILE:C	1:A:130:VAL:HG12	2.32	0.54
2:E:264:ARG:HG2	2:E:264:ARG:NH1	2.19	0.54
2:E:342:VAL:HG23	2:E:354:MET:HG3	1.88	0.54
3:F:104:ASP:O	3:F:107:ILE:HG23	2.08	0.54
3:F:194:PHE:CE2	3:F:384:MET:O	2.60	0.54
3:I:110:LEU:O	3:I:112:GLU:N	2.38	0.54
3:I:161:ALA:HB1	3:I:184:ILE:CD1	2.38	0.54
3:L:100:ILE:O	3:L:100:ILE:HG22	2.06	0.54
2:B:230:ASP:O	2:B:232:SER:N	2.35	0.54
3:I:172:LEU:HD13	3:I:239:GLN:HB2	1.88	0.54
3:I:317:ASN:HD22	3:I:317:ASN:C	2.16	0.54
2:K:190:MET:HE1	3:L:127:LYS:HD3	1.87	0.54
2:K:310:LEU:HB3	2:K:326:TYR:HB2	1.89	0.54
3:L:204:PHE:C	3:L:206:LYS:N	2.61	0.54
2:B:198:THR:O	2:B:199:VAL:HG13	2.07	0.54
3:C:246:LEU:O	3:C:261:ASP:HA	2.07	0.54
3:C:304:PHE:CG	3:C:338:LYS:HD3	2.43	0.54
3:F:354:TYR:O	3:F:376:TRP:HB3	2.08	0.54
2:H:198:THR:HA	3:I:140:LYS:O	2.07	0.54
2:H:328:GLY:O	2:H:343:ASN:N	2.37	0.54
2:H:359:GLN:O	2:H:359:GLN:HG2	2.07	0.54
3:I:196:LYS:CG	3:I:198:LEU:HD11	2.33	0.54
3:I:343:HIS:H	3:I:368:ILE:HG13	1.73	0.54
3:I:344:LEU:HD22	3:I:382:THR:HG21	1.90	0.54
3:L:200:GLY:H	3:L:225:GLU:CD	2.14	0.54
3:L:236:ILE:HG21	3:L:386:ILE:HD11	1.89	0.54
3:L:246:LEU:HD22	3:L:265:PHE:CE1	2.42	0.54
2:B:222:SER:OG	2:B:240:CYS:O	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:356:LYS:HG2	3:C:356:LYS:O	2.08	0.54
3:F:194:PHE:HD1	3:F:233:ILE:CG1	2.16	0.54
2:H:198:THR:O	2:H:199:VAL:HG13	2.08	0.54
2:H:421:GLN:HG2	2:H:445:TYR:HD1	1.72	0.54
2:H:428:LYS:C	2:H:429:HIS:HD2	2.14	0.54
3:I:191:TRP:CE3	3:I:385:LYS:HE2	2.42	0.54
3:I:202:VAL:O	3:I:202:VAL:HG12	2.06	0.54
1:J:144:LEU:HD13	1:J:182:GLN:CG	2.38	0.54
1:J:181:GLN:HE22	2:K:174:ASN:ND2	2.05	0.54
2:K:435:VAL:O	2:K:446:SER:HA	2.08	0.54
3:C:281:PHE:CD2	3:C:288:ASP:HB2	2.42	0.54
3:C:343:HIS:H	3:C:368:ILE:HG13	1.72	0.54
3:C:367:ILE:HG22	3:C:379:MET:CG	2.37	0.54
2:E:345:TYR:CD2	2:E:351:ASN:HB2	2.42	0.54
1:G:136:LEU:O	1:G:140:VAL:HG13	2.07	0.54
2:H:287:GLY:C	2:H:288:LEU:HD23	2.33	0.54
2:B:175:LEU:O	2:B:179:ILE:HG13	2.08	0.54
2:B:352:ALA:HB2	2:B:439:ASN:HB2	1.89	0.54
3:F:198:LEU:HA	3:F:381:LYS:HG2	1.90	0.54
1:G:186:GLU:OE2	1:G:189:ILE:HG21	2.07	0.54
2:H:442:GLY:O	2:H:444:TRP:N	2.41	0.54
3:I:163:GLN:O	3:I:167:TYR:OH	2.20	0.54
3:I:232:LYS:HA	3:I:235:LEU:CD1	2.38	0.54
3:I:247:ARG:O	3:I:249:GLU:N	2.41	0.54
2:K:456:PRO:O	2:K:457:PHE:O	2.25	0.54
3:L:172:LEU:HB2	3:L:239:GLN:HB2	1.90	0.54
2:B:162:PRO:CA	2:B:166:ARG:HD2	2.37	0.54
2:B:185:ASP:C	2:B:187:SER:H	2.15	0.54
2:B:200:SER:O	2:B:279:ASN:ND2	2.37	0.54
2:B:310:LEU:HB2	2:B:329:PHE:CD2	2.42	0.54
2:B:365:ARG:O	2:B:367:MET:N	2.41	0.54
2:B:440:TRP:CE3	2:B:447:MET:HE1	2.43	0.54
2:E:234:LYS:C	2:E:234:LYS:HD3	2.32	0.54
1:G:140:VAL:HG12	3:I:114:TYR:CD1	2.43	0.54
1:G:159:ARG:HH12	2:H:418:TRP:HB2	1.73	0.54
1:G:183:LYS:O	1:G:183:LYS:HD3	2.07	0.54
2:H:253:GLN:NE2	2:H:452:MET:HG3	2.23	0.54
2:H:258:GLY:O	2:H:260:VAL:N	2.40	0.54
2:H:300:SER:HA	2:H:331:VAL:O	2.07	0.54
2:H:351:ASN:ND2	2:H:354:MET:HB2	2.22	0.54
3:I:107:ILE:O	3:I:108:ARG:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:217:HIS:HB2	3:L:224:THR:OG1	2.07	0.54
3:L:307:HIS:O	3:L:308:ASN:C	2.50	0.54
2:B:276:VAL:O	2:B:277:ALA:HB3	2.08	0.54
2:B:455:ARG:CG	2:B:456:PRO:HD2	2.37	0.54
3:C:246:LEU:HB3	3:C:265:PHE:CD1	2.42	0.54
1:D:177:ASP:O	1:D:181:GLN:HG3	2.07	0.54
2:E:155:GLU:O	2:E:156:THR:C	2.51	0.54
2:H:237:ARG:HH21	3:I:143:VAL:CG2	2.20	0.54
2:H:352:ALA:HB2	2:H:439:ASN:HB2	1.90	0.54
3:I:205:LYS:HG2	3:I:205:LYS:O	2.08	0.54
2:B:238:VAL:HA	2:B:276:VAL:HG11	1.90	0.54
3:C:189:ASN:CG	3:C:391:ARG:HE	2.15	0.54
3:C:318:ASP:OD2	3:C:325:ASN:HB2	2.07	0.54
1:D:122:LEU:N	1:D:124:ARG:HE	2.06	0.54
2:E:373:MET:HE3	2:E:373:MET:CA	2.37	0.54
2:E:378:TYR:HB2	2:E:396:LYS:HD3	1.90	0.54
2:E:406:ARG:NE	4:N:3:ARG:HB2	2.23	0.54
2:H:266:TRP:HE1	2:H:380:ARG:CZ	2.21	0.54
3:L:312:PHE:CE1	3:L:334:TRP:HA	2.43	0.54
1:A:188:VAL:C	1:A:189:ILE:HD12	2.33	0.54
2:B:351:ASN:ND2	2:B:354:MET:HB2	2.22	0.54
3:C:336:MET:HE1	3:C:340:HIS:HD2	1.73	0.54
3:C:373:LYS:HG3	3:C:379:MET:HE1	1.89	0.54
3:F:355:SER:C	3:F:357:ALA:N	2.66	0.54
2:H:359:GLN:H	2:H:359:GLN:NE2	2.03	0.54
3:I:246:LEU:O	3:I:261:ASP:HA	2.08	0.54
3:L:321:LYS:HA	3:L:321:LYS:HE2	1.90	0.54
3:C:196:LYS:CG	3:C:198:LEU:HD11	2.34	0.53
3:C:368:ILE:CG2	3:C:375:ARG:HA	2.38	0.53
2:E:270:LYS:O	2:E:270:LYS:HG2	2.08	0.53
2:H:200:SER:O	2:H:279:ASN:ND2	2.37	0.53
2:H:215:ILE:CD1	2:H:242:MET:HB3	2.37	0.53
2:H:310:LEU:C	2:H:310:LEU:HD12	2.34	0.53
2:H:456:PRO:O	2:H:457:PHE:HB3	2.08	0.53
3:I:209:ILE:HG22	3:I:209:ILE:O	2.07	0.53
3:I:212:LYS:O	3:I:231:GLU:HB3	2.08	0.53
1:J:123:LYS:HA	1:J:126:VAL:HG12	1.89	0.53
3:L:224:THR:O	3:L:226:PHE:CD1	2.62	0.53
3:L:276:LEU:HD23	3:L:276:LEU:C	2.33	0.53
3:L:388:PRO:O	3:L:389:PHE:O	2.25	0.53
2:B:176:ARG:HD2	2:B:179:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:ASP:HB2	2:B:268:PRO:CD	2.37	0.53
2:E:170:SER:O	2:E:173:GLU:N	2.36	0.53
3:F:189:ASN:ND2	3:F:391:ARG:HD3	2.22	0.53
3:F:195:GLN:HG3	3:F:227:TRP:HE3	1.69	0.53
1:G:130:VAL:N	1:G:133:ILE:HD13	2.23	0.53
3:I:344:LEU:HD22	3:I:382:THR:CG2	2.38	0.53
3:L:94:MET:HB3	3:L:96:TYR:CE2	2.43	0.53
3:L:350:GLN:C	3:L:352:GLY:H	2.16	0.53
1:A:148:LYS:CE	2:B:425:ASP:HB2	2.38	0.53
2:B:226:LEU:O	2:B:227:ILE:O	2.26	0.53
3:C:329:GLN:HE22	3:C:363:TYR:HE2	1.57	0.53
2:E:177:SER:HA	2:E:180:GLN:HG2	1.91	0.53
2:E:264:ARG:CG	3:F:136:GLN:HE22	2.21	0.53
3:F:204:PHE:C	3:F:206:LYS:N	2.62	0.53
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.00	0.53
2:H:222:SER:OG	2:H:240:CYS:O	2.23	0.53
2:H:299:ILE:C	2:H:301:GLN:H	2.16	0.53
2:H:386:LEU:O	2:H:386:LEU:HD13	2.08	0.53
2:K:270:LYS:O	2:K:270:LYS:HG2	2.08	0.53
1:A:184:GLN:O	1:A:186:GLU:N	2.41	0.53
2:B:158:ASN:CA	2:B:162:PRO:HG2	2.38	0.53
2:B:215:ILE:CD1	2:B:242:MET:HB3	2.37	0.53
2:B:310:LEU:H	2:B:325:HIS:CE1	2.26	0.53
3:C:149:THR:HB	3:C:168:PHE:O	2.08	0.53
1:A:122:LEU:HB2	1:A:124:ARG:HD3	1.89	0.53
3:F:96:TYR:HD1	3:F:96:TYR:N	2.02	0.53
3:F:295:PHE:HE2	3:F:305:THR:HG21	1.73	0.53
2:H:255:ARG:HB2	2:H:450:MET:H	1.73	0.53
3:I:194:PHE:CE1	3:I:384:MET:HE2	2.43	0.53
2:K:266:TRP:CE3	2:K:380:ARG:HG2	2.44	0.53
3:L:101:LEU:O	3:L:104:ASP:HB3	2.07	0.53
1:A:183:LYS:O	1:A:183:LYS:HD3	2.09	0.53
2:B:351:ASN:HD21	2:B:354:MET:H	1.57	0.53
2:E:237:ARG:HG3	2:E:237:ARG:NH1	2.23	0.53
3:I:157:ALA:HA	3:I:161:ALA:HB3	1.91	0.53
2:K:242:MET:HA	2:K:248:GLY:H	1.74	0.53
3:L:194:PHE:H	3:L:194:PHE:HD2	1.55	0.53
3:L:295:PHE:HE2	3:L:305:THR:HG21	1.74	0.53
2:B:176:ARG:C	2:B:178:LYS:H	2.17	0.53
2:B:301:GLN:NE2	2:B:301:GLN:C	2.66	0.53
3:C:103:HIS:O	3:C:107:ILE:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:166:LEU:C	3:C:167:TYR:CD1	2.86	0.53
3:C:167:TYR:N	3:C:167:TYR:HD1	2.06	0.53
3:C:171:PRO:HG2	3:C:236:ILE:HG22	1.91	0.53
1:G:140:VAL:HA	3:I:114:TYR:HE1	1.73	0.53
2:H:185:ASP:HA	2:H:188:ALA:HB3	1.90	0.53
2:H:325:HIS:O	2:H:345:TYR:HA	2.09	0.53
3:I:149:THR:HB	3:I:168:PHE:O	2.09	0.53
3:I:304:PHE:CG	3:I:338:LYS:HD3	2.44	0.53
2:K:203:ILE:HD12	2:K:203:ILE:H	1.73	0.53
2:K:373:MET:HA	2:K:373:MET:CE	2.37	0.53
1:A:165:CYS:SG	3:C:135:CYS:SG	3.06	0.53
2:B:366:THR:O	2:B:369:ILE:HG13	2.09	0.53
3:C:191:TRP:HH2	3:C:247:ARG:HH11	1.57	0.53
2:H:242:MET:HA	2:H:247:GLY:CA	2.39	0.53
2:H:333:ASN:C	2:H:335:ALA:N	2.67	0.53
2:H:336:ASN:O	2:H:337:LYS:C	2.51	0.53
3:I:113:ILE:N	3:I:113:ILE:HD12	2.24	0.53
3:I:394:ILE:C	3:I:396:GLU:H	2.17	0.53
2:K:216:ARG:HH11	2:K:216:ARG:HB3	1.72	0.53
2:K:333:ASN:HB3	2:K:336:ASN:HD22	1.73	0.53
3:L:97:GLU:O	3:L:100:ILE:N	2.39	0.53
2:B:300:SER:HA	2:B:331:VAL:O	2.08	0.53
3:C:227:TRP:HE1	3:C:230:ASN:ND2	2.06	0.53
2:E:333:ASN:HB3	2:E:336:ASN:HD22	1.73	0.53
3:F:273:LYS:HE3	3:F:319:ASN:HD21	1.74	0.53
3:F:312:PHE:CE1	3:F:334:TRP:HA	2.44	0.53
2:H:326:TYR:C	2:H:328:GLY:H	2.17	0.53
3:I:149:THR:HA	3:I:156:ILE:CD1	2.38	0.53
3:I:196:LYS:HE3	3:I:198:LEU:HD11	1.91	0.53
3:I:197:ARG:HH21	3:I:367:ILE:HD11	1.72	0.53
1:J:123:LYS:O	1:J:127:ILE:HB	2.09	0.53
2:B:227:ILE:CD1	2:B:238:VAL:HG11	2.39	0.53
2:B:299:ILE:C	2:B:301:GLN:N	2.63	0.53
3:C:202:VAL:O	3:C:202:VAL:HG12	2.09	0.53
1:D:185:LEU:CD1	1:D:189:ILE:HD11	2.39	0.53
2:E:242:MET:HA	2:E:248:GLY:H	1.74	0.53
3:I:96:TYR:CD1	3:I:96:TYR:C	2.87	0.53
3:L:191:TRP:CE3	3:L:387:ILE:HB	2.44	0.53
2:B:168:LEU:HD23	3:C:110:LEU:HD23	1.90	0.52
2:B:191:GLU:C	2:B:193:CYS:N	2.67	0.52
2:B:385:TRP:CZ3	4:M:3:ARG:NE	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:428:LYS:C	2:B:429:HIS:HD2	2.16	0.52
3:C:154:GLN:NE2	3:C:190:GLY:H	2.06	0.52
3:C:195:GLN:HA	3:C:226:PHE:O	2.09	0.52
3:C:212:LYS:O	3:C:231:GLU:HB3	2.08	0.52
2:E:276:VAL:HA	2:E:292:TYR:CD1	2.44	0.52
3:I:100:ILE:C	3:I:102:THR:H	2.16	0.52
1:J:151:GLU:HG3	1:J:178:TYR:CZ	2.43	0.52
2:B:351:ASN:CG	2:B:354:MET:HB2	2.34	0.52
3:C:209:ILE:HD12	3:C:209:ILE:N	2.15	0.52
3:C:212:LYS:CG	3:C:231:GLU:HB2	2.28	0.52
2:E:315:GLU:OE2	2:E:448:ARG:NH2	2.42	0.52
2:H:169:ARG:NH2	3:I:109:TYR:HD2	2.07	0.52
2:H:224:MET:SD	2:H:237:ARG:HD3	2.48	0.52
2:H:228:GLN:O	2:H:228:GLN:HG2	2.08	0.52
3:I:227:TRP:NE1	3:I:229:GLY:HA2	2.25	0.52
3:I:274:TYR:HB2	3:I:312:PHE:HB3	1.90	0.52
3:L:251:GLU:CD	3:L:381:LYS:HD2	2.34	0.52
3:C:149:THR:HA	3:C:156:ILE:CD1	2.39	0.52
3:C:236:ILE:HG13	3:C:236:ILE:O	2.08	0.52
2:E:155:GLU:HG3	2:E:156:THR:H	1.73	0.52
2:E:236:TYR:CD2	2:E:298:LYS:HE2	2.43	0.52
3:F:194:PHE:HD2	3:F:384:MET:O	1.93	0.52
3:F:197:ARG:NE	3:F:204:PHE:CE1	2.77	0.52
3:F:304:PHE:CD1	3:F:338:LYS:HB3	2.45	0.52
2:H:238:VAL:HA	2:H:276:VAL:HG11	1.92	0.52
3:I:171:PRO:O	3:I:174:ALA:HB3	2.09	0.52
3:I:212:LYS:CG	3:I:231:GLU:HB2	2.29	0.52
3:I:274:TYR:HB2	3:I:312:PHE:CB	2.39	0.52
1:J:143:GLN:O	1:J:147:MET:HG2	2.09	0.52
2:K:180:GLN:HG3	2:K:181:LYS:H	1.70	0.52
2:K:211:CYS:SG	2:K:250:THR:HA	2.49	0.52
2:K:264:ARG:HG2	2:K:264:ARG:HH11	1.74	0.52
3:L:218:LEU:HD21	3:L:226:PHE:CE2	2.44	0.52
1:A:133:ILE:CG2	2:B:164:ASN:ND2	2.72	0.52
2:B:293:TRP:HE1	2:B:296:ASN:ND2	2.08	0.52
3:C:105:SER:C	3:C:107:ILE:N	2.66	0.52
1:D:140:VAL:HG22	1:D:144:LEU:HD11	1.90	0.52
2:E:170:SER:O	2:E:171:ILE:C	2.53	0.52
3:I:312:PHE:CZ	3:I:333:GLY:O	2.63	0.52
2:K:351:ASN:C	2:K:351:ASN:ND2	2.67	0.52
2:K:381:ASP:OD2	2:K:393:GLN:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:194:PHE:CE2	3:L:384:MET:O	2.62	0.52
2:B:176:ARG:O	2:B:180:GLN:CD	2.52	0.52
2:B:228:GLN:HG2	2:B:228:GLN:O	2.08	0.52
3:C:274:TYR:HB2	3:C:312:PHE:CB	2.39	0.52
2:E:167:VAL:O	2:E:168:LEU:C	2.50	0.52
2:E:351:ASN:C	2:E:351:ASN:ND2	2.66	0.52
2:H:183:GLU:O	2:H:183:GLU:CD	2.53	0.52
2:H:187:SER:HA	2:H:190:MET:HB3	1.92	0.52
2:K:162:PRO:HG3	3:L:103:HIS:CE1	2.44	0.52
3:L:145:ILE:HD13	3:L:168:PHE:HE2	1.74	0.52
2:B:287:GLY:C	2:B:288:LEU:HD23	2.35	0.52
3:C:264:MET:CE	3:F:279:ALA:HA	2.38	0.52
3:C:394:ILE:O	3:C:396:GLU:N	2.39	0.52
3:F:322:PHE:CD2	4:P:3:ARG:HG3	2.45	0.52
2:H:328:GLY:HA3	2:H:343:ASN:OD1	2.10	0.52
1:J:128:GLU:O	1:J:129:LYS:C	2.53	0.52
3:L:194:PHE:HD2	3:L:384:MET:O	1.93	0.52
2:B:253:GLN:NE2	2:B:452:MET:HG3	2.25	0.52
2:B:351:ASN:OD1	2:B:354:MET:HB2	2.10	0.52
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.18	0.52
3:C:245:ALA:O	3:C:386:ILE:HA	2.10	0.52
3:C:274:TYR:HB2	3:C:312:PHE:HB3	1.91	0.52
3:F:388:PRO:O	3:F:389:PHE:O	2.27	0.52
2:H:202:ASN:ND2	2:H:284:ASN:O	2.43	0.52
2:H:227:ILE:HD13	2:H:238:VAL:HG11	1.91	0.52
2:H:367:MET:O	2:H:405:ASN:O	2.27	0.52
3:I:165:GLY:C	3:I:166:LEU:HD23	2.35	0.52
1:A:128:GLU:HA	1:A:131:GLN:CD	2.34	0.52
2:B:359:GLN:H	2:B:359:GLN:NE2	2.05	0.52
2:B:406:ARG:O	2:B:406:ARG:HG2	2.09	0.52
2:E:164:ASN:O	2:E:164:ASN:ND2	2.33	0.52
2:E:266:TRP:CE3	2:E:380:ARG:HG2	2.45	0.52
3:F:307:HIS:O	3:F:308:ASN:C	2.52	0.52
2:H:173:GLU:C	2:H:175:LEU:N	2.68	0.52
3:I:169:ILE:HG12	3:I:180:VAL:HG11	1.91	0.52
3:I:252:ASP:C	3:I:254:ASN:H	2.18	0.52
3:I:261:ASP:O	3:I:262:TYR:CG	2.63	0.52
3:I:373:LYS:HG3	3:I:379:MET:HE1	1.92	0.52
2:K:213:GLU:O	2:K:217:LYS:HG3	2.09	0.52
3:L:314:THR:O	3:L:316:ASP:N	2.43	0.52
1:A:127:ILE:O	1:A:130:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:ASN:O	2:B:337:LYS:C	2.52	0.52
3:C:165:GLY:C	3:C:166:LEU:HD23	2.35	0.52
3:C:247:ARG:O	3:C:249:GLU:N	2.43	0.52
3:C:287:GLY:HA3	3:C:371:THR:HB	1.91	0.52
2:E:167:VAL:HG23	2:E:168:LEU:N	2.24	0.52
1:G:169:LEU:HD22	1:G:170:ALA:N	2.21	0.52
3:I:103:HIS:C	3:I:105:SER:N	2.67	0.52
3:I:107:ILE:CG1	3:I:108:ARG:H	2.17	0.52
1:J:186:GLU:OE1	1:J:186:GLU:HA	2.08	0.52
1:A:133:ILE:CG2	2:B:164:ASN:HD22	2.22	0.52
3:C:161:ALA:HB1	3:C:184:ILE:CD1	2.40	0.52
2:E:257:ASP:CG	2:E:259:SER:HG	2.18	0.52
3:F:236:ILE:HG21	3:F:386:ILE:HD11	1.92	0.52
3:F:304:PHE:C	3:F:306:SER:H	2.17	0.52
3:F:344:LEU:HD22	3:F:382:THR:HG21	1.91	0.52
2:H:226:LEU:O	2:H:227:ILE:C	2.53	0.52
2:H:267:ASP:HB2	2:H:268:PRO:CD	2.38	0.52
3:I:175:ASN:O	3:I:176:GLN:C	2.53	0.52
3:I:340:HIS:ND1	3:I:368:ILE:HD11	2.25	0.52
1:J:148:LYS:O	1:J:151:GLU:HB2	2.09	0.52
2:K:205:VAL:O	2:K:206:VAL:C	2.53	0.52
2:K:270:LYS:HG3	2:K:338:TYR:OH	2.09	0.52
2:K:345:TYR:CD2	2:K:351:ASN:HB2	2.45	0.52
2:K:441:LYS:HG3	2:K:447:MET:HE1	1.91	0.52
3:L:223:THR:O	3:L:224:THR:HB	2.10	0.52
2:B:299:ILE:C	2:B:301:GLN:H	2.18	0.51
2:B:456:PRO:O	2:B:457:PHE:HB3	2.10	0.51
3:C:149:THR:HA	3:C:156:ILE:HD13	1.92	0.51
3:C:175:ASN:O	3:C:176:GLN:C	2.54	0.51
3:C:219:SER:CB	3:C:224:THR:HG21	2.39	0.51
2:E:280:THR:O	2:E:281:ASP:C	2.51	0.51
2:E:436:VAL:HG12	2:E:445:TYR:O	2.10	0.51
1:G:126:VAL:HG12	1:G:127:ILE:N	2.25	0.51
1:G:144:LEU:CD2	1:G:182:GLN:HE21	2.23	0.51
2:H:299:ILE:C	2:H:301:GLN:N	2.63	0.51
3:I:149:THR:HA	3:I:156:ILE:HD13	1.93	0.51
1:J:130:VAL:O	1:J:134:GLN:HB2	2.10	0.51
2:K:202:ASN:ND2	3:L:219:SER:HB3	2.25	0.51
2:K:355:ASP:O	2:K:365:ARG:HD3	2.10	0.51
2:B:164:ASN:HB2	2:B:166:ARG:HH21	1.76	0.51
2:B:256:GLN:CA	2:B:449:LYS:HG2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:ILE:O	3:C:100:ILE:CG2	2.57	0.51
3:F:320:ASP:HB3	3:F:336:MET:HB2	1.92	0.51
2:H:442:GLY:C	2:H:444:TRP:H	2.18	0.51
3:I:356:LYS:O	3:I:356:LYS:HG2	2.10	0.51
3:L:195:GLN:NE2	3:L:344:LEU:O	2.43	0.51
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.92	0.51
2:B:397:GLU:O	2:B:398:ASP:C	2.53	0.51
3:C:355:SER:C	3:C:357:ALA:H	2.18	0.51
2:E:205:VAL:O	2:E:206:VAL:C	2.53	0.51
2:H:345:TYR:CB	2:H:354:MET:HE2	2.40	0.51
2:H:408:HIS:NE2	2:H:436:VAL:HG21	2.25	0.51
1:J:141:ARG:O	1:J:142:ALA:C	2.51	0.51
2:K:164:ASN:O	2:K:167:VAL:HG12	2.10	0.51
2:K:209:LYS:HG3	2:K:213:GLU:OE1	2.10	0.51
1:A:148:LYS:HZ2	2:B:425:ASP:HB2	1.72	0.51
2:B:210:GLU:OE1	2:B:212:GLU:N	2.32	0.51
2:B:333:ASN:C	2:B:335:ALA:N	2.68	0.51
2:E:406:ARG:HG2	2:E:406:ARG:O	2.10	0.51
2:H:210:GLU:HA	2:H:227:ILE:CB	2.32	0.51
2:H:351:ASN:C	2:H:351:ASN:HD22	2.18	0.51
3:I:368:ILE:CG2	3:I:375:ARG:HA	2.40	0.51
1:J:153:ASP:O	1:J:156:ILE:HB	2.10	0.51
3:C:227:TRP:NE1	3:C:229:GLY:HA2	2.26	0.51
3:F:321:LYS:HE2	3:F:321:LYS:HA	1.92	0.51
2:H:361:MET:HB2	5:H:470:NAG:O7	2.10	0.51
1:J:161:CYS:O	1:J:163:GLY:N	2.42	0.51
3:L:346:GLY:O	3:L:367:ILE:HG12	2.10	0.51
1:A:136:LEU:HD11	3:C:111:GLN:CB	2.40	0.51
2:B:165:LEU:CD2	2:B:166:ARG:NH2	2.70	0.51
2:B:210:GLU:CD	2:B:212:GLU:HB3	2.35	0.51
3:C:169:ILE:HG12	3:C:180:VAL:HG11	1.92	0.51
3:C:275:ARG:HB2	3:C:311:GLN:HG2	1.93	0.51
3:C:312:PHE:CZ	3:C:333:GLY:O	2.64	0.51
2:E:264:ARG:HD3	2:E:273:PHE:CD2	2.46	0.51
2:E:355:ASP:HA	2:E:369:ILE:CD1	2.41	0.51
3:F:259:THR:OG1	3:F:260:ALA:N	2.41	0.51
3:F:365:ASN:HD22	3:F:365:ASN:N	2.01	0.51
2:H:326:TYR:C	2:H:328:GLY:N	2.69	0.51
3:I:171:PRO:CG	3:I:236:ILE:HG22	2.40	0.51
3:I:219:SER:CB	3:I:224:THR:HG21	2.40	0.51
3:I:304:PHE:CD1	3:I:338:LYS:HD3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:186:VAL:HG12	2:K:190:MET:HE2	1.92	0.51
3:L:96:TYR:O	3:L:99:SER:HB2	2.11	0.51
3:L:109:TYR:HD1	3:L:110:LEU:HD23	1.75	0.51
2:B:421:GLN:HG2	2:B:445:TYR:CD1	2.46	0.51
3:C:157:ALA:HA	3:C:161:ALA:HB3	1.93	0.51
3:C:181:TYR:CG	3:C:181:TYR:O	2.63	0.51
3:C:252:ASP:C	3:C:254:ASN:H	2.18	0.51
2:E:326:TYR:OH	2:E:351:ASN:ND2	2.44	0.51
2:E:456:PRO:O	2:E:457:PHE:O	2.28	0.51
2:H:185:ASP:C	2:H:187:SER:H	2.18	0.51
2:H:310:LEU:H	2:H:325:HIS:CE1	2.29	0.51
3:I:389:PHE:C	3:I:391:ARG:N	2.69	0.51
1:J:122:LEU:HD21	3:L:98:ALA:HA	1.93	0.51
2:K:156:THR:O	2:K:158:ASN:N	2.43	0.51
2:K:242:MET:C	2:K:247:GLY:HA3	2.35	0.51
2:K:243:ASN:O	2:K:244:THR:C	2.53	0.51
2:K:280:THR:O	2:K:281:ASP:C	2.52	0.51
2:K:391:ARG:HG2	2:K:391:ARG:NH1	2.24	0.51
2:K:434:GLY:O	2:K:436:VAL:HG13	2.10	0.51
3:L:355:SER:C	3:L:357:ALA:H	2.17	0.51
1:D:161:CYS:C	1:D:163:GLY:N	2.65	0.51
2:E:242:MET:HA	2:E:247:GLY:HA3	1.92	0.51
3:F:350:GLN:C	3:F:352:GLY:H	2.19	0.51
3:F:355:SER:C	3:F:357:ALA:H	2.17	0.51
1:G:159:ARG:CZ	2:H:418:TRP:CE3	2.94	0.51
3:I:340:HIS:H	4:S:1:GLY:HA2	1.74	0.51
3:L:359:THR:OG1	3:L:362:GLY:HA2	2.10	0.51
2:B:311:LEU:HD11	2:B:323:LYS:HB2	1.93	0.51
2:E:406:ARG:HE	4:N:3:ARG:HB2	1.74	0.51
3:F:252:ASP:C	3:F:254:ASN:H	2.19	0.51
1:G:147:MET:CE	2:H:179:ILE:HG12	2.20	0.51
1:G:167:ARG:HD2	1:G:168:ALA:N	2.26	0.51
2:H:210:GLU:OE1	2:H:212:GLU:N	2.33	0.51
2:H:213:GLU:OE2	2:H:217:LYS:NZ	2.36	0.51
2:H:411:ASN:HD22	2:H:434:GLY:H	1.58	0.51
3:I:169:ILE:CD1	3:I:171:PRO:HD3	2.29	0.51
2:K:311:LEU:HD21	2:K:313:GLU:OE2	2.10	0.51
1:A:124:ARG:N	1:A:124:ARG:CD	2.73	0.51
1:A:158:ILE:CG2	1:A:159:ARG:N	2.74	0.51
2:B:218:GLY:CA	3:C:210:GLN:HE21	2.23	0.51
3:C:202:VAL:HG21	3:C:225:GLU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.75	0.51
2:E:202:ASN:ND2	3:F:219:SER:HB3	2.26	0.51
2:E:223:GLU:CB	2:E:287:GLY:HA2	2.40	0.51
2:E:391:ARG:HG2	2:E:391:ARG:NH1	2.25	0.51
2:H:218:GLY:CA	3:I:210:GLN:HE21	2.23	0.51
2:H:236:TYR:CE2	2:H:298:LYS:HD3	2.46	0.51
3:L:295:PHE:CE2	3:L:305:THR:HG21	2.46	0.51
3:L:295:PHE:CE2	4:T:2:PRO:HD3	2.45	0.51
2:B:325:HIS:O	2:B:345:TYR:HA	2.11	0.50
2:B:340:ILE:HD12	2:B:403:TRP:CE3	2.46	0.50
2:B:434:GLY:O	2:B:436:VAL:HG13	2.10	0.50
1:D:126:VAL:O	1:D:129:LYS:N	2.44	0.50
1:G:151:GLU:OE2	1:G:173:VAL:CG1	2.59	0.50
2:H:205:VAL:HG21	3:I:215:PHE:O	2.12	0.50
2:H:246:ASN:HB2	2:H:455:ARG:HH12	1.76	0.50
3:I:243:PRO:HB3	3:I:264:MET:HE3	1.93	0.50
2:K:333:ASN:HB3	2:K:336:ASN:ND2	2.26	0.50
2:K:402:TRP:CH2	2:K:412:PRO:HG2	2.46	0.50
1:A:140:VAL:HG12	3:C:114:TYR:CE1	2.46	0.50
2:B:449:LYS:NZ	2:B:449:LYS:HB3	2.26	0.50
3:C:389:PHE:C	3:C:391:ARG:N	2.69	0.50
1:D:127:ILE:HG23	1:D:128:GLU:N	2.25	0.50
1:D:175:LEU:HD21	2:E:426:MET:CE	2.40	0.50
2:E:245:GLU:O	2:E:246:ASN:HB2	2.11	0.50
2:E:373:MET:HA	2:E:373:MET:CE	2.41	0.50
3:F:295:PHE:CE2	3:F:305:THR:HG21	2.47	0.50
1:G:159:ARG:O	2:H:259:SER:N	2.44	0.50
2:H:173:GLU:O	2:H:175:LEU:N	2.44	0.50
2:H:179:ILE:O	2:H:179:ILE:HG22	2.11	0.50
2:H:345:TYR:HB3	2:H:354:MET:CE	2.40	0.50
2:H:411:ASN:CB	2:H:436:VAL:HG22	2.39	0.50
2:H:449:LYS:NZ	2:H:449:LYS:HB3	2.27	0.50
3:I:197:ARG:HB2	3:I:382:THR:HB	1.93	0.50
3:I:279:ALA:HB2	3:L:308:ASN:ND2	2.26	0.50
1:J:138:LYS:HB2	1:J:138:LYS:HZ2	1.76	0.50
2:K:373:MET:CG	2:K:405:ASN:HB2	2.36	0.50
2:B:204:PRO:HA	3:C:217:HIS:CB	2.41	0.50
2:B:345:TYR:CB	2:B:354:MET:HE2	2.41	0.50
3:C:381:LYS:O	3:C:382:THR:OG1	2.26	0.50
3:C:387:ILE:HG12	3:C:388:PRO:N	2.25	0.50
2:H:210:GLU:CD	2:H:212:GLU:HB3	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:267:ASP:O	2:H:268:PRO:C	2.54	0.50
2:H:326:TYR:O	2:H:328:GLY:N	2.45	0.50
1:J:127:ILE:HG22	1:J:128:GLU:N	2.27	0.50
2:K:242:MET:HA	2:K:247:GLY:HA3	1.93	0.50
2:K:313:GLU:CD	2:K:323:LYS:HZ3	2.19	0.50
1:A:190:ALA:C	1:A:191:LYS:HD2	2.36	0.50
2:B:210:GLU:CD	2:B:212:GLU:H	2.16	0.50
2:B:350:GLY:O	2:B:352:ALA:N	2.44	0.50
3:C:191:TRP:CH2	3:C:247:ARG:HD3	2.46	0.50
2:E:211:CYS:SG	2:E:250:THR:HA	2.51	0.50
3:F:93:ILE:O	3:F:95:LYS:N	2.45	0.50
3:F:330:ASP:HB3	3:F:343:HIS:HE1	1.76	0.50
1:G:141:ARG:HB3	1:G:141:ARG:HH11	1.76	0.50
1:G:191:LYS:O	1:G:192:ASP:HB3	2.12	0.50
3:I:97:GLU:C	3:I:99:SER:N	2.63	0.50
3:I:131:LEU:HD23	3:I:132:GLU:N	2.26	0.50
3:I:166:LEU:HD11	3:I:219:SER:O	2.11	0.50
3:L:252:ASP:C	3:L:254:ASN:H	2.19	0.50
3:L:304:PHE:C	3:L:306:SER:H	2.17	0.50
2:B:173:GLU:O	2:B:176:ARG:N	2.45	0.50
2:B:267:ASP:O	2:B:268:PRO:C	2.54	0.50
2:B:300:SER:HG	2:B:332:GLN:C	2.20	0.50
3:C:287:GLY:O	3:C:369:TRP:NE1	2.34	0.50
1:D:123:LYS:C	1:D:125:LYS:N	2.69	0.50
1:G:189:ILE:HG23	1:G:189:ILE:O	2.12	0.50
2:K:355:ASP:HA	2:K:369:ILE:CD1	2.42	0.50
2:K:405:ASN:C	2:K:407:CYS:H	2.16	0.50
3:L:354:TYR:O	3:L:376:TRP:HB3	2.11	0.50
3:I:166:LEU:C	3:I:167:TYR:CD1	2.89	0.50
3:I:235:LEU:HD12	3:I:235:LEU:N	2.25	0.50
3:I:310:MET:O	3:I:335:TRP:CD1	2.64	0.50
2:B:226:LEU:O	2:B:227:ILE:C	2.55	0.50
2:B:326:TYR:O	2:B:328:GLY:N	2.45	0.50
2:B:342:VAL:O	2:B:371:ASN:ND2	2.45	0.50
3:C:107:ILE:HG23	3:C:108:ARG:N	2.27	0.50
3:C:193:VAL:HA	3:C:385:LYS:HB3	1.93	0.50
3:C:197:ARG:NH2	3:C:348:TYR:HB2	2.27	0.50
3:C:326:CYS:O	3:C:327:ALA:C	2.55	0.50
2:E:264:ARG:HG2	3:F:136:GLN:NE2	2.25	0.50
3:F:109:TYR:CE1	3:F:113:ILE:HD11	2.46	0.50
2:H:249:TRP:HB3	2:H:453:LYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:317:TRP:CE3	2:H:448:ARG:HD3	2.47	0.50
3:I:287:GLY:HA3	3:I:371:THR:HB	1.93	0.50
3:I:326:CYS:O	3:I:327:ALA:C	2.55	0.50
1:J:128:GLU:HA	1:J:131:GLN:OE1	2.12	0.50
2:B:242:MET:HA	2:B:247:GLY:CA	2.42	0.50
2:B:408:HIS:NE2	2:B:436:VAL:HG21	2.27	0.50
3:C:171:PRO:O	3:C:174:ALA:HB3	2.12	0.50
3:C:253:TRP:O	3:C:254:ASN:CG	2.55	0.50
1:D:169:LEU:H	2:E:189:GLN:NE2	2.10	0.50
1:D:191:LYS:O	1:D:192:ASP:HB2	2.11	0.50
2:E:266:TRP:HA	2:E:377:THR:HG21	1.93	0.50
1:G:159:ARG:O	1:G:161:CYS:N	2.44	0.50
1:G:161:CYS:O	1:G:163:GLY:N	2.41	0.50
2:H:264:ARG:HD2	2:H:268:PRO:HB3	1.94	0.50
2:H:358:SER:C	2:H:360:LEU:H	2.19	0.50
2:H:360:LEU:O	2:H:361:MET:HG2	2.12	0.50
3:I:272:ASP:O	3:I:273:LYS:CB	2.59	0.50
2:K:164:ASN:O	2:K:168:LEU:HD23	2.11	0.50
2:K:280:THR:OG1	2:K:288:LEU:HG	2.12	0.50
2:K:405:ASN:O	2:K:407:CYS:N	2.45	0.50
3:L:97:GLU:HA	3:L:100:ILE:CG1	2.41	0.50
3:L:105:SER:O	3:L:108:ARG:N	2.45	0.50
3:L:227:TRP:HE1	3:L:230:ASN:ND2	2.09	0.50
1:A:128:GLU:C	1:A:130:VAL:H	2.18	0.50
1:A:173:VAL:HG23	1:A:174:ASP:N	2.27	0.50
1:A:185:LEU:HD13	1:A:185:LEU:O	2.12	0.50
2:B:179:ILE:CD1	3:C:117:ASN:ND2	2.75	0.50
2:B:246:ASN:HB2	2:B:455:ARG:HH12	1.77	0.50
3:C:97:GLU:O	3:C:101:LEU:HB2	2.12	0.50
3:C:209:ILE:O	3:C:209:ILE:HG22	2.10	0.50
3:C:334:TRP:CH2	3:C:344:LEU:HB2	2.47	0.50
3:C:353:THR:HA	3:C:377:TYR:HA	1.94	0.50
