



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:30 PM UTC

PDB ID : 2HOD / pdb_00002hod
Title : Crystal Structure of Fragment D from Human Fibrinogen Complexed with Gly-hydroxyPro-Arg-Pro-amide
Authors : Doolittle, R.F.; Kollman, J.M.; Chen, A.; Pandi, L.
Deposited on : 2006-07-14
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:

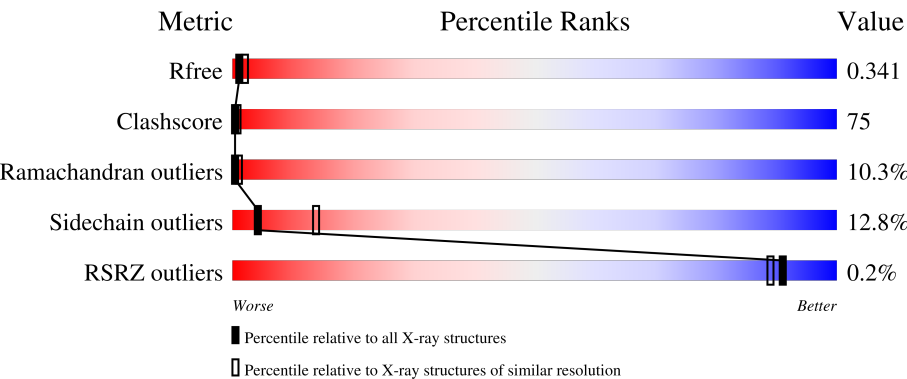
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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.



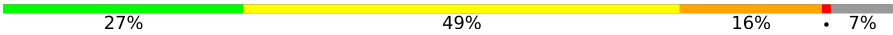
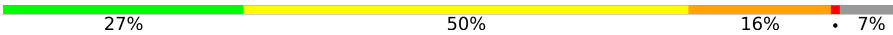
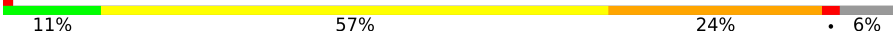
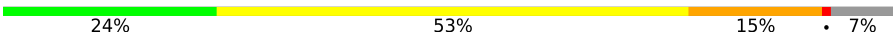
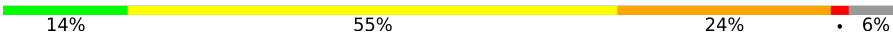
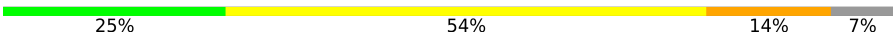
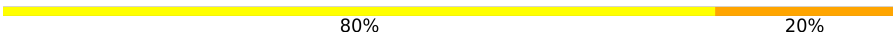
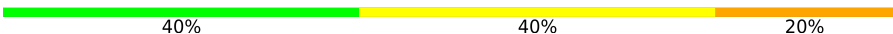
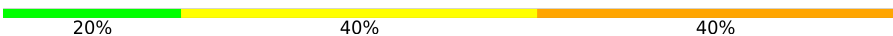
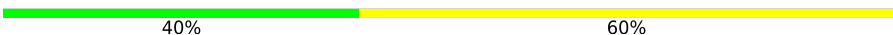
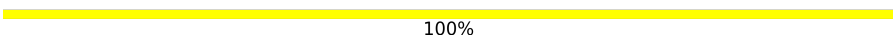
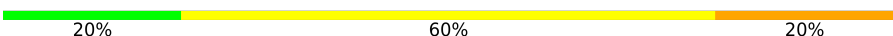
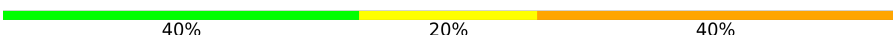
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	7%46%30%.15%
1	D	87	23%43%15%.18%
1	G	87	% 11%54%16%.15%
1	J	87	29%43%16%.9%
2	B	328	% 18%48%23%.6%

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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
4	HYP	S	2	-	-	X	-
5	NAG	E	470	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22278 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			

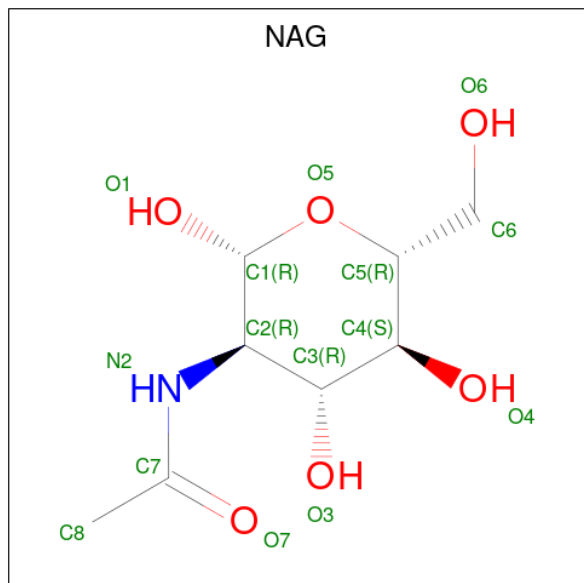
- Molecule 3 is a protein called Fibrinogen, gamma polypeptide.

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-hydroxyPro-Arg-Pro-amide peptide ligand.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	M	5	Total	C	N	O	0	0	1
			31	18	8	5			
4	N	5	Total	C	N	O	0	0	1
			31	18	8	5			
4	O	5	Total	C	N	O	0	0	1
			31	18	8	5			
4	P	5	Total	C	N	O	0	0	1
			31	18	8	5			
4	Q	5	Total	C	N	O	0	0	1
			31	18	8	5			
4	R	5	Total	C	N	O	0	0	1
			31	18	8	5			
4	S	5	Total	C	N	O	0	0	1
			31	18	8	5			
4	T	5	Total	C	N	O	0	0	1
			31	18	8	5			

- 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		

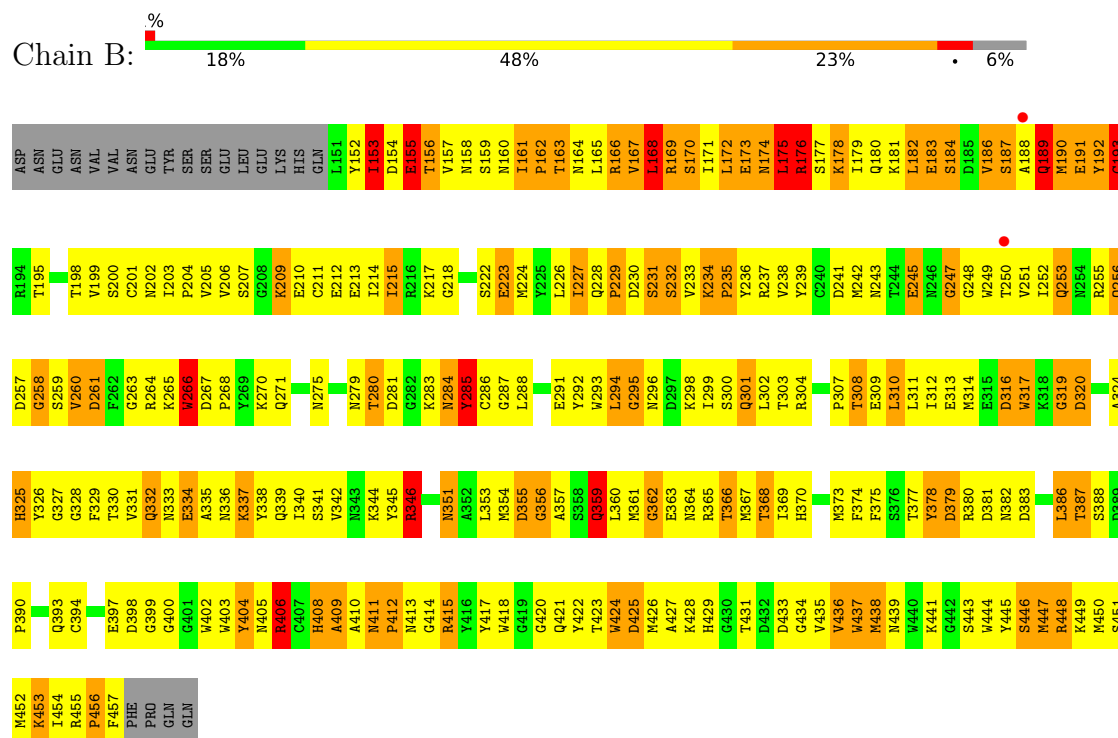
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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		

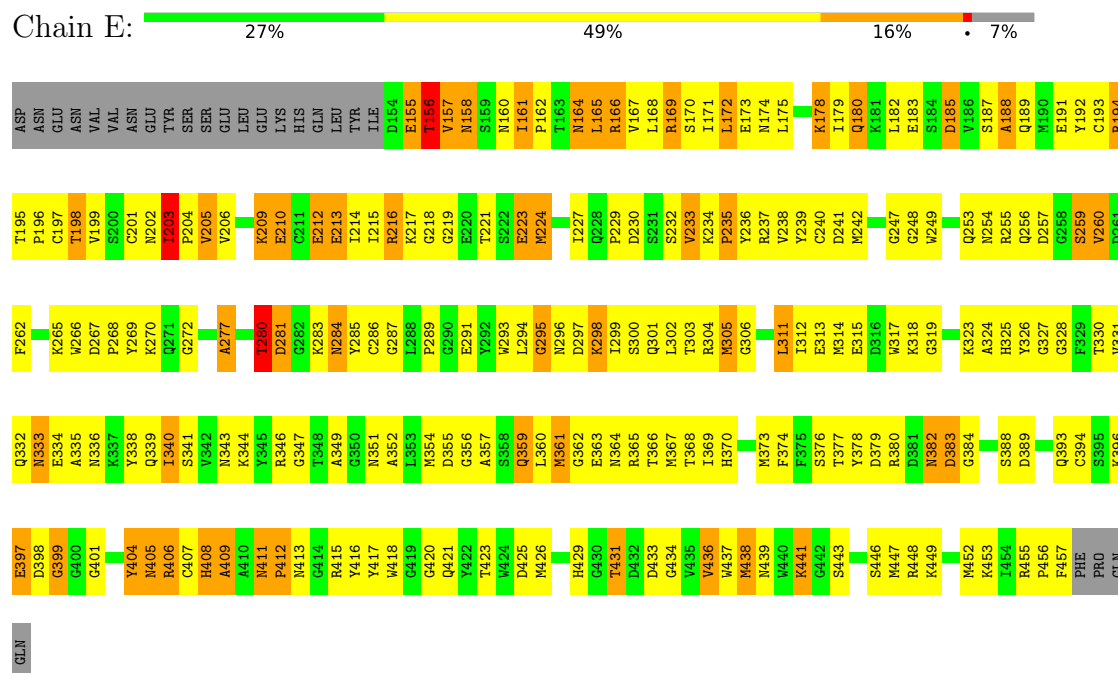
- Molecule 1: Fibrinogen alpha chain



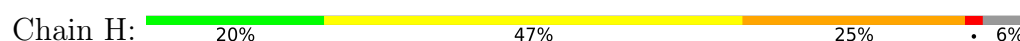
- Molecule 2: Fibrinogen beta chain

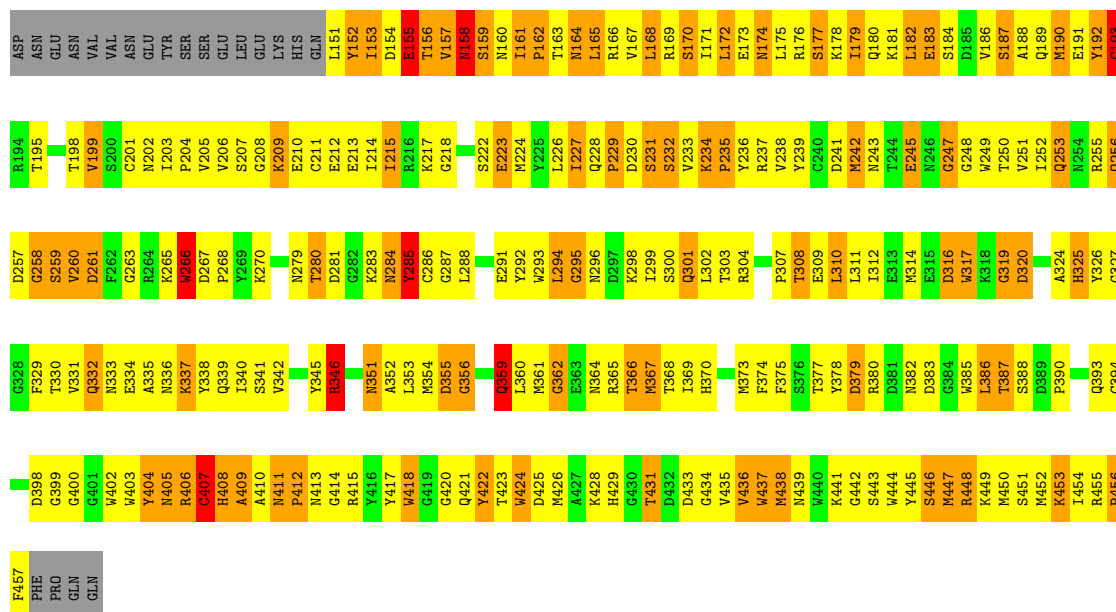


- Molecule 2: Fibrinogen beta chain



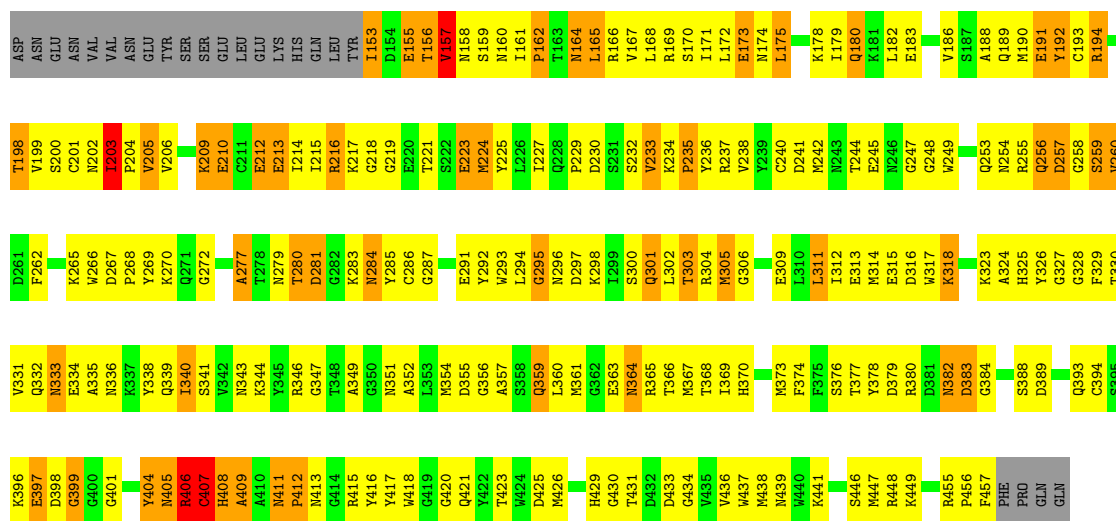
- Molecule 2: Fibrinogen beta chain





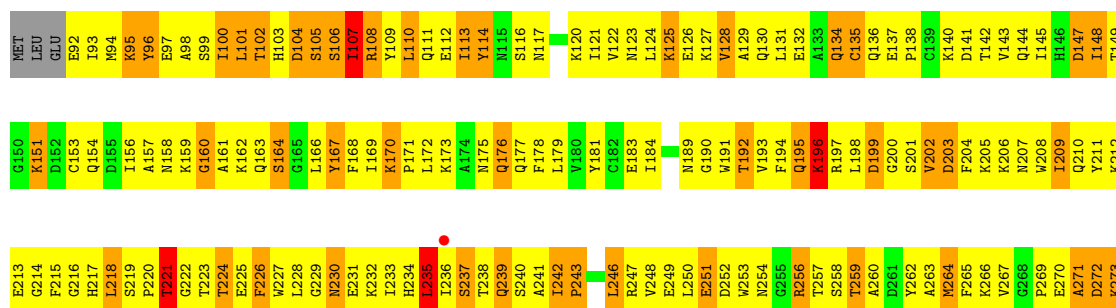
• Molecule 2: Fibrinogen beta chain

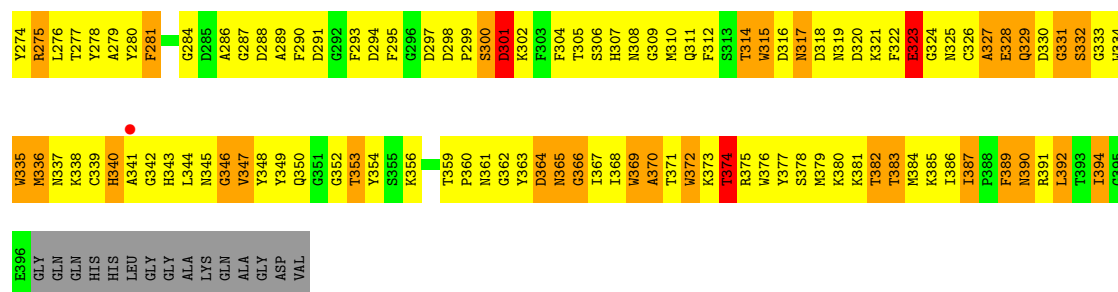
Chain K: 27% 50% 16% 7%



• Molecule 3: Fibrinogen, gamma polypeptide

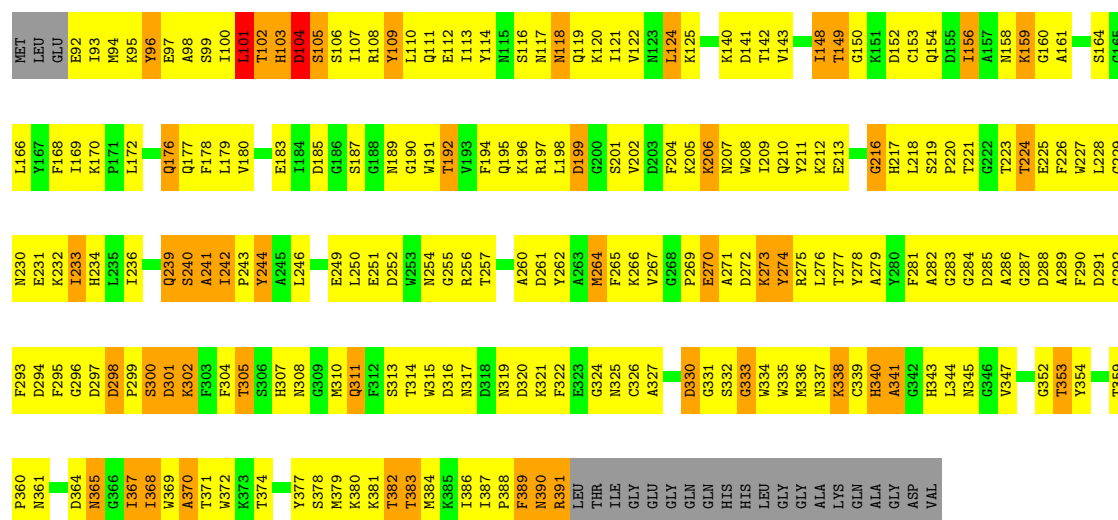
Chain C: 11% 57% 24% 6%





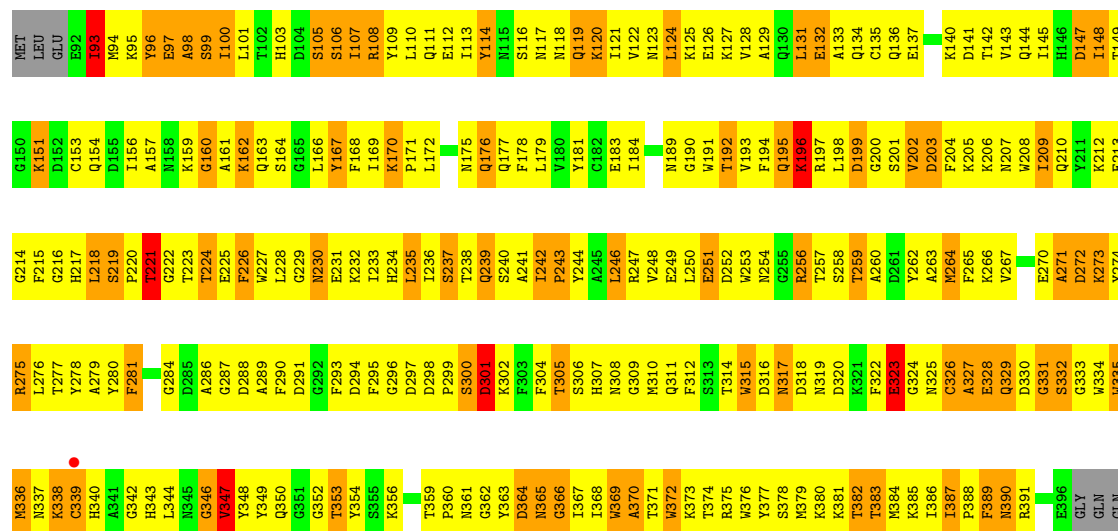
• Molecule 3: Fibrinogen, gamma polypeptide

Chain F: 24% 53% 15% 7%



• Molecule 3: Fibrinogen, gamma polypeptide

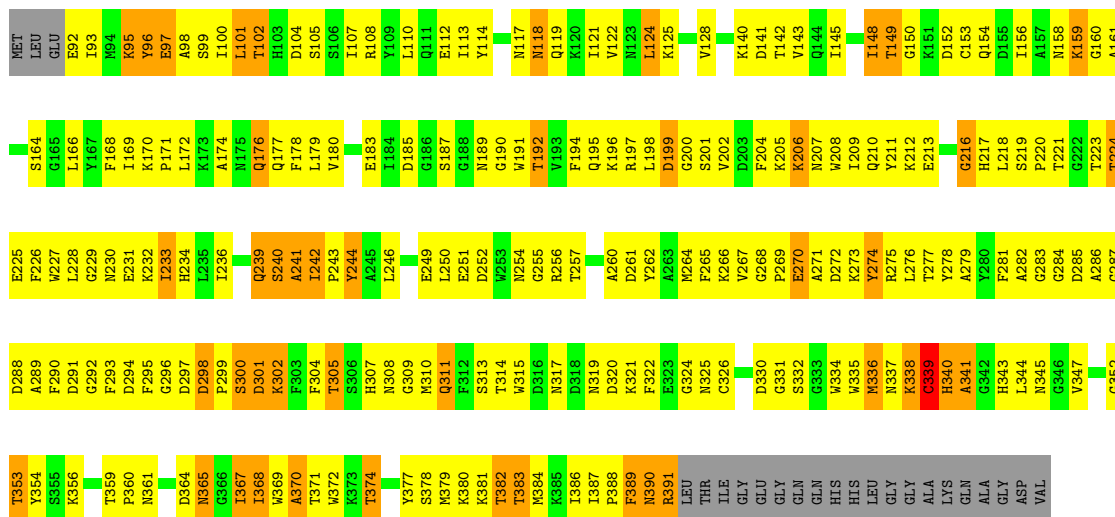
Chain I: 14% 55% 24% 6%



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

• Molecule 3: Fibrinogen, gamma polypeptide

Chain L: 25% 54% 14% 7%



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

Chain M: 80% 20%



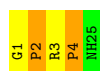
• Molecule 4: Gly-hydroxyPro-Arg-Pro-amide peptide ligand

Chain N: 40% 40% 20%



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

Chain O: 20% 40% 40%



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

Chain P: 40% 60%



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

Chain Q:  100%

G1
P2
R3
P4
NH25

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

Chain R:  20% 60% 20%

G1
P2
R3
P4
NH25

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

Chain S:  40% 20% 40%

G1
P2
R3
P4
NH25

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

Chain T:  40% 60%

G1
P2
R3
P4
NH25

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.65Å 47.07Å 431.46Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	89.5 (30.00-2.90) 90.3 (30.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.77Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.268 , 0.347 0.259 , 0.341	Depositor DCC
R_{free} test set	3441 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	75.8	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 112.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22278	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: CA, NAG, NH2, HYP

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	0.52	0/609	1.26	11/811 (1.4%)
1	D	0.59	0/585	1.19	5/778 (0.6%)
1	G	0.49	0/609	1.20	6/811 (0.7%)
1	J	0.60	0/653	1.19	4/869 (0.5%)
2	B	0.52	0/2523	1.19	37/3409 (1.1%)
2	E	0.64	0/2494	1.14	24/3369 (0.7%)
2	H	0.51	0/2523	1.20	34/3409 (1.0%)
2	K	0.65	0/2502	1.18	27/3380 (0.8%)
3	C	0.47	0/2512	1.08	31/3396 (0.9%)
3	F	0.53	0/2476	1.11	22/3347 (0.7%)
3	I	0.48	0/2512	1.12	29/3396 (0.9%)
3	L	0.52	0/2476	1.13	26/3347 (0.8%)
4	M	0.68	0/21	0.86	0/25
4	N	0.85	0/21	0.82	0/25
4	O	0.73	0/21	0.73	0/25
4	P	0.53	0/21	0.73	0/25
4	Q	0.59	0/21	0.82	0/25
4	R	0.81	0/21	1.02	0/25
4	S	0.64	0/21	0.76	0/25
4	T	0.62	0/21	0.70	0/25
All	All	0.55	0/22642	1.15	256/30522 (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	E	0	1
2	H	0	1
2	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

There are no bond length outliers.

All (256) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	GLN	N-CA-C	-12.10	100.83	114.62
1	J	135	LEU	N-CA-C	-11.86	99.30	113.88
3	F	101	LEU	N-CA-C	-11.21	99.61	113.28
2	H	155	GLU	N-CA-C	-11.13	101.93	114.62
3	I	96	TYR	N-CA-C	-10.63	99.57	112.54
3	L	338	LYS	N-CA-C	-10.52	95.61	111.81
2	K	178	LYS	N-CA-C	-10.29	100.47	113.43
1	G	134	GLN	N-CA-C	-10.27	100.42	113.16
3	L	102	THR	N-CA-C	-10.20	100.83	113.18
2	H	183	GLU	N-CA-C	-10.12	102.00	114.75
2	H	187	SER	N-CA-C	-10.09	101.75	114.56
2	B	190	MET	N-CA-C	-10.06	99.72	112.90
1	A	138	LYS	N-CA-C	-9.55	99.75	111.40
2	H	408	HIS	N-CA-C	9.51	123.79	108.76
2	B	175	LEU	N-CA-C	-9.49	102.79	114.75
3	L	272	ASP	N-CA-C	-9.33	102.02	112.57
1	D	179	GLU	N-CA-C	-9.25	101.15	111.14
3	L	101	LEU	N-CA-C	-9.18	102.19	112.57
2	B	408	HIS	N-CA-C	8.93	123.01	108.55
2	K	397	GLU	N-CA-C	-8.92	98.50	110.55
3	C	160	GLY	N-CA-C	-8.92	102.55	111.56
2	E	178	LYS	N-CA-C	-8.89	100.86	112.68
3	F	272	ASP	N-CA-C	-8.86	102.55	112.57
3	I	106	SER	N-CA-C	-8.85	102.63	112.72
2	E	409	ALA	N-CA-C	-8.84	102.30	113.43
2	B	156	THR	N-CA-C	-8.64	102.64	113.01
2	K	409	ALA	N-CA-C	-8.60	103.38	114.04
2	K	406	ARG	CA-C-N	8.56	137.89	121.54
2	K	406	ARG	C-N-CA	8.56	137.89	121.54
3	I	111	GLN	N-CA-C	-8.21	102.27	111.71
2	H	260	VAL	N-CA-C	8.21	119.73	107.75
2	H	215	ILE	N-CA-C	-8.19	103.14	113.22
2	B	337	LYS	N-CA-C	-8.18	102.89	112.86
3	L	340	HIS	N-CA-C	8.11	120.90	108.42
3	I	101	LEU	N-CA-C	-8.08	103.33	113.02
2	K	347	GLY	N-CA-C	8.02	121.77	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	408	HIS	N-CA-C	7.97	119.12	107.88
2	E	397	GLU	N-CA-C	-7.96	99.80	110.55
2	B	260	VAL	N-CA-C	7.89	119.28	107.75
2	B	346	ARG	N-CA-C	-7.83	97.09	109.23
2	H	156	THR	N-CA-C	-7.83	102.82	112.38
2	E	347	GLY	N-CA-C	7.82	121.49	110.38
3	C	106	SER	N-CA-C	-7.82	103.72	113.18
2	K	411	ASN	CA-C-N	-7.79	112.32	120.03
2	K	411	ASN	C-N-CA	-7.79	112.32	120.03
3	I	160	GLY	N-CA-C	-7.78	103.70	111.56
2	H	346	ARG	N-CA-C	-7.63	97.41	109.23
1	A	123	LYS	N-CA-C	-7.62	104.01	113.38
2	B	178	LYS	N-CA-C	-7.52	102.68	112.68
3	C	242	ILE	N-CA-C	-7.48	100.75	107.56
1	A	153	ASP	N-CA-C	-7.46	102.82	112.23
2	B	215	ILE	N-CA-C	-7.39	102.52	113.39
2	H	337	LYS	N-CA-C	-7.31	103.94	112.86
2	B	232	SER	N-CA-C	-7.29	103.70	112.59
2	E	411	ASN	CA-C-N	-7.27	112.84	120.03
2	E	411	ASN	C-N-CA	-7.27	112.84	120.03
2	H	172	LEU	N-CA-C	-7.25	103.90	112.89
3	L	274	TYR	N-CA-C	-7.20	95.63	109.24
2	E	412	PRO	N-CA-C	-7.18	100.64	111.41
3	C	145	ILE	N-CA-C	7.09	118.69	107.98
3	F	274	TYR	N-CA-C	-7.08	95.87	109.24
3	I	338	LYS	CA-C-N	7.05	135.00	121.54
3	I	338	LYS	C-N-CA	7.05	135.00	121.54
3	F	105	SER	N-CA-C	-7.03	103.61	111.28
3	L	338	LYS	CA-C-N	7.02	134.95	121.54
3	L	338	LYS	C-N-CA	7.02	134.95	121.54
2	B	163	THR	N-CA-C	-7.00	103.41	113.21
3	F	359	THR	CA-C-N	6.98	126.66	119.82
3	F	359	THR	C-N-CA	6.98	126.66	119.82
2	B	288	LEU	CA-C-N	6.96	126.89	119.85
2	B	288	LEU	C-N-CA	6.96	126.89	119.85
1	A	158	ILE	N-CA-C	-6.96	103.69	110.72
2	H	232	SER	N-CA-C	-6.94	104.12	112.59
3	C	241	ALA	N-CA-C	6.92	120.80	111.24
2	K	412	PRO	N-CA-C	-6.88	101.09	111.41
3	I	145	ILE	N-CA-C	6.87	118.45	107.73
3	L	370	ALA	N-CA-C	6.71	119.16	111.11
3	I	241	ALA	N-CA-C	6.70	120.48	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	169	ARG	N-CA-C	-6.68	102.53	111.96
2	E	260	VAL	N-CA-C	6.62	119.87	108.95
2	E	161	ILE	CB-CA-C	-6.61	107.42	113.70
2	K	203	ILE	CA-C-N	6.58	128.07	119.84
2	K	203	ILE	C-N-CA	6.58	128.07	119.84
2	H	181	LYS	N-CA-C	-6.58	104.25	113.20
2	B	193	CYS	N-CA-C	-6.58	104.86	114.39
2	K	260	VAL	N-CA-C	6.55	119.54	108.86
2	H	193	CYS	N-CA-C	-6.54	104.91	114.39
2	H	406	ARG	CA-C-N	6.53	134.02	121.54
2	H	406	ARG	C-N-CA	6.53	134.02	121.54
2	B	404	TYR	N-CA-C	6.53	119.34	108.96
2	E	277	ALA	N-CA-C	6.51	118.75	108.79
2	H	447	MET	N-CA-C	6.51	119.06	109.69
2	H	399	GLY	N-CA-C	6.50	128.59	113.18
3	L	302	LYS	N-CA-C	-6.49	104.04	112.68
2	H	288	LEU	CA-C-N	6.49	126.25	119.76
2	H	288	LEU	C-N-CA	6.49	126.25	119.76
3	C	242	ILE	CA-C-N	6.48	127.94	119.84
3	C	242	ILE	C-N-CA	6.48	127.94	119.84
2	H	437	TRP	N-CA-C	-6.48	94.67	107.69
2	H	367	MET	N-CA-C	-6.47	106.11	112.97
2	K	382	ASN	N-CA-C	-6.46	104.82	114.64
1	D	136	LEU	N-CA-C	-6.45	103.16	111.02
3	I	94	MET	N-CA-C	-6.45	105.28	113.01
2	B	176	ARG	N-CA-C	-6.40	104.40	111.82
3	F	340	HIS	N-CA-C	6.40	118.58	108.79
3	L	359	THR	CA-C-N	6.40	126.09	119.82
3	L	359	THR	C-N-CA	6.40	126.09	119.82
2	H	404	TYR	N-CA-C	6.38	119.10	108.96
2	B	399	GLY	N-CA-C	6.36	128.26	113.18
1	J	116	ARG	N-CA-C	-6.35	104.40	111.71
3	I	323	GLU	N-CA-C	-6.35	105.63	113.19
3	F	296	GLY	N-CA-C	-6.34	106.33	115.27
3	F	370	ALA	N-CA-C	6.32	118.73	111.02
3	C	107	ILE	N-CA-C	-6.32	106.81	112.12
2	B	447	MET	N-CA-C	6.28	118.73	109.69
2	E	169	ARG	N-CA-C	-6.28	101.95	111.56
3	C	114	TYR	N-CA-C	-6.28	103.71	112.12
3	C	256	ARG	N-CA-C	6.28	118.40	110.24
3	C	102	THR	N-CA-C	-6.27	105.76	113.41
3	I	242	ILE	CA-C-N	6.26	127.67	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	242	ILE	C-N-CA	6.26	127.67	119.84
1	J	134	GLN	N-CA-C	-6.26	102.91	112.99
3	I	356	LYS	N-CA-C	-6.24	105.25	112.92
1	A	181	GLN	N-CA-C	-6.22	104.79	113.37
3	I	108	ARG	N-CA-C	-6.20	105.43	112.87
2	K	213	GLU	N-CA-C	-6.20	105.74	113.55
2	B	438	MET	N-CA-C	6.17	118.00	111.28
1	A	187	GLN	N-CA-C	-6.16	105.42	113.12
3	C	281	PHE	N-CA-C	-6.15	101.83	110.50
3	C	346	GLY	N-CA-C	6.14	123.36	112.55
3	L	296	GLY	N-CA-C	-6.13	106.63	115.27
1	G	146	ASP	N-CA-C	-6.13	104.68	111.36
2	B	412	PRO	N-CA-C	-6.11	102.59	111.33
3	I	120	LYS	N-CA-C	-6.10	104.63	111.28
3	C	340	HIS	N-CA-C	6.10	117.46	108.86
1	G	187	GLN	N-CA-C	-6.08	103.39	111.96
1	G	138	LYS	N-CA-C	-6.08	104.60	112.68
3	C	323	GLU	N-CA-C	-6.07	105.97	113.19
2	B	437	TRP	N-CA-C	-6.04	95.56	107.69
3	C	205	LYS	N-CA-C	-6.03	103.29	110.41
2	E	319	GLY	N-CA-C	6.02	122.25	115.08
3	F	199	ASP	N-CA-C	6.02	117.52	110.41
2	K	407	CYS	N-CA-C	6.01	123.59	110.80
3	L	368	ILE	N-CA-C	5.99	118.39	109.17
3	I	346	GLY	N-CA-C	5.98	123.07	112.55
3	I	99	SER	N-CA-C	-5.97	106.12	113.41
3	I	205	LYS	N-CA-C	-5.96	103.37	110.41
1	A	177	ASP	N-CA-C	-5.95	103.58	111.96
1	J	128	GLU	N-CA-C	-5.95	104.71	111.07
3	L	268	GLY	N-CA-C	5.93	119.11	112.00
2	E	165	LEU	N-CA-C	-5.92	105.97	113.43
2	E	382	ASN	N-CA-C	-5.92	105.64	114.64
1	G	121	VAL	N-CA-C	5.91	121.64	109.34
3	I	256	ARG	N-CA-C	5.90	117.91	110.24
3	L	199	ASP	N-CA-C	5.90	117.37	110.41
3	F	302	LYS	N-CA-C	-5.90	103.65	111.96
2	K	277	ALA	N-CA-C	5.89	118.24	108.99
3	L	368	ILE	CB-CA-C	-5.88	103.14	111.38
2	H	190	MET	N-CA-C	-5.87	105.21	112.90
3	I	114	TYR	N-CA-C	-5.86	103.69	111.96
2	K	165	LEU	N-CA-C	-5.86	106.75	114.31
3	F	368	ILE	N-CA-C	5.86	118.19	109.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	407	CYS	N-CA-C	5.84	123.25	110.80
2	E	203	ILE	CA-C-N	5.84	127.14	119.84
2	E	203	ILE	C-N-CA	5.84	127.14	119.84
3	L	97	GLU	N-CA-C	-5.83	104.56	111.03
1	D	183	LYS	N-CA-C	-5.78	104.67	110.97
3	I	170	LYS	CA-C-N	5.77	127.05	119.84
3	I	170	LYS	C-N-CA	5.77	127.05	119.84
3	F	330	ASP	N-CA-C	-5.75	105.91	114.64
3	F	206	LYS	N-CA-C	-5.72	102.82	110.55
2	B	187	SER	N-CA-C	-5.69	105.06	112.23
2	K	173	GLU	N-CA-C	-5.67	105.18	111.36
2	E	213	GLU	N-CA-C	-5.66	106.04	113.12
3	F	341	ALA	N-CA-C	-5.66	104.95	113.89
3	C	356	LYS	N-CA-C	-5.64	105.98	112.92
3	C	147	ASP	N-CA-C	5.62	118.49	111.24
3	C	170	LYS	CA-C-N	5.60	126.84	119.84
3	C	170	LYS	C-N-CA	5.60	126.84	119.84
3	L	305	THR	N-CA-C	-5.59	106.35	112.72
2	B	446	SER	N-CA-C	-5.59	102.49	110.59
2	H	438	MET	N-CA-C	5.59	117.05	111.07
2	H	379	ASP	N-CA-C	-5.58	105.40	113.21
2	H	412	PRO	N-CA-C	-5.58	103.35	111.33
2	H	177	SER	N-CA-C	-5.57	105.11	111.07
3	C	336	MET	N-CA-C	5.56	118.66	110.59
2	H	409	ALA	N-CA-C	-5.56	106.54	113.38
3	C	134	GLN	N-CA-C	-5.55	106.56	113.55
3	I	159	LYS	N-CA-C	-5.55	104.05	111.87
2	B	411	ASN	CA-C-N	-5.54	113.91	120.11
2	B	411	ASN	C-N-CA	-5.54	113.91	120.11
3	C	159	LYS	N-CA-C	-5.54	104.07	111.87
3	L	216	GLY	N-CA-C	-5.53	103.85	111.76
1	G	177	ASP	N-CA-C	-5.51	105.36	112.68
2	B	418	TRP	N-CA-C	5.50	117.67	109.25
3	F	368	ILE	CB-CA-C	-5.49	103.70	111.38
1	A	176	LYS	N-CA-C	-5.46	106.69	113.19
3	C	96	TYR	N-CA-C	-5.45	106.58	113.18
2	E	408	HIS	N-CA-C	5.43	116.40	108.14
2	B	168	LEU	N-CA-C	-5.42	106.51	113.01
2	E	280	THR	N-CA-C	-5.42	104.88	112.25
2	B	409	ALA	N-CA-C	-5.41	106.73	113.38
2	H	248	GLY	N-CA-C	-5.41	107.75	115.64
3	C	104	ASP	N-CA-C	-5.40	105.92	113.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	336	MET	N-CA-C	5.39	118.41	110.59
3	L	341	ALA	N-CA-C	-5.39	105.53	113.61
2	K	166	ARG	N-CA-C	-5.38	105.49	111.36
2	K	399	GLY	N-CA-C	5.38	125.92	113.18
3	I	370	ALA	N-CA-C	5.37	119.32	112.34
1	A	133	ILE	N-CA-C	-5.36	106.58	111.67
2	B	379	ASP	N-CA-C	-5.35	105.72	113.21
3	F	305	THR	N-CA-C	-5.35	106.62	112.72
3	F	332	SER	N-CA-C	5.34	115.60	108.23
2	B	248	GLY	N-CA-C	-5.33	107.85	115.64
3	C	370	ALA	N-CA-C	5.32	119.26	112.34
3	I	281	PHE	N-CA-C	-5.32	102.41	110.28
2	E	188	ALA	N-CA-C	-5.31	104.54	111.02
2	B	415	ARG	N-CA-C	-5.31	101.04	109.59
2	K	329	PHE	N-CA-C	5.31	118.04	108.48
2	E	158	ASN	N-CA-C	5.30	119.44	112.92
1	D	130	VAL	N-CA-C	-5.29	105.34	110.42
1	A	182	GLN	N-CA-C	-5.28	105.91	112.93
2	B	406	ARG	CA-C-N	5.28	131.20	121.70
2	B	406	ARG	C-N-CA	5.28	131.20	121.70
2	K	188	ALA	N-CA-C	-5.27	105.23	110.97
2	E	443	SER	N-CA-C	5.26	117.92	111.82
2	E	399	GLY	N-CA-C	5.25	125.62	113.18
3	F	216	GLY	N-CA-C	-5.24	104.26	111.76
2	B	184	SER	N-CA-C	-5.22	105.99	112.93
3	F	327	ALA	N-CA-C	5.21	116.64	111.07
3	I	147	ASP	N-CA-C	5.20	117.94	111.24
2	K	393	GLN	N-CA-C	-5.20	99.98	108.76
2	H	418	TRP	N-CA-C	5.19	117.19	109.25
3	L	332	SER	N-CA-C	5.16	115.35	108.23
3	C	241	ALA	CA-C-N	-5.15	119.10	122.60
3	C	241	ALA	C-N-CA	-5.15	119.10	122.60
1	D	172	GLU	N-CA-C	-5.14	100.92	108.99
3	L	206	LYS	N-CA-C	-5.13	103.62	110.55
2	H	411	ASN	CA-C-N	-5.13	114.37	120.11
2	H	411	ASN	C-N-CA	-5.13	114.37	120.11
3	L	336	MET	N-CA-C	5.12	117.31	109.07
2	K	406	ARG	O-C-N	5.11	129.39	122.59
2	K	225	TYR	CB-CA-C	-5.11	108.01	114.40
3	F	333	GLY	N-CA-C	-5.11	101.08	113.18
2	E	393	GLN	N-CA-C	-5.09	100.15	108.76
3	C	314	THR	N-CA-C	-5.09	103.88	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	93	ILE	N-CA-C	-5.06	108.36	113.47
2	K	157	VAL	N-CA-C	5.06	119.86	109.34
2	B	368	THR	N-CA-C	-5.03	104.47	110.41
3	C	95	LYS	N-CA-C	-5.03	106.43	113.37
3	F	104	ASP	N-CA-C	-5.02	100.10	110.80
3	C	122	VAL	N-CA-C	-5.01	105.51	110.62
3	L	338	LYS	O-C-N	5.01	128.73	121.97
2	B	397	GLU	N-CA-C	-5.01	102.78	110.14
2	H	446	SER	N-CA-C	-5.00	103.33	110.59
3	L	339	CYS	N-CA-C	5.00	121.46	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	236	TYR	Sidechain
2	H	152	TYR	Sidechain
2	K	236	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	124	0
1	D	584	0	623	80	0
1	G	608	0	649	133	0
1	J	652	0	695	99	0
2	B	2462	0	2327	506	0
2	E	2434	0	2295	268	0
2	H	2462	0	2326	445	0
2	K	2442	0	2307	270	0
3	C	2446	0	2294	505	0
3	F	2410	0	2256	285	0
3	I	2446	0	2294	479	0
3	L	2410	0	2256	274	0
4	M	31	0	32	4	0
4	N	31	0	32	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	31	0	32	9	0
4	P	31	0	32	5	0
4	Q	31	0	32	5	0
4	R	31	0	32	4	0
4	S	31	0	32	13	0
4	T	31	0	32	5	0
5	B	14	0	13	4	0
5	E	14	0	13	5	0
5	H	14	0	13	3	0
5	K	14	0	13	2	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	22278	0	21279	3248	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 75.

