



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:27 PM UTC

PDB ID : 4F15 / pdb_00004f15
Title : Molecular basis of infectivity of 2009 pandemic H1N1 influenza A viruses
Authors : Kim, K.H.; Cho, K.J.; Lee, J.H.; Park, Y.H.; Khan, T.G.; Lee, J.Y.; Kang, S.H.; Alam, I.
Deposited on : 2012-05-06
Resolution : 2.81 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

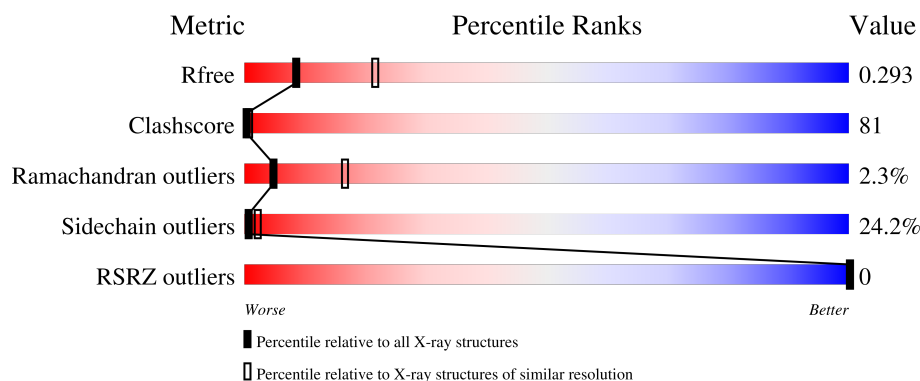
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	518	
1	D	518	
1	G	518	
1	J	518	
2	B	219	

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Mol	Chain	Length	Quality of chain
2	E	219	
2	H	219	
2	K	219	
3	C	218	
3	F	218	
3	I	218	
3	L	218	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19900 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1813	1152	311	344	6			
1	D	246	Total	C	N	O	S	0	0	0
			1872	1187	323	356	6			
1	G	227	Total	C	N	O	S	0	0	0
			1778	1131	304	337	6			
1	J	255	Total	C	N	O	S	0	0	0
			1918	1215	332	365	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ALA	-	expression tag	UNP C5MQE6
A	-7	ASP	-	expression tag	UNP C5MQE6
A	-6	PRO	-	expression tag	UNP C5MQE6
A	-5	GLY	-	expression tag	UNP C5MQE6
A	-4	TYR	-	expression tag	UNP C5MQE6
A	-3	LEU	-	expression tag	UNP C5MQE6
A	-2	LEU	-	expression tag	UNP C5MQE6
A	-1	GLU	-	expression tag	UNP C5MQE6
A	0	PHE	-	expression tag	UNP C5MQE6
A	507	ARG	-	expression tag	UNP C5MQE6
A	508	SER	-	expression tag	UNP C5MQE6
A	509	LEU	-	expression tag	UNP C5MQE6
A	510	VAL	-	expression tag	UNP C5MQE6
A	511	PRO	-	expression tag	UNP C5MQE6
A	512	ARG	-	expression tag	UNP C5MQE6
D	-8	ALA	-	expression tag	UNP C5MQE6
D	-7	ASP	-	expression tag	UNP C5MQE6
D	-6	PRO	-	expression tag	UNP C5MQE6
D	-5	GLY	-	expression tag	UNP C5MQE6
D	-4	TYR	-	expression tag	UNP C5MQE6
D	-3	LEU	-	expression tag	UNP C5MQE6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	LEU	-	expression tag	UNP C5MQE6
D	-1	GLU	-	expression tag	UNP C5MQE6
D	0	PHE	-	expression tag	UNP C5MQE6
D	507	ARG	-	expression tag	UNP C5MQE6
D	508	SER	-	expression tag	UNP C5MQE6
D	509	LEU	-	expression tag	UNP C5MQE6
D	510	VAL	-	expression tag	UNP C5MQE6
D	511	PRO	-	expression tag	UNP C5MQE6
D	512	ARG	-	expression tag	UNP C5MQE6
G	-8	ALA	-	expression tag	UNP C5MQE6
G	-7	ASP	-	expression tag	UNP C5MQE6
G	-6	PRO	-	expression tag	UNP C5MQE6
G	-5	GLY	-	expression tag	UNP C5MQE6
G	-4	TYR	-	expression tag	UNP C5MQE6
G	-3	LEU	-	expression tag	UNP C5MQE6
G	-2	LEU	-	expression tag	UNP C5MQE6
G	-1	GLU	-	expression tag	UNP C5MQE6
G	0	PHE	-	expression tag	UNP C5MQE6
G	507	ARG	-	expression tag	UNP C5MQE6
G	508	SER	-	expression tag	UNP C5MQE6
G	509	LEU	-	expression tag	UNP C5MQE6
G	510	VAL	-	expression tag	UNP C5MQE6
G	511	PRO	-	expression tag	UNP C5MQE6
G	512	ARG	-	expression tag	UNP C5MQE6
J	-8	ALA	-	expression tag	UNP C5MQE6
J	-7	ASP	-	expression tag	UNP C5MQE6
J	-6	PRO	-	expression tag	UNP C5MQE6
J	-5	GLY	-	expression tag	UNP C5MQE6
J	-4	TYR	-	expression tag	UNP C5MQE6
J	-3	LEU	-	expression tag	UNP C5MQE6
J	-2	LEU	-	expression tag	UNP C5MQE6
J	-1	GLU	-	expression tag	UNP C5MQE6
J	0	PHE	-	expression tag	UNP C5MQE6
J	507	ARG	-	expression tag	UNP C5MQE6
J	508	SER	-	expression tag	UNP C5MQE6
J	509	LEU	-	expression tag	UNP C5MQE6
J	510	VAL	-	expression tag	UNP C5MQE6
J	511	PRO	-	expression tag	UNP C5MQE6
J	512	ARG	-	expression tag	UNP C5MQE6

- Molecule 2 is a protein called Fab fragment, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			
2	E	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			
2	H	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			
2	K	208	Total	C	N	O	S	0	0	0
			1544	962	268	307	7			

- Molecule 3 is a protein called Fab fragment, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			
3	F	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			
3	I	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			
3	L	203	Total	C	N	O	S	0	0	0
			1557	975	263	313	6			

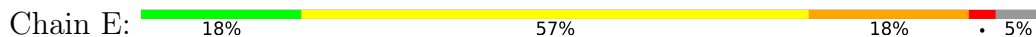
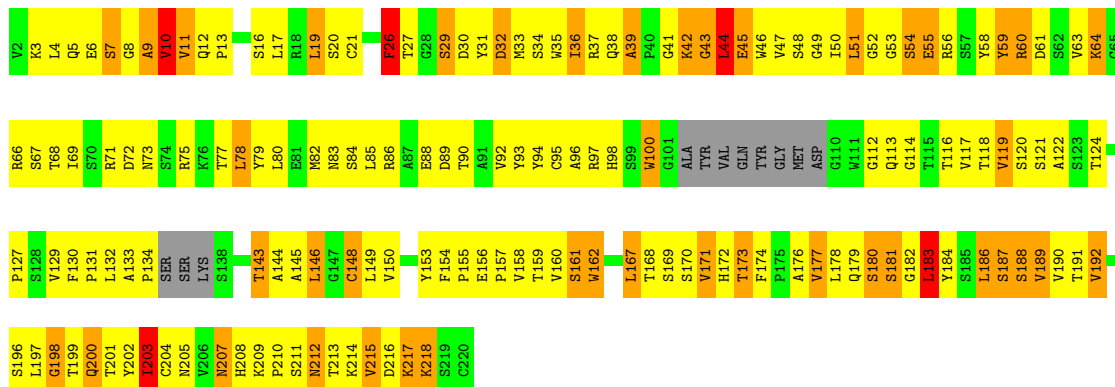
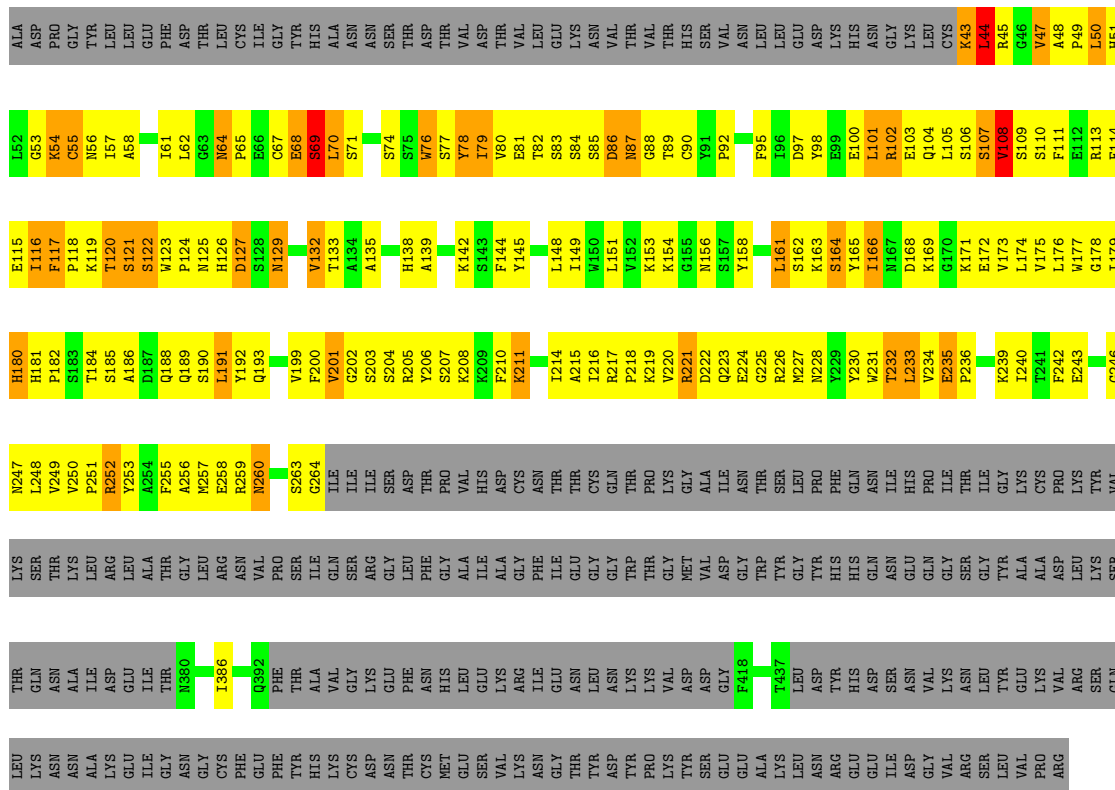
- Molecule 4 is water.

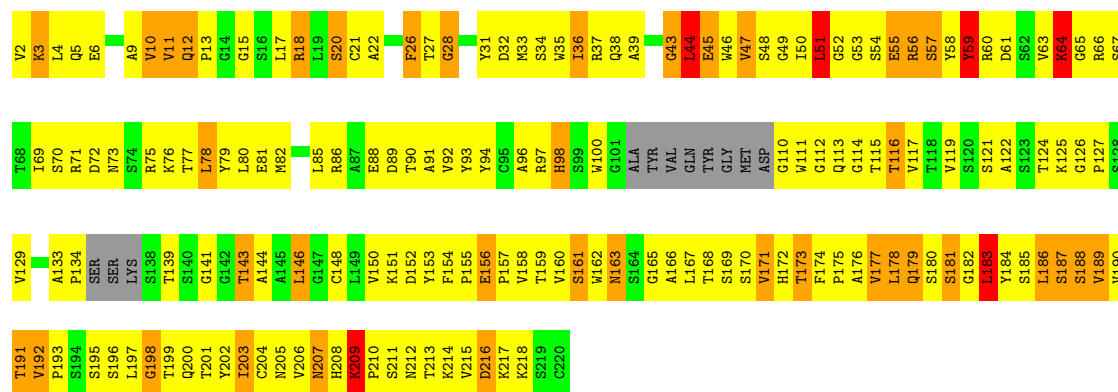
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		
4	B	8	Total	O	0	0
			8	8		
4	C	11	Total	O	0	0
			11	11		
4	D	7	Total	O	0	0
			7	7		
4	E	11	Total	O	0	0
			11	11		
4	F	9	Total	O	0	0
			9	9		
4	G	8	Total	O	0	0
			8	8		
4	H	10	Total	O	0	0
			10	10		
4	I	12	Total	O	0	0
			12	12		
4	J	7	Total	O	0	0
			7	7		

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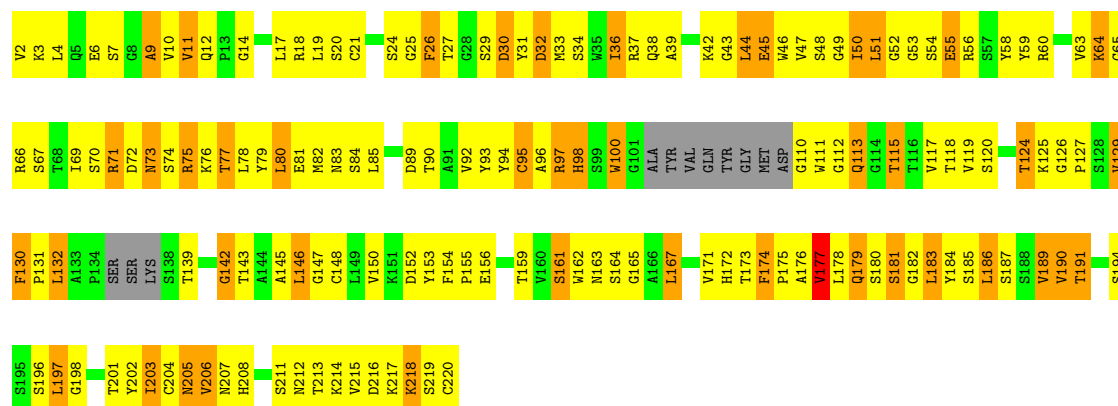
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	6	Total 6	O 6	0	0
4	L	15	Total 15	O 15	0	0





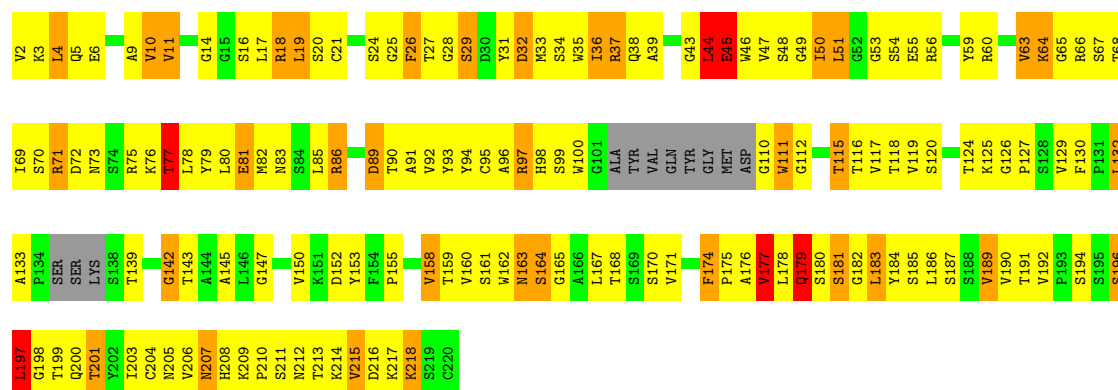
• Molecule 2: Fab fragment, heavy chain

Chain H: 23% 52% 20% 5%



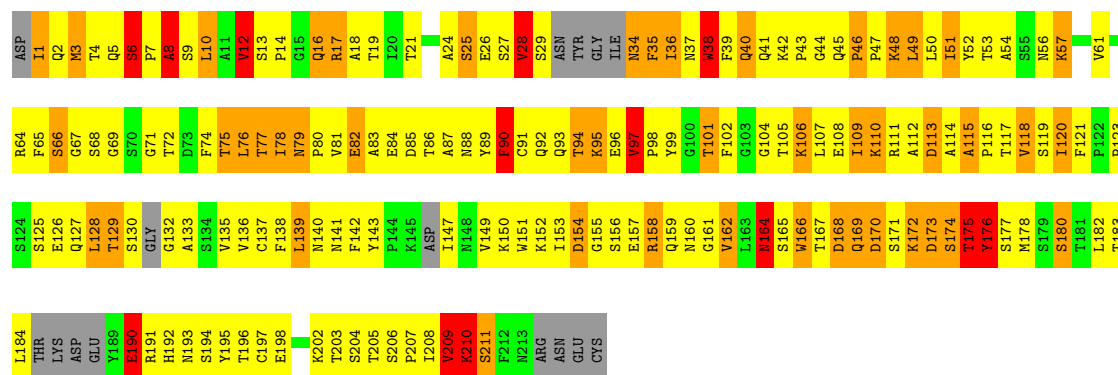
• Molecule 2: Fab fragment, heavy chain

Chain K: 23% 53% 16% 5%



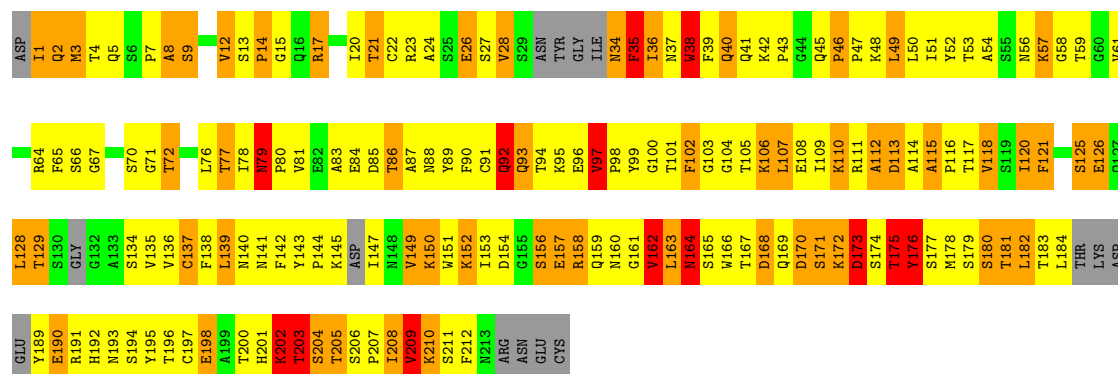
• Molecule 3: Fab fragment, light chain

Chain C: 14% 52% 22% 6% 7%



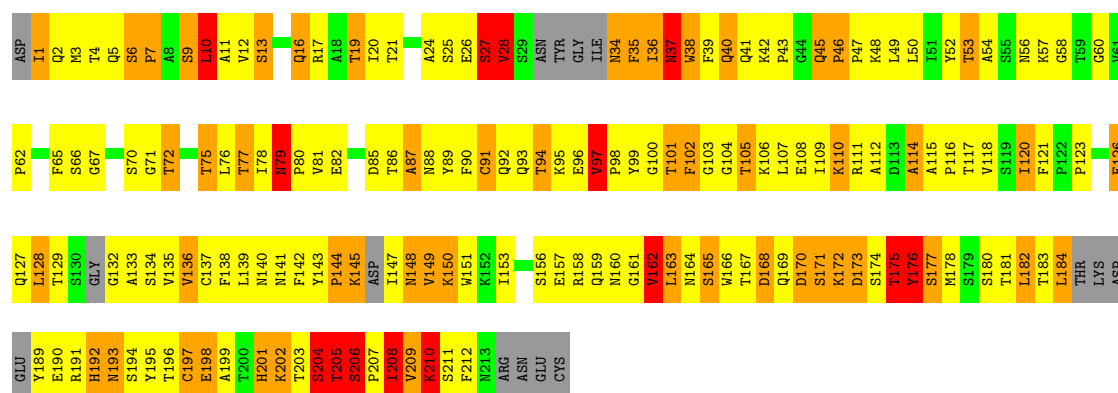
• Molecule 3: Fab fragment, light chain

Chain F: 14% 47% 26% 6% 7%



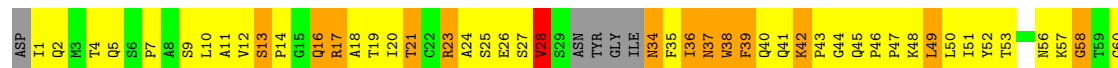
• Molecule 3: Fab fragment, light chain

Chain I: 15% 48% 24% 6% 7%



• Molecule 3: Fab fragment, light chain

Chain L: 13% 53% 23% 7%



ASP	P123	V61
GLU	S124	P62
Y189	A125	A63
E190	E126	R64
R191	O127	G65
H192	L128	S66
M193	T129	
S194	S130	G69
Y195	GLY	
T196	G132	T72
C197	A133	D73
E198		F74
A199	F136	T75
T200	L139	L76
H201	M140	T77
K202	N141	I78
T203	F142	N79
S204	Y143	P80
T205	P144	V81
S206	R145	E82
P207	ASP	A83
I208	L147	E84
V209	M148	D85
K210	V149	T86
S211	R150	A87
F212	M151	N88
N213	K152	Y89
ARG	I153	F90
ASN	D154	C91
GLU	G155	Q92
CYS	S156	Q93
	E157	T94
	R158	K95
		E96
	G161	V97
	V162	P98
	L163	P99
	M164	G100
	R165	T101
	W166	F102
	T167	G103
	D168	G104
	G169	T105
	D170	K106
	S171	L107
	K172	E108
	D173	T109
	T174	K110
	V175	R111
	S176	A112
	Y177	D113
	M178	A114
	R179	A115
	S180	P116
	L181	T117
	L182	V118
	T183	S119
	L184	T120
	T185	F121
	V186	E122

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.70Å 90.13Å 238.18Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	49.68 – 2.81 49.68 – 2.81	Depositor EDS
% Data completeness (in resolution range)	87.5 (49.68-2.81) 84.4 (49.68-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.233 , 0.289 0.236 , 0.293	Depositor DCC
R_{free} test set	3381 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 25.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
Reported twinning fraction	0.492 for h,-k,-l	Depositor
Outliers	2 of 66880 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19900	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1107e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/1861	1.07	12/2523 (0.5%)
1	D	0.52	0/1919	1.05	8/2602 (0.3%)
1	G	0.54	0/1826	1.11	10/2474 (0.4%)
1	J	0.54	0/1965	1.11	18/2667 (0.7%)
2	B	0.59	0/1577	1.21	18/2141 (0.8%)
2	E	0.56	0/1577	1.17	12/2141 (0.6%)
2	H	0.53	0/1577	1.14	16/2141 (0.7%)
2	K	0.54	0/1577	1.21	17/2141 (0.8%)
3	C	0.66	0/1590	1.42	29/2157 (1.3%)
3	F	0.71	0/1590	1.31	26/2157 (1.2%)
3	I	1.25	1/1591 (0.1%)	1.42	37/2160 (1.7%)
3	L	1.33	1/1591 (0.1%)	1.51	34/2160 (1.6%)
All	All	0.73	2/20241 (0.0%)	1.23	237/27464 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	3
1	G	0	3
1	J	0	2
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
3	C	0	8
3	F	0	13
3	I	0	6
3	L	0	2
All	All	0	43

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	145	LYS	C-N	46.17	1.98	1.33
3	I	145	LYS	C-N	41.07	1.89	1.33