2:H:316:ASP:HB2	2:H:445:TYR:CE2	2.42	0.50
2:H:398:ASP:CA	2:H:433:ASP:HB3	2.39	0.50
2:H:421:GLN:HG2	2:H:445:TYR:CD1	2.47	0.50
3:I:154:GLN:NE2	3:I:190:GLY:H	2.09	0.50
3:I:191:TRP:HH2	3:I:247:ARG:HH11	1.59	0.50
3:I:280:TYR:HD2	3:I:281:PHE:O	1.94	0.50
2:K:264:ARG:HG2	2:K:264:ARG:NH1	2.25	0.50
3:L:391:ARG:HB2	3:L:391:ARG:HH11	1.73	0.50
1:A:191:LYS:HD2	1:A:191:LYS:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:LEU:CD1	3:C:106:SER:O	2.59	0.49
2:B:169:ARG:HH12	3:C:109:TYR:HD2	1.58	0.49
3:C:261:ASP:O	3:C:262:TYR:CG	2.65	0.49
3:C:293:PHE:CA	3:C:302:LYS:HG3	2.42	0.49
1:D:148:LYS:HG3	1:D:178:TYR:CG	2.47	0.49
2:E:203:ILE:HG21	2:E:226:LEU:HD22	1.93	0.49
2:E:216:ARG:HH11	2:E:216:ARG:HB3	1.73	0.49
2:E:397:GLU:C	2:E:399:GLY:N	2.68	0.49
3:F:100:ILE:CG2	3:F:103:HIS:HB2	2.42	0.49
3:F:223:THR:O	3:F:224:THR:HB	2.12	0.49
3:F:227:TRP:NE1	3:F:230:ASN:ND2	2.60	0.49
3:F:311:GLN:O	3:F:335:TRP:HA	2.12	0.49
1:J:136:LEU:HD11	3:L:110:LEU:HB2	1.94	0.49
2:K:436:VAL:HG12	2:K:445:TYR:O	2.12	0.49
2:B:157:VAL:O	2:B:157:VAL:HG23	2.12	0.49
2:B:362:GLY:O	2:B:365:ARG:N	2.45	0.49
3:C:331:GLY:O	3:C:332:SER:HB3	2.12	0.49
3:C:390:ASN:OD1	3:C:391:ARG:HG3	2.12	0.49
3:L:236:ILE:HG22	3:L:386:ILE:HD11	1.93	0.49
3:L:365:ASN:HD22	3:L:365:ASN:N	2.02	0.49
3:L:391:ARG:HH11	3:L:391:ARG:CB	2.25	0.49
2:B:169:ARG:HH22	3:C:109:TYR:HD2	1.56	0.49
2:B:398:ASP:HA	2:B:433:ASP:HB2	1.92	0.49
3:C:96:TYR:O	3:C:97:GLU:C	2.55	0.49
3:C:280:TYR:HD2	3:C:281:PHE:O	1.95	0.49
1:D:130:VAL:O	1:D:133:ILE:HB	2.12	0.49
2:E:402:TRP:CH2	2:E:412:PRO:HG2	2.47	0.49
1:G:169:LEU:HD12	1:G:171:ARG:HB3	1.94	0.49
2:H:340:ILE:HD12	2:H:403:TRP:CE3	2.47	0.49
2:K:238:VAL:HG23	2:K:294:LEU:HD13	1.94	0.49
3:L:113:ILE:O	3:L:114:TYR:C	2.53	0.49
3:L:205:LYS:HZ2	3:L:331:GLY:HA2	1.76	0.49
3:L:314:THR:O	3:L:315:TRP:C	2.55	0.49
2:E:224:MET:SD	2:E:237:ARG:HD3	2.52	0.49
2:E:242:MET:C	2:E:247:GLY:HA3	2.37	0.49
2:H:156:THR:O	2:H:161:ILE:HB	2.12	0.49
2:H:175:LEU:C	2:H:175:LEU:HD12	2.37	0.49
3:I:163:GLN:HA	3:I:163:GLN:NE2	2.21	0.49
3:I:331:GLY:O	3:I:332:SER:HB3	2.11	0.49
3:I:394:ILE:HG23	3:I:395:GLY:N	2.26	0.49
1:A:158:ILE:HG21	1:A:171:ARG:HE	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.94	0.49
2:B:294:LEU:O	2:B:295:GLY:C	2.54	0.49
3:C:114:TYR:O	3:C:116:SER:N	2.45	0.49
3:C:344:LEU:HD22	3:C:382:THR:HG21	1.95	0.49
2:E:340:ILE:HG21	2:E:403:TRP:CG	2.47	0.49
3:F:96:TYR:C	3:F:98:ALA:N	2.64	0.49
3:F:98:ALA:C	3:F:100:ILE:H	2.20	0.49
3:F:200:GLY:H	3:F:225:GLU:CD	2.19	0.49
3:F:318:ASP:OD1	3:F:320:ASP:OD2	2.30	0.49
1:G:184:GLN:HE21	1:G:185:LEU:HB2	1.77	0.49
2:H:227:ILE:CD1	2:H:238:VAL:HG11	2.42	0.49
2:H:256:GLN:CA	2:H:449:LYS:HG2	2.41	0.49
2:H:310:LEU:HD12	2:H:311:LEU:N	2.27	0.49
3:I:128:VAL:O	3:I:129:ALA:C	2.56	0.49
3:I:219:SER:HB3	3:I:224:THR:HG21	1.95	0.49
2:K:216:ARG:HB2	2:K:216:ARG:HH11	1.59	0.49
2:K:373:MET:HE3	2:K:374:PHE:N	2.27	0.49
3:L:242:ILE:HG22	3:L:243:PRO:HD2	1.93	0.49
3:L:290:PHE:HD1	3:L:307:HIS:ND1	2.09	0.49
1:A:140:VAL:O	1:A:141:ARG:C	2.56	0.49
2:B:165:LEU:HD13	3:C:110:LEU:CD2	2.42	0.49
3:C:295:PHE:H	3:C:301:ASP:HB3	1.77	0.49
1:D:140:VAL:O	1:D:144:LEU:HD12	2.13	0.49
2:E:411:ASN:HB3	2:E:434:GLY:O	2.13	0.49
2:H:345:TYR:HB3	2:H:354:MET:HE2	1.94	0.49
3:I:281:PHE:CD2	3:I:288:ASP:HB2	2.47	0.49
3:I:355:SER:C	3:I:357:ALA:H	2.20	0.49
1:J:144:LEU:HD13	1:J:182:GLN:HG2	1.95	0.49
1:J:185:LEU:CD1	1:J:189:ILE:HD11	2.42	0.49
3:L:197:ARG:NE	3:L:204:PHE:CE1	2.80	0.49
3:L:311:GLN:O	3:L:335:TRP:HA	2.13	0.49
1:A:144:LEU:CG	1:A:182:GLN:HG2	2.42	0.49
2:B:175:LEU:O	2:B:175:LEU:HD23	2.12	0.49
3:C:171:PRO:CG	3:C:236:ILE:HG22	2.42	0.49
3:C:219:SER:OG	3:C:224:THR:HG21	2.13	0.49
3:C:340:HIS:HE1	3:C:364:ASP:OD2	1.96	0.49
2:E:213:GLU:O	2:E:217:LYS:HG3	2.12	0.49
1:G:133:ILE:C	1:G:135:LEU:N	2.67	0.49
2:H:422:TYR:CE1	2:H:444:TRP:HA	2.48	0.49
3:I:97:GLU:O	3:I:100:ILE:HG13	2.12	0.49
3:I:287:GLY:O	3:I:369:TRP:NE1	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:318:ASP:OD2	3:I:325:ASN:HB2	2.12	0.49
2:B:351:ASN:C	2:B:351:ASN:HD22	2.20	0.49
3:C:245:ALA:HA	3:C:265:PHE:HB2	1.95	0.49
3:C:272:ASP:O	3:C:273:LYS:CB	2.60	0.49
3:C:344:LEU:HD22	3:C:382:THR:CG2	2.42	0.49
3:F:230:ASN:C	3:F:232:LYS:N	2.70	0.49
3:F:243:PRO:HB2	3:F:389:PHE:HB3	1.95	0.49
1:G:139:ASN:HB3	3:I:114:TYR:OH	2.12	0.49
2:H:226:LEU:O	2:H:226:LEU:HD12	2.13	0.49
3:I:120:LYS:O	3:I:123:ASN:HB2	2.13	0.49
2:K:408:HIS:CD2	2:K:411:ASN:HB2	2.48	0.49
3:L:199:ASP:OD1	3:L:201:SER:HB3	2.12	0.49
1:A:126:VAL:O	1:A:127:ILE:C	2.55	0.49
2:B:236:TYR:CB	2:B:298:LYS:HZ3	2.24	0.49
2:B:304:ARG:HG3	2:B:304:ARG:HH11	1.77	0.49
2:E:161:ILE:O	2:E:162:PRO:C	2.55	0.49
2:E:314:MET:HE3	2:E:349:ALA:HB2	1.95	0.49
2:E:318:LYS:NZ	2:E:441:LYS:HZ3	2.11	0.49
3:F:224:THR:O	3:F:226:PHE:CD1	2.66	0.49
2:H:204:PRO:HA	3:I:217:HIS:CB	2.43	0.49
2:H:276:VAL:O	2:H:276:VAL:HG12	2.12	0.49
2:K:253:GLN:OE1	2:K:255:ARG:HG2	2.13	0.49
2:K:397:GLU:C	2:K:399:GLY:N	2.70	0.49
1:A:188:VAL:O	1:A:189:ILE:HD12	2.13	0.49
2:B:166:ARG:O	2:B:170:SER:HB2	2.12	0.49
2:B:210:GLU:HA	2:B:227:ILE:CB	2.34	0.49
2:B:326:TYR:OH	2:B:353:LEU:HB2	2.12	0.49
2:B:422:TYR:CE1	2:B:444:TRP:HA	2.48	0.49
3:C:235:LEU:HD12	3:C:235:LEU:N	2.26	0.49
2:E:162:PRO:HG3	3:F:103:HIS:CE1	2.47	0.49
2:E:270:LYS:HG3	2:E:338:TYR:OH	2.12	0.49
3:F:218:LEU:HD21	3:F:226:PHE:CE2	2.48	0.49
2:H:326:TYR:OH	2:H:353:LEU:HB2	2.12	0.49
3:I:191:TRP:CH2	3:I:247:ARG:HD3	2.48	0.49
3:L:216:GLY:O	3:L:217:HIS:CD2	2.65	0.49
2:B:164:ASN:N	2:B:166:ARG:HE	2.10	0.48
2:B:205:VAL:HG21	3:C:215:PHE:O	2.13	0.48
2:B:252:ILE:HG23	2:B:299:ILE:HG12	1.94	0.48
2:B:326:TYR:C	2:B:328:GLY:N	2.71	0.48
2:E:234:LYS:HG2	2:E:235:PRO:HD2	1.94	0.48
2:E:385:TRP:HZ3	2:E:397:GLU:OE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:92:GLU:HG2	3:F:93:ILE:H	1.76	0.48
3:F:278:TYR:HH	3:F:308:ASN:HB2	1.78	0.48
3:I:202:VAL:HG21	3:I:225:GLU:O	2.13	0.48
2:K:224:MET:SD	2:K:237:ARG:HD3	2.53	0.48
3:L:356:LYS:O	3:L:359:THR:OG1	2.28	0.48
2:B:317:TRP:CE3	2:B:448:ARG:HD3	2.48	0.48
2:B:399:GLY:H	2:B:433:ASP:HB2	1.79	0.48
2:B:405:ASN:O	2:B:405:ASN:CG	2.56	0.48
3:C:310:MET:O	3:C:335:TRP:CD1	2.65	0.48
1:D:131:GLN:HG3	1:D:132:HIS:H	1.78	0.48
1:D:176:LYS:HE2	1:D:176:LYS:HB2	1.68	0.48
2:E:223:GLU:HA	2:E:287:GLY:HA2	1.95	0.48
2:E:243:ASN:O	2:E:244:THR:C	2.55	0.48
3:F:238:THR:HG22	3:F:266:LYS:CE	2.41	0.48
2:H:189:GLN:O	2:H:193:CYS:SG	2.71	0.48
2:H:262:PHE:HB3	2:H:269:TYR:OH	2.12	0.48
2:H:317:TRP:CH2	2:H:418:TRP:HA	2.49	0.48
3:I:245:ALA:HA	3:I:265:PHE:HB2	1.95	0.48
2:K:237:ARG:HH11	2:K:237:ARG:HG3	1.77	0.48
2:K:266:TRP:HA	2:K:377:THR:HG21	1.94	0.48
2:B:262:PHE:HB3	2:B:269:TYR:OH	2.13	0.48
2:B:316:ASP:HB2	2:B:445:TYR:CE2	2.45	0.48
3:C:196:LYS:HE3	3:C:198:LEU:HD11	1.96	0.48
1:D:137:GLN:C	1:D:140:VAL:HG12	2.38	0.48
2:E:280:THR:OG1	2:E:288:LEU:HG	2.13	0.48
3:F:269:PRO:C	3:F:273:LYS:O	2.56	0.48
2:H:252:ILE:CG2	2:H:299:ILE:HG12	2.43	0.48
2:H:362:GLY:O	2:H:363:GLU:C	2.56	0.48
3:I:117:ASN:HD22	3:I:117:ASN:H	1.52	0.48
3:I:275:ARG:HB2	3:I:311:GLN:HG2	1.95	0.48
2:K:234:LYS:HD3	2:K:235:PRO:O	2.13	0.48
2:K:293:TRP:HE1	2:K:296:ASN:ND2	2.10	0.48
3:L:216:GLY:HA3	3:L:226:PHE:HA	1.95	0.48
1:A:159:ARG:C	1:A:161:CYS:H	2.21	0.48
2:B:236:TYR:CD2	2:B:298:LYS:HD3	2.48	0.48
2:B:338:TYR:O	2:B:339:GLN:C	2.56	0.48
3:C:169:ILE:CD1	3:C:171:PRO:HD3	2.31	0.48
2:E:310:LEU:HB3	2:E:326:TYR:HB2	1.95	0.48
3:F:94:MET:HE3	3:F:96:TYR:OH	2.14	0.48
2:H:362:GLY:O	2:H:365:ARG:N	2.47	0.48
3:I:264:MET:CE	3:L:279:ALA:HA	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:276:LEU:CD2	3:I:276:LEU:H	2.26	0.48
3:I:304:PHE:CB	3:I:338:LYS:HB3	2.43	0.48
3:I:353:THR:HA	3:I:377:TYR:HA	1.96	0.48
1:J:126:VAL:HG13	1:J:127:ILE:H	1.78	0.48
3:L:261:ASP:HB2	3:L:282:ALA:HB3	1.94	0.48
3:L:314:THR:HG22	3:L:333:GLY:HA3	1.95	0.48
2:B:161:ILE:O	2:B:166:ARG:CZ	2.62	0.48
2:B:267:ASP:O	2:B:270:LYS:N	2.47	0.48
3:C:383:THR:O	3:C:384:MET:HG3	2.13	0.48
1:D:143:GLN:O	1:D:147:MET:HG2	2.13	0.48
2:E:204:PRO:O	2:E:205:VAL:C	2.55	0.48
3:F:154:GLN:C	3:F:156:ILE:N	2.69	0.48
3:F:166:LEU:CD2	3:F:218:LEU:HB3	2.43	0.48
1:J:140:VAL:CG1	1:J:141:ARG:N	2.76	0.48
2:K:304:ARG:C	2:K:306:GLY:H	2.21	0.48
3:L:94:MET:HB3	3:L:96:TYR:HE2	1.78	0.48
3:L:230:ASN:C	3:L:232:LYS:N	2.71	0.48
3:L:320:ASP:HB3	3:L:336:MET:HB2	1.95	0.48
3:C:96:TYR:O	3:C:99:SER:N	2.46	0.48
2:E:423:THR:OG1	2:E:426:MET:HE3	2.13	0.48
3:F:145:ILE:HD13	3:F:168:PHE:CE2	2.44	0.48
3:F:198:LEU:N	3:F:198:LEU:HD12	2.28	0.48
3:F:391:ARG:HB2	3:F:391:ARG:HH11	1.75	0.48
1:G:126:VAL:C	1:G:128:GLU:H	2.20	0.48
1:A:184:GLN:C	1:A:186:GLU:N	2.62	0.48
2:B:177:SER:CA	2:B:180:GLN:HG2	2.42	0.48
2:B:276:VAL:O	2:B:276:VAL:HG12	2.13	0.48
3:C:198:LEU:C	3:C:348:TYR:OH	2.56	0.48
2:E:253:GLN:OE1	2:E:255:ARG:HG2	2.14	0.48
1:G:129:LYS:C	1:G:133:ILE:HD13	2.38	0.48
3:I:238:THR:HG22	3:I:266:LYS:CG	2.44	0.48
1:J:141:ARG:NH1	1:J:186:GLU:OE2	2.44	0.48
2:K:373:MET:CG	2:K:405:ASN:HD22	2.26	0.48
3:L:243:PRO:HB2	3:L:389:PHE:HB3	1.96	0.48
2:B:249:TRP:HB3	2:B:453:LYS:HB2	1.96	0.48
2:B:300:SER:OG	2:B:332:GLN:O	2.31	0.48
2:B:326:TYR:C	2:B:328:GLY:H	2.22	0.48
2:B:356:GLY:O	2:B:439:ASN:OD1	2.30	0.48
2:B:442:GLY:O	2:B:444:TRP:N	2.47	0.48
3:C:272:ASP:O	3:C:311:GLN:NE2	2.45	0.48
2:E:217:LYS:HE3	3:F:213:GLU:CD	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:355:ASP:O	2:E:365:ARG:HD3	2.14	0.48
1:G:127:ILE:O	1:G:131:GLN:HB2	2.14	0.48
3:I:295:PHE:H	3:I:301:ASP:HB3	1.78	0.48
1:J:167:ARG:HB2	2:K:192:TYR:CG	2.49	0.48
2:K:318:LYS:NZ	2:K:441:LYS:NZ	2.61	0.48
3:L:154:GLN:C	3:L:156:ILE:N	2.70	0.48
3:L:326:CYS:CB	3:L:336:MET:HE3	2.41	0.48
3:C:120:LYS:O	3:C:123:ASN:HB2	2.13	0.48
3:C:197:ARG:HB2	3:C:382:THR:HB	1.96	0.48
3:F:216:GLY:HA3	3:F:226:PHE:HA	1.95	0.48
3:F:275:ARG:HA	3:F:311:GLN:HA	1.95	0.48
2:H:199:VAL:C	2:H:200:SER:HG	2.22	0.48
2:H:210:GLU:CD	2:H:212:GLU:H	2.19	0.48
3:I:390:ASN:OD1	3:I:391:ARG:HG3	2.13	0.48
1:J:143:GLN:NE2	3:L:117:ASN:CB	2.77	0.48
1:J:186:GLU:OE1	1:J:189:ILE:HD12	2.14	0.48
2:K:278:THR:O	2:K:288:LEU:HB2	2.14	0.48
2:K:351:ASN:HD21	2:K:354:MET:HB2	1.79	0.48
2:B:252:ILE:CG2	2:B:299:ILE:HG12	2.43	0.48
2:B:385:TRP:CE3	4:M:3:ARG:HG3	2.48	0.48
2:B:442:GLY:C	2:B:444:TRP:H	2.22	0.48
3:C:263:ALA:HB1	3:C:264:MET:SD	2.54	0.48
3:C:334:TRP:CG	3:C:335:TRP:H	2.31	0.48
1:D:148:LYS:O	1:D:151:GLU:HB3	2.14	0.48
3:F:172:LEU:CD1	3:F:240:SER:HB3	2.37	0.48
3:F:284:GLY:C	3:F:286:ALA:H	2.22	0.48
3:F:391:ARG:HH11	3:F:391:ARG:CB	2.27	0.48
2:H:155:GLU:C	2:H:157:VAL:N	2.70	0.48
2:H:161:ILE:HG21	3:I:103:HIS:HE1	1.74	0.48
2:H:177:SER:OG	2:H:178:LYS:N	2.47	0.48
2:H:350:GLY:O	2:H:352:ALA:N	2.47	0.48
3:I:167:TYR:N	3:I:167:TYR:HD1	2.12	0.48
3:I:394:ILE:HG13	3:I:396:GLU:H	1.77	0.48
2:K:240:CYS:CB	2:K:242:MET:HE2	2.44	0.48
3:L:336:MET:HE1	3:L:340:HIS:HD2	1.79	0.48
2:B:156:THR:CA	2:B:160:ASN:HB2	2.44	0.47
2:B:187:SER:C	2:B:189:GLN:H	2.20	0.47
1:D:123:LYS:O	1:D:125:LYS:N	2.47	0.47
1:D:188:VAL:HG11	2:E:164:ASN:HA	1.96	0.47
2:H:152:TYR:C	2:H:154:ASP:N	2.72	0.47
2:H:252:ILE:HG23	2:H:299:ILE:HG12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:342:VAL:O	2:H:371:ASN:ND2	2.47	0.47
2:H:371:ASN:C	2:H:373:MET:H	2.22	0.47
2:H:398:ASP:HA	2:H:433:ASP:HB2	1.93	0.47
2:H:412:PRO:HG3	2:H:450:MET:CE	2.44	0.47
3:I:219:SER:HB2	3:I:220:PRO:HD2	1.95	0.47
3:I:243:PRO:HB2	3:I:389:PHE:HB3	1.95	0.47
3:I:253:TRP:O	3:I:254:ASN:CG	2.57	0.47
3:I:381:LYS:O	3:I:382:THR:OG1	2.28	0.47
2:K:204:PRO:O	2:K:205:VAL:O	2.32	0.47
3:L:261:ASP:O	3:L:262:TYR:CD2	2.67	0.47
1:A:128:GLU:HA	1:A:131:GLN:OE1	2.14	0.47
2:B:165:LEU:CB	2:B:166:ARG:NH2	2.76	0.47
3:C:239:GLN:C	3:C:241:ALA:H	2.21	0.47
1:D:143:GLN:NE2	3:F:117:ASN:CB	2.76	0.47
2:E:180:GLN:HG3	2:E:181:LYS:H	1.77	0.47
3:F:205:LYS:HZ2	3:F:331:GLY:HA2	1.78	0.47
3:F:290:PHE:HD1	3:F:307:HIS:ND1	2.11	0.47
2:H:267:ASP:O	2:H:270:LYS:N	2.47	0.47
2:H:280:THR:O	2:H:281:ASP:C	2.56	0.47
3:I:113:ILE:HD12	3:I:113:ILE:H	1.77	0.47
3:I:344:LEU:C	3:I:346:GLY:N	2.69	0.47
2:K:164:ASN:C	2:K:166:ARG:N	2.72	0.47
2:K:176:ARG:C	2:K:178:LYS:H	2.22	0.47
2:K:367:MET:O	2:K:405:ASN:O	2.32	0.47
3:L:246:LEU:HG	3:L:247:ARG:H	1.78	0.47
1:A:128:GLU:C	1:A:131:GLN:HG2	2.38	0.47
1:A:148:LYS:HZ1	2:B:425:ASP:CB	2.28	0.47
2:B:238:VAL:CG2	2:B:239:TYR:H	2.27	0.47
3:C:198:LEU:CD2	3:C:223:THR:HA	2.45	0.47
3:C:207:ASN:OD1	3:C:210:GLN:HG3	2.13	0.47
1:D:151:GLU:OE2	2:E:182:LEU:HD21	2.13	0.47
3:F:109:TYR:O	3:F:112:GLU:HB2	2.14	0.47
2:H:249:TRP:CZ2	2:H:455:ARG:CZ	2.97	0.47
3:I:133:ALA:HA	3:I:136:GLN:CG	2.44	0.47
3:I:370:ALA:HA	3:I:373:LYS:O	2.14	0.47
1:J:179:GLU:O	1:J:180:ASP:C	2.57	0.47
3:L:185:ASP:OD2	3:L:187:SER:HB3	2.14	0.47
3:L:198:LEU:HD12	3:L:198:LEU:N	2.29	0.47
2:B:161:ILE:HG22	2:B:166:ARG:NH1	2.28	0.47
2:B:173:GLU:C	2:B:175:LEU:N	2.73	0.47
2:B:253:GLN:HB2	2:B:293:TRP:HE3	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:SER:C	2:B:360:LEU:H	2.21	0.47
3:C:168:PHE:CE1	3:C:179:LEU:HD13	2.50	0.47
3:C:336:MET:HE1	3:C:340:HIS:CD2	2.50	0.47
1:D:124:ARG:H	1:D:124:ARG:CD	2.18	0.47
2:E:203:ILE:HD12	2:E:203:ILE:H	1.77	0.47
2:E:304:ARG:C	2:E:306:GLY:H	2.21	0.47
2:E:333:ASN:HB3	2:E:336:ASN:ND2	2.29	0.47
1:G:119:ILE:O	1:G:119:ILE:HG12	2.14	0.47
2:H:373:MET:HE3	2:H:374:PHE:N	2.28	0.47
3:I:109:TYR:O	3:I:112:GLU:N	2.48	0.47
3:I:295:PHE:H	3:I:301:ASP:CB	2.27	0.47
3:L:109:TYR:CD1	3:L:110:LEU:HD23	2.49	0.47
3:L:227:TRP:NE1	3:L:230:ASN:ND2	2.63	0.47
3:L:269:PRO:C	3:L:273:LYS:O	2.57	0.47
1:A:124:ARG:CD	1:A:124:ARG:H	2.27	0.47
2:B:213:GLU:OE2	2:B:217:LYS:NZ	2.41	0.47
2:B:249:TRP:CZ2	2:B:455:ARG:CZ	2.97	0.47
2:B:351:ASN:O	2:B:355:ASP:HB2	2.14	0.47
3:C:103:HIS:HA	3:C:106:SER:CB	2.44	0.47
2:E:410:ALA:C	2:E:412:PRO:HD3	2.40	0.47
3:F:208:TRP:HA	3:F:314:THR:HG21	1.97	0.47
3:F:292:GLY:HA2	3:F:305:THR:O	2.13	0.47
3:F:313:SER:HB3	3:F:319:ASN:H	1.80	0.47
1:G:155:ASP:HA	1:G:171:ARG:NH1	2.30	0.47
2:H:152:TYR:C	2:H:154:ASP:H	2.22	0.47
2:H:224:MET:HB2	2:H:286:CYS:HB2	1.95	0.47
3:I:166:LEU:HD23	3:I:166:LEU:N	2.29	0.47
3:I:387:ILE:HG12	3:I:388:PRO:N	2.28	0.47
1:J:125:LYS:O	1:J:128:GLU:HB2	2.15	0.47
2:K:201:CYS:O	3:L:143:VAL:HG21	2.14	0.47
3:L:131:LEU:O	3:L:134:GLN:N	2.36	0.47
2:B:167:VAL:HG23	2:B:167:VAL:O	2.13	0.47
2:B:266:TRP:HB3	2:B:267:ASP:H	1.54	0.47
2:B:411:ASN:HD22	2:B:434:GLY:H	1.63	0.47
3:C:126:GLU:C	3:C:128:VAL:N	2.69	0.47
3:C:145:ILE:HD12	3:C:145:ILE:O	2.15	0.47
1:D:128:GLU:O	1:D:129:LYS:C	2.55	0.47
3:F:194:PHE:CE2	3:F:384:MET:CB	2.97	0.47
2:H:266:TRP:HB3	2:H:267:ASP:H	1.55	0.47
2:H:294:LEU:O	2:H:295:GLY:C	2.57	0.47
2:K:340:ILE:HG21	2:K:403:TRP:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:385:TRP:HZ3	2:K:397:GLU:OE2	1.97	0.47
3:L:284:GLY:C	3:L:286:ALA:H	2.23	0.47
1:A:146:ASP:O	1:A:146:ASP:OD2	2.33	0.47
1:A:151:GLU:O	1:A:154:ILE:HG22	2.13	0.47
2:B:172:LEU:HD11	3:C:113:ILE:HG22	1.95	0.47
2:B:345:TYR:HB3	2:B:354:MET:CE	2.44	0.47
2:B:368:THR:HB	2:B:409:ALA:HB2	1.97	0.47
3:C:191:TRP:C	3:C:192:THR:HG22	2.40	0.47
3:C:198:LEU:HD12	3:C:198:LEU:N	2.29	0.47
3:C:276:LEU:H	3:C:276:LEU:CD2	2.28	0.47
3:C:344:LEU:C	3:C:346:GLY:N	2.69	0.47
1:D:169:LEU:HD22	1:D:170:ALA:O	2.14	0.47
3:F:216:GLY:O	3:F:217:HIS:CD2	2.67	0.47
3:F:244:TYR:CE2	3:F:388:PRO:HG3	2.49	0.47
3:F:333:GLY:O	3:F:334:TRP:HB2	2.14	0.47
3:F:334:TRP:CZ3	3:F:344:LEU:HB2	2.50	0.47
1:G:154:ILE:HG22	1:G:171:ARG:NH1	2.30	0.47
1:G:167:ARG:HH12	1:G:169:LEU:HD23	1.80	0.47
2:H:276:VAL:O	2:H:277:ALA:CB	2.62	0.47
2:H:311:LEU:HD11	2:H:323:LYS:HB2	1.97	0.47
3:I:263:ALA:HB1	3:I:264:MET:SD	2.55	0.47
3:I:337:ASN:C	3:I:339:CYS:N	2.64	0.47
1:J:167:ARG:NH1	1:J:168:ALA:H	2.13	0.47
2:K:313:GLU:HB3	2:K:323:LYS:HG3	1.96	0.47
3:L:166:LEU:CD2	3:L:218:LEU:HB3	2.45	0.47
1:A:159:ARG:NH2	2:B:418:TRP:CD2	2.83	0.47
2:B:161:ILE:CG2	2:B:166:ARG:HH12	2.28	0.47
2:B:284:ASN:ND2	2:B:284:ASN:N	2.63	0.47
3:C:94:MET:C	3:C:96:TYR:N	2.71	0.47
1:D:166:SER:HB2	2:E:195:THR:O	2.15	0.47
2:E:181:LYS:O	2:E:184:SER:HB3	2.15	0.47
1:G:149:ARG:HG2	2:H:426:MET:O	2.15	0.47
3:I:198:LEU:HD12	3:I:198:LEU:N	2.30	0.47
2:K:204:PRO:O	2:K:205:VAL:C	2.57	0.47
1:A:132:HIS:O	1:A:133:ILE:C	2.56	0.47
1:A:143:GLN:HA	1:A:143:GLN:NE2	2.16	0.47
2:B:155:GLU:C	2:B:157:VAL:N	2.70	0.47
2:H:242:MET:HA	2:H:247:GLY:HA3	1.97	0.47
2:H:351:ASN:O	2:H:355:ASP:HB2	2.15	0.47
3:I:298:ASP:N	3:I:301:ASP:OD1	2.48	0.47
1:J:126:VAL:CG1	1:J:127:ILE:H	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:191:LYS:NZ	1:J:191:LYS:CB	2.77	0.47
2:K:326:TYR:CD1	2:K:342:VAL:HB	2.50	0.47
3:L:172:LEU:CD1	3:L:240:SER:HB3	2.38	0.47
3:L:194:PHE:CE2	3:L:384:MET:CB	2.98	0.47
1:A:169:LEU:HD13	1:A:170:ALA:H	1.76	0.47
1:D:142:ALA:O	1:D:145:VAL:HB	2.15	0.47
2:E:441:LYS:HG3	2:E:447:MET:HE1	1.96	0.47
1:G:169:LEU:HD13	1:G:170:ALA:C	2.40	0.47
2:H:310:LEU:CD1	2:H:312:ILE:HG13	2.37	0.47
2:H:357:ALA:HA	2:H:439:ASN:CG	2.39	0.47
2:H:359:GLN:O	2:H:359:GLN:CG	2.63	0.47
3:I:239:GLN:C	3:I:241:ALA:H	2.22	0.47
1:J:139:ASN:HB3	3:L:114:TYR:CZ	2.50	0.47
2:K:217:LYS:HE3	3:L:213:GLU:CD	2.40	0.47
3:L:195:GLN:CB	3:L:384:MET:HE2	2.45	0.47
4:R:2:PRO:O	4:R:3:ARG:HD3	2.15	0.47
1:A:168:ALA:HA	2:B:189:GLN:CD	2.40	0.46
2:B:153:ILE:C	2:B:155:GLU:N	2.72	0.46
3:C:156:ILE:C	3:C:158:ASN:N	2.72	0.46
3:C:172:LEU:HD12	3:C:172:LEU:N	2.24	0.46
3:C:259:THR:H	3:C:286:ALA:HB2	1.79	0.46
3:C:311:GLN:OE1	3:C:319:ASN:HB3	2.15	0.46
1:D:180:ASP:O	1:D:184:GLN:HB2	2.15	0.46
1:D:186:GLU:OE1	1:D:189:ILE:HD12	2.15	0.46
2:E:240:CYS:CB	2:E:242:MET:HE2	2.44	0.46
3:F:290:PHE:HA	3:F:307:HIS:ND1	2.30	0.46
2:H:304:ARG:HH11	2:H:304:ARG:HG3	1.79	0.46
2:H:412:PRO:CG	2:H:450:MET:HE1	2.45	0.46
3:I:94:MET:HG3	3:I:94:MET:O	2.14	0.46
3:I:198:LEU:C	3:I:348:TYR:OH	2.57	0.46
2:K:326:TYR:OH	2:K:351:ASN:ND2	2.48	0.46
2:K:441:LYS:CG	2:K:447:MET:HE1	2.45	0.46
3:L:312:PHE:HD1	3:L:335:TRP:CD1	2.33	0.46
3:L:313:SER:HB3	3:L:319:ASN:H	1.80	0.46
3:C:243:PRO:HB2	3:C:389:PHE:HB3	1.97	0.46
3:C:287:GLY:CA	3:C:371:THR:HB	2.45	0.46
1:D:185:LEU:HB2	2:E:171:ILE:HD11	1.97	0.46
2:E:456:PRO:O	2:E:457:PHE:C	2.58	0.46
1:G:120:GLU:OE1	1:G:124:ARG:NH2	2.48	0.46
2:H:363:GLU:O	2:H:367:MET:HG2	2.16	0.46
3:I:191:TRP:C	3:I:192:THR:HG22	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:208:TRP:O	3:I:210:GLN:N	2.48	0.46
3:I:253:TRP:CD2	3:I:380:LYS:HB2	2.51	0.46
2:K:412:PRO:O	2:K:413:ASN:CB	2.50	0.46
3:L:203:ASP:OD2	3:L:205:LYS:HB2	2.16	0.46
1:A:161:CYS:HB3	1:A:165:CYS:SG	2.55	0.46
1:A:167:ARG:NH1	1:A:169:LEU:HD23	2.16	0.46
1:A:175:LEU:HD13	2:B:426:MET:HE3	1.98	0.46
2:B:197:CYS:O	3:C:140:LYS:N	2.42	0.46
2:B:362:GLY:O	2:B:363:GLU:C	2.59	0.46
2:B:412:PRO:CG	2:B:450:MET:HE1	2.45	0.46
3:C:208:TRP:CA	3:C:314:THR:HG21	2.44	0.46
3:C:219:SER:HB2	3:C:220:PRO:HD2	1.97	0.46
3:C:237:SER:O	3:C:266:LYS:HG3	2.15	0.46
3:C:271:ALA:C	3:C:273:LYS:N	2.71	0.46
2:E:432:ASP:HB3	2:E:444:TRP:CH2	2.50	0.46
3:F:172:LEU:H	3:F:239:GLN:HE21	1.63	0.46
3:F:203:ASP:OD2	3:F:205:LYS:HB2	2.16	0.46
1:G:158:ILE:HG13	2:H:189:GLN:HG2	1.97	0.46
2:H:180:GLN:C	2:H:182:LEU:N	2.74	0.46
2:H:284:ASN:H	2:H:284:ASN:ND2	2.06	0.46
2:H:360:LEU:HD22	5:H:470:NAG:H83	1.96	0.46
3:I:236:ILE:O	3:I:236:ILE:HG13	2.14	0.46
3:I:259:THR:H	3:I:286:ALA:HB2	1.80	0.46
2:K:156:THR:C	2:K:158:ASN:H	2.22	0.46
2:K:456:PRO:O	2:K:457:PHE:C	2.58	0.46
2:B:256:GLN:HE21	2:B:449:LYS:CE	2.18	0.46
2:B:266:TRP:NE1	2:B:380:ARG:CZ	2.78	0.46
2:B:386:LEU:O	2:B:386:LEU:HD13	2.15	0.46
2:E:182:LEU:O	2:E:186:VAL:HG23	2.14	0.46
3:F:314:THR:O	3:F:315:TRP:C	2.56	0.46
2:H:359:GLN:NE2	2:H:359:GLN:N	2.62	0.46
3:I:198:LEU:CD2	3:I:223:THR:HA	2.45	0.46
3:I:340:HIS:HE1	3:I:364:ASP:OD2	1.98	0.46
3:L:322:PHE:CE2	3:L:324:GLY:HA3	2.50	0.46
3:L:325:ASN:O	3:L:326:CYS:C	2.57	0.46
1:A:161:CYS:C	1:A:163:GLY:N	2.73	0.46
2:B:184:SER:O	2:B:185:ASP:C	2.58	0.46
2:B:280:THR:O	2:B:281:ASP:C	2.57	0.46
2:B:284:ASN:HD22	2:B:284:ASN:N	2.05	0.46
3:C:116:SER:O	3:C:120:LYS:N	2.37	0.46
3:C:394:ILE:C	3:C:396:GLU:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:GLU:O	1:D:131:GLN:HG2	2.16	0.46
1:G:184:GLN:OE1	2:H:167:VAL:HG22	2.15	0.46
2:H:356:GLY:O	2:H:439:ASN:OD1	2.34	0.46
3:I:124:LEU:N	3:I:124:LEU:CD1	2.77	0.46
3:I:392:LEU:O	3:I:393:THR:HB	2.16	0.46
1:J:144:LEU:CD2	2:K:175:LEU:HD21	2.44	0.46
3:L:246:LEU:HD13	3:L:265:PHE:CD2	2.50	0.46
3:L:310:MET:C	3:L:311:GLN:O	2.56	0.46
2:B:210:GLU:CD	2:B:210:GLU:C	2.83	0.46
2:B:226:LEU:O	2:B:226:LEU:HD12	2.16	0.46
2:B:236:TYR:O	2:B:236:TYR:CD1	2.69	0.46
3:C:93:ILE:C	3:C:95:LYS:H	2.23	0.46
3:C:97:GLU:C	3:C:99:SER:N	2.65	0.46
3:C:166:LEU:HD23	3:C:166:LEU:N	2.31	0.46
3:C:382:THR:O	3:C:382:THR:CG2	2.58	0.46
2:E:278:THR:O	2:E:288:LEU:HB2	2.16	0.46
1:G:165:CYS:O	1:G:166:SER:O	2.34	0.46
2:H:365:ARG:O	2:H:368:THR:HG23	2.15	0.46
2:H:368:THR:HB	2:H:409:ALA:HB2	1.98	0.46
3:I:162:LYS:HE3	3:I:186:GLY:HA2	1.96	0.46
1:J:149:ARG:O	1:J:152:VAL:CG2	2.64	0.46
1:J:178:TYR:CZ	2:K:178:LYS:HD3	2.51	0.46
2:K:351:ASN:OD1	2:K:354:MET:HB2	2.16	0.46
3:L:329:GLN:HE21	3:L:361:ASN:HD22	1.64	0.46
2:B:158:ASN:OD1	3:C:100:ILE:HG21	2.16	0.46
2:B:264:ARG:HD2	2:B:268:PRO:HB3	1.98	0.46
2:B:334:GLU:HG3	2:B:338:TYR:CE2	2.51	0.46
3:C:163:GLN:CA	3:C:163:GLN:NE2	2.78	0.46
3:C:195:GLN:OE1	3:C:197:ARG:HG2	2.15	0.46
3:C:238:THR:HG22	3:C:266:LYS:CG	2.46	0.46
3:C:248:VAL:HG22	3:C:384:MET:HG2	1.98	0.46
3:C:377:TYR:C	3:C:377:TYR:CD2	2.94	0.46
2:E:204:PRO:O	2:E:205:VAL:O	2.34	0.46
3:F:305:THR:CB	3:F:341:ALA:HB2	2.45	0.46
2:H:190:MET:HB2	3:I:131:LEU:HD12	1.98	0.46
2:H:236:TYR:O	2:H:236:TYR:CD1	2.69	0.46
2:K:155:GLU:O	2:K:157:VAL:N	2.49	0.46
2:K:327:GLY:HA3	2:K:344:LYS:CB	2.43	0.46
1:A:144:LEU:HD11	1:A:182:GLN:CG	2.46	0.46
1:A:188:VAL:HG11	2:B:167:VAL:HG21	1.97	0.46
2:B:184:SER:C	2:B:186:VAL:N	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:MET:HA	2:B:247:GLY:HA3	1.98	0.46
3:C:118:ASN:ND2	3:C:118:ASN:N	2.60	0.46
3:C:148:ILE:HD13	3:C:156:ILE:CG2	2.46	0.46
3:C:156:ILE:HA	3:C:159:LYS:CD	2.45	0.46
3:C:171:PRO:O	3:C:172:LEU:C	2.59	0.46
3:C:258:SER:O	3:C:259:THR:HB	2.16	0.46
2:E:432:ASP:HB3	2:E:444:TRP:CZ3	2.51	0.46
3:F:236:ILE:HG22	3:F:386:ILE:HD11	1.96	0.46
3:F:261:ASP:HB2	3:F:282:ALA:HB3	1.97	0.46
2:H:397:GLU:O	2:H:398:ASP:C	2.59	0.46