All (3248) 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)
3:F:305:THR:HB	3:F:341:ALA:HB2	1.23	1.17
2:E:355:ASP:HB3	2:E:365:ARG:HH22	1.12	1.15
2:H:245:GLU:HB3	2:H:249:TRP:HE1	1.09	1.15
1:J:127:ILE:HG23	2:K:153:ILE:HG21	1.27	1.15
2:H:412:PRO:HG3	2:H:450:MET:HE3	1.21	1.13
2:E:191:GLU:HA	2:E:194:ARG:HH21	1.09	1.13
3:L:305:THR:HB	3:L:341:ALA:HB2	1.29	1.13
3:I:330:ASP:HB2	3:I:365:ASN:HB3	1.14	1.12
2:K:355:ASP:HB3	2:K:365:ARG:HH22	1.09	1.11
2:B:245:GLU:HB3	2:B:249:TRP:HE1	1.06	1.11
2:B:412:PRO:HG3	2:B:450:MET:HE3	1.25	1.10
3:C:330:ASP:HB2	3:C:365:ASN:HB3	1.12	1.09
3:C:105:SER:HA	3:C:108:ARG:HB3	1.31	1.05
2:B:176:ARG:HA	2:B:179:ILE:HD12	1.34	1.04
1:G:148:LYS:NZ	2:H:425:ASP:HB2	1.74	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:326:CYS:HB3	3:I:336:MET:HE3	1.41	1.01
2:B:204:PRO:HG3	3:C:217:HIS:HB3	1.41	1.01
3:F:148:ILE:HD12	3:F:148:ILE:H	1.25	1.01
2:H:241:ASP:HB3	2:H:249:TRP:HB2	1.39	1.01
2:B:373:MET:HE3	2:B:374:PHE:H	1.28	0.98
3:L:148:ILE:H	3:L:148:ILE:HD12	1.29	0.98
1:D:191:LYS:HG3	1:D:192:ASP:H	1.27	0.97
1:A:133:ILE:HG21	2:B:164:ASN:HD21	1.29	0.97
1:A:169:LEU:HD12	1:A:171:ARG:HG3	1.46	0.97
1:J:167:ARG:HB3	1:J:167:ARG:NH1	1.79	0.96
2:E:398:ASP:HA	2:E:433:ASP:HB3	1.43	0.96
2:H:176:ARG:HA	2:H:179:ILE:HD12	1.44	0.96
2:K:398:ASP:HA	2:K:433:ASP:HB3	1.44	0.96
3:F:230:ASN:HA	3:F:233:ILE:HD12	1.47	0.96
2:H:256:GLN:HE21	2:H:449:LYS:HZ1	1.13	0.96
2:H:367:MET:SD	2:H:406:ARG:HG2	2.06	0.96
2:K:191:GLU:HA	2:K:194:ARG:HH21	1.26	0.96
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.42	0.96
1:G:148:LYS:HZ3	2:H:425:ASP:HB2	1.28	0.96
1:J:144:LEU:HD23	1:J:182:GLN:HG2	1.46	0.95
1:A:133:ILE:HG21	2:B:164:ASN:ND2	1.79	0.95
1:G:132:HIS:C	1:G:133:ILE:HD12	1.89	0.95
3:C:326:CYS:HB3	3:C:336:MET:HE3	1.46	0.95
2:H:415:ARG:H	2:H:434:GLY:HA2	1.33	0.94
2:H:373:MET:HE3	2:H:374:PHE:H	1.30	0.94
2:K:352:ALA:HB2	2:K:439:ASN:ND2	1.82	0.94
3:L:240:SER:HB2	3:L:242:ILE:HD11	1.49	0.93
2:B:267:ASP:HB2	2:B:268:PRO:HD3	1.50	0.93
2:H:205:VAL:HG12	3:I:232:LYS:NZ	1.84	0.93
3:I:154:GLN:HE22	3:I:189:ASN:HA	1.33	0.93
1:J:157:LYS:HA	1:J:157:LYS:HE2	1.49	0.93
2:E:352:ALA:HB2	2:E:439:ASN:ND2	1.83	0.92
3:F:194:PHE:HA	3:F:228:LEU:HD12	1.50	0.92
2:B:165:LEU:H	2:B:166:ARG:HH21	1.16	0.92
3:C:221:THR:HG23	3:C:222:GLY:H	1.32	0.92
1:A:143:GLN:HA	1:A:143:GLN:HE21	1.32	0.92
3:I:103:HIS:HA	3:I:106:SER:HB3	1.50	0.92
2:B:369:ILE:H	2:B:405:ASN:HD22	1.18	0.91
1:D:167:ARG:CB	1:D:167:ARG:HH11	1.82	0.91
3:I:221:THR:HG23	3:I:222:GLY:H	1.33	0.91
2:H:169:ARG:HG2	3:I:110:LEU:HD21	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:194:PHE:HA	3:L:228:LEU:HD12	1.52	0.91
2:H:204:PRO:HG3	3:I:217:HIS:HB3	1.51	0.91
2:H:267:ASP:HB2	2:H:268:PRO:HD3	1.53	0.91
3:L:230:ASN:HA	3:L:233:ILE:HD12	1.53	0.91
1:A:148:LYS:HE3	2:B:425:ASP:O	1.70	0.91
2:E:191:GLU:HA	2:E:194:ARG:NH2	1.84	0.91
2:K:355:ASP:HB3	2:K:365:ARG:NH2	1.85	0.90
2:K:367:MET:HB2	2:K:406:ARG:HB3	1.51	0.90
3:C:154:GLN:HE22	3:C:189:ASN:HA	1.35	0.90
3:C:273:LYS:HE3	3:C:319:ASN:HD21	1.36	0.90
2:B:415:ARG:H	2:B:434:GLY:HA2	1.37	0.90
2:B:245:GLU:HB3	2:B:249:TRP:NE1	1.87	0.90
1:J:140:VAL:HG13	1:J:185:LEU:HD11	1.54	0.90
3:L:208:TRP:HA	3:L:314:THR:HG21	1.54	0.89
2:B:205:VAL:HG12	3:C:232:LYS:NZ	1.87	0.89
2:H:223:GLU:HB3	2:H:287:GLY:HA2	1.54	0.89
2:H:369:ILE:H	2:H:405:ASN:HD22	1.16	0.89
4:S:3:ARG:HG2	4:S:3:ARG:HH21	1.37	0.89
3:I:251:GLU:HG2	3:I:252:ASP:H	1.37	0.89
2:K:327:GLY:HA3	2:K:344:LYS:HB2	1.54	0.89
2:H:367:MET:HB2	2:H:406:ARG:HB3	1.54	0.88
2:B:223:GLU:HB3	2:B:287:GLY:HA2	1.54	0.88
2:E:178:LYS:O	2:E:182:LEU:HD23	1.72	0.88
2:E:327:GLY:HA3	2:E:344:LYS:HB2	1.54	0.88
3:F:141:ASP:OD1	3:F:143:VAL:HG22	1.72	0.88
2:B:157:VAL:C	2:B:158:ASN:HD22	1.81	0.87
2:H:245:GLU:HB3	2:H:249:TRP:NE1	1.89	0.87
2:B:165:LEU:H	2:B:166:ARG:NH2	1.72	0.87
2:B:256:GLN:HE21	2:B:449:LYS:HZ1	1.21	0.87
2:H:359:GLN:NE2	2:H:359:GLN:H	1.73	0.86
2:K:191:GLU:HA	2:K:194:ARG:NH2	1.90	0.86
3:F:240:SER:HB2	3:F:242:ILE:HD11	1.55	0.86
3:L:340:HIS:O	4:T:1:GLY:HA2	1.75	0.86
2:B:204:PRO:HA	3:C:217:HIS:HA	1.56	0.86
2:B:300:SER:O	2:B:304:ARG:HG2	1.75	0.86
2:B:158:ASN:ND2	3:C:100:ILE:HG21	1.91	0.86
2:B:158:ASN:HD21	3:C:100:ILE:HG21	1.41	0.85
3:I:214:GLY:HA2	3:I:229:GLY:HA3	1.57	0.85
2:H:300:SER:O	2:H:304:ARG:HG2	1.75	0.85
2:E:241:ASP:HB3	2:E:249:TRP:HB2	1.58	0.85
2:K:333:ASN:HB3	2:K:336:ASN:ND2	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:THR:HG22	3:C:140:LYS:HB3	1.59	0.85
3:C:214:GLY:HA2	3:C:229:GLY:HA3	1.58	0.85
3:C:271:ALA:C	3:C:273:LYS:H	1.85	0.85
2:E:355:ASP:HB3	2:E:365:ARG:NH2	1.91	0.85
3:I:143:VAL:HG12	3:I:220:PRO:HD3	1.57	0.85
2:K:241:ASP:HB3	2:K:249:TRP:HB2	1.58	0.85
1:J:144:LEU:CD2	1:J:182:GLN:HG2	2.06	0.84
3:C:209:ILE:H	3:C:209:ILE:HD12	1.38	0.84
2:E:269:TYR:O	2:E:296:ASN:HB2	1.77	0.84
2:K:269:TYR:O	2:K:296:ASN:HB2	1.76	0.84
2:H:369:ILE:H	2:H:405:ASN:ND2	1.75	0.84
2:E:352:ALA:HB2	2:E:439:ASN:HD22	1.41	0.84
3:C:169:ILE:HD12	3:C:171:PRO:HD3	1.59	0.84
3:F:208:TRP:HA	3:F:314:THR:HG21	1.59	0.84
1:G:119:ILE:O	1:G:120:GLU:HB2	1.78	0.84
2:H:204:PRO:HA	3:I:217:HIS:HA	1.59	0.83
3:I:169:ILE:HD12	3:I:171:PRO:HD3	1.58	0.83
3:I:337:ASN:C	3:I:339:CYS:H	1.86	0.83
3:C:246:LEU:HD12	3:C:247:ARG:N	1.93	0.83
2:K:183:GLU:HG2	3:L:124:LEU:HG	1.60	0.83
2:K:412:PRO:O	2:K:413:ASN:HB2	1.77	0.83
2:H:159:SER:C	2:H:162:PRO:HD2	2.02	0.83
1:D:185:LEU:HD22	1:D:189:ILE:HG13	1.60	0.83
3:I:209:ILE:H	3:I:209:ILE:HD12	1.39	0.83
3:C:330:ASP:HB2	3:C:365:ASN:CB	2.03	0.83
1:A:164:SER:HB3	3:C:137:GLU:O	1.79	0.82
2:E:183:GLU:HG2	3:F:124:LEU:HG	1.59	0.82
2:H:266:TRP:NE1	2:H:380:ARG:HE	1.77	0.82
3:L:276:LEU:HD23	3:L:277:THR:N	1.93	0.82
2:B:369:ILE:H	2:B:405:ASN:ND2	1.76	0.82
2:E:333:ASN:HB3	2:E:336:ASN:ND2	1.93	0.82
3:F:119:GLN:HA	3:F:119:GLN:HE21	1.42	0.82
1:G:128:GLU:HA	1:G:131:GLN:HB3	1.59	0.82
3:I:271:ALA:C	3:I:273:LYS:H	1.87	0.82
2:B:317:TRP:CD1	2:B:317:TRP:H	1.93	0.82
2:B:359:GLN:NE2	2:B:359:GLN:H	1.77	0.82
3:C:172:LEU:HD13	3:C:239:GLN:HE21	1.44	0.82
1:J:137:GLN:NE2	1:J:189:ILE:HA	1.93	0.82
3:I:172:LEU:HD13	3:I:239:GLN:HE21	1.45	0.82
3:I:276:LEU:CD1	3:I:309:GLY:H	1.91	0.82
3:I:330:ASP:HB2	3:I:365:ASN:CB	2.03	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:172:LEU:HD13	3:I:239:GLN:HB2	1.61	0.82
1:J:158:ILE:HG23	2:K:189:GLN:HE21	1.44	0.82
2:K:352:ALA:HB2	2:K:439:ASN:HD22	1.42	0.82
2:H:293:TRP:HE1	2:H:296:ASN:ND2	1.79	0.81
1:D:167:ARG:HH11	1:D:167:ARG:HB2	1.45	0.81
1:J:137:GLN:HE22	1:J:189:ILE:HA	1.44	0.81
2:K:175:LEU:O	2:K:179:ILE:HG13	1.79	0.81
2:B:167:VAL:HA	2:B:170:SER:HB3	1.61	0.81
2:H:238:VAL:HG21	2:H:250:THR:HG23	1.63	0.81
3:I:235:LEU:HD12	3:I:235:LEU:H	1.43	0.81
2:B:266:TRP:NE1	2:B:380:ARG:HE	1.79	0.81
2:B:284:ASN:HD22	2:B:284:ASN:N	1.79	0.81
3:F:105:SER:HA	3:F:108:ARG:NH1	1.95	0.81
3:F:276:LEU:HD23	3:F:277:THR:N	1.95	0.81
2:B:156:THR:HG22	2:B:160:ASN:HD22	1.46	0.81
3:F:148:ILE:HD12	3:F:148:ILE:N	1.96	0.81
2:H:165:LEU:HD11	3:I:106:SER:O	1.81	0.81
2:B:202:ASN:HD22	2:B:284:ASN:HB3	1.44	0.81
3:C:276:LEU:CD1	3:C:309:GLY:H	1.93	0.81
3:L:229:GLY:O	3:L:233:ILE:HG13	1.80	0.81
2:B:176:ARG:O	2:B:180:GLN:HG2	1.81	0.81
3:C:251:GLU:HG2	3:C:252:ASP:H	1.43	0.81
3:C:143:VAL:HG12	3:C:220:PRO:HD3	1.62	0.80
2:K:253:GLN:OE1	2:K:255:ARG:HG2	1.81	0.80
2:E:412:PRO:O	2:E:413:ASN:HB2	1.80	0.80
2:H:198:THR:HG22	3:I:140:LYS:HB3	1.64	0.80
3:C:228:LEU:O	3:C:232:LYS:HD2	1.82	0.80
3:C:273:LYS:HE3	3:C:319:ASN:ND2	1.95	0.80
3:I:273:LYS:HE3	3:I:319:ASN:HD21	1.43	0.80
2:K:235:PRO:HG2	3:L:168:PHE:HE1	1.47	0.80
3:C:233:ILE:HA	3:C:236:ILE:HD11	1.63	0.80
2:B:361:MET:HB2	5:B:470:NAG:H81	1.64	0.80
2:E:398:ASP:CA	2:E:433:ASP:HB3	2.11	0.80
2:H:351:ASN:O	2:H:355:ASP:HB2	1.80	0.80
2:B:168:LEU:HD23	3:C:110:LEU:HD21	1.64	0.80
3:L:166:LEU:HD21	3:L:218:LEU:HB3	1.64	0.79
2:B:373:MET:HE2	2:B:404:TYR:O	1.81	0.79
2:H:351:ASN:C	2:H:351:ASN:HD22	1.91	0.79
3:L:141:ASP:OD1	3:L:143:VAL:HG22	1.81	0.79
1:A:150:LEU:HD12	1:A:150:LEU:O	1.81	0.79
1:D:137:GLN:NE2	2:E:164:ASN:HD21	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:246:LEU:HD12	3:I:247:ARG:N	1.98	0.79
3:L:148:ILE:HD12	3:L:148:ILE:N	1.98	0.79
2:E:253:GLN:OE1	2:E:255:ARG:HG2	1.81	0.79
3:C:365:ASN:HD22	3:C:365:ASN:N	1.81	0.79
3:F:166:LEU:HD21	3:F:218:LEU:HB3	1.65	0.79
3:F:270:GLU:HB2	3:F:274:TYR:OH	1.82	0.79
2:H:176:ARG:HA	2:H:179:ILE:CD1	2.13	0.79
3:C:214:GLY:CA	3:C:229:GLY:HA3	2.13	0.79
2:H:284:ASN:HD22	2:H:284:ASN:N	1.81	0.79
2:B:359:GLN:O	2:B:360:LEU:HD23	1.83	0.79
3:L:278:TYR:CZ	3:L:308:ASN:HB2	2.18	0.79
2:H:157:VAL:O	2:H:158:ASN:HB2	1.80	0.78
3:I:288:ASP:C	3:I:371:THR:HG21	2.08	0.78
2:B:238:VAL:HG21	2:B:250:THR:HG23	1.65	0.78
3:F:305:THR:CB	3:F:341:ALA:HB2	2.10	0.78
1:G:130:VAL:O	1:G:134:GLN:HG2	1.82	0.78
1:G:181:GLN:O	1:G:184:GLN:HG3	1.83	0.78
2:H:203:ILE:HG21	2:H:226:LEU:HD22	1.66	0.78
2:H:210:GLU:OE1	2:H:212:GLU:N	2.15	0.78
2:K:212:GLU:HG2	2:K:456:PRO:HG2	1.65	0.78
3:C:235:LEU:H	3:C:235:LEU:HD12	1.46	0.78
2:H:173:GLU:C	2:H:175:LEU:H	1.91	0.78
2:H:317:TRP:CD1	2:H:317:TRP:H	1.97	0.78
2:B:186:VAL:O	2:B:190:MET:HB2	1.83	0.78
3:C:212:LYS:HG2	3:C:231:GLU:HB2	1.65	0.78
3:C:232:LYS:O	3:C:236:ILE:HG12	1.83	0.78
2:H:359:GLN:O	2:H:360:LEU:HD23	1.83	0.78
3:L:391:ARG:HB2	3:L:391:ARG:HH11	1.48	0.78
2:H:214:ILE:HD12	2:H:227:ILE:HG22	1.65	0.78
3:C:228:LEU:HD11	3:C:232:LYS:HD3	1.66	0.78
1:J:156:ILE:HG21	2:K:415:ARG:NH1	1.99	0.78
1:J:178:TYR:O	1:J:182:GLN:HG3	1.82	0.78
1:D:124:ARG:HD3	1:D:124:ARG:H	1.47	0.78
2:E:212:GLU:HG2	2:E:456:PRO:HG2	1.65	0.78
2:B:351:ASN:C	2:B:351:ASN:HD22	1.92	0.77
3:F:251:GLU:HA	3:F:257:THR:HG22	1.66	0.77
3:I:298:ASP:O	3:I:301:ASP:HB2	1.84	0.77
3:I:365:ASN:HD22	3:I:365:ASN:N	1.83	0.77
3:C:288:ASP:C	3:C:371:THR:HG21	2.09	0.77
1:G:144:LEU:HD22	1:G:182:GLN:HB3	1.64	0.77
2:K:398:ASP:CA	2:K:433:ASP:HB3	2.13	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:SER:C	2:B:162:PRO:HD2	2.10	0.77
2:B:203:ILE:HG21	2:B:226:LEU:HD22	1.66	0.77
2:H:301:GLN:HE22	2:H:302:LEU:HD23	1.50	0.77
2:H:412:PRO:HG3	2:H:450:MET:CE	2.11	0.77
3:I:214:GLY:CA	3:I:229:GLY:HA3	2.15	0.77
3:I:252:ASP:HB2	3:I:377:TYR:OH	1.82	0.77
3:I:279:ALA:HB2	3:L:308:ASN:ND2	1.99	0.77
3:I:348:TYR:HA	3:I:367:ILE:HD11	1.66	0.77
3:L:251:GLU:HA	3:L:257:THR:HG22	1.66	0.77
3:C:298:ASP:O	3:C:301:ASP:HB2	1.84	0.77
3:L:270:GLU:HB2	3:L:274:TYR:OH	1.83	0.77
3:C:275:ARG:HB2	3:C:311:GLN:HA	1.66	0.77
3:F:278:TYR:CZ	3:F:308:ASN:HB2	2.20	0.77
2:H:256:GLN:HE21	2:H:449:LYS:NZ	1.82	0.77
2:B:178:LYS:C	2:B:180:GLN:H	1.89	0.77
2:E:175:LEU:O	2:E:179:ILE:HG13	1.85	0.77
3:F:229:GLY:O	3:F:233:ILE:HG13	1.84	0.77
1:G:189:ILE:HG23	1:G:189:ILE:O	1.85	0.77
3:I:97:GLU:C	3:I:99:SER:H	1.92	0.77
3:C:348:TYR:HA	3:C:367:ILE:HD11	1.66	0.76
3:L:227:TRP:HZ2	3:L:230:ASN:HD21	1.32	0.76
2:B:162:PRO:HA	2:B:166:ARG:HD2	1.67	0.76
2:B:214:ILE:HD12	2:B:227:ILE:HG22	1.66	0.76
2:K:157:VAL:C	2:K:158:ASN:HD22	1.94	0.76
2:B:293:TRP:HE1	2:B:296:ASN:ND2	1.84	0.76
3:I:93:ILE:HD12	3:I:93:ILE:N	2.01	0.76
3:I:273:LYS:HE3	3:I:319:ASN:ND2	1.99	0.76
2:H:202:ASN:HD22	2:H:284:ASN:HB3	1.49	0.76
3:I:212:LYS:HG2	3:I:231:GLU:HB2	1.67	0.76
3:I:250:LEU:HD21	3:I:379:MET:SD	2.26	0.76
2:B:176:ARG:CB	2:B:176:ARG:HH11	1.99	0.76
2:B:412:PRO:HG3	2:B:450:MET:CE	2.12	0.76
3:C:252:ASP:HB2	3:C:377:TYR:OH	1.84	0.76
3:C:250:LEU:HD21	3:C:379:MET:SD	2.26	0.76
3:C:278:TYR:OH	3:C:290:PHE:HB3	1.85	0.76
3:I:336:MET:HE1	3:I:340:HIS:HD2	1.50	0.76
2:K:210:GLU:OE1	2:K:212:GLU:HB3	1.86	0.76
1:A:147:MET:HG3	2:B:175:LEU:HD21	1.67	0.76
3:F:148:ILE:H	3:F:148:ILE:CD1	1.99	0.76
1:G:149:ARG:HH21	2:H:425:ASP:HA	1.51	0.76
3:C:99:SER:C	3:C:101:LEU:H	1.93	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:119:GLN:HA	3:F:119:GLN:NE2	1.97	0.75
1:G:120:GLU:CD	1:G:121:VAL:H	1.94	0.75
3:I:278:TYR:OH	3:I:290:PHE:HB3	1.85	0.75
3:L:227:TRP:HZ2	3:L:230:ASN:ND2	1.84	0.75
3:C:259:THR:H	3:C:286:ALA:HB2	1.52	0.75
2:E:235:PRO:HG2	3:F:168:PHE:HE1	1.51	0.75
3:I:276:LEU:HD12	3:I:309:GLY:H	1.51	0.75
3:F:322:PHE:CZ	4:P:3:ARG:HD2	2.21	0.75
3:F:391:ARG:HH11	3:F:391:ARG:HB2	1.51	0.75
2:B:351:ASN:HD21	2:B:354:MET:HG2	1.50	0.75
3:I:276:LEU:HD11	3:I:308:ASN:HA	1.67	0.75
3:I:327:ALA:HB1	3:I:332:SER:O	1.87	0.74
1:A:148:LYS:NZ	2:B:425:ASP:HB2	2.02	0.74
2:E:360:LEU:HD13	2:E:364:ASN:O	1.86	0.74
3:C:110:LEU:HD23	3:C:111:GLN:N	2.01	0.74
3:I:200:GLY:N	3:I:225:GLU:OE2	2.20	0.74
3:I:300:SER:C	3:I:302:LYS:H	1.90	0.74
1:A:185:LEU:HD13	1:A:185:LEU:O	1.87	0.74
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.35	0.74
3:F:153:CYS:HB2	3:F:192:THR:HG22	1.69	0.74
3:C:103:HIS:O	3:C:107:ILE:HG22	1.86	0.74
3:C:157:ALA:HA	3:C:161:ALA:HB3	1.68	0.74
2:E:210:GLU:OE1	2:E:212:GLU:HB3	1.88	0.74
1:J:130:VAL:O	1:J:133:ILE:HG22	1.88	0.74
2:B:351:ASN:O	2:B:355:ASP:HB2	1.88	0.74
3:I:325:ASN:HD21	3:I:327:ALA:HB3	1.52	0.74
2:K:360:LEU:HD13	2:K:364:ASN:O	1.86	0.74
3:I:232:LYS:O	3:I:236:ILE:HG12	1.86	0.74
3:C:105:SER:HA	3:C:108:ARG:CB	2.16	0.74
3:C:327:ALA:HB1	3:C:332:SER:O	1.88	0.74
2:H:351:ASN:HD21	2:H:354:MET:HG2	1.52	0.74
1:A:144:LEU:HD21	1:A:182:GLN:HA	1.70	0.73
2:B:224:MET:SD	2:B:237:ARG:HB3	2.27	0.73
3:C:209:ILE:HD12	3:C:209:ILE:N	2.02	0.73
2:E:317:TRP:CZ2	2:E:448:ARG:HG3	2.22	0.73
1:G:169:LEU:HD12	1:G:171:ARG:HD2	1.68	0.73
2:H:270:LYS:HA	2:H:296:ASN:HB2	1.69	0.73
3:I:228:LEU:O	3:I:232:LYS:HD2	1.87	0.73
1:J:167:ARG:O	2:K:192:TYR:HB3	1.88	0.73
3:C:276:LEU:HD12	3:C:309:GLY:H	1.53	0.73
3:I:157:ALA:HA	3:I:161:ALA:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:305:THR:HG21	4:S:2:HYP:HD23	1.70	0.73
1:J:116:ARG:H	1:J:116:ARG:HD2	1.53	0.73
2:K:235:PRO:HG2	3:L:168:PHE:CE1	2.21	0.73
3:I:275:ARG:HB2	3:I:311:GLN:HA	1.69	0.73
3:C:300:SER:C	3:C:302:LYS:H	1.91	0.73
3:C:336:MET:HE1	3:C:340:HIS:HD2	1.52	0.73
2:B:213:GLU:HG2	2:B:217:LYS:HE3	1.69	0.73
2:B:184:SER:O	2:B:187:SER:N	2.22	0.73
3:I:197:ARG:NH2	3:I:346:GLY:O	2.22	0.73
3:I:259:THR:H	3:I:286:ALA:HB2	1.54	0.73
3:L:320:ASP:HA	3:L:336:MET:O	1.88	0.73
2:E:210:GLU:HA	2:E:227:ILE:HG21	1.71	0.73
1:G:154:ILE:HD13	2:H:186:VAL:HG21	1.68	0.73
2:H:373:MET:HE2	2:H:404:TYR:O	1.88	0.73
3:L:305:THR:CB	3:L:341:ALA:HB2	2.16	0.73
1:A:140:VAL:HG23	1:A:141:ARG:N	2.04	0.73
3:I:193:VAL:HG12	3:I:195:GLN:H	1.53	0.73
3:L:338:LYS:HG2	4:T:3:ARG:HB2	1.71	0.73
2:B:284:ASN:N	2:B:284:ASN:ND2	2.36	0.73
3:I:228:LEU:HD11	3:I:232:LYS:HD3	1.70	0.73
2:B:255:ARG:HB2	2:B:450:MET:H	1.54	0.72
3:L:216:GLY:HA3	3:L:226:PHE:HA	1.71	0.72
2:B:212:GLU:O	2:B:215:ILE:HG22	1.89	0.72
2:B:253:GLN:HB2	2:B:293:TRP:CE3	2.24	0.72
3:C:365:ASN:HD22	3:C:365:ASN:H	1.37	0.72
3:I:233:ILE:HA	3:I:236:ILE:HD11	1.71	0.72
3:I:249:GLU:HB2	3:I:383:THR:HG23	1.71	0.72
3:L:185:ASP:OD2	3:L:187:SER:HB3	1.90	0.72
3:C:178:PHE:HE2	3:C:228:LEU:HD21	1.54	0.72
3:C:193:VAL:HG12	3:C:195:GLN:H	1.53	0.72
3:C:276:LEU:HD11	3:C:308:ASN:HA	1.69	0.72
3:F:191:TRP:CE3	3:F:387:ILE:HB	2.24	0.72
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	1.86	0.72
2:H:412:PRO:CG	2:H:450:MET:HE3	2.12	0.72
2:K:210:GLU:HA	2:K:227:ILE:HG21	1.72	0.72
3:L:148:ILE:H	3:L:148:ILE:CD1	2.02	0.72
3:L:196:LYS:HG2	3:L:198:LEU:HD11	1.70	0.72
3:I:195:GLN:HE22	3:I:382:THR:CG2	2.03	0.72
1:J:167:ARG:HB3	1:J:167:ARG:CZ	2.18	0.72
3:L:250:LEU:HG	3:L:379:MET:HG3	1.72	0.72
2:B:253:GLN:HB2	2:B:293:TRP:CZ3	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:TRP:HE1	2:B:447:MET:HA	1.54	0.72
2:B:370:HIS:O	2:B:373:MET:HB2	1.89	0.72
2:B:434:GLY:O	2:B:436:VAL:N	2.23	0.72
3:C:103:HIS:C	3:C:105:SER:H	1.96	0.72
2:H:266:TRP:HE1	2:H:380:ARG:NH2	1.87	0.72
2:K:230:ASP:OD2	2:K:232:SER:HB2	1.89	0.72
3:F:101:LEU:O	3:F:104:ASP:HB3	1.90	0.72
2:H:212:GLU:O	2:H:215:ILE:HG22	1.90	0.72
3:L:191:TRP:CE3	3:L:387:ILE:HB	2.24	0.72
3:F:338:LYS:HG2	4:P:3:ARG:HB2	1.70	0.72
2:B:251:VAL:C	2:B:252:ILE:HD13	2.14	0.72
2:B:292:TYR:HE2	2:B:294:LEU:HB2	1.55	0.72
2:H:236:TYR:HB2	2:H:298:LYS:NZ	2.05	0.72
3:I:103:HIS:O	3:I:107:ILE:HG12	1.90	0.72
1:J:167:ARG:HB3	1:J:167:ARG:HH11	1.54	0.72
2:K:317:TRP:CZ2	2:K:448:ARG:HG3	2.24	0.72
2:K:333:ASN:HB3	2:K:336:ASN:HD22	1.54	0.72
3:C:279:ALA:HB2	3:F:308:ASN:ND2	2.03	0.72
1:G:132:HIS:O	1:G:133:ILE:HD12	1.89	0.71
3:C:172:LEU:HD13	3:C:239:GLN:HB2	1.72	0.71
3:I:178:PHE:HE2	3:I:228:LEU:HD21	1.54	0.71
3:I:365:ASN:HD22	3:I:365:ASN:H	1.38	0.71
1:D:140:VAL:HG13	1:D:185:LEU:HD11	1.71	0.71
2:E:333:ASN:H	2:E:336:ASN:HD22	1.38	0.71
3:F:196:LYS:HG2	3:F:198:LEU:HD11	1.70	0.71
2:H:205:VAL:HG12	3:I:232:LYS:HZ2	1.52	0.71
3:I:370:ALA:HA	3:I:373:LYS:O	1.90	0.71
1:G:138:LYS:O	1:G:141:ARG:HG2	1.90	0.71
2:H:345:TYR:CE2	2:H:351:ASN:HB2	2.26	0.71
3:I:123:ASN:O	3:I:127:LYS:HD3	1.89	0.71
3:I:172:LEU:H	3:I:172:LEU:HD12	1.55	0.71
2:B:191:GLU:C	2:B:193:CYS:H	1.98	0.71
2:B:161:ILE:HG23	2:B:166:ARG:NH2	2.06	0.71
2:H:434:GLY:O	2:H:436:VAL:N	2.24	0.71
3:L:153:CYS:HB2	3:L:192:THR:HG22	1.72	0.71
1:A:136:LEU:O	2:B:168:LEU:HD11	1.91	0.71
2:B:152:TYR:C	2:B:154:ASP:H	1.98	0.71
2:B:193:CYS:HB3	3:C:134:GLN:OE1	1.89	0.71
5:E:470:NAG:C6	4:N:4:PRO:HG3	2.20	0.71
3:F:172:LEU:HD13	3:F:240:SER:OG	1.90	0.71
2:H:253:GLN:HB2	2:H:293:TRP:CZ3	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:O	1:A:161:CYS:N	2.23	0.71
2:B:301:GLN:HE22	2:B:302:LEU:HD23	1.56	0.71
2:E:230:ASP:O	2:E:233:VAL:HG12	1.91	0.71
1:G:124:ARG:O	1:G:126:VAL:N	2.23	0.71
2:B:398:ASP:HA	2:B:433:ASP:CB	2.21	0.70
1:D:131:GLN:HB2	1:D:134:GLN:HE21	1.56	0.70
3:F:172:LEU:HD22	3:F:240:SER:OG	1.91	0.70
3:I:209:ILE:HD12	3:I:209:ILE:N	2.06	0.70
3:L:219:SER:HB3	3:L:224:THR:CG2	2.20	0.70
2:B:204:PRO:CG	3:C:217:HIS:HB3	2.19	0.70
3:F:153:CYS:O	3:F:156:ILE:HB	1.92	0.70
3:L:149:THR:OG1	3:L:150:GLY:N	2.24	0.70
3:C:249:GLU:HB2	3:C:383:THR:HG23	1.73	0.70
2:H:213:GLU:HG2	2:H:217:LYS:HE3	1.74	0.70
2:H:270:LYS:HG3	2:H:338:TYR:OH	1.91	0.70
2:H:370:HIS:O	2:H:373:MET:HB2	1.91	0.70
3:C:94:MET:C	3:C:96:TYR:H	1.97	0.70
3:C:325:ASN:HD21	3:C:327:ALA:HB3	1.56	0.70
2:K:242:MET:HA	2:K:247:GLY:HA3	1.73	0.70
3:I:196:LYS:O	3:I:197:ARG:HG2	1.92	0.70
2:B:205:VAL:HG12	3:C:232:LYS:HZ2	1.53	0.70
2:B:284:ASN:ND2	2:B:284:ASN:H	1.89	0.70
2:B:434:GLY:O	2:B:436:VAL:HG13	1.92	0.70
3:C:256:ARG:HH11	3:C:256:ARG:HG3	1.56	0.70
3:C:281:PHE:CD1	3:C:288:ASP:HB2	2.26	0.70
3:C:338:LYS:O	3:C:338:LYS:HG2	1.91	0.70
2:E:266:TRP:CE3	2:E:380:ARG:HG2	2.27	0.70
2:B:266:TRP:HE1	2:B:380:ARG:NH2	1.89	0.70
2:B:412:PRO:CG	2:B:450:MET:HE3	2.14	0.70
2:H:242:MET:HA	2:H:247:GLY:CA	2.22	0.70
3:F:216:GLY:HA3	3:F:226:PHE:HA	1.74	0.70
3:I:219:SER:HB3	3:I:224:THR:HG21	1.73	0.70
3:C:195:GLN:HE22	3:C:382:THR:CG2	2.05	0.70
2:H:178:LYS:C	2:H:180:GLN:H	1.98	0.70
3:L:389:PHE:O	3:L:391:ARG:N	2.24	0.70
3:C:196:LYS:O	3:C:197:ARG:HG2	1.92	0.70
1:G:127:ILE:HD12	1:G:128:GLU:N	2.07	0.70
2:H:224:MET:SD	2:H:237:ARG:HB3	2.31	0.70
3:C:370:ALA:HA	3:C:373:LYS:O	1.91	0.69
2:E:326:TYR:OH	2:E:351:ASN:ND2	2.24	0.69
2:H:351:ASN:HD21	2:H:354:MET:H	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HG	1:A:182:GLN:CD	2.17	0.69
2:B:367:MET:SD	2:B:406:ARG:HG2	2.31	0.69
3:C:271:ALA:O	3:C:273:LYS:N	2.24	0.69
3:C:307:HIS:CD2	3:C:334:TRP:HE1	2.11	0.69
1:D:166:SER:HB2	2:E:195:THR:O	1.92	0.69
2:B:224:MET:HE2	2:B:237:ARG:HE	1.54	0.69
3:C:230:ASN:HD22	3:C:230:ASN:N	1.90	0.69
3:C:367:ILE:O	3:C:379:MET:HG2	1.93	0.69
3:F:219:SER:HB3	3:F:224:THR:CG2	2.22	0.69
2:H:242:MET:HA	2:H:247:GLY:HA3	1.73	0.69
2:K:214:ILE:HD11	2:K:227:ILE:HG22	1.74	0.69
3:C:278:TYR:HE2	3:C:290:PHE:HD2	1.39	0.69
2:B:210:GLU:OE1	2:B:212:GLU:N	2.19	0.69
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.27	0.69
2:B:454:ILE:C	2:B:454:ILE:HD12	2.18	0.69
3:I:154:GLN:NE2	3:I:189:ASN:HA	2.07	0.69
3:C:103:HIS:HA	3:C:106:SER:HB2	1.74	0.69
3:C:209:ILE:H	3:C:209:ILE:CD1	2.06	0.69
2:H:193:CYS:HB3	3:I:134:GLN:OE1	1.92	0.69
3:I:278:TYR:HE2	3:I:290:PHE:HD2	1.40	0.69
3:C:219:SER:HB3	3:C:224:THR:HG21	1.73	0.69
2:H:168:LEU:HB3	3:I:110:LEU:HD13	1.75	0.69
4:S:3:ARG:HG2	4:S:3:ARG:NH2	2.07	0.69
1:A:180:ASP:C	1:A:182:GLN:H	1.99	0.69
2:B:236:TYR:HB2	2:B:298:LYS:NZ	2.07	0.69
2:H:191:GLU:C	2:H:193:CYS:H	2.00	0.69
2:H:238:VAL:HG22	2:H:239:TYR:H	1.57	0.69
2:H:251:VAL:C	2:H:252:ILE:HD13	2.17	0.69
2:H:398:ASP:HA	2:H:433:ASP:CB	2.22	0.69
2:B:209:LYS:HA	2:B:228:GLN:O	1.93	0.69
2:H:310:LEU:HD13	2:H:312:ILE:HG13	1.75	0.69
2:H:314:MET:HE1	2:H:437:TRP:CD2	2.28	0.69
2:H:415:ARG:N	2:H:434:GLY:HA2	2.08	0.69
3:I:166:LEU:HD21	3:I:219:SER:O	1.92	0.69
3:I:256:ARG:HG3	3:I:256:ARG:HH11	1.57	0.69
3:L:251:GLU:HB3	3:L:381:LYS:HB2	1.75	0.69
3:I:293:PHE:N	3:I:302:LYS:HG3	2.08	0.69
1:J:140:VAL:CG1	1:J:185:LEU:HD11	2.23	0.69
2:B:165:LEU:N	2:B:166:ARG:HE	1.90	0.68
2:B:455:ARG:CG	2:B:456:PRO:HD2	2.22	0.68
3:C:344:LEU:HD12	3:C:384:MET:SD	2.33	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:LYS:HZ1	2:H:425:ASP:HB2	1.58	0.68
2:H:351:ASN:HB3	2:H:355:ASP:HB2	1.75	0.68
3:I:209:ILE:H	3:I:209:ILE:CD1	2.07	0.68
3:L:205:LYS:HE2	3:L:331:GLY:HA2	1.75	0.68
3:F:250:LEU:HG	3:F:379:MET:HG3	1.75	0.68
3:I:353:THR:HG23	3:I:377:TYR:HD1	1.58	0.68
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.28	0.68
3:F:242:ILE:HG22	3:F:243:PRO:HD2	1.74	0.68
2:H:249:TRP:HB3	2:H:453:LYS:HB2	1.75	0.68
3:I:183:GLU:O	3:I:191:TRP:HD1	1.76	0.68
3:C:200:GLY:N	3:C:225:GLU:OE2	2.26	0.68
3:C:304:PHE:O	3:C:306:SER:N	2.23	0.68
2:E:235:PRO:HG2	3:F:168:PHE:CE1	2.26	0.68
3:I:297:ASP:HB2	3:I:301:ASP:OD2	1.93	0.68
3:L:337:ASN:C	3:L:339:CYS:H	2.01	0.68
2:E:333:ASN:HB3	2:E:336:ASN:HD22	1.58	0.68
1:G:124:ARG:C	1:G:126:VAL:H	2.01	0.68
2:H:284:ASN:ND2	2:H:284:ASN:H	1.90	0.68
2:B:238:VAL:HG22	2:B:239:TYR:H	1.58	0.68
3:F:192:THR:HG23	3:F:386:ILE:O	1.93	0.68
3:I:281:PHE:CD1	3:I:288:ASP:HB2	2.28	0.68
2:K:230:ASP:O	2:K:233:VAL:HG12	1.94	0.68
3:L:172:LEU:HD13	3:L:240:SER:OG	1.93	0.68
1:A:157:LYS:HD3	1:A:160:SER:OG	1.94	0.68
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.75	0.68
2:E:346:ARG:HG2	2:E:346:ARG:HH11	1.59	0.68
3:I:344:LEU:HD12	3:I:384:MET:SD	2.34	0.68
2:K:212:GLU:HG2	2:K:456:PRO:CG	2.22	0.68
1:A:151:GLU:CD	1:A:173:VAL:HG12	2.19	0.68
2:H:213:GLU:O	2:H:217:LYS:HG3	1.94	0.68
2:H:317:TRP:HE1	2:H:447:MET:HA	1.59	0.68
1:J:181:GLN:HE22	2:K:174:ASN:HB3	1.58	0.68
3:C:154:GLN:NE2	3:C:189:ASN:HA	2.09	0.68
2:H:255:ARG:HB2	2:H:450:MET:H	1.59	0.68
3:I:170:LYS:HB2	3:I:177:GLN:HB3	1.75	0.68
3:I:271:ALA:O	3:I:273:LYS:N	2.26	0.68
2:K:326:TYR:OH	2:K:351:ASN:ND2	2.26	0.68
2:H:304:ARG:NH2	2:H:333:ASN:H	1.92	0.67
1:J:130:VAL:C	1:J:133:ILE:HG22	2.19	0.67
3:L:334:TRP:CD1	3:L:335:TRP:N	2.63	0.67
2:B:351:ASN:HD21	2:B:354:MET:H	1.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:ASN:HB3	2:B:355:ASP:HB2	1.76	0.67
2:B:390:PRO:HA	2:B:393:GLN:HE21	1.60	0.67
3:C:103:HIS:HA	3:C:106:SER:CB	2.23	0.67
3:F:160:GLY:O	3:F:161:ALA:HB3	1.94	0.67
1:G:178:TYR:C	1:G:180:ASP:H	2.03	0.67
2:H:180:GLN:C	2:H:182:LEU:H	2.01	0.67
2:H:454:ILE:HD12	2:H:454:ILE:C	2.20	0.67
2:H:253:GLN:HB2	2:H:293:TRP:CE3	2.30	0.67
3:L:265:PHE:O	3:L:266:LYS:HG3	1.93	0.67
3:I:208:TRP:HA	3:I:314:THR:HG21	1.75	0.67
2:B:270:LYS:HG3	2:B:338:TYR:OH	1.94	0.67
2:H:284:ASN:N	2:H:284:ASN:ND2	2.38	0.67
2:H:434:GLY:O	2:H:436:VAL:HG13	1.95	0.67
3:F:149:THR:OG1	3:F:150:GLY:N	2.23	0.67
3:F:305:THR:HB	3:F:341:ALA:CB	2.14	0.67
2:H:398:ASP:HA	2:H:433:ASP:HB3	1.77	0.67
3:I:304:PHE:O	3:I:306:SER:N	2.24	0.67
1:J:133:ILE:HD11	2:K:165:LEU:HD13	1.75	0.67
3:C:112:GLU:C	3:C:114:TYR:H	2.02	0.67
3:L:97:GLU:O	3:L:100:ILE:HG13	1.95	0.67
3:L:391:ARG:HB2	3:L:391:ARG:NH1	2.08	0.67
2:B:233:VAL:HG22	2:B:234:LYS:H	1.60	0.67
2:B:266:TRP:NE1	2:B:380:ARG:NE	2.42	0.67
2:B:310:LEU:HD13	2:B:312:ILE:HG13	1.74	0.67
3:C:172:LEU:H	3:C:172:LEU:HD12	1.60	0.67
2:E:230:ASP:OD2	2:E:232:SER:HB2	1.94	0.67
3:F:191:TRP:CZ3	3:F:387:ILE:HB	2.30	0.67