All (237) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	209	VAL	N-CA-C	14.42	125.30	107.70
3	I	209	VAL	N-CA-C	14.20	125.02	107.70
3	L	145	LYS	O-C-N	-13.77	102.07	122.99
3	L	145	LYS	CA-C-N	12.61	144.39	121.70
3	L	145	LYS	C-N-CA	12.61	144.39	121.70
2	E	43	GLY	N-CA-C	-11.84	96.09	111.37
3	L	175	THR	N-CA-C	11.81	125.48	108.00
3	I	176	TYR	N-CA-C	11.74	126.40	110.55
3	C	94	THR	N-CA-C	-11.65	93.11	110.24
2	K	174	PHE	CA-C-N	11.28	131.36	120.31
2	K	174	PHE	C-N-CA	11.28	131.36	120.31
3	L	79	ASN	CA-C-N	-10.49	107.32	120.23
3	L	79	ASN	C-N-CA	-10.49	107.32	120.23
3	I	94	THR	N-CA-C	-10.30	95.71	110.24
3	I	6	SER	CA-C-N	10.27	132.87	120.23
3	I	6	SER	C-N-CA	10.27	132.87	120.23
3	F	94	THR	N-CA-C	-10.21	95.24	110.24
3	F	209	VAL	N-CA-C	9.89	122.61	108.17
2	E	45	GLU	N-CA-C	9.81	123.48	110.53
3	L	176	TYR	N-CA-C	9.77	123.42	110.53
3	C	38	TRP	N-CA-C	-9.74	95.04	110.14
3	C	97	VAL	CA-C-N	-9.62	109.64	119.93
3	C	97	VAL	C-N-CA	-9.62	109.64	119.93
3	L	37	ASN	N-CA-C	9.46	125.44	108.69
2	B	198	GLY	N-CA-C	-9.32	103.58	115.42
2	H	26	PHE	CB-CA-C	-9.32	103.59	115.89
2	B	192	VAL	CA-C-N	9.31	129.89	119.83
2	B	192	VAL	C-N-CA	9.31	129.89	119.83
3	C	209	VAL	N-CA-C	9.29	121.63	107.78
3	L	94	THR	N-CA-C	-9.25	94.16	109.24
3	F	210	LYS	N-CA-C	9.14	121.53	108.00
3	C	206	SER	CA-C-N	9.07	129.76	120.14
3	C	206	SER	C-N-CA	9.07	129.76	120.14
3	I	58	GLY	N-CA-C	-8.89	102.55	112.33
3	C	210	LYS	N-CA-C	8.88	125.66	109.32
1	A	170	GLY	N-CA-C	-8.71	100.65	115.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	76	TRP	N-CA-C	8.68	119.72	108.34
3	F	46	PRO	N-CA-C	8.57	119.75	110.58
3	C	79	ASN	CA-C-N	-8.46	110.86	119.99
3	C	79	ASN	C-N-CA	-8.46	110.86	119.99
2	K	9	ALA	N-CA-C	8.40	119.82	108.23
2	E	26	PHE	CB-CA-C	-8.38	104.82	115.89
3	F	175	THR	CB-CA-C	-8.31	104.71	116.34
3	C	165	SER	N-CA-C	8.18	121.33	110.53
2	K	26	PHE	CB-CA-C	-8.18	105.10	115.89
3	F	115	ALA	CA-C-N	8.15	128.35	119.87
3	F	115	ALA	C-N-CA	8.15	128.35	119.87
1	A	123	TRP	CA-C-N	8.11	127.69	118.85
1	A	123	TRP	C-N-CA	8.11	127.69	118.85
3	I	175	THR	N-CA-C	8.08	128.00	110.80
3	F	17	ARG	N-CA-C	8.08	121.63	110.24
1	D	117	PHE	CA-C-N	-8.06	111.67	119.89
1	D	117	PHE	C-N-CA	-8.06	111.67	119.89
3	C	88	ASN	N-CA-C	-8.03	96.38	108.99
2	K	45	GLU	N-CA-C	8.02	121.06	108.79
3	L	210	LYS	N-CA-C	8.02	124.08	109.32
3	I	16	GLN	N-CA-C	7.99	118.78	108.24
3	L	209	VAL	CB-CA-C	-7.90	104.32	111.74
2	K	77	THR	N-CA-C	7.83	120.63	108.96
3	F	175	THR	N-CA-C	7.82	119.57	108.00
1	A	259	ARG	N-CA-C	7.78	118.85	107.88
3	F	97	VAL	CA-C-N	-7.76	111.62	119.93
3	F	97	VAL	C-N-CA	-7.76	111.62	119.93
3	L	206	SER	CA-C-N	7.75	128.36	120.14
3	L	206	SER	C-N-CA	7.75	128.36	120.14
2	B	45	GLU	N-CA-C	7.73	122.20	109.06
1	J	108	VAL	N-CA-C	7.59	120.56	109.63
2	H	11	VAL	N-CA-C	7.58	118.51	107.75
1	G	50	LEU	N-CA-C	7.57	119.77	110.91
2	K	198	GLY	N-CA-C	-7.54	105.85	115.42
3	I	208	ILE	CA-C-N	-7.54	114.43	121.97
3	I	208	ILE	C-N-CA	-7.54	114.43	121.97
1	J	50	LEU	N-CA-C	7.50	119.68	110.91
3	I	37	ASN	N-CA-C	7.43	120.36	109.07
1	D	56	ASN	N-CA-C	-7.36	98.56	109.81
3	L	42	LYS	CA-C-N	-7.35	110.66	119.84
3	L	42	LYS	C-N-CA	-7.35	110.66	119.84
3	C	46	PRO	CA-C-N	7.21	126.97	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	46	PRO	C-N-CA	7.21	126.97	119.76
3	I	28	VAL	N-CA-C	7.19	124.29	109.34
2	B	43	GLY	N-CA-C	-7.17	96.19	113.18
3	F	165	SER	N-CA-C	7.15	121.68	110.17
3	I	115	ALA	CA-C-N	-7.08	110.99	119.84
3	I	115	ALA	C-N-CA	-7.08	110.99	119.84
1	G	180	HIS	N-CA-C	6.98	119.78	108.41
2	K	139	THR	N-CA-C	6.97	117.47	108.34
3	F	112	ALA	N-CA-C	6.97	121.46	112.12
2	K	11	VAL	N-CA-C	6.97	118.39	108.42
3	C	172	LYS	N-CA-C	6.97	120.26	111.69
3	F	107	LEU	N-CA-C	6.95	119.04	110.91
3	I	210	LYS	N-CA-C	6.94	122.08	109.32
2	B	44	LEU	N-CA-C	6.91	125.52	110.80
3	I	27	SER	N-CA-C	6.86	125.40	110.80
1	G	211	LYS	CA-C-N	6.85	126.83	119.78
1	G	211	LYS	C-N-CA	6.85	126.83	119.78
3	L	175	THR	CB-CA-C	-6.81	106.81	116.34
1	G	188	GLN	N-CA-C	-6.80	103.94	111.36
2	E	183	LEU	N-CA-C	6.80	120.76	109.95
2	B	183	LEU	N-CA-C	-6.78	96.36	110.80
2	H	44	LEU	N-CA-C	6.73	116.87	108.19
3	C	170	ASP	N-CA-C	6.72	118.75	108.07
2	B	26	PHE	CB-CA-C	-6.68	107.07	115.89
3	I	210	LYS	CB-CA-C	-6.67	107.85	115.79
2	H	174	PHE	CA-C-N	6.64	128.14	119.84
2	H	174	PHE	C-N-CA	6.64	128.14	119.84
2	B	203	ILE	N-CA-C	6.63	117.10	108.35
2	B	9	ALA	N-CA-C	6.60	116.70	108.19
3	C	155	GLY	N-CA-C	6.59	121.38	111.42
2	E	178	LEU	N-CA-C	-6.58	100.56	110.24
1	J	70	LEU	N-CA-C	6.54	124.74	110.80
3	L	210	LYS	CB-CA-C	-6.53	108.02	115.79
1	A	82	THR	N-CA-C	-6.43	99.41	109.25
2	B	10	VAL	CB-CA-C	-6.42	104.26	111.45
3	L	172	LYS	N-CA-C	6.40	121.25	113.38
2	E	28	GLY	N-CA-C	-6.40	104.47	115.61
3	F	102	PHE	N-CA-C	6.37	116.69	108.34
2	K	177	VAL	N-CA-C	-6.37	101.37	109.58
1	D	169	LYS	N-CA-C	-6.36	102.09	110.43
3	L	58	GLY	N-CA-C	-6.36	98.10	113.18
3	L	112	ALA	N-CA-C	6.33	118.32	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	46	PRO	CA-C-N	6.30	126.25	119.76
3	F	46	PRO	C-N-CA	6.30	126.25	119.76
2	K	197	LEU	N-CA-C	6.27	118.93	108.96
1	G	122	SER	N-CA-C	-6.27	105.57	113.72
1	G	139	ALA	N-CA-C	-6.23	100.67	109.96
1	G	70	LEU	N-CA-C	6.22	124.05	110.80
3	L	115	ALA	CA-C-N	6.21	125.83	119.56
3	L	115	ALA	C-N-CA	6.21	125.83	119.56
3	I	46	PRO	N-CA-C	6.19	118.25	110.70
2	H	9	ALA	N-CA-C	6.13	123.87	110.80
2	B	7	SER	N-CA-C	6.11	118.40	108.26
3	I	46	PRO	CA-C-N	6.09	126.30	119.90
3	I	46	PRO	C-N-CA	6.09	126.30	119.90
2	K	142	GLY	N-CA-C	6.08	123.16	114.64
3	L	91	CYS	N-CA-C	-6.08	100.65	109.59
3	I	6	SER	N-CA-C	6.08	118.67	110.29
3	I	114	ALA	N-CA-C	6.03	120.76	113.17
1	D	257	MET	N-CA-C	6.00	116.16	108.24
3	F	35	PHE	N-CA-C	5.99	118.52	109.23
2	E	209	LYS	CA-C-N	5.96	125.67	119.05
2	E	209	LYS	C-N-CA	5.96	125.67	119.05
3	F	136	VAL	N-CA-C	5.95	116.57	107.77
3	F	205	THR	N-CA-C	5.95	123.47	110.80
3	I	205	THR	N-CA-C	5.94	123.46	110.80
3	L	168	ASP	N-CA-C	5.94	123.46	110.80
1	A	74	SER	N-CA-C	5.91	116.39	108.23
2	H	130	PHE	CA-C-N	5.91	125.85	119.76
2	H	130	PHE	C-N-CA	5.91	125.85	119.76
3	L	87	ALA	N-CA-C	5.89	118.91	109.02
2	H	142	GLY	N-CA-C	5.87	122.86	114.64
1	J	257	MET	N-CA-C	5.85	115.96	108.24
1	A	257	MET	N-CA-C	5.84	115.81	108.45
3	I	10	LEU	N-CA-C	5.83	118.14	108.99
1	J	74	SER	N-CA-C	5.80	117.67	108.79
2	E	59	TYR	N-CA-C	5.80	116.06	107.88
3	C	175	THR	CB-CA-C	-5.79	108.25	115.89
3	L	16	GLN	N-CA-C	5.78	118.66	109.65
3	L	97	VAL	CA-C-N	-5.73	113.34	119.98
3	L	97	VAL	C-N-CA	-5.73	113.34	119.98
2	H	177	VAL	N-CA-C	-5.70	101.67	109.37
1	J	235	GLU	CA-C-N	5.70	126.96	119.84
1	J	235	GLU	C-N-CA	5.70	126.96	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	113	ASP	N-CA-C	5.68	118.82	110.30
3	I	87	ALA	N-CA-C	5.67	119.76	109.32
3	I	171	SER	N-CA-C	5.64	118.28	111.40
3	I	97	VAL	CA-C-N	-5.64	113.89	119.93
3	I	97	VAL	C-N-CA	-5.64	113.89	119.93
2	H	45	GLU	N-CA-C	5.64	118.91	109.95
2	B	212	ASN	N-CA-C	-5.64	98.80	110.80
1	A	76	TRP	N-CA-C	5.63	116.70	108.14
1	J	64	ASN	CA-C-N	5.63	125.30	119.56
1	J	64	ASN	C-N-CA	5.63	125.30	119.56
2	B	162	TRP	N-CA-C	-5.62	106.01	112.92
3	I	87	ALA	CB-CA-C	-5.59	109.13	115.79
1	J	44	LEU	N-CA-C	5.59	117.89	107.99
3	L	87	ALA	CB-CA-C	-5.58	108.52	115.89
2	E	198	GLY	N-CA-C	-5.58	99.96	113.18
2	K	26	PHE	N-CA-C	5.58	118.39	109.02
3	C	210	LYS	CB-CA-C	-5.57	109.16	115.79
1	D	187	ASP	N-CA-C	-5.56	104.44	111.11
3	C	115	ALA	CA-C-N	5.54	125.16	119.56
3	C	115	ALA	C-N-CA	5.54	125.16	119.56
1	J	117	PHE	CA-C-N	-5.54	114.88	120.31
1	J	117	PHE	C-N-CA	-5.54	114.88	120.31
1	J	69	SER	N-CA-C	5.52	115.41	108.45
3	I	172	LYS	N-CA-C	5.52	120.07	113.23
1	J	107	SER	N-CA-C	5.52	119.76	113.19
2	E	44	LEU	N-CA-C	5.50	122.52	110.80
1	G	56	ASN	N-CA-C	-5.50	101.62	110.14
3	I	53	THR	N-CA-C	-5.49	106.17	112.86
1	A	108	VAL	N-CA-C	5.47	116.47	109.30
3	I	91	CYS	N-CA-C	-5.47	101.94	110.10
3	I	145	LYS	CA-C-N	5.46	131.80	121.97
3	I	145	LYS	C-N-CA	5.46	131.80	121.97
1	G	108	VAL	N-CA-C	5.46	116.45	109.30
3	L	204	SER	N-CA-C	5.45	118.95	111.54
3	L	126	GLU	N-CA-C	-5.44	106.64	113.28
1	A	203	SER	N-CA-C	5.42	116.02	108.00
3	L	205	THR	N-CA-C	5.40	117.23	110.91
3	F	180	SER	N-CA-C	5.39	117.19	108.34
3	I	165	SER	N-CA-C	5.38	117.52	108.96
1	J	180	HIS	N-CA-C	5.38	118.25	109.59
2	H	181	SER	N-CA-C	-5.37	104.66	111.11
3	F	79	ASN	CA-C-N	-5.35	113.15	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	79	ASN	C-N-CA	-5.35	113.15	119.84
1	A	128	SER	CA-C-N	-5.35	114.86	122.41
1	A	128	SER	C-N-CA	-5.35	114.86	122.41
3	C	175	THR	N-CA-C	5.34	118.00	109.02
2	B	39	ALA	CA-C-N	-5.34	115.08	120.21
2	B	39	ALA	C-N-CA	-5.34	115.08	120.21
3	C	6	SER	CA-C-N	-5.33	114.85	120.66
3	C	6	SER	C-N-CA	-5.33	114.85	120.66
2	B	8	GLY	N-CA-C	5.27	119.31	110.56
3	I	9	SER	N-CA-C	-5.26	99.01	108.48
2	B	116	THR	N-CA-C	5.21	116.80	108.41
2	K	44	LEU	N-CA-C	5.21	121.89	110.80
3	F	206	SER	N-CA-C	5.20	121.30	109.81
1	J	121	SER	N-CA-C	-5.20	99.73	110.80
3	C	166	TRP	N-CA-C	5.19	117.28	109.23
2	H	177	VAL	CA-C-N	-5.19	115.64	122.85
2	H	177	VAL	C-N-CA	-5.19	115.64	122.85
1	D	259	ARG	N-CA-C	5.17	115.35	108.38
2	E	51	LEU	N-CA-C	5.14	117.81	109.79
3	C	16	GLN	N-CA-C	5.13	117.66	109.65
2	K	192	VAL	CA-C-N	5.12	125.41	119.93
2	K	192	VAL	C-N-CA	5.12	125.41	119.93
2	H	167	LEU	N-CA-C	5.11	117.25	111.11
3	C	10	LEU	N-CA-C	5.11	117.02	108.99
2	H	139	THR	N-CA-C	5.10	115.03	108.34
1	D	203	SER	CB-CA-C	-5.09	109.22	116.34
1	J	79	ILE	N-CA-C	5.08	116.61	108.89
3	F	176	TYR	N-CA-C	5.08	117.24	110.53
3	I	206	SER	N-CA-C	5.07	121.01	109.81
3	C	90	PHE	CB-CA-C	-5.05	102.56	110.79
2	K	111	TRP	N-CA-C	5.03	117.03	109.23
3	C	176	TYR	N-CA-C	5.02	116.77	110.24
3	L	165	SER	N-CA-C	5.01	116.69	108.52

There are no chirality outliers.

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	ASN	Peptide
1	A	74	SER	Peptide
2	B	44	LEU	Peptide
3	C	164	ASN	Peptide

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Mol	Chain	Res	Type	Group
3	C	175	THR	Peptide
3	C	190	GLU	Peptide
3	C	209	VAL	Peptide
3	C	28	VAL	Peptide
3	C	35	PHE	Peptide
3	C	38	TRP	Peptide
3	C	8	ALA	Peptide
1	D	119	LYS	Peptide
1	D	139	ALA	Peptide
1	D	69	SER	Peptide
2	E	179	GLN	Peptide
3	F	112	ALA	Peptide
3	F	14	PRO	Peptide
3	F	164	ASN	Peptide
3	F	173	ASP	Peptide
3	F	175	THR	Peptide
3	F	202	LYS	Peptide
3	F	203	THR	Peptide
3	F	208	ILE	Peptide
3	F	209	VAL	Peptide
3	F	35	PHE	Peptide
3	F	38	TRP	Peptide
3	F	79	ASN	Peptide
3	F	92	GLN	Peptide
1	G	121	SER	Peptide
1	G	129	ASN	Peptide
1	G	69	SER	Peptide
2	H	181	SER	Peptide
3	I	175	THR	Peptide
3	I	201	HIS	Peptide
3	I	202	LYS	Peptide
3	I	35	PHE	Peptide
3	I	43	PRO	Peptide
3	I	79	ASN	Peptide
1	J	129	ASN	Peptide
1	J	44	LEU	Peptide
2	K	181	SER	Peptide
3	L	128	LEU	Peptide
3	L	175	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1813	0	1716	196	0
1	D	1872	0	1743	222	0
1	G	1778	0	1702	245	0
1	J	1918	0	1760	225	0
2	B	1544	0	1505	265	0
2	E	1544	0	1505	264	0
2	H	1544	0	1505	283	0
2	K	1544	0	1505	254	0
3	C	1557	0	1503	347	0
3	F	1557	0	1503	362	0
3	I	1557	0	1503	324	0
3	L	1557	0	1503	338	0
4	A	11	0	0	2	0
4	B	8	0	0	3	0
4	C	11	0	0	3	0
4	D	7	0	0	1	0
4	E	11	0	0	3	0
4	F	9	0	0	5	0
4	G	8	0	0	2	0
4	H	10	0	0	3	0
4	I	12	0	0	2	0
4	J	7	0	0	3	0
4	K	6	0	0	4	0
4	L	15	0	0	8	0
All	All	19900	0	18953	3136	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 81.