3:I:195:GLN:OE1	3:I:197:ARG:HG2	2.15	0.46
2:K:182:LEU:O	2:K:186:VAL:HG23	2.15	0.46
3:L:107:ILE:O	3:L:107:ILE:HD13	2.16	0.46
3:L:153:CYS:HA	3:L:156:ILE:HD12	1.97	0.46
3:L:246:LEU:HD12	3:L:386:ILE:HG22	1.96	0.46
3:L:275:ARG:HA	3:L:311:GLN:HA	1.96	0.46
3:L:330:ASP:HB3	3:L:343:HIS:HE1	1.80	0.46
2:B:365:ARG:HG2	2:B:366:THR:N	2.30	0.46
1:D:140:VAL:CG1	1:D:141:ARG:H	2.29	0.46
2:E:435:VAL:O	2:E:446:SER:HA	2.16	0.46
3:F:242:ILE:HG23	3:F:243:PRO:HD2	1.97	0.46
3:F:320:ASP:OD1	3:F:326:CYS:SG	2.73	0.46
1:G:140:VAL:HG12	3:I:114:TYR:CE1	2.51	0.46
3:I:248:VAL:O	3:I:248:VAL:HG12	2.16	0.46
3:I:272:ASP:O	3:I:311:GLN:NE2	2.47	0.46
3:I:322:PHE:CG	3:I:323:GLU:N	2.84	0.46
1:A:136:LEU:HA	1:A:139:ASN:HB2	1.98	0.46
1:A:154:ILE:CG2	1:A:155:ASP:N	2.79	0.46
2:B:157:VAL:O	2:B:158:ASN:CB	2.60	0.46
2:B:173:GLU:C	2:B:176:ARG:H	2.23	0.46
2:B:345:TYR:CZ	2:B:351:ASN:N	2.84	0.46
3:C:248:VAL:O	3:C:259:THR:HA	2.16	0.46
2:E:318:LYS:NZ	2:E:441:LYS:NZ	2.64	0.46
2:H:357:ALA:CA	2:H:439:ASN:HD21	2.17	0.46
3:I:137:GLU:HB3	3:I:138:PRO:HD2	1.98	0.46
3:I:156:ILE:C	3:I:158:ASN:N	2.73	0.46
3:I:334:TRP:CG	3:I:335:TRP:H	2.33	0.46
3:I:339:CYS:HB2	4:S:1:GLY:O	2.16	0.46
2:K:183:GLU:HG2	3:L:124:LEU:HG	1.98	0.46
2:K:434:GLY:O	2:K:436:VAL:N	2.49	0.46
2:B:314:MET:HE1	2:B:437:TRP:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:296:GLY:O	3:C:297:ASP:C	2.58	0.45
3:C:340:HIS:ND1	3:C:368:ILE:HD11	2.31	0.45
1:D:188:VAL:HB	2:E:164:ASN:CG	2.41	0.45
2:E:214:ILE:CD1	2:E:227:ILE:HG22	2.45	0.45
2:E:374:PHE:O	2:E:403:TRP:HA	2.16	0.45
2:E:408:HIS:CD2	2:E:411:ASN:HB2	2.52	0.45
3:F:162:LYS:HE3	3:F:186:GLY:CA	2.45	0.45
3:F:229:GLY:O	3:F:233:ILE:CG1	2.62	0.45
1:G:167:ARG:NE	2:H:192:TYR:CD2	2.77	0.45
2:H:236:TYR:CD2	2:H:298:LYS:HD3	2.52	0.45
2:H:309:GLU:O	2:H:454:ILE:HB	2.16	0.45
3:L:318:ASP:OD1	3:L:320:ASP:OD2	2.35	0.45
1:A:126:VAL:C	1:A:128:GLU:N	2.74	0.45
2:B:299:ILE:O	2:B:301:GLN:N	2.50	0.45
2:B:300:SER:HA	2:B:331:VAL:HB	1.97	0.45
2:B:349:ALA:O	2:B:440:TRP:HB2	2.16	0.45
2:B:369:ILE:O	2:B:405:ASN:HB3	2.15	0.45
3:C:96:TYR:O	3:C:98:ALA:N	2.49	0.45
3:C:320:ASP:OD2	3:C:322:PHE:HB3	2.16	0.45
2:E:326:TYR:CD1	2:E:342:VAL:HB	2.51	0.45
2:E:367:MET:HB2	2:E:406:ARG:HB3	1.98	0.45
1:G:189:ILE:O	1:G:189:ILE:HG13	2.15	0.45
2:H:447:MET:H	2:H:447:MET:HG2	1.43	0.45
3:I:207:ASN:OD1	3:I:210:GLN:HG3	2.16	0.45
2:B:224:MET:HB2	2:B:286:CYS:HB2	1.98	0.45
2:B:371:ASN:C	2:B:373:MET:H	2.24	0.45
3:C:310:MET:HE1	3:C:321:LYS:CE	2.44	0.45
3:C:322:PHE:CG	3:C:323:GLU:N	2.84	0.45
2:E:159:SER:O	2:E:160:ASN:HB2	2.16	0.45
2:E:191:GLU:C	2:E:193:CYS:H	2.24	0.45
2:E:234:LYS:HD3	2:E:235:PRO:O	2.16	0.45
3:F:242:ILE:HG22	3:F:243:PRO:HD2	1.96	0.45
3:F:310:MET:C	3:F:311:GLN:O	2.56	0.45
1:G:146:ASP:O	1:G:146:ASP:OD2	2.34	0.45
1:G:147:MET:HE1	3:I:121:ILE:HD11	1.99	0.45
2:H:300:SER:OG	2:H:332:GLN:O	2.33	0.45
2:H:366:THR:O	2:H:369:ILE:HG13	2.17	0.45
2:H:440:TRP:CE3	2:H:447:MET:HE1	2.52	0.45
3:I:156:ILE:HA	3:I:159:LYS:CD	2.46	0.45
2:K:203:ILE:HG21	2:K:226:LEU:HD22	1.98	0.45
2:K:204:PRO:HA	3:L:217:HIS:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:223:GLU:CB	2:K:287:GLY:HA2	2.46	0.45
3:L:154:GLN:HE21	3:L:158:ASN:ND2	2.13	0.45
1:A:136:LEU:CD2	1:A:139:ASN:HD22	2.29	0.45
2:B:164:ASN:O	2:B:168:LEU:HB2	2.17	0.45
2:B:187:SER:HA	2:B:190:MET:CB	2.40	0.45
2:B:209:LYS:HG2	2:B:229:PRO:HA	1.97	0.45
3:C:204:PHE:CE1	3:C:225:GLU:HB3	2.50	0.45
2:E:204:PRO:HA	3:F:217:HIS:CD2	2.50	0.45
3:F:281:PHE:CG	3:F:288:ASP:HB2	2.52	0.45
3:I:204:PHE:CE1	3:I:225:GLU:HB3	2.50	0.45
3:I:336:MET:HE1	3:I:340:HIS:HD2	1.81	0.45
3:L:229:GLY:O	3:L:233:ILE:CG1	2.63	0.45
1:A:187:GLN:O	1:A:189:ILE:N	2.41	0.45
3:C:114:TYR:C	3:C:116:SER:H	2.24	0.45
3:C:158:ASN:OD1	3:C:188:GLY:O	2.34	0.45
3:C:372:TRP:CE2	3:C:373:LYS:NZ	2.85	0.45
1:D:126:VAL:O	1:D:128:GLU:N	2.50	0.45
2:E:222:SER:O	2:E:223:GLU:HB3	2.16	0.45
2:E:373:MET:CG	2:E:405:ASN:HD22	2.28	0.45
3:F:168:PHE:HD1	3:F:177:GLN:CG	2.29	0.45
2:H:215:ILE:CB	2:H:242:MET:HE3	2.45	0.45
2:H:250:THR:O	2:H:252:ILE:CD1	2.65	0.45
2:H:338:TYR:O	2:H:339:GLN:C	2.58	0.45
3:I:261:ASP:N	3:I:261:ASP:OD1	2.49	0.45
3:I:307:HIS:O	3:I:310:MET:HB2	2.16	0.45
1:J:176:LYS:HE3	1:J:176:LYS:HB2	1.76	0.45
2:K:338:TYR:O	2:K:339:GLN:C	2.60	0.45
3:L:105:SER:O	3:L:106:SER:C	2.60	0.45
3:L:154:GLN:HA	3:L:190:GLY:HA3	1.98	0.45
3:L:290:PHE:HA	3:L:307:HIS:ND1	2.32	0.45
3:L:336:MET:SD	3:L:340:HIS:HD2	2.40	0.45
3:L:385:LYS:HG3	3:L:385:LYS:O	2.16	0.45
1:A:124:ARG:C	1:A:126:VAL:N	2.72	0.45
1:A:181:GLN:HE21	2:B:174:ASN:HB2	1.81	0.45
2:B:237:ARG:NH2	3:C:143:VAL:HG23	2.21	0.45
2:B:337:LYS:O	2:B:339:GLN:N	2.49	0.45
3:C:295:PHE:H	3:C:301:ASP:CB	2.30	0.45
1:G:144:LEU:HD21	1:G:182:GLN:CG	2.42	0.45
2:H:223:GLU:O	2:H:225:TYR:HD1	1.99	0.45
2:H:346:ARG:CB	2:H:346:ARG:NH1	2.77	0.45
3:I:197:ARG:NH2	3:I:348:TYR:HB2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:235:LEU:O	3:I:239:GLN:HG3	2.16	0.45
3:I:310:MET:HE1	3:I:321:LYS:CE	2.44	0.45
1:J:132:HIS:C	1:J:134:GLN:H	2.24	0.45
1:J:159:ARG:HD3	2:K:258:GLY:H	1.81	0.45
2:K:183:GLU:HA	3:L:124:LEU:HD21	1.98	0.45
2:K:296:ASN:HD22	2:K:296:ASN:HA	1.56	0.45
2:K:351:ASN:ND2	2:K:354:MET:HB2	2.32	0.45
2:K:370:HIS:CE1	2:K:402:TRP:HE1	2.35	0.45
2:B:191:GLU:O	2:B:193:CYS:N	2.42	0.45
2:B:357:ALA:HA	2:B:439:ASN:CG	2.41	0.45
3:C:196:LYS:HA	3:C:383:THR:HA	1.98	0.45
3:F:203:ASP:O	3:F:206:LYS:CE	2.65	0.45
3:F:209:ILE:O	3:F:213:GLU:HG2	2.16	0.45
3:F:322:PHE:CB	3:F:338:LYS:HD2	2.46	0.45
2:H:340:ILE:O	2:H:340:ILE:HG23	2.16	0.45
2:H:409:ALA:O	2:H:438:MET:HB2	2.17	0.45
3:I:111:GLN:O	3:I:111:GLN:CG	2.62	0.45
3:I:149:THR:O	3:I:159:LYS:NZ	2.49	0.45
3:I:171:PRO:O	3:I:172:LEU:C	2.60	0.45
3:I:250:LEU:CD1	3:I:382:THR:HA	2.39	0.45
3:I:264:MET:O	3:I:265:PHE:O	2.34	0.45
3:I:271:ALA:C	3:I:273:LYS:N	2.72	0.45
3:I:377:TYR:C	3:I:377:TYR:CD2	2.95	0.45
3:L:145:ILE:HD13	3:L:168:PHE:CE2	2.50	0.45
3:L:192:THR:HG23	3:L:386:ILE:CG1	2.47	0.45
3:L:207:ASN:N	3:L:210:GLN:OE1	2.46	0.45
1:A:174:ASP:OD2	1:A:177:ASP:HB2	2.17	0.45
2:B:177:SER:C	2:B:180:GLN:HG2	2.42	0.45
2:B:199:VAL:HG23	3:C:141:ASP:OD1	2.16	0.45
2:B:215:ILE:CB	2:B:242:MET:HE3	2.41	0.45
2:B:268:PRO:O	2:B:273:PHE:HD2	2.00	0.45
2:B:345:TYR:HB3	2:B:354:MET:HE2	1.98	0.45
2:B:354:MET:C	2:B:356:GLY:H	2.25	0.45
2:B:364:ASN:HD22	5:B:470:NAG:C7	2.28	0.45
3:C:124:LEU:HG	3:C:124:LEU:O	2.16	0.45
2:E:311:LEU:HD21	2:E:313:GLU:OE2	2.16	0.45
3:F:96:TYR:N	3:F:96:TYR:CD1	2.73	0.45
3:F:154:GLN:HE21	3:F:158:ASN:CG	2.25	0.45
3:F:236:ILE:O	3:F:244:TYR:CE1	2.70	0.45
3:F:246:LEU:HD13	3:F:265:PHE:CD2	2.51	0.45
1:G:128:GLU:OE1	1:G:129:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:GLN:HA	1:G:134:GLN:NE2	2.32	0.45
2:H:337:LYS:O	2:H:339:GLN:N	2.49	0.45
1:J:182:GLN:O	1:J:186:GLU:HG2	2.17	0.45
2:K:370:HIS:CE1	2:K:408:HIS:HB2	2.52	0.45
2:B:256:GLN:CB	2:B:449:LYS:HE2	2.38	0.45
2:B:317:TRP:CH2	2:B:448:ARG:HD3	2.51	0.45
2:B:346:ARG:CB	2:B:346:ARG:NH1	2.78	0.45
3:C:235:LEU:O	3:C:239:GLN:HG3	2.16	0.45
3:C:246:LEU:HD21	3:C:248:VAL:CG2	2.47	0.45
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.17	0.45
2:E:235:PRO:HG2	3:F:168:PHE:CE1	2.45	0.45
3:F:227:TRP:CE2	3:F:230:ASN:ND2	2.85	0.45
1:G:131:GLN:HA	1:G:134:GLN:HE21	1.82	0.45
2:H:242:MET:SD	2:H:248:GLY:CA	3.02	0.45
2:H:361:MET:O	2:H:362:GLY:C	2.60	0.45
3:I:208:TRP:CA	3:I:314:THR:HG21	2.46	0.45
3:I:390:ASN:O	3:I:390:ASN:CG	2.60	0.45
2:K:264:ARG:HG2	3:L:136:GLN:NE2	2.31	0.45
3:L:196:LYS:O	3:L:225:GLU:HA	2.17	0.45
3:L:339:CYS:O	3:L:340:HIS:HB3	2.17	0.45
2:B:328:GLY:HA3	2:B:343:ASN:OD1	2.17	0.45
2:B:340:ILE:HG23	2:B:340:ILE:O	2.16	0.45
2:B:389:ASP:OD1	2:B:390:PRO:HD2	2.17	0.45
3:F:270:GLU:HB2	3:F:274:TYR:CZ	2.53	0.45
2:H:334:GLU:HG3	2:H:338:TYR:CE2	2.52	0.45
3:L:227:TRP:CE2	3:L:230:ASN:ND2	2.85	0.45
2:B:301:GLN:HE21	2:B:302:LEU:HD23	1.81	0.44
3:C:356:LYS:HA	3:C:359:THR:CG2	2.48	0.44
1:D:131:GLN:C	1:D:133:ILE:N	2.74	0.44
3:F:322:PHE:CE2	3:F:324:GLY:HA3	2.52	0.44
3:F:349:TYR:HB2	3:F:378:SER:HB3	1.98	0.44
1:G:140:VAL:HG23	1:G:141:ARG:N	2.31	0.44
1:G:151:GLU:HG3	1:G:152:VAL:N	2.31	0.44
2:H:183:GLU:CD	2:H:183:GLU:C	2.85	0.44
2:H:209:LYS:HG2	2:H:229:PRO:HA	1.98	0.44
2:H:210:GLU:CD	2:H:210:GLU:C	2.85	0.44
2:H:215:ILE:HA	2:H:219:GLY:O	2.17	0.44
2:H:353:LEU:HD23	2:H:370:HIS:CD2	2.53	0.44
3:I:204:PHE:HE2	3:I:227:TRP:HB2	1.81	0.44
3:I:208:TRP:C	3:I:210:GLN:H	2.24	0.44
1:J:139:ASN:O	3:L:114:TYR:CE1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:167:ARG:CZ	1:J:167:ARG:CA	2.86	0.44
2:K:236:TYR:CD2	2:K:298:LYS:HE2	2.51	0.44
3:L:209:ILE:O	3:L:213:GLU:HG2	2.16	0.44
3:L:242:ILE:HG23	3:L:243:PRO:HD2	1.98	0.44
2:B:209:LYS:NZ	2:B:209:LYS:CB	2.80	0.44
2:B:296:ASN:HB3	2:B:338:TYR:CZ	2.52	0.44
2:B:329:PHE:CZ	2:B:331:VAL:HG23	2.52	0.44
2:B:447:MET:H	2:B:447:MET:HG2	1.47	0.44
3:C:184:ILE:HG22	3:C:185:ASP:N	2.32	0.44
3:C:269:PRO:O	3:C:270:GLU:C	2.60	0.44
3:C:315:TRP:CE3	3:C:328:GLU:HG2	2.52	0.44
3:F:95:LYS:HG3	3:F:95:LYS:O	2.17	0.44
3:F:192:THR:HG23	3:F:386:ILE:CG1	2.47	0.44
3:F:192:THR:CG2	3:F:386:ILE:HG13	2.46	0.44
3:F:239:GLN:O	3:F:240:SER:C	2.60	0.44
3:F:325:ASN:O	3:F:326:CYS:C	2.59	0.44
1:G:184:GLN:C	1:G:186:GLU:N	2.73	0.44
2:H:169:ARG:NH2	3:I:109:TYR:CD2	2.84	0.44
2:H:373:MET:HG3	2:H:405:ASN:HB2	1.97	0.44
3:I:163:GLN:CA	3:I:163:GLN:NE2	2.80	0.44
3:I:171:PRO:HD2	3:I:174:ALA:CB	2.46	0.44
3:I:296:GLY:O	3:I:297:ASP:C	2.59	0.44
2:K:234:LYS:HG2	2:K:235:PRO:HD2	1.98	0.44
1:A:164:SER:CB	3:C:137:GLU:O	2.65	0.44
1:A:184:GLN:NE2	1:A:185:LEU:HB2	2.29	0.44
2:B:153:ILE:O	2:B:155:GLU:N	2.47	0.44
2:B:294:LEU:CD2	2:B:298:LYS:HB2	2.47	0.44
3:C:107:ILE:CG2	3:C:108:ARG:N	2.80	0.44
1:D:162:ARG:O	1:D:162:ARG:CG	2.65	0.44
3:F:206:LYS:HB3	3:F:210:GLN:OE1	2.17	0.44
3:F:240:SER:O	3:F:241:ALA:C	2.61	0.44
3:F:312:PHE:HD1	3:F:335:TRP:CD1	2.35	0.44
2:H:314:MET:HE1	2:H:437:TRP:CD2	2.53	0.44
2:H:314:MET:HE2	2:H:450:MET:HG3	1.98	0.44
2:H:393:GLN:O	2:H:395:SER:N	2.51	0.44
3:I:124:LEU:C	3:I:126:GLU:N	2.75	0.44
3:I:179:LEU:O	3:I:218:LEU:HD11	2.17	0.44
3:I:253:TRP:CE2	3:I:380:LYS:HB2	2.53	0.44
1:J:149:ARG:O	1:J:152:VAL:HG23	2.17	0.44
2:K:239:TYR:HB3	2:K:251:VAL:HB	1.99	0.44
2:K:276:VAL:HA	2:K:292:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:322:PHE:CD2	4:T:3:ARG:HG3	2.52	0.44
3:L:383:THR:O	3:L:383:THR:OG1	2.35	0.44
2:B:166:ARG:H	2:B:166:ARG:HE	1.59	0.44
2:B:179:ILE:HG13	2:B:179:ILE:H	1.62	0.44
2:B:199:VAL:C	2:B:200:SER:HG	2.25	0.44
2:B:317:TRP:CH2	2:B:418:TRP:HA	2.53	0.44
2:B:385:TRP:HB2	2:B:406:ARG:HA	2.00	0.44
2:B:412:PRO:CB	2:B:450:MET:HE1	2.47	0.44
3:C:133:ALA:HA	3:C:136:GLN:CG	2.47	0.44
3:F:273:LYS:HA	3:F:273:LYS:HD3	1.78	0.44
1:G:128:GLU:OE2	1:G:129:LYS:HG2	2.17	0.44
2:H:176:ARG:CZ	2:H:176:ARG:HB3	2.47	0.44
2:H:185:ASP:HA	2:H:188:ALA:CB	2.48	0.44
2:H:236:TYR:CD1	2:H:236:TYR:C	2.95	0.44
2:H:345:TYR:CZ	2:H:351:ASN:N	2.86	0.44
3:I:158:ASN:OD1	3:I:188:GLY:O	2.35	0.44
3:I:178:PHE:CZ	3:I:232:LYS:HG2	2.52	0.44
3:I:227:TRP:HE1	3:I:230:ASN:ND2	2.15	0.44
2:K:242:MET:HA	2:K:247:GLY:CA	2.48	0.44
2:K:375:PHE:CD1	2:K:376:SER:N	2.85	0.44
3:L:145:ILE:HG21	3:L:168:PHE:CD2	2.52	0.44
3:L:292:GLY:HA2	3:L:305:THR:O	2.17	0.44
1:A:147:MET:CE	3:C:121:ILE:HD11	2.46	0.44
2:B:152:TYR:CD1	2:B:152:TYR:N	2.85	0.44
3:C:250:LEU:HD12	3:C:250:LEU:HA	1.85	0.44
3:C:258:SER:O	3:C:259:THR:CB	2.65	0.44
1:G:125:LYS:O	1:G:126:VAL:HG23	2.17	0.44
2:H:270:LYS:HG3	2:H:338:TYR:OH	2.17	0.44
2:H:296:ASN:HA	2:H:299:ILE:HD12	1.99	0.44
2:K:375:PHE:HD1	2:K:376:SER:N	2.16	0.44
3:L:197:ARG:O	3:L:381:LYS:HG2	2.17	0.44
1:A:148:LYS:HE2	1:A:148:LYS:HB3	1.74	0.44
2:B:152:TYR:O	2:B:155:GLU:HG3	2.18	0.44
2:B:152:TYR:C	2:B:154:ASP:N	2.76	0.44
2:B:161:ILE:CB	2:B:162:PRO:HD3	2.48	0.44
2:B:412:PRO:HG3	2:B:450:MET:CE	2.47	0.44
3:C:270:GLU:O	3:C:271:ALA:O	2.36	0.44
3:F:127:LYS:O	3:F:130:GLN:N	2.50	0.44
3:F:270:GLU:HA	3:F:273:LYS:O	2.17	0.44
1:G:121:VAL:HG12	1:G:124:ARG:NE	2.28	0.44
1:G:148:LYS:HE2	2:H:425:ASP:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:GLY:O	3:I:138:PRO:HA	2.17	0.44
1:G:174:ASP:HB3	1:G:177:ASP:HB3	1.99	0.44
2:H:268:PRO:O	2:H:273:PHE:HD2	2.01	0.44
3:I:204:PHE:CE2	3:I:227:TRP:HB2	2.53	0.44
3:I:212:LYS:HG3	3:I:274:TYR:OH	2.17	0.44
3:I:293:PHE:CA	3:I:302:LYS:HG3	2.47	0.44
3:I:356:LYS:HA	3:I:359:THR:CG2	2.48	0.44
1:J:127:ILE:CG2	1:J:128:GLU:N	2.79	0.44
1:J:151:GLU:O	1:J:152:VAL:C	2.60	0.44
3:L:238:THR:HG22	3:L:266:LYS:CE	2.46	0.44
1:A:157:LYS:O	1:A:160:SER:HB3	2.18	0.44
1:A:176:LYS:O	1:A:176:LYS:HG3	2.16	0.44
2:B:152:TYR:O	2:B:153:ILE:C	2.59	0.44
2:B:164:ASN:O	2:B:167:VAL:C	2.61	0.44
2:B:223:GLU:O	2:B:225:TYR:HD1	2.00	0.44
2:B:326:TYR:HE1	2:B:354:MET:HG3	1.83	0.44
2:B:363:GLU:O	2:B:367:MET:HG2	2.18	0.44
2:B:422:TYR:N	2:B:422:TYR:CD1	2.86	0.44
3:C:261:ASP:N	3:C:261:ASP:OD1	2.51	0.44
1:D:182:GLN:O	1:D:186:GLU:HG2	2.18	0.44
2:E:300:SER:O	2:E:301:GLN:C	2.59	0.44
3:F:295:PHE:CE2	4:P:1:GLY:HA2	2.52	0.44
3:F:313:SER:O	3:F:333:GLY:HA2	2.18	0.44
3:F:344:LEU:HA	3:F:344:LEU:HD23	1.72	0.44
2:H:178:LYS:C	2:H:180:GLN:N	2.76	0.44
2:H:213:GLU:CG	2:H:217:LYS:HE3	2.46	0.44
3:I:171:PRO:HB2	3:I:174:ALA:CB	2.24	0.44
3:I:196:LYS:HA	3:I:383:THR:HA	1.99	0.44
3:I:256:ARG:NH1	3:I:256:ARG:CG	2.81	0.44
3:L:328:GLU:C	3:L:330:ASP:N	2.76	0.44
3:L:372:TRP:HZ3	3:L:379:MET:HE2	1.82	0.44
1:A:128:GLU:HA	1:A:131:GLN:CG	2.46	0.44
2:B:210:GLU:O	2:B:212:GLU:N	2.51	0.44
2:B:434:GLY:C	2:B:436:VAL:HG13	2.43	0.44
3:C:208:TRP:C	3:C:210:GLN:H	2.25	0.44
3:C:296:GLY:O	3:C:298:ASP:N	2.50	0.44
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.15	0.44
2:E:425:ASP:OD1	2:E:425:ASP:N	2.49	0.44
3:F:154:GLN:HA	3:F:190:GLY:HA3	1.99	0.44
2:H:294:LEU:CD2	2:H:298:LYS:HB2	2.48	0.44
3:I:148:ILE:HD13	3:I:156:ILE:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:320:ASP:OD2	3:I:322:PHE:HB3	2.17	0.44
3:I:367:ILE:HB	3:I:379:MET:N	2.31	0.44
1:J:131:GLN:HE21	1:J:132:HIS:N	2.16	0.44
2:K:265:LYS:C	2:K:268:PRO:HD2	2.43	0.44
3:L:281:PHE:CG	3:L:288:ASP:HB2	2.53	0.44
2:B:206:VAL:HG13	2:B:206:VAL:O	2.18	0.44
2:B:361:MET:O	2:B:362:GLY:C	2.61	0.44
3:C:179:LEU:O	3:C:218:LEU:HD11	2.18	0.44
3:C:227:TRP:NE1	3:C:230:ASN:ND2	2.65	0.44
3:C:246:LEU:CB	3:C:265:PHE:CD1	3.01	0.44
3:C:264:MET:O	3:C:265:PHE:O	2.35	0.44
3:C:334:TRP:NE1	3:C:342:GLY:O	2.51	0.44
2:E:176:ARG:C	2:E:178:LYS:H	2.26	0.44
2:E:455:ARG:HG3	2:E:456:PRO:HD2	2.00	0.44
3:F:246:LEU:HG	3:F:247:ARG:H	1.83	0.44
3:F:340:HIS:CE1	3:F:368:ILE:HD11	2.53	0.44
2:H:262:PHE:N	2:H:262:PHE:CD1	2.86	0.44
3:I:172:LEU:HD12	3:I:172:LEU:N	2.27	0.44
3:I:269:PRO:O	3:I:270:GLU:C	2.61	0.44
3:L:154:GLN:HE21	3:L:158:ASN:CG	2.26	0.44
3:L:236:ILE:O	3:L:244:TYR:CE1	2.71	0.44
1:A:167:ARG:HD2	1:A:167:ARG:C	2.43	0.43
2:B:181:LYS:C	2:B:183:GLU:N	2.76	0.43
2:B:242:MET:SD	2:B:248:GLY:CA	3.04	0.43
3:C:162:LYS:HE3	3:C:186:GLY:HA2	1.99	0.43
3:C:171:PRO:HD2	3:C:174:ALA:CB	2.47	0.43
1:D:141:ARG:O	1:D:142:ALA:C	2.60	0.43
2:E:157:VAL:HG12	3:F:100:ILE:HG21	2.00	0.43
2:E:239:TYR:HB3	2:E:251:VAL:HB	1.99	0.43
1:G:179:GLU:HG2	1:G:182:GLN:OE1	2.18	0.43
2:H:237:ARG:NH2	3:I:143:VAL:HG23	2.24	0.43
2:H:329:PHE:CZ	2:H:331:VAL:HG23	2.53	0.43
3:I:100:ILE:O	3:I:100:ILE:HD12	2.18	0.43
3:I:206:LYS:HG3	3:I:215:PHE:CG	2.53	0.43
3:I:312:PHE:CE1	3:I:333:GLY:O	2.71	0.43
1:J:144:LEU:HD13	1:J:182:GLN:HG3	2.00	0.43
2:K:187:SER:CA	2:K:190:MET:HE3	2.36	0.43
3:L:98:ALA:O	3:L:101:LEU:HD23	2.18	0.43
3:L:172:LEU:H	3:L:239:GLN:HE21	1.66	0.43
3:L:239:GLN:O	3:L:240:SER:C	2.61	0.43
1:A:184:GLN:HE22	1:A:185:LEU:HD23	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:VAL:O	2:B:277:ALA:CB	2.66	0.43
2:B:330:THR:OG1	2:B:341:SER:HB2	2.19	0.43
2:B:374:PHE:O	2:B:403:TRP:HA	2.17	0.43
2:E:214:ILE:HD11	2:E:227:ILE:HG22	1.99	0.43
3:F:197:ARG:O	3:F:381:LYS:HG2	2.18	0.43
2:H:186:VAL:O	2:H:190:MET:HB2	2.18	0.43
2:H:387:THR:C	2:H:389:ASP:N	2.77	0.43
3:I:168:PHE:CE1	3:I:179:LEU:HD13	2.53	0.43
3:I:246:LEU:CB	3:I:265:PHE:CD1	3.01	0.43
2:K:163:THR:O	2:K:163:THR:HG22	2.18	0.43
2:K:237:ARG:HG3	2:K:237:ARG:NH1	2.33	0.43
2:K:318:LYS:NZ	2:K:441:LYS:HZ3	2.16	0.43
3:L:162:LYS:HE3	3:L:186:GLY:CA	2.47	0.43
3:L:240:SER:O	3:L:241:ALA:C	2.61	0.43
2:B:199:VAL:N	3:C:140:LYS:O	2.50	0.43
3:C:97:GLU:O	3:C:99:SER:N	2.48	0.43
3:C:178:PHE:CZ	3:C:232:LYS:HG2	2.52	0.43
3:C:339:CYS:HB2	4:O:1:GLY:H2	1.83	0.43
1:D:188:VAL:HG21	2:E:167:VAL:HG21	2.00	0.43
2:E:296:ASN:HD22	2:E:296:ASN:HA	1.57	0.43
3:F:169:ILE:O	3:F:177:GLN:HB2	2.17	0.43
2:H:152:TYR:CD1	2:H:152:TYR:N	2.86	0.43
2:H:362:GLY:O	2:H:364:ASN:N	2.51	0.43
3:I:105:SER:HA	3:I:108:ARG:HB3	2.00	0.43
3:I:258:SER:C	3:I:259:THR:HG22	2.43	0.43
3:I:298:ASP:OD2	3:I:300:SER:HB2	2.18	0.43
2:K:156:THR:C	2:K:158:ASN:N	2.77	0.43
3:L:107:ILE:HD13	3:L:107:ILE:C	2.44	0.43
3:L:192:THR:CG2	3:L:386:ILE:HG13	2.48	0.43
3:L:194:PHE:HB2	3:L:228:LEU:HB3	2.00	0.43
3:L:198:LEU:HB3	3:L:381:LYS:HG2	1.99	0.43
3:L:334:TRP:CZ3	3:L:344:LEU:HB2	2.54	0.43
3:L:349:TYR:HB2	3:L:378:SER:HB3	1.99	0.43
4:R:3:ARG:CB	4:R:4:PRO:CD	2.90	0.43
2:B:171:ILE:C	2:B:173:GLU:N	2.73	0.43
2:B:353:LEU:HD23	2:B:370:HIS:CD2	2.53	0.43
3:C:107:ILE:O	3:C:110:LEU:HB2	2.19	0.43
3:C:196:LYS:C	3:C:197:ARG:HG2	2.43	0.43
3:C:256:ARG:NH1	3:C:256:ARG:CG	2.81	0.43
2:E:265:LYS:C	2:E:268:PRO:HD2	2.40	0.43
3:F:207:ASN:N	3:F:210:GLN:OE1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:230:ASN:O	3:F:232:LYS:N	2.51	0.43
3:F:328:GLU:C	3:F:330:ASP:N	2.77	0.43
1:G:151:GLU:OE1	2:H:182:LEU:HD11	2.17	0.43
2:H:284:ASN:ND2	2:H:284:ASN:N	2.66	0.43
2:H:358:SER:O	2:H:360:LEU:N	2.43	0.43
2:H:428:LYS:C	2:H:429:HIS:CD2	2.95	0.43
3:I:99:SER:C	3:I:101:LEU:H	2.27	0.43
3:I:154:GLN:HG2	3:I:388:PRO:HG2	2.00	0.43
3:I:248:VAL:O	3:I:259:THR:HA	2.19	0.43
3:I:258:SER:O	3:I:259:THR:HB	2.18	0.43
2:K:381:ASP:O	2:K:382:ASN:OD1	2.36	0.43
3:L:95:LYS:O	3:L:95:LYS:HG2	2.18	0.43
2:B:398:ASP:CA	2:B:433:ASP:CB	2.88	0.43
2:B:401:GLY:O	2:B:402:TRP:HB2	2.18	0.43
3:C:117:ASN:O	3:C:118:ASN:C	2.62	0.43
3:C:373:LYS:HB2	3:C:379:MET:HE1	2.00	0.43
1:D:131:GLN:O	1:D:134:GLN:HG2	2.18	0.43
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.18	0.43
2:E:301:GLN:O	2:E:302:LEU:C	2.61	0.43
2:E:370:HIS:NE2	2:E:408:HIS:HA	2.34	0.43
1:G:120:GLU:CD	1:G:124:ARG:NH2	2.77	0.43
2:H:197:CYS:O	3:I:140:LYS:N	2.44	0.43
2:H:214:ILE:HD13	2:H:225:TYR:CD2	2.48	0.43
2:H:299:ILE:O	2:H:301:GLN:N	2.52	0.43
2:H:333:ASN:O	2:H:335:ALA:N	2.52	0.43
2:H:349:ALA:O	2:H:440:TRP:HB2	2.19	0.43
2:H:365:ARG:O	2:H:368:THR:N	2.51	0.43
2:H:371:ASN:C	2:H:373:MET:N	2.77	0.43
3:I:207:ASN:O	3:I:208:TRP:C	2.61	0.43
3:I:276:LEU:H	3:I:276:LEU:HD23	1.84	0.43
3:L:104:ASP:C	3:L:107:ILE:HG22	2.44	0.43
3:L:204:PHE:O	3:L:206:LYS:N	2.50	0.43
3:L:248:VAL:O	3:L:259:THR:HA	2.17	0.43
3:L:344:LEU:HA	3:L:344:LEU:HD23	1.72	0.43
1:A:126:VAL:O	1:A:128:GLU:N	2.51	0.43
2:B:417:TYR:HB2	2:B:446:SER:CB	2.49	0.43
3:C:253:TRP:CD2	3:C:380:LYS:HB2	2.54	0.43
2:E:376:SER:HB3	2:E:382:ASN:H	1.84	0.43
3:F:155:ASP:O	3:F:155:ASP:CG	2.61	0.43
3:F:383:THR:O	3:F:383:THR:OG1	2.36	0.43
3:I:100:ILE:C	3:I:102:THR:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:227:TRP:C	3:I:229:GLY:N	2.76	0.43
1:J:130:VAL:HA	1:J:133:ILE:CG2	2.47	0.43
3:L:270:GLU:HB2	3:L:274:TYR:CZ	2.54	0.43
3:L:279:ALA:O	3:L:280:TYR:HB3	2.18	0.43
3:L:304:PHE:O	3:L:337:ASN:HB3	2.18	0.43
2:B:387:THR:C	2:B:389:ASP:N	2.77	0.43
2:B:411:ASN:CB	2:B:436:VAL:HG22	2.43	0.43
3:C:212:LYS:HG3	3:C:274:TYR:OH	2.18	0.43
3:C:278:TYR:CD1	3:C:278:TYR:C	2.96	0.43
2:E:161:ILE:HB	2:E:162:PRO:HD3	2.01	0.43
2:E:191:GLU:C	2:E:193:CYS:N	2.77	0.43
2:E:370:HIS:CE1	2:E:408:HIS:HB2	2.54	0.43
3:F:203:ASP:O	3:F:206:LYS:CG	2.66	0.43
3:F:304:PHE:O	3:F:337:ASN:HB3	2.18	0.43
1:G:164:SER:HB3	3:I:137:GLU:C	2.44	0.43
2:H:222:SER:O	2:H:223:GLU:HB3	2.19	0.43
2:H:281:ASP:OD1	2:H:281:ASP:N	2.52	0.43
2:H:300:SER:HA	2:H:331:VAL:HB	1.99	0.43
3:I:120:LYS:O	3:I:124:LEU:HD13	2.18	0.43
3:I:233:ILE:O	3:I:237:SER:HB2	2.19	0.43
3:I:339:CYS:HB3	4:S:1:GLY:N	2.33	0.43
2:K:166:ARG:HD3	2:K:166:ARG:HA	1.90	0.43
3:L:168:PHE:CD1	3:L:177:GLN:HG3	2.52	0.43
3:L:313:SER:O	3:L:333:GLY:HA2	2.19	0.43
2:B:365:ARG:O	2:B:368:THR:HG23	2.19	0.43
3:C:93:ILE:C	3:C:95:LYS:N	2.77	0.43
3:C:114:TYR:C	3:C:116:SER:N	2.76	0.43
3:C:227:TRP:C	3:C:229:GLY:N	2.77	0.43
3:C:317:ASN:C	3:C:317:ASN:ND2	2.77	0.43
1:D:131:GLN:O	1:D:134:GLN:N	2.50	0.43
2:E:161:ILE:N	2:E:162:PRO:CD	2.82	0.43
2:E:215:ILE:HG23	2:E:216:ARG:N	2.34	0.43
3:F:248:VAL:O	3:F:259:THR:HA	2.18	0.43
2:H:295:GLY:O	2:H:299:ILE:HG13	2.18	0.43
3:I:196:LYS:C	3:I:197:ARG:HG2	2.43	0.43
3:I:297:ASP:HB3	4:S:4:PRO:HG3	2.00	0.43
3:I:310:MET:HE1	3:I:321:LYS:HG2	2.00	0.43
2:K:301:GLN:O	2:K:302:LEU:C	2.61	0.43
3:L:243:PRO:HB2	3:L:389:PHE:CB	2.49	0.43
3:L:304:PHE:CD1	3:L:338:LYS:CB	3.01	0.43
1:A:189:ILE:O	1:A:190:ALA:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:250:LEU:CD1	3:C:382:THR:HA	2.40	0.43
3:F:113:ILE:O	3:F:114:TYR:C	2.61	0.43
3:F:195:GLN:CB	3:F:384:MET:HE2	2.48	0.43
1:G:140:VAL:CA	3:I:114:TYR:HE1	2.32	0.43
2:H:326:TYR:CZ	2:H:353:LEU:HB2	2.54	0.43
3:I:204:PHE:CD2	3:I:215:PHE:CZ	3.07	0.43
3:I:246:LEU:HD21	3:I:248:VAL:CG2	2.49	0.43
3:I:269:PRO:O	3:I:271:ALA:N	2.52	0.43
3:I:273:LYS:NZ	3:I:317:ASN:HD21	2.17	0.43
2:K:432:ASP:HB3	2:K:444:TRP:CH2	2.53	0.43
3:L:121:ILE:O	3:L:125:LYS:HG3	2.18	0.43
3:L:278:TYR:HH	3:L:308:ASN:HB2	1.83	0.43
1:A:128:GLU:O	1:A:130:VAL:N	2.42	0.43
2:B:257:ASP:OD2	2:B:257:ASP:N	2.52	0.43
2:B:398:ASP:OD1	2:B:408:HIS:CE1	2.72	0.43
2:B:438:MET:O	2:B:440:TRP:N	2.52	0.43
3:C:96:TYR:C	3:C:98:ALA:N	2.75	0.43
3:C:191:TRP:CH2	3:C:247:ARG:CD	3.02	0.43
2:E:242:MET:HA	2:E:247:GLY:CA	2.49	0.43
2:E:381:ASP:O	2:E:382:ASN:OD1	2.37	0.43
3:F:92:GLU:O	3:F:93:ILE:C	2.62	0.43
3:F:145:ILE:HG21	3:F:168:PHE:CD2	2.54	0.43
2:H:160:ASN:O	2:H:164:ASN:HB2	2.18	0.43
2:H:206:VAL:O	2:H:206:VAL:HG13	2.19	0.43
2:H:209:LYS:NZ	2:H:209:LYS:CB	2.81	0.43
2:H:239:TYR:OH	2:H:289:PRO:HD3	2.19	0.43
2:H:434:GLY:C	2:H:436:VAL:HG13	2.44	0.43
3:I:145:ILE:O	3:I:145:ILE:HD12	2.19	0.43
3:I:326:CYS:SG	3:I:339:CYS:N	2.91	0.43
2:K:295:GLY:O	2:K:299:ILE:N	2.49	0.43