2:H:266:TRP:HA	2:H:266:TRP:CE3	2.30	0.67
4:O:3:ARG:HB3	4:O:4:PRO:CD	2.25	0.67
2:B:245:GLU:HG2	2:B:249:TRP:HZ2	1.60	0.67
3:C:170:LYS:HB2	3:C:177:GLN:HB3	1.77	0.67
3:C:208:TRP:HA	3:C:314:THR:HG21	1.75	0.67
3:F:273:LYS:HG3	3:F:311:GLN:HB3	1.76	0.67
2:H:266:TRP:NE1	2:H:380:ARG:NE	2.42	0.67
1:J:127:ILE:HA	1:J:130:VAL:HB	1.76	0.67
3:C:228:LEU:CD1	3:C:232:LYS:HD3	2.24	0.66
3:C:271:ALA:C	3:C:273:LYS:N	2.52	0.66
3:I:373:LYS:HG3	3:I:379:MET:HE1	1.75	0.66
2:K:203:ILE:HD12	2:K:203:ILE:N	2.10	0.66
2:K:234:LYS:HG2	2:K:235:PRO:HD2	1.76	0.66
3:C:183:GLU:O	3:C:191:TRP:HD1	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:278:TYR:CZ	3:C:308:ASN:HB2	2.30	0.66
1:D:191:LYS:O	1:D:192:ASP:HB2	1.95	0.66
1:G:149:ARG:HG2	2:H:426:MET:O	1.95	0.66
2:K:215:ILE:HG23	2:K:216:ARG:N	2.11	0.66
2:B:180:GLN:HA	2:B:180:GLN:HE21	1.59	0.66
2:B:304:ARG:NH2	2:B:333:ASN:H	1.93	0.66
2:B:314:MET:HE1	2:B:437:TRP:CD2	2.30	0.66
3:C:258:SER:OG	3:C:372:TRP:NE1	2.28	0.66
1:D:144:LEU:HD22	1:D:182:GLN:HG3	1.78	0.66
3:L:227:TRP:CZ2	3:L:230:ASN:ND2	2.63	0.66
2:E:212:GLU:HG2	2:E:456:PRO:CG	2.24	0.66
2:E:301:GLN:NE2	2:E:302:LEU:HG	2.11	0.66
3:I:238:THR:HG22	3:I:266:LYS:CG	2.24	0.66
1:A:149:ARG:HG2	2:B:426:MET:O	1.96	0.66
2:H:266:TRP:HE1	2:H:380:ARG:HH21	1.42	0.66
2:B:345:TYR:CE2	2:B:351:ASN:HB2	2.30	0.66
3:C:147:ASP:O	3:C:149:THR:HG23	1.96	0.66
3:C:197:ARG:NH2	3:C:346:GLY:O	2.28	0.66
1:D:122:LEU:N	1:D:124:ARG:HE	1.93	0.66
3:F:389:PHE:O	3:F:391:ARG:N	2.27	0.66
2:H:209:LYS:HA	2:H:228:GLN:O	1.96	0.66
3:I:147:ASP:O	3:I:149:THR:HG23	1.95	0.66
3:I:367:ILE:O	3:I:379:MET:HG2	1.96	0.66
2:K:284:ASN:HD22	2:K:285:TYR:N	1.93	0.66
1:A:125:LYS:O	1:A:129:LYS:HG2	1.95	0.66
2:B:255:ARG:O	2:B:449:LYS:HA	1.96	0.66
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.60	0.66
2:H:330:THR:OG1	2:H:341:SER:HB2	1.95	0.66
3:L:105:SER:HA	3:L:108:ARG:HG2	1.78	0.66
3:L:153:CYS:SG	3:L:192:THR:HB	2.36	0.66
2:B:161:ILE:HG21	3:C:103:HIS:CD2	2.30	0.66
3:C:198:LEU:O	3:C:348:TYR:OH	2.09	0.66
3:C:287:GLY:HA3	3:C:371:THR:O	1.96	0.66
2:H:255:ARG:O	2:H:449:LYS:HA	1.96	0.66
2:H:369:ILE:N	2:H:405:ASN:HD22	1.91	0.66
2:K:363:GLU:O	2:K:367:MET:HG2	1.96	0.66
2:B:242:MET:HA	2:B:247:GLY:CA	2.26	0.66
1:G:167:ARG:HD2	1:G:167:ARG:C	2.20	0.66
3:I:110:LEU:HD23	3:I:113:ILE:HD12	1.78	0.66
2:B:307:PRO:HB2	2:B:457:PHE:C	2.21	0.66
3:C:97:GLU:C	3:C:99:SER:H	2.04	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:230:ASN:HD22	3:I:230:ASN:N	1.94	0.66
2:K:333:ASN:H	2:K:336:ASN:HD22	1.44	0.66
3:L:304:PHE:HA	3:L:337:ASN:HD21	1.59	0.66
2:B:230:ASP:O	2:B:233:VAL:HG12	1.96	0.65
2:B:364:ASN:HD22	5:B:470:NAG:C7	2.08	0.65
3:C:197:ARG:HA	3:C:225:GLU:HG2	1.76	0.65
3:C:230:ASN:ND2	3:C:230:ASN:H	1.95	0.65
2:E:215:ILE:HG23	2:E:216:ARG:N	2.12	0.65
1:G:143:GLN:HA	1:G:146:ASP:HB3	1.77	0.65
2:H:152:TYR:O	2:H:154:ASP:N	2.29	0.65
2:H:172:LEU:HD21	3:I:113:ILE:O	1.95	0.65
3:I:198:LEU:O	3:I:348:TYR:OH	2.09	0.65
2:K:194:ARG:HH12	4:P:4:PRO:HB2	1.60	0.65
3:L:166:LEU:HB3	3:L:179:LEU:HD11	1.78	0.65
3:F:153:CYS:SG	3:F:192:THR:HB	2.37	0.65
3:F:166:LEU:HB3	3:F:179:LEU:HD11	1.77	0.65
2:H:186:VAL:HG11	3:I:128:VAL:HG22	1.78	0.65
2:H:202:ASN:HA	3:I:143:VAL:HG11	1.77	0.65
2:H:230:ASP:O	2:H:233:VAL:HG12	1.96	0.65
3:L:166:LEU:HD22	3:L:179:LEU:HD11	1.78	0.65
4:O:3:ARG:HB3	4:O:4:PRO:HD2	1.77	0.65
3:C:93:ILE:HD12	3:C:94:MET:N	2.12	0.65
3:C:166:LEU:HD21	3:C:219:SER:O	1.96	0.65
3:C:365:ASN:N	3:C:365:ASN:ND2	2.43	0.65
2:E:203:ILE:HD12	2:E:203:ILE:N	2.11	0.65
3:F:391:ARG:HB2	3:F:391:ARG:NH1	2.10	0.65
2:H:307:PRO:HB2	2:H:457:PHE:C	2.21	0.65
2:H:245:GLU:HG2	2:H:249:TRP:HZ2	1.62	0.65
3:I:365:ASN:HD22	3:I:366:GLY:H	1.45	0.65
2:B:249:TRP:HB3	2:B:453:LYS:HB2	1.77	0.65
3:C:117:ASN:O	3:C:120:LYS:HB3	1.96	0.65
3:C:197:ARG:HA	3:C:225:GLU:CG	2.26	0.65
3:F:104:ASP:O	3:F:107:ILE:HG22	1.96	0.65
1:G:147:MET:HG3	2:H:175:LEU:HD11	1.79	0.65
3:I:103:HIS:C	3:I:105:SER:H	2.05	0.65
3:L:288:ASP:C	3:L:371:THR:HG21	2.21	0.65
2:B:202:ASN:HD22	2:B:284:ASN:CB	2.09	0.65
2:H:266:TRP:HA	2:H:266:TRP:HE3	1.62	0.65
3:L:191:TRP:CZ3	3:L:387:ILE:HB	2.32	0.65
3:L:236:ILE:O	3:L:239:GLN:HG2	1.96	0.65
2:B:172:LEU:HD12	2:B:172:LEU:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:GLU:OE2	2:B:212:GLU:HB3	1.97	0.65
2:B:256:GLN:HE21	2:B:449:LYS:NZ	1.94	0.65
3:C:238:THR:HG22	3:C:266:LYS:CG	2.26	0.65
3:C:297:ASP:HB2	3:C:301:ASP:OD2	1.96	0.65
3:F:288:ASP:C	3:F:371:THR:HG21	2.21	0.65
1:G:130:VAL:CA	1:G:133:ILE:HB	2.26	0.65
2:H:394:CYS:SG	2:H:407:CYS:N	2.70	0.65
3:L:117:ASN:O	3:L:121:ILE:HG13	1.96	0.65
2:E:191:GLU:HG2	2:E:194:ARG:NH2	2.12	0.65
2:E:203:ILE:HD12	2:E:203:ILE:H	1.61	0.65
1:G:176:LYS:O	1:G:180:ASP:HB2	1.97	0.65
3:I:271:ALA:C	3:I:273:LYS:N	2.54	0.65
1:J:122:LEU:HD13	1:J:122:LEU:C	2.22	0.65
1:J:157:LYS:HA	1:J:157:LYS:CE	2.25	0.65
3:I:222:GLY:O	3:I:224:THR:HG22	1.96	0.65
2:K:202:ASN:ND2	2:K:284:ASN:HB2	2.12	0.65
3:C:235:LEU:HD12	3:C:235:LEU:N	2.11	0.65
2:E:363:GLU:O	2:E:367:MET:HG2	1.97	0.65
3:F:304:PHE:HA	3:F:337:ASN:HD21	1.61	0.65
1:A:148:LYS:CE	2:B:425:ASP:HB2	2.27	0.64
3:F:298:ASP:O	3:F:301:ASP:HB2	1.96	0.64
3:I:197:ARG:HA	3:I:225:GLU:HG2	1.76	0.64
2:K:373:MET:SD	2:K:405:ASN:HB2	2.37	0.64
2:B:324:ALA:O	2:B:325:HIS:HB2	1.98	0.64
2:H:233:VAL:HG22	2:H:234:LYS:H	1.63	0.64
2:B:267:ASP:HB2	2:B:268:PRO:CD	2.26	0.64
3:C:293:PHE:N	3:C:302:LYS:HG3	2.12	0.64
1:D:191:LYS:HG3	1:D:192:ASP:N	2.06	0.64
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.80	0.64
2:B:310:LEU:HD12	2:B:310:LEU:O	1.98	0.64
2:E:284:ASN:HD22	2:E:285:TYR:H	1.45	0.64
2:H:152:TYR:C	2:H:154:ASP:N	2.54	0.64
1:J:154:ILE:HG12	3:L:128:VAL:HG21	1.80	0.64
2:E:284:ASN:HD22	2:E:285:TYR:N	1.94	0.64
2:H:304:ARG:NH2	2:H:333:ASN:N	2.45	0.64
2:H:324:ALA:O	2:H:325:HIS:HB2	1.98	0.64
1:J:143:GLN:O	1:J:147:MET:HG2	1.97	0.64
3:L:204:PHE:C	3:L:206:LYS:H	2.04	0.64
3:L:211:TYR:HE1	3:L:345:ASN:HD22	1.44	0.64
2:B:173:GLU:O	2:B:176:ARG:HB3	1.96	0.64
2:B:408:HIS:CD2	2:B:411:ASN:HB2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:275:ARG:HB2	3:C:311:GLN:HG2	1.79	0.64
3:C:373:LYS:HG3	3:C:379:MET:HE1	1.78	0.64
2:H:210:GLU:OE2	2:H:212:GLU:HB3	1.98	0.64
2:H:364:ASN:ND2	5:H:470:NAG:H62	2.11	0.64
3:L:295:PHE:CE2	4:T:2:HYP:HD23	2.32	0.64
2:B:417:TYR:HB2	2:B:446:SER:CB	2.27	0.64
2:H:251:VAL:O	2:H:252:ILE:HD13	1.98	0.64
2:H:417:TYR:HB2	2:H:446:SER:CB	2.27	0.64
3:I:195:GLN:O	3:I:196:LYS:CB	2.46	0.64
2:B:165:LEU:HG	2:B:166:ARG:NH2	2.12	0.64
3:F:119:GLN:NE2	3:F:122:VAL:HG21	2.13	0.64
3:F:143:VAL:HA	3:F:220:PRO:HG2	1.80	0.64
2:H:345:TYR:CZ	2:H:351:ASN:HB2	2.32	0.64
3:I:258:SER:OG	3:I:372:TRP:NE1	2.31	0.64
3:C:125:LYS:HE3	3:C:125:LYS:HA	1.78	0.64
2:E:191:GLU:C	2:E:193:CYS:H	2.06	0.64
2:E:242:MET:HA	2:E:247:GLY:HA3	1.80	0.64
3:I:307:HIS:CD2	3:I:334:TRP:HE1	2.16	0.64
3:I:365:ASN:N	3:I:365:ASN:ND2	2.45	0.64
3:L:242:ILE:HG22	3:L:243:PRO:HD2	1.79	0.64
3:C:168:PHE:CD1	3:C:179:LEU:HD13	2.33	0.64
3:C:334:TRP:O	3:C:336:MET:HG2	1.97	0.64
3:C:390:ASN:O	3:C:391:ARG:HD2	1.98	0.64
2:H:199:VAL:O	3:I:142:THR:HG23	1.97	0.64
2:K:304:ARG:C	2:K:306:GLY:H	2.05	0.64
2:B:422:TYR:CE1	2:B:444:TRP:HA	2.33	0.63
3:C:113:ILE:O	3:C:113:ILE:HG22	1.98	0.63
3:C:222:GLY:O	3:C:224:THR:HG22	1.99	0.63
3:F:227:TRP:CZ2	3:F:230:ASN:ND2	2.66	0.63
3:I:154:GLN:CD	3:I:190:GLY:H	2.06	0.63
1:A:157:LYS:HD2	3:C:132:GLU:HB3	1.81	0.63
2:B:199:VAL:O	3:C:142:THR:HG23	1.97	0.63
2:B:369:ILE:N	2:B:405:ASN:HD22	1.92	0.63
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.79	0.63
2:B:455:ARG:HG3	2:B:456:PRO:HD2	1.80	0.63
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.79	0.63
2:K:327:GLY:HA3	2:K:344:LYS:HE3	1.79	0.63
2:B:242:MET:HA	2:B:247:GLY:HA3	1.79	0.63
3:C:195:GLN:O	3:C:196:LYS:CB	2.47	0.63
3:C:272:ASP:OD2	3:C:275:ARG:NE	2.31	0.63
2:H:238:VAL:HG22	2:H:239:TYR:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:422:TYR:CE1	2:H:444:TRP:HA	2.33	0.63
2:H:455:ARG:CG	2:H:456:PRO:HD2	2.28	0.63
3:L:192:THR:HG23	3:L:386:ILE:O	1.99	0.63
3:L:251:GLU:CD	3:L:381:LYS:HD2	2.23	0.63
3:C:178:PHE:CE2	3:C:228:LEU:HD11	2.33	0.63
3:F:293:PHE:CD2	3:F:370:ALA:HB1	2.34	0.63
2:H:408:HIS:CD2	2:H:411:ASN:HB2	2.33	0.63
5:K:470:NAG:H61	4:R:4:PRO:HG2	1.80	0.63
3:L:97:GLU:C	3:L:99:SER:H	2.06	0.63
2:B:153:ILE:O	2:B:153:ILE:HG12	1.99	0.63
2:B:402:TRP:CZ2	2:B:412:PRO:HD2	2.32	0.63
3:C:172:LEU:HD13	3:C:239:GLN:NE2	2.12	0.63
3:F:166:LEU:HD22	3:F:179:LEU:HD11	1.79	0.63
3:F:295:PHE:CE2	4:P:2:HYP:HD23	2.32	0.63
2:H:314:MET:HE1	2:H:437:TRP:CG	2.33	0.63
2:H:326:TYR:OH	2:H:351:ASN:ND2	2.32	0.63
3:I:117:ASN:C	3:I:119:GLN:H	2.04	0.63
3:I:227:TRP:HZ2	3:I:230:ASN:HD21	1.46	0.63
3:I:353:THR:HG23	3:I:377:TYR:CD1	2.34	0.63
1:J:126:VAL:O	1:J:129:LYS:N	2.32	0.63
2:K:313:GLU:HG2	2:K:323:LYS:CD	2.28	0.63
2:E:234:LYS:HG2	2:E:235:PRO:HD2	1.80	0.63
2:H:310:LEU:HD12	2:H:310:LEU:O	1.99	0.63
3:I:172:LEU:H	3:I:172:LEU:CD1	2.11	0.63
1:J:133:ILE:HG23	1:J:133:ILE:O	1.96	0.63
2:B:205:VAL:HG12	3:C:232:LYS:HZ3	1.64	0.63
3:C:93:ILE:O	3:C:96:TYR:HB3	1.98	0.63
1:D:126:VAL:O	1:D:130:VAL:HG23	1.97	0.63
2:E:283:LYS:HB3	2:E:285:TYR:CE2	2.34	0.63
2:E:327:GLY:HA3	2:E:344:LYS:CB	2.28	0.63
3:F:204:PHE:C	3:F:206:LYS:H	2.05	0.63
1:J:149:ARG:HH21	2:K:425:ASP:HA	1.64	0.63
2:K:203:ILE:HD12	2:K:203:ILE:H	1.62	0.63
2:K:266:TRP:HA	2:K:377:THR:HG21	1.81	0.63
2:K:397:GLU:HB3	2:K:431:THR:HG21	1.80	0.63
3:L:153:CYS:O	3:L:156:ILE:HB	1.99	0.63
3:L:273:LYS:HG3	3:L:311:GLN:HB3	1.80	0.63
3:L:295:PHE:HE2	4:T:2:HYP:HD23	1.64	0.63
3:C:172:LEU:H	3:C:172:LEU:CD1	2.11	0.63
3:C:264:MET:N	3:C:264:MET:SD	2.71	0.63
2:E:355:ASP:O	2:E:365:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:228:GLN:HE21	2:H:231:SER:HA	1.63	0.63
2:H:230:ASP:C	2:H:232:SER:H	2.07	0.63
3:I:168:PHE:CD1	3:I:179:LEU:HD13	2.33	0.63
1:J:182:GLN:O	1:J:186:GLU:HG2	1.98	0.63
2:K:301:GLN:NE2	2:K:302:LEU:HG	2.14	0.63
2:K:370:HIS:CE1	2:K:408:HIS:HB2	2.34	0.63
2:B:373:MET:SD	2:B:405:ASN:HB2	2.39	0.62
2:B:420:GLY:HA2	2:B:446:SER:O	1.98	0.62
3:C:315:TRP:HE3	3:C:328:GLU:HG2	1.63	0.62
2:E:304:ARG:C	2:E:306:GLY:H	2.06	0.62
2:B:238:VAL:HG22	2:B:239:TYR:N	2.15	0.62
3:F:304:PHE:HA	3:F:337:ASN:ND2	2.14	0.62
3:F:320:ASP:HA	3:F:336:MET:O	1.99	0.62
1:G:191:LYS:O	1:G:192:ASP:HB3	1.99	0.62
1:A:123:LYS:O	1:A:126:VAL:HB	2.00	0.62
2:B:326:TYR:OH	2:B:351:ASN:ND2	2.32	0.62
2:B:340:ILE:HD12	2:B:403:TRP:CE3	2.34	0.62
3:C:110:LEU:HD23	3:C:110:LEU:C	2.24	0.62
3:C:160:GLY:O	3:C:161:ALA:HB3	1.98	0.62
2:H:166:ARG:NE	2:H:166:ARG:HA	2.14	0.62
3:I:373:LYS:CG	3:I:379:MET:HE1	2.29	0.62
1:J:127:ILE:HG23	2:K:153:ILE:CG2	2.18	0.62
2:K:327:GLY:HA3	2:K:344:LYS:CB	2.28	0.62
1:A:121:VAL:HG23	1:A:122:LEU:N	2.13	0.62
2:B:310:LEU:HD12	2:B:310:LEU:C	2.25	0.62
2:E:314:MET:HE1	2:E:437:TRP:CE3	2.35	0.62
2:E:364:ASN:ND2	5:E:470:NAG:C7	2.62	0.62
2:H:359:GLN:H	2:H:359:GLN:HE21	1.44	0.62
3:I:197:ARG:NH2	3:I:348:TYR:HB2	2.14	0.62
3:I:305:THR:CG2	4:S:2:HYP:HD23	2.29	0.62
3:I:340:HIS:C	4:S:1:GLY:H2	2.07	0.62
2:K:183:GLU:CG	3:L:124:LEU:HG	2.29	0.62
3:L:304:PHE:HA	3:L:337:ASN:ND2	2.14	0.62
2:B:157:VAL:HG23	2:B:158:ASN:ND2	2.14	0.62
2:B:202:ASN:ND2	2:B:284:ASN:HB3	2.11	0.62
1:D:165:CYS:O	2:E:196:PRO:HA	2.00	0.62
2:E:214:ILE:HD11	2:E:227:ILE:HG22	1.82	0.62
3:F:265:PHE:O	3:F:266:LYS:HG3	1.99	0.62
3:L:101:LEU:N	3:L:101:LEU:HD22	2.15	0.62
3:L:160:GLY:O	3:L:161:ALA:HB3	2.00	0.62
2:B:373:MET:HE3	2:B:374:PHE:N	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:ASN:OD1	3:C:394:ILE:HD12	1.99	0.62
2:H:292:TYR:HE2	2:H:294:LEU:HB2	1.64	0.62
3:I:334:TRP:O	3:I:336:MET:HG2	1.99	0.62
3:L:293:PHE:CD2	3:L:370:ALA:HB1	2.35	0.62
1:A:159:ARG:C	1:A:161:CYS:H	2.06	0.62
2:H:152:TYR:C	2:H:154:ASP:H	2.08	0.62
3:I:275:ARG:HB2	3:I:311:GLN:HG2	1.80	0.62
2:B:178:LYS:C	2:B:180:GLN:N	2.52	0.62
3:C:272:ASP:CG	3:C:275:ARG:HE	2.07	0.62
3:C:365:ASN:HD22	3:C:366:GLY:H	1.48	0.62
3:F:211:TYR:HE1	3:F:345:ASN:HD22	1.47	0.62
1:G:130:VAL:N	1:G:133:ILE:HD13	2.14	0.62
2:H:204:PRO:CG	3:I:217:HIS:HB3	2.27	0.62
3:I:153:CYS:HB2	3:I:192:THR:HG22	1.81	0.62
3:I:272:ASP:O	3:I:273:LYS:HB2	2.00	0.62
3:I:315:TRP:HE3	3:I:328:GLU:HG2	1.65	0.62
2:E:359:GLN:O	2:E:360:LEU:HD23	2.00	0.62
3:F:344:LEU:HA	3:F:367:ILE:HG23	1.82	0.62
2:H:402:TRP:CZ2	2:H:412:PRO:HD2	2.33	0.62
3:I:300:SER:C	3:I:302:LYS:N	2.56	0.62
2:K:284:ASN:HD22	2:K:285:TYR:H	1.46	0.62
2:E:357:ALA:HB3	2:E:360:LEU:HD12	1.80	0.62
3:F:205:LYS:HE2	3:F:331:GLY:HA2	1.82	0.62
1:G:143:GLN:HE22	3:I:117:ASN:HB2	1.65	0.62
3:I:235:LEU:HD12	3:I:235:LEU:N	2.15	0.62
2:K:215:ILE:CG2	2:K:216:ARG:N	2.63	0.62
2:K:266:TRP:CE3	2:K:380:ARG:HG2	2.35	0.62
3:C:168:PHE:CE1	3:C:179:LEU:HD13	2.34	0.61
3:C:273:LYS:CE	3:C:319:ASN:HD21	2.12	0.61
2:E:317:TRP:CH2	2:E:448:ARG:HG3	2.34	0.61
1:J:147:MET:HG3	2:K:175:LEU:HD13	1.82	0.61
2:B:330:THR:OG1	2:B:341:SER:HB2	1.99	0.61
2:E:313:GLU:HG2	2:E:323:LYS:HD3	1.80	0.61
2:H:236:TYR:HB2	2:H:298:LYS:HZ3	1.63	0.61
3:I:228:LEU:CD1	3:I:232:LYS:HD3	2.30	0.61
2:K:160:ASN:O	2:K:161:ILE:C	2.42	0.61
2:K:234:LYS:HD3	2:K:234:LYS:C	2.25	0.61
2:K:242:MET:HA	2:K:247:GLY:CA	2.30	0.61
2:B:165:LEU:N	2:B:166:ARG:NE	2.47	0.61
2:B:253:GLN:HA	2:B:292:TYR:O	2.00	0.61
3:C:151:LYS:HD2	3:C:172:LEU:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:194:PHE:CA	3:F:228:LEU:HD12	2.27	0.61
2:H:210:GLU:HA	2:H:227:ILE:HB	1.82	0.61
2:H:263:GLY:HA2	2:H:400:GLY:HA2	1.81	0.61
2:K:247:GLY:O	2:K:455:ARG:NH1	2.32	0.61
2:K:313:GLU:HG2	2:K:323:LYS:HD3	1.81	0.61
1:A:128:GLU:HA	1:A:131:GLN:HG2	1.83	0.61
2:B:230:ASP:C	2:B:232:SER:H	2.08	0.61
2:E:191:GLU:O	2:E:193:CYS:N	2.34	0.61
2:E:313:GLU:HG2	2:E:323:LYS:CD	2.30	0.61
1:G:140:VAL:HA	3:I:114:TYR:HE1	1.66	0.61
3:I:197:ARG:HA	3:I:225:GLU:CG	2.30	0.61
3:I:227:TRP:CD1	3:I:229:GLY:HA2	2.35	0.61
3:I:367:ILE:O	3:I:367:ILE:HG22	2.00	0.61
2:K:394:CYS:SG	2:K:407:CYS:N	2.73	0.61
1:A:164:SER:CB	3:C:137:GLU:O	2.46	0.61
2:H:390:PRO:HA	2:H:393:GLN:HE21	1.66	0.61
3:I:287:GLY:HA3	3:I:371:THR:O	2.00	0.61
2:K:314:MET:HE1	2:K:437:TRP:CE3	2.35	0.61
3:L:199:ASP:OD1	3:L:201:SER:HB3	1.99	0.61
2:B:365:ARG:HG2	2:B:366:THR:N	2.16	0.61
3:F:209:ILE:O	3:F:213:GLU:HG2	2.00	0.61
3:F:334:TRP:CD1	3:F:335:TRP:N	2.69	0.61
1:G:129:LYS:O	1:G:130:VAL:HG23	1.99	0.61
1:G:166:SER:HB3	2:H:195:THR:O	2.00	0.61
3:I:199:ASP:N	3:I:225:GLU:OE2	2.34	0.61
3:L:298:ASP:O	3:L:301:ASP:HB2	1.99	0.61
3:F:185:ASP:OD2	3:F:187:SER:HB3	2.01	0.61
1:G:125:LYS:O	1:G:125:LYS:HG2	2.00	0.61
2:H:223:GLU:CB	2:H:287:GLY:HA2	2.27	0.61
1:J:149:ARG:NH2	2:K:425:ASP:HA	2.15	0.61
2:K:277:ALA:HB1	2:K:286:CYS:HB3	1.81	0.61
3:L:143:VAL:HA	3:L:220:PRO:HG2	1.82	0.61
2:E:370:HIS:CE1	2:E:408:HIS:HB2	2.35	0.61
3:F:265:PHE:CE2	3:F:267:VAL:HG23	2.36	0.61
3:I:230:ASN:H	3:I:230:ASN:ND2	1.98	0.61
3:I:279:ALA:HB2	3:L:308:ASN:HD21	1.63	0.61
3:L:204:PHE:HB3	3:L:211:TYR:OH	2.00	0.61
2:B:314:MET:HE1	2:B:437:TRP:CG	2.36	0.61
3:C:107:ILE:HD13	3:C:107:ILE:O	2.01	0.61
3:C:295:PHE:H	3:C:301:ASP:HB3	1.65	0.61
2:B:205:VAL:HG23	3:C:216:GLY:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:GLN:CD	3:C:190:GLY:H	2.09	0.61
3:C:272:ASP:O	3:C:273:LYS:HB2	2.01	0.61
2:H:279:ASN:C	2:H:281:ASP:H	2.07	0.61
2:H:411:ASN:N	2:H:436:VAL:O	2.32	0.61
3:I:251:GLU:HG2	3:I:252:ASP:N	2.14	0.61
3:I:264:MET:N	3:I:264:MET:SD	2.73	0.61
3:I:329:GLN:OE1	3:I:361:ASN:HB2	2.01	0.61
2:B:152:TYR:C	2:B:154:ASP:N	2.56	0.60
2:B:173:GLU:C	2:B:175:LEU:H	2.08	0.60
2:B:202:ASN:HA	3:C:143:VAL:HG11	1.82	0.60
3:C:300:SER:C	3:C:302:LYS:N	2.57	0.60
3:C:367:ILE:HG22	3:C:379:MET:CG	2.30	0.60
2:E:191:GLU:CA	2:E:194:ARG:HH21	2.00	0.60
2:E:429:HIS:O	2:E:431:THR:HG23	2.01	0.60
2:H:267:ASP:HB2	2:H:268:PRO:CD	2.29	0.60
2:B:304:ARG:NH2	2:B:333:ASN:N	2.48	0.60
3:C:353:THR:HA	3:C:376:TRP:O	2.01	0.60
3:F:287:GLY:HA3	3:F:371:THR:HB	1.84	0.60
3:F:343:HIS:O	3:F:367:ILE:HA	2.01	0.60
1:G:154:ILE:HD13	2:H:186:VAL:CG2	2.31	0.60
3:I:96:TYR:CD1	3:I:96:TYR:C	2.79	0.60
3:I:167:TYR:N	3:I:167:TYR:CD1	2.69	0.60
2:B:236:TYR:HB2	2:B:298:LYS:HZ3	1.64	0.60
1:D:143:GLN:HE21	3:F:118:ASN:ND2	1.99	0.60
3:F:199:ASP:N	3:F:225:GLU:OE2	2.32	0.60
3:I:336:MET:HE1	3:I:340:HIS:CD2	2.35	0.60
2:K:283:LYS:HB3	2:K:285:TYR:CE2	2.36	0.60
1:A:143:GLN:HA	1:A:143:GLN:NE2	2.11	0.60
3:C:170:LYS:HE2	3:C:177:GLN:HB3	1.84	0.60
1:G:158:ILE:HD11	2:H:189:GLN:HB3	1.83	0.60
3:I:160:GLY:O	3:I:161:ALA:HB3	2.02	0.60
2:K:215:ILE:HA	2:K:219:GLY:O	2.01	0.60
1:A:127:ILE:O	1:A:130:VAL:HG12	2.01	0.60
2:B:181:LYS:C	2:B:183:GLU:H	2.08	0.60
3:C:100:ILE:O	3:C:100:ILE:HG22	2.01	0.60
3:F:231:GLU:O	3:F:234:HIS:HB3	2.02	0.60
2:H:205:VAL:HG12	3:I:232:LYS:HZ3	1.64	0.60
2:H:253:GLN:HA	2:H:292:TYR:O	2.02	0.60
2:H:261:ASP:C	2:H:261:ASP:OD2	2.45	0.60
2:H:412:PRO:O	2:H:413:ASN:HB2	2.01	0.60
3:L:304:PHE:CD1	3:L:338:LYS:HB2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:329:GLN:NE2	4:O:3:ARG:NH1	2.50	0.60
3:C:353:THR:HG23	3:C:377:TYR:CD1	2.37	0.60
2:E:303:THR:HB	2:E:330:THR:HA	1.83	0.60
2:E:397:GLU:HB3	2:E:431:THR:HG21	1.82	0.60
3:F:104:ASP:HA	3:F:107:ILE:HG22	1.84	0.60
2:H:310:LEU:HD12	2:H:310:LEU:C	2.27	0.60
3:L:340:HIS:ND1	3:L:368:ILE:HD11	2.16	0.60
2:B:279:ASN:C	2:B:281:ASP:H	2.08	0.60
2:B:409:ALA:O	2:B:438:MET:HB2	2.01	0.60
3:C:197:ARG:NH2	3:C:348:TYR:HB2	2.16	0.60
2:H:187:SER:O	2:H:191:GLU:HB2	2.02	0.60
3:I:316:ASP:O	3:I:317:ASN:HB2	2.01	0.60
2:K:317:TRP:CH2	2:K:448:ARG:HG3	2.36	0.60
2:K:346:ARG:HG2	2:K:346:ARG:HH11	1.67	0.60
2:K:357:ALA:HB3	2:K:360:LEU:HD12	1.81	0.60
1:A:149:ARG:HH21	2:B:425:ASP:HA	1.67	0.60
2:B:161:ILE:O	2:B:166:ARG:CZ	2.50	0.60
2:B:228:GLN:HG3	2:B:235:PRO:HG3	1.84	0.60
2:B:310:LEU:HD23	2:B:329:PHE:CD2	2.37	0.60
3:C:195:GLN:HE21	3:C:384:MET:HG3	1.65	0.60
3:C:336:MET:HE1	3:C:340:HIS:CD2	2.35	0.60
2:E:352:ALA:CB	2:E:439:ASN:ND2	2.63	0.60
3:I:259:THR:O	3:I:284:GLY:HA3	2.02	0.60
2:K:205:VAL:HG12	2:K:206:VAL:N	2.17	0.60
3:C:214:GLY:HA2	3:C:229:GLY:CA	2.29	0.60
3:C:353:THR:HG23	3:C:377:TYR:HD1	1.65	0.60
2:E:242:MET:HA	2:E:247:GLY:CA	2.32	0.60
3:L:194:PHE:CA	3:L:228:LEU:HD12	2.29	0.60
3:L:246:LEU:HD13	3:L:265:PHE:CE1	2.37	0.60
2:B:204:PRO:HA	3:C:217:HIS:CA	2.29	0.60
2:B:356:GLY:HA2	2:B:368:THR:O	2.00	0.60
3:C:178:PHE:CE2	3:C:228:LEU:HD21	2.35	0.60
3:C:248:VAL:O	3:C:259:THR:HA	2.02	0.60
2:E:215:ILE:HA	2:E:219:GLY:O	2.02	0.60
2:E:327:GLY:HA3	2:E:344:LYS:HE3	1.83	0.60
2:E:331:VAL:HA	2:E:339:GLN:O	2.01	0.60
3:F:199:ASP:OD1	3:F:201:SER:HB3	2.01	0.60
2:H:224:MET:HE2	2:H:237:ARG:HE	1.64	0.60
3:I:172:LEU:HD13	3:I:239:GLN:NE2	2.16	0.60
3:I:178:PHE:CE2	3:I:228:LEU:HD21	2.35	0.60
3:L:199:ASP:N	3:L:225:GLU:OE2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LEU:HB2	2:B:189:GLN:HG2	1.83	0.59
2:B:205:VAL:HG21	3:C:215:PHE:O	2.03	0.59
2:B:280:THR:O	2:B:281:ASP:OD2	2.19	0.59
3:C:293:PHE:CD2	3:C:370:ALA:HB1	2.36	0.59
2:E:205:VAL:HG12	2:E:206:VAL:N	2.17	0.59
1:G:140:VAL:HG23	1:G:141:ARG:N	2.16	0.59
3:I:195:GLN:HE21	3:I:384:MET:HG3	1.65	0.59
3:I:251:GLU:HB3	3:I:381:LYS:HB2	1.84	0.59
1:A:127:ILE:HA	1:A:130:VAL:HG12	1.85	0.59
2:B:210:GLU:HA	2:B:227:ILE:HB	1.84	0.59
2:B:252:ILE:HG12	2:B:452:MET:O	2.03	0.59
1:A:148:LYS:HE3	2:B:425:ASP:HB2	1.83	0.59
2:B:211:CYS:O	2:B:242:MET:HE1	2.03	0.59
3:C:167:TYR:CD1	3:C:167:TYR:N	2.70	0.59
2:E:234:LYS:C	2:E:234:LYS:HD3	2.26	0.59
2:E:294:LEU:O	2:E:295:GLY:C	2.45	0.59
2:H:211:CYS:O	2:H:242:MET:HE1	2.02	0.59
2:H:293:TRP:HE1	2:H:296:ASN:HD21	1.51	0.59
2:B:165:LEU:HD21	3:C:107:ILE:HG12	1.84	0.59
2:B:176:ARG:NH1	2:B:179:ILE:HD12	2.16	0.59
2:B:228:GLN:HE21	2:B:231:SER:HA	1.67	0.59
2:E:179:ILE:O	2:E:183:GLU:HG3	2.02	0.59
2:E:277:ALA:HB1	2:E:286:CYS:HB3	1.84	0.59
3:F:195:GLN:OE1	3:F:382:THR:HG22	2.03	0.59
2:H:356:GLY:HA2	2:H:368:THR:O	2.01	0.59
3:I:178:PHE:CE2	3:I:228:LEU:HD11	2.37	0.59
3:I:331:GLY:O	3:I:332:SER:HB3	2.03	0.59
3:I:367:ILE:HG21	3:I:379:MET:HB2	1.85	0.59
2:K:325:HIS:HB3	2:K:346:ARG:HB3	1.85	0.59
3:L:95:LYS:HG2	3:L:98:ALA:HB3	1.83	0.59
3:L:195:GLN:OE1	3:L:382:THR:HG22	2.03	0.59
3:L:265:PHE:CE2	3:L:267:VAL:HG23	2.38	0.59
3:C:293:PHE:CE2	3:C:370:ALA:HB1	2.38	0.59
3:C:334:TRP:HZ3	3:C:344:LEU:HB2	1.68	0.59
2:H:359:GLN:NE2	2:H:359:GLN:N	2.48	0.59
2:H:373:MET:CG	2:H:405:ASN:HB2	2.32	0.59
2:H:409:ALA:O	2:H:438:MET:HB2	2.02	0.59
3:I:117:ASN:N	3:I:117:ASN:HD22	1.99	0.59
3:I:168:PHE:CE1	3:I:179:LEU:HD13	2.37	0.59
3:I:251:GLU:OE1	3:I:381:LYS:HD2	2.02	0.59
3:I:367:ILE:HG22	3:I:379:MET:CG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:322:PHE:CZ	4:T:3:ARG:HD2	2.37	0.59
2:B:161:ILE:HG22	2:B:162:PRO:HD3	1.84	0.59
3:C:96:TYR:CD1	3:C:96:TYR:C	2.80	0.59
3:C:141:ASP:OD2	3:C:143:VAL:HG22	2.02	0.59
3:I:278:TYR:CZ	3:I:308:ASN:HB2	2.37	0.59
3:I:368:ILE:HG21	3:I:375:ARG:C	2.28	0.59
2:K:301:GLN:NE2	2:K:302:LEU:N	2.51	0.59
1:A:149:ARG:HG2	2:B:426:MET:C	2.27	0.59
2:B:152:TYR:O	2:B:154:ASP:N	2.36	0.59
2:B:266:TRP:HE1	2:B:380:ARG:HH21	1.48	0.59
2:E:215:ILE:CG2	2:E:216:ARG:N	2.65	0.59
3:I:214:GLY:HA2	3:I:229:GLY:CA	2.30	0.59
3:I:353:THR:HA	3:I:376:TRP:O	2.03	0.59
1:J:124:ARG:HG2	1:J:124:ARG:HH11	1.68	0.59
2:K:209:LYS:HG3	2:K:213:GLU:OE1	2.01	0.59
2:K:429:HIS:O	2:K:431:THR:HG23	2.01	0.59
3:L:343:HIS:O	3:L:367:ILE:HA	2.02	0.59
4:N:3:ARG:HG2	4:N:3:ARG:HH21	1.67	0.59
2:B:365:ARG:O	2:B:368:THR:HG23	2.02	0.59
3:C:169:ILE:CD1	3:C:171:PRO:HD3	2.32	0.59
3:C:368:ILE:HG21	3:C:375:ARG:C	2.28	0.59
3:F:246:LEU:HD22	3:F:265:PHE:CD1	2.38	0.59
1:G:139:ASN:HB3	3:I:114:TYR:CZ	2.37	0.59
2:H:373:MET:SD	2:H:405:ASN:HB2	2.42	0.59
3:I:103:HIS:HA	3:I:106:SER:CB	2.29	0.59
3:I:272:ASP:CG	3:I:275:ARG:HE	2.10	0.59
3:L:92:GLU:HG2	3:L:93:ILE:N	2.17	0.59
1:A:190:ALA:O	1:A:191:LYS:HG3	2.02	0.59
3:C:198:LEU:HD22	3:C:223:THR:HG23	1.85	0.59
3:C:329:GLN:OE1	3:C:361:ASN:HB2	2.02	0.59
3:C:373:LYS:CG	3:C:379:MET:HE1	2.32	0.59
3:F:96:TYR:C	3:F:98:ALA:H	2.11	0.59
3:F:246:LEU:HD13	3:F:265:PHE:CE1	2.38	0.59
3:F:344:LEU:HD22	3:F:382:THR:OG1	2.03	0.59
2:H:177:SER:O	2:H:180:GLN:HB2	2.02	0.59
2:H:280:THR:O	2:H:281:ASP:OD2	2.20	0.59
2:K:164:ASN:O	2:K:168:LEU:HD23	2.02	0.59
2:K:356:GLY:HA3	2:K:368:THR:OG1	2.01	0.59
3:L:251:GLU:OE1	3:L:381:LYS:HD2	2.02	0.59
2:B:340:ILE:HG23	2:B:340:ILE:O	2.03	0.59
2:E:160:ASN:H	2:E:162:PRO:HD2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:266:TRP:NE1	2:H:380:ARG:HH21	2.00	0.59
2:H:374:PHE:HB3	2:H:382:ASN:HB3	1.85	0.59
1:J:151:GLU:HG3	1:J:178:TYR:OH	2.03	0.59
2:K:191:GLU:C	2:K:193:CYS:H	2.11	0.59
2:B:180:GLN:HA	2:B:183:GLU:OE1	2.02	0.58
2:E:240:CYS:HB3	2:E:242:MET:HE2	1.85	0.58
2:K:315:GLU:OE2	2:K:448:ARG:NH2	2.35	0.58
2:B:251:VAL:O	2:B:252:ILE:HD13	2.03	0.58
2:E:202:ASN:ND2	2:E:284:ASN:HB2	2.18	0.58
2:H:171:ILE:HA	2:H:174:ASN:HB2	1.85	0.58
2:K:303:THR:HB	2:K:330:THR:HG22	1.84	0.58
2:B:176:ARG:HH11	2:B:176:ARG:CA	2.16	0.58
2:B:209:LYS:HZ2	2:B:209:LYS:HB3	1.65	0.58
2:B:218:GLY:CA	3:C:210:GLN:HE21	2.16	0.58
2:B:263:GLY:HA2	2:B:400:GLY:HA2	1.84	0.58
2:B:365:ARG:O	2:B:367:MET:N	2.37	0.58
3:F:251:GLU:OE1	3:F:381:LYS:HD2	2.03	0.58
3:F:270:GLU:HB2	3:F:274:TYR:CZ	2.37	0.58
3:I:181:TYR:CG	3:I:181:TYR:O	2.55	0.58
3:I:329:GLN:HE22	3:I:363:TYR:HB2	1.69	0.58
2:K:405:ASN:C	2:K:407:CYS:N	2.56	0.58
1:A:119:ILE:O	1:A:119:ILE:HG12	2.02	0.58
1:A:134:GLN:HA	1:A:137:GLN:OE1	2.03	0.58
1:D:127:ILE:HG23	1:D:128:GLU:H	1.67	0.58
2:E:303:THR:HB	2:E:330:THR:HG22	1.84	0.58
3:L:246:LEU:HD13	3:L:265:PHE:CD1	2.39	0.58
1:A:128:GLU:OE1	1:A:129:LYS:HD3	2.02	0.58
2:H:420:GLY:HA2	2:H:446:SER:O	2.03	0.58
3:I:198:LEU:HD22	3:I:223:THR:HG23	1.86	0.58
2:K:199:VAL:O	3:L:142:THR:HG23	2.03	0.58
3:L:231:GLU:O	3:L:234:HIS:HB3	2.03	0.58
3:I:312:PHE:CE1	3:I:334:TRP:HA	2.38	0.58
2:K:212:GLU:HG3	2:K:212:GLU:O	2.03	0.58
2:K:331:VAL:HA	2:K:339:GLN:O	2.02	0.58
1:A:140:VAL:HG23	1:A:141:ARG:H	1.67	0.58
2:B:412:PRO:HB3	2:B:450:MET:HG2	1.86	0.58