All (3136) 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:38:TRP:CD1	3:F:40:GLN:H	1.45	1.35
3:I:145:LYS:C	3:I:147:ILE:N	1.89	1.30
3:C:38:TRP:CD2	3:C:39:PHE:HA	1.74	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:145:LYS:C	3:L:147:ILE:N	1.98	1.20
2:B:171:VAL:HG21	3:C:176:TYR:CE1	1.76	1.19
3:I:184:LEU:C	3:I:189:TYR:N	2.02	1.17
2:E:32:ASP:HB3	2:E:51:LEU:HA	1.27	1.15
3:F:141:ASN:HA	3:F:175:THR:HG22	1.14	1.14
3:C:138:PHE:CD1	3:C:178:MET:HG2	1.82	1.14
1:G:54:LYS:HG3	1:G:67:CYS:HA	1.17	1.13
3:F:92:GLN:HG2	3:F:101:THR:HG23	1.20	1.13
3:F:158:ARG:HH22	2:H:97:ARG:HD2	1.11	1.12
3:F:38:TRP:CD2	3:F:39:PHE:HA	1.83	1.12
3:C:9:SER:HB3	3:C:106:LYS:HB3	1.12	1.11
3:F:111:ARG:HD3	3:F:173:ASP:HA	1.32	1.11
2:B:32:ASP:HB3	2:B:51:LEU:HA	1.28	1.11
3:I:11:ALA:HB2	3:I:108:GLU:HG3	1.13	1.10
3:C:1:ILE:HD11	3:C:98:PRO:HB2	1.31	1.10
1:J:177:TRP:HB3	4:J:601:HOH:O	1.51	1.10
2:B:181:SER:HB2	3:L:62:PRO:HG3	1.33	1.09
3:L:38:TRP:HB2	3:L:47:PRO:HB2	1.09	1.07
3:L:45:GLN:HB3	3:L:46:PRO:HD2	1.36	1.07
3:L:140:ASN:HA	3:L:176:TYR:HB3	1.33	1.07
1:G:54:LYS:H	1:G:54:LYS:HD3	1.19	1.06
2:B:59:TYR:HE1	2:B:69:ILE:HG22	1.18	1.04
2:E:46:TRP:H	2:E:60:ARG:NH2	1.54	1.04
3:I:140:ASN:HA	3:I:176:TYR:HB3	1.35	1.04
1:D:91:TYR:HD1	1:D:227:MET:HB2	1.18	1.03
1:G:171:LYS:HD3	1:G:258:GLU:HG3	1.36	1.03
3:L:142:PHE:CZ	3:L:177:SER:HB3	1.94	1.02
1:A:202:GLY:HA3	1:A:241:THR:H	1.18	1.02
3:F:141:ASN:CA	3:F:175:THR:HG22	1.89	1.02
3:I:141:ASN:HA	3:I:175:THR:HG22	1.41	1.02
3:C:39:PHE:O	3:C:50:LEU:HG	1.60	1.01
1:J:201:VAL:HG12	1:J:202:GLY:H	1.23	1.01
3:I:194:SER:HB2	3:I:210:LYS:HD2	1.38	1.01
2:B:50:ILE:HD11	2:B:71:ARG:HB2	1.39	1.01
2:B:39:ALA:HB3	2:B:44:LEU:HD13	1.42	1.01
3:F:38:TRP:CD1	3:F:40:GLN:N	2.29	1.00
2:B:59:TYR:CE1	2:B:69:ILE:HG22	1.97	1.00
3:I:38:TRP:CB	3:I:47:PRO:HB2	1.90	1.00
3:F:92:GLN:OE1	3:F:101:THR:OG1	1.80	0.99
3:F:9:SER:H	3:F:105:THR:HG23	1.24	0.99
3:L:11:ALA:HB2	3:L:108:GLU:HB3	1.45	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:TYR:CD1	1:A:227:MET:HB2	1.97	0.99
3:C:203:THR:HG23	3:C:205:THR:H	1.28	0.99
2:E:179:GLN:HB3	3:I:60:GLY:HA2	1.40	0.99
2:K:14:GLY:N	2:K:85:LEU:O	1.94	0.99
2:H:97:ARG:HB3	2:H:110:GLY:HA3	1.44	0.98
3:L:38:TRP:HB2	3:L:47:PRO:CB	1.93	0.98
3:L:142:PHE:HZ	3:L:177:SER:HB3	1.25	0.98
1:A:75:SER:OG	1:A:108:VAL:O	1.81	0.98
1:J:67:CYS:O	1:J:68:GLU:HG3	1.61	0.98
3:I:57:LYS:NZ	3:I:65:PHE:O	1.97	0.98
2:E:46:TRP:N	2:E:60:ARG:HH22	1.61	0.97
1:A:91:TYR:HD1	1:A:227:MET:HB2	1.25	0.97
1:G:119:LYS:NZ	1:G:129:ASN:HD22	1.61	0.97
3:I:100:GLY:HA3	4:I:306:HOH:O	1.62	0.97
3:C:113:ASP:OD1	3:C:115:ALA:N	1.96	0.97
2:K:32:ASP:HB2	2:K:98:HIS:HD1	1.29	0.97
1:A:149:ILE:HB	1:A:250:VAL:HG23	1.43	0.97
2:E:162:TRP:H	2:E:167:LEU:HG	1.28	0.97
1:G:217:ARG:HD3	1:G:226:ARG:HG2	1.45	0.97
3:L:145:LYS:NZ	3:L:167:THR:OG1	1.98	0.97
3:C:42:LYS:NZ	3:C:84:GLU:OE2	1.97	0.97
1:D:84:SER:O	1:D:87:ASN:N	1.97	0.97
3:F:92:GLN:HG2	3:F:101:THR:CG2	1.94	0.97
3:C:4:THR:HG22	3:C:24:ALA:HA	1.46	0.96
1:D:137:PRO:HA	1:D:142:LYS:HA	1.48	0.96
3:C:35:PHE:HE1	3:C:49:LEU:HD11	1.30	0.96
1:D:160:LYS:H	1:D:160:LYS:HE3	1.31	0.96
2:K:96:ALA:HB1	3:L:36:ILE:CD1	1.96	0.96
3:F:97:VAL:HG12	3:F:98:PRO:O	1.66	0.95
1:D:91:TYR:CD1	1:D:227:MET:HB2	2.00	0.95
3:C:38:TRP:O	3:C:39:PHE:CD2	2.20	0.95
2:E:5:GLN:O	2:E:21:CYS:HA	1.66	0.95
3:C:138:PHE:HD1	3:C:178:MET:HG2	1.30	0.95
1:J:102:ARG:HG3	1:J:102:ARG:HH11	1.30	0.95
3:C:38:TRP:CE3	3:C:39:PHE:HA	2.03	0.94
2:B:5:GLN:O	2:B:21:CYS:HA	1.66	0.94
1:A:225:GLY:O	1:A:226:ARG:NH1	1.99	0.94
1:D:119:LYS:NZ	1:D:128:SER:O	2.01	0.94
3:I:194:SER:HB2	3:I:210:LYS:CD	1.97	0.94
2:B:162:TRP:H	2:B:167:LEU:HD11	1.32	0.94
2:B:171:VAL:HG21	3:C:176:TYR:CZ	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:7:PRO:HD3	3:C:21:THR:O	1.68	0.94
3:F:86:THR:HG22	3:F:109:ILE:HD13	1.50	0.94
1:G:199:VAL:HG12	1:G:200:PHE:H	1.32	0.94
3:F:39:PHE:O	3:F:50:LEU:HG	1.66	0.93
2:H:10:VAL:HG21	2:H:155:PRO:HG3	1.47	0.93
1:J:235:GLU:HG3	1:J:236:PRO:HD2	1.48	0.93
3:L:91:CYS:SG	3:L:102:PHE:HD2	1.90	0.93
2:B:38:GLN:HA	2:B:44:LEU:H	1.31	0.93
2:E:165:GLY:O	2:E:168:THR:OG1	1.86	0.93
3:F:141:ASN:HA	3:F:175:THR:CG2	1.96	0.93
2:B:54:SER:HB3	2:B:56:ARG:HD3	1.51	0.93
3:F:190:GLU:OE1	3:F:191:ARG:HG2	1.68	0.93
2:B:203:ILE:HD11	2:B:216:ASP:HB3	1.50	0.93
3:I:196:THR:OG1	3:I:210:LYS:HD3	1.68	0.93
2:B:180:SER:O	2:B:182:GLY:N	2.01	0.93
1:A:219:LYS:HG3	1:A:224:GLU:HG3	1.52	0.92
3:F:38:TRP:CE2	3:F:39:PHE:HA	2.03	0.92
3:F:116:PRO:HA	3:F:142:PHE:HB3	1.51	0.92
3:F:153:ILE:HG13	3:F:154:ASP:H	1.34	0.92
3:I:38:TRP:HB2	3:I:47:PRO:HB2	1.50	0.92
2:B:32:ASP:HA	2:B:71:ARG:HH22	1.35	0.92
3:C:106:LYS:HG3	3:C:107:LEU:H	1.32	0.92
2:K:71:ARG:HA	2:K:78:LEU:HA	1.52	0.92
3:I:11:ALA:HB2	3:I:108:GLU:CG	1.99	0.92
3:I:37:ASN:HD22	3:I:38:TRP:N	1.66	0.92
2:E:6:GLU:HA	2:E:20:SER:O	1.70	0.91
3:I:38:TRP:HZ3	3:I:92:GLN:HE21	1.10	0.91
3:I:38:TRP:CD1	3:I:47:PRO:HB3	2.04	0.91
2:H:90:THR:HG23	2:H:118:THR:HA	1.52	0.91
3:C:50:LEU:HD11	3:C:89:TYR:HE1	1.36	0.91
3:C:9:SER:HB3	3:C:106:LYS:CB	1.99	0.91
2:H:146:LEU:HD13	2:H:147:GLY:H	1.33	0.91
1:A:201:VAL:CG1	1:A:202:GLY:H	1.82	0.91
2:H:44:LEU:O	4:H:305:HOH:O	1.89	0.91
1:J:84:SER:O	1:J:87:ASN:N	2.02	0.91
3:F:4:THR:HG22	3:F:24:ALA:HA	1.53	0.91
3:F:38:TRP:HA	3:F:49:LEU:HA	1.51	0.91
2:H:51:LEU:HD21	2:H:56:ARG:HB2	1.53	0.90
3:I:141:ASN:HA	3:I:175:THR:CG2	2.00	0.90
2:E:212:ASN:OD1	2:E:213:THR:N	2.03	0.90
3:I:196:THR:OG1	3:I:209:VAL:HG23	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:GLN:HG3	3:C:93:GLN:H	1.37	0.90
3:C:210:LYS:HD2	3:C:211:SER:H	1.37	0.90
3:F:173:ASP:CG	3:F:175:THR:HG23	1.96	0.90
3:I:45:GLN:HB3	3:I:46:PRO:HD2	1.55	0.89
3:I:38:TRP:CZ3	3:I:92:GLN:NE2	2.41	0.89
3:C:92:GLN:NE2	3:C:101:THR:OG1	2.05	0.89
3:C:109:ILE:HG22	3:C:110:LYS:H	1.36	0.89
3:C:38:TRP:CE3	3:C:40:GLN:N	2.41	0.89
3:F:8:ALA:HB1	3:F:105:THR:HG23	1.54	0.89
3:F:24:ALA:HB3	3:F:72:THR:HA	1.52	0.89
1:J:78:TYR:HB3	1:J:264:GLY:HA3	1.54	0.89
1:D:202:GLY:HA3	1:D:241:THR:H	1.37	0.89
2:H:174:PHE:CD1	2:H:175:PRO:HD2	2.06	0.89
3:L:141:ASN:HA	3:L:175:THR:CB	2.03	0.89
2:H:54:SER:HB3	2:H:56:ARG:HE	1.37	0.89
3:C:39:PHE:HB2	3:C:50:LEU:H	1.36	0.89
1:J:219:LYS:HD3	1:J:222:ASP:HA	1.54	0.89
1:G:133:THR:HG23	1:G:136:CYS:HB2	1.55	0.88
1:J:199:VAL:HG12	1:J:200:PHE:H	1.39	0.88
2:K:51:LEU:HD21	2:K:56:ARG:HB2	1.52	0.88
2:K:51:LEU:HD11	2:K:56:ARG:H	1.38	0.88
1:A:259:ARG:NH1	1:A:259:ARG:HB3	1.86	0.88
2:E:46:TRP:H	2:E:60:ARG:HH22	0.89	0.88
1:D:93:GLY:HA3	1:D:227:MET:O	1.74	0.88
3:F:108:GLU:HG3	3:F:109:ILE:H	1.38	0.88
2:H:82:MET:HE1	2:H:117:VAL:HG21	1.54	0.88
3:C:38:TRP:O	3:C:38:TRP:CD1	2.26	0.88
3:F:182:LEU:C	3:F:182:LEU:HD12	1.99	0.88
3:I:38:TRP:HZ3	3:I:92:GLN:NE2	1.70	0.88
2:K:28:GLY:H	2:K:76:LYS:HZ2	1.17	0.88
3:L:162:VAL:HG21	3:L:182:LEU:H	1.37	0.88
3:I:11:ALA:CB	3:I:108:GLU:HG3	2.01	0.88
1:J:153:LYS:HD3	1:J:193:GLN:HB2	1.54	0.88
3:I:92:GLN:OE1	3:I:93:GLN:N	2.05	0.88
3:I:159:GLN:HG3	3:I:160:ASN:N	1.87	0.88
3:F:210:LYS:HG2	3:F:211:SER:N	1.88	0.87
3:I:159:GLN:HG3	3:I:160:ASN:H	1.39	0.87
2:K:3:LYS:H	2:K:24:SER:HB2	1.40	0.87
3:L:162:VAL:HG23	3:L:182:LEU:HG	1.57	0.87
1:A:49:PRO:HG2	1:A:77:SER:H	1.38	0.87
2:E:45:GLU:HB3	2:E:60:ARG:CZ	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:9:SER:HB3	3:F:106:LYS:NZ	1.89	0.87
2:H:4:LEU:HD23	2:H:95:CYS:HB3	1.53	0.87
3:L:86:THR:OG1	3:L:87:ALA:N	2.02	0.87
3:C:106:LYS:HG3	3:C:107:LEU:N	1.86	0.87
1:D:49:PRO:HB2	1:D:76:TRP:HB2	1.55	0.87
2:H:14:GLY:N	2:H:85:LEU:O	2.08	0.87
1:J:201:VAL:CG1	1:J:202:GLY:H	1.86	0.87
3:L:64:ARG:NH1	3:L:82:GLU:OE1	2.08	0.87
1:A:201:VAL:HG12	1:A:202:GLY:H	1.39	0.86
2:K:27:THR:C	2:K:29:SER:H	1.82	0.86
3:C:128:LEU:HD13	3:C:129:THR:H	1.37	0.86
3:I:27:SER:O	3:I:28:VAL:HG22	1.76	0.86
2:H:44:LEU:HG	2:H:45:GLU:H	1.37	0.86
2:E:50:ILE:HD11	2:E:71:ARG:HB2	1.56	0.86
2:K:96:ALA:HB1	3:L:36:ILE:HD12	1.57	0.86
1:A:49:PRO:HB2	1:A:76:TRP:HB2	1.58	0.86
2:E:38:GLN:HG3	2:E:43:GLY:HA2	1.57	0.86
1:D:145:TYR:OH	1:D:229:TYR:OH	1.91	0.86
3:F:8:ALA:HB1	3:F:105:THR:CG2	2.05	0.85
3:C:194:SER:HA	3:C:210:LYS:HB2	1.57	0.85
1:J:54:LYS:HZ2	1:J:54:LYS:HB3	1.41	0.85
3:L:102:PHE:HD1	3:L:104:GLY:H	1.20	0.85
2:K:63:VAL:C	2:K:65:GLY:H	1.84	0.85
1:A:149:ILE:HB	1:A:250:VAL:CG2	2.05	0.85
3:C:170:ASP:OD2	3:C:172:LYS:N	2.10	0.85
3:C:1:ILE:HD11	3:C:98:PRO:CB	2.05	0.85
3:C:86:THR:OG1	3:C:87:ALA:N	2.05	0.85
2:E:174:PHE:O	3:F:166:TRP:CE2	2.30	0.85
2:H:176:ALA:HB2	3:I:166:TRP:CE2	2.11	0.85
3:I:6:SER:HB3	3:I:7:PRO:HD2	1.55	0.85
3:I:173:ASP:N	3:I:173:ASP:OD1	2.05	0.85
3:I:196:THR:HA	3:I:209:VAL:HA	1.55	0.85
2:K:150:VAL:HB	2:K:186:LEU:HB3	1.58	0.85
2:E:46:TRP:N	2:E:60:ARG:NH2	2.21	0.85
2:E:173:THR:HG23	2:E:187:SER:O	1.76	0.85
1:G:119:LYS:HZ1	1:G:129:ASN:HD22	1.23	0.85
1:G:201:VAL:CG1	1:G:202:GLY:H	1.90	0.85
1:J:153:LYS:NZ	1:J:189:GLN:O	2.10	0.85
3:I:45:GLN:HB3	3:I:46:PRO:CD	2.06	0.85
3:C:35:PHE:HB3	3:C:95:LYS:HD3	1.58	0.85
3:C:39:PHE:CB	3:C:50:LEU:HB2	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:THR:HB	1:D:150:TRP:CZ3	2.12	0.84
2:K:10:VAL:CG2	2:K:155:PRO:HG3	2.06	0.84
3:C:45:GLN:HB3	3:C:46:PRO:HD2	1.55	0.84
3:C:162:VAL:O	3:C:164:ASN:ND2	2.10	0.84
2:B:63:VAL:HG11	2:B:67:SER:HB2	1.56	0.84
3:F:170:ASP:OD2	3:F:171:SER:N	2.11	0.84
3:F:202:LYS:O	3:F:203:THR:HG23	1.76	0.84
1:A:93:GLY:HA3	1:A:227:MET:O	1.78	0.84
3:I:10:LEU:O	3:I:107:LEU:HA	1.78	0.84
3:C:43:PRO:HD3	3:C:87:ALA:HA	1.57	0.84
3:C:64:ARG:NH2	3:C:85:ASP:OD1	2.09	0.84
2:E:32:ASP:CB	2:E:51:LEU:HA	2.05	0.84
2:K:37:ARG:HB3	2:K:93:TYR:CE2	2.13	0.84
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.60	0.84
2:E:181:SER:HB3	3:I:62:PRO:HG3	1.60	0.84
3:F:9:SER:N	3:F:105:THR:HG23	1.93	0.84
2:B:180:SER:C	2:B:182:GLY:H	1.83	0.83
3:F:110:LYS:HZ2	3:F:110:LYS:HB3	1.42	0.83
1:J:133:THR:O	1:J:142:LYS:HB2	1.78	0.83
3:L:194:SER:HB3	3:L:210:LYS:HD3	1.60	0.83
1:G:164:SER:O	2:H:56:ARG:NH2	2.11	0.83
2:K:10:VAL:HG13	2:K:118:THR:HB	1.58	0.83
2:B:162:TRP:CD1	2:B:170:SER:HG	1.96	0.83
3:C:35:PHE:CE1	3:C:49:LEU:HD11	2.14	0.83
2:E:10:VAL:HG22	2:E:155:PRO:HG3	1.60	0.83
2:H:129:VAL:HG11	2:H:206:VAL:HG21	1.59	0.83
2:K:11:VAL:O	2:K:120:SER:N	2.11	0.83
3:C:71:GLY:O	3:C:72:THR:HG22	1.78	0.83
1:J:206:TYR:HE2	1:J:208:LYS:HB2	1.43	0.83
3:C:141:ASN:HA	3:C:175:THR:HG22	1.57	0.83
3:L:195:TYR:O	3:L:210:LYS:HA	1.77	0.83
1:J:180:HIS:O	1:J:247:ASN:ND2	2.11	0.83
3:L:184:LEU:O	3:L:189:TYR:HB2	1.78	0.82
2:B:86:ARG:HG2	2:B:89:ASP:OD2	1.79	0.82
1:J:58:ALA:HB2	1:J:98:TYR:CE1	2.13	0.82
1:D:148:LEU:HD23	1:D:251:PRO:HA	1.60	0.82
3:I:38:TRP:HA	3:I:48:LYS:O	1.78	0.82
1:D:153:LYS:HE3	1:D:156:ASN:HA	1.61	0.82
2:B:180:SER:HB3	3:L:62:PRO:HA	1.61	0.82
2:E:168:THR:O	2:E:169:SER:OG	1.97	0.82
2:H:59:TYR:CE1	2:H:69:ILE:HG22	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:146:LEU:HD11	2:H:219:SER:OG	1.78	0.82
2:K:171:VAL:HG22	3:L:176:TYR:CZ	2.14	0.82
3:L:162:VAL:O	3:L:164:ASN:ND2	2.12	0.82
1:D:144:PHE:CE2	1:D:150:TRP:HB2	2.15	0.82
1:D:258:GLU:HG2	1:D:259:ARG:H	1.44	0.82
2:E:45:GLU:OE1	2:E:60:ARG:NH2	2.13	0.82
3:F:9:SER:HA	3:F:106:LYS:H	1.45	0.82
3:C:39:PHE:HB2	3:C:50:LEU:HB2	1.62	0.82
2:K:32:ASP:HB2	2:K:98:HIS:ND1	1.95	0.82
1:A:104:GLN:HE22	1:A:233:LEU:HD22	1.45	0.81
2:K:46:TRP:O	2:K:60:ARG:HG3	1.80	0.81
2:K:95:CYS:O	2:K:112:GLY:N	2.12	0.81
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.12	0.81
3:I:193:ASN:O	3:I:211:SER:HB3	1.80	0.81
2:B:51:LEU:CD1	2:B:56:ARG:H	1.93	0.81
1:G:119:LYS:NZ	1:G:129:ASN:HB3	1.93	0.81
2:E:66:ARG:NH2	2:E:86:ARG:HD3	1.95	0.81
1:J:204:SER:HB3	4:J:603:HOH:O	1.79	0.81
3:L:128:LEU:HD12	3:L:129:THR:H	1.46	0.81
1:D:116:ILE:HG13	1:D:165:TYR:CD1	2.15	0.81
3:F:3:MET:HG3	3:F:5:GLN:HE21	1.43	0.81
3:F:158:ARG:NH2	2:H:97:ARG:HD2	1.94	0.81
2:H:203:ILE:HD11	2:H:216:ASP:HB3	1.63	0.81
3:L:42:LYS:HD3	3:L:87:ALA:HB2	1.62	0.81
3:F:158:ARG:HH22	2:H:97:ARG:CD	1.92	0.81
3:L:198:GLU:HA	3:L:207:PRO:HA	1.63	0.81
2:B:178:LEU:N	2:B:183:LEU:O	2.12	0.81
2:E:61:ASP:HB3	2:H:142:GLY:O	1.81	0.81
2:E:151:LYS:HG2	2:E:185:SER:OG	1.81	0.81
3:F:96:GLU:O	3:F:97:VAL:HG23	1.81	0.81
2:K:176:ALA:HB2	3:L:166:TRP:CE2	2.15	0.81
2:B:82:MET:HB3	2:B:85:LEU:HD21	1.63	0.80
2:B:155:PRO:O	2:B:208:HIS:NE2	2.14	0.80
3:C:176:TYR:H	3:C:176:TYR:HD2	1.29	0.80
2:E:45:GLU:HB3	2:E:60:ARG:NH2	1.97	0.80
2:E:178:LEU:N	2:E:183:LEU:O	2.15	0.80
3:I:116:PRO:HB2	3:I:139:LEU:HB3	1.64	0.80
2:E:51:LEU:HG	2:E:56:ARG:HB2	1.63	0.80
3:F:38:TRP:NE1	3:F:40:GLN:H	1.77	0.80
3:L:163:LEU:C	3:L:163:LEU:HD12	2.06	0.80
2:K:171:VAL:HB	2:K:189:VAL:HG22	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:LYS:HZ2	3:C:110:LYS:HB3	1.44	0.80
1:D:148:LEU:HD21	1:D:176:LEU:O	1.82	0.80
2:H:207:ASN:HB3	2:H:214:LYS:HG3	1.64	0.80
3:F:116:PRO:O	3:F:140:ASN:N	2.15	0.80
2:H:100:TRP:CD1	3:I:34:ASN:HA	2.16	0.80
3:L:191:ARG:O	3:L:191:ARG:HD2	1.82	0.80
1:A:51:HIS:CE1	1:A:80:VAL:HG21	2.16	0.80
2:B:50:ILE:HD11	2:B:71:ARG:CB	2.12	0.80
3:C:204:SER:O	3:C:205:THR:HG22	1.82	0.80
2:E:60:ARG:O	2:E:64:LYS:HB2	1.82	0.79
3:C:167:THR:HG22	3:C:168:ASP:H	1.47	0.79
1:G:235:GLU:HG3	1:G:236:PRO:HD2	1.62	0.79
3:L:98:PRO:HB2	4:L:309:HOH:O	1.82	0.79
2:E:32:ASP:HA	2:E:71:ARG:NH2	1.98	0.79
3:F:166:TRP:O	3:F:177:SER:HA	1.82	0.79
2:H:34:SER:OG	2:H:49:GLY:HA3	1.81	0.79
2:H:67:SER:HA	2:H:81:GLU:O	1.83	0.79
2:K:111:TRP:CZ2	3:L:38:TRP:HB3	2.17	0.79
3:F:86:THR:OG1	3:F:87:ALA:N	2.05	0.79
2:B:173:THR:HB	3:C:178:MET:HE3	1.63	0.79
3:L:2:GLN:O	3:L:2:GLN:HG2	1.80	0.79
1:A:167:ASN:ND2	1:A:236:PRO:HA	1.97	0.79
1:D:91:TYR:CD1	1:D:227:MET:HE2	2.17	0.79
2:H:197:LEU:HD12	2:H:198:GLY:N	1.98	0.79
3:F:38:TRP:NE1	3:F:40:GLN:N	2.30	0.79
3:I:170:ASP:OD2	3:I:171:SER:N	2.15	0.79
3:L:141:ASN:HA	3:L:175:THR:HB	1.65	0.79
2:H:45:GLU:HB3	2:H:60:ARG:HH11	1.48	0.79
2:K:5:GLN:O	2:K:21:CYS:HA	1.83	0.79
2:K:97:ARG:O	3:L:36:ILE:HB	1.82	0.79
3:C:116:PRO:O	3:C:140:ASN:N	2.16	0.79
3:F:38:TRP:CE3	3:F:38:TRP:C	2.60	0.79
1:J:120:THR:OG1	1:J:121:SER:N	2.14	0.79
3:L:162:VAL:HG21	3:L:181:THR:HA	1.65	0.79
3:C:38:TRP:CZ3	3:C:89:TYR:HA	2.18	0.78
2:E:174:PHE:O	3:F:166:TRP:NE1	2.15	0.78
1:G:138:HIS:HB2	1:G:143:SER:HB2	1.65	0.78
2:K:178:LEU:O	2:K:180:SER:N	2.16	0.78
1:A:116:ILE:HG22	1:A:252:ARG:O	1.82	0.78
1:D:160:LYS:H	1:D:160:LYS:CE	1.96	0.78
2:E:45:GLU:HB3	2:E:60:ARG:NH1	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:82:MET:HE1	2:E:117:VAL:HG21	1.64	0.78
3:F:45:GLN:HB3	3:F:46:PRO:CD	2.12	0.78
1:J:84:SER:HB3	1:J:88:GLY:H	1.48	0.78
3:C:210:LYS:CD	3:C:211:SER:H	1.95	0.78
1:A:57:ILE:O	1:A:61:ILE:HG22	1.83	0.78
2:H:2:VAL:HG22	2:H:25:GLY:HA3	1.64	0.78
1:A:55:CYS:SG	1:A:66:GLU:HG3	2.24	0.78
1:G:49:PRO:HD2	1:G:77:SER:OG	1.83	0.78
1:J:49:PRO:HB2	1:J:76:TRP:HB2	1.66	0.78
2:K:111:TRP:CH2	3:L:38:TRP:HB3	2.18	0.78
2:B:32:ASP:CB	2:B:51:LEU:HA	2.12	0.78
2:E:97:ARG:O	3:F:36:ILE:HG23	1.83	0.78
1:G:118:PRO:HG2	2:H:58:TYR:CE1	2.17	0.78
3:I:1:ILE:HD11	3:I:98:PRO:HB2	1.66	0.78
1:J:119:LYS:NZ	1:J:129:ASN:HB3	1.99	0.78
3:I:37:ASN:ND2	3:I:38:TRP:N	2.32	0.78
2:K:45:GLU:CD	2:K:46:TRP:H	1.92	0.78
1:D:133:THR:O	1:D:142:LYS:HB2	1.84	0.77
1:G:206:TYR:HE2	1:G:208:LYS:HB2	1.49	0.77
3:C:16:GLN:HG3	3:C:17:ARG:H	1.48	0.77
3:C:24:ALA:HB3	3:C:72:THR:HA	1.65	0.77
3:C:57:LYS:HD3	3:C:61:VAL:O	1.83	0.77
1:G:153:LYS:NZ	1:G:156:ASN:HA	1.98	0.77
1:J:211:LYS:HB2	1:J:211:LYS:NZ	1.98	0.77
3:F:27:SER:O	3:F:28:VAL:HG22	1.84	0.77
3:F:156:SER:OG	3:F:158:ARG:O	2.02	0.77
1:G:153:LYS:HG2	1:G:193:GLN:HB2	1.66	0.77
3:C:39:PHE:H	3:C:49:LEU:HA	1.47	0.77
3:I:109:ILE:HG22	3:I:110:LYS:H	1.50	0.77
3:I:194:SER:CB	3:I:210:LYS:HD2	2.13	0.77
1:J:103:GLU:O	1:J:106:SER:OG	2.03	0.77
3:C:38:TRP:CH2	3:C:89:TYR:HD1	2.03	0.77
3:F:111:ARG:HD3	3:F:173:ASP:CA	2.14	0.77
2:H:59:TYR:HE1	2:H:69:ILE:HG22	1.49	0.77
1:J:57:ILE:N	1:J:81:GLU:OE2	2.15	0.77
2:K:63:VAL:O	2:K:65:GLY:N	2.17	0.77
3:L:102:PHE:HE1	3:L:104:GLY:CA	1.98	0.77
2:K:18:ARG:HG3	2:K:81:GLU:HA	1.66	0.77
3:L:123:PRO:HB3	3:L:133:ALA:HB1	1.67	0.77
3:L:195:TYR:O	3:L:210:LYS:N	2.18	0.77
2:B:171:VAL:HG11	3:C:176:TYR:CD2	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:LYS:H	1:G:54:LYS:CD	1.92	0.77
1:G:119:LYS:HZ1	1:G:129:ASN:ND2	1.81	0.77
3:I:49:LEU:HD23	3:I:50:LEU:N	2.00	0.77
3:L:108:GLU:CD	3:L:109:ILE:H	1.93	0.77
2:E:32:ASP:HB3	2:E:51:LEU:CA	2.11	0.76
1:A:144:PHE:CE2	1:A:150:TRP:HB2	2.20	0.76
1:D:133:THR:HB	1:D:150:TRP:HZ3	1.48	0.76
2:E:32:ASP:HA	2:E:71:ARG:HH22	1.48	0.76
3:F:108:GLU:HG3	3:F:109:ILE:N	1.99	0.76
1:G:199:VAL:HG11	1:G:248:LEU:HD13	1.66	0.76
2:H:21:CYS:O	2:H:77:THR:HB	1.84	0.76
1:J:199:VAL:HG12	1:J:200:PHE:N	2.00	0.76
1:D:101:LEU:O	1:D:104:GLN:N	2.19	0.76
3:F:137:CYS:HB2	3:F:151:TRP:CZ2	2.20	0.76
3:F:183:THR:HG22	3:F:184:LEU:H	1.50	0.76
1:D:51:HIS:HA	1:D:80:VAL:HB	1.67	0.76
1:J:182:PRO:HD2	1:J:214:ILE:HG13	1.68	0.76
2:K:178:LEU:HD23	2:K:179:GLN:HB2	1.66	0.76
1:A:75:SER:HB2	1:A:109:SER:O	1.86	0.76
3:C:129:THR:O	3:C:130:SER:OG	2.04	0.76