2:K:394:CYS:O	2:K:397:GLU:O	2.37	0.43
1:A:145:VAL:O	1:A:145:VAL:HG12	2.18	0.42
1:A:167:ARG:NH2	2:B:192:TYR:CD2	2.87	0.42
2:B:213:GLU:CG	2:B:217:LYS:HE3	2.47	0.42
2:B:236:TYR:CD1	2:B:236:TYR:C	2.97	0.42
2:B:358:SER:O	2:B:360:LEU:N	2.51	0.42
2:B:428:LYS:C	2:B:429:HIS:CD2	2.96	0.42
3:C:103:HIS:O	3:C:105:SER:N	2.52	0.42
2:H:374:PHE:O	2:H:403:TRP:HA	2.18	0.42
2:H:399:GLY:H	2:H:433:ASP:HB2	1.84	0.42
2:H:405:ASN:O	2:H:406:ARG:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:258:SER:O	3:I:259:THR:CB	2.66	0.42
3:I:356:LYS:HB3	3:I:356:LYS:HE2	1.77	0.42
2:K:203:ILE:N	2:K:203:ILE:CD1	2.78	0.42
3:L:99:SER:C	3:L:101:LEU:H	2.27	0.42
3:L:109:TYR:CD1	3:L:109:TYR:C	2.96	0.42
3:L:244:TYR:CE2	3:L:388:PRO:HG3	2.53	0.42
2:B:190:MET:CB	3:C:131:LEU:HD12	2.49	0.42
2:B:304:ARG:HG3	2:B:304:ARG:NH1	2.34	0.42
3:C:208:TRP:O	3:C:210:GLN:N	2.52	0.42
3:C:258:SER:C	3:C:259:THR:HG22	2.44	0.42
1:D:171:ARG:HD2	2:E:185:ASP:OD2	2.19	0.42
2:E:203:ILE:HA	2:E:204:PRO:HD3	1.84	0.42
2:E:229:PRO:CG	2:E:301:GLN:HE22	2.29	0.42
2:E:386:LEU:HD13	2:E:387:THR:N	2.34	0.42
3:F:196:LYS:HG3	3:F:383:THR:HG22	2.01	0.42
1:G:137:GLN:CD	1:G:189:ILE:HD12	2.44	0.42
1:G:140:VAL:C	1:G:142:ALA:N	2.76	0.42
3:I:150:GLY:N	3:I:156:ILE:HG12	2.34	0.42
3:I:208:TRP:C	3:I:210:GLN:N	2.77	0.42
3:I:242:ILE:CG2	3:I:243:PRO:HD2	2.49	0.42
3:I:334:TRP:NE1	3:I:342:GLY:O	2.53	0.42
3:L:230:ASN:HD22	3:L:233:ILE:HD12	1.84	0.42
1:A:124:ARG:O	1:A:126:VAL:N	2.51	0.42
1:A:141:ARG:HD2	1:A:186:GLU:OE1	2.19	0.42
1:A:144:LEU:CD1	1:A:182:GLN:HG2	2.48	0.42
2:B:304:ARG:HH22	2:B:333:ASN:CB	2.31	0.42
3:C:197:ARG:HH22	3:C:348:TYR:N	2.17	0.42
3:F:197:ARG:NE	3:F:204:PHE:CZ	2.87	0.42
3:F:338:LYS:O	4:P:2:PRO:HA	2.19	0.42
2:H:191:GLU:C	2:H:193:CYS:N	2.72	0.42
2:H:199:VAL:HG23	3:I:141:ASP:OD1	2.19	0.42
2:H:296:ASN:HB3	2:H:338:TYR:CZ	2.54	0.42
2:H:328:GLY:HA3	2:H:343:ASN:CG	2.45	0.42
2:H:360:LEU:HA	5:H:470:NAG:H81	2.01	0.42
3:I:101:LEU:C	3:I:103:HIS:N	2.76	0.42
3:I:287:GLY:CA	3:I:371:THR:HB	2.49	0.42
3:I:328:GLU:C	3:I:331:GLY:H	2.27	0.42
3:L:97:GLU:O	3:L:98:ALA:C	2.62	0.42
3:L:114:TYR:HD2	3:L:115:ASN:ND2	2.18	0.42
3:L:167:TYR:CD1	3:L:182:CYS:HB2	2.54	0.42
3:L:230:ASN:O	3:L:231:GLU:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:GLN:C	2:B:183:GLU:HB3	2.41	0.42
2:B:294:LEU:CD2	2:B:298:LYS:HD2	2.49	0.42
2:B:365:ARG:O	2:B:368:THR:N	2.52	0.42
2:B:385:TRP:CA	2:B:406:ARG:HB2	2.50	0.42
3:C:110:LEU:HD12	3:C:110:LEU:N	2.34	0.42
3:C:165:GLY:C	3:C:167:TYR:CE1	2.97	0.42
3:C:206:LYS:HG3	3:C:215:PHE:CG	2.54	0.42
3:C:328:GLU:O	3:C:331:GLY:N	2.51	0.42
1:D:141:ARG:HA	1:D:144:LEU:HD13	2.01	0.42
2:E:364:ASN:O	2:E:368:THR:HG23	2.19	0.42
2:E:367:MET:O	2:E:405:ASN:O	2.37	0.42
3:F:305:THR:HB	3:F:341:ALA:CB	2.48	0.42
2:H:160:ASN:N	2:H:160:ASN:HD22	2.18	0.42
2:H:230:ASP:O	2:H:233:VAL:HG12	2.19	0.42
2:H:257:ASP:OD2	2:H:257:ASP:N	2.52	0.42
3:I:148:ILE:N	3:I:148:ILE:HD12	2.35	0.42
3:I:250:LEU:HD12	3:I:250:LEU:HA	1.86	0.42
2:K:363:GLU:O	2:K:367:MET:HE3	2.18	0.42
3:L:127:LYS:O	3:L:130:GLN:N	2.44	0.42
1:A:128:GLU:CA	1:A:131:GLN:HG2	2.49	0.42
1:A:140:VAL:HG12	3:C:114:TYR:CD1	2.54	0.42
2:B:179:ILE:HD13	3:C:117:ASN:ND2	2.34	0.42
2:B:184:SER:O	2:B:186:VAL:N	2.52	0.42
2:B:359:GLN:NE2	2:B:359:GLN:N	2.66	0.42
2:B:409:ALA:O	2:B:438:MET:HB2	2.19	0.42
3:C:307:HIS:O	3:C:310:MET:HB2	2.20	0.42
3:C:367:ILE:HB	3:C:379:MET:N	2.32	0.42
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.38	0.42
2:E:394:CYS:O	2:E:397:GLU:O	2.37	0.42
2:E:441:LYS:CG	2:E:447:MET:HE1	2.49	0.42
3:F:197:ARG:C	3:F:198:LEU:HG	2.44	0.42
3:F:359:THR:OG1	3:F:362:GLY:HA2	2.19	0.42
2:H:284:ASN:HD22	2:H:284:ASN:N	2.09	0.42
3:I:298:ASP:O	3:I:301:ASP:OD1	2.37	0.42
1:J:139:ASN:O	3:L:114:TYR:HE1	2.03	0.42
2:K:245:GLU:O	2:K:246:ASN:HB2	2.18	0.42
2:K:410:ALA:C	2:K:412:PRO:HD3	2.45	0.42
3:L:322:PHE:HB2	3:L:338:LYS:HA	2.00	0.42
1:A:126:VAL:HG12	1:A:127:ILE:N	2.35	0.42
1:A:150:LEU:O	1:A:150:LEU:HD12	2.20	0.42
2:B:230:ASP:O	2:B:233:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:GLY:O	2:B:299:ILE:HG13	2.19	0.42
2:B:385:TRP:CD1	2:B:406:ARG:NH1	2.87	0.42
3:C:164:SER:HB2	3:C:183:GLU:HA	2.00	0.42
3:C:307:HIS:CE1	3:C:341:ALA:H	2.38	0.42
3:C:328:GLU:C	3:C:331:GLY:H	2.27	0.42
3:C:340:HIS:CE1	3:C:364:ASP:OD2	2.72	0.42
2:E:429:HIS:C	2:E:431:THR:H	2.28	0.42
3:F:117:ASN:O	3:F:121:ILE:CG1	2.62	0.42
3:F:194:PHE:HB2	3:F:228:LEU:HB3	2.02	0.42
3:F:198:LEU:HB3	3:F:381:LYS:HG2	2.01	0.42
2:H:167:VAL:HG12	2:H:168:LEU:N	2.32	0.42
2:H:366:THR:HA	2:H:369:ILE:HG13	2.00	0.42
3:I:269:PRO:C	3:I:271:ALA:N	2.75	0.42
2:K:235:PRO:HG2	3:L:168:PHE:CE1	2.49	0.42
2:K:309:GLU:OE1	2:K:325:HIS:CE1	2.72	0.42
3:L:131:LEU:O	3:L:132:GLU:C	2.63	0.42
1:A:120:GLU:OE1	1:A:122:LEU:HB3	2.20	0.42
1:A:140:VAL:C	1:A:142:ALA:N	2.77	0.42
2:B:180:GLN:O	2:B:181:LYS:C	2.63	0.42
2:B:427:ALA:O	2:B:428:LYS:C	2.62	0.42
3:C:154:GLN:HG2	3:C:388:PRO:HG2	2.02	0.42
3:C:171:PRO:HB2	3:C:174:ALA:CB	2.25	0.42
3:C:298:ASP:N	3:C:301:ASP:OD1	2.52	0.42
2:E:236:TYR:CG	2:E:298:LYS:HE2	2.55	0.42
3:F:95:LYS:O	3:F:95:LYS:CG	2.67	0.42
3:F:336:MET:HE1	3:F:340:HIS:HD2	1.84	0.42
2:H:230:ASP:C	2:H:232:SER:N	2.75	0.42
2:H:371:ASN:OD1	2:H:372:GLY:N	2.52	0.42
3:I:113:ILE:H	3:I:113:ILE:CD1	2.33	0.42
3:I:278:TYR:CD1	3:I:278:TYR:C	2.98	0.42
3:I:372:TRP:CE2	3:I:373:LYS:NZ	2.88	0.42
2:K:215:ILE:HG23	2:K:216:ARG:N	2.35	0.42
1:A:140:VAL:HG23	1:A:141:ARG:N	2.34	0.42
2:B:193:CYS:HB3	3:C:134:GLN:CD	2.44	0.42
2:B:399:GLY:N	2:B:433:ASP:HB2	2.34	0.42
2:B:421:GLN:HA	2:B:444:TRP:O	2.20	0.42
1:D:185:LEU:HD13	1:D:189:ILE:HD11	2.02	0.42
3:F:92:GLU:C	3:F:94:MET:N	2.77	0.42
3:F:143:VAL:HA	3:F:220:PRO:HG2	2.02	0.42
3:F:196:LYS:O	3:F:225:GLU:HA	2.20	0.42
2:H:166:ARG:HD3	2:H:166:ARG:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:330:THR:OG1	2:H:341:SER:HB2	2.20	0.42
3:I:334:TRP:HH2	3:I:344:LEU:HD12	1.84	0.42
3:I:340:HIS:CE1	3:I:364:ASP:OD2	2.72	0.42
1:J:115:LEU:C	1:J:117:SER:N	2.75	0.42
2:K:374:PHE:O	2:K:403:TRP:HA	2.20	0.42
3:L:246:LEU:HD13	3:L:265:PHE:CZ	2.55	0.42
2:B:215:ILE:HA	2:B:219:GLY:O	2.20	0.42
3:C:193:VAL:HA	3:C:385:LYS:CB	2.50	0.42
3:C:263:ALA:HB2	3:C:280:TYR:CE1	2.54	0.42
2:E:191:GLU:O	2:E:193:CYS:N	2.52	0.42
2:E:201:CYS:O	3:F:143:VAL:HG21	2.20	0.42
2:E:325:HIS:N	2:E:346:ARG:O	2.45	0.42
3:F:372:TRP:HZ3	3:F:379:MET:HE2	1.85	0.42
1:G:144:LEU:HD11	1:G:181:GLN:HB2	2.00	0.42
1:G:159:ARG:O	2:H:259:SER:HA	2.20	0.42
1:G:175:LEU:O	1:G:179:GLU:HB2	2.20	0.42
2:H:252:ILE:HG12	2:H:452:MET:O	2.19	0.42
3:I:154:GLN:OE1	3:I:190:GLY:N	2.53	0.42
3:I:359:THR:O	3:I:360:PRO:C	2.62	0.42
1:J:130:VAL:HA	1:J:133:ILE:HG22	2.02	0.42
1:J:131:GLN:HE21	1:J:131:GLN:C	2.28	0.42
2:K:361:MET:HB2	5:K:470:NAG:C8	2.49	0.42
3:L:194:PHE:HE2	3:L:384:MET:CB	2.33	0.42
3:L:333:GLY:O	3:L:334:TRP:HB2	2.19	0.42
1:A:158:ILE:HA	1:A:158:ILE:HD12	1.75	0.42
3:C:99:SER:C	3:C:101:LEU:N	2.76	0.42
3:C:103:HIS:O	3:C:104:ASP:C	2.63	0.42
3:C:250:LEU:HD23	3:C:372:TRP:CE3	2.54	0.42
3:C:269:PRO:C	3:C:271:ALA:N	2.76	0.42
1:D:136:LEU:HD13	3:F:111:GLN:NE2	2.35	0.42
2:E:321:LYS:HB2	2:E:321:LYS:HZ3	1.84	0.42
3:F:243:PRO:HB2	3:F:389:PHE:CB	2.50	0.42
3:F:367:ILE:HB	3:F:378:SER:OG	2.20	0.42
3:F:388:PRO:O	3:F:389:PHE:C	2.63	0.42
1:G:161:CYS:C	1:G:163:GLY:N	2.77	0.42
2:H:238:VAL:CG2	2:H:239:TYR:H	2.33	0.42
2:H:354:MET:C	2:H:356:GLY:H	2.28	0.42
2:H:448:ARG:HD2	2:H:448:ARG:HA	1.82	0.42
3:I:184:ILE:HG22	3:I:185:ASP:N	2.34	0.42
2:K:340:ILE:HG12	2:K:341:SER:N	2.35	0.42
2:K:422:TYR:C	2:K:423:THR:HG23	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASN:HB3	3:C:114:TYR:OH	2.19	0.41
1:A:144:LEU:O	1:A:144:LEU:HG	2.20	0.41
2:B:245:GLU:C	2:B:247:GLY:H	2.27	0.41
2:B:322:VAL:HB	2:B:348:THR:OG1	2.19	0.41
2:B:326:TYR:CZ	2:B:353:LEU:HB2	2.55	0.41
2:B:359:GLN:O	2:B:359:GLN:CG	2.67	0.41
3:C:143:VAL:HG12	3:C:220:PRO:CD	2.42	0.41
3:C:153:CYS:CB	3:C:191:TRP:O	2.67	0.41
3:C:165:GLY:C	3:C:167:TYR:HE1	2.28	0.41
3:C:298:ASP:OD2	3:C:300:SER:HB2	2.20	0.41
3:C:370:ALA:HA	3:C:373:LYS:O	2.20	0.41
1:D:181:GLN:OE1	2:E:174:ASN:ND2	2.53	0.41
2:E:215:ILE:CG2	2:E:216:ARG:N	2.83	0.41
2:E:252:ILE:HG12	2:E:454:ILE:HG12	2.02	0.41
2:E:310:LEU:HD21	2:E:312:ILE:CD1	2.50	0.41
2:E:434:GLY:O	2:E:436:VAL:N	2.53	0.41
3:F:261:ASP:O	3:F:262:TYR:CD2	2.73	0.41
3:I:289:ALA:HB2	3:I:371:THR:OG1	2.20	0.41
3:I:317:ASN:C	3:I:317:ASN:ND2	2.78	0.41
2:K:215:ILE:HD12	2:K:247:GLY:C	2.44	0.41
2:K:318:LYS:HZ1	2:K:441:LYS:NZ	2.18	0.41
3:L:101:LEU:HD12	3:L:104:ASP:HB2	2.02	0.41
3:L:203:ASP:O	3:L:206:LYS:CG	2.67	0.41
3:L:203:ASP:O	3:L:206:LYS:CE	2.68	0.41
3:L:203:ASP:O	3:L:206:LYS:HE3	2.21	0.41
2:B:222:SER:O	2:B:223:GLU:HB3	2.20	0.41
2:B:266:TRP:CE3	2:B:266:TRP:CA	3.03	0.41
3:C:169:ILE:HG12	3:C:180:VAL:CG1	2.50	0.41
3:C:270:GLU:O	3:C:271:ALA:C	2.61	0.41
3:C:312:PHE:CE1	3:C:333:GLY:O	2.73	0.41
3:C:394:ILE:HG12	3:C:396:GLU:O	2.20	0.41
2:E:203:ILE:N	2:E:203:ILE:CD1	2.78	0.41
3:F:194:PHE:HE2	3:F:384:MET:CB	2.33	0.41
1:G:173:VAL:O	1:G:173:VAL:HG23	2.20	0.41
2:H:304:ARG:HH22	2:H:333:ASN:CB	2.32	0.41
2:H:315:GLU:CB	2:H:321:LYS:HB3	2.44	0.41
2:H:385:TRP:CZ3	4:Q:3:ARG:HG3	2.55	0.41
3:I:164:SER:HB2	3:I:183:GLU:HA	2.01	0.41
3:I:288:ASP:OD1	3:I:291:ASP:HB2	2.20	0.41
2:B:173:GLU:O	2:B:176:ARG:HB3	2.20	0.41
2:B:253:GLN:HB2	2:B:293:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:CZ2	2:B:380:ARG:NE	2.88	0.41
3:C:131:LEU:HD23	3:C:131:LEU:C	2.45	0.41
3:C:253:TRP:CE2	3:C:380:LYS:HB2	2.55	0.41
3:C:269:PRO:O	3:C:271:ALA:N	2.53	0.41
1:D:131:GLN:HA	1:D:134:GLN:HG2	2.02	0.41
2:E:309:GLU:OE1	2:E:325:HIS:CE1	2.73	0.41
3:F:233:ILE:HG13	3:F:233:ILE:H	1.65	0.41
3:F:299:PRO:O	3:F:301:ASP:N	2.46	0.41
3:F:322:PHE:HA	3:F:338:LYS:HD2	2.01	0.41
3:I:227:TRP:O	3:I:228:LEU:C	2.62	0.41
2:K:203:ILE:H	2:K:203:ILE:CD1	2.33	0.41
3:L:340:HIS:CE1	3:L:368:ILE:HD11	2.55	0.41
3:L:359:THR:HA	3:L:360:PRO:HD3	1.74	0.41
1:A:128:GLU:CD	1:A:129:LYS:HZ2	2.28	0.41
1:A:143:GLN:C	1:A:145:VAL:H	2.28	0.41
2:B:162:PRO:HA	2:B:166:ARG:CD	2.48	0.41
2:B:207:SER:OG	2:B:208:GLY:N	2.52	0.41
2:B:254:ASN:HD21	2:B:256:GLN:NE2	2.17	0.41
3:C:248:VAL:O	3:C:248:VAL:HG12	2.21	0.41
3:C:288:ASP:OD1	3:C:291:ASP:HB2	2.20	0.41
1:D:159:ARG:O	1:D:159:ARG:CG	2.69	0.41
1:D:181:GLN:OE1	2:E:174:ASN:CG	2.63	0.41
2:E:357:ALA:C	2:E:359:GLN:H	2.27	0.41
1:G:185:LEU:O	1:G:189:ILE:HB	2.19	0.41
2:H:246:ASN:HB2	2:H:455:ARG:NH1	2.35	0.41
3:I:153:CYS:CB	3:I:191:TRP:O	2.68	0.41
1:J:167:ARG:HB2	2:K:192:TYR:CB	2.50	0.41
2:K:241:ASP:C	2:K:241:ASP:OD2	2.63	0.41
2:K:456:PRO:C	2:K:457:PHE:O	2.62	0.41
3:L:117:ASN:O	3:L:121:ILE:CG1	2.63	0.41
3:L:205:LYS:NZ	3:L:331:GLY:HA2	2.34	0.41
3:L:325:ASN:ND2	3:L:327:ALA:HB3	2.28	0.41
1:A:143:GLN:CD	3:C:118:ASN:ND2	2.74	0.41
2:B:236:TYR:HB2	2:B:298:LYS:HZ3	1.85	0.41
2:B:255:ARG:NH1	2:B:262:PHE:CD1	2.88	0.41
2:B:412:PRO:O	2:B:413:ASN:C	2.62	0.41
3:C:110:LEU:O	3:C:112:GLU:N	2.53	0.41
3:C:228:LEU:HD12	3:C:228:LEU:C	2.44	0.41
3:C:230:ASN:O	3:C:231:GLU:C	2.60	0.41
3:C:390:ASN:O	3:C:390:ASN:CG	2.64	0.41
2:E:232:SER:O	2:E:233:VAL:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:265:LYS:HB3	2:E:379:ASP:OD2	2.21	0.41
2:E:301:GLN:HE21	2:E:301:GLN:HB3	1.54	0.41
3:F:336:MET:SD	3:F:340:HIS:HD2	2.43	0.41
1:G:184:GLN:C	1:G:186:GLU:H	2.28	0.41
1:G:190:ALA:O	1:G:191:LYS:HB2	2.20	0.41
2:H:172:LEU:HD23	2:H:172:LEU:C	2.45	0.41
2:H:179:ILE:HD13	3:I:117:ASN:HB3	2.03	0.41
2:H:190:MET:O	2:H:190:MET:SD	2.78	0.41
2:H:296:ASN:O	2:H:299:ILE:N	2.53	0.41
2:H:301:GLN:HE21	2:H:302:LEU:HD23	1.85	0.41
2:H:398:ASP:OD1	2:H:408:HIS:CE1	2.73	0.41
3:I:109:TYR:O	3:I:110:LEU:C	2.63	0.41
3:I:196:LYS:CE	3:I:198:LEU:HD21	2.39	0.41
3:I:248:VAL:HG22	3:I:384:MET:HG2	2.02	0.41
3:I:310:MET:HE1	3:I:321:LYS:CG	2.51	0.41
1:J:171:ARG:HH21	1:J:173:VAL:HG22	1.85	0.41
2:K:161:ILE:O	2:K:164:ASN:HB3	2.21	0.41
2:K:254:ASN:O	2:K:291:GLU:HA	2.21	0.41
3:L:110:LEU:C	3:L:112:GLU:N	2.78	0.41
1:A:158:ILE:C	1:A:160:SER:N	2.76	0.41
1:A:167:ARG:NE	2:B:192:TYR:CD2	2.89	0.41
2:B:173:GLU:HA	2:B:176:ARG:CB	2.49	0.41
2:B:230:ASP:C	2:B:232:SER:N	2.76	0.41
2:B:250:THR:O	2:B:252:ILE:CD1	2.69	0.41
2:B:371:ASN:C	2:B:373:MET:N	2.79	0.41
2:B:448:ARG:HD2	2:B:448:ARG:HA	1.85	0.41
3:C:150:GLY:N	3:C:156:ILE:HG12	2.36	0.41
3:C:233:ILE:O	3:C:237:SER:HB2	2.21	0.41
3:C:261:ASP:OD2	3:C:392:LEU:HD11	2.20	0.41
2:E:205:VAL:HG12	2:E:206:VAL:H	1.78	0.41
2:E:313:GLU:HB3	2:E:323:LYS:HG3	2.02	0.41
2:H:184:SER:O	2:H:188:ALA:N	2.54	0.41
2:H:314:MET:HB3	2:H:450:MET:HG3	2.02	0.41
3:I:101:LEU:O	3:I:104:ASP:N	2.54	0.41
3:I:169:ILE:HG12	3:I:180:VAL:CG1	2.50	0.41
3:I:235:LEU:H	3:I:235:LEU:CD1	2.28	0.41
3:I:311:GLN:OE1	3:I:319:ASN:HB3	2.21	0.41
1:J:171:ARG:HH21	1:J:173:VAL:CG2	2.34	0.41
2:K:222:SER:O	2:K:223:GLU:HB3	2.20	0.41
3:L:97:GLU:HA	3:L:100:ILE:CD1	2.51	0.41
3:L:169:ILE:O	3:L:177:GLN:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:388:PRO:O	3:L:389:PHE:C	2.64	0.41
2:B:186:VAL:O	2:B:186:VAL:HG13	2.20	0.41
2:B:193:CYS:O	2:B:194:ARG:C	2.63	0.41
2:B:254:ASN:ND2	2:B:256:GLN:OE1	2.54	0.41
2:B:314:MET:HE2	2:B:450:MET:HG3	2.02	0.41
3:C:156:ILE:HA	3:C:159:LYS:HD3	2.03	0.41
3:C:207:ASN:O	3:C:208:TRP:C	2.63	0.41
3:C:239:GLN:HB2	3:C:239:GLN:HE21	1.53	0.41
3:C:258:SER:OG	3:C:372:TRP:CE2	2.73	0.41
2:E:156:THR:O	2:E:157:VAL:C	2.64	0.41
2:E:241:ASP:O	2:E:247:GLY:HA2	2.21	0.41
2:H:310:LEU:HB2	2:H:454:ILE:HG22	2.03	0.41
2:H:324:ALA:HB1	2:H:345:TYR:HE1	1.86	0.41
2:H:369:ILE:O	2:H:405:ASN:HB3	2.19	0.41
2:H:422:TYR:N	2:H:422:TYR:CD1	2.89	0.41
3:I:93:ILE:HD12	3:I:93:ILE:N	2.35	0.41
3:I:107:ILE:O	3:I:109:TYR:N	2.53	0.41
3:I:114:TYR:C	3:I:116:SER:H	2.29	0.41
3:I:156:ILE:HA	3:I:159:LYS:HD3	2.03	0.41
1:J:122:LEU:HA	1:J:122:LEU:HD23	1.80	0.41
1:J:137:GLN:C	1:J:140:VAL:HG12	2.46	0.41
1:J:176:LYS:O	1:J:179:GLU:N	2.54	0.41
2:K:211:CYS:SG	2:K:250:THR:HG23	2.61	0.41
3:L:154:GLN:OE1	3:L:190:GLY:N	2.46	0.41
3:L:273:LYS:HA	3:L:273:LYS:HD3	1.81	0.41
3:L:336:MET:HE1	3:L:340:HIS:CD2	2.56	0.41
3:L:367:ILE:HB	3:L:378:SER:OG	2.21	0.41
2:B:257:ASP:O	2:B:291:GLU:OE1	2.38	0.41
2:B:333:ASN:O	2:B:335:ALA:N	2.54	0.41
2:B:354:MET:C	2:B:356:GLY:N	2.79	0.41
3:C:149:THR:O	3:C:159:LYS:NZ	2.50	0.41
3:C:191:TRP:CZ3	3:C:385:LYS:HE2	2.56	0.41
3:C:206:LYS:HB3	3:C:210:GLN:OE1	2.20	0.41
3:C:208:TRP:C	3:C:210:GLN:N	2.78	0.41
1:D:181:GLN:O	1:D:184:GLN:HB3	2.21	0.41
2:E:375:PHE:CD1	2:E:376:SER:N	2.88	0.41
3:F:284:GLY:O	3:F:286:ALA:N	2.45	0.41
3:F:295:PHE:CZ	4:P:1:GLY:HA2	2.56	0.41
3:F:314:THR:O	3:F:316:ASP:N	2.54	0.41
2:H:266:TRP:CE3	2:H:266:TRP:CA	3.03	0.41
2:H:389:ASP:OD1	2:H:390:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:315:TRP:CE3	3:I:328:GLU:HG2	2.55	0.41
3:I:322:PHE:CD1	3:I:338:LYS:HG3	2.51	0.41
2:K:217:LYS:HB3	3:L:213:GLU:HG3	2.02	0.41
2:K:314:MET:HE3	2:K:349:ALA:HB2	2.03	0.41
2:K:341:SER:HA	2:K:371:ASN:OD1	2.20	0.41
3:L:192:THR:HG23	3:L:386:ILE:HG12	2.02	0.41
3:L:233:ILE:HG13	3:L:233:ILE:H	1.65	0.41
3:L:265:PHE:CZ	3:L:267:VAL:HG23	2.56	0.41
1:A:174:ASP:OD2	1:A:177:ASP:CB	2.69	0.41
2:B:227:ILE:HG12	2:B:238:VAL:HG11	2.02	0.41
2:B:254:ASN:HD21	2:B:256:GLN:HE22	1.69	0.41
2:B:266:TRP:CE2	2:B:380:ARG:NE	2.89	0.41
2:B:366:THR:HA	2:B:369:ILE:HG13	2.02	0.41
3:C:124:LEU:O	3:C:128:VAL:HG23	2.21	0.41
1:D:137:GLN:NE2	1:D:189:ILE:HA	2.36	0.41
2:E:373:MET:HE3	2:E:374:PHE:N	2.36	0.41
2:E:408:HIS:CE1	4:N:1:GLY:N	2.89	0.41
3:F:92:GLU:CG	3:F:93:ILE:H	2.32	0.41
3:F:154:GLN:HE21	3:F:158:ASN:ND2	2.18	0.41
3:F:227:TRP:C	3:F:229:GLY:N	2.78	0.41
3:F:230:ASN:O	3:F:231:GLU:C	2.64	0.41
3:F:288:ASP:O	3:F:371:THR:HG21	2.20	0.41
1:G:147:MET:CE	3:I:121:ILE:HD11	2.51	0.41
1:G:158:ILE:HA	1:G:158:ILE:HD12	1.80	0.41
1:G:184:GLN:NE2	1:G:185:LEU:N	2.68	0.41
2:H:202:ASN:O	2:H:204:PRO:HD3	2.20	0.41
2:H:398:ASP:CA	2:H:433:ASP:CB	2.91	0.41
3:I:252:ASP:OD1	3:I:256:ARG:O	2.38	0.41
2:K:223:GLU:HA	2:K:287:GLY:HA2	2.03	0.41
3:L:103:HIS:O	3:L:104:ASP:C	2.63	0.41
3:L:198:LEU:CA	3:L:381:LYS:HG2	2.51	0.41
2:B:171:ILE:O	2:B:175:LEU:HB3	2.21	0.41
2:B:176:ARG:HD2	2:B:179:ILE:CD1	2.50	0.41
2:B:179:ILE:HD11	3:C:117:ASN:ND2	2.36	0.41
2:B:236:TYR:CB	2:B:298:LYS:NZ	2.84	0.41
2:B:281:ASP:OD1	2:B:281:ASP:N	2.53	0.41
3:C:111:GLN:HG2	3:C:111:GLN:O	2.21	0.41
3:C:230:ASN:HA	3:C:233:ILE:HB	2.03	0.41
1:D:126:VAL:C	1:D:128:GLU:N	2.78	0.41
2:E:456:PRO:C	2:E:457:PHE:O	2.63	0.41
3:F:115:ASN:N	3:F:115:ASN:HD22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:211:TYR:CE2	3:F:333:GLY:HA3	2.56	0.41
3:F:293:PHE:HD2	3:F:370:ALA:HB1	1.86	0.41
2:H:155:GLU:C	2:H:157:VAL:H	2.29	0.41
2:H:314:MET:HE2	2:H:450:MET:SD	2.61	0.41
2:H:317:TRP:CH2	2:H:448:ARG:HD3	2.55	0.41
3:I:191:TRP:CH2	3:I:247:ARG:CD	3.04	0.41
1:J:137:GLN:NE2	1:J:189:ILE:HA	2.35	0.41
2:K:316:ASP:OD1	2:K:320:ASP:O	2.38	0.41
3:L:196:LYS:HG3	3:L:383:THR:HG22	2.03	0.41
3:L:205:LYS:HG2	3:L:331:GLY:CA	2.51	0.41
3:L:270:GLU:HA	3:L:273:LYS:O	2.21	0.41
1:A:142:ALA:O	1:A:146:ASP:N	2.54	0.40
1:A:167:ARG:HH21	2:B:192:TYR:HD2	1.69	0.40
2:B:223:GLU:HG2	2:B:225:TYR:HE1	1.85	0.40
2:B:322:VAL:HG21	2:B:349:ALA:HA	2.03	0.40
2:B:362:GLY:O	2:B:364:ASN:N	2.54	0.40
3:C:101:LEU:HD22	3:C:101:LEU:HA	1.93	0.40
3:C:356:LYS:HE2	3:C:356:LYS:HB3	1.78	0.40
3:C:373:LYS:CG	3:C:379:MET:HE1	2.51	0.40
3:F:302:LYS:O	3:F:303:PHE:C	2.63	0.40
3:F:329:GLN:HE21	3:F:361:ASN:HD22	1.70	0.40
2:H:207:SER:OG	2:H:208:GLY:N	2.53	0.40
2:H:326:TYR:HE1	2:H:354:MET:HG3	1.87	0.40
3:I:96:TYR:CD1	3:I:97:GLU:N	2.89	0.40
3:I:339:CYS:HB3	4:S:1:GLY:H2	1.85	0.40
2:K:156:THR:HG22	2:K:157:VAL:N	2.36	0.40
2:K:161:ILE:O	2:K:162:PRO:C	2.64	0.40
2:K:215:ILE:CG2	2:K:216:ARG:N	2.85	0.40
3:L:191:TRP:CE3	3:L:386:ILE:O	2.74	0.40
2:E:238:VAL:HG23	2:E:294:LEU:HD13	2.02	0.40
2:E:375:PHE:HD1	2:E:376:SER:N	2.20	0.40
3:F:205:LYS:HG2	3:F:331:GLY:CA	2.51	0.40
3:F:251:GLU:HG3	3:F:257:THR:CG2	2.51	0.40
1:G:140:VAL:HG12	3:I:114:TYR:HD1	1.86	0.40
1:G:174:ASP:CG	1:G:177:ASP:HB2	2.47	0.40
2:H:190:MET:SD	2:H:190:MET:C	3.04	0.40
2:H:205:VAL:H	3:I:217:HIS:HA	1.86	0.40
2:H:366:THR:C	2:H:368:THR:H	2.27	0.40
2:H:453:LYS:H	2:H:453:LYS:HG2	1.79	0.40
1:J:124:ARG:HG2	1:J:124:ARG:NH1	2.36	0.40
2:K:210:GLU:OE1	2:K:212:GLU:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:402:TRP:CG	2:K:403:TRP:N	2.89	0.40
3:L:97:GLU:C	3:L:99:SER:N	2.76	0.40
3:L:107:ILE:HG23	3:L:108:ARG:N	2.36	0.40
3:L:299:PRO:O	3:L:301:ASP:N	2.45	0.40
1:A:184:GLN:NE2	1:A:185:LEU:N	2.69	0.40
2:B:252:ILE:HG12	2:B:452:MET:O	2.20	0.40
2:B:324:ALA:HB1	2:B:345:TYR:HE1	1.86	0.40
2:B:442:GLY:C	2:B:444:TRP:N	2.79	0.40
3:C:191:TRP:HH2	3:C:247:ARG:CD	2.34	0.40
3:C:289:ALA:HB2	3:C:371:THR:OG1	2.22	0.40
1:D:122:LEU:CD2	3:F:98:ALA:HB2	2.52	0.40
2:E:156:THR:HA	2:E:160:ASN:HB3	2.03	0.40
2:E:241:ASP:C	2:E:241:ASP:OD2	2.64	0.40
2:E:328:GLY:HA3	2:E:343:ASN:OD1	2.22	0.40
3:F:246:LEU:HB2	3:F:265:PHE:CB	2.51	0.40
2:H:153:ILE:O	2:H:156:THR:HG23	2.21	0.40
2:H:175:LEU:HD12	2:H:179:ILE:HD11	2.03	0.40
2:H:188:ALA:C	2:H:190:MET:N	2.79	0.40
2:H:199:VAL:N	3:I:140:LYS:O	2.53	0.40
2:H:214:ILE:C	2:H:216:ARG:N	2.77	0.40
2:H:223:GLU:HB3	2:H:287:GLY:HA2	1.98	0.40
2:H:266:TRP:CZ2	2:H:380:ARG:NE	2.89	0.40
2:H:310:LEU:CA	2:H:454:ILE:HG22	2.47	0.40
2:H:385:TRP:CE3	4:Q:3:ARG:HG3	2.57	0.40
2:H:421:GLN:HA	2:H:444:TRP:O	2.22	0.40
2:H:427:ALA:O	2:H:428:LYS:C	2.64	0.40
3:I:250:LEU:HD23	3:I:372:TRP:CE3	2.55	0.40
3:I:252:ASP:HB2	3:I:377:TYR:OH	2.22	0.40
3:L:92:GLU:O	3:L:93:ILE:C	2.63	0.40
3:L:194:PHE:CE2	3:L:384:MET:HE3	2.57	0.40
3:L:341:ALA:HB1	3:L:370:ALA:HB3	2.03	0.40
3:L:350:GLN:C	3:L:352:GLY:N	2.80	0.40
1:A:144:LEU:HD11	1:A:182:GLN:CA	2.52	0.40
2:B:357:ALA:CA	2:B:439:ASN:HD21	2.21	0.40
2:B:393:GLN:O	2:B:395:SER:N	2.55	0.40
3:C:235:LEU:H	3:C:235:LEU:CD1	2.27	0.40
3:C:271:ALA:C	3:C:273:LYS:H	2.28	0.40
3:C:310:MET:HE1	3:C:321:LYS:HG2	2.03	0.40
2:E:225:TYR:HB3	2:E:226:LEU:H	1.64	0.40
2:E:302:LEU:O	2:E:305:MET:HB3	2.22	0.40
2:E:338:TYR:O	2:E:339:GLN:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:204:PHE:O	3:F:206:LYS:N	2.53	0.40
3:F:307:HIS:O	3:F:310:MET:HB2	2.22	0.40
3:F:359:THR:HA	3:F:360:PRO:HD3	1.76	0.40
2:H:210:GLU:OE1	2:H:212:GLU:CB	2.69	0.40
2:H:278:THR:O	2:H:279:ASN:C	2.65	0.40
2:H:304:ARG:HG3	2:H:304:ARG:NH1	2.37	0.40
2:H:373:MET:HE2	2:H:404:TYR:C	2.45	0.40
3:I:328:GLU:O	3:I:331:GLY:N	2.53	0.40
2:K:190:MET:HG3	3:L:131:LEU:HD13	2.04	0.40
2:K:265:LYS:HB3	2:K:379:ASP:OD2	2.21	0.40
2:K:381:ASP:OD1	2:K:381:ASP:C	2.64	0.40
3:L:386:ILE:O	3:L:387:ILE:HB	2.21	0.40
1:A:132:HIS:O	1:A:135:LEU:N	2.53	0.40
1:A:140:VAL:HA	1:A:143:GLN:HB2	2.04	0.40
2:B:163:THR:O	2:B:167:VAL:CG2	2.70	0.40
3:C:103:HIS:C	3:C:105:SER:N	2.79	0.40
3:C:196:LYS:O	3:C:225:GLU:HA	2.22	0.40
3:C:204:PHE:CE2	3:C:227:TRP:HB2	2.56	0.40
3:C:227:TRP:O	3:C:228:LEU:C	2.64	0.40
2:E:265:LYS:HB3	2:E:379:ASP:CG	2.47	0.40
3:F:246:LEU:HD12	3:F:386:ILE:HG22	2.03	0.40
2:H:165:LEU:HD13	2:H:165:LEU:HA	1.88	0.40
3:I:237:SER:O	3:I:266:LYS:HG3	2.22	0.40
3:I:336:MET:HE1	3:I:340:HIS:CD2	2.57	0.40
2:K:263:GLY:HA2	2:K:400:GLY:HA2	2.03	0.40
3:L:230:ASN:O	3:L:232:LYS:N	2.55	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	72/87 (83%)	44 (61%)	15 (21%)	13 (18%)	0	0
1	D	69/87 (79%)	50 (72%)	15 (22%)	4 (6%)	1	4
1	G	72/87 (83%)	44 (61%)	14 (19%)	14 (19%)	0	0
1	J	77/87 (88%)	55 (71%)	18 (23%)	4 (5%)	1	5
2	B	305/328 (93%)	186 (61%)	76 (25%)	43 (14%)	0	0
2	E	302/328 (92%)	235 (78%)	41 (14%)	26 (9%)	0	1
2	H	305/328 (93%)	196 (64%)	64 (21%)	45 (15%)	0	0
2	K	303/328 (92%)	236 (78%)	47 (16%)	20 (7%)	1	3
3	C	303/323 (94%)	167 (55%)	86 (28%)	50 (16%)	0	0
3	F	298/323 (92%)	207 (70%)	69 (23%)	22 (7%)	1	2
3	I	303/323 (94%)	170 (56%)	81 (27%)	52 (17%)	0	0
3	L	298/323 (92%)	207 (70%)	68 (23%)	23 (8%)	1	2
4	M	3/5 (60%)	1 (33%)	2 (67%)	0	100	100
4	N	3/5 (60%)	0	2 (67%)	1 (33%)	0	0
4	O	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
4	P	3/5 (60%)	1 (33%)	1 (33%)	1 (33%)	0	0
4	Q	3/5 (60%)	1 (33%)	1 (33%)	1 (33%)	0	0
4	R	3/5 (60%)	0	2 (67%)	1 (33%)	0	0
4	S	3/5 (60%)	3 (100%)	0	0	100	100
4	T	3/5 (60%)	1 (33%)	1 (33%)	1 (33%)	0	0
All	All	2731/2992 (91%)	1806 (66%)	604 (22%)	321 (12%)	0	1