3:C:259:THR:O	3:C:284:GLY:HA3	2.04	0.58
3:C:334:TRP:O	3:C:336:MET:N	2.37	0.58
1:D:131:GLN:C	1:D:133:ILE:N	2.60	0.58
1:D:137:GLN:OE1	1:D:189:ILE:HA	2.03	0.58
3:F:93:ILE:O	3:F:95:LYS:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:236:ILE:O	3:F:239:GLN:HG2	2.03	0.58
3:I:97:GLU:C	3:I:99:SER:N	2.61	0.58
3:I:242:ILE:HD12	3:I:242:ILE:N	2.18	0.58
1:J:181:GLN:HE22	2:K:174:ASN:CB	2.17	0.58
3:L:154:GLN:HA	3:L:190:GLY:HA3	1.85	0.58
3:L:194:PHE:CZ	3:L:384:MET:HE3	2.39	0.58
2:B:223:GLU:CB	2:B:287:GLY:HA2	2.28	0.58
3:C:99:SER:C	3:C:101:LEU:N	2.62	0.58
3:C:170:LYS:NZ	3:C:177:GLN:H	2.02	0.58
3:C:316:ASP:O	3:C:317:ASN:HB2	2.02	0.58
3:F:117:ASN:O	3:F:121:ILE:HG13	2.03	0.58
3:F:154:GLN:HA	3:F:190:GLY:HA3	1.85	0.58
3:F:304:PHE:CD1	3:F:338:LYS:HB3	2.39	0.58
2:H:202:ASN:HD22	2:H:284:ASN:CB	2.15	0.58
3:I:272:ASP:OD2	3:I:275:ARG:NE	2.36	0.58
1:J:134:GLN:OE1	1:J:137:GLN:HB2	2.04	0.58
1:J:139:ASN:HB3	3:L:114:TYR:CZ	2.39	0.58
2:K:172:LEU:HB3	3:L:113:ILE:HG21	1.85	0.58
2:K:191:GLU:O	2:K:193:CYS:N	2.37	0.58
2:K:356:GLY:HA2	2:K:409:ALA:CB	2.33	0.58
2:B:161:ILE:HG21	3:C:103:HIS:NE2	2.19	0.58
2:B:345:TYR:CZ	2:B:351:ASN:HB2	2.38	0.58
3:C:97:GLU:C	3:C:99:SER:N	2.61	0.58
3:F:251:GLU:CD	3:F:381:LYS:HD2	2.28	0.58
1:G:131:GLN:C	1:G:133:ILE:H	2.12	0.58
3:I:132:GLU:C	3:I:134:GLN:H	2.11	0.58
3:I:295:PHE:H	3:I:301:ASP:HB3	1.67	0.58
1:J:115:LEU:C	1:J:115:LEU:HD13	2.29	0.58
2:K:240:CYS:HB3	2:K:242:MET:HE2	1.86	0.58
2:K:270:LYS:O	2:K:270:LYS:HG2	2.04	0.58
2:B:171:ILE:O	2:B:175:LEU:HB3	2.03	0.58
2:B:337:LYS:HG3	2:B:374:PHE:CD2	2.38	0.58
2:B:412:PRO:O	2:B:413:ASN:HB2	2.03	0.58
3:C:126:GLU:C	3:C:128:VAL:H	2.10	0.58
3:F:250:LEU:HD21	3:F:369:TRP:CD1	2.39	0.58
1:G:130:VAL:HA	1:G:133:ILE:HB	1.85	0.58
1:G:174:ASP:OD1	1:G:177:ASP:HB2	2.03	0.58
2:H:455:ARG:HG3	2:H:456:PRO:HD2	1.85	0.58
3:I:246:LEU:HD11	3:I:248:VAL:HG23	1.85	0.58
3:L:307:HIS:O	3:L:308:ASN:C	2.45	0.58
3:L:334:TRP:CD1	3:L:335:TRP:H	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:141:ASP:OD2	3:I:143:VAL:HG22	2.03	0.57
3:I:293:PHE:CE2	3:I:370:ALA:HB1	2.40	0.57
3:L:276:LEU:HD21	3:L:278:TYR:HD2	1.69	0.57
1:A:140:VAL:CG2	1:A:141:ARG:N	2.68	0.57
2:B:303:THR:HA	2:B:308:THR:HG21	1.85	0.57
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.50	0.57
2:E:247:GLY:O	2:E:455:ARG:NH1	2.36	0.57
2:H:337:LYS:HG3	2:H:374:PHE:CD2	2.38	0.57
3:I:128:VAL:O	3:I:129:ALA:C	2.47	0.57
3:L:246:LEU:HD22	3:L:265:PHE:CD1	2.40	0.57
3:C:230:ASN:HD22	3:C:230:ASN:H	1.48	0.57
3:C:329:GLN:HE22	3:C:363:TYR:HB2	1.69	0.57
2:H:204:PRO:HA	3:I:217:HIS:CA	2.32	0.57
2:K:234:LYS:HD3	2:K:235:PRO:N	2.19	0.57
2:K:267:ASP:HB3	2:K:268:PRO:HD3	1.85	0.57
1:A:158:ILE:CG1	2:B:189:GLN:HG3	2.35	0.57
1:A:189:ILE:O	1:A:190:ALA:HB3	2.04	0.57
2:B:224:MET:CE	2:B:237:ARG:HE	2.17	0.57
3:C:181:TYR:CG	3:C:181:TYR:O	2.56	0.57
3:C:352:GLY:HA2	3:C:378:SER:HB3	1.85	0.57
3:I:151:LYS:HD2	3:I:172:LEU:HD11	1.87	0.57
3:I:170:LYS:HE2	3:I:177:GLN:HB3	1.87	0.57
3:I:248:VAL:O	3:I:259:THR:HA	2.04	0.57
3:I:293:PHE:CD2	3:I:370:ALA:HB1	2.39	0.57
2:K:169:ARG:HG2	2:K:173:GLU:OE2	2.04	0.57
2:K:355:ASP:O	2:K:365:ARG:NH1	2.37	0.57
2:K:455:ARG:HG3	2:K:456:PRO:HD2	1.86	0.57
2:B:172:LEU:HD21	3:C:114:TYR:HB2	1.87	0.57
1:D:149:ARG:NH2	2:E:425:ASP:HA	2.19	0.57
5:E:470:NAG:O6	4:N:4:PRO:HG3	2.05	0.57
3:F:204:PHE:HB3	3:F:211:TYR:OH	2.03	0.57
3:F:295:PHE:HE2	4:P:2:HYP:HD23	1.69	0.57
1:G:159:ARG:NH1	2:H:418:TRP:CE3	2.73	0.57
2:H:202:ASN:ND2	2:H:284:ASN:HB3	2.17	0.57
2:H:228:GLN:HG3	2:H:235:PRO:HG3	1.87	0.57
2:H:340:ILE:HG12	2:H:342:VAL:HG13	1.87	0.57
1:J:116:ARG:O	1:J:120:GLU:HG3	2.05	0.57
1:J:156:ILE:HG21	2:K:415:ARG:HH11	1.68	0.57
3:L:204:PHE:O	3:L:211:TYR:HE2	1.87	0.57
3:L:340:HIS:CE1	3:L:368:ILE:HD11	2.40	0.57
1:A:167:ARG:HH12	1:A:169:LEU:HD22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:ILE:HG23	2:B:166:ARG:HH22	1.69	0.57
2:B:402:TRP:HB3	2:B:404:TYR:CE1	2.40	0.57
3:C:92:GLU:O	3:C:95:LYS:HE3	2.03	0.57
2:E:203:ILE:H	2:E:203:ILE:CD1	2.18	0.57
2:E:301:GLN:NE2	2:E:302:LEU:N	2.53	0.57
3:L:299:PRO:O	3:L:301:ASP:N	2.35	0.57
2:E:255:ARG:HG3	2:E:255:ARG:NH1	2.20	0.57
3:I:220:PRO:HG2	3:I:221:THR:H	1.70	0.57
3:I:334:TRP:O	3:I:336:MET:N	2.38	0.57
3:I:334:TRP:HZ3	3:I:344:LEU:HB2	1.69	0.57
2:K:158:ASN:HD21	3:L:100:ILE:HD12	1.70	0.57
2:B:213:GLU:O	2:B:217:LYS:HG3	2.05	0.57
2:B:340:ILE:HG12	2:B:342:VAL:HG13	1.87	0.57
2:B:415:ARG:N	2:B:434:GLY:HA2	2.15	0.57
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.86	0.57
3:C:251:GLU:OE1	3:C:381:LYS:HD2	2.04	0.57
3:C:284:GLY:C	3:C:286:ALA:H	2.11	0.57
3:F:307:HIS:O	3:F:308:ASN:C	2.46	0.57
1:G:168:ALA:HA	2:H:189:GLN:OE1	2.04	0.57
3:I:274:TYR:O	3:I:335:TRP:NE1	2.37	0.57
3:I:284:GLY:C	3:I:286:ALA:H	2.11	0.57
1:J:149:ARG:O	1:J:152:VAL:HG22	2.05	0.57
1:A:158:ILE:HD13	1:A:171:ARG:HE	1.70	0.57
1:A:169:LEU:HD13	1:A:170:ALA:N	2.20	0.57
3:I:195:GLN:HE22	3:I:382:THR:HG22	1.69	0.57
1:J:185:LEU:HD22	1:J:189:ILE:HG13	1.86	0.57
2:K:201:CYS:O	3:L:143:VAL:HG21	2.05	0.57
3:C:315:TRP:CE3	3:C:328:GLU:HG2	2.39	0.57
1:D:169:LEU:HD13	2:E:185:ASP:OD1	2.05	0.57
2:E:265:LYS:O	2:E:268:PRO:HD2	2.05	0.57
2:E:356:GLY:HA3	2:E:368:THR:OG1	2.04	0.57
3:I:170:LYS:NZ	3:I:177:GLN:H	2.03	0.57
3:I:337:ASN:C	3:I:339:CYS:N	2.57	0.57
3:L:197:ARG:C	3:L:198:LEU:HD12	2.30	0.57
2:B:199:VAL:N	3:C:140:LYS:O	2.38	0.56
3:C:367:ILE:HG21	3:C:379:MET:HB2	1.87	0.56
3:F:204:PHE:O	3:F:211:TYR:HE2	1.88	0.56
2:H:205:VAL:HG23	3:I:216:GLY:O	2.05	0.56
3:I:304:PHE:C	3:I:306:SER:H	2.11	0.56
1:A:155:ASP:O	1:A:158:ILE:HG22	2.05	0.56
2:B:158:ASN:ND2	3:C:100:ILE:HD13	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:LYS:NZ	2:B:209:LYS:CB	2.68	0.56
3:C:94:MET:C	3:C:96:TYR:N	2.62	0.56
3:C:193:VAL:HG22	3:C:385:LYS:HB3	1.87	0.56
3:C:199:ASP:N	3:C:225:GLU:OE2	2.37	0.56
1:G:186:GLU:HA	1:G:189:ILE:HG22	1.87	0.56
2:H:410:ALA:HB1	2:H:437:TRP:CE3	2.39	0.56
1:J:154:ILE:HD12	2:K:182:LEU:HD13	1.88	0.56
2:K:255:ARG:HG3	2:K:255:ARG:NH1	2.20	0.56
2:B:176:ARG:HH12	2:B:179:ILE:CD1	2.18	0.56
2:B:233:VAL:HG22	2:B:234:LYS:N	2.20	0.56
2:B:410:ALA:HB1	2:B:437:TRP:CE3	2.39	0.56
3:C:153:CYS:HB2	3:C:192:THR:HG22	1.86	0.56
2:E:210:GLU:HA	2:E:227:ILE:CG2	2.35	0.56
2:E:351:ASN:HD21	2:E:354:MET:HB2	1.70	0.56
3:F:143:VAL:O	3:F:143:VAL:HG23	2.05	0.56
3:F:194:PHE:CD2	3:F:384:MET:O	2.58	0.56
3:F:196:LYS:HG2	3:F:198:LEU:CD1	2.36	0.56
3:F:367:ILE:O	3:F:378:SER:HA	2.05	0.56
2:H:310:LEU:HD23	2:H:329:PHE:CD2	2.41	0.56
3:I:97:GLU:O	3:I:99:SER:N	2.38	0.56
3:I:134:GLN:C	3:I:136:GLN:H	2.13	0.56
1:J:151:GLU:HG3	1:J:178:TYR:CE2	2.41	0.56
1:J:157:LYS:HE2	1:J:157:LYS:CA	2.28	0.56
2:K:210:GLU:HA	2:K:227:ILE:CG2	2.35	0.56
2:K:294:LEU:O	2:K:295:GLY:C	2.46	0.56
2:K:359:GLN:O	2:K:360:LEU:HD23	2.05	0.56
3:L:289:ALA:HB3	3:L:369:TRP:CZ2	2.40	0.56
3:C:169:ILE:O	3:C:177:GLN:HB2	2.05	0.56
2:E:356:GLY:HA2	2:E:409:ALA:CB	2.35	0.56
1:D:127:ILE:HG23	1:D:128:GLU:N	2.20	0.56
3:F:104:ASP:CA	3:F:107:ILE:HG22	2.35	0.56
3:F:278:TYR:CE2	3:F:308:ASN:HB2	2.40	0.56
2:H:218:GLY:CA	3:I:210:GLN:HE21	2.19	0.56
1:J:116:ARG:H	1:J:116:ARG:CD	2.17	0.56
2:K:280:THR:O	2:K:281:ASP:C	2.49	0.56
2:K:352:ALA:CB	2:K:439:ASN:ND2	2.62	0.56
3:C:227:TRP:CD1	3:C:229:GLY:HA2	2.40	0.56
1:D:144:LEU:HD22	1:D:182:GLN:CG	2.36	0.56
3:I:169:ILE:HD11	3:I:178:PHE:CE1	2.41	0.56
3:I:390:ASN:O	3:I:391:ARG:HD2	2.06	0.56
1:G:128:GLU:O	1:G:133:ILE:HD13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:173:GLU:C	2:H:175:LEU:N	2.62	0.56
2:H:402:TRP:HB3	2:H:404:TYR:CE1	2.41	0.56
3:I:297:ASP:HB2	3:I:301:ASP:CG	2.31	0.56
3:L:196:LYS:HG2	3:L:198:LEU:CD1	2.36	0.56
1:A:174:ASP:OD2	1:A:177:ASP:HB2	2.06	0.56
2:B:176:ARG:HA	2:B:176:ARG:HH11	1.70	0.56
3:C:242:ILE:N	3:C:242:ILE:HD12	2.21	0.56
3:C:304:PHE:C	3:C:306:SER:H	2.12	0.56
3:C:322:PHE:CD2	3:C:324:GLY:N	2.74	0.56
2:E:198:THR:HG22	3:F:140:LYS:O	2.06	0.56
2:E:406:ARG:NH2	4:N:4:PRO:O	2.39	0.56
1:G:144:LEU:HD13	1:G:182:GLN:HA	1.88	0.56
2:B:310:LEU:HB3	2:B:329:PHE:CD2	2.41	0.56
2:B:359:GLN:H	2:B:359:GLN:HE21	1.50	0.56
2:B:411:ASN:ND2	2:B:434:GLY:H	2.04	0.56
3:C:312:PHE:CZ	3:C:333:GLY:O	2.59	0.56
3:I:304:PHE:CG	3:I:338:LYS:HB3	2.41	0.56
3:L:278:TYR:CE2	3:L:308:ASN:HB2	2.40	0.56
1:A:133:ILE:HD13	2:B:164:ASN:HD22	1.69	0.56
2:B:168:LEU:C	3:C:110:LEU:HD11	2.31	0.56
3:C:246:LEU:HD12	3:C:247:ARG:H	1.70	0.56
3:C:367:ILE:O	3:C:367:ILE:HG22	2.06	0.56
2:H:173:GLU:O	2:H:175:LEU:N	2.36	0.56
2:H:362:GLY:O	2:H:365:ARG:N	2.39	0.56
2:K:156:THR:O	2:K:158:ASN:N	2.39	0.56
2:K:311:LEU:HD22	2:K:325:HIS:CD2	2.40	0.56
3:L:209:ILE:O	3:L:213:GLU:HG2	2.05	0.56
3:L:267:VAL:HA	3:L:275:ARG:O	2.06	0.56
3:C:149:THR:C	3:C:156:ILE:HG12	2.32	0.55
3:C:251:GLU:HG2	3:C:252:ASP:N	2.19	0.55
2:E:280:THR:O	2:E:281:ASP:C	2.49	0.55
2:H:176:ARG:HH11	2:H:176:ARG:HG2	1.69	0.55
3:I:195:GLN:O	3:I:196:LYS:HB3	2.06	0.55
2:K:265:LYS:O	2:K:268:PRO:HD2	2.06	0.55
3:L:194:PHE:CD2	3:L:384:MET:O	2.59	0.55
2:B:155:GLU:C	2:B:157:VAL:N	2.63	0.55
2:B:173:GLU:O	2:B:176:ARG:N	2.39	0.55
2:B:229:PRO:HG2	2:B:233:VAL:HG11	1.87	0.55
3:F:196:LYS:O	3:F:197:ARG:HD2	2.05	0.55
1:G:129:LYS:HA	1:G:133:ILE:CD1	2.35	0.55
3:I:169:ILE:O	3:I:177:GLN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:407:CYS:HB2	4:R:1:GLY:O	2.06	0.55
3:L:172:LEU:HD22	3:L:240:SER:OG	2.06	0.55
2:B:155:GLU:C	2:B:157:VAL:H	2.14	0.55
2:B:309:GLU:HG3	2:B:309:GLU:O	2.06	0.55
3:C:224:THR:HG23	3:C:224:THR:O	2.05	0.55
2:E:366:THR:HA	2:E:369:ILE:CD1	2.36	0.55
2:E:408:HIS:C	2:E:408:HIS:CD2	2.84	0.55
3:F:276:LEU:HD11	3:F:290:PHE:CE2	2.42	0.55
2:H:175:LEU:O	2:H:179:ILE:HG13	2.07	0.55
3:I:172:LEU:CD1	3:I:239:GLN:HE21	2.17	0.55
2:B:258:GLY:O	2:B:260:VAL:N	2.37	0.55
2:B:351:ASN:ND2	2:B:354:MET:H	2.04	0.55
2:E:234:LYS:HD3	2:E:235:PRO:N	2.21	0.55
3:F:246:LEU:HD13	3:F:265:PHE:CD1	2.42	0.55
2:K:203:ILE:H	2:K:203:ILE:CD1	2.19	0.55
3:L:108:ARG:O	3:L:112:GLU:HG3	2.06	0.55
2:B:173:GLU:HA	2:B:176:ARG:HB3	1.88	0.55
3:C:318:ASP:OD2	3:C:325:ASN:HB2	2.06	0.55
3:C:331:GLY:O	3:C:332:SER:HB3	2.04	0.55
2:E:394:CYS:O	2:E:397:GLU:O	2.25	0.55
3:F:109:TYR:CD1	3:F:110:LEU:HD23	2.41	0.55
3:F:169:ILE:HD11	3:F:236:ILE:HD11	1.88	0.55
3:I:166:LEU:C	3:I:167:TYR:CD1	2.84	0.55
3:I:288:ASP:OD2	3:I:291:ASP:HB2	2.06	0.55
2:K:332:GLN:HB3	2:K:336:ASN:HB2	1.88	0.55
3:L:228:LEU:O	3:L:232:LYS:HD2	2.06	0.55
2:B:373:MET:CG	2:B:405:ASN:HB2	2.36	0.55
3:C:312:PHE:CE1	3:C:334:TRP:HA	2.41	0.55
3:F:267:VAL:HA	3:F:275:ARG:O	2.07	0.55
2:H:156:THR:HG22	2:H:160:ASN:HD22	1.72	0.55
2:H:178:LYS:C	2:H:180:GLN:N	2.64	0.55
2:H:209:LYS:NZ	2:H:209:LYS:CB	2.70	0.55
2:H:256:GLN:NE2	2:H:449:LYS:HZ1	1.95	0.55
2:H:312:ILE:HG12	2:H:452:MET:HG2	1.89	0.55
2:H:340:ILE:HD12	2:H:403:TRP:CE3	2.42	0.55
3:I:126:GLU:O	3:I:129:ALA:HB3	2.07	0.55
3:I:276:LEU:HD12	3:I:276:LEU:O	2.07	0.55
3:L:270:GLU:HB2	3:L:274:TYR:CZ	2.40	0.55
1:A:163:GLY:O	3:C:138:PRO:HA	2.07	0.55
2:B:176:ARG:HH11	2:B:176:ARG:CG	2.19	0.55
3:C:274:TYR:O	3:C:335:TRP:NE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:ASN:HB3	3:F:114:TYR:CZ	2.42	0.55
2:E:340:ILE:HG12	2:E:341:SER:N	2.21	0.55
2:E:360:LEU:O	2:E:365:ARG:HD2	2.07	0.55
2:E:404:TYR:O	2:E:405:ASN:HB2	2.05	0.55
3:F:212:LYS:HG3	3:F:231:GLU:HB2	1.88	0.55
3:L:287:GLY:HA3	3:L:371:THR:HB	1.89	0.55
3:L:344:LEU:HA	3:L:367:ILE:HG23	1.88	0.55
2:B:374:PHE:HB3	2:B:382:ASN:HB3	1.89	0.55
3:C:195:GLN:HE22	3:C:382:THR:HG22	1.71	0.55
3:C:256:ARG:HG3	3:C:256:ARG:NH1	2.22	0.55
3:F:211:TYR:HE1	3:F:345:ASN:ND2	2.05	0.55
2:H:151:LEU:HD23	2:H:152:TYR:N	2.21	0.55
2:H:190:MET:SD	2:H:190:MET:O	2.64	0.55
2:H:233:VAL:HG22	2:H:234:LYS:N	2.22	0.55
2:K:215:ILE:HD12	2:K:248:GLY:N	2.21	0.55
2:K:415:ARG:O	2:K:434:GLY:HA2	2.06	0.55
2:B:176:ARG:HA	2:B:179:ILE:CD1	2.23	0.55
2:B:369:ILE:O	2:B:405:ASN:HB3	2.06	0.55
3:C:219:SER:CB	3:C:224:THR:HG21	2.36	0.55
3:C:279:ALA:HB2	3:F:308:ASN:HD21	1.71	0.55
2:E:199:VAL:O	3:F:142:THR:HG23	2.06	0.55
2:E:374:PHE:HB2	2:E:382:ASN:HB3	1.88	0.55
2:H:199:VAL:HG23	3:I:141:ASP:OD1	2.07	0.55
2:H:301:GLN:HE21	2:H:302:LEU:N	2.04	0.55
2:H:373:MET:HE3	2:H:374:PHE:N	2.12	0.55
2:H:411:ASN:ND2	2:H:434:GLY:H	2.05	0.55
3:I:326:CYS:O	3:I:327:ALA:C	2.49	0.55
1:J:152:VAL:HG23	1:J:153:ASP:N	2.21	0.55
2:B:175:LEU:HD13	2:B:179:ILE:HD11	1.87	0.55
2:B:261:ASP:C	2:B:261:ASP:OD2	2.50	0.55
2:B:266:TRP:NE1	2:B:380:ARG:HH21	2.04	0.55
3:C:189:ASN:HB3	3:C:387:ILE:HD11	1.89	0.55
3:C:221:THR:HG23	3:C:222:GLY:N	2.12	0.55
2:H:369:ILE:O	2:H:405:ASN:HB3	2.07	0.55
3:I:219:SER:CB	3:I:224:THR:HG21	2.36	0.55
3:I:237:SER:OG	3:I:266:LYS:HA	2.07	0.55
3:I:372:TRP:CE3	3:I:373:LYS:HE3	2.42	0.55
3:L:113:ILE:O	3:L:114:TYR:C	2.50	0.55
1:A:180:ASP:C	1:A:182:GLN:N	2.64	0.54
3:C:96:TYR:O	3:C:99:SER:N	2.35	0.54
3:F:185:ASP:C	3:F:187:SER:H	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:196:LYS:HA	3:F:382:THR:O	2.07	0.54
3:F:299:PRO:O	3:F:301:ASP:N	2.37	0.54
3:F:372:TRP:HZ3	3:F:379:MET:CE	2.20	0.54
2:H:365:ARG:O	2:H:367:MET:N	2.41	0.54
3:I:193:VAL:HG22	3:I:385:LYS:HB3	1.87	0.54
2:K:255:ARG:HG3	2:K:255:ARG:HH11	1.72	0.54
2:B:293:TRP:HE1	2:B:296:ASN:HD21	1.56	0.54
2:E:189:GLN:O	2:E:193:CYS:SG	2.65	0.54
2:E:325:HIS:HB3	2:E:346:ARG:HB3	1.89	0.54
3:F:96:TYR:HD1	3:F:97:GLU:N	2.03	0.54
3:I:252:ASP:OD2	3:I:254:ASN:HB2	2.06	0.54
1:J:131:GLN:HE21	1:J:132:HIS:H	1.55	0.54
3:L:205:LYS:HZ3	3:L:315:TRP:CG	2.24	0.54
1:D:133:ILE:C	1:D:135:LEU:N	2.64	0.54
1:D:137:GLN:HE21	2:E:164:ASN:HD21	1.54	0.54
2:E:169:ARG:O	2:E:173:GLU:HG3	2.07	0.54
1:G:180:ASP:O	1:G:183:LYS:HB3	2.06	0.54
3:I:189:ASN:HB3	3:I:387:ILE:HD11	1.89	0.54
3:I:315:TRP:CE3	3:I:328:GLU:HG2	2.41	0.54
3:I:322:PHE:CD2	3:I:324:GLY:N	2.76	0.54
3:I:389:PHE:O	3:I:391:ARG:N	2.36	0.54
3:L:252:ASP:C	3:L:254:ASN:H	2.15	0.54
3:L:288:ASP:OD2	3:L:291:ASP:HB2	2.07	0.54
1:A:163:GLY:CA	2:B:275:ASN:HD21	2.21	0.54
2:B:359:GLN:NE2	2:B:359:GLN:N	2.53	0.54
2:B:424:TRP:C	2:B:426:MET:H	2.16	0.54
3:C:389:PHE:O	3:C:391:ARG:N	2.35	0.54
1:D:185:LEU:HD22	1:D:189:ILE:CG1	2.36	0.54
3:F:205:LYS:HZ3	3:F:315:TRP:CG	2.24	0.54
2:H:301:GLN:NE2	2:H:302:LEU:N	2.55	0.54
2:H:351:ASN:ND2	2:H:354:MET:H	2.04	0.54
1:J:137:GLN:HB3	1:J:189:ILE:HG12	1.88	0.54
2:K:158:ASN:HD21	3:L:100:ILE:CD1	2.20	0.54
2:B:175:LEU:O	2:B:175:LEU:HD22	2.08	0.54
2:B:266:TRP:HE1	2:B:380:ARG:CZ	2.21	0.54
3:C:275:ARG:HB2	3:C:311:GLN:CA	2.34	0.54
3:F:223:THR:O	3:F:223:THR:HG22	2.08	0.54
2:H:252:ILE:HG12	2:H:452:MET:O	2.08	0.54
3:L:307:HIS:O	3:L:310:MET:HG2	2.08	0.54
1:A:157:LYS:NZ	3:C:132:GLU:HB2	2.23	0.54
2:B:176:ARG:HH12	2:B:179:ILE:HD12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:254:ASN:O	2:E:291:GLU:HA	2.07	0.54
2:E:332:GLN:HB3	2:E:336:ASN:HB2	1.89	0.54
1:G:128:GLU:HA	1:G:131:GLN:CB	2.34	0.54
2:H:199:VAL:N	3:I:140:LYS:O	2.41	0.54
3:I:276:LEU:HD11	3:I:309:GLY:H	1.72	0.54
3:I:312:PHE:CZ	3:I:333:GLY:O	2.61	0.54
3:I:359:THR:HB	3:I:362:GLY:C	2.32	0.54
2:K:167:VAL:HG23	2:K:168:LEU:HD22	1.90	0.54
2:K:303:THR:HB	2:K:330:THR:HA	1.88	0.54
1:A:150:LEU:HD12	1:A:150:LEU:C	2.30	0.54
2:B:237:ARG:HH22	3:C:143:VAL:HG21	1.73	0.54
2:B:265:LYS:HB3	2:B:379:ASP:CG	2.33	0.54
3:C:166:LEU:C	3:C:167:TYR:CD1	2.86	0.54
3:C:237:SER:OG	3:C:266:LYS:HA	2.07	0.54
3:C:248:VAL:HB	3:C:260:ALA:HB3	1.90	0.54
2:E:166:ARG:HD3	2:E:167:VAL:N	2.22	0.54
2:E:266:TRP:N	2:E:379:ASP:OD1	2.38	0.54
2:H:168:LEU:HB3	3:I:110:LEU:CD1	2.38	0.54
2:H:337:LYS:HB3	2:H:382:ASN:OD1	2.08	0.54
3:I:149:THR:C	3:I:156:ILE:HG12	2.33	0.54
3:I:352:GLY:HA2	3:I:378:SER:HB3	1.88	0.54
3:I:367:ILE:HG22	3:I:379:MET:HG2	1.90	0.54
2:B:180:GLN:HA	2:B:180:GLN:NE2	2.22	0.54
1:D:181:GLN:HE22	2:E:174:ASN:CB	2.21	0.54
2:E:333:ASN:OD1	2:E:334:GLU:N	2.41	0.54
5:E:470:NAG:H62	4:N:4:PRO:HG3	1.89	0.54
3:F:288:ASP:OD2	3:F:291:ASP:HB2	2.07	0.54
3:F:330:ASP:HB3	3:F:343:HIS:HE1	1.72	0.54
1:G:130:VAL:H	1:G:133:ILE:HD13	1.72	0.54
2:H:351:ASN:C	2:H:351:ASN:ND2	2.62	0.54
3:L:211:TYR:HE1	3:L:345:ASN:ND2	2.06	0.54
3:L:234:HIS:CE1	3:L:269:PRO:HD3	2.41	0.54
1:A:140:VAL:CG2	1:A:141:ARG:H	2.21	0.54
1:A:175:LEU:C	1:A:177:ASP:H	2.16	0.54
3:C:275:ARG:CB	3:C:311:GLN:HA	2.35	0.54
3:C:276:LEU:HD12	3:C:276:LEU:O	2.07	0.54
3:C:350:GLN:C	3:C:352:GLY:H	2.15	0.54
1:D:124:ARG:H	1:D:124:ARG:CD	2.10	0.54
2:E:370:HIS:HE1	2:E:408:HIS:HB2	1.73	0.54
2:H:354:MET:C	2:H:356:GLY:H	2.16	0.54
2:H:365:ARG:HG2	2:H:366:THR:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:124:LEU:O	3:I:124:LEU:HG	2.08	0.54
1:J:152:VAL:CG2	1:J:153:ASP:N	2.71	0.54
1:D:174:ASP:OD1	1:D:177:ASP:HB2	2.07	0.54
3:F:276:LEU:HD21	3:F:278:TYR:HD2	1.73	0.54
3:F:290:PHE:HA	3:F:307:HIS:HD1	1.71	0.54
2:H:152:TYR:CD2	2:H:155:GLU:HG2	2.43	0.54
3:I:208:TRP:HE3	3:I:314:THR:HG23	1.73	0.54
3:I:221:THR:HG23	3:I:222:GLY:N	2.13	0.54
1:J:140:VAL:HG13	1:J:185:LEU:CD1	2.34	0.54
2:K:394:CYS:O	2:K:397:GLU:O	2.25	0.54
3:L:276:LEU:O	3:L:277:THR:HG23	2.08	0.54
1:A:136:LEU:HA	1:A:139:ASN:HB2	1.90	0.53
2:B:165:LEU:H	2:B:166:ARG:CZ	2.19	0.53
3:C:148:ILE:HD12	3:C:148:ILE:N	2.23	0.53
3:C:170:LYS:HZ3	3:C:177:GLN:N	2.06	0.53
1:D:131:GLN:O	1:D:134:GLN:HG2	2.08	0.53
1:D:164:SER:O	2:E:197:CYS:SG	2.66	0.53
2:E:367:MET:O	2:E:405:ASN:O	2.25	0.53
3:F:242:ILE:CG2	3:F:243:PRO:HD2	2.39	0.53
3:I:105:SER:HA	3:I:108:ARG:HB3	1.89	0.53
3:I:191:TRP:HH2	3:I:247:ARG:HH11	1.54	0.53
3:I:208:TRP:CA	3:I:314:THR:HG21	2.38	0.53
2:K:215:ILE:CG2	2:K:216:ARG:H	2.22	0.53
3:L:223:THR:O	3:L:223:THR:HG22	2.08	0.53
3:L:372:TRP:HZ3	3:L:379:MET:CE	2.21	0.53
2:B:231:SER:HB2	3:C:176:GLN:NE2	2.23	0.53
2:B:346:ARG:HB2	2:B:346:ARG:HH11	1.72	0.53
2:B:364:ASN:HA	2:B:367:MET:HE3	1.90	0.53
3:C:111:GLN:O	3:C:114:TYR:HB3	2.07	0.53
1:D:126:VAL:HG23	1:D:127:ILE:N	2.23	0.53
2:E:156:THR:HG22	2:E:157:VAL:N	2.22	0.53
2:E:189:GLN:HA	2:E:189:GLN:OE1	2.09	0.53
2:H:237:ARG:HH22	3:I:143:VAL:HG21	1.73	0.53
3:I:248:VAL:HB	3:I:260:ALA:HB3	1.90	0.53
2:K:204:PRO:HA	3:L:217:HIS:HD2	1.72	0.53
2:K:304:ARG:O	2:K:306:GLY:N	2.42	0.53
3:L:281:PHE:HB2	3:L:288:ASP:OD1	2.07	0.53
3:L:367:ILE:O	3:L:378:SER:HA	2.08	0.53
3:L:380:LYS:O	3:L:381:LYS:HG3	2.08	0.53
2:B:156:THR:HA	2:B:160:ASN:HB2	1.90	0.53
2:B:163:THR:HG22	2:B:163:THR:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:LYS:O	2:B:183:GLU:N	2.38	0.53
3:C:93:ILE:CD1	3:C:94:MET:HE2	2.38	0.53
2:E:253:GLN:HB2	2:E:293:TRP:CE3	2.43	0.53
2:E:346:ARG:HG2	2:E:346:ARG:NH1	2.22	0.53
2:H:293:TRP:NE1	2:H:296:ASN:ND2	2.54	0.53
2:H:364:ASN:HA	2:H:367:MET:HE3	1.90	0.53
1:J:151:GLU:HG3	1:J:178:TYR:CZ	2.42	0.53
3:C:311:GLN:OE1	3:C:319:ASN:HB3	2.09	0.53
3:I:218:LEU:O	3:I:219:SER:HB3	2.09	0.53
2:B:209:LYS:HB3	2:B:209:LYS:NZ	2.23	0.53
3:C:202:VAL:HG11	3:C:216:GLY:HA3	1.91	0.53
3:C:246:LEU:HB2	3:C:265:PHE:CE1	2.44	0.53
3:C:278:TYR:HH	3:C:290:PHE:HB3	1.71	0.53
1:D:143:GLN:O	1:D:147:MET:HG2	2.09	0.53
2:E:209:LYS:HG3	2:E:213:GLU:OE1	2.08	0.53
2:B:183:GLU:HG2	2:B:183:GLU:O	2.08	0.53
2:B:317:TRP:CD1	2:B:317:TRP:N	2.69	0.53
3:F:249:GLU:O	3:F:250:LEU:HD12	2.09	0.53
2:H:237:ARG:HH22	3:I:143:VAL:CG2	2.22	0.53
1:G:191:LYS:O	1:G:192:ASP:CB	2.57	0.53
2:H:249:TRP:CZ3	2:H:455:ARG:HB2	2.43	0.53
3:I:256:ARG:HG3	3:I:256:ARG:NH1	2.23	0.53
1:J:140:VAL:HG13	1:J:141:ARG:N	2.24	0.53
2:K:408:HIS:C	2:K:408:HIS:CD2	2.87	0.53
3:L:360:PRO:O	3:L:361:ASN:ND2	2.42	0.53
3:C:276:LEU:HD11	3:C:309:GLY:H	1.73	0.53
3:C:317:ASN:HD22	3:C:317:ASN:C	2.16	0.53
2:H:408:HIS:O	4:Q:1:GLY:N	2.40	0.53
3:I:337:ASN:OD1	3:I:338:LYS:N	2.35	0.53
1:A:136:LEU:HD12	3:C:107:ILE:HD11	1.91	0.53
2:B:164:ASN:C	2:B:166:ARG:H	2.17	0.53
2:B:402:TRP:CH2	2:B:412:PRO:HD2	2.44	0.53
2:E:204:PRO:HA	3:F:217:HIS:HD2	1.71	0.53
2:E:300:SER:OG	2:E:332:GLN:O	2.27	0.53
2:E:301:GLN:HE22	2:E:302:LEU:HG	1.73	0.53
3:F:194:PHE:CZ	3:F:384:MET:HE3	2.44	0.53
2:H:229:PRO:HG2	2:H:233:VAL:HG11	1.90	0.53
3:I:193:VAL:HG12	3:I:195:GLN:N	2.24	0.53
1:J:126:VAL:HG12	1:J:127:ILE:N	2.23	0.53
2:K:266:TRP:N	2:K:379:ASP:OD1	2.39	0.53
3:L:212:LYS:HG3	3:L:231:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:GLU:O	2:B:193:CYS:N	2.41	0.53
2:B:354:MET:C	2:B:356:GLY:H	2.17	0.53
2:B:394:CYS:SG	2:B:406:ARG:HA	2.49	0.53
3:C:170:LYS:HZ3	3:C:177:GLN:H	1.57	0.53
3:C:193:VAL:HG12	3:C:195:GLN:N	2.23	0.53
2:H:309:GLU:O	2:H:309:GLU:HG3	2.09	0.53
2:H:424:TRP:C	2:H:426:MET:H	2.17	0.53
3:I:246:LEU:HB2	3:I:265:PHE:CE1	2.44	0.53
3:I:354:TYR:OH	3:I:364:ASP:HA	2.08	0.53
2:K:198:THR:HG22	3:L:140:LYS:O	2.09	0.53
2:K:374:PHE:HB2	2:K:382:ASN:HB3	1.90	0.53
2:K:405:ASN:O	2:K:406:ARG:C	2.52	0.53
3:L:365:ASN:HD22	3:L:365:ASN:C	2.16	0.53
2:B:213:GLU:CG	2:B:217:LYS:HE3	2.39	0.52
2:E:166:ARG:O	2:E:169:ARG:HB3	2.09	0.52
2:E:314:MET:HA	2:E:449:LYS:O	2.09	0.52
1:G:139:ASN:O	1:G:142:ALA:HB3	2.09	0.52
3:I:365:ASN:HD22	3:I:366:GLY:N	2.05	0.52
2:B:202:ASN:O	2:B:204:PRO:HD3	2.10	0.52
2:B:310:LEU:HD23	2:B:329:PHE:CG	2.44	0.52
2:B:388:SER:O	2:B:390:PRO:HD3	2.10	0.52
3:C:191:TRP:HH2	3:C:247:ARG:HH11	1.55	0.52
2:E:212:GLU:HB2	2:E:455:ARG:HG3	1.90	0.52
2:E:234:LYS:HD3	2:E:235:PRO:O	2.09	0.52
2:H:161:ILE:N	2:H:162:PRO:CD	2.73	0.52
2:H:179:ILE:O	2:H:179:ILE:HG22	2.09	0.52
2:H:266:TRP:HE1	2:H:380:ARG:CZ	2.23	0.52
2:K:270:LYS:HG3	2:K:338:TYR:OH	2.09	0.52
2:K:351:ASN:HD21	2:K:354:MET:HB2	1.73	0.52
3:L:143:VAL:HG23	3:L:143:VAL:O	2.09	0.52
3:L:242:ILE:CG2	3:L:243:PRO:HD2	2.39	0.52
3:L:311:GLN:O	3:L:335:TRP:HA	2.10	0.52
1:A:181:GLN:NE2	2:B:174:ASN:HB2	2.25	0.52
2:B:161:ILE:HG22	2:B:162:PRO:CD	2.39	0.52
3:C:347:VAL:HB	3:C:349:TYR:CE2	2.43	0.52
2:E:283:LYS:HD2	2:E:283:LYS:N	2.24	0.52
3:F:96:TYR:HD1	3:F:97:GLU:H	1.57	0.52
2:H:303:THR:HA	2:H:308:THR:HG21	1.91	0.52
2:H:411:ASN:HB3	2:H:436:VAL:HG22	1.92	0.52
3:C:178:PHE:HE2	3:C:228:LEU:HD11	1.73	0.52
3:C:295:PHE:CD2	4:O:2:HYP:HD23	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:354:TYR:OH	3:C:364:ASP:HA	2.09	0.52
2:E:161:ILE:N	2:E:162:PRO:CD	2.72	0.52
2:E:333:ASN:N	2:E:336:ASN:HD22	2.05	0.52
3:F:234:HIS:CE1	3:F:269:PRO:HD3	2.44	0.52
3:F:281:PHE:HB2	3:F:288:ASP:OD1	2.09	0.52
1:G:120:GLU:OE1	1:G:121:VAL:N	2.38	0.52
1:G:150:LEU:HD12	1:G:150:LEU:O	2.09	0.52
2:H:213:GLU:CG	2:H:217:LYS:HE3	2.38	0.52
2:H:242:MET:HA	2:H:247:GLY:HA2	1.91	0.52
2:H:249:TRP:CZ2	2:H:455:ARG:CZ	2.92	0.52
1:J:156:ILE:CG2	2:K:415:ARG:NH1	2.72	0.52
2:K:156:THR:HG22	2:K:157:VAL:N	2.23	0.52
1:A:121:VAL:O	1:A:122:LEU:HB3	2.10	0.52
3:C:377:TYR:HD2	3:C:379:MET:HE2	1.74	0.52
2:E:218:GLY:HA3	3:F:210:GLN:HG2	1.92	0.52
3:F:228:LEU:O	3:F:232:LYS:HD2	2.09	0.52
3:F:281:PHE:O	3:F:283:GLY:N	2.43	0.52
3:F:380:LYS:O	3:F:381:LYS:HG3	2.10	0.52
1:G:133:ILE:C	1:G:135:LEU:H	2.17	0.52
2:H:227:ILE:HD13	2:H:238:VAL:HG11	1.92	0.52
2:H:255:ARG:NH1	2:H:413:ASN:HA	2.24	0.52
2:H:304:ARG:HH22	2:H:333:ASN:H	1.57	0.52
2:H:428:LYS:HG2	2:H:429:HIS:HD2	1.73	0.52
3:I:93:ILE:N	3:I:93:ILE:CD1	2.72	0.52
3:I:171:PRO:HB3	3:I:235:LEU:O	2.09	0.52
1:J:119:ILE:HA	1:J:122:LEU:HB3	1.90	0.52
1:J:167:ARG:CZ	1:J:167:ARG:CB	2.87	0.52
2:K:283:LYS:N	2:K:283:LYS:HD2	2.24	0.52
3:L:185:ASP:C	3:L:187:SER:H	2.16	0.52
2:B:175:LEU:O	2:B:179:ILE:HG13	2.09	0.52
2:B:303:THR:HB	2:B:330:THR:HA	1.91	0.52
2:B:332:GLN:HB3	2:B:336:ASN:HD22	1.75	0.52
2:E:215:ILE:HD12	2:E:248:GLY:N	2.25	0.52
3:F:195:GLN:HG3	3:F:227:TRP:CZ3	2.44	0.52
1:G:172:GLU:O	1:G:173:VAL:HG23	2.09	0.52
3:I:322:PHE:CG	3:I:323:GLU:N	2.78	0.52
2:K:216:ARG:HB2	2:K:216:ARG:CZ	2.39	0.52
3:L:344:LEU:HD22	3:L:382:THR:OG1	2.10	0.52
2:B:165:LEU:HB2	2:B:166:ARG:CZ	2.40	0.52
2:B:175:LEU:HA	2:B:178:LYS:HG3	1.92	0.52
2:B:255:ARG:HB2	2:B:450:MET:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:373:MET:SD	2:E:405:ASN:HB2	2.50	0.52
5:E:470:NAG:H83	5:E:470:NAG:C1	2.40	0.52
3:F:239:GLN:O	3:F:242:ILE:HD12	2.10	0.52
3:F:310:MET:O	3:F:311:GLN:O	2.28	0.52
2:H:205:VAL:HG21	3:I:215:PHE:O	2.10	0.52
2:H:417:TYR:HB2	2:H:446:SER:HB3	1.90	0.52