3:I:162:VAL:HG23	3:I:164:ASN:OD1	1.85	0.76
2:K:10:VAL:HG21	2:K:155:PRO:HG3	1.66	0.76
3:C:39:PHE:HB3	3:C:50:LEU:HD12	1.67	0.76
3:I:45:GLN:NE2	3:I:46:PRO:HD3	2.00	0.76
2:K:96:ALA:HB1	3:L:36:ILE:HD11	1.68	0.76
3:L:143:TYR:HD1	3:L:174:SER:HG	1.34	0.76
1:A:127:ASP:OD2	1:A:130:LYS:HG2	1.86	0.76
1:D:204:SER:OG	1:D:238:ASP:OD2	2.04	0.76
3:F:182:LEU:HD12	3:F:182:LEU:O	1.86	0.76
1:G:120:THR:OG1	1:G:121:SER:N	2.16	0.76
3:F:183:THR:HG22	3:F:184:LEU:N	2.01	0.75
1:G:126:HIS:CE1	1:G:159:PRO:HD2	2.21	0.75
2:K:163:ASN:C	2:K:165:GLY:H	1.90	0.75
3:I:123:PRO:HB3	3:I:133:ALA:HB1	1.68	0.75
2:K:75:ARG:O	2:K:77:THR:HG23	1.87	0.75
3:L:7:PRO:HG2	3:L:21:THR:HG23	1.69	0.75
3:L:203:THR:HG23	3:L:203:THR:O	1.86	0.75
3:F:41:GLN:O	3:F:88:ASN:N	2.18	0.75
1:G:118:PRO:CB	1:G:120:THR:HG23	2.17	0.75
1:A:260:ASN:HB3	4:A:608:HOH:O	1.86	0.75
2:B:41:GLY:O	2:B:42:LYS:HD2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:TRP:CZ2	3:C:39:PHE:CD1	2.75	0.75
2:E:45:GLU:C	2:E:60:ARG:HH12	1.95	0.75
3:F:41:GLN:N	3:F:88:ASN:O	2.19	0.75
3:F:198:GLU:HG3	3:F:198:GLU:O	1.87	0.75
1:A:259:ARG:HB3	1:A:259:ARG:CZ	2.17	0.75
3:C:166:TRP:HE3	3:C:167:THR:H	1.33	0.75
1:G:135:ALA:HB2	1:G:223:GLN:HE21	1.52	0.75
2:B:11:VAL:HG11	2:B:85:LEU:HD12	1.68	0.75
2:E:196:SER:HB3	2:E:202:TYR:CE2	2.22	0.75
3:F:38:TRP:CE3	3:F:38:TRP:O	2.39	0.75
1:G:171:LYS:CD	1:G:258:GLU:HG3	2.16	0.75
3:I:17:ARG:HB3	3:I:79:ASN:OD1	1.87	0.75
3:L:162:VAL:HG21	3:L:182:LEU:N	2.00	0.75
2:B:124:THR:HG23	2:B:155:PRO:HD2	1.67	0.75
1:G:49:PRO:HB2	1:G:76:TRP:HB2	1.69	0.75
2:K:11:VAL:HG21	2:K:85:LEU:HD12	1.68	0.75
3:L:39:PHE:O	3:L:89:TYR:HA	1.87	0.75
3:L:18:ALA:HB3	3:L:78:ILE:HG23	1.68	0.74
3:F:174:SER:O	3:F:175:THR:OG1	2.04	0.74
3:I:95:LYS:O	3:I:99:TYR:HE1	1.70	0.74
1:A:96:ILE:HG22	1:A:97:ASP:OD2	1.87	0.74
3:C:150:LYS:HB3	3:C:198:GLU:HG3	1.70	0.74
1:G:84:SER:O	1:G:88:GLY:N	2.19	0.74
1:J:171:LYS:NZ	1:J:258:GLU:OE2	2.20	0.74
2:B:100:TRP:HA	3:C:34:ASN:N	2.02	0.74
2:E:198:GLY:HA3	4:E:305:HOH:O	1.86	0.74
3:F:210:LYS:HG2	3:F:211:SER:H	1.51	0.74
1:J:50:LEU:HD23	1:J:79:ILE:HG12	1.68	0.74
3:F:182:LEU:HD23	4:F:302:HOH:O	1.86	0.74
2:H:63:VAL:C	2:H:65:GLY:H	1.95	0.74
3:L:42:LYS:O	3:L:44:GLY:N	2.21	0.74
3:F:93:GLN:HA	3:F:100:GLY:O	1.86	0.74
3:I:111:ARG:HE	3:I:173:ASP:HA	1.51	0.74
1:J:54:LYS:HZ1	1:J:69:SER:HB3	1.53	0.74
1:J:182:PRO:HG2	1:J:188:GLN:HB2	1.70	0.74
1:J:201:VAL:HG12	1:J:202:GLY:N	1.94	0.74
1:A:137:PRO:HA	1:A:143:SER:H	1.52	0.73
2:B:196:SER:HB3	2:B:202:TYR:OH	1.89	0.73
3:C:86:THR:HA	3:C:107:LEU:O	1.88	0.73
3:C:207:PRO:C	3:C:208:ILE:HD12	2.13	0.73
1:G:201:VAL:HG12	1:G:202:GLY:H	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:167:THR:HG22	3:L:168:ASP:H	1.53	0.73
3:C:38:TRP:O	3:C:39:PHE:HD2	1.69	0.73
2:E:160:VAL:O	2:E:172:HIS:NE2	2.17	0.73
3:C:18:ALA:HB3	3:C:78:ILE:HG23	1.70	0.73
3:I:37:ASN:ND2	3:I:38:TRP:H	1.86	0.73
3:I:116:PRO:HG3	3:I:139:LEU:HD23	1.71	0.73
2:E:203:ILE:HB	2:E:218:LYS:HA	1.71	0.73
3:F:26:GLU:CD	3:F:27:SER:HB2	2.14	0.73
2:B:36:ILE:HB	2:B:46:TRP:HA	1.69	0.73
3:C:153:ILE:HG13	3:C:154:ASP:H	1.51	0.73
2:H:50:ILE:HG23	2:H:69:ILE:HD13	1.69	0.73
3:L:45:GLN:HB3	3:L:46:PRO:CD	2.16	0.73
1:A:202:GLY:HA3	1:A:241:THR:N	1.99	0.73
3:F:92:GLN:CG	3:F:101:THR:HG23	2.11	0.73
3:L:156:SER:O	3:L:157:GLU:HB2	1.89	0.73
2:E:46:TRP:O	2:E:60:ARG:CZ	2.36	0.73
1:J:111:PHE:CZ	1:J:255:PHE:CD1	2.76	0.73
3:L:52:TYR:N	3:L:56:ASN:O	2.20	0.73
1:A:120:THR:OG1	1:A:121:SER:N	2.20	0.73
1:A:169:LYS:HB3	1:A:171:LYS:H	1.53	0.73
1:A:201:VAL:CG1	1:A:202:GLY:N	2.51	0.73
2:B:160:VAL:HG21	2:B:186:LEU:HD11	1.71	0.73
1:D:137:PRO:CA	1:D:142:LYS:HA	2.17	0.73
2:K:16:SER:OG	2:K:83:ASN:OD1	2.04	0.73
3:L:108:GLU:OE1	3:L:108:GLU:HA	1.85	0.73
1:A:201:VAL:HG12	1:A:202:GLY:N	2.01	0.73
2:H:10:VAL:HG22	2:H:118:THR:HB	1.69	0.73
1:J:199:VAL:CG1	1:J:200:PHE:H	2.01	0.73
1:J:251:PRO:HG3	4:J:601:HOH:O	1.88	0.73
3:L:79:ASN:HB3	3:L:80:PRO:HD3	1.70	0.73
3:L:81:VAL:O	3:L:82:GLU:HG3	1.89	0.73
2:B:6:GLU:OE1	2:B:113:GLN:HG2	1.89	0.72
3:F:39:PHE:CD1	3:F:76:LEU:HB2	2.23	0.72
1:G:179:ILE:HD11	1:G:212:PRO:HB3	1.71	0.72
1:A:137:PRO:HA	1:A:142:LYS:HA	1.70	0.72
2:B:178:LEU:HD12	2:B:179:GLN:H	1.54	0.72
1:A:54:LYS:HG2	1:A:55:CYS:H	1.53	0.72
3:C:38:TRP:HH2	3:C:89:TYR:HB3	1.54	0.72
1:G:54:LYS:HD3	1:G:54:LYS:N	2.00	0.72
1:J:102:ARG:HG3	1:J:102:ARG:NH1	2.03	0.72
2:K:197:LEU:O	2:K:197:LEU:HD13	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:162:VAL:CG2	3:L:182:LEU:H	2.02	0.72
3:I:9:SER:HB3	3:I:106:LYS:HG3	1.70	0.72
3:L:66:SER:O	3:L:76:LEU:HD12	1.90	0.72
3:L:170:ASP:HB3	3:L:174:SER:O	1.88	0.72
2:H:171:VAL:C	2:H:172:HIS:HD1	1.97	0.72
3:F:38:TRP:CD2	3:F:39:PHE:CA	2.67	0.72
2:H:3:LYS:H	2:H:24:SER:HB2	1.51	0.72
2:H:208:HIS:O	2:H:212:ASN:N	2.22	0.72
1:D:109:SER:HB3	1:D:258:GLU:HB3	1.72	0.72
3:F:108:GLU:CG	3:F:109:ILE:H	2.02	0.72
2:H:97:ARG:O	3:I:36:ILE:HB	1.89	0.72
2:B:144:ALA:N	2:B:192:VAL:O	2.23	0.72
3:C:92:GLN:HG3	3:C:93:GLN:N	2.04	0.72
2:K:178:LEU:C	2:K:180:SER:H	1.96	0.72
1:G:135:ALA:CB	1:G:223:GLN:HE21	2.02	0.71
2:K:130:PHE:HB3	3:L:124:SER:OG	1.90	0.71
3:L:138:PHE:C	3:L:139:LEU:HD12	2.16	0.71
3:C:156:SER:O	3:C:157:GLU:HB2	1.87	0.71
1:J:57:ILE:HG13	1:J:81:GLU:OE2	1.89	0.71
2:K:171:VAL:HG22	3:L:176:TYR:CE2	2.26	0.71
1:A:227:MET:HG2	1:A:229:TYR:CE2	2.25	0.71
2:H:176:ALA:O	2:H:184:TYR:HA	1.89	0.71
3:I:1:ILE:HG22	3:I:3:MET:HE2	1.71	0.71
2:B:162:TRP:N	2:B:167:LEU:HD11	2.05	0.71
3:I:168:ASP:OD1	3:I:168:ASP:N	2.21	0.71
2:K:178:LEU:HD11	3:L:182:LEU:HD13	1.72	0.71
1:A:167:ASN:OD1	1:A:169:LYS:N	2.23	0.71
1:D:162:SER:C	1:D:163:LYS:HD2	2.14	0.71
2:E:63:VAL:CG1	2:E:67:SER:H	2.04	0.71
2:E:156:GLU:HB2	2:E:157:PRO:HA	1.71	0.71
3:F:168:ASP:OD1	3:F:168:ASP:N	2.21	0.71
2:H:72:ASP:HB3	2:H:79:TYR:CE2	2.26	0.71
2:H:93:TYR:HE1	2:H:117:VAL:HG12	1.56	0.71
3:L:17:ARG:HG2	3:L:17:ARG:O	1.90	0.71
2:B:19:LEU:HD22	2:B:82:MET:HE1	1.71	0.71
3:C:38:TRP:CH2	3:C:89:TYR:HB3	2.26	0.71
2:H:96:ALA:HB1	3:I:36:ILE:CD1	2.21	0.71
2:K:48:SER:HG	2:K:59:TYR:HD1	1.36	0.71
2:B:203:ILE:HD12	2:B:217:LYS:C	2.15	0.71
3:C:64:ARG:HH22	3:C:85:ASP:CG	1.98	0.71
3:I:17:ARG:HA	3:I:78:ILE:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:140:ASN:HB3	3:F:141:ASN:ND2	2.05	0.71
1:G:79:ILE:HG22	1:G:80:VAL:N	2.05	0.71
2:H:3:LYS:N	2:H:24:SER:HB2	2.06	0.71
3:L:208:ILE:C	3:L:209:VAL:HG12	2.14	0.71
3:F:170:ASP:HB3	3:F:175:THR:OG1	1.89	0.71
1:G:118:PRO:HB2	1:G:120:THR:HG23	1.71	0.71
3:L:162:VAL:O	3:L:164:ASN:CG	2.34	0.71
3:L:209:VAL:HG23	3:L:210:LYS:N	2.05	0.71
1:D:148:LEU:HD23	1:D:251:PRO:CA	2.21	0.70
1:G:115:GLU:HG2	3:I:96:GLU:HG2	1.71	0.70
3:I:142:PHE:H	3:I:175:THR:HA	1.55	0.70
2:B:127:PRO:CB	2:B:153:TYR:HB3	2.19	0.70
1:G:96:ILE:HG13	1:G:230:TYR:CE2	2.25	0.70
2:K:50:ILE:HD11	2:K:71:ARG:HG2	1.73	0.70
1:J:54:LYS:NZ	1:J:69:SER:HB3	2.06	0.70
3:L:102:PHE:HD1	3:L:103:GLY:N	1.89	0.70
1:A:115:GLU:HB2	3:C:96:GLU:HG2	1.73	0.70
2:B:173:THR:HG22	3:C:178:MET:SD	2.32	0.70
3:C:123:PRO:HD3	3:C:135:VAL:HG22	1.73	0.70
2:E:63:VAL:HG13	2:E:66:ARG:HB2	1.73	0.70
3:F:175:THR:HB	3:F:176:TYR:CD2	2.27	0.70
2:H:153:TYR:OH	2:H:156:GLU:OE2	2.08	0.70
3:I:109:ILE:HG22	3:I:110:LYS:N	2.06	0.70
3:I:141:ASN:HA	3:I:175:THR:CB	2.20	0.70
3:C:158:ARG:HH22	2:K:97:ARG:CD	2.03	0.70
3:F:39:PHE:HB3	3:F:76:LEU:HD22	1.74	0.70
2:B:32:ASP:HB3	2:B:50:ILE:O	1.90	0.70
3:C:38:TRP:HE3	3:C:40:GLN:H	1.37	0.70
3:C:170:ASP:OD2	3:C:171:SER:N	2.24	0.70
3:F:153:ILE:HG22	3:F:195:TYR:CD2	2.27	0.70
3:F:170:ASP:OD2	3:F:170:ASP:C	2.33	0.70
2:H:33:MET:HB3	2:H:78:LEU:HD13	1.71	0.70
3:I:161:GLY:O	3:I:162:VAL:HG22	1.91	0.70
2:B:203:ILE:HG13	2:B:204:CYS:N	2.07	0.70
3:I:120:ILE:HD11	3:I:151:TRP:CH2	2.27	0.70
1:J:162:SER:HA	1:J:242:PHE:O	1.92	0.70
2:B:6:GLU:HA	2:B:20:SER:O	1.91	0.70
3:C:210:LYS:CG	3:C:211:SER:H	2.02	0.70
3:I:111:ARG:HE	3:I:173:ASP:CA	2.05	0.70
3:L:126:GLU:N	3:L:126:GLU:OE1	2.25	0.70
3:C:35:PHE:HE1	3:C:49:LEU:CD1	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:79:ASN:O	3:F:80:PRO:C	2.34	0.70
2:H:6:GLU:OE2	2:H:112:GLY:HA3	1.92	0.70
1:J:201:VAL:HG13	1:J:240:ILE:HD11	1.72	0.70
1:A:55:CYS:HB2	1:A:60:TRP:HB2	1.73	0.69
1:A:91:TYR:CD1	1:A:227:MET:HE2	2.27	0.69
2:B:51:LEU:HD12	2:B:56:ARG:H	1.56	0.69
1:D:54:LYS:HE2	1:D:55:CYS:H	1.57	0.69
1:J:164:SER:O	2:K:56:ARG:NH2	2.22	0.69
3:C:140:ASN:CG	3:C:176:TYR:CD1	2.70	0.69
2:H:202:TYR:CE1	2:H:219:SER:HB2	2.27	0.69
3:I:191:ARG:HG2	3:I:192:HIS:N	2.04	0.69
2:K:34:SER:OG	2:K:49:GLY:HA3	1.92	0.69
3:C:97:VAL:HG13	3:C:98:PRO:HD2	1.74	0.69
2:E:51:LEU:CD1	2:E:56:ARG:H	2.05	0.69
3:F:34:ASN:HD22	3:F:34:ASN:N	1.89	0.69
3:F:153:ILE:HA	3:F:194:SER:O	1.92	0.69
1:A:206:TYR:C	1:A:206:TYR:CD2	2.71	0.69
2:E:6:GLU:N	2:E:6:GLU:OE1	2.26	0.69
2:E:32:ASP:CG	2:E:98:HIS:CE1	2.70	0.69
2:E:53:GLY:O	2:E:54:SER:HB2	1.90	0.69
3:F:23:ARG:HG3	3:F:72:THR:O	1.92	0.69
3:L:11:ALA:CB	3:L:108:GLU:HB3	2.21	0.69
2:B:127:PRO:CA	2:B:153:TYR:HB3	2.23	0.69
3:C:109:ILE:HG22	3:C:110:LYS:N	2.07	0.69
3:C:110:LYS:O	3:C:111:ARG:HD3	1.92	0.69
1:G:54:LYS:HG3	1:G:67:CYS:CA	2.11	0.69
1:G:201:VAL:CG1	1:G:202:GLY:N	2.53	0.69
2:H:98:HIS:HA	3:I:36:ILE:CG2	2.22	0.69
3:L:102:PHE:CD1	3:L:102:PHE:C	2.70	0.69
3:F:140:ASN:CG	3:F:176:TYR:HD1	1.99	0.69
1:J:248:LEU:HD12	1:J:249:VAL:N	2.08	0.69
3:L:173:ASP:N	3:L:173:ASP:OD2	2.26	0.69
1:A:91:TYR:CG	1:A:227:MET:HE2	2.28	0.69
1:A:91:TYR:HH	1:A:180:HIS:HE2	1.38	0.69
3:C:195:TYR:H	3:C:210:LYS:CB	2.05	0.69
3:F:38:TRP:CE3	3:F:39:PHE:HA	2.28	0.69
3:F:101:THR:HG22	3:F:102:PHE:H	1.57	0.69
1:G:58:ALA:HB2	1:G:98:TYR:CE1	2.28	0.69
1:G:121:SER:OG	2:H:64:LYS:HD2	1.92	0.69
1:G:199:VAL:HG12	1:G:200:PHE:N	2.07	0.69
2:H:83:ASN:OD1	2:H:84:SER:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:171:VAL:HG22	3:I:176:TYR:CZ	2.28	0.69
2:K:2:VAL:HA	2:K:24:SER:O	1.93	0.69
2:B:3:LYS:C	2:B:4:LEU:HD12	2.18	0.69
3:C:120:ILE:HD12	3:C:208:ILE:HG22	1.73	0.69
3:C:158:ARG:HG3	2:K:31:TYR:OH	1.92	0.69
2:K:160:VAL:HG22	2:K:206:VAL:HG22	1.75	0.69
1:D:48:ALA:HB2	1:D:78:TYR:OH	1.93	0.69
1:G:127:ASP:HB3	1:G:152:VAL:HG23	1.75	0.69
3:I:1:ILE:HG12	3:I:1:ILE:O	1.93	0.69
3:I:162:VAL:O	3:I:164:ASN:ND2	2.26	0.69
3:L:170:ASP:OD2	3:L:171:SER:N	2.26	0.69
2:B:27:THR:HG23	2:B:30:ASP:OD1	1.93	0.68
3:C:2:GLN:OE1	3:C:97:VAL:HG21	1.93	0.68
3:F:210:LYS:HE2	3:F:212:PHE:CZ	2.28	0.68
1:J:161:LEU:O	1:J:243:GLU:HA	1.93	0.68
1:D:49:PRO:HG2	1:D:77:SER:H	1.57	0.68
3:L:92:GLN:CD	3:L:101:THR:HB	2.17	0.68
1:A:123:TRP:CZ3	1:A:163:LYS:HG3	2.28	0.68
2:H:44:LEU:HG	2:H:45:GLU:N	2.07	0.68
2:H:127:PRO:CB	2:H:150:VAL:HG13	2.23	0.68
2:K:125:LYS:HD2	2:K:126:GLY:N	2.07	0.68
2:E:176:ALA:HB2	3:F:166:TRP:CZ2	2.29	0.68
2:E:208:HIS:O	2:E:212:ASN:O	2.11	0.68
3:F:7:PRO:HG2	3:F:21:THR:HG23	1.75	0.68
3:F:41:GLN:NE2	4:F:307:HOH:O	1.97	0.68
3:F:170:ASP:OD2	3:F:172:LYS:N	2.26	0.68
1:G:235:GLU:HG3	1:G:236:PRO:CD	2.22	0.68
3:L:36:ILE:O	3:L:36:ILE:HD13	1.93	0.68
2:B:186:LEU:HD12	2:B:187:SER:N	2.09	0.68
3:C:86:THR:HG22	3:C:109:ILE:HD13	1.73	0.68
3:C:96:GLU:O	3:C:97:VAL:HG23	1.92	0.68
3:C:109:ILE:N	3:C:109:ILE:HD12	2.09	0.68
1:G:92:PRO:HG3	1:G:223:GLN:HB2	1.75	0.68
1:J:49:PRO:HG2	1:J:77:SER:HB3	1.74	0.68
1:A:219:LYS:HG3	1:A:224:GLU:CG	2.23	0.68
2:H:162:TRP:CE3	2:H:190:VAL:HG11	2.28	0.68
3:I:38:TRP:HB2	3:I:47:PRO:CB	2.24	0.68
2:K:67:SER:HB3	2:K:80:LEU:HD11	1.76	0.68
2:K:203:ILE:HD11	2:K:216:ASP:C	2.17	0.68
1:A:118:PRO:O	1:A:122:SER:OG	2.08	0.68
3:C:125:SER:O	3:C:128:LEU:HD12	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:51:LEU:CD1	2:K:56:ARG:H	2.07	0.68
3:C:64:ARG:O	3:C:78:ILE:HA	1.94	0.68
3:C:128:LEU:HD22	3:C:129:THR:N	2.09	0.68
2:E:66:ARG:HH22	2:E:86:ARG:HD3	1.58	0.68
2:B:197:LEU:C	2:B:199:THR:H	2.01	0.68
3:C:85:ASP:O	3:C:86:THR:C	2.37	0.68
3:F:182:LEU:C	3:F:182:LEU:CD1	2.67	0.68
2:K:10:VAL:HG22	2:K:155:PRO:HG3	1.75	0.68
1:G:201:VAL:HG12	1:G:202:GLY:N	2.07	0.68
3:I:170:ASP:HB3	3:I:175:THR:OG1	1.95	0.67
2:K:152:ASP:C	2:K:183:LEU:HD12	2.19	0.67
2:H:203:ILE:HG12	2:H:204:CYS:N	2.09	0.67
2:K:133:ALA:C	3:L:121:PHE:HE1	2.02	0.67
3:C:39:PHE:N	3:C:48:LYS:O	2.27	0.67
3:C:190:GLU:OE2	3:C:191:ARG:NE	2.27	0.67
3:F:38:TRP:CD2	3:F:38:TRP:C	2.72	0.67
1:J:97:ASP:CB	1:J:231:TRP:HE1	2.07	0.67
2:K:33:MET:HB2	2:K:78:LEU:HD13	1.76	0.67
3:C:38:TRP:CD2	3:C:39:PHE:CA	2.68	0.67
3:C:39:PHE:HB2	3:C:50:LEU:N	2.07	0.67
3:F:9:SER:HB3	3:F:106:LYS:HZ2	1.58	0.67
3:F:64:ARG:NH2	3:F:85:ASP:OD1	2.21	0.67
1:J:133:THR:HG23	1:J:135:ALA:H	1.57	0.67
3:C:120:ILE:HG13	3:C:197:CYS:SG	2.35	0.67
2:E:156:GLU:CB	2:E:157:PRO:HA	2.25	0.67
3:F:89:TYR:O	3:F:104:GLY:HA2	1.93	0.67
1:J:220:VAL:HG12	1:J:221:ARG:HD2	1.77	0.67
1:A:54:LYS:HD3	1:A:54:LYS:H	1.59	0.67
2:B:98:HIS:HB3	3:C:36:ILE:HG13	1.75	0.67
2:B:174:PHE:O	3:C:166:TRP:CE2	2.47	0.67
3:C:176:TYR:CD2	3:C:176:TYR:N	2.61	0.67
2:K:197:LEU:C	2:K:199:THR:H	2.02	0.67
3:L:194:SER:HB3	3:L:210:LYS:CD	2.24	0.67
1:G:180:HIS:O	1:G:247:ASN:ND2	2.27	0.67
2:H:93:TYR:HE1	2:H:117:VAL:CG1	2.08	0.67
2:H:178:LEU:C	2:H:180:SER:H	2.01	0.67
1:J:174:LEU:N	1:J:255:PHE:O	2.26	0.67
1:D:169:LYS:HB2	4:D:604:HOH:O	1.95	0.67
2:H:154:PHE:O	2:H:208:HIS:HE1	1.78	0.67
1:A:60:TRP:HA	1:A:67:CYS:SG	2.34	0.67
2:H:27:THR:C	2:H:29:SER:H	2.01	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:ASP:OD1	3:C:168:ASP:N	2.26	0.67
3:F:140:ASN:HB3	3:F:141:ASN:HD22	1.57	0.67
3:I:108:GLU:C	3:I:109:ILE:HD12	2.20	0.67
3:I:194:SER:HB2	3:I:210:LYS:CG	2.25	0.67
1:J:69:SER:OG	1:J:70:LEU:N	2.26	0.67
3:L:125:SER:O	3:L:128:LEU:HD23	1.94	0.67
1:G:57:ILE:O	1:G:61:ILE:HG22	1.95	0.66
1:G:119:LYS:HZ1	1:G:129:ASN:HB3	1.57	0.66
2:H:111:TRP:CE3	3:I:47:PRO:HG2	2.30	0.66
1:J:78:TYR:HB3	1:J:264:GLY:CA	2.25	0.66
3:L:196:THR:OG1	3:L:210:LYS:HG3	1.95	0.66
1:A:179:ILE:HD11	1:A:199:VAL:HG11	1.76	0.66
1:D:56:ASN:O	1:D:57:ILE:C	2.38	0.66
1:D:219:LYS:HG3	1:D:224:GLU:HG3	1.77	0.66
1:J:67:CYS:C	1:J:68:GLU:HG3	2.20	0.66
2:B:49:GLY:HA3	4:B:306:HOH:O	1.93	0.66
2:B:181:SER:OG	3:L:84:GLU:OE2	2.14	0.66
3:I:116:PRO:CG	3:I:139:LEU:HD23	2.24	0.66
1:J:115:GLU:H	3:L:96:GLU:HG2	1.59	0.66
1:A:54:LYS:HD3	1:A:54:LYS:N	2.10	0.66
3:C:150:LYS:HB3	3:C:198:GLU:CG	2.25	0.66
1:D:121:SER:HB2	2:E:58:TYR:HA	1.78	0.66
2:E:32:ASP:HB2	2:E:50:ILE:O	1.94	0.66
2:E:196:SER:HB3	2:E:202:TYR:HE2	1.59	0.66
3:F:53:THR:HG22	3:F:53:THR:O	1.95	0.66
2:H:63:VAL:O	2:H:65:GLY:N	2.29	0.66
2:H:71:ARG:HA	2:H:78:LEU:HA	1.76	0.66
2:H:82:MET:HB3	2:H:85:LEU:HD21	1.76	0.66
2:H:213:THR:HG22	2:H:213:THR:O	1.95	0.66
3:I:6:SER:HB2	3:I:102:PHE:CE1	2.30	0.66
1:A:54:LYS:HD2	1:A:69:SER:OG	1.95	0.66
3:C:39:PHE:HB2	3:C:50:LEU:CB	2.25	0.66
1:D:97:ASP:HA	1:D:99:GLU:OE2	1.95	0.66
3:F:194:SER:HA	3:F:210:LYS:HG3	1.78	0.66
1:G:76:TRP:NE1	1:G:105:LEU:O	2.29	0.66
2:H:159:THR:HB	2:H:207:ASN:OD1	1.95	0.66
3:I:140:ASN:HB2	3:I:141:ASN:HD22	1.61	0.66
3:C:39:PHE:N	3:C:49:LEU:HA	2.10	0.66
1:D:258:GLU:HG2	1:D:259:ARG:N	2.10	0.66
2:H:131:PRO:HD2	3:I:126:GLU:HG3	1.77	0.66
3:I:7:PRO:HD3	3:I:21:THR:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:66:ARG:HH21	2:K:85:LEU:HA	1.61	0.66
3:I:38:TRP:CG	3:I:47:PRO:HB2	2.31	0.66
2:K:28:GLY:H	2:K:76:LYS:NZ	1.91	0.66
2:B:54:SER:HB3	2:B:56:ARG:HH11	1.59	0.66
3:F:9:SER:HA	3:F:106:LYS:HB2	1.75	0.66
3:F:158:ARG:HD3	2:H:31:TYR:CE2	2.31	0.66
2:E:28:GLY:O	2:E:71:ARG:NH1	2.29	0.66
2:E:72:ASP:OD1	2:E:75:ARG:N	2.19	0.66
2:E:171:VAL:HG23	2:E:189:VAL:HG22	1.77	0.66
3:F:210:LYS:CG	3:F:211:SER:H	2.07	0.66
3:I:170:ASP:OD2	3:I:170:ASP:C	2.39	0.66
2:K:147:GLY:C	2:K:162:TRP:HH2	2.03	0.66
3:L:202:LYS:O	3:L:203:THR:HG22	1.96	0.66
1:D:149:ILE:HB	1:D:250:VAL:HG23	1.78	0.66
2:E:127:PRO:CA	2:E:153:TYR:HB3	2.26	0.66
1:J:51:HIS:CD2	1:J:80:VAL:HB	2.30	0.66
2:K:178:LEU:HA	3:L:163:LEU:HD21	1.78	0.66
3:L:91:CYS:SG	3:L:102:PHE:CD2	2.82	0.66
3:F:168:ASP:OD1	3:F:176:TYR:O	2.14	0.65
3:I:91:CYS:N	3:I:102:PHE:CD2	2.63	0.65
3:I:116:PRO:HB3	3:I:142:PHE:CD2	2.31	0.65
3:L:92:GLN:HA	3:L:101:THR:HA	1.77	0.65
1:A:182:PRO:HG2	1:A:188:GLN:HA	1.78	0.65
2:B:203:ILE:HB	2:B:218:LYS:HA	1.77	0.65
3:C:79:ASN:HB3	3:C:80:PRO:HD3	1.76	0.65
2:H:146:LEU:HD11	2:H:219:SER:CB	2.27	0.65
3:I:38:TRP:CG	3:I:47:PRO:CB	2.79	0.65
2:K:36:ILE:HB	2:K:46:TRP:HA	1.79	0.65
2:K:163:ASN:HD22	2:K:163:ASN:N	1.92	0.65
3:L:120:ILE:HD13	3:L:197:CYS:HB3	1.79	0.65
3:C:36:ILE:HD12	3:C:93:GLN:NE2	2.11	0.65
2:H:9:ALA:H	2:H:17:LEU:HD21	1.60	0.65
1:G:219:LYS:HG3	1:G:223:GLN:N	2.10	0.65
2:K:3:LYS:N	2:K:24:SER:HB2	2.08	0.65
3:L:110:LYS:O	3:L:111:ARG:HD3	1.97	0.65
3:C:110:LYS:HB3	3:C:110:LYS:NZ	2.12	0.65
3:C:196:THR:HG23	3:C:208:ILE:O	1.97	0.65
3:F:164:ASN:N	3:F:164:ASN:OD1	2.28	0.65
3:I:102:PHE:CE1	3:I:104:GLY:N	2.65	0.65
2:K:207:ASN:N	2:K:207:ASN:OD1	2.29	0.65
2:B:56:ARG:N	2:B:56:ARG:HD2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:TRP:CH2	3:C:89:TYR:CD1	2.83	0.65
2:E:212:ASN:CG	2:E:213:THR:H	2.05	0.65
1:G:241:THR:HG22	1:G:242:PHE:N	2.10	0.65
1:J:84:SER:O	1:J:88:GLY:N	2.30	0.65