All (321) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	SER
1	A	190	ALA
2	B	227	ILE
2	B	230	ASP
2	B	259	SER
2	B	266	TRP
2	B	295	GLY
2	B	338	TYR
2	B	339	GLN
2	B	351	ASN
2	B	366	THR

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Mol	Chain	Res	Type
2	B	447	MET
3	C	162	LYS
3	C	164	SER
3	C	203	ASP
3	C	218	LEU
3	C	219	SER
3	C	221	THR
3	C	224	THR
3	C	259	THR
3	C	271	ALA
3	C	273	LYS
3	C	317	ASN
2	E	156	THR
2	E	160	ASN
2	E	164	ASN
2	E	205	VAL
2	E	206	VAL
2	E	229	PRO
2	E	233	VAL
2	E	235	PRO
2	E	399	GLY
3	F	104	ASP
3	F	159	LYS
3	F	240	SER
3	F	241	ALA
3	F	371	THR
3	F	374	THR
3	F	389	PHE
3	F	390	ASN
1	G	124	ARG
1	G	125	LYS
1	G	126	VAL
1	G	164	SER
1	G	166	SER
2	H	163	THR
2	H	167	VAL
2	H	174	ASN
2	H	182	LEU
2	H	227	ILE
2	H	230	ASP
2	H	266	TRP
2	H	295	GLY