1:J:185:LEU:O	1:J:189:ILE:HG13	2.09	0.52
3:F:153:CYS:SG	3:F:192:THR:HA	2.50	0.52
2:K:357:ALA:HB3	2:K:360:LEU:CD1	2.39	0.52
3:L:196:LYS:O	3:L:197:ARG:HD2	2.08	0.52
2:B:337:LYS:HB3	2:B:382:ASN:OD1	2.10	0.52
2:B:411:ASN:N	2:B:436:VAL:O	2.33	0.52
3:C:350:GLN:C	3:C:352:GLY:N	2.67	0.52
2:E:266:TRP:HA	2:E:377:THR:HG21	1.92	0.52
2:E:270:LYS:HA	2:E:296:ASN:CB	2.40	0.52
2:E:369:ILE:O	2:E:405:ASN:ND2	2.38	0.52
3:F:297:ASP:O	3:F:298:ASP:CB	2.57	0.52
3:F:340:HIS:ND1	3:F:368:ILE:HD11	2.25	0.52
2:H:230:ASP:O	2:H:232:SER:N	2.43	0.52
2:H:310:LEU:HB3	2:H:329:PHE:CD2	2.45	0.52
2:K:366:THR:HA	2:K:369:ILE:CD1	2.40	0.52
3:L:297:ASP:O	3:L:298:ASP:CB	2.57	0.52
1:D:122:LEU:N	1:D:124:ARG:NE	2.57	0.52
2:E:215:ILE:CG2	2:E:216:ARG:H	2.23	0.52
2:E:255:ARG:HG3	2:E:255:ARG:HH11	1.74	0.52
1:G:167:ARG:HH22	1:G:169:LEU:HD23	1.75	0.52
2:H:236:TYR:CB	2:H:298:LYS:NZ	2.73	0.52
3:I:131:LEU:O	3:I:134:GLN:HB3	2.10	0.52
3:I:329:GLN:HE21	4:S:3:ARG:CZ	2.22	0.52
2:K:363:GLU:C	2:K:365:ARG:H	2.18	0.52
2:B:280:THR:O	2:B:281:ASP:CG	2.54	0.51
3:C:195:GLN:CD	3:C:196:LYS:H	2.18	0.51
3:C:297:ASP:HB2	3:C:301:ASP:CG	2.35	0.51
3:C:326:CYS:O	3:C:327:ALA:C	2.52	0.51
2:E:357:ALA:HB3	2:E:360:LEU:CD1	2.40	0.51
2:E:397:GLU:O	2:E:398:ASP:HB2	2.10	0.51
2:H:251:VAL:HG12	2:H:252:ILE:N	2.24	0.51
2:H:304:ARG:HH11	2:H:304:ARG:HG3	1.76	0.51
3:I:275:ARG:HB2	3:I:311:GLN:CA	2.37	0.51
1:A:158:ILE:HG12	2:B:189:GLN:HG3	1.91	0.51
2:B:429:HIS:C	2:B:431:THR:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:MET:SD	4:M:1:GLY:N	2.74	0.51
3:C:170:LYS:NZ	3:C:175:ASN:O	2.42	0.51
2:E:398:ASP:HA	2:E:433:ASP:CB	2.27	0.51
3:F:313:SER:N	3:F:334:TRP:O	2.40	0.51
2:H:189:GLN:HE21	2:H:189:GLN:HA	1.75	0.51
2:H:319:GLY:O	2:H:320:ASP:O	2.29	0.51
2:H:365:ARG:O	2:H:368:THR:HG23	2.09	0.51
3:I:347:VAL:HB	3:I:349:TYR:CE2	2.44	0.51
2:K:255:ARG:HD3	2:K:262:PHE:CZ	2.45	0.51
1:A:127:ILE:HG22	1:A:128:GLU:N	2.26	0.51
1:A:147:MET:SD	3:C:121:ILE:HD11	2.51	0.51
2:B:351:ASN:HD21	2:B:354:MET:CG	2.23	0.51
2:B:361:MET:CB	5:B:470:NAG:H81	2.36	0.51
2:B:408:HIS:O	4:M:1:GLY:N	2.37	0.51
2:B:433:ASP:OD1	2:B:433:ASP:O	2.29	0.51
2:E:161:ILE:HB	2:E:162:PRO:HD3	1.92	0.51
2:E:332:GLN:HB2	2:E:339:GLN:H	1.75	0.51
1:G:164:SER:CB	3:I:137:GLU:O	2.58	0.51
2:H:191:GLU:C	2:H:193:CYS:N	2.69	0.51
2:H:209:LYS:NZ	2:H:209:LYS:HB3	2.24	0.51
3:I:350:GLN:C	3:I:352:GLY:H	2.18	0.51
3:L:250:LEU:HD21	3:L:369:TRP:CD1	2.45	0.51
1:A:172:GLU:O	1:A:173:VAL:HG13	2.09	0.51
3:C:169:ILE:HD11	3:C:178:PHE:CE1	2.46	0.51
3:C:349:TYR:HB2	3:C:378:SER:CB	2.41	0.51
3:F:205:LYS:HZ3	3:F:315:TRP:CD1	2.28	0.51
3:F:294:ASP:HA	3:F:301:ASP:HB3	1.91	0.51
3:F:307:HIS:O	3:F:310:MET:HG2	2.11	0.51
2:H:412:PRO:HB3	2:H:450:MET:HG2	1.93	0.51
3:I:169:ILE:HD11	3:I:178:PHE:HE1	1.76	0.51
3:I:208:TRP:NE1	3:I:270:GLU:OE2	2.43	0.51
3:I:263:ALA:O	3:I:264:MET:C	2.52	0.51
1:J:125:LYS:O	1:J:129:LYS:HG2	2.11	0.51
1:J:128:GLU:O	1:J:131:GLN:NE2	2.43	0.51
2:K:270:LYS:HA	2:K:296:ASN:HB3	1.91	0.51
2:K:324:ALA:HB2	2:K:349:ALA:HB3	1.92	0.51
2:K:340:ILE:HG12	2:K:341:SER:N	2.25	0.51
3:L:232:LYS:O	3:L:234:HIS:N	2.44	0.51
2:B:351:ASN:ND2	2:B:355:ASP:H	2.09	0.51
3:C:101:LEU:HD12	3:C:104:ASP:OD1	2.11	0.51
3:C:322:PHE:C	3:C:324:GLY:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:340:HIS:O	4:O:1:GLY:HA2	2.10	0.51
3:C:348:TYR:HA	3:C:367:ILE:CD1	2.40	0.51
3:C:365:ASN:HD22	3:C:366:GLY:N	2.07	0.51
1:D:140:VAL:CG1	1:D:185:LEU:HD11	2.38	0.51
2:E:270:LYS:O	2:E:270:LYS:HG2	2.10	0.51
2:E:304:ARG:O	2:E:306:GLY:N	2.44	0.51
3:F:311:GLN:O	3:F:335:TRP:HA	2.11	0.51
3:I:202:VAL:HG11	3:I:216:GLY:HA3	1.93	0.51
2:K:280:THR:O	2:K:281:ASP:O	2.28	0.51
2:K:328:GLY:HA3	2:K:343:ASN:OD1	2.11	0.51
3:L:388:PRO:O	3:L:389:PHE:C	2.54	0.51
3:C:96:TYR:C	3:C:98:ALA:N	2.67	0.51
3:C:131:LEU:HD23	3:C:131:LEU:C	2.35	0.51
3:C:220:PRO:HG2	3:C:221:THR:H	1.76	0.51
2:E:216:ARG:CZ	2:E:216:ARG:HB2	2.41	0.51
2:E:356:GLY:HA2	2:E:409:ALA:HB2	1.92	0.51
3:F:197:ARG:NH1	3:F:344:LEU:O	2.44	0.51
1:G:178:TYR:C	1:G:180:ASP:N	2.69	0.51
2:H:178:LYS:O	2:H:182:LEU:HB3	2.11	0.51
2:H:346:ARG:HH11	2:H:346:ARG:HB2	1.75	0.51
2:K:210:GLU:OE2	2:K:213:GLU:HB2	2.11	0.51
2:K:300:SER:OG	2:K:332:GLN:O	2.27	0.51
2:K:356:GLY:HA2	2:K:409:ALA:HB2	1.93	0.51
3:C:109:TYR:O	3:C:110:LEU:C	2.53	0.51
3:I:170:LYS:NZ	3:I:175:ASN:O	2.42	0.51
3:L:170:LYS:HE2	3:L:176:GLN:C	2.36	0.51
3:C:221:THR:CG2	3:C:222:GLY:H	2.09	0.51
1:D:156:ILE:HG21	2:E:415:ARG:NH1	2.26	0.51
3:F:240:SER:O	3:F:241:ALA:C	2.54	0.51
3:F:374:THR:OG1	3:F:377:TYR:HB2	2.11	0.51
1:G:189:ILE:O	1:G:189:ILE:CG2	2.58	0.51
3:I:193:VAL:HG12	3:I:194:PHE:N	2.26	0.51
2:K:346:ARG:HG2	2:K:346:ARG:NH1	2.25	0.51
3:L:196:LYS:HA	3:L:382:THR:O	2.11	0.51
3:L:249:GLU:O	3:L:250:LEU:HD12	2.11	0.51
2:B:222:SER:HB2	2:B:243:ASN:OD1	2.11	0.51
2:B:227:ILE:HD13	2:B:238:VAL:HG11	1.93	0.51
3:F:217:HIS:O	3:F:224:THR:OG1	2.27	0.51
2:H:424:TRP:N	2:H:444:TRP:CZ3	2.79	0.51
3:I:369:TRP:NE1	3:I:371:THR:OG1	2.44	0.51
2:K:253:GLN:HB2	2:K:293:TRP:CE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:239:GLN:O	3:L:242:ILE:HD12	2.10	0.51
3:C:112:GLU:C	3:C:114:TYR:N	2.69	0.51
3:C:218:LEU:O	3:C:219:SER:HB3	2.11	0.51
3:I:195:GLN:CD	3:I:196:LYS:H	2.19	0.51
3:I:276:LEU:CD1	3:I:308:ASN:HA	2.38	0.51
3:I:317:ASN:HD22	3:I:317:ASN:C	2.19	0.51
1:J:151:GLU:OE2	2:K:182:LEU:HD21	2.09	0.51
2:K:204:PRO:HG2	2:K:224:MET:O	2.11	0.51
2:K:270:LYS:HA	2:K:296:ASN:CB	2.42	0.51
4:R:3:ARG:HH21	4:R:3:ARG:HG2	1.75	0.51
2:B:237:ARG:HH22	3:C:143:VAL:CG2	2.24	0.50
2:B:301:GLN:NE2	2:B:302:LEU:N	2.59	0.50
2:B:437:TRP:HB3	2:B:447:MET:HE1	1.92	0.50
3:C:252:ASP:OD2	3:C:254:ASN:HB2	2.10	0.50
3:F:153:CYS:HB2	3:F:192:THR:CG2	2.39	0.50
3:F:232:LYS:O	3:F:234:HIS:N	2.44	0.50
2:H:162:PRO:C	2:H:164:ASN:N	2.69	0.50
2:H:317:TRP:CD1	2:H:317:TRP:N	2.72	0.50
2:H:388:SER:O	2:H:390:PRO:HD3	2.12	0.50
3:I:156:ILE:HD11	3:I:169:ILE:HG22	1.92	0.50
3:I:170:LYS:HZ3	3:I:177:GLN:N	2.09	0.50
2:K:270:LYS:HE2	2:K:297:ASP:OD2	2.10	0.50
2:K:303:THR:CG2	2:K:330:THR:HA	2.41	0.50
2:K:327:GLY:CA	2:K:344:LYS:HB2	2.35	0.50
3:L:217:HIS:O	3:L:224:THR:OG1	2.26	0.50
3:L:278:TYR:OH	3:L:308:ASN:HB2	2.10	0.50
2:B:301:GLN:HE21	2:B:302:LEU:N	2.08	0.50
3:C:148:ILE:HD12	3:C:148:ILE:H	1.77	0.50
1:D:167:ARG:HH11	1:D:167:ARG:CG	2.23	0.50
2:E:404:TYR:O	2:E:405:ASN:CB	2.60	0.50
3:I:275:ARG:CB	3:I:311:GLN:HA	2.40	0.50
3:L:322:PHE:HB2	3:L:338:LYS:HA	1.94	0.50
1:A:128:GLU:CA	1:A:131:GLN:HG2	2.42	0.50
1:A:158:ILE:CG2	1:A:159:ARG:N	2.73	0.50
3:F:179:LEU:HG	3:F:218:LEU:HD12	1.93	0.50
2:H:215:ILE:HD13	2:H:242:MET:HB3	1.93	0.50
2:H:316:ASP:OD1	2:H:320:ASP:HB3	2.11	0.50
2:H:333:ASN:OD1	2:H:335:ALA:HB3	2.10	0.50
3:I:93:ILE:HD12	3:I:93:ILE:H	1.74	0.50
3:I:179:LEU:O	3:I:218:LEU:HD11	2.11	0.50
3:I:349:TYR:HB2	3:I:378:SER:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:363:TYR:CD2	4:S:3:ARG:HD3	2.46	0.50
2:K:397:GLU:O	2:K:398:ASP:HB2	2.11	0.50
2:B:242:MET:HA	2:B:247:GLY:HA2	1.93	0.50
3:C:116:SER:O	3:C:120:LYS:N	2.40	0.50
3:C:128:VAL:C	3:C:130:GLN:N	2.67	0.50
3:C:208:TRP:CA	3:C:314:THR:HG21	2.40	0.50
2:E:212:GLU:HG3	2:E:212:GLU:O	2.11	0.50
2:E:351:ASN:ND2	2:E:354:MET:HB2	2.26	0.50
2:E:455:ARG:HG3	2:E:456:PRO:HD2	1.93	0.50
3:F:158:ASN:O	3:F:159:LYS:HB2	2.11	0.50
2:H:155:GLU:C	2:H:157:VAL:N	2.66	0.50
3:L:93:ILE:O	3:L:95:LYS:N	2.40	0.50
3:L:240:SER:O	3:L:241:ALA:C	2.55	0.50
3:L:276:LEU:HD11	3:L:290:PHE:CE2	2.46	0.50
2:B:158:ASN:HD21	3:C:100:ILE:HD13	1.77	0.50
2:B:207:SER:C	2:B:214:ILE:HG12	2.37	0.50
3:C:125:LYS:HA	3:C:125:LYS:CE	2.41	0.50
2:E:155:GLU:O	2:E:156:THR:C	2.54	0.50
2:E:367:MET:HB2	2:E:406:ARG:HB3	1.94	0.50
2:H:215:ILE:HB	2:H:242:MET:HE3	1.94	0.50
2:H:229:PRO:O	2:H:230:ASP:C	2.53	0.50
2:K:160:ASN:C	2:K:162:PRO:HD2	2.37	0.50
3:L:374:THR:OG1	3:L:377:TYR:HB2	2.11	0.50
2:B:230:ASP:O	2:B:232:SER:N	2.45	0.50
2:B:264:ARG:NH2	3:C:136:GLN:O	2.38	0.50
3:C:275:ARG:CA	3:C:311:GLN:HA	2.42	0.50
3:C:288:ASP:OD2	3:C:291:ASP:HB2	2.12	0.50
3:C:322:PHE:CG	3:C:323:GLU:N	2.80	0.50
2:E:363:GLU:C	2:E:365:ARG:H	2.20	0.50
3:F:260:ALA:HB2	3:F:286:ALA:HB3	1.94	0.50
3:F:310:MET:C	3:F:311:GLN:O	2.52	0.50
1:G:140:VAL:HG23	1:G:185:LEU:HD21	1.93	0.50
2:H:212:GLU:O	2:H:215:ILE:CG2	2.59	0.50
3:I:123:ASN:C	3:I:125:LYS:H	2.19	0.50
3:I:194:PHE:HB2	3:I:233:ILE:CD1	2.42	0.50
3:I:253:TRP:CZ3	3:I:380:LYS:HG3	2.47	0.50
1:J:185:LEU:HD22	1:J:189:ILE:CG1	2.41	0.50
2:K:257:ASP:HA	2:K:416:TYR:CE2	2.45	0.50
3:L:195:GLN:CB	3:L:384:MET:HE2	2.42	0.50
2:B:165:LEU:HD13	3:C:106:SER:O	2.12	0.50
3:C:193:VAL:CG1	3:C:195:GLN:H	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:PHE:HE2	3:C:227:TRP:HB2	1.76	0.50
3:C:284:GLY:C	3:C:286:ALA:N	2.67	0.50
3:F:340:HIS:CE1	3:F:368:ILE:HD11	2.46	0.50
3:I:119:GLN:NE2	3:I:120:LYS:N	2.60	0.50
3:I:224:THR:HG23	3:I:224:THR:O	2.11	0.50
3:I:284:GLY:C	3:I:286:ALA:N	2.67	0.50
2:B:229:PRO:HB2	2:B:301:GLN:OE1	2.12	0.50
2:B:245:GLU:HG2	2:B:249:TRP:CZ2	2.42	0.50
2:B:428:LYS:HG2	2:B:429:HIS:HD2	1.76	0.50
3:C:124:LEU:HD12	3:C:127:LYS:HB3	1.94	0.50
3:C:193:VAL:HG12	3:C:194:PHE:N	2.26	0.50
3:C:310:MET:O	3:C:335:TRP:HD1	1.93	0.50
3:C:377:TYR:CD2	3:C:379:MET:HE2	2.47	0.50
2:E:415:ARG:O	2:E:434:GLY:HA2	2.12	0.50
2:H:266:TRP:HB2	2:H:379:ASP:OD2	2.12	0.50
2:H:280:THR:O	2:H:281:ASP:CG	2.55	0.50
2:H:374:PHE:CB	2:H:382:ASN:HB3	2.42	0.50
2:H:407:CYS:SG	4:Q:3:ARG:NH2	2.85	0.50
3:I:197:ARG:HB2	3:I:382:THR:HB	1.94	0.50
3:I:334:TRP:O	3:I:335:TRP:C	2.55	0.50
2:K:398:ASP:HA	2:K:433:ASP:CB	2.28	0.50
3:L:100:ILE:C	3:L:102:THR:H	2.19	0.50
3:L:251:GLU:CB	3:L:381:LYS:HB2	2.41	0.50
1:A:183:LYS:HD3	1:A:183:LYS:C	2.37	0.50
3:C:207:ASN:ND2	3:C:210:GLN:HG3	2.26	0.50
3:C:212:LYS:C	3:C:214:GLY:H	2.19	0.50
3:C:238:THR:HG22	3:C:266:LYS:HG3	1.94	0.50
3:C:251:GLU:HA	3:C:256:ARG:O	2.11	0.50
2:E:201:CYS:O	3:F:143:VAL:HG21	2.11	0.50
2:H:310:LEU:HD23	2:H:329:PHE:CE2	2.47	0.50
3:I:350:GLN:C	3:I:352:GLY:N	2.69	0.50
1:J:125:LYS:HA	1:J:125:LYS:HE3	1.94	0.50
3:L:179:LEU:HG	3:L:218:LEU:HD12	1.94	0.50
1:A:160:SER:O	3:C:135:CYS:HB3	2.12	0.49
3:C:263:ALA:O	3:C:264:MET:C	2.54	0.49
3:C:359:THR:HB	3:C:362:GLY:C	2.37	0.49
2:E:164:ASN:O	2:E:164:ASN:ND2	2.45	0.49
1:G:139:ASN:O	3:I:114:TYR:OH	2.30	0.49
1:G:171:ARG:HH11	1:G:171:ARG:HG2	1.75	0.49
2:H:207:SER:C	2:H:214:ILE:HG12	2.38	0.49
3:I:310:MET:HE2	3:I:310:MET:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:310:MET:SD	3:I:337:ASN:ND2	2.85	0.49
3:I:377:TYR:HD2	3:I:379:MET:HE2	1.75	0.49
1:J:152:VAL:HG21	2:K:426:MET:O	2.12	0.49
2:K:189:GLN:O	2:K:193:CYS:SG	2.70	0.49
2:K:212:GLU:O	2:K:212:GLU:CG	2.60	0.49
1:A:154:ILE:O	1:A:157:LYS:N	2.46	0.49
2:B:226:LEU:O	2:B:227:ILE:C	2.55	0.49
3:C:196:LYS:HD2	3:C:198:LEU:HD11	1.94	0.49
3:C:253:TRP:NE1	3:C:378:SER:O	2.28	0.49
3:C:309:GLY:C	3:C:310:MET:HE2	2.37	0.49
3:F:195:GLN:HG3	3:F:227:TRP:CE3	2.48	0.49
3:F:198:LEU:HD23	3:F:381:LYS:HE2	1.92	0.49
2:H:258:GLY:O	2:H:260:VAL:N	2.40	0.49
1:J:149:ARG:O	1:J:150:LEU:C	2.54	0.49
2:K:333:ASN:ND2	2:K:335:ALA:HB3	2.27	0.49
2:K:367:MET:O	2:K:405:ASN:O	2.29	0.49
2:B:226:LEU:O	2:B:227:ILE:O	2.30	0.49
3:C:195:GLN:O	3:C:196:LYS:HB3	2.12	0.49
3:C:250:LEU:HG	3:C:251:GLU:H	1.76	0.49
1:G:136:LEU:O	1:G:140:VAL:HG13	2.11	0.49
2:H:223:GLU:OE2	2:H:285:TYR:HD1	1.96	0.49
3:I:127:LYS:O	3:I:128:VAL:C	2.55	0.49
3:I:204:PHE:HE2	3:I:227:TRP:HB2	1.77	0.49
3:I:353:THR:HA	3:I:377:TYR:HA	1.94	0.49
2:K:272:GLY:N	2:K:295:GLY:HA2	2.28	0.49
2:K:420:GLY:HA2	2:K:446:SER:O	2.12	0.49
3:L:194:PHE:CD1	3:L:233:ILE:HD13	2.48	0.49
3:L:292:GLY:C	3:L:302:LYS:HD2	2.37	0.49
3:L:305:THR:HB	3:L:341:ALA:CB	2.21	0.49
1:A:158:ILE:HG21	1:A:171:ARG:HE	1.77	0.49
2:B:158:ASN:CG	3:C:100:ILE:HD13	2.37	0.49
2:B:249:TRP:CZ2	2:B:455:ARG:CZ	2.95	0.49
3:C:304:PHE:O	3:C:337:ASN:ND2	2.45	0.49
3:I:93:ILE:O	3:I:96:TYR:HD2	1.96	0.49
3:I:169:ILE:CD1	3:I:171:PRO:HD3	2.34	0.49
3:I:194:PHE:CZ	3:I:384:MET:HB3	2.47	0.49
3:I:251:GLU:CG	3:I:252:ASP:H	2.17	0.49
2:K:257:ASP:OD2	2:K:259:SER:OG	2.30	0.49
3:L:249:GLU:HB2	3:L:383:THR:HG23	1.94	0.49
1:A:167:ARG:HH22	1:A:169:LEU:HD23	1.78	0.49
2:B:158:ASN:HD22	2:B:158:ASN:N	2.05	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:VAL:HG12	2:B:252:ILE:N	2.26	0.49
2:B:362:GLY:O	2:B:365:ARG:N	2.45	0.49
2:E:327:GLY:CA	2:E:344:LYS:HB2	2.36	0.49
2:E:417:TYR:HE1	2:E:433:ASP:O	1.95	0.49
3:F:252:ASP:C	3:F:254:ASN:H	2.18	0.49
3:F:289:ALA:HB2	3:F:371:THR:OG1	2.13	0.49
1:G:166:SER:CB	2:H:195:THR:O	2.61	0.49
2:H:210:GLU:CD	2:H:212:GLU:HB3	2.38	0.49
1:J:130:VAL:O	1:J:133:ILE:CG2	2.60	0.49
3:L:97:GLU:C	3:L:99:SER:N	2.70	0.49
3:L:195:GLN:HG3	3:L:227:TRP:CZ3	2.47	0.49
3:L:284:GLY:C	3:L:286:ALA:H	2.20	0.49
2:B:424:TRP:N	2:B:444:TRP:CZ3	2.81	0.49
3:C:208:TRP:NE1	3:C:270:GLU:OE2	2.45	0.49
1:D:183:LYS:O	1:D:186:GLU:HB2	2.12	0.49
2:E:170:SER:O	2:E:171:ILE:C	2.55	0.49
2:E:272:GLY:N	2:E:295:GLY:HA2	2.28	0.49
3:F:197:ARG:C	3:F:198:LEU:HD12	2.38	0.49
3:L:310:MET:O	3:L:311:GLN:O	2.31	0.49
2:B:411:ASN:HB3	2:B:436:VAL:HG22	1.95	0.49
3:C:208:TRP:HE3	3:C:314:THR:HG23	1.77	0.49
1:G:185:LEU:HG	1:G:185:LEU:O	2.11	0.49
2:H:222:SER:HB2	2:H:243:ASN:OD1	2.13	0.49
2:H:303:THR:HA	2:H:308:THR:OG1	2.12	0.49
3:I:230:ASN:HD22	3:I:230:ASN:H	1.55	0.49
3:I:304:PHE:O	3:I:337:ASN:ND2	2.46	0.49
3:L:229:GLY:O	3:L:230:ASN:C	2.55	0.49
3:L:281:PHE:O	3:L:283:GLY:N	2.46	0.49
3:L:313:SER:N	3:L:334:TRP:O	2.38	0.49
3:C:195:GLN:NE2	3:C:384:MET:HG3	2.25	0.49
3:F:284:GLY:C	3:F:286:ALA:H	2.21	0.49
3:F:353:THR:HG23	3:F:377:TYR:CD1	2.47	0.49
2:H:351:ASN:ND2	2:H:355:ASP:H	2.11	0.49
3:I:195:GLN:NE2	3:I:384:MET:HG3	2.26	0.49
3:I:250:LEU:O	3:I:257:THR:HB	2.13	0.49
3:I:253:TRP:NE1	3:I:378:SER:O	2.29	0.49
3:I:339:CYS:HB2	4:S:2:HYP:HA	1.93	0.49
3:I:377:TYR:CD2	3:I:379:MET:HE2	2.48	0.49
2:K:191:GLU:C	2:K:193:CYS:N	2.71	0.49
2:K:332:GLN:HB2	2:K:339:GLN:H	1.78	0.49
2:K:333:ASN:OD1	2:K:334:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:351:ASN:ND2	2:K:354:MET:HB2	2.28	0.49
2:K:373:MET:HA	2:K:373:MET:HE3	1.95	0.49
2:K:398:ASP:OD1	2:K:431:THR:OG1	2.28	0.49
2:K:417:TYR:HE1	2:K:433:ASP:O	1.95	0.49
3:L:158:ASN:O	3:L:159:LYS:HB2	2.12	0.49
2:B:310:LEU:HD23	2:B:329:PHE:CE2	2.47	0.49
3:C:194:PHE:CZ	3:C:384:MET:HB3	2.47	0.49
3:C:276:LEU:HD12	3:C:276:LEU:C	2.38	0.49
3:I:238:THR:HG22	3:I:266:LYS:HG3	1.95	0.49
2:K:360:LEU:O	2:K:365:ARG:HD2	2.12	0.49
2:K:367:MET:O	2:K:405:ASN:ND2	2.46	0.49
2:B:402:TRP:HB3	2:B:404:TYR:CZ	2.48	0.49
2:B:454:ILE:C	2:B:454:ILE:CD1	2.86	0.49
3:C:156:ILE:HD11	3:C:169:ILE:HG22	1.94	0.49
3:F:170:LYS:HE2	3:F:176:GLN:C	2.38	0.49
3:F:249:GLU:HB2	3:F:383:THR:HG23	1.95	0.49
3:F:278:TYR:OH	3:F:308:ASN:HB2	2.12	0.49
2:H:245:GLU:HG2	2:H:249:TRP:CZ2	2.45	0.49
2:H:310:LEU:HA	2:H:454:ILE:HG22	1.95	0.49
2:K:254:ASN:O	2:K:291:GLU:HA	2.12	0.49
2:B:417:TYR:HB2	2:B:446:SER:HB3	1.92	0.48
3:C:171:PRO:O	3:C:172:LEU:C	2.55	0.48
3:C:207:ASN:CG	3:C:210:GLN:HG3	2.38	0.48
2:E:360:LEU:HB3	2:E:364:ASN:O	2.13	0.48
3:I:178:PHE:HE2	3:I:228:LEU:HD11	1.77	0.48
1:J:158:ILE:HG23	2:K:189:GLN:NE2	2.21	0.48
2:K:157:VAL:HG23	2:K:158:ASN:ND2	2.28	0.48
2:K:305:MET:O	2:K:305:MET:HG2	2.13	0.48
3:L:105:SER:CA	3:L:108:ARG:HG2	2.43	0.48
3:L:269:PRO:C	3:L:273:LYS:O	2.56	0.48
1:A:131:GLN:C	1:A:133:ILE:H	2.21	0.48
1:A:183:LYS:HD3	1:A:183:LYS:O	2.13	0.48
2:B:339:GLN:HG2	2:B:340:ILE:N	2.26	0.48
2:B:374:PHE:CB	2:B:382:ASN:HB3	2.43	0.48
3:C:197:ARG:HB2	3:C:382:THR:HB	1.96	0.48
3:C:289:ALA:HB2	3:C:371:THR:HG23	1.96	0.48
1:D:137:GLN:OE1	1:D:189:ILE:HG12	2.13	0.48
2:B:184:SER:C	2:B:186:VAL:N	2.71	0.48
2:B:337:LYS:HG3	2:B:374:PHE:CE2	2.49	0.48
1:D:126:VAL:O	1:D:127:ILE:C	2.55	0.48
1:D:147:MET:O	1:D:148:LYS:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:LYS:O	1:G:129:LYS:HG2	2.13	0.48
3:I:193:VAL:CG1	3:I:195:GLN:H	2.26	0.48
2:K:405:ASN:C	2:K:407:CYS:H	2.21	0.48
3:L:153:CYS:HB2	3:L:192:THR:CG2	2.42	0.48
2:B:210:GLU:CD	2:B:212:GLU:HB3	2.39	0.48
2:B:319:GLY:O	2:B:320:ASP:O	2.32	0.48
3:C:179:LEU:O	3:C:218:LEU:HD11	2.14	0.48
3:C:353:THR:HA	3:C:377:TYR:HA	1.95	0.48
1:G:120:GLU:CD	1:G:121:VAL:N	2.68	0.48
2:H:184:SER:O	2:H:188:ALA:N	2.47	0.48
2:H:326:TYR:O	2:H:327:GLY:C	2.56	0.48
3:I:163:GLN:O	3:I:167:TYR:OH	2.26	0.48
2:K:234:LYS:HD3	2:K:235:PRO:O	2.14	0.48
3:L:294:ASP:HA	3:L:301:ASP:HB3	1.94	0.48
3:L:310:MET:C	3:L:311:GLN:O	2.54	0.48
2:B:158:ASN:OD1	3:C:100:ILE:HD13	2.13	0.48
2:B:229:PRO:O	2:B:230:ASP:C	2.54	0.48
3:C:321:LYS:O	3:C:338:LYS:HB2	2.13	0.48
1:D:131:GLN:C	1:D:133:ILE:H	2.22	0.48
3:F:269:PRO:C	3:F:273:LYS:O	2.56	0.48
2:H:159:SER:H	2:H:162:PRO:CD	2.26	0.48
2:H:433:ASP:OD1	2:H:433:ASP:O	2.31	0.48
3:I:322:PHE:C	3:I:324:GLY:H	2.21	0.48
3:L:353:THR:HG23	3:L:377:TYR:CD1	2.47	0.48
1:A:189:ILE:O	1:A:190:ALA:CB	2.61	0.48
2:B:455:ARG:HG2	2:B:456:PRO:HD2	1.94	0.48
3:C:124:LEU:HG	3:C:124:LEU:O	2.13	0.48
2:E:191:GLU:C	2:E:193:CYS:N	2.69	0.48
2:E:315:GLU:OE2	2:E:448:ARG:NH2	2.45	0.48
3:F:240:SER:O	3:F:242:ILE:HG13	2.12	0.48
1:G:167:ARG:NH1	1:G:169:LEU:HA	2.28	0.48
2:H:236:TYR:OH	2:H:302:LEU:HD11	2.14	0.48
3:L:205:LYS:HZ3	3:L:315:TRP:CD1	2.31	0.48
3:L:219:SER:CB	3:L:224:THR:HG21	2.44	0.48
2:B:326:TYR:O	2:B:327:GLY:C	2.56	0.48
3:C:178:PHE:HD1	3:C:178:PHE:H	1.60	0.48
3:C:367:ILE:HG22	3:C:379:MET:HG2	1.94	0.48
3:C:386:ILE:O	3:C:387:ILE:HB	2.14	0.48
1:D:147:MET:HG3	2:E:175:LEU:HD13	1.95	0.48
2:E:332:GLN:HB3	2:E:336:ASN:CB	2.43	0.48
2:E:333:ASN:ND2	2:E:335:ALA:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:167:ARG:NE	2:H:192:TYR:CD2	2.77	0.48
2:H:153:ILE:O	2:H:153:ILE:HG12	2.12	0.48
2:H:229:PRO:HB2	2:H:301:GLN:OE1	2.14	0.48
2:H:454:ILE:C	2:H:454:ILE:CD1	2.86	0.48
3:I:117:ASN:N	3:I:117:ASN:ND2	2.61	0.48
3:I:121:ILE:HG23	3:I:122:VAL:N	2.29	0.48
2:K:269:TYR:CE2	2:K:401:GLY:HA3	2.49	0.48
1:A:154:ILE:O	1:A:158:ILE:N	2.41	0.48
1:A:157:LYS:HE3	3:C:132:GLU:OE1	2.14	0.48
1:A:161:CYS:HA	3:C:135:CYS:HB3	1.96	0.48
2:B:292:TYR:CE2	2:B:294:LEU:HB2	2.41	0.48
2:B:317:TRP:H	2:B:317:TRP:HD1	1.54	0.48
2:B:441:LYS:HB3	2:B:445:TYR:HB3	1.96	0.48
3:C:169:ILE:HD11	3:C:178:PHE:HE1	1.79	0.48
3:C:276:LEU:CD1	3:C:308:ASN:HA	2.41	0.48
3:C:312:PHE:HZ	3:C:333:GLY:O	1.96	0.48
2:E:378:TYR:HB2	2:E:396:LYS:HG2	1.95	0.48
2:E:398:ASP:C	2:E:433:ASP:HB3	2.39	0.48
3:F:118:ASN:O	3:F:122:VAL:HG23	2.14	0.48
3:F:124:LEU:O	3:F:125:LYS:C	2.55	0.48
1:G:140:VAL:O	1:G:143:GLN:N	2.46	0.48
2:H:429:HIS:C	2:H:431:THR:H	2.22	0.48
2:H:439:ASN:HD22	2:H:439:ASN:H	1.62	0.48
3:I:116:SER:O	3:I:119:GLN:HB3	2.14	0.48
3:I:171:PRO:O	3:I:172:LEU:C	2.56	0.48
3:I:276:LEU:HD12	3:I:276:LEU:C	2.39	0.48
1:J:174:ASP:OD1	1:J:177:ASP:HB2	2.13	0.48
2:K:212:GLU:HB2	2:K:455:ARG:HG3	1.94	0.48
2:K:448:ARG:O	2:K:449:LYS:HG3	2.14	0.48
3:C:307:HIS:CE1	3:C:341:ALA:H	2.32	0.48
1:D:131:GLN:HG3	1:D:132:HIS:N	2.29	0.48
2:E:311:LEU:HD22	2:E:325:HIS:CD2	2.49	0.48
3:F:102:THR:O	3:F:104:ASP:N	2.46	0.48
2:H:189:GLN:HA	2:H:189:GLN:NE2	2.28	0.48
2:H:224:MET:CE	2:H:237:ARG:HE	2.27	0.48
2:H:236:TYR:HB2	2:H:298:LYS:HZ1	1.77	0.48
2:H:301:GLN:NE2	2:H:301:GLN:C	2.72	0.48
2:H:402:TRP:HB3	2:H:404:TYR:CZ	2.49	0.48
3:I:316:ASP:O	3:I:317:ASN:CB	2.61	0.48
3:L:205:LYS:HG2	3:L:331:GLY:C	2.38	0.48
2:B:191:GLU:C	2:B:193:CYS:N	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:ASP:HB2	2:B:445:TYR:OH	2.13	0.48
3:C:196:LYS:C	3:C:197:ARG:HG2	2.38	0.48
3:C:280:TYR:N	3:C:280:TYR:CD1	2.82	0.48
1:D:185:LEU:CD2	1:D:189:ILE:HG13	2.39	0.48
2:E:332:GLN:HG3	2:E:339:GLN:HB3	1.96	0.48
2:E:456:PRO:O	2:E:457:PHE:C	2.57	0.48
3:F:109:TYR:CD1	3:F:109:TYR:C	2.92	0.48
3:F:334:TRP:CD1	3:F:335:TRP:H	2.30	0.48
1:G:135:LEU:O	1:G:138:LYS:HB3	2.13	0.48
2:H:161:ILE:HG21	3:I:103:HIS:CE1	2.48	0.48
2:H:337:LYS:HG3	2:H:374:PHE:CE2	2.49	0.48
2:H:373:MET:HG3	2:H:405:ASN:HB2	1.94	0.48
3:I:386:ILE:O	3:I:387:ILE:HB	2.14	0.48
2:K:158:ASN:HD22	2:K:158:ASN:N	2.06	0.48
2:B:165:LEU:HD13	3:C:106:SER:C	2.39	0.47
2:B:293:TRP:NE1	2:B:296:ASN:ND2	2.59	0.47
3:F:92:GLU:HG2	3:F:93:ILE:N	2.29	0.47
3:F:205:LYS:HG2	3:F:331:GLY:C	2.39	0.47
3:F:229:GLY:O	3:F:230:ASN:C	2.57	0.47
2:H:176:ARG:HA	2:H:179:ILE:CG1	2.44	0.47
3:I:96:TYR:O	3:I:98:ALA:N	2.47	0.47
3:L:153:CYS:SG	3:L:192:THR:HA	2.54	0.47
1:A:148:LYS:HZ2	2:B:425:ASP:HB2	1.77	0.47
2:B:177:SER:HA	2:B:180:GLN:CG	2.43	0.47
2:B:186:VAL:HG12	3:C:127:LYS:HE2	1.96	0.47
2:B:191:GLU:HG3	2:B:192:TYR:N	2.28	0.47
2:B:296:ASN:O	2:B:299:ILE:N	2.47	0.47
3:C:103:HIS:C	3:C:105:SER:N	2.64	0.47
3:C:196:LYS:CD	3:C:198:LEU:HD11	2.43	0.47
2:E:359:GLN:OE1	2:E:438:MET:HB3	2.14	0.47
3:F:103:HIS:HD1	3:F:103:HIS:N	2.11	0.47
3:F:317:ASN:ND2	3:F:319:ASN:OD1	2.47	0.47
2:H:253:GLN:HE21	2:H:253:GLN:HB3	1.53	0.47
2:H:293:TRP:O	2:H:295:GLY:N	2.47	0.47
2:H:340:ILE:O	2:H:340:ILE:HG23	2.14	0.47
2:H:441:LYS:HB3	2:H:445:TYR:HB3	1.96	0.47
3:I:170:LYS:HZ3	3:I:177:GLN:H	1.62	0.47
3:L:344:LEU:HB3	3:L:382:THR:HG21	1.96	0.47
2:B:253:GLN:HE21	2:B:253:GLN:HB3	1.54	0.47
3:C:171:PRO:HB3	3:C:235:LEU:O	2.13	0.47
3:C:178:PHE:CD2	3:C:228:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:334:TRP:CH2	3:C:344:LEU:HG	2.50	0.47
2:E:223:GLU:CB	2:E:287:GLY:HA2	2.44	0.47
3:F:195:GLN:CB	3:F:384:MET:HE2	2.44	0.47
2:H:252:ILE:HD11	2:H:454:ILE:HG13	1.96	0.47
2:K:224:MET:SD	2:K:237:ARG:HD3	2.53	0.47
2:K:312:ILE:HB	2:K:324:ALA:HB3	1.96	0.47
2:K:313:GLU:OE2	2:K:323:LYS:NZ	2.43	0.47
2:K:364:ASN:ND2	5:K:470:NAG:O7	2.46	0.47
3:L:197:ARG:NH1	3:L:344:LEU:O	2.47	0.47
3:L:298:ASP:OD2	3:L:300:SER:HB2	2.14	0.47
1:A:137:GLN:HA	1:A:140:VAL:HG22	1.96	0.47
2:B:265:LYS:HB3	2:B:379:ASP:OD2	2.15	0.47
2:B:310:LEU:HA	2:B:454:ILE:HG22	1.97	0.47
2:E:332:GLN:CG	2:E:339:GLN:HB3	2.43	0.47
1:G:143:GLN:NE2	3:I:117:ASN:HB2	2.30	0.47
2:H:296:ASN:O	2:H:299:ILE:N	2.47	0.47
2:H:303:THR:HB	2:H:330:THR:HA	1.96	0.47
2:H:310:LEU:CB	2:H:454:ILE:HG22	2.44	0.47
3:I:373:LYS:HG3	3:I:377:TYR:CD2	2.49	0.47
1:J:164:SER:C	1:J:165:CYS:O	2.53	0.47
4:N:3:ARG:HG2	4:N:3:ARG:NH2	2.29	0.47
2:B:161:ILE:HD13	3:C:103:HIS:CD2	2.49	0.47
2:B:161:ILE:C	2:B:163:THR:H	2.23	0.47
2:B:164:ASN:H	2:B:166:ARG:HE	1.62	0.47
2:E:160:ASN:O	2:E:161:ILE:C	2.57	0.47
2:H:265:LYS:HB3	2:H:379:ASP:CG	2.40	0.47
2:H:353:LEU:HA	2:H:370:HIS:HD2	1.80	0.47
3:I:325:ASN:ND2	3:I:327:ALA:HB3	2.24	0.47
2:B:156:THR:HG22	2:B:160:ASN:ND2	2.23	0.47
2:B:161:ILE:O	2:B:166:ARG:NE	2.48	0.47
2:B:357:ALA:HA	2:B:439:ASN:HD21	1.79	0.47
2:B:367:MET:O	2:B:406:ARG:O	2.31	0.47
3:C:202:VAL:HG22	3:C:217:HIS:CE1	2.49	0.47
1:D:157:LYS:HA	1:D:157:LYS:CE	2.45	0.47
3:F:230:ASN:CA	3:F:233:ILE:HD12	2.31	0.47
2:H:361:MET:HB2	5:H:470:NAG:O7	2.14	0.47
2:H:383:ASP:HA	2:H:404:TYR:O	2.15	0.47
3:I:114:TYR:C	3:I:116:SER:N	2.72	0.47
3:I:280:TYR:CD1	3:I:280:TYR:N	2.82	0.47
1:J:147:MET:O	1:J:148:LYS:C	2.56	0.47
2:K:214:ILE:HD11	2:K:227:ILE:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:145:ILE:HD13	3:L:168:PHE:HE2	1.80	0.47
3:L:246:LEU:HD22	3:L:265:PHE:HD1	1.79	0.47
3:L:322:PHE:CE2	3:L:324:GLY:HA3	2.50	0.47
1:A:127:ILE:CG2	1:A:128:GLU:N	2.78	0.47
1:A:188:VAL:O	1:A:189:ILE:HG13	2.15	0.47
2:B:199:VAL:HG23	3:C:141:ASP:OD1	2.15	0.47
2:B:212:GLU:O	2:B:215:ILE:CG2	2.60	0.47
2:B:223:GLU:OE2	2:B:285:TYR:HD1	1.98	0.47
2:B:303:THR:HA	2:B:308:THR:OG1	2.14	0.47
2:B:304:ARG:HH22	2:B:333:ASN:H	1.60	0.47
2:B:383:ASP:HA	2:B:404:TYR:O	2.15	0.47
3:C:231:GLU:O	3:C:234:HIS:HB3	2.15	0.47
3:C:275:ARG:HA	3:C:311:GLN:HA	1.96	0.47
3:C:327:ALA:O	3:C:328:GLU:C	2.56	0.47
1:D:188:VAL:HB	2:E:164:ASN:OD1	2.15	0.47
2:E:164:ASN:O	2:E:168:LEU:HD12	2.15	0.47
2:E:333:ASN:CG	2:E:334:GLU:N	2.73	0.47
3:F:113:ILE:O	3:F:114:TYR:C	2.56	0.47
3:F:179:LEU:HG	3:F:218:LEU:CD1	2.45	0.47
1:G:142:ALA:O	1:G:146:ASP:N	2.47	0.47
1:G:150:LEU:HD22	3:I:125:LYS:HZ3	1.80	0.47
2:H:226:LEU:O	2:H:227:ILE:C	2.57	0.47
2:H:294:LEU:O	2:H:295:GLY:O	2.33	0.47
3:I:143:VAL:HG12	3:I:220:PRO:CD	2.36	0.47