2:K:67:SER:HA	2:K:81:GLU:O	1.97	0.65
3:L:37:ASN:ND2	3:L:93:GLN:HB2	2.12	0.65
3:L:92:GLN:CG	3:L:101:THR:HB	2.27	0.65
3:L:111:ARG:NH2	4:L:311:HOH:O	2.29	0.65
1:G:171:LYS:HB3	1:G:257:MET:O	1.97	0.65
3:L:62:PRO:HG2	3:L:65:PHE:CE2	2.32	0.65
3:L:145:LYS:HD3	3:L:167:THR:HG21	1.79	0.65
1:A:126:HIS:HA	1:A:154:LYS:HG2	1.79	0.65
1:D:101:LEU:HA	1:D:104:GLN:HB3	1.77	0.65
2:E:162:TRP:N	2:E:167:LEU:HG	2.08	0.65
2:H:127:PRO:HB2	2:H:150:VAL:HG13	1.76	0.65
3:I:198:GLU:HB3	3:I:207:PRO:HA	1.77	0.65
3:I:202:LYS:O	3:I:203:THR:OG1	2.11	0.65
3:L:102:PHE:CE1	3:L:104:GLY:CA	2.80	0.65
3:L:109:ILE:HG22	3:L:110:LYS:N	2.12	0.65
1:A:84:SER:O	1:A:87:ASN:N	2.22	0.65
3:C:108:GLU:HG3	3:C:109:ILE:H	1.61	0.65
2:E:63:VAL:O	2:E:65:GLY:N	2.28	0.65
2:K:210:PRO:HD2	4:K:306:HOH:O	1.97	0.65
3:L:195:TYR:O	3:L:210:LYS:CA	2.45	0.65
1:A:57:ILE:HG13	1:A:81:GLU:OE2	1.97	0.65
2:B:27:THR:HG22	2:B:31:TYR:HB2	1.79	0.65
1:D:162:SER:O	1:D:163:LYS:HD2	1.97	0.65
2:E:4:LEU:HD12	2:E:112:GLY:N	2.11	0.65
1:G:153:LYS:HG3	1:G:191:LEU:O	1.97	0.65
3:I:120:ILE:HD11	3:I:151:TRP:CZ3	2.32	0.65
1:A:101:LEU:HA	1:A:104:GLN:HB3	1.78	0.64
2:E:169:SER:N	4:E:308:HOH:O	2.29	0.64
3:F:3:MET:O	3:F:3:MET:HG2	1.96	0.64
1:G:169:LYS:HE2	1:G:256:ALA:HB2	1.79	0.64
1:G:193:GLN:NE2	1:G:193:GLN:HA	2.12	0.64
1:G:206:TYR:CE2	1:G:208:LYS:HB2	2.31	0.64
2:B:27:THR:HG23	2:B:30:ASP:CG	2.22	0.64
1:D:60:TRP:HA	1:D:67:CYS:SG	2.37	0.64
3:L:42:LYS:C	3:L:44:GLY:H	2.06	0.64
3:L:142:PHE:H	3:L:175:THR:HA	1.61	0.64
1:A:166:ILE:HD12	1:A:166:ILE:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:PRO:HA	1:D:143:SER:H	1.61	0.64
1:G:121:SER:H	2:H:64:LYS:HE3	1.62	0.64
3:L:52:TYR:O	3:L:56:ASN:HB2	1.97	0.64
2:B:156:GLU:HB3	2:B:157:PRO:HA	1.79	0.64
3:C:7:PRO:O	3:C:105:THR:OG1	2.14	0.64
1:D:54:LYS:HD2	1:D:67:CYS:HA	1.80	0.64
1:D:153:LYS:HD2	1:D:193:GLN:HB2	1.78	0.64
2:E:51:LEU:HD12	2:E:56:ARG:H	1.60	0.64
1:G:173:VAL:HA	1:G:255:PHE:O	1.98	0.64
2:B:51:LEU:HG	2:B:56:ARG:HG2	1.80	0.64
3:F:38:TRP:HZ2	3:F:89:TYR:HB3	1.62	0.64
3:F:152:LYS:O	3:F:196:THR:N	2.26	0.64
1:G:70:LEU:O	1:G:71:SER:OG	2.14	0.64
1:G:211:LYS:HB2	1:G:211:LYS:NZ	2.12	0.64
3:I:2:GLN:O	3:I:2:GLN:HG2	1.98	0.64
1:J:184:THR:C	1:J:214:ILE:HG21	2.21	0.64
2:K:59:TYR:CE1	2:K:69:ILE:HG22	2.32	0.64
3:C:38:TRP:CD1	3:C:90:PHE:O	2.50	0.64
3:C:38:TRP:CE2	3:C:39:PHE:HA	2.32	0.64
1:D:79:ILE:HD12	1:D:79:ILE:H	1.61	0.64
2:E:180:SER:O	2:E:182:GLY:N	2.30	0.64
3:I:92:GLN:NE2	3:I:101:THR:HG22	2.12	0.64
2:K:97:ARG:NE	2:K:110:GLY:HA3	2.13	0.64
3:L:34:ASN:O	3:L:95:LYS:HB3	1.98	0.64
2:B:181:SER:CB	3:L:62:PRO:HG3	2.21	0.64
1:G:153:LYS:HZ1	1:G:156:ASN:HA	1.61	0.64
3:I:16:GLN:HA	3:I:80:PRO:HA	1.79	0.64
3:I:163:LEU:O	3:I:182:LEU:HD11	1.97	0.64
2:K:6:GLU:OE2	2:K:112:GLY:HA3	1.96	0.64
2:B:34:SER:O	2:B:96:ALA:N	2.30	0.64
2:E:181:SER:HB3	3:I:62:PRO:CG	2.28	0.64
2:H:45:GLU:HB3	2:H:60:ARG:NH1	2.13	0.64
3:C:158:ARG:HH22	2:K:97:ARG:HD2	1.63	0.64
1:D:91:TYR:HH	1:D:180:HIS:CD2	2.15	0.64
2:E:146:LEU:O	2:E:190:VAL:N	2.27	0.64
3:F:38:TRP:CH2	3:F:91:CYS:HA	2.32	0.64
1:G:166:ILE:HA	1:G:239:LYS:HB2	1.80	0.64
3:I:120:ILE:HD13	3:I:197:CYS:SG	2.38	0.64
2:K:45:GLU:OE2	3:L:99:TYR:O	2.15	0.64
3:L:153:ILE:HG22	3:L:192:HIS:CD2	2.33	0.64
1:A:115:GLU:HB2	3:C:96:GLU:CG	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:HD11	2:B:56:ARG:H	1.61	0.63
2:B:201:THR:CG2	2:B:218:LYS:HE3	2.29	0.63
3:C:111:ARG:NH1	3:C:172:LYS:O	2.31	0.63
3:C:195:TYR:H	3:C:210:LYS:HB2	1.63	0.63
2:E:49:GLY:HA3	4:E:304:HOH:O	1.98	0.63
2:H:11:VAL:O	2:H:120:SER:N	2.29	0.63
3:I:208:ILE:HG23	3:I:209:VAL:N	2.12	0.63
1:A:76:TRP:CH2	1:A:108:VAL:HG21	2.33	0.63
3:C:38:TRP:CZ3	3:C:89:TYR:CD1	2.86	0.63
3:C:156:SER:OG	3:C:157:GLU:N	2.30	0.63
2:H:18:ARG:HG3	2:H:81:GLU:HA	1.80	0.63
2:K:2:VAL:HG22	2:K:25:GLY:HA3	1.80	0.63
1:D:91:TYR:OH	1:D:180:HIS:NE2	2.32	0.63
1:D:116:ILE:HG13	1:D:165:TYR:HD1	1.61	0.63
2:E:28:GLY:H	2:E:76:LYS:NZ	1.97	0.63
3:I:2:GLN:HA	3:I:25:SER:OG	1.99	0.63
3:I:66:SER:O	3:I:76:LEU:HD12	1.98	0.63
1:J:149:ILE:HB	1:J:250:VAL:HG23	1.79	0.63
1:J:165:TYR:HE2	1:J:173:VAL:HG21	1.63	0.63
3:L:87:ALA:O	3:L:106:LYS:O	2.17	0.63
3:L:141:ASN:CA	3:L:175:THR:HB	2.28	0.63
3:C:7:PRO:HG2	4:C:309:HOH:O	1.99	0.63
1:G:186:ALA:O	1:G:190:SER:OG	2.17	0.63
3:L:141:ASN:HA	3:L:175:THR:CG2	2.27	0.63
3:C:92:GLN:HA	3:C:101:THR:HG23	1.81	0.63
1:J:153:LYS:HG2	1:J:191:LEU:O	1.99	0.63
2:K:203:ILE:HD12	2:K:218:LYS:HG3	1.81	0.63
2:B:32:ASP:HA	2:B:71:ARG:NH2	2.11	0.63
3:F:41:GLN:HG2	3:F:42:LYS:N	2.14	0.63
1:G:153:LYS:CG	1:G:193:GLN:HB2	2.28	0.63
3:I:203:THR:O	3:I:205:THR:N	2.32	0.63
1:J:49:PRO:HD2	1:J:77:SER:OG	1.99	0.63
2:E:89:ASP:O	2:E:93:TYR:OH	2.10	0.63
3:I:17:ARG:O	3:I:17:ARG:HG3	1.99	0.63
3:I:162:VAL:O	3:I:164:ASN:CG	2.41	0.63
2:K:18:ARG:HG3	2:K:81:GLU:CA	2.28	0.63
2:K:55:GLU:HG3	2:K:71:ARG:HD2	1.80	0.63
2:B:178:LEU:HD12	2:B:179:GLN:N	2.13	0.63
2:B:180:SER:C	2:B:182:GLY:N	2.50	0.63
2:E:21:CYS:HB3	2:E:78:LEU:HD23	1.80	0.63
2:B:161:SER:O	2:B:205:ASN:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:TRP:CZ3	2:B:204:CYS:HB3	2.34	0.62
2:B:181:SER:HB2	3:L:62:PRO:CG	2.18	0.62
3:F:7:PRO:O	3:F:8:ALA:HB2	1.99	0.62
2:K:97:ARG:HE	2:K:110:GLY:HA3	1.63	0.62
2:K:163:ASN:N	2:K:163:ASN:ND2	2.43	0.62
3:L:102:PHE:HD1	3:L:102:PHE:C	2.06	0.62
1:D:121:SER:CB	2:E:58:TYR:HA	2.29	0.62
1:D:127:ASP:HB2	1:D:154:LYS:HB3	1.81	0.62
1:D:138:HIS:O	1:D:139:ALA:C	2.41	0.62
1:D:164:SER:OG	1:D:241:THR:HG23	1.98	0.62
1:G:188:GLN:HE22	1:G:197:ALA:CB	2.12	0.62
3:I:91:CYS:H	3:I:102:PHE:HE2	1.45	0.62
3:I:109:ILE:CG2	3:I:110:LYS:H	2.11	0.62
1:A:48:ALA:HB2	1:A:78:TYR:CZ	2.34	0.62
3:I:147:ILE:HG12	3:I:148:ASN:H	1.63	0.62
3:I:91:CYS:SG	3:I:102:PHE:HB3	2.40	0.62
3:I:132:GLY:N	3:I:184:LEU:O	2.32	0.62
3:I:196:THR:HG1	3:I:209:VAL:HG23	1.64	0.62
2:K:86:ARG:O	2:K:89:ASP:HB2	1.99	0.62
3:F:39:PHE:CE1	3:F:76:LEU:HB2	2.34	0.62
2:H:36:ILE:HB	2:H:46:TRP:HA	1.81	0.62
3:C:176:TYR:HB2	3:C:178:MET:HE2	1.81	0.62
3:F:108:GLU:C	3:F:109:ILE:HD12	2.25	0.62
1:G:57:ILE:N	1:G:81:GLU:OE2	2.23	0.62
1:G:161:LEU:O	1:G:243:GLU:HA	2.00	0.62
3:I:156:SER:O	3:I:157:GLU:HB2	2.00	0.62
1:J:43:LYS:HB3	1:J:43:LYS:NZ	2.14	0.62
2:K:132:LEU:HD12	2:K:147:GLY:HA3	1.82	0.62
2:B:45:GLU:CD	2:B:46:TRP:N	2.58	0.62
3:C:153:ILE:HG22	3:C:195:TYR:CD1	2.34	0.62
1:G:131:GLY:O	1:G:144:PHE:HB2	1.99	0.62
2:H:194:SER:O	2:H:197:LEU:N	2.19	0.62
1:J:102:ARG:HG2	1:J:103:GLU:N	2.15	0.62
3:L:28:VAL:HG23	3:L:74:PHE:HE2	1.65	0.62
3:C:86:THR:HG22	3:C:109:ILE:CD1	2.30	0.62
1:D:168:ASP:OD1	1:D:168:ASP:N	2.33	0.62
3:F:45:GLN:HB3	3:F:46:PRO:HD3	1.81	0.62
1:G:202:GLY:O	1:G:203:SER:OG	2.16	0.62
3:I:92:GLN:NE2	3:I:101:THR:CG2	2.63	0.62
2:E:162:TRP:HB3	2:E:166:ALA:CB	2.29	0.62
3:F:35:PHE:HB3	3:F:95:LYS:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:95:PHE:HB3	1:J:98:TYR:HB2	1.82	0.62
1:J:118:PRO:HB2	1:J:120:THR:HG23	1.80	0.62
3:L:147:ILE:HG13	3:L:201:HIS:CG	2.35	0.62
1:D:55:CYS:HB2	1:D:60:TRP:HB2	1.82	0.61
1:D:215:ALA:O	1:D:217:ARG:NH1	2.32	0.61
1:D:258:GLU:O	1:D:259:ARG:HG3	1.99	0.61
2:E:98:HIS:CD2	2:E:98:HIS:N	2.67	0.61
2:E:162:TRP:H	2:E:167:LEU:CG	2.06	0.61
2:H:37:ARG:NH1	2:H:93:TYR:OH	2.31	0.61
1:D:187:ASP:O	1:D:191:LEU:HD13	2.00	0.61
1:D:219:LYS:HG2	1:D:222:ASP:HA	1.80	0.61
2:E:93:TYR:O	2:E:114:GLY:HA2	2.00	0.61
3:F:2:GLN:CD	3:F:97:VAL:HG21	2.24	0.61
3:F:150:LYS:O	3:F:198:GLU:N	2.17	0.61
3:I:7:PRO:HG3	3:I:21:THR:N	2.14	0.61
3:I:7:PRO:CD	3:I:21:THR:O	2.47	0.61
3:I:10:LEU:HD23	3:I:11:ALA:H	1.64	0.61
3:I:34:ASN:OD1	3:I:34:ASN:N	2.32	0.61
2:B:90:THR:OG1	2:B:119:VAL:HG23	2.00	0.61
1:D:116:ILE:HG23	1:D:117:PHE:H	1.64	0.61
3:F:9:SER:HB3	3:F:106:LYS:HZ1	1.63	0.61
1:D:146:LYS:HD2	1:D:252:ARG:NH2	2.14	0.61
3:F:38:TRP:CZ3	3:F:91:CYS:HA	2.36	0.61
3:L:17:ARG:NE	4:L:308:HOH:O	2.23	0.61
3:L:151:TRP:CZ2	3:L:180:SER:HA	2.36	0.61
3:F:101:THR:HG22	3:F:102:PHE:N	2.15	0.61
1:J:153:LYS:HD2	1:J:156:ASN:HA	1.82	0.61
1:A:127:ASP:N	1:A:154:LYS:HB3	2.15	0.61
3:C:37:ASN:HD22	3:C:39:PHE:HE2	1.47	0.61
3:F:38:TRP:HE1	3:F:89:TYR:HA	1.66	0.61
1:G:121:SER:N	2:H:64:LYS:HE3	2.15	0.61
2:H:150:VAL:HB	2:H:186:LEU:HG	1.82	0.61
3:I:159:GLN:CG	3:I:160:ASN:H	2.11	0.61
3:I:170:ASP:CG	3:I:171:SER:N	2.59	0.61
1:J:119:LYS:HZ3	1:J:129:ASN:HB3	1.65	0.61
1:A:104:GLN:HE22	1:A:233:LEU:CD2	2.13	0.61
1:A:123:TRP:HE1	1:A:149:ILE:HD13	1.65	0.61
1:D:160:LYS:HE3	1:D:160:LYS:N	2.09	0.61
2:E:178:LEU:O	2:E:179:GLN:C	2.42	0.61
3:F:139:LEU:HD12	3:F:139:LEU:N	2.15	0.61
3:I:45:GLN:CB	3:I:46:PRO:CD	2.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:57:ILE:O	1:J:61:ILE:HG22	2.01	0.61
2:K:38:GLN:HG3	2:K:43:GLY:HA2	1.82	0.61
1:A:161:LEU:C	1:A:161:LEU:HD23	2.25	0.61
2:B:45:GLU:CD	2:B:46:TRP:H	2.08	0.61
1:D:55:CYS:HB2	1:D:60:TRP:CB	2.31	0.61
1:D:75:SER:HB2	1:D:109:SER:O	2.00	0.61
3:F:135:VAL:HG12	3:F:151:TRP:CH2	2.36	0.61
1:G:87:ASN:N	1:G:87:ASN:OD1	2.34	0.61
2:H:50:ILE:HB	2:H:56:ARG:O	2.01	0.61
2:K:177:VAL:HG22	2:K:184:TYR:CE2	2.36	0.61
3:L:142:PHE:CD1	3:L:144:PRO:O	2.53	0.61
1:A:235:GLU:HG3	1:A:236:PRO:HD2	1.82	0.61
3:C:78:ILE:O	3:C:78:ILE:HG12	2.00	0.61
3:C:153:ILE:HG13	3:C:154:ASP:N	2.16	0.61
2:E:122:ALA:HB3	2:E:154:PHE:CZ	2.35	0.61
2:E:162:TRP:O	2:E:166:ALA:HB3	2.00	0.61
3:F:153:ILE:HG13	3:F:154:ASP:N	2.12	0.61
3:I:20:ILE:HG22	3:I:21:THR:N	2.16	0.61
2:B:71:ARG:HG2	2:B:72:ASP:N	2.15	0.61
1:D:91:TYR:HH	1:D:180:HIS:HE2	1.45	0.61
2:E:10:VAL:CG2	2:E:155:PRO:HG3	2.30	0.61
2:E:33:MET:HE1	2:E:97:ARG:HB2	1.82	0.61
1:G:51:HIS:HB3	4:G:604:HOH:O	1.99	0.61
3:C:109:ILE:O	3:C:143:TYR:OH	2.15	0.60
2:H:51:LEU:HD11	2:H:56:ARG:CD	2.31	0.60
2:H:93:TYR:N	2:H:115:THR:O	2.32	0.60
2:K:33:MET:CB	2:K:78:LEU:HD13	2.30	0.60
2:K:127:PRO:CB	2:K:150:VAL:HG13	2.31	0.60
3:L:38:TRP:NE1	3:L:90:PHE:CD2	2.67	0.60
3:L:178:MET:SD	3:L:178:MET:C	2.85	0.60
2:E:113:GLN:HG3	2:E:114:GLY:O	2.01	0.60
3:F:173:ASP:OD2	3:F:175:THR:HG23	2.00	0.60
2:H:6:GLU:N	2:H:6:GLU:OE1	2.34	0.60
2:H:153:TYR:N	2:H:183:LEU:HD12	2.16	0.60
3:I:39:PHE:O	3:I:89:TYR:HA	2.01	0.60
3:I:164:ASN:HB3	3:I:180:SER:H	1.66	0.60
2:E:36:ILE:HD12	2:E:45:GLU:C	2.26	0.60
1:G:101:LEU:HG	1:G:231:TRP:CE2	2.37	0.60
3:I:107:LEU:HG	3:I:107:LEU:O	2.01	0.60
3:F:41:GLN:HB2	3:F:47:PRO:HB3	1.83	0.60
3:F:107:LEU:HD23	3:F:107:LEU:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:11:VAL:HG11	2:H:85:LEU:HD13	1.83	0.60
2:H:206:VAL:O	2:H:214:LYS:HA	2.01	0.60
3:I:164:ASN:OD1	3:I:180:SER:O	2.19	0.60
3:L:9:SER:HA	3:L:105:THR:HG23	1.82	0.60
2:B:127:PRO:HB3	2:B:153:TYR:CB	2.30	0.60
3:C:38:TRP:CE3	3:C:39:PHE:CA	2.82	0.60
3:F:38:TRP:O	3:F:39:PHE:CD2	2.53	0.60
3:F:38:TRP:HD1	3:F:40:GLN:O	1.84	0.60
2:H:9:ALA:O	2:H:10:VAL:HG23	2.01	0.60
2:H:51:LEU:HD11	2:H:56:ARG:H	1.66	0.60
3:I:193:ASN:OD1	3:I:194:SER:HB3	2.01	0.60
3:C:53:THR:HG22	3:C:53:THR:O	2.01	0.60
2:H:69:ILE:CG1	2:H:70:SER:H	2.15	0.60
1:A:56:ASN:O	1:A:57:ILE:C	2.43	0.60
1:A:169:LYS:CB	1:A:171:LYS:H	2.14	0.60
1:A:183:SER:HA	1:A:215:ALA:O	2.01	0.60
2:B:148:CYS:HB2	2:B:162:TRP:CH2	2.37	0.60
3:C:45:GLN:OE1	3:C:45:GLN:HA	2.01	0.60
2:E:207:ASN:N	2:E:207:ASN:OD1	2.34	0.60
3:F:149:VAL:HG21	3:F:179:SER:OG	2.02	0.60
1:G:153:LYS:HZ3	1:G:156:ASN:HA	1.67	0.60
2:H:72:ASP:CB	2:H:79:TYR:HE2	2.15	0.60
3:I:175:THR:HB	3:I:176:TYR:CD1	2.37	0.60
3:L:102:PHE:HE1	3:L:104:GLY:C	2.09	0.60
3:C:64:ARG:NH2	3:C:85:ASP:CG	2.56	0.60
3:C:113:ASP:OD1	3:C:113:ASP:C	2.45	0.60
2:E:61:ASP:OD1	2:E:64:LYS:HD2	2.02	0.60
3:I:120:ILE:HB	3:I:208:ILE:HG21	1.84	0.60
3:L:195:TYR:N	3:L:210:LYS:HG2	2.16	0.60
1:D:149:ILE:HB	1:D:250:VAL:CG2	2.31	0.60
1:D:167:ASN:ND2	1:D:236:PRO:HA	2.16	0.60
2:E:6:GLU:OE1	2:E:113:GLN:HG2	2.02	0.60
2:E:179:GLN:O	2:E:180:SER:C	2.45	0.60
3:F:38:TRP:CZ2	3:F:89:TYR:HB3	2.36	0.60
2:H:186:LEU:C	2:H:186:LEU:HD12	2.26	0.60
1:J:77:SER:O	1:J:106:SER:O	2.20	0.60
1:D:75:SER:OG	1:D:108:VAL:O	2.20	0.59
3:F:96:GLU:N	4:F:309:HOH:O	2.22	0.59
1:G:201:VAL:HG13	1:G:240:ILE:HD11	1.84	0.59
3:I:37:ASN:OD1	3:I:92:GLN:HB3	2.02	0.59
1:D:108:VAL:HG12	1:D:257:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:92:PRO:CG	1:G:223:GLN:HB2	2.31	0.59
3:I:199:ALA:HB3	3:I:206:SER:HB3	1.84	0.59
1:J:97:ASP:HB2	1:J:231:TRP:NE1	2.18	0.59
3:F:39:PHE:C	3:F:50:LEU:HG	2.27	0.59
1:G:72:THR:HG21	3:I:70:SER:OG	2.03	0.59
2:H:152:ASP:C	2:H:183:LEU:HD12	2.27	0.59
3:I:20:ILE:HG22	3:I:21:THR:H	1.66	0.59
3:I:38:TRP:CB	3:I:47:PRO:CB	2.75	0.59
3:I:93:GLN:HA	3:I:100:GLY:O	2.02	0.59
3:I:102:PHE:CE1	3:I:104:GLY:CA	2.86	0.59
1:J:84:SER:HB3	1:J:87:ASN:HB2	1.84	0.59
1:J:97:ASP:HB2	1:J:231:TRP:HE1	1.66	0.59
3:L:141:ASN:HA	3:L:175:THR:HG22	1.82	0.59
1:A:48:ALA:HB2	1:A:78:TYR:CE2	2.38	0.59
3:C:110:LYS:C	3:C:111:ARG:HD3	2.27	0.59
3:C:169:GLN:OE1	3:C:169:GLN:HA	2.02	0.59
1:D:58:ALA:O	1:D:62:LEU:HB2	2.01	0.59
2:E:127:PRO:HB3	2:E:153:TYR:CD2	2.38	0.59
2:E:178:LEU:O	2:E:180:SER:HB2	2.02	0.59
3:F:39:PHE:H	3:F:50:LEU:H	1.47	0.59
2:H:38:GLN:HG3	2:H:43:GLY:HA2	1.84	0.59
2:H:100:TRP:CD1	3:I:34:ASN:CA	2.85	0.59
1:J:235:GLU:CG	1:J:236:PRO:HD2	2.27	0.59
2:K:55:GLU:CG	2:K:71:ARG:HD2	2.32	0.59
2:K:125:LYS:HE3	2:K:126:GLY:O	2.03	0.59
3:L:27:SER:C	3:L:28:VAL:HG22	2.27	0.59
1:A:167:ASN:CG	1:A:236:PRO:HA	2.28	0.59
3:C:204:SER:O	3:C:205:THR:CG2	2.50	0.59
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.82	0.59
2:E:152:ASP:HB3	2:E:183:LEU:HD23	1.84	0.59
1:J:161:LEU:HD23	1:J:161:LEU:C	2.27	0.59
2:K:4:LEU:HD23	2:K:95:CYS:O	2.03	0.59
1:A:58:ALA:HB2	1:A:98:TYR:CE1	2.38	0.59
3:F:36:ILE:H	3:F:93:GLN:NE2	2.00	0.59
1:G:132:VAL:HB	1:G:142:LYS:O	2.02	0.59
1:G:179:ILE:HG12	1:G:180:HIS:N	2.18	0.59
3:L:89:TYR:O	3:L:102:PHE:CZ	2.55	0.59
2:B:161:SER:OG	2:B:205:ASN:HB2	2.02	0.59
3:C:108:GLU:HG3	3:C:109:ILE:N	2.18	0.59
1:D:153:LYS:O	1:D:153:LYS:HG2	1.99	0.59
2:E:171:VAL:HG21	3:F:176:TYR:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:86:THR:HA	3:F:107:LEU:HD23	1.85	0.59
1:G:69:SER:OG	1:G:70:LEU:HB2	2.02	0.59
2:H:27:THR:CG2	2:H:31:TYR:HD2	2.15	0.59
3:I:2:GLN:OE1	3:I:94:THR:HG21	2.03	0.59
2:K:211:SER:C	2:K:213:THR:H	2.11	0.59
3:L:96:GLU:O	3:L:97:VAL:HB	2.02	0.59
1:A:49:PRO:HB2	1:A:76:TRP:CB	2.32	0.59
2:B:10:VAL:HG22	2:B:155:PRO:HG3	1.85	0.59
2:B:53:GLY:O	2:B:54:SER:HB2	2.03	0.59
3:C:45:GLN:HB3	3:C:46:PRO:CD	2.30	0.59
3:C:97:VAL:HG12	3:C:98:PRO:O	2.03	0.59
1:D:228:ASN:HB3	1:D:230:TYR:CE1	2.37	0.59
2:E:21:CYS:O	2:E:77:THR:HA	2.03	0.59
3:F:110:LYS:O	3:F:111:ARG:HG3	2.03	0.59
1:G:193:GLN:HA	1:G:193:GLN:HE21	1.68	0.59
1:J:153:LYS:HB3	1:J:158:TYR:HB2	1.85	0.59
3:C:39:PHE:HB3	3:C:50:LEU:HB2	1.82	0.59
3:F:23:ARG:CG	3:F:72:THR:O	2.50	0.59
1:G:182:PRO:HG2	1:G:188:GLN:HB2	1.85	0.59
3:I:149:VAL:HG23	3:I:150:LYS:N	2.17	0.59
1:J:54:LYS:HE3	1:J:67:CYS:HA	1.84	0.59
2:B:10:VAL:CG2	2:B:155:PRO:HG3	2.33	0.59
3:C:38:TRP:CG	3:C:90:PHE:O	2.56	0.59
3:C:140:ASN:OD1	3:C:176:TYR:HB3	2.02	0.59
1:G:134:ALA:N	1:G:142:LYS:HD2	2.18	0.59
2:H:163:ASN:O	2:H:164:SER:OG	2.20	0.59
2:K:203:ILE:HG13	2:K:217:LYS:O	2.02	0.59
3:L:167:THR:HG22	3:L:168:ASP:N	2.18	0.59
1:A:94:ASP:N	1:A:94:ASP:OD1	2.34	0.58
1:D:219:LYS:HD2	1:D:222:ASP:OD1	2.03	0.58
1:G:118:PRO:HB3	1:G:120:THR:HG23	1.84	0.58
2:H:34:SER:CB	2:H:98:HIS:NE2	2.65	0.58
3:I:208:ILE:HG23	3:I:209:VAL:H	1.68	0.58
1:J:221:ARG:O	1:J:223:GLN:HG2	2.03	0.58
2:B:86:ARG:HG3	2:B:88:GLU:OE1	2.03	0.58
1:D:51:HIS:ND1	1:D:80:VAL:HG11	2.17	0.58
1:D:181:HIS:ND1	1:D:212:PRO:HA	2.18	0.58
3:F:34:ASN:N	3:F:34:ASN:ND2	2.51	0.58
3:F:158:ARG:HG3	3:F:159:GLN:H	1.68	0.58
1:G:201:VAL:HG13	1:G:202:GLY:H	1.67	0.58
1:J:120:THR:O	1:J:122:SER:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:171:LYS:HZ2	1:J:258:GLU:HG3	1.68	0.58
3:L:162:VAL:CG2	3:L:182:LEU:HG	2.32	0.58
3:C:193:ASN:O	3:C:211:SER:HB3	2.04	0.58
1:D:94:ASP:HB2	1:D:228:ASN:OD1	2.04	0.58
2:E:129:VAL:HG13	2:E:150:VAL:HG22	1.83	0.58
3:F:114:ALA:HA	3:F:201:HIS:CD2	2.39	0.58
3:F:192:HIS:O	3:F:195:TYR:OH	2.13	0.58
1:G:131:GLY:HA3	1:G:150:TRP:HB3	1.85	0.58
1:G:180:HIS:O	1:G:182:PRO:HD3	2.03	0.58
2:H:33:MET:CB	2:H:78:LEU:HD13	2.33	0.58
2:H:92:VAL:HA	2:H:115:THR:O	2.03	0.58
2:H:132:LEU:HB3	3:I:121:PHE:CD1	2.39	0.58
1:J:138:HIS:O	1:J:139:ALA:C	2.47	0.58
2:B:127:PRO:HA	2:B:153:TYR:HB3	1.85	0.58
3:C:113:ASP:O	3:C:143:TYR:O	2.21	0.58
3:C:158:ARG:HG3	2:K:31:TYR:CZ	2.38	0.58
2:E:160:VAL:HG22	2:E:206:VAL:HG22	1.85	0.58
3:F:20:ILE:HG12	3:F:105:THR:HG21	1.85	0.58
3:I:167:THR:HG22	3:I:168:ASP:H	1.67	0.58
3:I:170:ASP:HB3	3:I:175:THR:HG1	1.69	0.58
1:J:48:ALA:CB	1:J:78:TYR:CE1	2.86	0.58
2:K:66:ARG:NH2	2:K:85:LEU:HA	2.18	0.58
3:L:94:THR:O	3:L:99:TYR:HD1	1.86	0.58
3:L:140:ASN:HB2	3:L:141:ASN:HD22	1.69	0.58
2:B:176:ALA:HB2	3:C:166:TRP:CZ2	2.38	0.58
3:C:159:GLN:HG3	3:C:160:ASN:H	1.67	0.58
2:E:67:SER:HA	2:E:81:GLU:O	2.03	0.58
3:F:38:TRP:CZ2	3:F:89:TYR:C	2.81	0.58
3:F:108:GLU:OE2	3:F:173:ASP:O	2.21	0.58
3:F:150:LYS:HA	3:F:150:LYS:HE3	1.85	0.58
3:F:169:GLN:OE1	3:F:169:GLN:HA	2.03	0.58