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Mol	Chain	Res	Type
2	H	338	TYR
2	H	351	ASN
2	H	366	THR
2	H	435	VAL
2	H	443	SER
2	H	447	MET
3	I	97	GLU
3	I	162	LYS
3	I	164	SER
3	I	203	ASP
3	I	218	LEU
3	I	219	SER
3	I	221	THR
3	I	224	THR
3	I	248	VAL
3	I	259	THR
3	I	271	ALA
3	I	273	LYS
3	I	317	ASN
3	I	339	CYS
1	J	151	GLU
2	K	156	THR
2	K	205	VAL
2	K	206	VAL
2	K	229	PRO
2	K	233	VAL
2	K	235	PRO
2	K	399	GLY
3	L	159	LYS
3	L	240	SER
3	L	241	ALA
3	L	371	THR
3	L	374	THR
3	L	389	PHE
3	L	390	ASN
1	A	162	ARG
1	A	185	LEU
1	A	188	VAL
2	B	153	ILE
2	B	199	VAL
2	B	211	CYS
2	B	231	SER

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Mol	Chain	Res	Type
2	B	256	GLN
2	B	320	ASP
2	B	362	GLY
2	B	365	ARG
2	B	394	CYS
2	B	399	GLY
2	B	424	TRP
2	B	435	VAL
2	B	443	SER
3	C	115	ASN
3	C	151	LYS
3	C	161	ALA
3	C	205	LYS
3	C	248	VAL
3	C	265	PHE
3	C	284	GLY
3	C	297	ASP
3	C	370	ALA
3	C	372	TRP
3	C	390	ASN
1	D	124	ARG
1	D	162	ARG
2	E	157	VAL
2	E	301	GLN
2	E	398	ASP
2	E	405	ASN
2	E	406	ARG
3	F	161	ALA
3	F	234	HIS
3	F	285	ASP
3	F	325	ASN
1	G	121	VAL
1	G	130	VAL
1	G	160	SER
1	G	162	ARG
1	G	191	LYS
2	H	170	SER
2	H	211	CYS
2	H	231	SER
2	H	256	GLN
2	H	259	SER
2	H	320	ASP