3:I:147:ASP:O	3:I:148:ILE:C	2.57	0.47
3:I:300:SER:O	3:I:302:LYS:N	2.47	0.47
3:I:354:TYR:CE1	3:I:366:GLY:HA3	2.49	0.47
3:I:377:TYR:HD2	3:I:379:MET:CE	2.28	0.47
1:J:144:LEU:HD21	1:J:182:GLN:HG2	1.94	0.47
1:J:183:LYS:O	1:J:184:GLN:C	2.57	0.47
1:A:139:ASN:O	1:A:142:ALA:HB3	2.15	0.47
2:B:164:ASN:HB3	2:B:166:ARG:HH21	1.78	0.47
2:B:175:LEU:HD13	2:B:175:LEU:C	2.39	0.47
2:B:178:LYS:O	2:B:180:GLN:N	2.48	0.47
2:B:179:ILE:CD1	3:C:117:ASN:ND2	2.78	0.47
2:B:223:GLU:OE1	2:B:224:MET:O	2.33	0.47
2:B:405:ASN:CG	2:B:405:ASN:O	2.57	0.47
2:E:255:ARG:HD3	2:E:262:PHE:CZ	2.50	0.47
2:E:269:TYR:CE2	2:E:401:GLY:HA3	2.50	0.47
3:F:276:LEU:HD23	3:F:276:LEU:C	2.39	0.47
3:F:292:GLY:C	3:F:302:LYS:HD2	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:388:PRO:O	3:F:389:PHE:C	2.58	0.47
2:H:172:LEU:CD2	3:I:113:ILE:HG22	2.45	0.47
3:I:251:GLU:HA	3:I:256:ARG:O	2.14	0.47
3:I:318:ASP:OD2	3:I:325:ASN:HB2	2.15	0.47
3:L:179:LEU:HG	3:L:218:LEU:CD1	2.45	0.47
3:C:99:SER:O	3:C:102:THR:HG23	2.15	0.47
3:C:213:GLU:O	3:C:232:LYS:HE3	2.14	0.47
2:E:210:GLU:OE2	2:E:213:GLU:HB2	2.15	0.47
1:G:158:ILE:HG13	2:H:189:GLN:HG2	1.96	0.47
2:H:223:GLU:OE1	2:H:224:MET:O	2.33	0.47
3:I:203:ASP:O	3:I:206:LYS:HE3	2.15	0.47
2:K:333:ASN:N	2:K:336:ASN:HD22	2.10	0.47
3:L:330:ASP:HB3	3:L:343:HIS:HE1	1.79	0.47
2:B:157:VAL:C	2:B:158:ASN:ND2	2.63	0.47
1:D:179:GLU:O	1:D:180:ASP:C	2.57	0.47
2:E:157:VAL:HG23	2:E:158:ASN:N	2.30	0.47
2:E:270:LYS:HA	2:E:296:ASN:HB3	1.96	0.47
2:E:270:LYS:HG3	2:E:338:TYR:OH	2.15	0.47
2:E:280:THR:O	2:E:281:ASP:O	2.32	0.47
3:F:360:PRO:O	3:F:361:ASN:ND2	2.48	0.47
1:G:171:ARG:HH11	1:G:171:ARG:CG	2.28	0.47
2:H:249:TRP:CE3	2:H:455:ARG:HB2	2.50	0.47
2:H:339:GLN:HG2	2:H:340:ILE:N	2.29	0.47
3:I:107:ILE:C	3:I:109:TYR:N	2.72	0.47
3:I:134:GLN:O	3:I:136:GLN:N	2.43	0.47
3:I:262:TYR:OH	3:I:288:ASP:OD1	2.23	0.47
1:J:183:LYS:O	1:J:186:GLU:HB2	2.15	0.47
2:K:218:GLY:HA3	3:L:210:GLN:HG2	1.97	0.47
1:A:149:ARG:HD3	2:B:427:ALA:O	2.14	0.46
2:B:252:ILE:HD11	2:B:454:ILE:HG13	1.96	0.46
2:B:266:TRP:HB2	2:B:379:ASP:OD2	2.15	0.46
3:C:316:ASP:O	3:C:317:ASN:CB	2.62	0.46
3:C:334:TRP:O	3:C:335:TRP:C	2.58	0.46
1:D:169:LEU:CD1	2:E:185:ASP:OD1	2.63	0.46
3:F:246:LEU:HD22	3:F:265:PHE:HD1	1.79	0.46
1:G:149:ARG:NH2	2:H:425:ASP:HA	2.24	0.46
3:I:172:LEU:HD12	3:I:172:LEU:N	2.27	0.46
3:I:196:LYS:C	3:I:197:ARG:HG2	2.40	0.46
2:K:215:ILE:C	2:K:217:LYS:H	2.22	0.46
1:A:167:ARG:HD2	1:A:167:ARG:C	2.40	0.46
2:B:207:SER:O	2:B:214:ILE:HG12	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:TRP:CZ3	2:B:455:ARG:HB2	2.50	0.46
2:B:270:LYS:HD2	2:B:334:GLU:OE1	2.15	0.46
2:B:301:GLN:NE2	2:B:301:GLN:C	2.73	0.46
3:C:253:TRP:CD1	3:C:253:TRP:H	2.33	0.46
3:C:262:TYR:OH	3:C:288:ASP:OD1	2.25	0.46
3:C:310:MET:O	3:C:335:TRP:CD1	2.68	0.46
2:E:328:GLY:HA3	2:E:343:ASN:OD1	2.15	0.46
2:H:226:LEU:O	2:H:227:ILE:O	2.33	0.46
3:I:167:TYR:N	3:I:167:TYR:HD1	2.11	0.46
3:I:196:LYS:HA	3:I:382:THR:O	2.16	0.46
2:K:301:GLN:HE22	2:K:302:LEU:HG	1.77	0.46
2:K:374:PHE:CB	2:K:382:ASN:HB3	2.45	0.46
3:L:290:PHE:HA	3:L:307:HIS:HD1	1.78	0.46
3:L:365:ASN:C	3:L:365:ASN:ND2	2.73	0.46
2:B:177:SER:HA	2:B:180:GLN:HG3	1.98	0.46
2:B:257:ASP:O	2:B:291:GLU:OE2	2.33	0.46
3:C:170:LYS:CE	3:C:177:GLN:HB3	2.44	0.46
3:C:212:LYS:CG	3:C:231:GLU:HB2	2.40	0.46
3:C:298:ASP:CG	3:C:299:PRO:HD2	2.40	0.46
2:E:215:ILE:C	2:E:217:LYS:H	2.23	0.46
2:H:421:GLN:NE2	2:H:444:TRP:O	2.48	0.46
3:I:340:HIS:O	4:S:1:GLY:N	2.43	0.46
1:J:122:LEU:HD21	3:L:98:ALA:HA	1.98	0.46
2:K:233:VAL:HG13	2:K:233:VAL:O	2.14	0.46
3:L:96:TYR:CD2	3:L:96:TYR:N	2.79	0.46
3:L:219:SER:CB	3:L:224:THR:CG2	2.91	0.46
1:A:185:LEU:HD13	1:A:185:LEU:C	2.39	0.46
2:B:181:LYS:C	2:B:183:GLU:N	2.73	0.46
3:C:219:SER:HB2	3:C:220:PRO:HD2	1.97	0.46
3:C:233:ILE:HA	3:C:236:ILE:CD1	2.42	0.46
1:D:143:GLN:HE21	3:F:118:ASN:HD22	1.64	0.46
3:F:344:LEU:HB3	3:F:382:THR:HG21	1.97	0.46
2:H:214:ILE:CD1	2:H:227:ILE:HG22	2.41	0.46
3:I:191:TRP:HH2	3:I:247:ARG:NH1	2.13	0.46
3:I:344:LEU:HD12	3:I:384:MET:CE	2.45	0.46
3:C:128:VAL:O	3:C:129:ALA:C	2.56	0.46
3:C:189:ASN:OD1	3:C:391:ARG:NE	2.39	0.46
3:C:354:TYR:CE1	3:C:366:GLY:HA3	2.50	0.46
3:C:372:TRP:CE3	3:C:373:LYS:HE3	2.50	0.46
1:D:159:ARG:HH11	1:D:159:ARG:HB3	1.81	0.46
1:D:164:SER:O	1:D:165:CYS:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:100:ILE:O	3:F:100:ILE:HG22	2.16	0.46
3:F:160:GLY:O	3:F:161:ALA:CB	2.61	0.46
1:G:122:LEU:C	1:G:124:ARG:H	2.23	0.46
1:G:133:ILE:HD12	1:G:133:ILE:N	2.29	0.46
3:I:103:HIS:C	3:I:105:SER:N	2.73	0.46
3:I:298:ASP:CG	3:I:299:PRO:HD2	2.41	0.46
3:I:304:PHE:O	3:I:337:ASN:CG	2.58	0.46
2:K:370:HIS:HE1	2:K:408:HIS:HB2	1.77	0.46
2:B:215:ILE:HB	2:B:242:MET:CE	2.45	0.46
2:E:224:MET:SD	2:E:237:ARG:HD3	2.55	0.46
3:F:103:HIS:HD1	3:F:103:HIS:H	1.64	0.46
1:G:164:SER:HA	3:I:137:GLU:O	2.15	0.46
2:H:365:ARG:O	2:H:368:THR:N	2.49	0.46
3:I:213:GLU:O	3:I:232:LYS:HE3	2.15	0.46
3:I:312:PHE:HZ	3:I:333:GLY:O	1.98	0.46
1:A:128:GLU:OE1	1:A:129:LYS:CD	2.63	0.46
1:A:128:GLU:C	1:A:131:GLN:HG2	2.40	0.46
1:A:175:LEU:C	1:A:177:ASP:N	2.74	0.46
2:B:283:LYS:HB3	2:B:285:TYR:CE2	2.51	0.46
2:B:353:LEU:HA	2:B:370:HIS:HD2	1.81	0.46
3:C:160:GLY:O	3:C:161:ALA:CB	2.63	0.46
3:C:197:ARG:HA	3:C:225:GLU:HG3	1.96	0.46
1:D:126:VAL:C	1:D:130:VAL:HG23	2.41	0.46
3:F:109:TYR:HA	3:F:112:GLU:OE1	2.16	0.46
2:H:202:ASN:O	2:H:204:PRO:HD3	2.15	0.46
2:H:230:ASP:C	2:H:232:SER:N	2.74	0.46
3:I:93:ILE:O	3:I:96:TYR:CD2	2.69	0.46
3:I:208:TRP:HZ2	3:I:270:GLU:HG3	1.80	0.46
3:I:250:LEU:HD23	3:I:372:TRP:CE3	2.51	0.46
3:I:334:TRP:CH2	3:I:344:LEU:HG	2.51	0.46
3:I:367:ILE:HB	3:I:379:MET:N	2.30	0.46
1:J:159:ARG:HD3	2:K:418:TRP:HZ3	1.80	0.46
2:K:161:ILE:HB	2:K:162:PRO:HD3	1.98	0.46
3:L:152:ASP:OD1	3:L:154:GLN:N	2.48	0.46
3:L:391:ARG:HH11	3:L:391:ARG:CB	2.24	0.46
2:B:215:ILE:HD13	2:B:242:MET:HB3	1.98	0.46
2:B:336:ASN:C	2:B:338:TYR:N	2.72	0.46
2:B:363:GLU:O	2:B:367:MET:HE2	2.15	0.46
3:C:246:LEU:HD11	3:C:248:VAL:HG23	1.97	0.46
3:F:119:GLN:HE21	3:F:119:GLN:CA	2.13	0.46
3:F:322:PHE:CE2	3:F:324:GLY:HA3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:352:GLY:O	3:F:377:TYR:HA	2.15	0.46
2:H:201:CYS:O	3:I:143:VAL:HG21	2.16	0.46
2:H:301:GLN:O	2:H:304:ARG:HB2	2.16	0.46
2:H:332:GLN:HB3	2:H:336:ASN:HD22	1.80	0.46
3:I:114:TYR:C	3:I:116:SER:H	2.22	0.46
3:I:184:ILE:HD12	3:I:184:ILE:N	2.31	0.46
3:I:318:ASP:HB2	3:I:320:ASP:OD1	2.15	0.46
3:I:325:ASN:HD21	3:I:327:ALA:CB	2.27	0.46
2:K:180:GLN:NE2	2:K:180:GLN:C	2.74	0.46
2:K:369:ILE:O	2:K:405:ASN:ND2	2.46	0.46
3:L:334:TRP:CG	3:L:335:TRP:N	2.83	0.46
1:A:157:LYS:HD2	3:C:132:GLU:CB	2.45	0.46
2:B:184:SER:O	2:B:188:ALA:N	2.46	0.46
2:B:365:ARG:O	2:B:368:THR:N	2.49	0.46
2:B:406:ARG:O	2:B:406:ARG:CG	2.62	0.46
2:E:255:ARG:HH11	2:E:255:ARG:CG	2.28	0.46
2:E:312:ILE:HB	2:E:324:ALA:HB3	1.97	0.46
3:F:95:LYS:HD2	3:F:98:ALA:CB	2.46	0.46
2:H:198:THR:HA	3:I:140:LYS:O	2.15	0.46
2:H:336:ASN:C	2:H:338:TYR:N	2.73	0.46
2:H:364:ASN:ND2	5:H:470:NAG:C6	2.78	0.46
2:H:377:THR:O	2:H:379:ASP:N	2.47	0.46
3:I:219:SER:HB2	3:I:220:PRO:HD2	1.97	0.46
2:K:266:TRP:H	2:K:379:ASP:CG	2.23	0.46
1:A:165:CYS:HB3	2:B:193:CYS:HA	1.97	0.46
2:B:214:ILE:CD1	2:B:227:ILE:HG22	2.41	0.46
2:B:310:LEU:CB	2:B:454:ILE:HG22	2.46	0.46
2:B:311:LEU:HB3	2:B:453:LYS:O	2.16	0.46
3:C:242:ILE:HA	3:C:243:PRO:HD2	1.72	0.46
3:C:253:TRP:CZ3	3:C:380:LYS:HG3	2.51	0.46
3:C:367:ILE:HB	3:C:379:MET:N	2.31	0.46
1:D:136:LEU:HD23	2:E:168:LEU:HD22	1.96	0.46
3:F:333:GLY:O	3:F:334:TRP:HB2	2.16	0.46
1:G:154:ILE:CD1	2:H:186:VAL:HG21	2.44	0.46
2:H:152:TYR:HE2	2:H:155:GLU:OE2	1.98	0.46
2:H:155:GLU:C	2:H:157:VAL:H	2.24	0.46
2:H:311:LEU:HB3	2:H:453:LYS:O	2.16	0.46
2:H:398:ASP:HA	2:H:433:ASP:HA	1.98	0.46
3:I:170:LYS:CE	3:I:177:GLN:HB3	2.45	0.46
3:I:253:TRP:CD1	3:I:253:TRP:H	2.34	0.46
2:K:161:ILE:N	2:K:162:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:255:ARG:HH11	2:K:255:ARG:CG	2.27	0.46
4:R:3:ARG:HG2	4:R:3:ARG:NH2	2.31	0.46
1:A:139:ASN:O	3:C:114:TYR:OH	2.28	0.45
2:B:366:THR:C	2:B:368:THR:H	2.22	0.45
3:C:131:LEU:HD23	3:C:132:GLU:N	2.32	0.45
3:C:197:ARG:NH1	3:C:204:PHE:CD1	2.84	0.45
3:C:250:LEU:O	3:C:257:THR:HB	2.16	0.45
1:D:147:MET:SD	3:F:121:ILE:HD11	2.56	0.45
2:E:266:TRP:H	2:E:379:ASP:CG	2.23	0.45
3:F:104:ASP:O	3:F:108:ARG:N	2.39	0.45
3:L:276:LEU:HD23	3:L:276:LEU:C	2.40	0.45
1:A:145:VAL:HG13	1:A:148:LYS:HE2	1.99	0.45
2:B:201:CYS:O	3:C:143:VAL:HG21	2.16	0.45
2:B:329:PHE:HD1	2:B:342:VAL:HG12	1.81	0.45
2:B:377:THR:O	2:B:379:ASP:N	2.46	0.45
3:C:178:PHE:CE2	3:C:232:LYS:HB3	2.51	0.45
3:C:250:LEU:HD23	3:C:372:TRP:CE3	2.52	0.45
2:H:210:GLU:OE1	2:H:212:GLU:CB	2.64	0.45
2:H:359:GLN:O	2:H:359:GLN:HG2	2.17	0.45
3:I:178:PHE:HD1	3:I:178:PHE:H	1.63	0.45
3:I:342:GLY:HA2	3:I:368:ILE:O	2.17	0.45
1:J:154:ILE:O	1:J:155:ASP:C	2.59	0.45
2:K:223:GLU:CB	2:K:287:GLY:HA2	2.46	0.45
3:L:169:ILE:HD11	3:L:236:ILE:HD11	1.97	0.45
3:L:219:SER:HB3	3:L:224:THR:HG21	1.96	0.45
2:B:398:ASP:HA	2:B:433:ASP:CA	2.45	0.45
3:C:103:HIS:HA	3:C:106:SER:OG	2.17	0.45
3:C:243:PRO:HG3	3:F:279:ALA:HB1	1.99	0.45
3:C:337:ASN:OD1	3:C:338:LYS:N	2.47	0.45
3:C:352:GLY:O	3:C:353:THR:C	2.59	0.45
2:E:204:PRO:HG2	2:E:224:MET:O	2.17	0.45
2:E:420:GLY:HA2	2:E:446:SER:O	2.17	0.45
3:F:304:PHE:O	3:F:337:ASN:ND2	2.46	0.45
2:H:152:TYR:O	2:H:153:ILE:C	2.59	0.45
2:H:184:SER:O	2:H:187:SER:N	2.41	0.45
2:H:283:LYS:HB3	2:H:285:TYR:CE2	2.51	0.45
2:H:310:LEU:HB3	2:H:454:ILE:HG22	1.98	0.45
3:I:96:TYR:C	3:I:98:ALA:N	2.74	0.45
3:I:189:ASN:OD1	3:I:391:ARG:NE	2.40	0.45
3:I:242:ILE:HA	3:I:243:PRO:HD2	1.71	0.45
3:I:301:ASP:HA	4:S:2:HYP:OD1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:304:PHE:HB3	3:I:338:LYS:HB3	1.98	0.45
2:K:359:GLN:OE1	2:K:438:MET:HB3	2.16	0.45
3:L:317:ASN:ND2	3:L:319:ASN:OD1	2.49	0.45
2:B:255:ARG:NH1	2:B:413:ASN:HA	2.31	0.45
2:B:351:ASN:ND2	2:B:354:MET:HG2	2.25	0.45
1:D:132:HIS:O	1:D:135:LEU:HB3	2.15	0.45
3:F:152:ASP:OD1	3:F:154:GLN:N	2.48	0.45
3:F:281:PHE:C	3:F:283:GLY:H	2.24	0.45
1:G:148:LYS:NZ	2:H:425:ASP:O	2.49	0.45
1:G:150:LEU:HD22	3:I:121:ILE:HD11	1.98	0.45
2:H:182:LEU:HD23	2:H:182:LEU:O	2.15	0.45
2:H:215:ILE:HB	2:H:242:MET:CE	2.46	0.45
2:H:292:TYR:CE2	2:H:294:LEU:HB2	2.49	0.45
2:H:398:ASP:HA	2:H:433:ASP:CA	2.45	0.45
3:I:304:PHE:CE2	3:I:338:LYS:HD3	2.51	0.45
1:J:121:VAL:O	1:J:121:VAL:HG12	2.16	0.45
1:J:131:GLN:NE2	1:J:132:HIS:N	2.64	0.45
2:K:313:GLU:HG2	2:K:323:LYS:HD2	1.98	0.45
2:K:378:TYR:HB2	2:K:396:LYS:HG2	1.98	0.45
3:L:195:GLN:HG3	3:L:227:TRP:CE3	2.52	0.45
4:M:3:ARG:O	4:M:5:NH2:N	2.50	0.45
1:A:151:GLU:HB2	2:B:182:LEU:HD13	1.98	0.45
2:B:398:ASP:C	2:B:433:ASP:HB2	2.42	0.45
3:C:196:LYS:HD2	3:C:198:LEU:CD1	2.46	0.45
3:C:322:PHE:C	3:C:324:GLY:N	2.72	0.45
2:E:257:ASP:HA	2:E:416:TYR:CE2	2.51	0.45
2:H:252:ILE:HG22	2:H:299:ILE:HD11	1.99	0.45
2:H:279:ASN:C	2:H:281:ASP:N	2.75	0.45
2:K:327:GLY:CA	2:K:344:LYS:HE3	2.45	0.45
3:L:124:LEU:O	3:L:125:LYS:C	2.59	0.45
2:B:176:ARG:HA	2:B:176:ARG:NH1	2.31	0.45
2:B:236:TYR:CB	2:B:298:LYS:NZ	2.76	0.45
3:C:132:GLU:C	3:C:134:GLN:H	2.24	0.45
3:C:377:TYR:HD2	3:C:379:MET:CE	2.29	0.45
2:E:305:MET:O	2:E:305:MET:HG2	2.16	0.45
2:E:382:ASN:O	2:E:383:ASP:O	2.34	0.45
2:E:406:ARG:HG2	2:E:406:ARG:O	2.16	0.45
1:G:127:ILE:O	1:G:131:GLN:N	2.49	0.45
3:I:191:TRP:CG	3:I:385:LYS:HD2	2.52	0.45
3:I:200:GLY:H	3:I:225:GLU:CD	2.20	0.45
3:I:251:GLU:CD	3:I:381:LYS:HD2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:118:ASN:O	3:L:122:VAL:HG23	2.16	0.45
3:L:183:GLU:HB3	3:L:191:TRP:HB2	1.99	0.45
3:L:304:PHE:CD1	3:L:338:LYS:CB	2.99	0.45
3:L:352:GLY:O	3:L:377:TYR:HA	2.16	0.45
1:A:144:LEU:HG	1:A:182:GLN:OE1	2.16	0.45
1:A:149:ARG:HA	1:A:152:VAL:HG23	1.99	0.45
1:A:191:LYS:O	1:A:192:ASP:OD2	2.34	0.45
2:B:166:ARG:CD	2:B:166:ARG:N	2.80	0.45
2:B:294:LEU:O	2:B:295:GLY:O	2.35	0.45
3:C:197:ARG:HD3	3:C:204:PHE:CE1	2.52	0.45
3:C:226:PHE:HE2	3:C:228:LEU:HB2	1.82	0.45
2:E:160:ASN:N	2:E:162:PRO:HD2	2.31	0.45
3:F:119:GLN:O	3:F:122:VAL:HB	2.17	0.45
3:F:344:LEU:HA	3:F:367:ILE:CG2	2.46	0.45
1:G:126:VAL:O	1:G:127:ILE:C	2.59	0.45
1:G:159:ARG:HG2	2:H:258:GLY:HA3	1.99	0.45
2:H:176:ARG:CZ	2:H:176:ARG:HB3	2.46	0.45
2:H:326:TYR:OH	2:H:353:LEU:HB2	2.17	0.45
3:I:129:ALA:O	3:I:132:GLU:HB3	2.16	0.45
3:I:208:TRP:HE3	3:I:314:THR:CG2	2.28	0.45
3:I:250:LEU:HG	3:I:251:GLU:H	1.80	0.45
3:I:270:GLU:HB2	3:I:274:TYR:OH	2.16	0.45
2:K:314:MET:HE1	2:K:437:TRP:CD2	2.52	0.45
1:A:133:ILE:HG22	1:A:137:GLN:OE1	2.17	0.45
2:B:205:VAL:CG1	3:C:232:LYS:HZ3	2.29	0.45
3:C:197:ARG:C	3:C:198:LEU:HD12	2.41	0.45
3:F:251:GLU:CB	3:F:381:LYS:HB2	2.46	0.45
3:F:321:LYS:N	3:F:337:ASN:O	2.38	0.45
2:H:257:ASP:O	2:H:291:GLU:OE2	2.34	0.45
2:H:351:ASN:ND2	2:H:354:MET:HG2	2.25	0.45
2:H:423:THR:HA	2:H:444:TRP:CE3	2.52	0.45
2:K:168:LEU:HB3	3:L:110:LEU:HD13	1.99	0.45
1:A:133:ILE:C	1:A:135:LEU:N	2.73	0.45
3:C:214:GLY:HA3	3:C:228:LEU:O	2.17	0.45
1:D:122:LEU:N	1:D:124:ARG:HG2	2.31	0.45
2:E:257:ASP:OD2	2:E:259:SER:OG	2.34	0.45
3:F:118:ASN:HD22	3:F:118:ASN:HA	1.66	0.45
3:F:219:SER:CB	3:F:224:THR:HG21	2.46	0.45
1:G:129:LYS:HA	1:G:133:ILE:HD13	1.99	0.45
2:H:366:THR:C	2:H:368:THR:H	2.24	0.45
2:H:437:TRP:HB3	2:H:447:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:207:ASN:ND2	3:I:210:GLN:HG3	2.31	0.45
3:I:212:LYS:C	3:I:214:GLY:H	2.25	0.45
1:J:176:LYS:HB2	1:J:176:LYS:HE3	1.68	0.45
2:K:204:PRO:O	2:K:205:VAL:C	2.60	0.45
2:K:301:GLN:NE2	2:K:301:GLN:C	2.75	0.45
2:K:304:ARG:C	2:K:306:GLY:N	2.73	0.45
3:L:293:PHE:N	3:L:305:THR:OG1	2.50	0.45
2:B:230:ASP:C	2:B:232:SER:N	2.75	0.45
3:C:173:LYS:HE3	3:C:238:THR:O	2.17	0.45
3:C:304:PHE:O	3:C:337:ASN:CG	2.59	0.45
3:C:340:HIS:O	4:O:1:GLY:CA	2.65	0.45
2:E:314:MET:HE1	2:E:437:TRP:CD2	2.51	0.45
3:F:325:ASN:O	3:F:326:CYS:C	2.60	0.45
2:H:153:ILE:HG23	2:H:154:ASP:OD2	2.17	0.45
3:I:95:LYS:C	3:I:97:GLU:N	2.70	0.45
3:I:223:THR:O	3:I:224:THR:HB	2.17	0.45
3:I:364:ASP:OD2	4:S:1:GLY:N	2.42	0.45
3:I:367:ILE:CG2	3:I:379:MET:HB2	2.46	0.45
3:L:166:LEU:HD22	3:L:179:LEU:CD1	2.45	0.45
3:L:207:ASN:OD1	3:L:208:TRP:N	2.50	0.45
3:L:261:ASP:C	3:L:262:TYR:HD2	2.24	0.45
2:B:164:ASN:C	2:B:166:ARG:N	2.75	0.44
2:B:164:ASN:C	2:B:166:ARG:HE	2.26	0.44
3:C:184:ILE:HD12	3:C:184:ILE:N	2.32	0.44
3:C:212:LYS:C	3:C:214:GLY:N	2.74	0.44
2:E:172:LEU:HG	3:F:113:ILE:CG2	2.47	0.44
2:E:367:MET:O	2:E:405:ASN:ND2	2.50	0.44
2:E:388:SER:O	2:E:389:ASP:C	2.60	0.44
3:I:226:PHE:HE2	3:I:228:LEU:HB2	1.82	0.44
3:I:275:ARG:CA	3:I:311:GLN:HA	2.48	0.44
2:K:203:ILE:HA	2:K:204:PRO:HD3	1.77	0.44
3:L:97:GLU:HA	3:L:100:ILE:CD1	2.47	0.44
1:A:167:ARG:NE	2:B:192:TYR:CD2	2.73	0.44
2:B:214:ILE:HG22	2:B:214:ILE:O	2.17	0.44
2:B:398:ASP:HA	2:B:433:ASP:HA	1.99	0.44
3:C:124:LEU:O	3:C:124:LEU:CG	2.65	0.44
3:C:167:TYR:N	3:C:167:TYR:HD1	2.12	0.44
1:D:131:GLN:HA	1:D:134:GLN:HG2	1.99	0.44
2:H:374:PHE:O	2:H:375:PHE:C	2.60	0.44
2:H:455:ARG:HG2	2:H:456:PRO:HD2	1.97	0.44
3:I:178:PHE:CD2	3:I:228:LEU:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:LEU:C	1:J:122:LEU:CD1	2.90	0.44
2:K:170:SER:O	2:K:171:ILE:C	2.59	0.44
3:L:105:SER:O	3:L:108:ARG:HG2	2.18	0.44
3:L:293:PHE:O	3:L:301:ASP:O	2.35	0.44
2:B:161:ILE:HG23	2:B:166:ARG:CZ	2.47	0.44
2:B:167:VAL:O	2:B:171:ILE:HG12	2.17	0.44
2:B:329:PHE:CZ	2:B:331:VAL:HG23	2.52	0.44
2:B:411:ASN:HD22	2:B:434:GLY:H	1.64	0.44
3:C:191:TRP:HH2	3:C:247:ARG:NH1	2.14	0.44
3:C:253:TRP:CZ2	3:C:349:TYR:O	2.70	0.44
3:C:310:MET:HE2	3:C:310:MET:HA	1.97	0.44
2:E:406:ARG:NH2	4:N:4:PRO:C	2.76	0.44
2:E:415:ARG:H	2:E:434:GLY:HA2	1.82	0.44
3:F:148:ILE:N	3:F:148:ILE:CD1	2.68	0.44
3:F:293:PHE:N	3:F:305:THR:OG1	2.50	0.44
1:G:129:LYS:HA	1:G:133:ILE:HD11	1.99	0.44
3:I:196:LYS:CD	3:I:198:LEU:HD11	2.47	0.44
2:K:405:ASN:O	2:K:407:CYS:N	2.50	0.44
2:K:408:HIS:CE1	2:K:411:ASN:HB2	2.51	0.44
3:L:121:ILE:O	3:L:125:LYS:HG2	2.18	0.44
3:L:325:ASN:O	3:L:326:CYS:C	2.60	0.44
1:A:119:ILE:O	1:A:119:ILE:HG23	2.18	0.44
2:B:265:LYS:HE3	2:B:378:TYR:CE1	2.53	0.44
2:B:266:TRP:CD1	2:B:380:ARG:HE	2.35	0.44
2:B:279:ASN:C	2:B:281:ASP:N	2.75	0.44
2:B:293:TRP:O	2:B:295:GLY:N	2.50	0.44
3:C:134:GLN:C	3:C:136:GLN:H	2.25	0.44
3:C:143:VAL:O	3:C:144:GLN:HG3	2.17	0.44
3:C:367:ILE:CG2	3:C:379:MET:HB2	2.47	0.44
2:E:303:THR:CB	2:E:330:THR:HA	2.46	0.44
2:E:407:CYS:HB2	4:N:3:ARG:HH22	1.81	0.44
2:E:423:THR:HG23	2:E:426:MET:HE3	1.99	0.44
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.99	0.44
3:F:298:ASP:OD2	3:F:300:SER:HB2	2.17	0.44
2:H:154:ASP:C	2:H:157:VAL:HG22	2.43	0.44
2:H:193:CYS:O	3:I:134:GLN:OE1	2.36	0.44
2:H:206:VAL:HG22	2:H:214:ILE:HG23	1.99	0.44
2:H:301:GLN:HE22	2:H:302:LEU:CD2	2.24	0.44
3:I:154:GLN:OE1	3:I:190:GLY:N	2.49	0.44
3:I:340:HIS:CE1	3:I:364:ASP:OD2	2.70	0.44
1:J:130:VAL:CA	1:J:133:ILE:HG22	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:181:GLN:HE21	2:K:171:ILE:HA	1.82	0.44
3:L:197:ARG:NE	3:L:204:PHE:CE1	2.85	0.44
3:L:244:TYR:CD2	3:L:387:ILE:C	2.95	0.44
3:L:307:HIS:HA	3:L:310:MET:HG2	1.98	0.44
1:A:119:ILE:HD11	3:C:95:LYS:NZ	2.31	0.44
2:B:164:ASN:H	2:B:166:ARG:NE	2.15	0.44
2:B:165:LEU:CG	2:B:166:ARG:NH2	2.80	0.44
3:C:169:ILE:HD12	3:C:171:PRO:CD	2.38	0.44
3:C:251:GLU:HA	3:C:257:THR:HA	1.99	0.44
1:D:133:ILE:C	1:D:135:LEU:H	2.25	0.44
3:F:261:ASP:C	3:F:262:TYR:HD2	2.25	0.44
3:F:293:PHE:O	3:F:301:ASP:O	2.36	0.44
1:G:125:LYS:HG2	1:G:129:LYS:HE2	1.98	0.44
1:G:154:ILE:HD12	2:H:182:LEU:CD2	2.47	0.44
2:H:236:TYR:O	2:H:236:TYR:CD1	2.70	0.44
2:H:310:LEU:HD23	2:H:329:PHE:CG	2.52	0.44
3:I:207:ASN:OD1	3:I:207:ASN:C	2.60	0.44
3:I:310:MET:O	3:I:335:TRP:HD1	1.99	0.44
3:I:316:ASP:O	3:I:316:ASP:OD2	2.35	0.44
2:K:366:THR:HA	2:K:369:ILE:HG13	1.99	0.44
3:L:230:ASN:O	3:L:231:GLU:C	2.60	0.44
1:A:131:GLN:C	1:A:133:ILE:N	2.75	0.44
2:B:256:GLN:NE2	2:B:449:LYS:HZ1	2.02	0.44
3:C:143:VAL:C	3:C:144:GLN:HG3	2.43	0.44
3:C:163:GLN:O	3:C:167:TYR:OH	2.30	0.44
3:C:191:TRP:CG	3:C:385:LYS:HD2	2.52	0.44
3:C:369:TRP:NE1	3:C:371:THR:OG1	2.51	0.44
1:D:135:LEU:CD2	1:D:139:ASN:HD21	2.31	0.44
3:F:290:PHE:CD1	3:F:307:HIS:ND1	2.86	0.44
2:H:351:ASN:OD1	2:H:354:MET:HG3	2.18	0.44
2:H:402:TRP:CH2	2:H:412:PRO:HD2	2.52	0.44
3:I:154:GLN:NE2	3:I:190:GLY:H	2.14	0.44
2:K:309:GLU:HB2	2:K:325:HIS:HE1	1.82	0.44
2:K:333:ASN:CG	2:K:334:GLU:N	2.76	0.44
2:K:398:ASP:C	2:K:433:ASP:HB3	2.42	0.44
3:L:271:ALA:C	3:L:273:LYS:H	2.24	0.44
2:B:155:GLU:O	2:B:159:SER:N	2.49	0.44
2:B:390:PRO:O	2:B:393:GLN:NE2	2.51	0.44
3:C:278:TYR:CD1	3:C:278:TYR:C	2.96	0.44
2:E:157:VAL:C	2:E:158:ASN:HD22	2.25	0.44
2:E:201:CYS:CB	2:E:224:MET:HE1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:253:GLN:HB2	2:E:293:TRP:CZ3	2.53	0.44
2:E:324:ALA:HB2	2:E:349:ALA:HB3	1.98	0.44
2:E:327:GLY:CA	2:E:344:LYS:HE3	2.46	0.44
2:E:366:THR:HA	2:E:369:ILE:HG13	2.00	0.44
2:E:434:GLY:O	2:E:436:VAL:HG13	2.18	0.44
3:F:230:ASN:O	3:F:231:GLU:C	2.59	0.44
3:I:169:ILE:HD12	3:I:171:PRO:CD	2.39	0.44
3:I:212:LYS:CG	3:I:231:GLU:HB2	2.43	0.44
3:I:251:GLU:HA	3:I:257:THR:HA	1.99	0.44
3:I:295:PHE:HB2	3:I:301:ASP:OD2	2.18	0.44
2:K:332:GLN:CG	2:K:339:GLN:HB3	2.47	0.44
3:L:195:GLN:CG	3:L:384:MET:HE2	2.48	0.44
2:B:198:THR:HA	3:C:140:LYS:O	2.18	0.44
2:B:411:ASN:C	2:B:412:PRO:O	2.56	0.44
3:C:123:ASN:C	3:C:125:LYS:H	2.25	0.44
1:D:133:ILE:HG13	3:F:107:ILE:HD12	1.99	0.44
2:E:360:LEU:CD1	2:E:364:ASN:O	2.62	0.44
2:E:433:ASP:O	2:E:433:ASP:OD1	2.36	0.44
2:H:170:SER:O	2:H:173:GLU:HB2	2.18	0.44
2:H:191:GLU:O	2:H:193:CYS:N	2.49	0.44
2:H:228:GLN:NE2	2:H:231:SER:OG	2.51	0.44
1:J:167:ARG:NH1	2:K:192:TYR:CZ	2.86	0.44
2:K:382:ASN:O	2:K:383:ASP:O	2.35	0.44
3:L:96:TYR:O	3:L:99:SER:HB2	2.18	0.44
3:L:250:LEU:HD23	3:L:372:TRP:HE3	1.83	0.44
1:A:119:ILE:HD11	3:C:95:LYS:HZ3	1.82	0.44
1:A:166:SER:CB	2:B:195:THR:O	2.66	0.44
2:B:159:SER:CA	2:B:162:PRO:HD2	2.48	0.44
2:B:236:TYR:HB2	2:B:298:LYS:HZ1	1.80	0.44
3:C:143:VAL:HG12	3:C:220:PRO:CD	2.40	0.44
3:C:204:PHE:CE2	3:C:227:TRP:HB2	2.53	0.44
2:E:214:ILE:HD11	2:E:227:ILE:CG2	2.47	0.44
2:E:373:MET:HA	2:E:373:MET:HE3	2.00	0.44
2:H:207:SER:O	2:H:214:ILE:HG12	2.16	0.44
2:H:319:GLY:O	2:H:320:ASP:C	2.60	0.44
2:H:329:PHE:CZ	2:H:331:VAL:HG23	2.53	0.44
3:I:178:PHE:CE2	3:I:232:LYS:HB3	2.53	0.44
3:I:195:GLN:HE21	3:I:195:GLN:HB3	1.64	0.44
3:I:239:GLN:O	3:I:240:SER:HB3	2.17	0.44
3:I:331:GLY:O	3:I:332:SER:CB	2.65	0.44
1:J:124:ARG:O	1:J:128:GLU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:332:GLN:HB3	2:K:336:ASN:CB	2.47	0.44
1:A:137:GLN:CA	1:A:140:VAL:HG22	2.48	0.43
2:B:165:LEU:N	2:B:166:ARG:CZ	2.81	0.43
2:B:303:THR:O	2:B:308:THR:OG1	2.35	0.43
3:C:208:TRP:HZ2	3:C:270:GLU:HG3	1.83	0.43
3:C:211:TYR:HD1	3:C:227:TRP:NE1	2.16	0.43
3:C:273:LYS:HG3	3:C:319:ASN:ND2	2.33	0.43
3:C:328:GLU:O	3:C:329:GLN:C	2.60	0.43
2:E:187:SER:O	2:E:188:ALA:C	2.61	0.43
2:E:270:LYS:HE2	2:E:297:ASP:OD2	2.17	0.43
3:F:189:ASN:ND2	3:F:391:ARG:HG2	2.33	0.43
3:F:204:PHE:O	3:F:206:LYS:N	2.48	0.43
3:F:250:LEU:HD21	3:F:369:TRP:CG	2.53	0.43
1:G:136:LEU:C	1:G:138:LYS:H	2.25	0.43
1:G:140:VAL:O	1:G:141:ARG:C	2.60	0.43
1:G:188:VAL:HG21	2:H:167:VAL:HG21	1.99	0.43
2:H:167:VAL:O	2:H:171:ILE:HG12	2.18	0.43
2:H:445:TYR:CD1	2:H:445:TYR:C	2.96	0.43
3:I:231:GLU:O	3:I:234:HIS:HB3	2.18	0.43
3:I:289:ALA:HB2	3:I:371:THR:HG23	2.00	0.43
3:I:327:ALA:O	3:I:328:GLU:C	2.59	0.43
1:J:159:ARG:HG2	2:K:258:GLY:HA3	2.00	0.43
2:K:388:SER:O	2:K:389:ASP:C	2.61	0.43
1:A:165:CYS:O	1:A:166:SER:O	2.36	0.43
3:C:234:HIS:HA	3:C:267:VAL:HG12	2.00	0.43
1:D:133:ILE:HG22	1:D:134:GLN:N	2.33	0.43
2:E:204:PRO:O	2:E:205:VAL:C	2.60	0.43
2:E:304:ARG:HB3	2:E:304:ARG:HH11	1.83	0.43
2:H:180:GLN:C	2:H:182:LEU:N	2.69	0.43
3:I:258:SER:OG	3:I:372:TRP:CE2	2.69	0.43
3:I:348:TYR:HA	3:I:367:ILE:CD1	2.41	0.43
3:I:365:ASN:ND2	3:I:366:GLY:N	2.66	0.43
1:J:157:LYS:O	1:J:158:ILE:C	2.60	0.43
2:K:257:ASP:HA	2:K:416:TYR:CZ	2.54	0.43
2:B:301:GLN:HE22	2:B:302:LEU:CD2	2.28	0.43
2:B:411:ASN:O	2:B:412:PRO:C	2.60	0.43
3:C:278:TYR:OH	3:C:308:ASN:HB2	2.18	0.43
3:C:329:GLN:NE2	4:O:3:ARG:HH11	2.14	0.43
2:E:241:ASP:N	2:E:249:TRP:O	2.46	0.43
2:E:374:PHE:CB	2:E:382:ASN:HB3	2.47	0.43
3:F:354:TYR:OH	3:F:364:ASP:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:LEU:HA	1:G:139:ASN:HB2	2.01	0.43
2:H:251:VAL:CG1	2:H:252:ILE:N	2.81	0.43
2:H:317:TRP:CE3	2:H:448:ARG:HD2	2.52	0.43
2:H:351:ASN:HB3	2:H:355:ASP:CB	2.44	0.43
2:K:256:GLN:O	2:K:257:ASP:HB3	2.18	0.43
3:L:176:GLN:H	3:L:176:GLN:CD	2.26	0.43
3:L:260:ALA:HB2	3:L:286:ALA:HB3	2.00	0.43
1:A:178:TYR:O	1:A:180:ASP:N	2.42	0.43
2:B:313:GLU:HB2	2:B:453:LYS:NZ	2.33	0.43
3:F:195:GLN:CG	3:F:227:TRP:CE3	3.02	0.43
3:F:234:HIS:HE1	3:F:269:PRO:HD3	1.81	0.43
1:G:175:LEU:C	1:G:177:ASP:H	2.25	0.43
2:H:266:TRP:CD1	2:H:380:ARG:HE	2.36	0.43
3:I:220:PRO:HG2	3:I:221:THR:N	2.30	0.43
3:I:352:GLY:O	3:I:353:THR:C	2.61	0.43
2:K:186:VAL:O	2:K:190:MET:HG3	2.18	0.43
2:K:423:THR:HG23	2:K:426:MET:HE3	2.00	0.43
1:A:124:ARG:N	1:A:124:ARG:HD2	2.32	0.43
2:B:190:MET:O	2:B:190:MET:SD	2.76	0.43
2:B:351:ASN:OD1	2:B:354:MET:HG3	2.19	0.43
3:C:157:ALA:HA	3:C:161:ALA:CB	2.42	0.43
3:C:194:PHE:HB2	3:C:233:ILE:CD1	2.48	0.43
3:C:281:PHE:CG	3:C:288:ASP:HB2	2.53	0.43
3:C:340:HIS:CE1	3:C:364:ASP:OD2	2.71	0.43
1:D:124:ARG:HD3	1:D:124:ARG:N	2.24	0.43
2:E:209:LYS:C	2:E:210:GLU:HG3	2.43	0.43
3:F:108:ARG:O	3:F:111:GLN:HB3	2.18	0.43
3:F:109:TYR:CE1	3:F:110:LEU:HD23	2.53	0.43
3:F:219:SER:CB	3:F:224:THR:CG2	2.95	0.43
3:F:250:LEU:HD23	3:F:372:TRP:HE3	1.84	0.43
3:F:307:HIS:HA	3:F:310:MET:HG2	1.99	0.43
2:H:214:ILE:HG22	2:H:214:ILE:O	2.18	0.43
2:H:253:GLN:HB2	2:H:293:TRP:HZ3	1.80	0.43
2:H:390:PRO:O	2:H:393:GLN:NE2	2.52	0.43
3:I:172:LEU:CD1	3:I:239:GLN:NE2	2.78	0.43
3:I:207:ASN:CG	3:I:210:GLN:HG3	2.44	0.43
3:I:214:GLY:HA3	3:I:228:LEU:O	2.19	0.43
2:K:382:ASN:O	2:K:383:ASP:C	2.61	0.43
3:L:252:ASP:OD1	3:L:255:GLY:N	2.51	0.43
2:B:304:ARG:HG3	2:B:304:ARG:HH11	1.84	0.43