1:G:199:VAL:HG13	1:G:244:ALA:HB2	1.86	0.58
2:H:171:VAL:HG22	3:I:176:TYR:CE2	2.37	0.58
2:B:197:LEU:HG	2:B:198:GLY:N	2.19	0.58
1:D:99:GLU:CD	1:D:99:GLU:H	2.12	0.58
1:G:187:ASP:O	1:G:191:LEU:HD13	2.03	0.58
1:A:76:TRP:CZ3	1:A:108:VAL:HG21	2.39	0.58
2:B:171:VAL:CG2	3:C:176:TYR:CZ	2.83	0.58
3:C:108:GLU:C	3:C:109:ILE:HD12	2.28	0.58
1:D:51:HIS:CE1	1:D:80:VAL:HG21	2.39	0.58
2:E:59:TYR:CE1	2:E:69:ILE:HG22	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:59:TYR:HE1	2:E:69:ILE:HG22	1.67	0.58
2:H:208:HIS:N	2:H:212:ASN:O	2.36	0.58
3:I:72:THR:HG23	3:I:72:THR:O	2.04	0.58
1:J:199:VAL:CG1	1:J:200:PHE:N	2.64	0.58
1:A:177:TRP:CE2	1:A:230:TYR:HB2	2.39	0.58
2:B:157:PRO:O	2:B:208:HIS:HD2	1.87	0.58
2:B:208:HIS:C	2:B:210:PRO:HD2	2.29	0.58
3:C:38:TRP:CZ3	3:C:89:TYR:CA	2.87	0.58
3:C:106:LYS:CG	3:C:107:LEU:N	2.65	0.58
3:F:71:GLY:O	3:F:72:THR:HG22	2.04	0.58
3:F:145:LYS:HD2	3:F:167:THR:HG21	1.84	0.58
1:J:100:GLU:HG2	1:J:231:TRP:HZ2	1.68	0.58
3:L:20:ILE:HG22	3:L:21:THR:N	2.17	0.58
2:E:171:VAL:HG11	3:F:176:TYR:CD2	2.39	0.58
3:F:151:TRP:CZ3	3:F:197:CYS:HB3	2.38	0.58
3:I:102:PHE:CD1	3:I:103:GLY:N	2.71	0.58
1:J:119:LYS:HZ2	1:J:129:ASN:HB3	1.68	0.58
2:K:27:THR:C	2:K:29:SER:N	2.48	0.58
2:K:36:ILE:HG13	2:K:36:ILE:O	2.03	0.58
2:K:209:LYS:O	2:K:212:ASN:N	2.26	0.58
2:B:63:VAL:HG13	2:B:67:SER:H	1.69	0.58
2:B:160:VAL:O	2:B:172:HIS:NE2	2.36	0.58
2:E:200:GLN:HG2	2:E:202:TYR:CE2	2.39	0.58
2:H:34:SER:OG	2:H:98:HIS:CE1	2.56	0.58
2:K:28:GLY:HA2	4:K:301:HOH:O	2.04	0.58
3:L:14:PRO:HG3	3:L:111:ARG:NH1	2.19	0.58
3:L:62:PRO:HG2	3:L:65:PHE:CD2	2.38	0.58
1:A:165:TYR:O	1:A:239:LYS:HA	2.04	0.57
1:D:108:VAL:HG12	1:D:257:MET:HE3	1.85	0.57
2:E:11:VAL:HG22	2:E:12:GLN:O	2.03	0.57
1:G:231:TRP:HZ3	1:G:233:LEU:HD13	1.68	0.57
3:I:102:PHE:CE1	3:I:104:GLY:C	2.81	0.57
1:J:106:SER:OG	1:J:263:SER:OG	2.22	0.57
1:J:114:PHE:HA	3:L:96:GLU:OE1	2.04	0.57
1:J:158:TYR:CZ	1:J:246:GLY:HA2	2.39	0.57
2:B:29:SER:HA	2:B:73:ASN:HD22	1.69	0.57
1:D:202:GLY:HA3	1:D:241:THR:N	2.16	0.57
3:F:13:SER:HB3	3:F:110:LYS:HD3	1.84	0.57
1:J:48:ALA:HB2	1:J:78:TYR:CE1	2.38	0.57
1:J:118:PRO:HB2	1:J:120:THR:CG2	2.34	0.57
2:K:111:TRP:CZ2	3:L:38:TRP:N	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:49:LEU:O	3:L:50:LEU:HD23	2.04	0.57
3:C:157:GLU:O	2:K:27:THR:HG21	2.03	0.57
1:D:126:HIS:HA	1:D:154:LYS:HG2	1.85	0.57
3:F:126:GLU:OE1	3:F:126:GLU:N	2.38	0.57
1:G:242:PHE:CE1	1:G:251:PRO:HG2	2.39	0.57
2:H:66:ARG:HH22	2:H:89:ASP:CG	2.12	0.57
3:I:37:ASN:O	3:I:49:LEU:HB2	2.04	0.57
1:J:123:TRP:HZ3	1:J:163:LYS:HG3	1.70	0.57
3:L:94:THR:O	3:L:99:TYR:CD1	2.58	0.57
1:A:121:SER:HB2	2:B:58:TYR:HD1	1.68	0.57
3:F:38:TRP:HZ2	3:F:89:TYR:C	2.12	0.57
3:F:39:PHE:O	3:F:40:GLN:HB2	2.03	0.57
3:F:45:GLN:CB	3:F:46:PRO:CD	2.82	0.57
1:G:54:LYS:HZ1	1:G:60:TRP:HD1	1.52	0.57
2:H:208:HIS:ND1	2:H:211:SER:OG	2.35	0.57
2:K:163:ASN:C	2:K:165:GLY:N	2.56	0.57
2:B:63:VAL:CG1	2:B:67:SER:HB2	2.30	0.57
3:C:38:TRP:CH2	3:C:89:TYR:CB	2.87	0.57
3:C:203:THR:HG23	3:C:205:THR:N	2.10	0.57
1:D:57:ILE:CD1	1:D:102:ARG:HG3	2.34	0.57
1:G:119:LYS:NZ	1:G:129:ASN:ND2	2.40	0.57
2:H:98:HIS:N	2:H:98:HIS:CD2	2.72	0.57
2:H:145:ALA:HB2	2:H:191:THR:HG23	1.85	0.57
2:K:17:LEU:HD23	2:K:82:MET:SD	2.44	0.57
3:C:38:TRP:CE2	3:C:90:PHE:O	2.58	0.57
3:C:138:PHE:CE1	3:C:178:MET:HG2	2.38	0.57
1:G:219:LYS:HA	1:G:223:GLN:O	2.05	0.57
2:H:177:VAL:HG12	2:H:182:GLY:HA2	1.87	0.57
3:I:106:LYS:O	3:I:107:LEU:HB3	2.05	0.57
3:I:209:VAL:HG22	3:I:210:LYS:CG	2.35	0.57
1:J:56:ASN:HB3	1:J:84:SER:H	1.69	0.57
1:J:233:LEU:HD12	1:J:233:LEU:N	2.20	0.57
3:L:130:SER:HB3	3:L:132:GLY:N	2.20	0.57
2:B:35:TRP:HE1	2:B:78:LEU:HD13	1.69	0.57
2:B:190:VAL:HG22	2:B:192:VAL:HG23	1.84	0.57
3:C:52:TYR:O	3:C:56:ASN:HB2	2.05	0.57
3:F:113:ASP:O	3:F:143:TYR:O	2.22	0.57
3:F:116:PRO:CA	3:F:142:PHE:HB3	2.31	0.57
3:I:38:TRP:CD1	3:I:47:PRO:CB	2.82	0.57
1:J:51:HIS:HD2	1:J:80:VAL:HB	1.70	0.57
1:J:227:MET:SD	1:J:249:VAL:HG21	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:28:VAL:HG23	3:L:74:PHE:CE2	2.40	0.57
3:L:141:ASN:HA	3:L:175:THR:CA	2.35	0.57
2:B:13:PRO:HD3	2:B:120:SER:C	2.30	0.57
2:B:32:ASP:HB3	2:B:51:LEU:CA	2.18	0.57
2:B:180:SER:HB3	3:L:62:PRO:CA	2.33	0.57
3:C:190:GLU:CD	3:C:191:ARG:HG3	2.30	0.57
2:E:46:TRP:N	2:E:60:ARG:CZ	2.67	0.57
3:F:39:PHE:O	3:F:50:LEU:CG	2.46	0.57
2:H:69:ILE:HG12	2:H:70:SER:N	2.19	0.57
2:H:177:VAL:HG12	2:H:182:GLY:CA	2.35	0.57
2:B:61:ASP:HB3	2:K:142:GLY:O	2.04	0.57
2:B:174:PHE:O	3:C:166:TRP:NE1	2.38	0.57
3:C:4:THR:O	3:C:102:PHE:HB2	2.05	0.57
3:C:90:PHE:N	3:C:90:PHE:CD2	2.72	0.57
1:D:57:ILE:O	1:D:61:ILE:HG22	2.04	0.57
1:G:89:THR:HB	1:G:145:TYR:OH	2.05	0.57
2:H:49:GLY:HA3	4:H:302:HOH:O	2.03	0.57
3:I:6:SER:CB	3:I:7:PRO:HD2	2.25	0.57
3:L:20:ILE:HG22	3:L:21:THR:H	1.70	0.57
3:L:142:PHE:HZ	3:L:177:SER:CB	2.07	0.57
3:L:142:PHE:CE2	3:L:177:SER:HB3	2.39	0.57
1:A:52:LEU:HD12	1:A:81:GLU:HG3	1.86	0.56
3:C:38:TRP:NE1	3:C:91:CYS:HA	2.19	0.56
3:F:4:THR:HG22	3:F:24:ALA:CA	2.31	0.56
3:F:45:GLN:HB3	3:F:46:PRO:HD2	1.85	0.56
3:L:143:TYR:C	3:L:143:TYR:CD2	2.83	0.56
2:E:43:GLY:O	2:E:44:LEU:HD12	2.04	0.56
3:F:116:PRO:HB2	3:F:139:LEU:HB3	1.86	0.56
2:H:54:SER:HB3	2:H:56:ARG:NE	2.14	0.56
3:I:9:SER:HB2	3:I:106:LYS:HZ3	1.70	0.56
3:I:162:VAL:HG23	3:I:162:VAL:O	2.04	0.56
1:A:147:ASN:HD22	1:A:253:TYR:HB2	1.70	0.56
2:B:10:VAL:CG1	2:B:155:PRO:HG3	2.35	0.56
2:B:122:ALA:HB3	2:B:154:PHE:CE2	2.41	0.56
2:B:134:PRO:HD3	2:B:146:LEU:HD11	1.87	0.56
3:C:140:ASN:CG	3:C:176:TYR:HD1	2.14	0.56
2:E:122:ALA:HB3	2:E:154:PHE:CE2	2.40	0.56
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.35	0.56
3:F:142:PHE:H	3:F:175:THR:HA	1.70	0.56
3:F:167:THR:HG22	3:F:168:ASP:N	2.20	0.56
3:F:183:THR:CG2	3:F:184:LEU:H	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:PHE:CG	1:G:145:TYR:N	2.73	0.56
2:H:34:SER:N	2:H:98:HIS:NE2	2.53	0.56
2:H:178:LEU:O	2:H:180:SER:N	2.38	0.56
3:I:45:GLN:CD	3:I:46:PRO:HD3	2.29	0.56
3:I:159:GLN:CG	3:I:160:ASN:N	2.64	0.56
1:A:239:LYS:HG3	1:A:239:LYS:O	2.06	0.56
2:B:207:ASN:N	2:B:207:ASN:OD1	2.38	0.56
2:E:173:THR:HG21	3:F:178:MET:HG2	1.86	0.56
2:K:110:GLY:N	4:K:304:HOH:O	2.37	0.56
2:K:150:VAL:O	2:K:186:LEU:N	2.28	0.56
1:A:225:GLY:O	1:A:226:ARG:HD3	2.06	0.56
2:B:211:SER:O	2:B:212:ASN:HB3	2.05	0.56
3:C:140:ASN:HA	3:C:176:TYR:HA	1.88	0.56
3:F:151:TRP:CH2	3:F:197:CYS:HB3	2.40	0.56
1:G:92:PRO:HD2	1:G:223:GLN:HG3	1.88	0.56
2:H:98:HIS:HA	3:I:36:ILE:HG21	1.87	0.56
1:J:116:ILE:HG23	1:J:252:ARG:O	2.05	0.56
1:J:260:ASN:C	1:J:260:ASN:OD1	2.49	0.56
2:K:34:SER:OG	2:K:98:HIS:CE1	2.59	0.56
2:K:178:LEU:HD23	2:K:178:LEU:C	2.31	0.56
3:L:45:GLN:CB	3:L:46:PRO:HD2	2.23	0.56
3:L:49:LEU:HD23	3:L:50:LEU:H	1.71	0.56
3:C:9:SER:HA	3:C:105:THR:HG23	1.86	0.56
3:C:162:VAL:HG11	3:C:182:LEU:O	2.06	0.56
2:E:208:HIS:CE1	2:E:210:PRO:HG2	2.39	0.56
2:H:63:VAL:C	2:H:65:GLY:N	2.64	0.56
2:H:152:ASP:N	2:H:184:TYR:O	2.39	0.56
3:I:6:SER:CB	3:I:102:PHE:CE1	2.89	0.56
3:I:195:TYR:N	3:I:210:LYS:HA	2.21	0.56
3:L:50:LEU:O	3:L:58:GLY:N	2.30	0.56
3:L:142:PHE:N	3:L:175:THR:HA	2.20	0.56
3:L:162:VAL:HG21	3:L:181:THR:CA	2.35	0.56
1:A:206:TYR:C	1:A:206:TYR:HD2	2.14	0.56
2:B:162:TRP:CD1	2:B:170:SER:OG	2.56	0.56
2:B:171:VAL:HG21	3:C:176:TYR:CD1	2.37	0.56
3:C:36:ILE:O	3:C:93:GLN:HG3	2.06	0.56
2:E:203:ILE:HD11	2:E:216:ASP:HB2	1.88	0.56
2:H:69:ILE:HG12	2:H:70:SER:H	1.70	0.56
3:I:27:SER:C	3:I:28:VAL:HG22	2.30	0.56
3:I:195:TYR:O	3:I:210:LYS:N	2.39	0.56
3:L:120:ILE:HD13	3:L:197:CYS:CB	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:198:GLU:HB3	3:L:207:PRO:HB3	1.88	0.56
2:B:178:LEU:O	2:B:180:SER:N	2.39	0.56
3:C:64:ARG:NH2	3:C:82:GLU:H	2.03	0.56
3:F:109:ILE:HG22	3:F:110:LYS:N	2.21	0.56
3:F:118:VAL:HB	3:F:208:ILE:HD13	1.87	0.56
3:I:140:ASN:CB	3:I:141:ASN:HD22	2.18	0.56
1:J:235:GLU:HG3	1:J:236:PRO:CD	2.30	0.56
2:B:11:VAL:O	2:B:120:SER:N	2.37	0.56
3:C:128:LEU:HD13	3:C:129:THR:HG23	1.87	0.56
3:I:13:SER:HB3	3:I:110:LYS:HZ1	1.70	0.56
2:B:12:GLN:HG3	2:B:121:SER:HA	1.88	0.56
3:I:118:VAL:HG22	3:I:139:LEU:HG	1.88	0.56
2:B:32:ASP:CB	2:B:50:ILE:O	2.54	0.55
3:C:13:SER:HB3	3:C:110:LYS:HZ2	1.70	0.55
2:E:46:TRP:N	2:E:60:ARG:NH1	2.54	0.55
1:G:84:SER:O	1:G:87:ASN:N	2.37	0.55
1:G:199:VAL:HG13	1:G:248:LEU:HD22	1.87	0.55
2:K:71:ARG:NH1	2:K:73:ASN:OD1	2.39	0.55
3:L:128:LEU:CD1	3:L:129:THR:H	2.18	0.55
1:A:216:ILE:H	1:D:96:ILE:HG23	1.71	0.55
2:B:182:GLY:O	2:B:183:LEU:HB2	2.06	0.55
3:C:150:LYS:O	3:C:198:GLU:HG2	2.07	0.55
1:G:79:ILE:CG2	1:G:80:VAL:N	2.69	0.55
2:B:63:VAL:CG1	2:B:67:SER:H	2.19	0.55
3:C:166:TRP:O	3:C:177:SER:HA	2.07	0.55
1:D:48:ALA:HB3	1:D:51:HIS:CE1	2.42	0.55
1:D:165:TYR:C	1:D:165:TYR:CD2	2.85	0.55
1:G:52:LEU:HD12	1:G:81:GLU:HB3	1.87	0.55
2:H:34:SER:OG	2:H:98:HIS:NE2	2.39	0.55
2:K:207:ASN:HA	2:K:213:THR:O	2.06	0.55
2:K:211:SER:C	2:K:213:THR:N	2.65	0.55
1:A:138:HIS:O	1:A:139:ALA:C	2.49	0.55
1:D:101:LEU:CD2	1:D:105:LEU:HG	2.37	0.55
2:E:18:ARG:HD2	2:E:79:TYR:HB3	1.89	0.55
2:E:186:LEU:HG	2:E:187:SER:N	2.20	0.55
1:J:77:SER:OG	1:J:78:TYR:N	2.37	0.55
2:K:178:LEU:HD23	2:K:179:GLN:CB	2.37	0.55
3:L:12:VAL:HG12	3:L:13:SER:N	2.21	0.55
3:L:102:PHE:CE1	3:L:104:GLY:N	2.73	0.55
3:L:116:PRO:O	3:L:140:ASN:N	2.36	0.55
3:L:172:LYS:HG2	3:L:172:LYS:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:205:THR:O	3:L:207:PRO:HD3	2.06	0.55
3:C:153:ILE:CG1	3:C:154:ASP:H	2.20	0.55
1:D:178:GLY:C	1:D:179:ILE:HD12	2.30	0.55
2:H:97:ARG:O	3:I:36:ILE:CB	2.55	0.55
3:I:79:ASN:HB3	3:I:80:PRO:CD	2.36	0.55
3:I:148:ASN:C	3:I:148:ASN:OD1	2.49	0.55
1:J:200:PHE:O	1:J:201:VAL:HG23	2.07	0.55
2:K:176:ALA:CB	3:L:166:TRP:CE2	2.88	0.55
3:L:102:PHE:CD1	3:L:103:GLY:N	2.74	0.55
1:D:70:LEU:O	1:D:71:SER:OG	2.22	0.55
2:E:129:VAL:HG11	2:E:206:VAL:HG21	1.89	0.55
2:E:173:THR:HG22	3:F:178:MET:HE2	1.88	0.55
2:H:207:ASN:HB3	2:H:214:LYS:CG	2.36	0.55
3:I:95:LYS:O	3:I:99:TYR:CE1	2.56	0.55
3:I:207:PRO:O	3:I:208:ILE:HD12	2.07	0.55
3:I:208:ILE:CG2	3:I:209:VAL:N	2.70	0.55
1:J:84:SER:CB	1:J:88:GLY:H	2.16	0.55
1:A:59:GLY:HA2	1:A:89:THR:HG22	1.88	0.55
2:B:129:VAL:HG22	2:B:150:VAL:HG22	1.89	0.55
3:C:38:TRP:CD2	3:C:90:PHE:O	2.60	0.55
3:C:210:LYS:CG	3:C:211:SER:N	2.65	0.55
3:F:86:THR:HG22	3:F:109:ILE:CD1	2.31	0.55
3:F:193:ASN:O	3:F:211:SER:HB3	2.06	0.55
1:G:54:LYS:HG2	1:G:55:CYS:N	2.22	0.55
1:G:166:ILE:HD13	1:G:166:ILE:N	2.21	0.55
1:G:200:PHE:CE2	1:G:201:VAL:O	2.60	0.55
3:I:42:LYS:HG2	3:I:87:ALA:HB2	1.87	0.55
3:I:81:VAL:O	3:I:82:GLU:HG3	2.07	0.55
1:J:107:SER:HB2	1:J:260:ASN:OD1	2.06	0.55
2:K:32:ASP:CB	2:K:98:HIS:HD1	2.13	0.55
2:K:97:ARG:N	2:K:110:GLY:O	2.35	0.55
2:K:207:ASN:ND2	2:K:214:LYS:HD2	2.22	0.55
2:E:32:ASP:CB	2:E:50:ILE:O	2.55	0.55
3:F:78:ILE:HD12	3:F:107:LEU:HD11	1.89	0.55
1:G:149:ILE:HD11	1:G:252:ARG:HG3	1.87	0.55
2:H:11:VAL:HG11	2:H:85:LEU:CD1	2.36	0.55
2:H:66:ARG:NH2	2:H:85:LEU:HA	2.21	0.55
2:H:146:LEU:HD13	2:H:147:GLY:N	2.13	0.55
2:K:36:ILE:HD11	3:L:38:TRP:CE3	2.42	0.55
3:L:41:GLN:OE1	3:L:47:PRO:HG3	2.07	0.55
2:B:168:THR:O	2:B:169:SER:OG	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:TRP:CZ3	1:D:108:VAL:HG21	2.41	0.55
2:E:124:THR:HA	2:E:154:PHE:O	2.07	0.55
3:F:38:TRP:CZ2	3:F:90:PHE:N	2.75	0.55
3:F:203:THR:O	3:F:205:THR:N	2.39	0.55
2:H:130:PHE:CD2	3:I:127:GLN:HB2	2.42	0.55
2:K:125:LYS:HD2	2:K:126:GLY:H	1.71	0.55
3:L:109:ILE:HG22	3:L:110:LYS:H	1.72	0.55
2:B:196:SER:C	2:B:202:TYR:HE2	2.15	0.55
2:E:173:THR:CG2	3:F:178:MET:SD	2.95	0.55
3:F:209:VAL:HG22	3:F:210:LYS:HB3	1.87	0.55
1:G:203:SER:HB3	1:G:239:LYS:O	2.06	0.55
2:H:202:TYR:HE1	2:H:219:SER:HB2	1.70	0.55
3:I:79:ASN:O	3:I:80:PRO:C	2.48	0.55
1:J:178:GLY:HA2	1:J:228:ASN:O	2.07	0.55
3:L:34:ASN:ND2	3:L:96:GLU:OE2	2.34	0.55
3:L:142:PHE:CD1	3:L:142:PHE:O	2.59	0.55
1:A:121:SER:CB	2:B:58:TYR:HA	2.37	0.54
2:B:122:ALA:O	2:B:154:PHE:HE2	1.90	0.54
1:D:252:ARG:HD2	1:D:253:TYR:N	2.22	0.54
3:F:38:TRP:CZ2	3:F:90:PHE:C	2.85	0.54
3:F:153:ILE:HG22	3:F:195:TYR:CE2	2.42	0.54
1:G:54:LYS:HB2	1:G:66:GLU:O	2.06	0.54
1:G:219:LYS:HG2	1:G:222:ASP:HA	1.89	0.54
3:I:10:LEU:HD23	3:I:11:ALA:N	2.22	0.54
3:I:138:PHE:C	3:I:139:LEU:HD12	2.32	0.54
1:J:54:LYS:HB3	1:J:54:LYS:NZ	2.06	0.54
2:K:34:SER:HA	2:K:49:GLY:HA2	1.89	0.54
2:K:48:SER:OG	2:K:59:TYR:HD1	1.90	0.54
3:L:38:TRP:HE1	3:L:90:PHE:CB	2.19	0.54
3:C:24:ALA:HB1	3:C:26:GLU:O	2.07	0.54
3:C:35:PHE:CD1	3:C:36:ILE:HA	2.43	0.54
3:C:128:LEU:CD1	3:C:129:THR:HG23	2.37	0.54
3:F:42:LYS:HD2	3:F:87:ALA:HB2	1.89	0.54
1:G:132:VAL:HG23	1:G:132:VAL:O	2.07	0.54
1:G:188:GLN:NE2	1:G:197:ALA:CB	2.70	0.54
2:H:75:ARG:O	2:H:76:LYS:HB2	2.07	0.54
2:H:78:LEU:HD23	2:H:78:LEU:H	1.73	0.54
3:I:38:TRP:HB3	3:I:47:PRO:HB2	1.86	0.54
3:L:108:GLU:CG	3:L:109:ILE:H	2.20	0.54
3:L:109:ILE:CG2	3:L:110:LYS:N	2.70	0.54
1:G:127:ASP:N	1:G:154:LYS:HB2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:145:LYS:HE2	3:I:169:GLN:HG2	1.89	0.54
3:I:209:VAL:HG22	3:I:210:LYS:HG2	1.88	0.54
2:K:174:PHE:CD2	3:L:166:TRP:HE3	2.25	0.54
3:L:208:ILE:C	3:L:209:VAL:CG1	2.78	0.54
2:B:54:SER:CB	2:B:56:ARG:HH11	2.21	0.54
1:D:63:GLY:O	1:D:146:LYS:N	2.25	0.54
2:E:46:TRP:N	2:E:60:ARG:HH12	2.05	0.54
2:E:196:SER:O	2:E:200:GLN:N	2.40	0.54
3:F:141:ASN:CB	3:F:175:THR:HG22	2.36	0.54
2:H:54:SER:CB	2:H:56:ARG:HE	2.16	0.54
2:H:164:SER:HA	2:H:167:LEU:HB2	1.89	0.54
2:K:38:GLN:HG3	2:K:43:GLY:CA	2.37	0.54
3:L:28:VAL:HG23	3:L:72:THR:H	1.72	0.54
3:L:143:TYR:CD2	3:L:144:PRO:HD3	2.41	0.54
3:L:209:VAL:HG23	3:L:210:LYS:CB	2.37	0.54
1:D:228:ASN:HB3	1:D:230:TYR:HE1	1.73	0.54
1:G:182:PRO:HD2	1:G:214:ILE:HG13	1.90	0.54
2:H:72:ASP:HB3	2:H:79:TYR:OH	2.08	0.54
3:I:86:THR:HG22	3:I:109:ILE:HD13	1.90	0.54
2:K:18:ARG:HA	2:K:80:LEU:O	2.07	0.54
2:B:32:ASP:OD2	2:B:32:ASP:N	2.25	0.54
3:C:111:ARG:O	3:C:112:ALA:HB3	2.07	0.54
1:D:48:ALA:HB1	1:D:80:VAL:CG2	2.37	0.54
1:G:119:LYS:HZ3	1:G:129:ASN:HB3	1.67	0.54
3:I:20:ILE:CG2	3:I:105:THR:HG21	2.38	0.54
2:B:20:SER:O	2:B:35:TRP:HH2	1.90	0.54
3:C:51:ILE:HG12	3:C:67:GLY:N	2.23	0.54
2:E:82:MET:HE1	2:E:117:VAL:HG11	1.89	0.54
2:E:144:ALA:N	2:E:192:VAL:O	2.39	0.54
2:E:205:ASN:HD22	2:E:214:LYS:CE	2.21	0.54
3:F:138:PHE:C	3:F:139:LEU:HD12	2.33	0.54
2:H:69:ILE:CG1	2:H:70:SER:N	2.71	0.54
1:J:121:SER:N	2:K:64:LYS:HE3	2.23	0.54
3:L:69:GLY:HA2	3:L:73:ASP:O	2.08	0.54
1:A:252:ARG:HD2	1:A:253:TYR:N	2.23	0.54
2:B:10:VAL:HG13	2:B:155:PRO:HG3	1.88	0.54
3:F:166:TRP:O	3:F:177:SER:CA	2.55	0.54
1:G:101:LEU:HD22	1:G:105:LEU:HD11	1.90	0.54
2:H:32:ASP:HB2	2:H:98:HIS:ND1	2.22	0.54
3:I:27:SER:O	3:I:28:VAL:CG2	2.54	0.54
3:I:38:TRP:CG	3:I:47:PRO:HB3	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:37:ARG:HB3	2:K:93:TYR:CD2	2.43	0.54
3:L:38:TRP:CD1	3:L:38:TRP:C	2.84	0.54
4:B:307:HOH:O	3:L:172:LYS:HD2	2.07	0.54
3:F:84:GLU:O	3:F:86:THR:N	2.41	0.54
2:H:72:ASP:HB3	2:H:79:TYR:HE2	1.68	0.54
2:K:201:THR:HG22	2:K:218:LYS:HD3	1.89	0.54
1:A:216:ILE:O	1:D:96:ILE:HA	2.08	0.54
2:B:3:LYS:O	2:B:4:LEU:HD12	2.07	0.54
3:C:8:ALA:HB3	4:C:309:HOH:O	2.06	0.54
2:E:143:THR:HG23	2:E:191:THR:HG23	1.90	0.54
3:I:109:ILE:CG2	3:I:110:LYS:N	2.70	0.54
3:I:167:THR:HG23	3:I:177:SER:HB2	1.90	0.54
2:K:98:HIS:HD2	3:L:36:ILE:HG21	1.73	0.54
3:L:109:ILE:CG2	3:L:110:LYS:H	2.21	0.54
2:B:78:LEU:HD12	2:B:78:LEU:O	2.08	0.53
2:B:177:VAL:HG12	2:B:183:LEU:H	1.73	0.53
3:F:152:LYS:N	3:F:196:THR:O	2.41	0.53
3:F:164:ASN:HB3	3:F:180:SER:O	2.08	0.53
3:I:143:TYR:CZ	3:I:144:PRO:HB3	2.43	0.53
3:I:170:ASP:OD2	3:I:172:LYS:N	2.41	0.53
1:J:98:TYR:O	1:J:98:TYR:CG	2.60	0.53
3:L:36:ILE:HD13	3:L:36:ILE:C	2.33	0.53
3:L:209:VAL:HG23	3:L:210:LYS:HG3	1.90	0.53
2:B:21:CYS:O	2:B:77:THR:HA	2.08	0.53
2:B:43:GLY:O	2:B:44:LEU:HG	2.07	0.53
2:B:83:ASN:OD1	2:B:84:SER:N	2.41	0.53
3:C:38:TRP:CE2	3:C:39:PHE:CD1	2.97	0.53
3:C:83:ALA:O	3:C:171:SER:O	2.26	0.53
3:C:135:VAL:HG12	3:C:151:TRP:HH2	1.74	0.53
1:D:94:ASP:N	1:D:94:ASP:OD1	2.38	0.53
2:H:218:LYS:HB2	2:H:218:LYS:NZ	2.23	0.53
3:I:89:TYR:O	3:I:102:PHE:CE2	2.61	0.53
3:I:140:ASN:CB	3:I:141:ASN:ND2	2.72	0.53
1:J:149:ILE:HB	1:J:250:VAL:CG2	2.38	0.53
3:L:27:SER:O	3:L:28:VAL:HG13	2.07	0.53
3:C:108:GLU:HG2	3:C:169:GLN:NE2	2.24	0.53
1:D:133:THR:CB	1:D:150:TRP:HZ3	2.21	0.53
3:F:57:LYS:HD3	3:F:61:VAL:O	2.07	0.53
3:F:172:LYS:N	3:F:172:LYS:HD3	2.23	0.53
1:G:83:SER:O	1:G:85:SER:N	2.42	0.53
3:I:92:GLN:HG2	3:I:101:THR:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:144:PRO:O	3:I:201:HIS:CE1	2.61	0.53
3:I:147:ILE:HG23	3:I:148:ASN:N	2.22	0.53
1:J:64:ASN:OD1	1:J:65:PRO:HD2	2.08	0.53
2:K:99:SER:HB3	3:L:35:PHE:O	2.09	0.53
3:L:151:TRP:HZ2	3:L:180:SER:HA	1.71	0.53
2:B:78:LEU:HD12	2:B:78:LEU:C	2.33	0.53
2:B:97:ARG:O	3:C:36:ILE:HG12	2.09	0.53
2:H:162:TRP:CD2	2:H:190:VAL:HG11	2.43	0.53
2:H:174:PHE:CD2	3:I:166:TRP:HE3	2.26	0.53
1:J:48:ALA:CB	1:J:78:TYR:HE1	2.20	0.53
1:J:115:GLU:OE1	3:L:99:TYR:OH	2.22	0.53
1:J:149:ILE:O	1:J:250:VAL:HG22	2.09	0.53
1:J:201:VAL:CG1	1:J:202:GLY:N	2.54	0.53
2:K:90:THR:HG23	2:K:117:VAL:O	2.09	0.53
3:L:10:LEU:O	3:L:107:LEU:HA	2.08	0.53