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Mol	Chain	Res	Type
2	H	339	GLN
2	H	362	GLY
2	H	365	ARG
2	H	394	CYS
2	H	399	GLY
2	H	424	TRP
3	I	98	ALA
3	I	100	ILE
3	I	111	GLN
3	I	118	ASN
3	I	126	GLU
3	I	151	LYS
3	I	161	ALA
3	I	265	PHE
3	I	284	GLY
3	I	370	ALA
3	I	372	TRP
3	I	390	ASN
2	K	157	VAL
2	K	164	ASN
2	K	247	GLY
2	K	398	ASP
2	K	407	CYS
3	L	161	ALA
3	L	285	ASP
3	L	315	TRP
3	L	325	ASN
3	L	339	CYS
1	A	125	LYS
1	A	130	VAL
1	A	160	SER
2	B	158	ASN
2	B	192	TYR
2	B	202	ASN
2	B	281	ASP
2	B	284	ASN
2	B	355	ASP
2	B	359	GLN
2	B	439	ASN
3	C	194	PHE
3	C	208	TRP
3	C	220	PRO

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Mol	Chain	Res	Type
3	C	332	SER
3	C	369	TRP
1	D	127	ILE
1	D	151	GLU
2	E	223	GLU
2	E	256	GLN
3	F	132	GLU
3	F	224	THR
3	F	278	TYR
3	F	298	ASP
1	G	151	GLU
2	H	162	PRO
2	H	192	TYR
2	H	199	VAL
2	H	277	ALA
2	H	281	ASP
2	H	284	ASN
2	H	355	ASP
2	H	359	GLN
3	I	115	ASN
3	I	205	LYS
3	I	208	TRP
3	I	209	ILE
3	I	220	PRO
3	I	297	ASP
3	I	331	GLY
3	I	332	SER
3	I	369	TRP
1	J	162	ARG
2	K	256	GLN
2	K	301	GLN
2	K	405	ASN
3	L	100	ILE
3	L	224	THR
3	L	234	HIS
3	L	278	TYR
3	L	298	ASP
3	L	323	GLU
4	P	2	PRO
1	A	151	GLU
1	A	163	GLY
1	A	174	ASP