2:B:423:THR:HA	2:B:444:TRP:CE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:LEU:CD1	3:C:239:GLN:HE21	2.23	0.43
3:C:278:TYR:HE2	3:C:290:PHE:CD2	2.27	0.43
3:C:329:GLN:NE2	3:C:363:TYR:HB2	2.31	0.43
2:E:167:VAL:C	2:E:169:ARG:H	2.26	0.43
2:E:303:THR:CG2	2:E:330:THR:HA	2.48	0.43
2:E:382:ASN:O	2:E:383:ASP:C	2.61	0.43
3:F:176:GLN:H	3:F:176:GLN:CD	2.26	0.43
3:F:219:SER:HB3	3:F:224:THR:HG21	1.97	0.43
1:G:136:LEU:C	1:G:138:LYS:N	2.76	0.43
2:H:386:LEU:C	2:H:387:THR:HG22	2.43	0.43
3:I:204:PHE:CE2	3:I:227:TRP:HB2	2.53	0.43
3:I:253:TRP:CZ2	3:I:349:TYR:O	2.71	0.43
3:I:273:LYS:CE	3:I:319:ASN:HD21	2.20	0.43
1:J:126:VAL:C	1:J:128:GLU:N	2.72	0.43
2:K:303:THR:CB	2:K:330:THR:HA	2.47	0.43
2:K:303:THR:HG21	2:K:330:THR:HA	2.00	0.43
1:A:149:ARG:HA	1:A:152:VAL:CG2	2.48	0.43
3:C:126:GLU:HA	3:C:129:ALA:HB3	2.00	0.43
3:C:251:GLU:CG	3:C:252:ASP:H	2.21	0.43
1:D:135:LEU:C	1:D:135:LEU:HD13	2.44	0.43
1:D:140:VAL:HG13	1:D:141:ARG:N	2.32	0.43
3:F:334:TRP:CG	3:F:335:TRP:N	2.86	0.43
1:G:140:VAL:C	1:G:142:ALA:N	2.76	0.43
1:G:183:LYS:HD3	1:G:183:LYS:C	2.44	0.43
2:H:209:LYS:HB3	2:H:209:LYS:HZ2	1.81	0.43
2:H:266:TRP:NE1	2:H:380:ARG:NH2	2.59	0.43
3:I:134:GLN:C	3:I:136:GLN:N	2.76	0.43
3:I:196:LYS:HD2	3:I:198:LEU:HD11	2.00	0.43
3:I:309:GLY:C	3:I:310:MET:HE2	2.43	0.43
2:K:244:THR:O	2:K:245:GLU:C	2.60	0.43
2:K:456:PRO:O	2:K:457:PHE:C	2.62	0.43
3:L:156:ILE:O	3:L:160:GLY:O	2.36	0.43
3:L:185:ASP:C	3:L:187:SER:N	2.76	0.43
3:L:281:PHE:C	3:L:283:GLY:H	2.27	0.43
3:L:334:TRP:CG	3:L:335:TRP:H	2.36	0.43
2:B:359:GLN:O	2:B:359:GLN:HG2	2.19	0.43
3:C:154:GLN:HE21	3:C:158:ASN:HD21	1.67	0.43
3:C:344:LEU:HD12	3:C:384:MET:CE	2.49	0.43
1:D:150:LEU:HD13	3:F:125:LYS:HE2	1.99	0.43
2:E:212:GLU:O	2:E:212:GLU:CG	2.67	0.43
1:G:148:LYS:CE	1:G:182:GLN:HE22	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:337:LYS:O	2:H:338:TYR:HB2	2.18	0.43
3:I:276:LEU:HD11	3:I:309:GLY:N	2.34	0.43
3:I:281:PHE:CG	3:I:288:ASP:HB2	2.53	0.43
2:K:301:GLN:HE21	2:K:302:LEU:N	2.16	0.43
3:L:321:LYS:HD3	3:L:321:LYS:HA	1.88	0.43
1:A:175:LEU:O	1:A:179:GLU:N	2.51	0.43
2:B:250:THR:O	2:B:252:ILE:HD11	2.19	0.43
2:B:266:TRP:O	2:B:267:ASP:C	2.62	0.43
2:B:317:TRP:CE3	2:B:448:ARG:HD2	2.53	0.43
2:B:423:THR:O	2:B:426:MET:HG3	2.19	0.43
2:B:429:HIS:O	2:B:431:THR:N	2.46	0.43
3:C:203:ASP:O	3:C:206:LYS:HE3	2.19	0.43
3:F:178:PHE:CZ	3:F:236:ILE:HD11	2.54	0.43
3:F:244:TYR:CD2	3:F:387:ILE:C	2.96	0.43
3:F:391:ARG:HH11	3:F:391:ARG:CB	2.27	0.43
2:H:316:ASP:HB2	2:H:445:TYR:OH	2.18	0.43
2:H:405:ASN:O	2:H:406:ARG:C	2.61	0.43
3:I:131:LEU:HD23	3:I:132:GLU:N	2.34	0.43
3:I:234:HIS:HA	3:I:267:VAL:HG12	2.00	0.43
2:K:332:GLN:HG3	2:K:339:GLN:HB3	2.01	0.43
2:K:365:ARG:O	2:K:365:ARG:HG2	2.18	0.43
3:L:198:LEU:HD12	3:L:198:LEU:N	2.33	0.43
3:L:250:LEU:O	3:L:257:THR:HG22	2.19	0.43
3:L:275:ARG:NH1	3:L:309:GLY:O	2.47	0.43
3:L:289:ALA:HB2	3:L:371:THR:OG1	2.19	0.43
2:B:180:GLN:O	2:B:181:LYS:C	2.62	0.43
2:B:236:TYR:OH	2:B:302:LEU:HD11	2.19	0.43
2:B:257:ASP:O	2:B:291:GLU:CD	2.62	0.43
2:B:333:ASN:OD1	2:B:335:ALA:HB3	2.18	0.43
2:B:346:ARG:HH11	2:B:346:ARG:CB	2.32	0.43
3:C:99:SER:O	3:C:102:THR:CG2	2.67	0.43
3:C:279:ALA:CB	3:C:280:TYR:CD1	3.02	0.43
3:C:317:ASN:C	3:C:317:ASN:ND2	2.76	0.43
2:E:203:ILE:HA	2:E:204:PRO:HD3	1.79	0.43
3:F:252:ASP:OD1	3:F:255:GLY:N	2.51	0.43
2:H:199:VAL:HG23	3:I:141:ASP:HA	2.01	0.43
2:K:241:ASP:N	2:K:249:TRP:O	2.48	0.43
2:K:384:GLY:H	2:K:405:ASN:HA	1.84	0.43
3:L:208:TRP:CA	3:L:314:THR:HG21	2.38	0.43
2:B:210:GLU:OE1	2:B:212:GLU:CB	2.67	0.42
2:B:223:GLU:HB2	2:B:286:CYS:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:GLN:NE2	2:B:231:SER:OG	2.52	0.42
2:B:304:ARG:HH22	2:B:333:ASN:ND2	2.17	0.42
3:C:220:PRO:HG2	3:C:221:THR:N	2.34	0.42
3:C:267:VAL:O	3:C:267:VAL:HG13	2.17	0.42
3:C:300:SER:O	3:C:302:LYS:N	2.51	0.42
3:F:170:LYS:HE3	3:F:177:GLN:HB3	2.00	0.42
3:F:195:GLN:CG	3:F:384:MET:HE2	2.49	0.42
1:G:147:MET:C	1:G:149:ARG:N	2.77	0.42
1:G:147:MET:C	1:G:149:ARG:H	2.27	0.42
2:H:152:TYR:C	2:H:152:TYR:CD2	2.95	0.42
2:H:231:SER:HB2	3:I:176:GLN:NE2	2.34	0.42
2:H:310:LEU:CA	2:H:454:ILE:HG22	2.49	0.42
3:I:288:ASP:O	3:I:371:THR:HG21	2.18	0.42
3:I:322:PHE:C	3:I:324:GLY:N	2.75	0.42
1:A:178:TYR:C	1:A:180:ASP:H	2.26	0.42
2:B:206:VAL:HG22	2:B:214:ILE:HG23	2.01	0.42
2:B:271:GLN:O	2:B:295:GLY:HA3	2.19	0.42
2:B:293:TRP:O	2:B:294:LEU:C	2.62	0.42
2:B:345:TYR:C	2:B:346:ARG:HG3	2.44	0.42
3:C:108:ARG:O	3:C:111:GLN:HB3	2.18	0.42
3:C:207:ASN:OD1	3:C:207:ASN:C	2.62	0.42
3:C:235:LEU:H	3:C:235:LEU:CD1	2.12	0.42
3:C:295:PHE:HB2	3:C:301:ASP:OD2	2.18	0.42
3:C:318:ASP:HB2	3:C:320:ASP:OD1	2.18	0.42
1:D:176:LYS:HE2	1:D:176:LYS:HB2	1.85	0.42
3:F:236:ILE:HG21	3:F:386:ILE:HD11	2.01	0.42
1:G:124:ARG:C	1:G:126:VAL:N	2.68	0.42
2:H:176:ARG:HH11	2:H:176:ARG:CG	2.32	0.42
2:H:442:GLY:O	2:H:444:TRP:N	2.52	0.42
3:I:107:ILE:C	3:I:109:TYR:H	2.27	0.42
3:I:148:ILE:N	3:I:148:ILE:HD12	2.34	0.42
3:I:328:GLU:C	3:I:328:GLU:OE1	2.62	0.42
2:K:249:TRP:CZ2	2:K:311:LEU:HD23	2.54	0.42
3:L:101:LEU:N	3:L:101:LEU:CD2	2.81	0.42
3:L:205:LYS:HG2	3:L:331:GLY:O	2.19	0.42
3:L:250:LEU:HD21	3:L:369:TRP:CG	2.54	0.42
2:B:190:MET:CB	3:C:131:LEU:HD12	2.50	0.42
2:B:373:MET:HG3	2:B:405:ASN:HB2	2.01	0.42
2:B:412:PRO:HB3	2:B:450:MET:CG	2.47	0.42
3:C:128:VAL:O	3:C:130:GLN:N	2.52	0.42
3:C:227:TRP:CZ3	3:C:345:ASN:OD1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:ARG:CG	1:D:167:ARG:NH1	2.82	0.42
3:F:95:LYS:HD2	3:F:98:ALA:HB2	2.00	0.42
3:F:207:ASN:OD1	3:F:208:TRP:N	2.53	0.42
3:F:276:LEU:O	3:F:277:THR:HG23	2.20	0.42
1:G:150:LEU:HD13	3:I:125:LYS:NZ	2.35	0.42
2:H:317:TRP:CZ3	2:H:448:ARG:HD2	2.54	0.42
3:I:197:ARG:HD3	3:I:204:PHE:CE1	2.55	0.42
3:I:342:GLY:HA2	3:I:369:TRP:HA	2.02	0.42
3:L:204:PHE:C	3:L:206:LYS:N	2.70	0.42
3:L:270:GLU:HA	3:L:273:LYS:O	2.19	0.42
4:S:3:ARG:NH2	4:S:3:ARG:CG	2.75	0.42
2:B:176:ARG:HH11	2:B:176:ARG:HB2	1.80	0.42
2:B:319:GLY:O	2:B:320:ASP:C	2.62	0.42
3:C:223:THR:O	3:C:224:THR:HB	2.19	0.42
3:C:239:GLN:O	3:C:240:SER:HB3	2.19	0.42
3:C:276:LEU:HD11	3:C:309:GLY:N	2.34	0.42
3:C:368:ILE:HB	3:C:374:THR:O	2.20	0.42
1:D:159:ARG:HH11	1:D:159:ARG:CB	2.32	0.42
2:E:257:ASP:HA	2:E:416:TYR:CZ	2.55	0.42
1:G:150:LEU:HD22	3:I:125:LYS:NZ	2.34	0.42
2:H:207:SER:OG	2:H:208:GLY:N	2.53	0.42
3:I:195:GLN:HE22	3:I:382:THR:HG23	1.83	0.42
3:I:196:LYS:HE2	3:I:198:LEU:HD11	2.01	0.42
3:I:212:LYS:C	3:I:214:GLY:N	2.77	0.42
3:I:338:LYS:NZ	4:S:3:ARG:O	2.51	0.42
3:L:288:ASP:OD2	3:L:291:ASP:CB	2.67	0.42
1:A:159:ARG:HB3	2:B:258:GLY:HA3	2.02	0.42
2:B:161:ILE:O	2:B:163:THR:N	2.45	0.42
2:B:180:GLN:O	2:B:183:GLU:HB3	2.20	0.42
2:B:249:TRP:CE3	2:B:455:ARG:HB2	2.54	0.42
2:B:266:TRP:CD1	2:B:380:ARG:HH21	2.38	0.42
3:C:112:GLU:O	3:C:114:TYR:N	2.51	0.42
3:C:154:GLN:OE1	3:C:190:GLY:N	2.51	0.42
3:C:325:ASN:ND2	3:C:327:ALA:HB3	2.30	0.42
3:F:195:GLN:CG	3:F:227:TRP:HE3	2.32	0.42
3:F:197:ARG:NE	3:F:204:PHE:CE1	2.87	0.42
1:G:150:LEU:HD13	3:I:125:LYS:HZ3	1.82	0.42
2:H:329:PHE:HD1	2:H:342:VAL:HG12	1.84	0.42
3:I:96:TYR:CD1	3:I:97:GLU:N	2.86	0.42
3:I:329:GLN:NE2	3:I:363:TYR:HB2	2.32	0.42
2:K:191:GLU:CA	2:K:194:ARG:HH21	2.14	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:200:SER:H	2:K:279:ASN:HD21	1.67	0.42
3:L:178:PHE:CZ	3:L:236:ILE:HD11	2.54	0.42
3:L:251:GLU:O	3:L:379:MET:HE3	2.20	0.42
3:L:252:ASP:HB2	3:L:254:ASN:ND2	2.34	0.42
2:B:179:ILE:HG13	2:B:179:ILE:H	1.66	0.42
2:B:215:ILE:HB	2:B:242:MET:HE3	2.01	0.42
2:B:374:PHE:O	2:B:375:PHE:C	2.62	0.42
2:B:429:HIS:O	2:B:431:THR:HG23	2.18	0.42
3:C:173:LYS:CE	3:C:239:GLN:HA	2.49	0.42
3:C:337:ASN:HB3	3:C:339:CYS:O	2.20	0.42
3:C:373:LYS:HG3	3:C:377:TYR:CD2	2.54	0.42
2:E:297:ASP:O	2:E:299:ILE:N	2.52	0.42
3:F:104:ASP:C	3:F:107:ILE:HG22	2.44	0.42
3:F:271:ALA:C	3:F:273:LYS:H	2.27	0.42
1:G:147:MET:HE1	3:I:121:ILE:HD13	2.01	0.42
1:G:159:ARG:NH1	2:H:418:TRP:CD2	2.88	0.42
2:H:162:PRO:O	2:H:164:ASN:N	2.52	0.42
2:H:367:MET:HB2	2:H:406:ARG:CB	2.37	0.42
3:I:120:LYS:HB2	3:I:120:LYS:HE3	1.86	0.42
3:I:197:ARG:NH1	3:I:204:PHE:CD1	2.87	0.42
1:J:127:ILE:O	1:J:131:GLN:HG3	2.19	0.42
1:J:150:LEU:HD12	1:J:150:LEU:HA	1.77	0.42
3:L:204:PHE:O	3:L:206:LYS:N	2.50	0.42
3:L:289:ALA:HA	3:L:371:THR:HG23	2.02	0.42
2:B:158:ASN:O	2:B:162:PRO:HG2	2.19	0.42
2:B:252:ILE:HG22	2:B:299:ILE:HD11	2.02	0.42
3:C:202:VAL:HG21	3:C:225:GLU:O	2.20	0.42
2:E:253:GLN:H	2:E:452:MET:HB2	1.84	0.42
2:E:255:ARG:HH12	2:E:413:ASN:N	2.18	0.42
2:E:313:GLU:OE1	2:E:453:LYS:HE2	2.19	0.42
3:F:289:ALA:HB3	3:F:369:TRP:CZ2	2.54	0.42
1:G:143:GLN:C	1:G:145:VAL:N	2.78	0.42
2:H:223:GLU:HB2	2:H:286:CYS:O	2.19	0.42
2:H:411:ASN:HD22	2:H:434:GLY:H	1.66	0.42
3:I:278:TYR:CD1	3:I:278:TYR:C	2.98	0.42
3:I:365:ASN:ND2	3:I:366:GLY:H	2.14	0.42
3:L:160:GLY:O	3:L:161:ALA:CB	2.66	0.42
4:M:3:ARG:HA	4:M:4:PRO:HD3	1.95	0.42
1:A:128:GLU:OE1	1:A:129:LYS:CE	2.67	0.42
2:B:169:ARG:O	2:B:173:GLU:HB2	2.19	0.42
2:B:200:SER:OG	3:C:142:THR:HG21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:GLN:NE2	2:B:444:TRP:O	2.53	0.42
3:C:170:LYS:HE2	3:C:177:GLN:OE1	2.20	0.42
3:C:195:GLN:HE21	3:C:195:GLN:HB3	1.66	0.42
3:C:234:HIS:C	3:C:236:ILE:N	2.78	0.42
1:D:122:LEU:HD13	1:D:122:LEU:C	2.45	0.42
2:E:172:LEU:HG	3:F:113:ILE:HG22	2.01	0.42
2:E:295:GLY:O	2:E:299:ILE:HG13	2.20	0.42
3:F:264:MET:O	3:F:278:TYR:HA	2.20	0.42
1:G:140:VAL:CG2	1:G:141:ARG:N	2.82	0.42
1:G:158:ILE:CD1	2:H:189:GLN:HB3	2.50	0.42
2:H:209:LYS:NZ	2:H:213:GLU:OE1	2.53	0.42
2:H:411:ASN:O	2:H:412:PRO:C	2.61	0.42
3:I:202:VAL:HG21	3:I:225:GLU:O	2.19	0.42
3:I:202:VAL:HG22	3:I:217:HIS:CE1	2.55	0.42
3:I:242:ILE:N	3:I:242:ILE:CD1	2.83	0.42
2:K:314:MET:HA	2:K:449:LYS:O	2.20	0.42
4:Q:3:ARG:O	4:Q:5:NH2:N	2.53	0.42
2:B:251:VAL:CG1	2:B:252:ILE:N	2.83	0.42
2:B:266:TRP:NE1	2:B:380:ARG:NH2	2.60	0.42
3:C:96:TYR:O	3:C:97:GLU:C	2.63	0.42
3:C:147:ASP:O	3:C:148:ILE:C	2.61	0.42
2:E:161:ILE:O	2:E:162:PRO:C	2.61	0.42
2:E:239:TYR:CZ	2:E:289:PRO:HD3	2.55	0.42
3:F:95:LYS:O	3:F:98:ALA:HB3	2.19	0.42
3:F:99:SER:O	3:F:101:LEU:HG	2.20	0.42
3:F:314:THR:C	3:F:316:ASP:N	2.78	0.42
3:F:338:LYS:N	3:F:339:CYS:HA	2.34	0.42
3:F:365:ASN:C	3:F:365:ASN:ND2	2.77	0.42
2:H:152:TYR:HD2	2:H:155:GLU:HG2	1.84	0.42
2:H:295:GLY:O	2:H:299:ILE:HG13	2.19	0.42
2:H:317:TRP:H	2:H:317:TRP:HD1	1.59	0.42
2:H:445:TYR:C	2:H:445:TYR:HD1	2.28	0.42
2:K:317:TRP:CE2	2:K:448:ARG:HB2	2.55	0.42
3:L:92:GLU:HG2	3:L:93:ILE:H	1.85	0.42
3:L:204:PHE:O	3:L:211:TYR:CE2	2.70	0.42
3:L:230:ASN:HA	3:L:233:ILE:CD1	2.38	0.42
3:L:382:THR:HG22	3:L:382:THR:O	2.19	0.42
1:A:147:MET:SD	3:C:121:ILE:CD1	3.08	0.42
2:B:175:LEU:HA	2:B:178:LYS:CG	2.49	0.42
2:B:301:GLN:O	2:B:304:ARG:HB2	2.20	0.42
2:B:351:ASN:C	2:B:351:ASN:ND2	2.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:LEU:HD12	3:C:172:LEU:N	2.29	0.42
3:C:172:LEU:CD1	3:C:239:GLN:NE2	2.81	0.42
3:C:267:VAL:O	3:C:267:VAL:CG1	2.68	0.42
1:D:133:ILE:O	1:D:134:GLN:C	2.62	0.42
2:E:165:LEU:O	2:E:166:ARG:C	2.62	0.42
2:E:180:GLN:NE2	2:E:180:GLN:C	2.78	0.42
2:E:297:ASP:O	2:E:298:LYS:C	2.63	0.42
2:E:370:HIS:HE1	2:E:408:HIS:CB	2.33	0.42
3:F:252:ASP:HB2	3:F:254:ASN:ND2	2.34	0.42
3:F:288:ASP:O	3:F:371:THR:HG21	2.19	0.42
2:H:351:ASN:OD1	2:H:354:MET:CG	2.68	0.42
2:H:398:ASP:CA	2:H:433:ASP:CB	2.97	0.42
3:I:278:TYR:HE2	3:I:290:PHE:CD2	2.28	0.42
2:K:213:GLU:O	2:K:217:LYS:HG3	2.20	0.42
2:K:433:ASP:O	2:K:433:ASP:OD1	2.38	0.42
3:L:171:PRO:HD2	3:L:174:ALA:HB2	2.02	0.42
2:B:236:TYR:O	2:B:236:TYR:CD1	2.72	0.41
3:C:251:GLU:CD	3:C:381:LYS:HD2	2.45	0.41
3:C:316:ASP:O	3:C:316:ASP:OD2	2.38	0.41
3:F:365:ASN:C	3:F:365:ASN:HD22	2.27	0.41
1:G:126:VAL:O	1:G:129:LYS:N	2.53	0.41
1:G:191:LYS:HE2	2:H:160:ASN:ND2	2.35	0.41
2:H:385:TRP:CE2	4:Q:3:ARG:HG3	2.55	0.41
2:H:451:SER:C	2:H:452:MET:HG3	2.45	0.41
3:I:143:VAL:C	3:I:144:GLN:HG3	2.45	0.41
3:I:310:MET:O	3:I:335:TRP:CD1	2.73	0.41
1:J:130:VAL:HA	1:J:133:ILE:HG22	2.02	0.41
3:L:119:GLN:HA	3:L:122:VAL:HG23	2.02	0.41
3:L:356:LYS:HE3	3:L:356:LYS:HB3	1.88	0.41
1:A:124:ARG:HD2	1:A:124:ARG:H	1.85	0.41
1:A:154:ILE:O	1:A:155:ASP:C	2.62	0.41
2:B:307:PRO:CB	2:B:457:PHE:C	2.92	0.41
3:C:99:SER:O	3:C:101:LEU:N	2.52	0.41
3:C:200:GLY:H	3:C:225:GLU:CD	2.24	0.41
3:C:298:ASP:O	3:C:301:ASP:CB	2.63	0.41
2:E:158:ASN:N	2:E:158:ASN:HD22	2.17	0.41
2:E:255:ARG:HH12	2:E:413:ASN:H	1.68	0.41
2:E:361:MET:O	2:E:362:GLY:C	2.63	0.41
3:F:321:LYS:HD3	3:F:321:LYS:HA	1.88	0.41
2:H:307:PRO:CB	2:H:457:PHE:C	2.92	0.41
3:I:100:ILE:O	3:I:100:ILE:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:189:ASN:CG	3:I:391:ARG:HG3	2.45	0.41
3:I:234:HIS:CE1	3:I:238:THR:OG1	2.73	0.41
3:I:311:GLN:HB2	3:I:319:ASN:HB2	2.02	0.41
2:K:158:ASN:N	2:K:158:ASN:ND2	2.67	0.41
2:K:242:MET:SD	2:K:248:GLY:HA2	2.60	0.41
3:L:195:GLN:HG3	3:L:384:MET:HE2	2.03	0.41
2:B:211:CYS:SG	2:B:250:THR:OG1	2.73	0.41
2:B:365:ARG:C	2:B:367:MET:N	2.78	0.41
3:C:173:LYS:HE3	3:C:239:GLN:HA	2.02	0.41
3:C:193:VAL:CG1	3:C:194:PHE:N	2.83	0.41
3:C:253:TRP:O	3:C:254:ASN:OD1	2.38	0.41
1:D:159:ARG:CB	1:D:159:ARG:NH1	2.83	0.41
2:E:242:MET:SD	2:E:248:GLY:HA2	2.60	0.41
3:F:116:SER:O	3:F:120:LYS:HG3	2.20	0.41
3:F:204:PHE:C	3:F:206:LYS:N	2.70	0.41
1:G:140:VAL:HG23	1:G:141:ARG:H	1.83	0.41
2:H:159:SER:H	2:H:162:PRO:HD3	1.84	0.41
2:H:258:GLY:C	2:H:259:SER:HG	2.25	0.41
3:I:275:ARG:HA	3:I:311:GLN:HA	2.01	0.41
1:J:167:ARG:NH1	2:K:192:TYR:CE1	2.88	0.41
3:L:93:ILE:C	3:L:95:LYS:H	2.27	0.41
1:A:140:VAL:C	1:A:142:ALA:N	2.77	0.41
2:B:312:ILE:HG12	2:B:452:MET:HG2	2.03	0.41
2:B:386:LEU:C	2:B:387:THR:HG22	2.45	0.41
2:E:167:VAL:HG23	2:E:168:LEU:N	2.35	0.41
2:E:233:VAL:O	2:E:233:VAL:HG13	2.19	0.41
2:E:423:THR:OG1	2:E:426:MET:HE3	2.20	0.41
3:F:204:PHE:O	3:F:211:TYR:CE2	2.71	0.41
3:F:304:PHE:C	3:F:337:ASN:HD22	2.28	0.41
2:H:224:MET:HB2	2:H:286:CYS:HB2	2.02	0.41
2:H:256:GLN:NE2	2:H:449:LYS:NZ	2.58	0.41
2:H:365:ARG:C	2:H:367:MET:N	2.78	0.41
1:J:126:VAL:O	1:J:127:ILE:C	2.63	0.41
2:K:224:MET:HE3	2:K:277:ALA:HB3	2.02	0.41
2:K:253:GLN:HA	2:K:292:TYR:O	2.19	0.41
2:K:363:GLU:C	2:K:365:ARG:N	2.75	0.41
3:L:189:ASN:ND2	3:L:391:ARG:HG2	2.35	0.41
2:B:164:ASN:N	2:B:166:ARG:HE	2.18	0.41
2:B:229:PRO:HG2	2:B:233:VAL:CG1	2.51	0.41
3:F:103:HIS:O	3:F:104:ASP:HB2	2.20	0.41
3:F:293:PHE:N	3:F:302:LYS:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:164:SER:HB3	3:I:137:GLU:O	2.20	0.41
2:H:236:TYR:CE1	2:H:294:LEU:HD21	2.55	0.41
2:H:238:VAL:CG2	2:H:250:THR:HG23	2.44	0.41
2:H:266:TRP:CD1	2:H:380:ARG:HH21	2.39	0.41
2:H:346:ARG:HH11	2:H:346:ARG:CB	2.34	0.41
2:H:385:TRP:CH2	4:Q:3:ARG:NE	2.88	0.41
3:I:276:LEU:HD11	3:I:308:ASN:CA	2.43	0.41
3:I:328:GLU:O	3:I:329:GLN:C	2.63	0.41
2:K:404:TYR:O	2:K:405:ASN:HB2	2.21	0.41
2:B:310:LEU:C	2:B:310:LEU:CD1	2.91	0.41
3:C:154:GLN:NE2	3:C:190:GLY:H	2.17	0.41
3:C:234:HIS:C	3:C:236:ILE:H	2.27	0.41
3:F:281:PHE:CD2	3:F:288:ASP:HB2	2.56	0.41
3:F:353:THR:HG23	3:F:377:TYR:CE1	2.55	0.41
1:G:128:GLU:OE2	1:G:129:LYS:NZ	2.46	0.41
1:G:131:GLN:C	1:G:133:ILE:N	2.76	0.41
1:G:133:ILE:O	1:G:133:ILE:HG22	2.20	0.41
1:G:151:GLU:OE1	2:H:182:LEU:HD11	2.21	0.41
2:H:261:ASP:OD2	2:H:263:GLY:N	2.53	0.41
3:I:194:PHE:HB2	3:I:233:ILE:HD11	2.03	0.41
3:I:223:THR:O	3:I:224:THR:CB	2.68	0.41
3:I:223:THR:C	3:I:224:THR:HG22	2.45	0.41
3:I:246:LEU:HD12	3:I:246:LEU:C	2.44	0.41
3:I:304:PHE:CB	3:I:338:LYS:HB3	2.50	0.41
3:I:322:PHE:HB3	3:I:324:GLY:O	2.20	0.41
1:A:188:VAL:C	1:A:189:ILE:HD12	2.46	0.41
2:B:218:GLY:HA3	3:C:210:GLN:HE21	1.86	0.41
2:B:294:LEU:O	2:B:295:GLY:C	2.63	0.41
2:B:337:LYS:O	2:B:338:TYR:HB2	2.21	0.41
2:B:456:PRO:HB2	2:B:457:PHE:H	1.67	0.41
2:E:160:ASN:C	2:E:162:PRO:HD2	2.45	0.41
3:F:156:ILE:O	3:F:160:GLY:O	2.38	0.41
1:G:137:GLN:OE1	1:G:189:ILE:HG13	2.20	0.41
1:G:158:ILE:CG1	2:H:189:GLN:HB3	2.51	0.41
2:H:180:GLN:O	2:H:183:GLU:N	2.54	0.41
3:I:96:TYR:O	3:I:97:GLU:C	2.63	0.41
3:I:265:PHE:CD2	3:I:265:PHE:C	2.99	0.41
1:J:148:LYS:HG3	1:J:178:TYR:CG	2.56	0.41
2:K:201:CYS:CB	2:K:224:MET:HE1	2.51	0.41
3:L:97:GLU:HA	3:L:100:ILE:HD11	2.03	0.41
3:L:240:SER:O	3:L:242:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:ASN:HA	2:B:299:ILE:HD12	2.03	0.41
2:B:317:TRP:HE1	2:B:447:MET:CA	2.27	0.41
2:B:377:THR:C	2:B:379:ASP:H	2.29	0.41
2:B:381:ASP:OD1	2:B:383:ASP:CG	2.64	0.41
3:C:340:HIS:O	4:O:1:GLY:N	2.54	0.41
1:D:130:VAL:O	1:D:133:ILE:HB	2.21	0.41
1:G:149:ARG:HG2	2:H:426:MET:C	2.46	0.41
1:G:181:GLN:C	1:G:183:LYS:N	2.78	0.41
1:G:186:GLU:HA	1:G:189:ILE:CG2	2.51	0.41
3:I:317:ASN:C	3:I:317:ASN:ND2	2.78	0.41
1:J:124:ARG:HG2	1:J:124:ARG:NH1	2.36	0.41
1:J:132:HIS:O	1:J:135:LEU:HB3	2.20	0.41
3:L:293:PHE:N	3:L:302:LYS:HD2	2.36	0.41
2:B:161:ILE:O	2:B:164:ASN:N	2.50	0.41
2:B:169:ARG:HB2	3:C:110:LEU:HD12	2.02	0.41
2:B:176:ARG:NH1	2:B:176:ARG:CG	2.79	0.41
2:B:303:THR:HA	2:B:308:THR:CG2	2.50	0.41
2:B:307:PRO:HB2	2:B:457:PHE:O	2.20	0.41
2:B:386:LEU:HA	2:B:386:LEU:HD22	1.80	0.41
3:C:93:ILE:HD12	3:C:93:ILE:C	2.46	0.41
3:C:164:SER:HB2	3:C:183:GLU:HA	2.03	0.41
3:C:171:PRO:HG3	3:C:236:ILE:HG22	2.01	0.41
3:C:197:ARG:N	3:C:382:THR:O	2.54	0.41
3:C:269:PRO:O	3:C:270:GLU:C	2.64	0.41
3:C:311:GLN:HB2	3:C:319:ASN:HB2	2.02	0.41
3:C:315:TRP:CD1	3:C:316:ASP:N	2.88	0.41
3:C:365:ASN:ND2	3:C:366:GLY:N	2.68	0.41
1:D:125:LYS:O	1:D:126:VAL:C	2.63	0.41
1:D:148:LYS:O	1:D:152:VAL:HG12	2.21	0.41
3:F:102:THR:O	3:F:103:HIS:C	2.64	0.41
3:F:105:SER:HA	3:F:108:ARG:CZ	2.49	0.41
3:F:166:LEU:HD22	3:F:179:LEU:CD1	2.49	0.41
3:F:243:PRO:O	3:F:389:PHE:N	2.53	0.41
3:F:304:PHE:CD1	3:F:338:LYS:HD2	2.56	0.41
1:G:122:LEU:HD11	3:I:98:ALA:HB2	2.02	0.41
1:G:125:LYS:O	1:G:125:LYS:CG	2.69	0.41
1:G:128:GLU:CA	1:G:131:GLN:HB3	2.40	0.41
1:G:158:ILE:HD12	1:G:158:ILE:HA	1.84	0.41
2:H:224:MET:HE2	2:H:237:ARG:HH21	1.85	0.41
2:H:255:ARG:HH11	2:H:413:ASN:HA	1.84	0.41
2:H:256:GLN:HB3	2:H:449:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:279:ASN:O	2:H:281:ASP:N	2.53	0.41
2:H:352:ALA:O	2:H:409:ALA:HB3	2.21	0.41
2:H:405:ASN:C	2:H:407:CYS:N	2.75	0.41
3:I:156:ILE:H	3:I:156:ILE:HG13	1.74	0.41
3:I:170:LYS:HE2	3:I:177:GLN:OE1	2.21	0.41
3:I:232:LYS:O	3:I:235:LEU:HD12	2.21	0.41
3:I:267:VAL:O	3:I:267:VAL:HG13	2.19	0.41
3:I:267:VAL:O	3:I:267:VAL:CG1	2.69	0.41
3:I:279:ALA:CB	3:I:280:TYR:CD1	3.04	0.41
3:I:334:TRP:CZ3	3:I:344:LEU:HB2	2.53	0.41
2:K:155:GLU:O	2:K:156:THR:C	2.64	0.41
3:L:170:LYS:HE3	3:L:177:GLN:HB3	2.02	0.41
3:L:347:VAL:O	3:L:367:ILE:HG13	2.21	0.41
1:A:137:GLN:C	1:A:140:VAL:HG22	2.46	0.41
2:B:304:ARG:HH21	2:B:332:GLN:HA	1.85	0.41
2:B:361:MET:HB2	5:B:470:NAG:C8	2.43	0.41
2:B:423:THR:O	2:B:425:ASP:N	2.54	0.41
3:C:102:THR:C	3:C:104:ASP:N	2.77	0.41
3:C:392:LEU:O	3:C:392:LEU:HG	2.20	0.41
1:D:148:LYS:O	1:D:149:ARG:C	2.64	0.41
1:D:159:ARG:NE	2:E:418:TRP:CE3	2.88	0.41
1:D:169:LEU:HD23	1:D:170:ALA:N	2.36	0.41
2:E:218:GLY:CA	3:F:210:GLN:HG2	2.50	0.41
2:E:363:GLU:HB3	2:E:367:MET:HE2	2.03	0.41
3:F:233:ILE:HG13	3:F:233:ILE:H	1.54	0.41
3:F:250:LEU:HD23	3:F:372:TRP:CE3	2.56	0.41
1:G:128:GLU:C	1:G:130:VAL:H	2.29	0.41
1:G:178:TYR:O	1:G:182:GLN:HG2	2.21	0.41
3:I:197:ARG:C	3:I:198:LEU:HD12	2.45	0.41
3:I:243:PRO:HG3	3:L:279:ALA:C	2.45	0.41
1:J:115:LEU:C	1:J:115:LEU:CD1	2.94	0.41
1:J:140:VAL:CG1	1:J:141:ARG:N	2.83	0.41
2:K:253:GLN:HB2	2:K:293:TRP:CZ3	2.56	0.41
2:K:316:ASP:C	2:K:318:LYS:H	2.29	0.41
1:A:181:GLN:HE22	2:B:174:ASN:HB2	1.86	0.40
1:A:190:ALA:C	1:A:191:LYS:HD2	2.46	0.40
2:B:304:ARG:HH22	2:B:333:ASN:CG	2.29	0.40
2:B:351:ASN:HB3	2:B:355:ASP:CB	2.47	0.40
3:C:196:LYS:HA	3:C:382:THR:O	2.21	0.40
3:C:234:HIS:CE1	3:C:238:THR:OG1	2.74	0.40
3:C:262:TYR:OH	3:C:290:PHE:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:VAL:O	1:D:144:LEU:HB2	2.21	0.40
2:E:441:LYS:CG	2:E:447:MET:HE1	2.51	0.40
3:F:205:LYS:HG2	3:F:331:GLY:O	2.21	0.40
1:G:169:LEU:HD13	1:G:170:ALA:N	2.36	0.40
2:H:361:MET:O	2:H:362:GLY:C	2.63	0.40
2:H:422:TYR:HE1	2:H:444:TRP:HA	1.84	0.40
3:I:112:GLU:HA	3:I:112:GLU:OE1	2.21	0.40
3:I:157:ALA:HA	3:I:161:ALA:CB	2.46	0.40
3:I:193:VAL:CG1	3:I:194:PHE:N	2.84	0.40
3:L:207:ASN:OD1	3:L:209:ILE:N	2.54	0.40
2:B:171:ILE:HG13	2:B:172:LEU:N	2.35	0.40
3:C:212:LYS:O	3:C:231:GLU:HB3	2.21	0.40
3:C:248:VAL:HG22	3:C:384:MET:HE3	2.04	0.40
2:E:223:GLU:HB2	2:E:286:CYS:O	2.21	0.40
2:E:249:TRP:CZ2	2:E:311:LEU:HD23	2.57	0.40
2:E:384:GLY:H	2:E:405:ASN:HA	1.87	0.40
2:H:175:LEU:O	2:H:178:LYS:HB2	2.21	0.40
2:H:303:THR:O	2:H:308:THR:OG1	2.39	0.40
2:H:304:ARG:HH22	2:H:333:ASN:CG	2.29	0.40
2:H:345:TYR:C	2:H:346:ARG:HG3	2.47	0.40
3:I:162:LYS:HA	3:I:184:ILE:HG21	2.03	0.40
3:L:93:ILE:C	3:L:95:LYS:N	2.79	0.40
3:L:242:ILE:HD12	3:L:242:ILE:N	2.36	0.40
1:A:158:ILE:HD13	1:A:171:ARG:NE	2.35	0.40
2:B:165:LEU:CD2	3:C:107:ILE:HG12	2.51	0.40
2:B:238:VAL:CG2	2:B:239:TYR:N	2.84	0.40
2:B:252:ILE:CG2	2:B:299:ILE:HG12	2.51	0.40
3:C:148:ILE:H	3:C:148:ILE:CD1	2.29	0.40
3:C:329:GLN:HE21	4:O:3:ARG:CZ	2.33	0.40
2:E:284:ASN:N	2:E:284:ASN:ND2	2.67	0.40
2:E:411:ASN:C	2:E:412:PRO:O	2.63	0.40
3:F:347:VAL:O	3:F:367:ILE:HG13	2.21	0.40
2:H:189:GLN:HG3	2:H:189:GLN:O	2.21	0.40
2:H:205:VAL:CG1	3:I:232:LYS:NZ	2.70	0.40
2:H:252:ILE:CG2	2:H:299:ILE:HG12	2.51	0.40
2:H:298:LYS:O	2:H:302:LEU:HG	2.21	0.40
2:H:456:PRO:HB2	2:H:457:PHE:H	1.68	0.40
3:I:265:PHE:CD2	3:I:266:LYS:N	2.89	0.40
2:K:363:GLU:HB3	2:K:367:MET:HE2	2.02	0.40
3:L:269:PRO:O	3:L:273:LYS:O	2.40	0.40
2:B:200:SER:OG	3:C:142:THR:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:ARG:HG2	2:B:450:MET:O	2.22	0.40
2:B:300:SER:O	2:B:304:ARG:CG	2.59	0.40
2:B:300:SER:HA	2:B:331:VAL:O	2.21	0.40
2:B:451:SER:C	2:B:452:MET:HG3	2.46	0.40
2:E:167:VAL:C	2:E:169:ARG:N	2.77	0.40
2:E:448:ARG:O	2:E:449:LYS:HG3	2.22	0.40
1:G:143:GLN:O	1:G:146:ASP:N	2.53	0.40
1:G:178:TYR:O	1:G:180:ASP:N	2.45	0.40
2:H:162:PRO:C	2:H:164:ASN:H	2.27	0.40
2:H:317:TRP:CZ3	2:H:448:ARG:CD	3.05	0.40
2:H:353:LEU:O	2:H:370:HIS:N	2.44	0.40
2:H:398:ASP:C	2:H:433:ASP:HB2	2.46	0.40
3:I:244:TYR:CE2	3:I:388:PRO:HG3	2.56	0.40
3:I:248:VAL:HG22	3:I:384:MET:HE3	2.04	0.40
2:K:441:LYS:HG2	2:K:447:MET:HE1	2.03	0.40
2:K:448:ARG:O	2:K:448:ARG:HG2	2.21	0.40
3:L:304:PHE:C	3:L:337:ASN:HD22	2.29	0.40
3:L:354:TYR:OH	3:L:364:ASP:HB2	2.21	0.40
1:A:120:GLU:C	1:A:121:VAL:O	2.65	0.40
1:A:140:VAL:O	1:A:143:GLN:N	2.54	0.40
2:B:152:TYR:C	2:B:152:TYR:CD2	2.99	0.40
2:B:224:MET:HE2	2:B:237:ARG:HH21	1.85	0.40
2:B:307:PRO:O	2:B:456:PRO:C	2.64	0.40
2:B:310:LEU:CA	2:B:454:ILE:HG22	2.51	0.40
2:B:328:GLY:H	2:B:344:LYS:HB2	1.86	0.40
3:C:154:GLN:HG3	3:C:158:ASN:ND2	2.36	0.40
3:C:242:ILE:N	3:C:242:ILE:CD1	2.85	0.40
3:C:342:GLY:HA2	3:C:368:ILE:O	2.22	0.40
1:G:123:LYS:C	1:G:124:ARG:HD2	2.46	0.40
2:H:369:ILE:O	2:H:405:ASN:CB	2.68	0.40
3:I:105:SER:C	3:I:107:ILE:H	2.28	0.40
3:I:296:GLY:C	3:I:298:ASP:N	2.79	0.40
1:J:147:MET:SD	3:L:121:ILE:HD11	2.61	0.40
1:J:184:GLN:O	1:J:185:LEU:C	2.63	0.40
2:K:262:PHE:O	2:K:269:TYR:OH	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	72/87 (83%)	43 (60%)	17 (24%)	12 (17%)	0	0
1	D	69/87 (79%)	47 (68%)	19 (28%)	3 (4%)	2	8
1	G	72/87 (83%)	43 (60%)	19 (26%)	10 (14%)	0	0
1	J	77/87 (88%)	58 (75%)	15 (20%)	4 (5%)	1	5
2	B	305/328 (93%)	195 (64%)	70 (23%)	40 (13%)	0	0
2	E	302/328 (92%)	229 (76%)	53 (18%)	20 (7%)	1	3
2	H	305/328 (93%)	191 (63%)	70 (23%)	44 (14%)	0	0
2	K	303/328 (92%)	230 (76%)	47 (16%)	26 (9%)	0	1
3	C	303/323 (94%)	168 (55%)	96 (32%)	39 (13%)	0	0
3	F	298/323 (92%)	210 (70%)	70 (24%)	18 (6%)	1	4
3	I	303/323 (94%)	175 (58%)	85 (28%)	43 (14%)	0	0
3	L	298/323 (92%)	215 (72%)	66 (22%)	17 (6%)	1	4
4	M	2/5 (40%)	1 (50%)	0	1 (50%)	0	0
4	N	2/5 (40%)	1 (50%)	0	1 (50%)	0	0
4	O	2/5 (40%)	0	1 (50%)	1 (50%)	0	0
4	P	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
4	Q	2/5 (40%)	1 (50%)	0	1 (50%)	0	0
4	R	2/5 (40%)	1 (50%)	0	1 (50%)	0	0
4	S	2/5 (40%)	2 (100%)	0	0	100	100
4	T	2/5 (40%)	2 (100%)	0	0	100	100
All	All	2723/2992 (91%)	1813 (67%)	629 (23%)	281 (10%)	0	1