1:A:104:GLN:O	1:A:104:GLN:HG3	2.04	0.53
3:F:9:SER:CA	3:F:106:LYS:HB2	2.39	0.53
3:F:26:GLU:OE2	3:F:27:SER:HB2	2.08	0.53
3:F:114:ALA:HB1	3:F:202:LYS:O	2.08	0.53
3:I:24:ALA:HB3	3:I:72:THR:OG1	2.08	0.53
3:I:102:PHE:HE1	3:I:104:GLY:C	2.17	0.53
3:L:81:VAL:HG12	3:L:82:GLU:N	2.24	0.53
3:L:118:VAL:O	3:L:208:ILE:HD12	2.08	0.53
3:L:161:GLY:O	3:L:162:VAL:HG12	2.09	0.53
2:E:4:LEU:HB2	2:E:112:GLY:CA	2.39	0.53
2:E:28:GLY:H	2:E:76:LYS:HZ3	1.57	0.53
2:E:162:TRP:HB3	2:E:166:ALA:HB1	1.90	0.53
3:F:36:ILE:H	3:F:93:GLN:HE22	1.57	0.53
3:F:134:SER:HB2	3:F:181:THR:O	2.09	0.53
3:F:159:GLN:NE2	2:H:26:PHE:HE2	2.07	0.53
1:G:169:LYS:HE2	1:G:256:ALA:CB	2.39	0.53
1:J:122:SER:C	1:J:124:PRO:HD3	2.33	0.53
3:C:38:TRP:CZ3	3:C:89:TYR:HD1	2.24	0.53
3:C:81:VAL:HG13	3:C:85:ASP:OD2	2.09	0.53
1:D:178:GLY:O	1:D:179:ILE:HD12	2.09	0.53
3:F:173:ASP:CG	3:F:175:THR:CG2	2.79	0.53
1:G:57:ILE:HD13	1:G:102:ARG:HB2	1.89	0.53
2:H:53:GLY:O	2:H:54:SER:HB2	2.09	0.53
2:H:176:ALA:CB	3:I:166:TRP:CZ2	2.91	0.53
2:K:100:TRP:NE1	3:L:34:ASN:HA	2.22	0.53
2:B:161:SER:HG	2:B:205:ASN:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:ARG:HA	3:C:79:ASN:O	2.08	0.53
2:E:13:PRO:CD	2:E:121:SER:HB2	2.38	0.53
3:F:170:ASP:CG	3:F:171:SER:N	2.67	0.53
2:H:2:VAL:HG13	2:H:24:SER:O	2.08	0.53
3:L:17:ARG:HA	3:L:79:ASN:HA	1.90	0.53
1:A:259:ARG:HB3	1:A:259:ARG:HH11	1.70	0.53
2:B:98:HIS:H	2:B:98:HIS:CD2	2.27	0.53
2:B:203:ILE:HD12	2:B:218:LYS:N	2.23	0.53
3:C:38:TRP:CD1	3:C:38:TRP:H	2.27	0.53
1:D:231:TRP:HZ3	1:D:233:LEU:CD2	2.22	0.53
2:E:12:GLN:HG3	2:E:121:SER:OG	2.09	0.53
2:E:161:SER:HA	2:E:167:LEU:HD11	1.90	0.53
2:H:163:ASN:C	2:H:165:GLY:H	2.16	0.53
2:H:186:LEU:C	2:H:186:LEU:CD1	2.82	0.53
3:I:202:LYS:O	3:I:202:LYS:HG2	2.09	0.53
1:J:115:GLU:HG3	1:J:115:GLU:O	2.09	0.53
1:J:203:SER:OG	1:J:204:SER:N	2.39	0.53
2:K:63:VAL:C	2:K:65:GLY:N	2.54	0.53
3:L:205:THR:O	3:L:205:THR:HG23	2.09	0.53
1:A:219:LYS:HG2	1:A:222:ASP:C	2.34	0.53
2:B:86:ARG:H	2:B:89:ASP:HB2	1.74	0.53
3:C:7:PRO:HG3	3:C:21:THR:OG1	2.08	0.53
3:C:93:GLN:O	3:C:94:THR:C	2.46	0.53
2:E:82:MET:HE1	2:E:117:VAL:CG2	2.35	0.53
2:E:208:HIS:CD2	2:E:210:PRO:HD2	2.44	0.53
2:E:209:LYS:N	2:E:210:PRO:HD2	2.23	0.53
3:F:8:ALA:CB	3:F:105:THR:OG1	2.56	0.53
1:G:119:LYS:HZ1	1:G:129:ASN:CB	2.22	0.53
1:G:221:ARG:O	1:G:223:GLN:HG2	2.08	0.53
3:L:170:ASP:HB3	3:L:175:THR:OG1	2.09	0.53
2:B:51:LEU:HD12	2:B:56:ARG:N	2.21	0.52
2:E:46:TRP:C	2:E:60:ARG:NH1	2.67	0.52
3:I:92:GLN:O	3:I:93:GLN:C	2.52	0.52
2:K:174:PHE:CD1	2:K:175:PRO:HD2	2.43	0.52
1:A:49:PRO:HD3	1:A:77:SER:OG	2.09	0.52
2:H:51:LEU:HD11	2:H:56:ARG:HD3	1.90	0.52
1:J:76:TRP:NE1	1:J:105:LEU:O	2.42	0.52
2:K:72:ASP:HB2	2:K:79:TYR:HE2	1.74	0.52
2:K:94:TYR:HE1	3:L:46:PRO:HB3	1.75	0.52
3:L:193:ASN:O	3:L:211:SER:OG	2.19	0.52
2:B:50:ILE:HG23	2:B:69:ILE:HG12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:THR:HB	3:C:178:MET:CE	2.38	0.52
3:C:9:SER:C	3:C:106:LYS:HG2	2.34	0.52
2:E:189:VAL:HG12	3:F:138:PHE:CZ	2.45	0.52
3:F:8:ALA:O	3:F:9:SER:HB2	2.09	0.52
3:F:9:SER:H	3:F:105:THR:CG2	2.09	0.52
1:G:118:PRO:HG2	2:H:58:TYR:CZ	2.45	0.52
3:I:111:ARG:HH21	3:I:173:ASP:HA	1.74	0.52
3:L:1:ILE:O	3:L:1:ILE:HG22	2.10	0.52
3:L:127:GLN:HG2	3:L:132:GLY:O	2.08	0.52
3:L:163:LEU:HD12	3:L:163:LEU:O	2.09	0.52
1:A:201:VAL:HG13	1:A:202:GLY:H	1.68	0.52
2:E:213:THR:O	2:E:213:THR:HG22	2.07	0.52
1:G:172:GLU:OE2	1:G:258:GLU:HA	2.09	0.52
2:H:52:GLY:O	2:H:53:GLY:C	2.52	0.52
3:I:140:ASN:HB3	3:I:141:ASN:ND2	2.24	0.52
3:I:167:THR:HG22	3:I:168:ASP:N	2.24	0.52
1:J:114:PHE:HA	3:L:96:GLU:CD	2.35	0.52
2:B:35:TRP:CD1	2:B:80:LEU:HB2	2.44	0.52
3:F:3:MET:HG3	3:F:5:GLN:NE2	2.20	0.52
3:F:105:THR:HG22	3:F:106:LYS:N	2.24	0.52
3:F:110:LYS:HG2	3:F:111:ARG:N	2.24	0.52
2:H:34:SER:HG	2:H:49:GLY:HA3	1.74	0.52
2:H:90:THR:HG23	2:H:117:VAL:O	2.09	0.52
2:H:125:LYS:HD2	2:H:126:GLY:N	2.24	0.52
2:H:129:VAL:O	2:H:217:LYS:HE3	2.10	0.52
2:H:132:LEU:HB3	3:I:121:PHE:CG	2.45	0.52
3:I:19:THR:CG2	3:I:77:THR:HG22	2.39	0.52
1:J:120:THR:O	1:J:121:SER:C	2.51	0.52
2:K:153:TYR:N	2:K:183:LEU:HD12	2.25	0.52
3:L:26:GLU:O	3:L:27:SER:HB2	2.09	0.52
2:B:51:LEU:CG	2:B:56:ARG:HG2	2.39	0.52
3:C:38:TRP:CE2	3:C:39:PHE:CG	2.97	0.52
3:C:116:PRO:HA	3:C:142:PHE:HB3	1.92	0.52
2:E:32:ASP:OD2	2:E:98:HIS:CE1	2.62	0.52
3:F:27:SER:O	3:F:28:VAL:CG2	2.57	0.52
1:G:182:PRO:HG3	1:G:192:TYR:HE1	1.75	0.52
2:H:2:VAL:HA	2:H:24:SER:C	2.34	0.52
2:K:97:ARG:N	3:L:36:ILE:HG13	2.25	0.52
3:L:138:PHE:O	3:L:139:LEU:HD12	2.09	0.52
1:A:91:TYR:HD1	1:A:227:MET:CB	2.11	0.52
2:B:196:SER:HB3	2:B:202:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:TYR:OH	1:D:180:HIS:CD2	2.63	0.52
1:D:227:MET:HG2	1:D:229:TYR:CE2	2.45	0.52
2:E:2:VAL:C	2:E:3:LYS:HE2	2.34	0.52
1:G:202:GLY:O	1:G:206:TYR:O	2.27	0.52
3:I:97:VAL:HG13	3:I:98:PRO:HD2	1.91	0.52
3:I:197:CYS:O	3:I:208:ILE:N	2.35	0.52
1:J:182:PRO:HG2	1:J:188:GLN:CB	2.39	0.52
3:L:139:LEU:HD21	3:L:199:ALA:HB1	1.91	0.52
1:A:56:ASN:HA	1:A:81:GLU:HG2	1.92	0.52
3:C:9:SER:O	3:C:10:LEU:HD23	2.09	0.52
1:D:90:CYS:SG	1:D:145:TYR:CZ	3.03	0.52
1:D:116:ILE:HG23	1:D:117:PHE:N	2.25	0.52
2:E:162:TRP:HB3	2:E:166:ALA:HB3	1.91	0.52
3:F:125:SER:O	3:F:128:LEU:HD23	2.10	0.52
3:I:139:LEU:HD21	3:I:199:ALA:HB2	1.92	0.52
2:K:17:LEU:HB3	2:K:82:MET:CG	2.40	0.52
2:K:21:CYS:O	2:K:77:THR:HB	2.10	0.52
2:K:180:SER:OG	2:K:183:LEU:N	2.42	0.52
3:L:168:ASP:OD2	3:L:176:TYR:HD2	1.93	0.52
3:F:86:THR:HA	3:F:107:LEU:CD2	2.40	0.52
3:F:111:ARG:HB2	3:F:143:TYR:CD1	2.45	0.52
1:G:248:LEU:HD12	1:G:249:VAL:N	2.25	0.52
2:H:17:LEU:HB3	2:H:82:MET:CE	2.40	0.52
1:J:76:TRP:CD1	1:J:106:SER:O	2.63	0.52
1:J:92:PRO:CG	1:J:223:GLN:HB2	2.39	0.52
1:J:201:VAL:CG1	1:J:240:ILE:HD11	2.39	0.52
2:K:66:ARG:HH22	2:K:89:ASP:CG	2.18	0.52
2:B:4:LEU:HB2	2:B:112:GLY:HA2	1.91	0.52
2:B:134:PRO:HB3	3:C:121:PHE:HE1	1.74	0.52
2:B:197:LEU:C	2:B:199:THR:N	2.66	0.52
3:C:38:TRP:HE1	3:C:91:CYS:HA	1.74	0.52
1:D:77:SER:O	1:D:106:SER:O	2.28	0.52
2:E:152:ASP:CB	2:E:183:LEU:HD23	2.40	0.52
1:G:127:ASP:HB2	1:G:153:LYS:O	2.10	0.52
1:G:184:THR:C	1:G:214:ILE:HG21	2.35	0.52
1:G:232:THR:HG23	1:G:233:LEU:N	2.24	0.52
2:H:174:PHE:HD2	3:I:166:TRP:HE3	1.58	0.52
2:K:100:TRP:HD1	3:L:34:ASN:N	2.08	0.52
2:K:111:TRP:HZ2	3:L:38:TRP:H	1.58	0.52
3:L:43:PRO:HD3	3:L:87:ALA:HA	1.91	0.52
1:A:133:THR:CG2	1:A:150:TRP:HZ3	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ASN:HB3	1:A:230:TYR:CE1	2.45	0.51
3:C:39:PHE:CB	3:C:50:LEU:CB	2.83	0.51
3:C:83:ALA:HB1	3:C:171:SER:O	2.10	0.51
2:E:203:ILE:HD12	2:E:217:LYS:C	2.34	0.51
1:G:188:GLN:NE2	1:G:197:ALA:HB2	2.25	0.51
3:I:196:THR:HG23	3:I:208:ILE:O	2.09	0.51
3:L:161:GLY:O	3:L:162:VAL:CG1	2.58	0.51
1:A:129:ASN:HB2	4:A:604:HOH:O	2.09	0.51
1:D:165:TYR:HE2	1:D:167:ASN:HB2	1.74	0.51
3:F:110:LYS:HG2	3:F:111:ARG:H	1.74	0.51
3:F:153:ILE:CG1	3:F:154:ASP:H	2.15	0.51
3:F:183:THR:CG2	3:F:184:LEU:N	2.70	0.51
1:G:118:PRO:O	1:G:122:SER:OG	2.28	0.51
1:G:146:LYS:HG2	1:G:147:ASN:OD1	2.10	0.51
1:J:118:PRO:O	1:J:122:SER:OG	2.23	0.51
1:J:181:HIS:O	1:J:225:GLY:HA3	2.10	0.51
2:K:6:GLU:HB3	2:K:115:THR:HB	1.92	0.51
2:K:63:VAL:HG13	2:K:67:SER:H	1.74	0.51
1:A:175:VAL:C	1:A:176:LEU:HD12	2.34	0.51
2:B:44:LEU:N	4:B:302:HOH:O	2.42	0.51
2:B:50:ILE:HB	2:B:56:ARG:O	2.11	0.51
3:C:161:GLY:C	3:C:162:VAL:HG22	2.36	0.51
3:F:39:PHE:HB2	3:F:50:LEU:HB2	1.93	0.51
2:K:100:TRP:CD1	3:L:34:ASN:N	2.78	0.51
3:C:48:LYS:HG2	3:C:49:LEU:H	1.75	0.51
3:C:50:LEU:HD11	3:C:89:TYR:CE1	2.28	0.51
3:C:83:ALA:O	3:C:86:THR:CG2	2.59	0.51
2:K:11:VAL:HG11	2:K:85:LEU:HD13	1.92	0.51
1:A:51:HIS:ND1	1:A:80:VAL:HG11	2.26	0.51
1:A:54:LYS:HD2	1:A:69:SER:CB	2.40	0.51
2:E:180:SER:C	2:E:182:GLY:N	2.68	0.51
3:F:151:TRP:N	4:F:305:HOH:O	2.38	0.51
3:F:164:ASN:HB3	3:F:180:SER:H	1.75	0.51
3:F:172:LYS:N	3:F:172:LYS:CD	2.73	0.51
1:G:163:LYS:HZ1	2:H:56:ARG:HG2	1.76	0.51
2:K:97:ARG:H	3:L:36:ILE:HG13	1.76	0.51
3:L:203:THR:O	3:L:203:THR:CG2	2.57	0.51
3:C:141:ASN:HA	3:C:175:THR:CG2	2.36	0.51
3:F:42:LYS:HD3	3:F:84:GLU:OE2	2.10	0.51
1:G:134:ALA:HA	1:G:142:LYS:HB3	1.92	0.51
2:H:147:GLY:O	2:H:148:CYS:SG	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:LEU:C	2:H:180:SER:N	2.69	0.51
3:I:41:GLN:HB2	3:I:47:PRO:HA	1.93	0.51
1:A:96:ILE:HA	1:D:216:ILE:O	2.11	0.51
2:B:85:LEU:HB3	2:B:119:VAL:HG13	1.93	0.51
3:C:37:ASN:OD1	3:C:95:LYS:NZ	2.30	0.51
2:E:94:TYR:CE1	3:F:46:PRO:HB3	2.45	0.51
3:F:13:SER:HB2	3:F:110:LYS:NZ	2.26	0.51
2:H:93:TYR:CE1	2:H:117:VAL:CG1	2.92	0.51
2:H:164:SER:HA	2:H:167:LEU:HD12	1.92	0.51
3:I:11:ALA:HA	3:I:108:GLU:O	2.09	0.51
1:J:44:LEU:HD11	1:J:47:VAL:HG23	1.92	0.51
2:K:171:VAL:HB	2:K:189:VAL:CG2	2.38	0.51
3:L:92:GLN:HG3	3:L:100:GLY:O	2.11	0.51
3:L:92:GLN:O	3:L:93:GLN:C	2.54	0.51
3:L:192:HIS:HB3	3:L:194:SER:H	1.76	0.51
3:L:193:ASN:OD1	3:L:194:SER:OG	2.27	0.51
1:A:232:THR:HG21	1:A:240:ILE:HD12	1.93	0.51
1:A:259:ARG:CZ	1:A:259:ARG:CB	2.89	0.51
2:B:98:HIS:CD2	2:B:98:HIS:N	2.78	0.51
3:C:9:SER:CB	3:C:106:LYS:HB3	2.07	0.51
3:C:29:SER:HB3	4:C:310:HOH:O	2.10	0.51
1:D:173:VAL:O	1:D:233:LEU:HA	2.11	0.51
2:E:208:HIS:NE2	2:E:210:PRO:HG2	2.26	0.51
3:F:35:PHE:CE1	3:F:49:LEU:HD11	2.46	0.51
2:H:10:VAL:HG13	2:H:118:THR:O	2.11	0.51
3:I:9:SER:HB2	3:I:106:LYS:NZ	2.25	0.51
3:I:16:GLN:O	3:I:81:VAL:HG23	2.10	0.51
1:J:153:LYS:CB	1:J:158:TYR:HB2	2.41	0.51
1:J:166:ILE:HD13	1:J:166:ILE:N	2.26	0.51
3:L:1:ILE:O	3:L:2:GLN:HB3	2.10	0.51
3:L:17:ARG:HB2	3:L:79:ASN:OD1	2.11	0.51
3:C:57:LYS:HZ1	3:C:65:PHE:HB2	1.76	0.51
1:D:211:LYS:HB2	1:D:211:LYS:NZ	2.26	0.51
2:E:47:VAL:O	2:E:48:SER:HB3	2.11	0.51
2:E:50:ILE:HG23	2:E:69:ILE:HD13	1.92	0.51
3:F:38:TRP:O	3:F:38:TRP:HE3	1.88	0.51
3:F:121:PHE:CD2	3:F:121:PHE:N	2.79	0.51
2:H:72:ASP:HB3	2:H:79:TYR:CZ	2.46	0.51
2:H:125:LYS:HE3	2:H:126:GLY:O	2.11	0.51
3:I:26:GLU:O	3:I:27:SER:HB2	2.10	0.51
1:J:144:PHE:CZ	1:J:145:TYR:HD2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ALA:CB	1:A:78:TYR:CZ	2.93	0.51
1:A:120:THR:HG1	1:A:121:SER:N	2.08	0.51
1:D:175:VAL:O	1:D:231:TRP:HA	2.11	0.51
3:F:149:VAL:HG22	3:F:149:VAL:O	2.11	0.51
2:H:171:VAL:C	2:H:172:HIS:ND1	2.67	0.51
3:I:164:ASN:CG	3:I:180:SER:O	2.54	0.51
2:K:20:SER:OG	2:K:21:CYS:N	2.42	0.51
1:A:122:SER:C	1:A:124:PRO:HD3	2.36	0.50
1:A:184:THR:O	1:A:187:ASP:N	2.45	0.50
2:B:38:GLN:OE1	3:C:41:GLN:NE2	2.44	0.50
2:B:93:TYR:O	2:B:114:GLY:HA2	2.11	0.50
2:B:215:VAL:C	2:B:216:ASP:OD1	2.55	0.50
3:C:13:SER:HB3	3:C:110:LYS:NZ	2.25	0.50
3:C:154:ASP:OD1	3:C:191:ARG:NH1	2.45	0.50
1:D:91:TYR:HD1	1:D:227:MET:CB	2.08	0.50
2:E:173:THR:HG22	3:F:178:MET:CE	2.40	0.50
1:G:144:PHE:CZ	1:G:145:TYR:HD2	2.28	0.50
1:G:199:VAL:HA	1:G:243:GLU:O	2.11	0.50
2:H:32:ASP:HB2	2:H:98:HIS:HD1	1.76	0.50
1:J:53:GLY:HA2	1:J:82:THR:HG23	1.93	0.50
1:J:62:LEU:HD22	1:J:148:LEU:HD11	1.92	0.50
1:J:100:GLU:HG2	1:J:231:TRP:CZ2	2.46	0.50
2:K:145:ALA:HA	2:K:191:THR:HA	1.93	0.50
2:K:162:TRP:CE2	2:K:204:CYS:HB3	2.45	0.50
2:K:207:ASN:HA	2:K:214:LYS:HA	1.92	0.50
3:L:102:PHE:HE1	3:L:104:GLY:HA2	1.75	0.50
2:K:97:ARG:O	2:K:97:ARG:NE	2.45	0.50
3:L:141:ASN:H	3:L:175:THR:HB	1.75	0.50
2:B:178:LEU:C	2:B:180:SER:H	2.20	0.50
3:C:175:THR:HB	3:C:176:TYR:CD2	2.47	0.50
3:F:189:TYR:O	3:F:190:GLU:CB	2.59	0.50
2:H:27:THR:C	2:H:29:SER:N	2.64	0.50
2:H:27:THR:HG23	2:H:30:ASP:HB3	1.92	0.50
2:H:34:SER:OG	2:H:49:GLY:CA	2.55	0.50
2:K:178:LEU:C	2:K:180:SER:N	2.65	0.50
3:L:102:PHE:CE1	3:L:104:GLY:HA2	2.45	0.50
1:A:64:ASN:CG	1:A:66:GLU:HG2	2.37	0.50
2:B:4:LEU:HD22	2:B:112:GLY:N	2.26	0.50
2:B:51:LEU:HD13	2:B:51:LEU:C	2.36	0.50
2:B:69:ILE:HD11	2:B:78:LEU:HD22	1.94	0.50
2:B:98:HIS:H	2:B:98:HIS:HD2	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:GLU:CG	3:C:109:ILE:H	2.23	0.50
1:D:54:LYS:HZ3	1:D:54:LYS:H	1.59	0.50
3:F:13:SER:CB	3:F:110:LYS:HZ2	2.24	0.50
3:F:159:GLN:NE2	2:H:26:PHE:CE2	2.80	0.50
3:F:172:LYS:O	3:F:173:ASP:HB3	2.11	0.50
2:H:60:ARG:HH22	3:I:99:TYR:C	2.18	0.50
3:I:89:TYR:O	3:I:102:PHE:CZ	2.64	0.50
2:K:50:ILE:HD11	2:K:71:ARG:CG	2.41	0.50
2:K:92:VAL:HG12	2:K:93:TYR:N	2.26	0.50
2:K:218:LYS:HB2	2:K:218:LYS:NZ	2.27	0.50
3:L:40:GLN:HA	3:L:88:ASN:O	2.11	0.50
3:L:161:GLY:C	3:L:162:VAL:HG12	2.36	0.50
3:L:163:LEU:C	3:L:163:LEU:CD1	2.77	0.50
2:B:98:HIS:CB	3:C:36:ILE:HG13	2.40	0.50
2:B:200:GLN:HB3	2:B:202:TYR:CZ	2.46	0.50
3:C:3:MET:O	3:C:25:SER:N	2.44	0.50
1:D:132:VAL:HA	1:D:144:PHE:HB2	1.93	0.50
3:F:109:ILE:CG2	3:F:110:LYS:N	2.74	0.50
2:H:51:LEU:HD11	2:H:56:ARG:HD2	1.92	0.50
3:I:13:SER:HB3	3:I:110:LYS:NZ	2.27	0.50
1:J:204:SER:OG	1:J:205:ARG:N	2.44	0.50
2:K:125:LYS:HG3	2:K:126:GLY:O	2.12	0.50
3:L:37:ASN:HD21	3:L:93:GLN:H	1.59	0.50
2:B:50:ILE:HG23	2:B:69:ILE:CG1	2.42	0.50
2:B:78:LEU:C	2:B:78:LEU:CD1	2.85	0.50
3:C:13:SER:OG	3:C:110:LYS:HD3	2.11	0.50
3:C:64:ARG:HH21	3:C:82:GLU:H	1.58	0.50
3:C:69:GLY:HA3	3:C:74:PHE:HA	1.93	0.50
3:C:83:ALA:O	3:C:86:THR:HG21	2.12	0.50
1:D:201:VAL:HG23	1:D:208:LYS:H	1.77	0.50
2:E:13:PRO:HD3	2:E:121:SER:HB2	1.94	0.50
3:F:52:TYR:CE2	3:F:58:GLY:HA2	2.47	0.50
3:F:162:VAL:HB	3:F:182:LEU:HG	1.94	0.50
3:F:173:ASP:OD2	3:F:175:THR:CG2	2.59	0.50
1:G:101:LEU:HG	1:G:231:TRP:CD2	2.46	0.50
1:G:167:ASN:C	1:G:167:ASN:OD1	2.55	0.50
2:H:18:ARG:HA	2:H:80:LEU:O	2.12	0.50
3:I:53:THR:HG22	3:I:53:THR:O	2.12	0.50
3:I:91:CYS:N	3:I:102:PHE:HD2	2.07	0.50
3:I:111:ARG:O	3:I:112:ALA:HB3	2.12	0.50
2:K:127:PRO:HB2	2:K:150:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:178:LEU:HA	3:L:163:LEU:CD2	2.42	0.50
2:K:182:GLY:O	2:K:183:LEU:HD22	2.12	0.50
1:A:150:TRP:CD1	1:A:150:TRP:C	2.90	0.50
1:A:167:ASN:OD1	1:A:167:ASN:C	2.54	0.50
2:B:167:LEU:HA	2:B:170:SER:HB2	1.93	0.50
2:B:208:HIS:CD2	2:B:210:PRO:HD2	2.47	0.50
3:C:50:LEU:CD1	3:C:89:TYR:HE1	2.16	0.50
3:C:162:VAL:O	3:C:164:ASN:CG	2.55	0.50
1:D:49:PRO:HD2	1:D:78:TYR:O	2.11	0.50
3:F:38:TRP:CE2	3:F:90:PHE:O	2.65	0.50
2:H:19:LEU:HD13	2:H:80:LEU:HD23	1.93	0.50
2:H:66:ARG:HH21	2:H:85:LEU:HA	1.75	0.50
2:H:95:CYS:O	2:H:112:GLY:N	2.39	0.50
3:I:54:ALA:O	3:I:67:GLY:HA3	2.12	0.50
3:I:120:ILE:CD1	3:I:137:CYS:HB2	2.42	0.50
1:J:54:LYS:HB2	1:J:55:CYS:SG	2.52	0.50
1:J:186:ALA:O	1:J:189:GLN:HG2	2.11	0.50
2:K:60:ARG:O	2:K:64:LYS:NZ	2.44	0.50
3:L:142:PHE:HD1	3:L:144:PRO:O	1.93	0.50
3:L:143:TYR:HD2	3:L:144:PRO:HD3	1.76	0.50
2:B:63:VAL:HG12	2:B:64:LYS:N	2.26	0.50
2:B:174:PHE:O	3:C:166:TRP:CD1	2.64	0.50
3:C:92:GLN:CG	3:C:93:GLN:N	2.74	0.50
3:F:138:PHE:CD1	3:F:178:MET:HG3	2.47	0.50
1:G:198:TYR:HB2	1:G:210:PHE:O	2.12	0.50
1:G:201:VAL:HG11	1:G:206:TYR:CD2	2.47	0.50
2:H:150:VAL:HG21	2:H:206:VAL:HG11	1.94	0.50
2:K:21:CYS:HB2	2:K:35:TRP:CZ2	2.46	0.50
2:K:162:TRP:HA	2:K:203:ILE:O	2.11	0.50
3:L:28:VAL:CG2	3:L:74:PHE:CE2	2.94	0.50
3:L:78:ILE:HD11	3:L:80:PRO:O	2.12	0.50
1:A:101:LEU:O	1:A:104:GLN:N	2.44	0.50
2:E:197:LEU:HG	2:E:198:GLY:N	2.26	0.50
2:E:200:GLN:HG2	2:E:202:TYR:CZ	2.46	0.50
3:F:138:PHE:HD1	3:F:178:MET:HG3	1.77	0.50
3:F:156:SER:OG	3:F:157:GLU:N	2.44	0.50
1:G:162:SER:HA	1:G:242:PHE:O	2.12	0.50
2:H:27:THR:CG2	2:H:31:TYR:CD2	2.95	0.50
2:K:116:THR:HG21	4:K:302:HOH:O	2.11	0.50
3:L:162:VAL:O	3:L:163:LEU:C	2.53	0.50
3:L:213:ASN:C	3:L:213:ASN:OD1	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:THR:HG23	2:B:30:ASP:OD2	2.11	0.49
2:B:36:ILE:HG13	2:B:45:GLU:C	2.36	0.49
2:B:100:TRP:NE1	3:C:34:ASN:OD1	2.44	0.49
1:D:201:VAL:C	1:D:241:THR:O	2.55	0.49
2:E:35:TRP:CD1	2:E:80:LEU:HB2	2.47	0.49
3:F:162:VAL:O	3:F:162:VAL:CG2	2.59	0.49
3:I:40:GLN:HB3	3:I:50:LEU:HD11	1.94	0.49
2:K:147:GLY:C	2:K:162:TRP:CH2	2.89	0.49
3:L:81:VAL:HG12	3:L:82:GLU:H	1.74	0.49
3:L:196:THR:HA	3:L:209:VAL:HB	1.94	0.49
1:D:149:ILE:HD11	1:D:252:ARG:HB2	1.94	0.49
2:E:125:LYS:HD2	2:E:126:GLY:N	2.27	0.49
1:G:248:LEU:HD12	1:G:249:VAL:H	1.76	0.49
2:K:72:ASP:N	2:K:77:THR:O	2.44	0.49
1:A:104:GLN:NE2	1:A:233:LEU:HD22	2.22	0.49
2:B:127:PRO:HD2	2:B:213:THR:HG21	1.93	0.49
3:C:101:THR:HG22	3:C:102:PHE:H	1.76	0.49
3:C:109:ILE:CG2	3:C:110:LYS:H	2.16	0.49
2:E:205:ASN:ND2	2:E:214:LYS:HE3	2.27	0.49
3:F:12:VAL:HG22	3:F:13:SER:N	2.27	0.49
3:F:141:ASN:ND2	3:F:176:TYR:CE1	2.81	0.49
1:J:122:SER:O	1:J:124:PRO:HD3	2.12	0.49
2:K:63:VAL:CG1	2:K:67:SER:H	2.24	0.49
3:L:97:VAL:HG22	3:L:98:PRO:HD2	1.93	0.49
3:L:191:ARG:HD2	3:L:191:ARG:C	2.36	0.49
1:A:109:SER:HB3	1:A:258:GLU:HG2	1.93	0.49
1:A:229:TYR:C	1:A:230:TYR:CD1	2.90	0.49
2:E:203:ILE:HG13	2:E:204:CYS:N	2.25	0.49
2:E:209:LYS:N	2:E:210:PRO:CD	2.75	0.49
3:F:159:GLN:HG3	3:F:160:ASN:H	1.77	0.49
2:H:194:SER:O	2:H:196:SER:N	2.45	0.49
3:I:120:ILE:HB	3:I:208:ILE:CG2	2.42	0.49
1:J:54:LYS:HZ2	1:J:54:LYS:CB	2.17	0.49
2:K:45:GLU:OE1	2:K:46:TRP:N	2.46	0.49
3:C:35:PHE:HB2	3:C:95:LYS:HE2	1.94	0.49
1:D:153:LYS:HG3	1:D:157:SER:N	2.27	0.49
2:E:63:VAL:HG11	2:E:67:SER:H	1.76	0.49
3:F:26:GLU:O	3:F:72:THR:HB	2.13	0.49
2:H:96:ALA:HB1	3:I:36:ILE:HD11	1.95	0.49
1:J:144:PHE:CG	1:J:145:TYR:N	2.78	0.49
1:A:115:GLU:CB	3:C:96:GLU:HG2	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PHE:HB3	1:A:243:GLU:HB3	1.95	0.49
2:B:30:ASP:OD1	2:B:30:ASP:N	2.44	0.49