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Mol	Chain	Res	Type
2	B	154	ASP
2	B	182	LEU
2	B	277	ALA
2	B	327	GLY
2	B	334	GLU
2	B	388	SER
3	C	104	ASP
3	C	157	ALA
3	C	209	ILE
3	C	222	GLY
3	C	243	PRO
3	C	251	GLU
3	C	331	GLY
3	C	341	ALA
3	C	382	THR
2	E	170	SER
2	E	171	ILE
2	E	192	TYR
3	F	172	LEU
3	F	198	LEU
3	F	323	GLU
1	G	120	GLU
2	H	317	TRP
2	H	327	GLY
2	H	334	GLU
2	H	388	SER
2	H	407	CYS
2	H	439	ASN
3	I	108	ARG
3	I	157	ALA
3	I	171	PRO
3	I	178	PHE
3	I	194	PHE
3	I	222	GLY
3	I	251	GLU
3	I	264	MET
3	I	341	ALA
2	K	223	GLU
3	L	132	GLU
3	L	171	PRO
1	A	173	VAL
2	B	162	PRO

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Mol	Chain	Res	Type
2	B	235	PRO
2	B	267	ASP
3	C	97	GLU
3	C	98	ALA
3	C	127	LYS
3	C	171	PRO
3	C	172	LEU
3	C	193	VAL
3	C	270	GLU
2	E	281	ASP
2	E	383	ASP
1	G	122	LEU
2	H	179	ILE
2	H	202	ASN
3	I	243	PRO
3	I	270	GLU
3	I	382	THR
2	K	305	MET
2	K	435	VAL
3	L	198	LEU
3	L	353	THR
4	N	2	PRO
2	B	317	TRP
3	C	111	GLN
3	C	178	PHE
3	C	264	MET
2	E	247	GLY
2	E	302	LEU
2	E	305	MET
3	F	175	ASN
2	H	235	PRO
3	I	360	PRO
2	K	170	SER
3	L	279	ALA
4	R	2	PRO
3	C	128	VAL
3	F	171	PRO
1	G	189	ILE
2	H	267	ASP
2	H	276	VAL
3	I	128	VAL
3	I	193	VAL

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Mol	Chain	Res	Type
1	J	133	ILE
2	K	161	ILE
4	Q	2	PRO
2	B	276	VAL
3	C	360	PRO
3	C	387	ILE
2	E	435	VAL
3	I	188	GLY
3	C	188	GLY
2	E	414	GLY
1	J	152	VAL
4	T	2	PRO
2	B	186	VAL
3	F	138	PRO
3	I	387	ILE
1	A	127	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	69/82 (84%)	57 (83%)	12 (17%)	2	7
1	D	66/82 (80%)	57 (86%)	9 (14%)	3	12
1	G	69/82 (84%)	54 (78%)	15 (22%)	1	3
1	J	74/82 (90%)	60 (81%)	14 (19%)	1	5
2	B	265/286 (93%)	234 (88%)	31 (12%)	5	17
2	E	262/286 (92%)	229 (87%)	33 (13%)	4	14
2	H	265/286 (93%)	236 (89%)	29 (11%)	6	20
2	K	263/286 (92%)	233 (89%)	30 (11%)	5	18
3	C	257/269 (96%)	229 (89%)	28 (11%)	6	20
3	F	253/269 (94%)	221 (87%)	32 (13%)	4	14
3	I	257/269 (96%)	229 (89%)	28 (11%)	6	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	253/269 (94%)	219 (87%)	34 (13%)	4	12
4	M	3/3 (100%)	3 (100%)	0	100	100
4	N	3/3 (100%)	3 (100%)	0	100	100
4	O	3/3 (100%)	3 (100%)	0	100	100
4	P	3/3 (100%)	3 (100%)	0	100	100
4	Q	3/3 (100%)	3 (100%)	0	100	100
4	R	3/3 (100%)	3 (100%)	0	100	100
4	S	3/3 (100%)	3 (100%)	0	100	100
4	T	3/3 (100%)	3 (100%)	0	100	100
All	All	2377/2572 (92%)	2082 (88%)	295 (12%)	4	15

All (295) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	144	LEU
1	A	154	ILE
1	A	155	ASP
1	A	158	ILE
1	A	159	ARG
1	A	171	ARG
1	A	172	GLU
1	A	178	TYR
1	A	179	GLU
1	A	185	LEU
1	A	186	GLU
2	B	153	ILE
2	B	155	GLU
2	B	161	ILE
2	B	166	ARG
2	B	172	LEU
2	B	175	LEU
2	B	180	GLN
2	B	189	GLN
2	B	190	MET
2	B	194	ARG
2	B	209	LYS
2	B	238	VAL
2	B	253	GLN

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Mol	Chain	Res	Type
2	B	256	GLN
2	B	261	ASP
2	B	266	TRP
2	B	281	ASP
2	B	284	ASN
2	B	285	TYR
2	B	288	LEU
2	B	301	GLN
2	B	310	LEU
2	B	315	GLU
2	B	323	LYS
2	B	346	ARG
2	B	359	GLN
2	B	376	SER
2	B	387	THR
2	B	422	TYR
2	B	439	ASN
2	B	447	MET
3	C	96	TYR
3	C	101	LEU
3	C	118	ASN
3	C	121	ILE
3	C	134	GLN
3	C	144	GLN
3	C	145	ILE
3	C	148	ILE
3	C	163	GLN
3	C	166	LEU
3	C	167	TYR
3	C	192	THR
3	C	230	ASN
3	C	232	LYS
3	C	235	LEU
3	C	239	GLN
3	C	246	LEU
3	C	257	THR
3	C	264	MET
3	C	276	LEU
3	C	294	ASP
3	C	315	TRP
3	C	323	GLU
3	C	329	GLN

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Mol	Chain	Res	Type
3	C	347	VAL
3	C	365	ASN
3	C	377	TYR
3	C	383	THR
1	D	124	ARG
1	D	132	HIS
1	D	135	LEU
1	D	143	GLN
1	D	152	VAL
1	D	161	CYS
1	D	167	ARG
1	D	169	LEU
1	D	182	GLN
2	E	154	ASP
2	E	157	VAL
2	E	158	ASN
2	E	164	ASN
2	E	180	GLN
2	E	195	THR
2	E	203	ILE
2	E	206	VAL
2	E	209	LYS
2	E	210	GLU
2	E	212	GLU
2	E	221	THR
2	E	224	MET
2	E	253	GLN
2	E	257	ASP
2	E	264	ARG
2	E	271	GLN
2	E	279	ASN
2	E	301	GLN
2	E	313	GLU
2	E	323	LYS
2	E	340	ILE
2	E	348	THR
2	E	359	GLN
2	E	363	GLU
2	E	366	THR
2	E	369	ILE
2	E	376	SER
2	E	386	LEU

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Mol	Chain	Res	Type
2	E	391	ARG
2	E	395	SER
2	E	421	GLN
2	E	433	ASP
3	F	96	TYR
3	F	102	THR
3	F	106	SER
3	F	107	ILE
3	F	124	LEU
3	F	147	ASP
3	F	148	ILE
3	F	164	SER
3	F	171	PRO
3	F	173	LYS
3	F	176	GLN
3	F	180	VAL
3	F	194	PHE
3	F	198	LEU
3	F	202	VAL
3	F	205	LYS
3	F	221	THR
3	F	225	GLU
3	F	239	GLN
3	F	250	LEU
3	F	259	THR
3	F	264	MET
3	F	266	LYS
3	F	276	LEU
3	F	290	PHE
3	F	294	ASP
3	F	313	SER
3	F	317	ASN
3	F	325	ASN
3	F	347	VAL
3	F	365	ASN
3	F	383	THR
1	G	122	LEU
1	G	128	GLU
1	G	130	VAL
1	G	134	GLN
1	G	136	LEU
1	G	137	GLN

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Mol	Chain	Res	Type
1	G	141	ARG
1	G	148	LYS
1	G	155	ASP
1	G	156	ILE
1	G	158	ILE
1	G	164	SER
1	G	179	GLU
1	G	182	GLN
1	G	186	GLU
2	H	153	ILE
2	H	155	GLU
2	H	161	ILE
2	H	166	ARG
2	H	167	VAL
2	H	175	LEU
2	H	182	LEU
2	H	190	MET
2	H	209	LYS
2	H	238	VAL
2	H	253	GLN
2	H	256	GLN
2	H	261	ASP
2	H	266	TRP
2	H	281	ASP
2	H	284	ASN
2	H	285	TYR
2	H	294	LEU
2	H	301	GLN
2	H	310	LEU
2	H	315	GLU
2	H	323	LYS
2	H	346	ARG
2	H	359	GLN
2	H	376	SER
2	H	387	THR
2	H	422	TYR
2	H	439	ASN
2	H	447	MET
3	I	97	GLU
3	I	110	LEU
3	I	117	ASN
3	I	121	ILE

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Mol	Chain	Res	Type
3	I	134	GLN
3	I	144	GLN
3	I	145	ILE
3	I	148	ILE
3	I	163	GLN
3	I	166	LEU
3	I	167	TYR
3	I	192	THR
3	I	230	ASN
3	I	232	LYS
3	I	235	LEU
3	I	239	GLN
3	I	246	LEU
3	I	257	THR
3	I	264	MET
3	I	276	LEU
3	I	294	ASP
3	I	315	TRP
3	I	323	GLU
3	I	329	GLN
3	I	347	VAL
3	I	365	ASN
3	I	377	TYR
3	I	383	THR
1	J	118	ARG
1	J	127	ILE
1	J	131	GLN
1	J	132	HIS
1	J	133	ILE
1	J	134	GLN
1	J	135	LEU
1	J	138	LYS
1	J	157	LYS
1	J	161	CYS
1	J	167	ARG
1	J	169	LEU
1	J	188	VAL
1	J	191	LYS
2	K	157	VAL
2	K	165	LEU
2	K	167	VAL
2	K	191	GLU

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Mol	Chain	Res	Type
2	K	195	THR
2	K	203	ILE
2	K	206	VAL
2	K	209	LYS
2	K	210	GLU
2	K	212	GLU
2	K	221	THR
2	K	224	MET
2	K	253	GLN
2	K	257	ASP
2	K	264	ARG
2	K	279	ASN
2	K	301	GLN
2	K	323	LYS
2	K	340	ILE
2	K	348	THR
2	K	359	GLN
2	K	363	GLU
2	K	366	THR
2	K	369	ILE
2	K	376	SER
2	K	386	LEU
2	K	391	ARG
2	K	395	SER
2	K	421	GLN
2	K	433	ASP
3	L	96	TYR
3	L	102	THR
3	L	104	ASP
3	L	106	SER
3	L	107	ILE
3	L	109	TYR
3	L	124	LEU
3	L	147	ASP
3	L	148	ILE
3	L	164	SER
3	L	171	PRO
3	L	173	LYS
3	L	176	GLN
3	L	180	VAL
3	L	194	PHE
3	L	198	LEU

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Mol	Chain	Res	Type
3	L	202	VAL
3	L	205	LYS
3	L	221	THR
3	L	225	GLU
3	L	239	GLN
3	L	250	LEU
3	L	259	THR
3	L	264	MET
3	L	266	LYS
3	L	276	LEU
3	L	290	PHE
3	L	294	ASP
3	L	313	SER
3	L	325	ASN
3	L	347	VAL
3	L	365	ASN
3	L	374	THR
3	L	383	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	132	HIS
1	A	139	ASN
1	A	143	GLN
1	A	181	GLN
1	A	182	GLN
1	A	184	GLN
2	B	164	ASN
2	B	174	ASN
2	B	253	GLN
2	B	254	ASN
2	B	256	GLN
2	B	275	ASN
2	B	296	ASN
2	B	301	GLN
2	B	351	ASN
2	B	359	GLN
2	B	405	ASN
2	B	411	ASN
2	B	429	HIS

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Mol	Chain	Res	Type
2	B	439	ASN
3	C	118	ASN
3	C	134	GLN
3	C	158	ASN
3	C	163	GLN
3	C	177	GLN
3	C	210	GLN
3	C	230	ASN
3	C	317	ASN
3	C	319	ASN
3	C	329	GLN
3	C	340	HIS
3	C	345	ASN
3	C	365	ASN
1	D	134	GLN
1	D	137	GLN
1	D	187	GLN
2	E	158	ASN
2	E	174	ASN
2	E	189	GLN
2	E	256	GLN
2	E	271	GLN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	333	ASN
2	E	336	ASN
2	E	339	GLN
2	E	351	ASN
2	E	405	ASN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	111	GLN
3	F	115	ASN
3	F	119	GLN
3	F	136	GLN
3	F	158	ASN
3	F	163	GLN
3	F	189	ASN
3	F	217	HIS
3	F	230	ASN

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Mol	Chain	Res	Type
3	F	254	ASN
3	F	308	ASN
3	F	311	GLN
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	329	GLN
3	F	365	ASN
1	G	134	GLN
1	G	137	GLN
1	G	182	GLN
2	H	158	ASN
2	H	164	ASN
2	H	174	ASN
2	H	180	GLN
2	H	189	GLN
2	H	253	GLN
2	H	254	ASN
2	H	256	GLN
2	H	296	ASN
2	H	301	GLN
2	H	351	ASN
2	H	359	GLN
2	H	405	ASN
2	H	411	ASN
2	H	429	HIS
2	H	439	ASN
3	I	103	HIS
3	I	111	GLN
3	I	117	ASN
3	I	123	ASN
3	I	130	GLN
3	I	136	GLN
3	I	158	ASN
3	I	163	GLN
3	I	177	GLN
3	I	210	GLN
3	I	230	ASN
3	I	317	ASN
3	I	319	ASN
3	I	329	GLN
3	I	340	HIS

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Mol	Chain	Res	Type
3	I	345	ASN
3	I	365	ASN
1	J	131	GLN
1	J	137	GLN
1	J	139	ASN
1	J	143	GLN
1	J	181	GLN
1	J	184	GLN
1	J	187	GLN
2	K	160	ASN
2	K	174	ASN
2	K	189	GLN
2	K	256	GLN
2	K	271	GLN
2	K	296	ASN
2	K	301	GLN
2	K	325	HIS
2	K	336	ASN
2	K	339	GLN
2	K	351	ASN
2	K	405	ASN
2	K	439	ASN
3	L	111	GLN
3	L	115	ASN
3	L	118	ASN
3	L	136	GLN
3	L	158	ASN
3	L	163	GLN
3	L	189	ASN
3	L	217	HIS
3	L	230	ASN
3	L	254	ASN
3	L	308	ASN
3	L	311	GLN
3	L	317	ASN
3	L	319	ASN
3	L	325	ASN
3	L	329	GLN
3	L	365	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	NAG	B	470	2	14,14,15	0.82	0	17,19,21	0.81	1 (5%)
5	NAG	K	470	2	14,14,15	0.51	0	17,19,21	0.97	1 (5%)
5	NAG	H	470	2	14,14,15	0.72	0	17,19,21	0.99	1 (5%)
5	NAG	E	470	2	14,14,15	0.63	0	17,19,21	0.90	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	470	2	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	K	470	2	-	4/6/23/26	0/1/1/1
5	NAG	H	470	2	-	5/6/23/26	0/1/1/1
5	NAG	E	470	2	1/1/5/7	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	470	NAG	C2-N2-C7	-2.66	119.34	122.90
5	B	470	NAG	C2-N2-C7	-2.24	119.89	122.90
5	K	470	NAG	C2-N2-C7	-2.16	120.00	122.90
5	E	470	NAG	C2-N2-C7	-2.10	120.08	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	470	NAG	C1
5	E	470	NAG	C1

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	470	NAG	C8-C7-N2-C2
5	E	470	NAG	O7-C7-N2-C2
5	H	470	NAG	C1-C2-N2-C7
5	H	470	NAG	C8-C7-N2-C2
5	H	470	NAG	O7-C7-N2-C2
5	K	470	NAG	C8-C7-N2-C2
5	K	470	NAG	O7-C7-N2-C2
5	B	470	NAG	C8-C7-N2-C2
5	B	470	NAG	O7-C7-N2-C2
5	K	470	NAG	C4-C5-C6-O6
5	K	470	NAG	O5-C5-C6-O6
5	H	470	NAG	O5-C5-C6-O6
5	B	470	NAG	O5-C5-C6-O6
5	E	470	NAG	C4-C5-C6-O6
5	H	470	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	470	NAG	1	0
5	K	470	NAG	3	0
5	H	470	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	74/87 (85%)	-1.03	0 100 100	62, 83, 105, 111	0
1	D	71/87 (81%)	-1.07	0 100 100	29, 56, 89, 96	0
1	G	74/87 (85%)	-1.01	0 100 100	62, 81, 100, 115	0
1	J	79/87 (90%)	-1.06	0 100 100	35, 58, 108, 122	0
2	B	307/328 (93%)	-0.93	0 100 100	42, 76, 99, 108	0
2	E	304/328 (92%)	-1.07	0 100 100	27, 51, 79, 99	0
2	H	307/328 (93%)	-0.95	1 (0%) 90 87	42, 76, 99, 107	0
2	K	305/328 (92%)	-1.01	0 100 100	25, 51, 80, 97	0
3	C	305/323 (94%)	-0.87	0 100 100	49, 83, 107, 116	0
3	F	300/323 (92%)	-1.02	1 (0%) 90 87	39, 66, 92, 116	0
3	I	305/323 (94%)	-0.86	4 (1%) 75 67	54, 84, 109, 136	0
3	L	300/323 (92%)	-0.99	1 (0%) 90 87	36, 66, 91, 117	0
4	M	4/5 (80%)	-0.68	0 100 100	63, 64, 65, 97	0
4	N	4/5 (80%)	-0.85	0 100 100	41, 48, 60, 86	0
4	O	4/5 (80%)	-0.83	0 100 100	90, 94, 99, 106	0
4	P	4/5 (80%)	-0.84	0 100 100	64, 73, 79, 93	0
4	Q	4/5 (80%)	-1.16	0 100 100	63, 64, 64, 94	0
4	R	4/5 (80%)	-1.06	0 100 100	44, 50, 62, 87	0
4	S	4/5 (80%)	-0.68	0 100 100	89, 100, 101, 104	0
4	T	4/5 (80%)	-0.54	0 100 100	66, 73, 74, 91	0
All	All	2763/2992 (92%)	-0.97	7 (0%) 90 87	25, 71, 100, 136	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	289	ALA	3.3
3	I	290	PHE	2.7
3	I	179	LEU	2.6
3	L	271	ALA	2.6
2	H	445	TYR	2.5
3	I	236	ILE	2.2
3	F	179	LEU	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	K	470	14/15	0.96	0.06	65,75,82,89	0
5	NAG	H	470	14/15	0.97	0.09	94,105,117,117	0
5	NAG	B	470	14/15	0.97	0.06	60,83,88,91	0
5	NAG	E	470	14/15	0.98	0.06	68,77,92,92	0
6	CA	B	2	1/1	0.98	0.05	90,90,90,90	0
6	CA	K	3	1/1	0.98	0.03	89,89,89,89	0
6	CA	H	2	1/1	0.99	0.03	83,83,83,83	0
6	CA	I	1	1/1	0.99	0.03	76,76,76,76	0
6	CA	K	2	1/1	0.99	0.03	60,60,60,60	0
6	CA	C	1	1/1	0.99	0.02	78,78,78,78	0
6	CA	L	1	1/1	0.99	0.02	58,58,58,58	0
6	CA	F	1	1/1	1.00	0.03	54,54,54,54	0
6	CA	E	2	1/1	1.00	0.02	57,57,57,57	0
6	CA	E	3	1/1	1.00	0.02	90,90,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.