All (281) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	VAL

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Mol	Chain	Res	Type
1	A	122	LEU
1	A	160	SER
1	A	166	SER
2	B	170	SER
2	B	189	GLN
2	B	227	ILE
2	B	285	TYR
2	B	295	GLY
2	B	320	ASP
2	B	366	THR
2	B	435	VAL
3	C	151	LYS
3	C	162	LYS
3	C	196	LYS
3	C	201	SER
3	C	224	THR
3	C	271	ALA
3	C	272	ASP
3	C	305	THR
3	C	317	ASN
3	C	335	TRP
3	C	353	THR
1	D	165	CYS
2	E	192	TYR
2	E	205	VAL
2	E	229	PRO
2	E	233	VAL
2	E	259	SER
2	E	281	ASP
2	E	399	GLY
2	E	405	ASN
3	F	104	ASP
3	F	159	LYS
3	F	282	ALA
3	F	298	ASP
3	F	311	GLN
3	F	390	ASN
1	G	120	GLU
1	G	121	VAL
1	G	125	LYS
1	G	130	VAL
1	G	166	SER

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Mol	Chain	Res	Type
2	H	158	ASN
2	H	174	ASN
2	H	227	ILE
2	H	285	TYR
2	H	295	GLY
2	H	320	ASP
2	H	435	VAL
3	I	98	ALA
3	I	151	LYS
3	I	162	LYS
3	I	196	LYS
3	I	201	SER
3	I	224	THR
3	I	271	ALA
3	I	305	THR
3	I	317	ASN
3	I	335	TRP
3	I	353	THR
2	K	156	THR
2	K	157	VAL
2	K	205	VAL
2	K	229	PRO
2	K	233	VAL
2	K	259	SER
2	K	281	ASP
2	K	405	ASN
3	L	159	LYS
3	L	256	ARG
3	L	298	ASP
3	L	311	GLN
3	L	390	ASN
4	M	4	PRO
1	A	173	VAL
1	A	190	ALA
2	B	153	ILE
2	B	182	LEU
2	B	231	SER
2	B	258	GLY
2	B	280	THR
2	B	332	GLN
2	B	359	GLN
2	B	362	GLY

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Mol	Chain	Res	Type
2	B	378	TYR
2	B	424	TRP
2	B	443	SER
2	B	456	PRO
3	C	100	ILE
3	C	164	SER
3	C	218	LEU
3	C	237	SER
3	C	243	PRO
3	C	331	GLY
3	C	360	PRO
1	D	164	SER
2	E	156	THR
2	E	157	VAL
2	E	295	GLY
2	E	305	MET
2	E	383	ASP
3	F	233	ILE
3	F	240	SER
3	F	241	ALA
3	F	256	ARG
3	F	270	GLU
3	F	285	ASP
1	G	191	LYS
2	H	153	ILE
2	H	159	SER
2	H	170	SER
2	H	231	SER
2	H	258	GLY
2	H	280	THR
2	H	359	GLN
2	H	362	GLY
2	H	366	THR
2	H	378	TYR
2	H	407	CYS
2	H	424	TRP
2	H	443	SER
2	H	456	PRO
3	I	97	GLU
3	I	105	SER
3	I	164	SER
3	I	218	LEU

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Mol	Chain	Res	Type
3	I	237	SER
3	I	243	PRO
3	I	272	ASP
3	I	327	ALA
3	I	331	GLY
3	I	332	SER
3	I	339	CYS
3	I	360	PRO
3	I	366	GLY
3	I	390	ASN
1	J	165	CYS
2	K	192	TYR
2	K	295	GLY
2	K	305	MET
2	K	399	GLY
3	L	233	ILE
3	L	240	SER
3	L	241	ALA
3	L	270	GLU
3	L	282	ALA
3	L	285	ASP
3	L	300	SER
3	L	339	CYS
4	N	4	PRO
1	A	164	SER
2	B	155	GLU
2	B	247	GLY
2	B	259	SER
2	B	266	TRP
2	B	317	TRP
2	B	325	HIS
2	B	334	GLU
2	B	355	ASP
3	C	113	ILE
3	C	251	GLU
3	C	273	LYS
3	C	327	ALA
3	C	332	SER
3	C	374	THR
3	C	389	PHE
3	C	390	ASN
1	D	166	SER

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Mol	Chain	Res	Type
2	E	216	ARG
2	E	298	LYS
2	E	404	TYR
2	E	406	ARG
3	F	94	MET
3	F	102	THR
3	F	300	SER
3	F	367	ILE
3	F	389	PHE
2	H	182	LEU
2	H	247	GLY
2	H	259	SER
2	H	294	LEU
2	H	317	TRP
2	H	325	HIS
2	H	332	GLN
2	H	334	GLU
2	H	355	ASP
2	H	356	GLY
3	I	135	CYS
3	I	221	THR
3	I	251	GLU
3	I	273	LYS
3	I	301	ASP
3	I	374	THR
2	K	162	PRO
2	K	216	ARG
2	K	298	LYS
2	K	364	ASN
2	K	383	ASP
2	K	407	CYS
3	L	389	PHE
4	Q	4	PRO
4	R	4	PRO
1	A	180	ASP
2	B	174	ASN
2	B	192	TYR
2	B	229	PRO
2	B	356	GLY
3	C	105	SER
3	C	128	VAL
3	C	221	THR

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Mol	Chain	Res	Type
3	C	259	THR
3	C	301	ASP
3	C	366	GLY
2	E	223	GLU
1	G	179	GLU
2	H	192	TYR
2	H	229	PRO
2	H	266	TRP
3	I	118	ASN
3	I	133	ALA
3	I	369	TRP
3	I	389	PHE
1	J	164	SER
2	K	159	SER
2	K	164	ASN
2	K	223	GLU
1	A	174	ASP
1	A	179	GLU
1	A	188	VAL
2	B	256	GLN
2	B	294	LEU
2	B	406	ARG
2	B	425	ASP
3	C	135	CYS
3	C	202	VAL
3	C	235	LEU
3	C	369	TRP
2	E	438	MET
1	G	164	SER
1	G	173	VAL
1	G	190	ALA
2	H	162	PRO
2	H	163	THR
2	H	256	GLN
2	H	431	THR
3	I	100	ILE
3	I	124	LEU
3	I	202	VAL
3	I	259	THR
1	J	184	GLN
3	L	367	ILE
3	L	374	THR

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Mol	Chain	Res	Type
2	B	162	PRO
3	C	387	ILE
3	F	273	LYS
2	H	179	ILE
3	I	387	ILE
2	K	257	ASP
2	K	404	TYR
2	K	406	ARG
2	B	235	PRO
1	A	126	VAL
2	B	414	GLY
2	E	235	PRO
2	H	414	GLY
3	I	107	ILE
2	K	235	PRO
2	K	430	GLY
2	H	235	PRO
3	I	219	SER
3	I	347	VAL
4	O	4	PRO
3	C	394	ILE
2	H	157	VAL
2	H	199	VAL
1	J	126	VAL
2	B	319	GLY
3	C	347	VAL
2	H	319	GLY
3	L	200	GLY

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%)	55 (83%)	11 (17%)	2	7
1	G	69/82 (84%)	61 (88%)	8 (12%)	5	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	74/82 (90%)	59 (80%)	15 (20%)	1	4
2	B	265/286 (93%)	229 (86%)	36 (14%)	3	12
2	E	262/286 (92%)	231 (88%)	31 (12%)	5	17
2	H	265/286 (93%)	234 (88%)	31 (12%)	5	17
2	K	263/286 (92%)	234 (89%)	29 (11%)	6	20
3	C	257/269 (96%)	219 (85%)	38 (15%)	3	10
3	F	253/269 (94%)	224 (88%)	29 (12%)	5	18
3	I	257/269 (96%)	220 (86%)	37 (14%)	3	11
3	L	253/269 (94%)	227 (90%)	26 (10%)	7	23
4	M	2/2 (100%)	2 (100%)	0	100	100
4	N	2/2 (100%)	2 (100%)	0	100	100
4	O	2/2 (100%)	2 (100%)	0	100	100
4	P	2/2 (100%)	2 (100%)	0	100	100
4	Q	2/2 (100%)	2 (100%)	0	100	100
4	R	2/2 (100%)	2 (100%)	0	100	100
4	S	2/2 (100%)	1 (50%)	1 (50%)	0	0
4	T	2/2 (100%)	2 (100%)	0	100	100
All	All	2369/2564 (92%)	2065 (87%)	304 (13%)	4	14

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	ILE
1	A	128	GLU
1	A	132	HIS
1	A	138	LYS
1	A	143	GLN
1	A	150	LEU
1	A	151	GLU
1	A	152	VAL
1	A	169	LEU
1	A	171	ARG
1	A	173	VAL
1	A	182	GLN
2	B	153	ILE
2	B	155	GLU

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Mol	Chain	Res	Type
2	B	161	ILE
2	B	166	ARG
2	B	167	VAL
2	B	168	LEU
2	B	172	LEU
2	B	173	GLU
2	B	175	LEU
2	B	176	ARG
2	B	183	GLU
2	B	186	VAL
2	B	189	GLN
2	B	191	GLU
2	B	193	CYS
2	B	209	LYS
2	B	223	GLU
2	B	234	LYS
2	B	245	GLU
2	B	253	GLN
2	B	261	ASP
2	B	266	TRP
2	B	284	ASN
2	B	285	TYR
2	B	301	GLN
2	B	308	THR
2	B	310	LEU
2	B	316	ASP
2	B	346	ARG
2	B	351	ASN
2	B	359	GLN
2	B	386	LEU
2	B	387	THR
2	B	436	VAL
2	B	448	ARG
2	B	453	LYS
3	C	101	LEU
3	C	107	ILE
3	C	108	ARG
3	C	110	LEU
3	C	125	LYS
3	C	148	ILE
3	C	167	TYR
3	C	176	GLN

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Mol	Chain	Res	Type
3	C	192	THR
3	C	195	GLN
3	C	196	LYS
3	C	199	ASP
3	C	203	ASP
3	C	209	ILE
3	C	221	THR
3	C	226	PHE
3	C	230	ASN
3	C	235	LEU
3	C	239	GLN
3	C	246	LEU
3	C	264	MET
3	C	275	ARG
3	C	277	THR
3	C	294	ASP
3	C	300	SER
3	C	301	ASP
3	C	315	TRP
3	C	323	GLU
3	C	328	GLU
3	C	329	GLN
3	C	343	HIS
3	C	364	ASP
3	C	365	ASN
3	C	372	TRP
3	C	374	THR
3	C	382	THR
3	C	383	THR
3	C	392	LEU
1	D	124	ARG
1	D	127	ILE
1	D	133	ILE
1	D	135	LEU
1	D	138	LYS
1	D	152	VAL
1	D	161	CYS
1	D	162	ARG
1	D	167	ARG
1	D	179	GLU
1	D	185	LEU
2	E	155	GLU

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Mol	Chain	Res	Type
2	E	156	THR
2	E	164	ASN
2	E	166	ARG
2	E	172	LEU
2	E	180	GLN
2	E	185	ASP
2	E	194	ARG
2	E	198	THR
2	E	203	ILE
2	E	209	LYS
2	E	210	GLU
2	E	212	GLU
2	E	221	THR
2	E	224	MET
2	E	238	VAL
2	E	256	GLN
2	E	260	VAL
2	E	280	THR
2	E	284	ASN
2	E	311	LEU
2	E	318	LYS
2	E	333	ASN
2	E	340	ILE
2	E	359	GLN
2	E	361	MET
2	E	376	SER
2	E	421	GLN
2	E	431	THR
2	E	436	VAL
2	E	441	LYS
3	F	96	TYR
3	F	101	LEU
3	F	103	HIS
3	F	106	SER
3	F	109	TYR
3	F	118	ASN
3	F	124	LEU
3	F	148	ILE
3	F	149	THR
3	F	156	ILE
3	F	164	SER
3	F	176	GLN

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Mol	Chain	Res	Type
3	F	180	VAL
3	F	192	THR
3	F	202	VAL
3	F	221	THR
3	F	224	THR
3	F	239	GLN
3	F	242	ILE
3	F	244	TYR
3	F	264	MET
3	F	301	ASP
3	F	338	LYS
3	F	353	THR
3	F	365	ASN
3	F	382	THR
3	F	383	THR
3	F	390	ASN
3	F	391	ARG
1	G	120	GLU
1	G	121	VAL
1	G	130	VAL
1	G	137	GLN
1	G	144	LEU
1	G	171	ARG
1	G	175	LEU
1	G	186	GLU
2	H	155	GLU
2	H	158	ASN
2	H	161	ILE
2	H	164	ASN
2	H	165	LEU
2	H	168	LEU
2	H	193	CYS
2	H	209	LYS
2	H	223	GLU
2	H	234	LYS
2	H	242	MET
2	H	245	GLU
2	H	253	GLN
2	H	261	ASP
2	H	266	TRP
2	H	284	ASN
2	H	285	TYR

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Mol	Chain	Res	Type
2	H	301	GLN
2	H	308	THR
2	H	310	LEU
2	H	316	ASP
2	H	346	ARG
2	H	351	ASN
2	H	359	GLN
2	H	386	LEU
2	H	387	THR
2	H	405	ASN
2	H	422	TYR
2	H	436	VAL
2	H	448	ARG
2	H	453	LYS
3	I	93	ILE
3	I	119	GLN
3	I	131	LEU
3	I	132	GLU
3	I	148	ILE
3	I	167	TYR
3	I	176	GLN
3	I	192	THR
3	I	195	GLN
3	I	196	LYS
3	I	199	ASP
3	I	203	ASP
3	I	209	ILE
3	I	221	THR
3	I	226	PHE
3	I	230	ASN
3	I	235	LEU
3	I	239	GLN
3	I	246	LEU
3	I	264	MET
3	I	275	ARG
3	I	277	THR
3	I	294	ASP
3	I	300	SER
3	I	301	ASP
3	I	315	TRP
3	I	323	GLU
3	I	326	CYS

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Mol	Chain	Res	Type
3	I	328	GLU
3	I	329	GLN
3	I	343	HIS
3	I	347	VAL
3	I	364	ASP
3	I	365	ASN
3	I	372	TRP
3	I	382	THR
3	I	383	THR
1	J	115	LEU
1	J	116	ARG
1	J	118	ARG
1	J	122	LEU
1	J	125	LYS
1	J	127	ILE
1	J	131	GLN
1	J	134	GLN
1	J	135	LEU
1	J	138	LYS
1	J	148	LYS
1	J	157	LYS
1	J	161	CYS
1	J	167	ARG
1	J	185	LEU
2	K	153	ILE
2	K	155	GLU
2	K	175	LEU
2	K	180	GLN
2	K	191	GLU
2	K	194	ARG
2	K	198	THR
2	K	203	ILE
2	K	209	LYS
2	K	210	GLU
2	K	212	GLU
2	K	221	THR
2	K	224	MET
2	K	238	VAL
2	K	256	GLN
2	K	260	VAL
2	K	280	THR
2	K	284	ASN

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Mol	Chain	Res	Type
2	K	301	GLN
2	K	303	THR
2	K	311	LEU
2	K	318	LYS
2	K	333	ASN
2	K	340	ILE
2	K	359	GLN
2	K	361	MET
2	K	376	SER
2	K	421	GLN
2	K	436	VAL
3	L	95	LYS
3	L	96	TYR
3	L	104	ASP
3	L	107	ILE
3	L	118	ASN
3	L	124	LEU
3	L	148	ILE
3	L	149	THR
3	L	164	SER
3	L	176	GLN
3	L	180	VAL
3	L	192	THR
3	L	202	VAL
3	L	221	THR
3	L	224	THR
3	L	239	GLN
3	L	242	ILE
3	L	244	TYR
3	L	264	MET
3	L	301	ASP
3	L	353	THR
3	L	365	ASN
3	L	382	THR
3	L	383	THR
3	L	390	ASN
3	L	391	ARG
4	S	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (176) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	143	GLN
1	A	181	GLN
1	A	182	GLN
1	A	184	GLN
1	A	187	GLN
2	B	158	ASN
2	B	160	ASN
2	B	164	ASN
2	B	174	ASN
2	B	180	GLN
2	B	202	ASN
2	B	228	GLN
2	B	253	GLN
2	B	254	ASN
2	B	256	GLN
2	B	279	ASN
2	B	284	ASN
2	B	296	ASN
2	B	301	GLN
2	B	336	ASN
2	B	339	GLN
2	B	351	ASN
2	B	359	GLN
2	B	393	GLN
2	B	405	ASN
2	B	408	HIS
2	B	411	ASN
2	B	421	GLN
2	B	429	HIS
2	B	439	ASN
3	C	130	GLN
3	C	158	ASN
3	C	176	GLN
3	C	195	GLN
3	C	210	GLN
3	C	217	HIS
3	C	230	ASN
3	C	234	HIS
3	C	239	GLN
3	C	307	HIS
3	C	308	ASN
3	C	317	ASN

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Mol	Chain	Res	Type
3	C	319	ASN
3	C	329	GLN
3	C	340	HIS
3	C	365	ASN
1	D	134	GLN
1	D	139	ASN
1	D	181	GLN
1	D	182	GLN
1	D	187	GLN
2	E	158	ASN
2	E	164	ASN
2	E	180	GLN
2	E	202	ASN
2	E	256	GLN
2	E	271	GLN
2	E	284	ASN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	336	ASN
2	E	351	ASN
2	E	359	GLN
2	E	382	ASN
2	E	405	ASN
2	E	408	HIS
2	E	439	ASN
3	F	111	GLN
3	F	115	ASN
3	F	118	ASN
3	F	119	GLN
3	F	134	GLN
3	F	144	GLN
3	F	163	GLN
3	F	189	ASN
3	F	210	GLN
3	F	217	HIS
3	F	230	ASN
3	F	239	GLN
3	F	254	ASN
3	F	308	ASN
3	F	325	ASN
3	F	337	ASN

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Mol	Chain	Res	Type
3	F	361	ASN
3	F	365	ASN
1	G	143	GLN
2	H	160	ASN
2	H	164	ASN
2	H	174	ASN
2	H	189	GLN
2	H	202	ASN
2	H	228	GLN
2	H	253	GLN
2	H	254	ASN
2	H	256	GLN
2	H	279	ASN
2	H	284	ASN
2	H	296	ASN
2	H	301	GLN
2	H	336	ASN
2	H	339	GLN
2	H	351	ASN
2	H	359	GLN
2	H	370	HIS
2	H	393	GLN
2	H	405	ASN
2	H	408	HIS
2	H	411	ASN
2	H	421	GLN
2	H	429	HIS
2	H	439	ASN
3	I	103	HIS
3	I	111	GLN
3	I	119	GLN
3	I	123	ASN
3	I	136	GLN
3	I	158	ASN
3	I	176	GLN
3	I	195	GLN
3	I	210	GLN
3	I	217	HIS
3	I	230	ASN
3	I	234	HIS
3	I	239	GLN
3	I	307	HIS

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Mol	Chain	Res	Type
3	I	308	ASN
3	I	317	ASN
3	I	319	ASN
3	I	329	GLN
3	I	340	HIS
3	I	345	ASN
3	I	365	ASN
1	J	131	GLN
1	J	137	GLN
1	J	139	ASN
1	J	181	GLN
1	J	182	GLN
1	J	184	GLN
1	J	187	GLN
2	K	158	ASN
2	K	160	ASN
2	K	180	GLN
2	K	189	GLN
2	K	202	ASN
2	K	246	ASN
2	K	256	GLN
2	K	271	GLN
2	K	284	ASN
2	K	296	ASN
2	K	301	GLN
2	K	325	HIS
2	K	336	ASN
2	K	351	ASN
2	K	359	GLN
2	K	382	ASN
2	K	405	ASN
2	K	421	GLN
2	K	439	ASN
3	L	111	GLN
3	L	115	ASN
3	L	117	ASN
3	L	136	GLN
3	L	144	GLN
3	L	163	GLN
3	L	189	ASN
3	L	217	HIS
3	L	230	ASN

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Mol	Chain	Res	Type
3	L	239	GLN
3	L	254	ASN
3	L	308	ASN
3	L	325	ASN
3	L	337	ASN
3	L	361	ASN
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 ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
4	HYP	M	2	4	7,8,9	1.16	1 (14%)	5,10,12	1.37	1 (20%)
4	HYP	O	2	4	7,8,9	0.70	0	5,10,12	2.03	2 (40%)
4	HYP	N	2	4	7,8,9	0.90	0	5,10,12	1.78	1 (20%)
4	HYP	P	2	4	7,8,9	0.97	0	5,10,12	1.13	0
4	HYP	R	2	4	7,8,9	0.91	0	5,10,12	2.24	1 (20%)
4	HYP	T	2	4	7,8,9	0.82	0	5,10,12	1.14	0
4	HYP	Q	2	4	7,8,9	1.05	1 (14%)	5,10,12	1.41	1 (20%)
4	HYP	S	2	4	7,8,9	1.00	0	5,10,12	1.24	1 (20%)

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
4	HYP	M	2	4	-	0/0/11/13	0/1/1/1
4	HYP	O	2	4	-	0/0/11/13	0/1/1/1
4	HYP	N	2	4	-	0/0/11/13	0/1/1/1
4	HYP	P	2	4	-	0/0/11/13	0/1/1/1
4	HYP	R	2	4	-	0/0/11/13	0/1/1/1
4	HYP	T	2	4	-	0/0/11/13	0/1/1/1
4	HYP	Q	2	4	-	0/0/11/13	0/1/1/1
4	HYP	S	2	4	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	2	HYP	CB-CG	-2.41	1.48	1.52
4	Q	2	HYP	CB-CG	-2.07	1.49	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	2	HYP	CG-CB-CA	-3.94	99.20	103.75
4	N	2	HYP	CG-CB-CA	-3.33	99.91	103.75
4	O	2	HYP	CG-CB-CA	-3.16	100.10	103.75
4	M	2	HYP	CG-CB-CA	-2.46	100.91	103.75
4	O	2	HYP	CB-CG-CD	-2.43	100.45	103.16
4	S	2	HYP	CG-CB-CA	-2.39	100.98	103.75
4	Q	2	HYP	CG-CB-CA	-2.34	101.05	103.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	O	2	HYP	1	0
4	P	2	HYP	2	0
4	T	2	HYP	2	0
4	S	2	HYP	4	0

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	E	470	2	14,14,15	0.79	1 (7%)	17,19,21	0.82	0
5	NAG	K	470	2	14,14,15	0.65	0	17,19,21	0.96	1 (5%)
5	NAG	H	470	2	14,14,15	0.79	0	17,19,21	0.84	1 (5%)
5	NAG	B	470	2	14,14,15	0.65	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	E	470	2	1/1/5/7	5/6/23/26	0/1/1/1
5	NAG	K	470	2	-	3/6/23/26	0/1/1/1
5	NAG	H	470	2	-	5/6/23/26	0/1/1/1
5	NAG	B	470	2	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	470	NAG	C1-C2	2.33	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	470	NAG	C2-N2-C7	-2.96	118.94	122.90
5	B	470	NAG	C2-N2-C7	-2.76	119.20	122.90
5	H	470	NAG	C2-N2-C7	-2.18	119.98	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	470	NAG	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	470	NAG	C1-C2-N2-C7
5	E	470	NAG	C8-C7-N2-C2
5	E	470	NAG	O7-C7-N2-C2
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	E	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	O5-C5-C6-O6
5	H	470	NAG	C3-C2-N2-C7
5	H	470	NAG	C1-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	470	NAG	5	0
5	K	470	NAG	2	0
5	H	470	NAG	3	0
5	B	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%)	-0.87	0 100 100	61, 81, 96, 116	0
1	D	71/87 (81%)	-0.97	0 100 100	36, 59, 88, 90	0
1	G	74/87 (85%)	-0.86	1 (1%) 73 65	56, 82, 101, 110	0
1	J	79/87 (90%)	-1.04	0 100 100	37, 60, 102, 108	0
2	B	307/328 (93%)	-0.80	2 (0%) 84 79	49, 78, 102, 115	0
2	E	304/328 (92%)	-1.05	0 100 100	30, 52, 82, 104	0
2	H	307/328 (93%)	-0.77	0 100 100	49, 78, 101, 115	0
2	K	305/328 (92%)	-1.07	0 100 100	29, 52, 83, 105	0
3	C	305/323 (94%)	-0.72	2 (0%) 84 79	49, 85, 110, 121	0
3	F	300/323 (92%)	-0.93	0 100 100	35, 70, 93, 123	0
3	I	305/323 (94%)	-0.76	1 (0%) 90 87	47, 85, 108, 123	0
3	L	300/323 (92%)	-0.93	0 100 100	38, 70, 92, 113	0
4	M	3/5 (60%)	-1.05	0 100 100	70, 70, 73, 91	0
4	N	3/5 (60%)	-1.00	0 100 100	57, 57, 66, 82	0
4	O	3/5 (60%)	-0.95	0 100 100	94, 94, 110, 115	0
4	P	3/5 (60%)	-0.73	0 100 100	67, 67, 70, 99	0
4	Q	3/5 (60%)	-1.03	0 100 100	66, 66, 67, 87	0
4	R	3/5 (60%)	-0.55	0 100 100	51, 51, 63, 77	0
4	S	3/5 (60%)	0.14	0 100 100	89, 89, 98, 123	0
4	T	3/5 (60%)	-0.47	0 100 100	65, 65, 69, 91	0
All	All	2755/2992 (92%)	-0.88	6 (0%) 91 89	29, 73, 102, 123	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	188	ALA	3.2
3	C	236	ILE	2.9
1	G	170	ALA	2.6
3	I	339	CYS	2.6
3	C	341	ALA	2.2
2	B	250	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
4	HYP	S	2	8/9	0.96	0.06	90,94,98,103	0
4	HYP	O	2	8/9	0.97	0.06	97,105,109,110	0
4	HYP	P	2	8/9	0.98	0.06	72,76,81,85	0
4	HYP	Q	2	8/9	0.98	0.06	70,72,73,76	0
4	HYP	M	2	8/9	0.98	0.05	70,73,74,74	0
4	HYP	R	2	8/9	0.99	0.04	43,49,56,59	0
4	HYP	N	2	8/9	0.99	0.04	49,56,63,64	0
4	HYP	T	2	8/9	0.99	0.08	73,75,76,79	0

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(Å ²)	Q<0.9
5	NAG	B	470	14/15	0.97	0.06	85,88,92,100	0
5	NAG	E	470	14/15	0.97	0.05	66,77,88,93	0
5	NAG	K	470	14/15	0.97	0.07	65,89,100,103	0
5	NAG	H	470	14/15	0.98	0.07	82,95,103,105	0
6	CA	B	2	1/1	0.98	0.04	86,86,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	E	3	1/1	0.98	0.06	88,88,88,88	0
6	CA	F	1	1/1	0.98	0.05	64,64,64,64	0
6	CA	K	3	1/1	0.98	0.08	94,94,94,94	0
6	CA	E	2	1/1	0.99	0.04	60,60,60,60	0
6	CA	H	2	1/1	0.99	0.03	87,87,87,87	0
6	CA	I	1	1/1	0.99	0.04	69,69,69,69	0
6	CA	K	2	1/1	0.99	0.02	60,60,60,60	0
6	CA	C	1	1/1	0.99	0.03	70,70,70,70	0
6	CA	L	1	1/1	0.99	0.03	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.