1:D:91:TYR:CG	1:D:227:MET:HE2	2.46	0.49
2:E:61:ASP:OD1	2:H:142:GLY:HA2	2.13	0.49
1:G:54:LYS:HZ1	1:G:60:TRP:CD1	2.31	0.49
1:G:206:TYR:OH	1:G:208:LYS:HD2	2.12	0.49
1:G:219:LYS:HD3	1:G:224:GLU:CG	2.42	0.49
1:G:241:THR:CG2	1:G:242:PHE:N	2.76	0.49
2:H:97:ARG:NE	2:H:110:GLY:HA3	2.27	0.49
3:I:209:VAL:HG22	3:I:210:LYS:CB	2.43	0.49
3:L:108:GLU:CG	3:L:109:ILE:N	2.75	0.49
1:D:179:ILE:HG22	1:D:181:HIS:CE1	2.48	0.49
2:E:186:LEU:HD12	2:E:187:SER:H	1.78	0.49
1:G:231:TRP:CE3	1:G:232:THR:HA	2.47	0.49
2:H:162:TRP:CE2	2:H:204:CYS:HB3	2.47	0.49
3:I:141:ASN:N	3:I:176:TYR:HD1	2.10	0.49
3:I:204:SER:C	3:I:205:THR:CG2	2.86	0.49
3:L:165:SER:C	3:L:166:TRP:CD1	2.90	0.49
1:A:127:ASP:OD2	1:A:127:ASP:C	2.56	0.49
3:C:64:ARG:NH2	3:C:82:GLU:HB2	2.28	0.49
3:C:183:THR:CG2	3:C:184:LEU:N	2.75	0.49
1:D:103:GLU:OE1	1:D:104:GLN:N	2.46	0.49
1:D:150:TRP:CD1	1:D:150:TRP:C	2.90	0.49
1:D:221:ARG:O	1:D:223:GLN:HG2	2.12	0.49
3:F:140:ASN:CG	3:F:176:TYR:CD1	2.87	0.49
1:G:56:ASN:HB3	1:G:82:THR:O	2.11	0.49
1:G:101:LEU:HD22	1:G:105:LEU:CD1	2.42	0.49
2:H:176:ALA:CB	3:I:166:TRP:CE2	2.90	0.49
2:H:178:LEU:C	2:H:178:LEU:HD23	2.38	0.49
3:I:1:ILE:HG22	3:I:3:MET:CE	2.39	0.49
3:I:141:ASN:HA	3:I:175:THR:HB	1.92	0.49
1:J:56:ASN:HD21	1:J:88:GLY:HA2	1.77	0.49
2:K:54:SER:HB3	2:K:56:ARG:NE	2.28	0.49
2:K:176:ALA:O	2:K:185:SER:N	2.45	0.49
3:L:141:ASN:N	3:L:175:THR:HB	2.27	0.49
1:A:151:LEU:HD12	1:A:250:VAL:HG13	1.94	0.49
2:E:152:ASP:OD1	2:E:178:LEU:HD22	2.13	0.49
2:K:34:SER:OG	2:K:98:HIS:NE2	2.46	0.49
2:K:39:ALA:CB	2:K:44:LEU:HG	2.43	0.49
2:K:201:THR:CG2	2:K:218:LYS:HD3	2.42	0.49
3:L:88:ASN:ND2	3:L:90:PHE:CE2	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ILE:HD11	3:C:81:VAL:HA	1.94	0.49
2:H:46:TRP:O	2:H:60:ARG:NH1	2.46	0.49
2:H:90:THR:CG2	2:H:118:THR:HA	2.36	0.49
3:I:209:VAL:HG23	3:I:210:LYS:HD3	1.94	0.49
3:I:209:VAL:HG22	3:I:210:LYS:N	2.27	0.49
2:K:162:TRP:CZ2	2:K:204:CYS:HB3	2.48	0.49
3:L:62:PRO:HB2	3:L:64:ARG:HG3	1.94	0.49
1:A:183:SER:OG	1:A:224:GLU:HB2	2.13	0.48
1:D:101:LEU:O	1:D:102:ARG:C	2.54	0.48
1:D:151:LEU:HD12	1:D:250:VAL:HG13	1.94	0.48
1:D:179:ILE:HG22	1:D:181:HIS:NE2	2.27	0.48
2:E:72:ASP:OD1	2:E:75:ARG:HB2	2.12	0.48
2:E:173:THR:HG21	3:F:178:MET:CG	2.43	0.48
2:H:37:ARG:HB3	2:H:93:TYR:CE2	2.48	0.48
3:I:178:MET:HE2	3:I:180:SER:OG	2.12	0.48
2:K:34:SER:OG	2:K:49:GLY:CA	2.61	0.48
2:K:34:SER:CB	2:K:98:HIS:NE2	2.76	0.48
2:K:162:TRP:CH2	2:K:204:CYS:HB3	2.47	0.48
3:L:204:SER:C	3:L:205:THR:HG22	2.38	0.48
1:A:226:ARG:HD3	1:A:226:ARG:HA	1.46	0.48
2:B:32:ASP:HB2	2:B:98:HIS:NE2	2.28	0.48
3:C:12:VAL:HG13	3:C:13:SER:N	2.27	0.48
3:C:39:PHE:O	3:C:40:GLN:HB2	2.12	0.48
3:C:66:SER:N	3:C:77:THR:O	2.45	0.48
1:D:97:ASP:HB2	1:D:231:TRP:HE1	1.79	0.48
2:E:63:VAL:C	2:E:65:GLY:H	2.18	0.48
2:E:172:HIS:ND1	2:E:188:SER:HB2	2.28	0.48
3:F:162:VAL:O	3:F:164:ASN:CG	2.56	0.48
1:G:56:ASN:HA	1:G:81:GLU:HB2	1.95	0.48
1:G:161:LEU:HD23	1:G:161:LEU:C	2.38	0.48
3:I:197:CYS:O	3:I:208:ILE:O	2.31	0.48
1:J:113:ARG:HB2	1:J:255:PHE:CE1	2.47	0.48
3:L:57:LYS:O	3:L:58:GLY:C	2.56	0.48
2:B:35:TRP:CZ3	2:B:95:CYS:HB2	2.48	0.48
2:B:177:VAL:HA	2:B:184:TYR:CD2	2.48	0.48
1:D:119:LYS:HG2	1:D:120:THR:H	1.77	0.48
2:E:96:ALA:HB1	3:F:36:ILE:HG21	1.94	0.48
3:F:13:SER:CB	3:F:110:LYS:NZ	2.76	0.48
1:G:57:ILE:CD1	1:G:102:ARG:HB2	2.43	0.48
1:J:184:THR:O	1:J:186:ALA:N	2.46	0.48
1:J:192:TYR:HB3	1:J:246:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:90:PHE:HA	3:L:102:PHE:CZ	2.49	0.48
1:A:57:ILE:HG22	1:A:58:ALA:N	2.29	0.48
1:A:122:SER:O	1:A:124:PRO:HD3	2.13	0.48
1:D:51:HIS:ND1	1:D:80:VAL:HG21	2.27	0.48
1:D:57:ILE:HG13	1:D:81:GLU:OE2	2.14	0.48
3:F:38:TRP:NE1	3:F:90:PHE:H	2.11	0.48
3:F:38:TRP:HB2	3:F:48:LYS:O	2.14	0.48
3:F:193:ASN:ND2	3:F:211:SER:OG	2.46	0.48
2:H:97:ARG:HE	2:H:110:GLY:HA3	1.79	0.48
1:J:165:TYR:CE2	1:J:173:VAL:HG21	2.48	0.48
2:K:163:ASN:HD22	2:K:163:ASN:H	1.61	0.48
3:L:143:TYR:HD1	3:L:174:SER:OG	1.94	0.48
3:L:170:ASP:CB	3:L:175:THR:OG1	2.61	0.48
3:C:38:TRP:HZ3	3:C:89:TYR:HA	1.70	0.48
3:C:64:ARG:NH2	3:C:85:ASP:OD2	2.47	0.48
3:C:194:SER:HA	3:C:210:LYS:CB	2.36	0.48
3:C:205:THR:O	3:C:205:THR:HG23	2.13	0.48
1:D:227:MET:HB3	1:D:229:TYR:CZ	2.48	0.48
2:E:151:LYS:HG2	2:E:185:SER:HG	1.79	0.48
3:F:140:ASN:OD1	3:F:176:TYR:HD1	1.96	0.48
3:F:149:VAL:O	3:F:149:VAL:CG2	2.60	0.48
1:G:153:LYS:CD	1:G:193:GLN:HB2	2.43	0.48
1:G:219:LYS:HG3	1:G:223:GLN:H	1.78	0.48
3:L:127:GLN:O	3:L:130:SER:OG	2.32	0.48
1:A:54:LYS:HG2	1:A:55:CYS:N	2.23	0.48
2:B:51:LEU:HD13	2:B:52:GLY:O	2.13	0.48
2:B:145:ALA:HA	2:B:191:THR:HA	1.96	0.48
2:B:171:VAL:HG11	3:C:176:TYR:CE2	2.48	0.48
3:C:164:ASN:ND2	3:C:164:ASN:N	2.61	0.48
1:D:90:CYS:SG	1:D:145:TYR:CE1	3.07	0.48
2:E:38:GLN:OE1	3:F:41:GLN:NE2	2.42	0.48
2:E:125:LYS:HD2	2:E:126:GLY:H	1.78	0.48
3:I:162:VAL:O	3:I:162:VAL:CG2	2.61	0.48
3:I:209:VAL:CG2	3:I:210:LYS:N	2.76	0.48
1:J:133:THR:HG23	1:J:135:ALA:N	2.25	0.48
3:L:102:PHE:CD1	3:L:104:GLY:N	2.63	0.48
1:A:105:LEU:HD23	1:A:257:MET:SD	2.54	0.48
2:B:180:SER:O	2:B:182:GLY:O	2.32	0.48
3:C:38:TRP:CG	3:C:39:PHE:HA	2.41	0.48
3:C:45:GLN:CB	3:C:46:PRO:HD2	2.35	0.48
2:E:10:VAL:HG13	2:E:155:PRO:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:92:VAL:HA	2:E:115:THR:O	2.12	0.48
3:F:2:GLN:OE1	3:F:97:VAL:HG21	2.14	0.48
3:F:38:TRP:CD1	3:F:40:GLN:O	2.65	0.48
3:I:52:TYR:O	3:I:56:ASN:HB2	2.14	0.48
3:I:178:MET:C	3:I:178:MET:SD	2.96	0.48
1:J:185:SER:N	1:J:214:ILE:HG21	2.29	0.48
1:A:57:ILE:H	1:A:81:GLU:CD	2.22	0.48
3:C:140:ASN:ND2	3:C:176:TYR:HD1	2.12	0.48
2:H:30:ASP:O	2:H:30:ASP:CG	2.56	0.48
3:I:93:GLN:C	3:I:94:THR:O	2.54	0.48
1:J:151:LEU:HD12	1:J:250:VAL:CG1	2.43	0.48
2:K:178:LEU:HD11	3:L:182:LEU:CD1	2.42	0.48
3:L:52:TYR:O	3:L:56:ASN:CB	2.62	0.48
3:L:56:ASN:ND2	4:L:303:HOH:O	2.46	0.48
1:A:232:THR:HG23	1:A:233:LEU:N	2.28	0.48
2:B:36:ILE:CB	2:B:46:TRP:HA	2.41	0.48
2:E:2:VAL:N	2:E:3:LYS:HE2	2.29	0.48
1:J:92:PRO:HB2	1:J:226:ARG:HD2	1.94	0.48
1:J:110:SER:HB2	1:J:171:LYS:NZ	2.29	0.48
1:A:215:ALA:HB1	1:D:96:ILE:HG21	1.95	0.48
2:E:33:MET:HE1	2:E:97:ARG:CB	2.42	0.48
3:F:84:GLU:C	3:F:86:THR:H	2.22	0.48
1:G:114:PHE:CD2	1:G:114:PHE:N	2.79	0.48
1:G:188:GLN:O	1:G:192:TYR:N	2.41	0.48
2:H:197:LEU:HD12	2:H:198:GLY:H	1.75	0.48
1:J:125:ASN:O	1:J:154:LYS:HB3	2.14	0.48
1:J:217:ARG:N	1:J:224:GLU:O	2.38	0.48
2:K:38:GLN:O	2:K:91:ALA:HB1	2.13	0.48
2:K:205:ASN:HA	2:K:215:VAL:O	2.14	0.48
3:L:79:ASN:HB3	3:L:80:PRO:CD	2.41	0.48
1:A:137:PRO:CA	1:A:142:LYS:HA	2.41	0.47
3:C:39:PHE:CB	3:C:50:LEU:H	2.19	0.47
3:C:157:GLU:O	3:C:158:ARG:HG2	2.14	0.47
1:D:82:THR:O	1:D:82:THR:OG1	2.31	0.47
1:D:153:LYS:HE3	1:D:156:ASN:CA	2.40	0.47
2:E:28:GLY:O	2:E:71:ARG:CZ	2.62	0.47
2:E:56:ARG:HB3	2:E:58:TYR:CE1	2.49	0.47
2:E:116:THR:O	2:E:116:THR:HG22	2.14	0.47
2:E:146:LEU:N	2:E:190:VAL:O	2.48	0.47
2:E:205:ASN:HD22	2:E:214:LYS:HE3	1.79	0.47
3:F:37:ASN:OD1	3:F:95:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:83:ALA:O	3:F:171:SER:O	2.32	0.47
3:F:158:ARG:HG3	3:F:159:GLN:N	2.29	0.47
2:H:6:GLU:HA	2:H:20:SER:O	2.14	0.47
2:K:45:GLU:CD	2:K:46:TRP:N	2.68	0.47
2:K:50:ILE:HB	2:K:56:ARG:O	2.14	0.47
1:A:49:PRO:CD	1:A:77:SER:OG	2.62	0.47
1:A:133:THR:HG21	1:A:150:TRP:HZ3	1.77	0.47
2:B:177:VAL:HG12	2:B:182:GLY:HA2	1.97	0.47
3:C:35:PHE:CD1	3:C:35:PHE:C	2.91	0.47
3:C:204:SER:C	3:C:205:THR:HG22	2.38	0.47
1:D:64:ASN:OD1	1:D:65:PRO:HD2	2.14	0.47
2:E:86:ARG:O	2:E:119:VAL:HG21	2.14	0.47
3:F:97:VAL:CG1	3:F:98:PRO:N	2.76	0.47
3:F:209:VAL:HG22	3:F:210:LYS:CB	2.44	0.47
2:H:117:VAL:CG1	2:H:117:VAL:O	2.60	0.47
3:I:123:PRO:CB	3:I:133:ALA:HB1	2.41	0.47
3:I:209:VAL:CG2	3:I:210:LYS:HG2	2.43	0.47
1:J:57:ILE:O	1:J:58:ALA:C	2.58	0.47
1:J:176:LEU:HA	1:J:230:TYR:O	2.15	0.47
2:K:175:PRO:O	3:L:166:TRP:CE3	2.66	0.47
1:A:92:PRO:C	1:A:226:ARG:HD2	2.39	0.47
3:C:7:PRO:CD	3:C:21:THR:O	2.53	0.47
1:D:211:LYS:HG3	1:D:212:PRO:HD2	1.96	0.47
2:E:48:SER:CB	2:E:59:TYR:HD1	2.27	0.47
2:E:56:ARG:HA	2:E:56:ARG:HD2	1.46	0.47
3:F:38:TRP:CD2	3:F:90:PHE:O	2.66	0.47
3:F:135:VAL:HG12	3:F:151:TRP:CZ3	2.48	0.47
1:G:241:THR:HG22	1:G:242:PHE:H	1.76	0.47
2:H:63:VAL:CG1	2:H:66:ARG:H	2.26	0.47
2:H:93:TYR:CE1	2:H:117:VAL:HG12	2.45	0.47
2:H:162:TRP:CZ2	2:H:204:CYS:HB3	2.50	0.47
2:K:11:VAL:O	2:K:119:VAL:HA	2.15	0.47
3:L:23:ARG:HD2	3:L:72:THR:HG23	1.96	0.47
2:B:143:THR:O	2:B:143:THR:HG22	2.13	0.47
2:B:150:VAL:HB	2:B:186:LEU:HG	1.95	0.47
1:D:164:SER:H	2:E:56:ARG:HH22	1.60	0.47
1:D:186:ALA:O	1:D:187:ASP:C	2.57	0.47
2:E:26:PHE:O	2:E:27:THR:C	2.57	0.47
2:E:48:SER:HB3	2:E:59:TYR:HD1	1.78	0.47
3:F:13:SER:HB3	3:F:110:LYS:HB3	1.96	0.47
3:F:38:TRP:CE2	3:F:90:PHE:N	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:151:LEU:HD12	1:G:250:VAL:HG11	1.97	0.47
3:I:9:SER:HB3	3:I:106:LYS:CG	2.42	0.47
1:J:101:LEU:HG	1:J:231:TRP:CE2	2.48	0.47
1:J:182:PRO:O	1:J:214:ILE:HG23	2.13	0.47
1:J:200:PHE:CG	1:J:201:VAL:N	2.82	0.47
1:J:232:THR:HG23	1:J:233:LEU:N	2.29	0.47
2:K:76:LYS:O	2:K:77:THR:HG22	2.14	0.47
3:L:86:THR:HG22	3:L:109:ILE:HD13	1.97	0.47
2:B:43:GLY:C	2:B:44:LEU:HD12	2.39	0.47
2:B:186:LEU:HD12	2:B:186:LEU:C	2.40	0.47
2:B:196:SER:O	2:B:200:GLN:N	2.48	0.47
3:C:34:ASN:N	3:C:34:ASN:ND2	2.62	0.47
3:C:84:GLU:C	3:C:86:THR:HG23	2.40	0.47
1:D:64:ASN:HD21	1:D:90:CYS:HB3	1.79	0.47
1:D:114:PHE:CE2	1:D:254:ALA:HB3	2.49	0.47
2:E:181:SER:CB	3:I:62:PRO:HG3	2.38	0.47
3:F:38:TRP:CH2	3:F:39:PHE:CD1	3.02	0.47
3:F:114:ALA:HA	3:F:201:HIS:HD2	1.79	0.47
3:F:173:ASP:OD1	3:F:175:THR:OG1	2.32	0.47
3:F:204:SER:C	3:F:205:THR:HG22	2.38	0.47
1:G:54:LYS:CG	1:G:67:CYS:HA	2.12	0.47
2:H:37:ARG:HB3	2:H:93:TYR:CD2	2.48	0.47
2:H:51:LEU:HD12	2:H:52:GLY:O	2.13	0.47
1:J:248:LEU:HD12	1:J:249:VAL:H	1.75	0.47
3:L:12:VAL:O	3:L:109:ILE:HA	2.15	0.47
2:B:27:THR:CG2	2:B:31:TYR:CG	2.98	0.47
2:B:178:LEU:C	2:B:180:SER:N	2.72	0.47
3:C:68:SER:OG	3:C:75:THR:HB	2.14	0.47
3:C:116:PRO:HB2	3:C:139:LEU:HB3	1.96	0.47
2:E:32:ASP:HB3	2:E:51:LEU:C	2.39	0.47
2:E:45:GLU:OE2	3:F:101:THR:N	2.43	0.47
2:E:46:TRP:O	2:E:46:TRP:CE3	2.67	0.47
2:E:51:LEU:HD12	2:E:56:ARG:N	2.28	0.47
2:E:173:THR:HG22	3:F:178:MET:SD	2.55	0.47
3:F:95:LYS:O	3:F:96:GLU:HG3	2.15	0.47
3:F:126:GLU:O	3:F:129:THR:HG23	2.15	0.47
1:G:131:GLY:CA	1:G:150:TRP:HB3	2.44	0.47
1:G:153:LYS:HD2	1:G:193:GLN:HB2	1.95	0.47
2:H:46:TRP:HE3	2:H:60:ARG:CZ	2.27	0.47
2:H:202:TYR:CD1	2:H:219:SER:HB2	2.48	0.47
2:K:63:VAL:HG13	2:K:66:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TRP:CZ2	1:A:230:TYR:HB2	2.50	0.47
1:A:212:PRO:HB3	1:A:247:ASN:ND2	2.29	0.47
2:B:17:LEU:HD21	2:B:19:LEU:HD13	1.95	0.47
2:B:211:SER:CB	2:B:213:THR:HG1	2.28	0.47
3:C:97:VAL:HG13	3:C:98:PRO:CD	2.42	0.47
1:D:161:LEU:O	1:D:243:GLU:HA	2.15	0.47
1:D:184:THR:H	1:D:187:ASP:CB	2.28	0.47
2:E:44:LEU:HD23	2:E:45:GLU:HG2	1.95	0.47
2:E:45:GLU:HB3	2:E:60:ARG:HH22	1.76	0.47
2:E:189:VAL:HG12	3:F:138:PHE:CE2	2.49	0.47
3:F:14:PRO:O	3:F:15:GLY:C	2.58	0.47
3:F:43:PRO:HD3	3:F:87:ALA:HA	1.97	0.47
3:F:52:TYR:O	3:F:56:ASN:HB2	2.14	0.47
3:F:143:TYR:CE2	3:F:144:PRO:HB3	2.49	0.47
3:F:167:THR:HG22	3:F:168:ASP:H	1.79	0.47
1:G:77:SER:OG	1:G:78:TYR:N	2.48	0.47
1:G:94:ASP:O	1:G:228:ASN:HA	2.15	0.47
1:G:119:LYS:HZ2	1:G:129:ASN:HD22	1.53	0.47
1:G:235:GLU:CG	1:G:236:PRO:CD	2.91	0.47
2:H:63:VAL:HG11	2:H:67:SER:H	1.80	0.47
2:H:208:HIS:O	2:H:212:ASN:CA	2.62	0.47
3:I:6:SER:HB3	3:I:7:PRO:CD	2.38	0.47
3:I:81:VAL:HG12	3:I:82:GLU:H	1.78	0.47
3:I:148:ASN:OD1	3:I:149:VAL:N	2.47	0.47
1:J:217:ARG:HD3	1:J:226:ARG:HG2	1.97	0.47
3:L:2:GLN:HA	3:L:25:SER:OG	2.14	0.47
3:L:204:SER:HA	4:L:310:HOH:O	2.15	0.47
2:B:6:GLU:HG2	2:B:35:TRP:HZ3	1.80	0.47
2:B:174:PHE:N	2:B:174:PHE:CD1	2.80	0.47
3:C:5:GLN:HB3	3:C:102:PHE:CD1	2.50	0.47
3:C:89:TYR:O	3:C:104:GLY:HA2	2.15	0.47
3:C:153:ILE:HA	3:C:194:SER:O	2.15	0.47
3:F:41:GLN:O	3:F:87:ALA:HB1	2.15	0.47
1:G:184:THR:O	1:G:185:SER:C	2.58	0.47
1:G:187:ASP:O	1:G:191:LEU:HB2	2.14	0.47
3:I:37:ASN:HD21	3:I:92:GLN:CB	2.28	0.47
3:I:97:VAL:HG13	3:I:98:PRO:CD	2.45	0.47
3:I:196:THR:OG1	3:I:210:LYS:CD	2.52	0.47
2:K:197:LEU:C	2:K:199:THR:N	2.72	0.47
3:L:170:ASP:OD2	3:L:170:ASP:C	2.58	0.47
1:A:161:LEU:HD23	1:A:161:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ARG:NE	2:B:88:GLU:OE1	2.45	0.47
2:B:173:THR:CG2	3:C:178:MET:SD	3.02	0.47
2:B:181:SER:OG	3:L:84:GLU:CD	2.58	0.47
1:D:57:ILE:HD11	1:D:102:ARG:HG3	1.97	0.47
2:E:36:ILE:O	2:E:94:TYR:HB2	2.15	0.47
2:E:37:ARG:HG3	2:E:37:ARG:O	2.14	0.47
3:F:158:ARG:HD3	2:H:31:TYR:CZ	2.50	0.47
1:J:64:ASN:O	1:J:67:CYS:HB2	2.15	0.47
2:K:17:LEU:HB3	2:K:82:MET:HG2	1.96	0.47
2:K:162:TRP:N	2:K:162:TRP:CD1	2.82	0.47
3:L:14:PRO:HG3	3:L:111:ARG:HH12	1.79	0.47
3:L:173:ASP:HA	4:L:311:HOH:O	2.14	0.47
1:A:57:ILE:HD11	1:A:79:ILE:HD13	1.97	0.47
2:B:173:THR:HG23	2:B:187:SER:O	2.15	0.47
3:C:89:TYR:O	3:C:104:GLY:CA	2.63	0.47
3:C:138:PHE:HD1	3:C:178:MET:CG	2.14	0.47
1:D:98:TYR:HE2	1:D:102:ARG:HH21	1.54	0.47
1:D:115:GLU:HB2	3:F:96:GLU:CG	2.45	0.47
1:D:188:GLN:NE2	1:D:194:ASN:O	2.48	0.47
3:F:84:GLU:C	3:F:86:THR:N	2.72	0.47
3:F:108:GLU:HG2	3:F:169:GLN:NE2	2.29	0.47
2:H:47:VAL:O	2:H:48:SER:HB2	2.15	0.47
3:I:41:GLN:HA	4:I:305:HOH:O	2.14	0.47
3:I:116:PRO:HA	3:I:140:ASN:O	2.15	0.47
2:K:17:LEU:O	2:K:82:MET:N	2.42	0.47
3:L:156:SER:O	3:L:157:GLU:CB	2.61	0.47
1:A:123:TRP:NE1	1:A:149:ILE:HD13	2.29	0.46
3:C:50:LEU:HD13	3:C:65:PHE:CD1	2.50	0.46
1:D:99:GLU:HG2	1:D:100:GLU:N	2.29	0.46
1:D:127:ASP:CG	1:D:130:LYS:HG2	2.39	0.46
2:E:38:GLN:HB3	2:E:94:TYR:HE2	1.80	0.46
2:E:64:LYS:HG3	2:E:64:LYS:O	2.15	0.46
3:F:27:SER:C	3:F:28:VAL:HG22	2.40	0.46
3:F:161:GLY:C	3:F:162:VAL:HG13	2.40	0.46
3:F:167:THR:CG2	3:F:168:ASP:H	2.28	0.46
1:G:135:ALA:HB3	1:G:223:GLN:HE21	1.80	0.46
2:H:46:TRP:CH2	2:H:59:TYR:O	2.68	0.46
2:H:146:LEU:HD12	2:H:162:TRP:CZ3	2.51	0.46
3:I:9:SER:CB	3:I:106:LYS:HG3	2.42	0.46
2:K:162:TRP:CD2	2:K:204:CYS:HB3	2.50	0.46
3:L:16:GLN:O	3:L:81:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:139:LEU:HD21	3:L:199:ALA:CB	2.45	0.46
1:A:152:VAL:HG11	1:A:191:LEU:HD12	1.98	0.46
2:B:132:LEU:HD11	2:B:149:LEU:HB2	1.98	0.46
2:E:46:TRP:O	2:E:60:ARG:NH1	2.48	0.46
3:F:110:LYS:O	3:F:111:ARG:CG	2.64	0.46
1:G:186:ALA:O	1:G:189:GLN:HB3	2.15	0.46
1:J:177:TRP:N	1:J:177:TRP:CE3	2.83	0.46
3:C:128:LEU:HD13	3:C:129:THR:N	2.18	0.46
2:E:178:LEU:C	2:E:180:SER:HB2	2.40	0.46
1:G:132:VAL:O	1:G:132:VAL:CG2	2.63	0.46
2:H:132:LEU:HD13	2:H:132:LEU:N	2.31	0.46
2:H:142:GLY:C	2:H:194:SER:OG	2.58	0.46
1:J:90:CYS:HB2	1:J:135:ALA:O	2.15	0.46
1:J:182:PRO:HG2	1:J:188:GLN:CA	2.45	0.46
2:K:78:LEU:H	2:K:78:LEU:HD23	1.80	0.46
2:K:176:ALA:CB	3:L:166:TRP:CZ2	2.98	0.46
3:L:111:ARG:HB2	3:L:143:TYR:CD1	2.51	0.46
1:D:165:TYR:HB3	1:D:240:ILE:HG22	1.97	0.46
2:E:208:HIS:C	2:E:210:PRO:HD2	2.40	0.46
3:F:196:THR:CG2	3:F:209:VAL:HG23	2.45	0.46
1:G:75:SER:OG	1:G:109:SER:O	2.30	0.46
1:G:149:ILE:HB	1:G:250:VAL:CG2	2.45	0.46
1:G:197:ALA:O	1:G:212:PRO:HD2	2.15	0.46
1:G:231:TRP:CZ3	1:G:233:LEU:HD13	2.49	0.46
2:H:44:LEU:N	4:H:305:HOH:O	2.48	0.46
2:H:73:ASN:OD1	2:H:73:ASN:N	2.37	0.46
3:I:143:TYR:HB2	3:I:174:SER:HB2	1.97	0.46
2:K:171:VAL:HG22	3:L:176:TYR:CE1	2.50	0.46
1:A:153:LYS:HB2	1:A:157:SER:O	2.16	0.46
2:B:156:GLU:CB	2:B:157:PRO:HA	2.46	0.46
3:C:37:ASN:HB3	3:C:38:TRP:O	2.15	0.46
3:C:38:TRP:CZ3	3:C:40:GLN:N	2.84	0.46
3:C:90:PHE:N	3:C:90:PHE:HD2	2.12	0.46
1:D:99:GLU:CG	1:D:100:GLU:H	2.29	0.46
1:D:116:ILE:HG22	1:D:252:ARG:O	2.16	0.46
1:D:192:TYR:C	1:D:194:ASN:H	2.23	0.46
2:E:173:THR:O	2:E:174:PHE:C	2.57	0.46
2:E:186:LEU:CG	2:E:187:SER:N	2.78	0.46
3:F:42:LYS:HD2	3:F:87:ALA:CB	2.45	0.46
3:F:193:ASN:HA	3:F:195:TYR:HE1	1.80	0.46
1:G:133:THR:O	1:G:142:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:216:ILE:O	1:G:216:ILE:HG22	2.16	0.46
1:G:220:VAL:HG23	1:G:226:ARG:HH22	1.80	0.46
1:G:222:ASP:O	1:G:222:ASP:CG	2.57	0.46
2:H:63:VAL:CG1	2:H:67:SER:H	2.28	0.46
2:K:158:VAL:HG23	2:K:208:HIS:HD2	1.80	0.46
2:K:162:TRP:CZ3	2:K:204:CYS:HB3	2.50	0.46
3:L:179:SER:HB2	4:L:302:HOH:O	2.15	0.46
1:A:153:LYS:HG3	1:A:153:LYS:O	2.15	0.46
2:B:162:TRP:HD1	2:B:170:SER:OG	1.98	0.46
2:E:100:TRP:CD1	3:F:34:ASN:CG	2.93	0.46
2:E:171:VAL:HG21	3:F:176:TYR:CD1	2.50	0.46
1:G:117:PHE:HB2	1:G:251:PRO:O	2.16	0.46
1:G:149:ILE:CD1	1:G:252:ARG:HB2	2.45	0.46
2:H:119:VAL:O	2:H:119:VAL:HG12	2.16	0.46
1:J:49:PRO:HG2	1:J:77:SER:CB	2.44	0.46
1:J:231:TRP:HZ3	1:J:233:LEU:HD11	1.79	0.46
2:K:147:GLY:O	2:K:162:TRP:HH2	1.98	0.46
2:K:174:PHE:HD2	3:L:166:TRP:HE3	1.64	0.46
1:D:144:PHE:CZ	1:D:150:TRP:HB2	2.49	0.46
1:D:199:VAL:HG13	1:D:244:ALA:HB2	1.98	0.46
2:E:174:PHE:CD1	2:E:175:PRO:HD2	2.51	0.46
2:E:212:ASN:CG	2:E:213:THR:N	2.66	0.46
3:F:13:SER:HB3	3:F:110:LYS:CD	2.46	0.46
3:F:24:ALA:N	3:F:72:THR:O	2.48	0.46
3:F:96:GLU:O	3:F:97:VAL:CG2	2.60	0.46
2:H:179:GLN:HG2	3:I:163:LEU:HB2	1.96	0.46
3:I:191:ARG:HG2	3:I:192:HIS:H	1.79	0.46
1:J:101:LEU:HG	1:J:231:TRP:CD2	2.50	0.46
1:J:211:LYS:HB2	1:J:211:LYS:HZ2	1.79	0.46
1:A:51:HIS:HA	1:A:80:VAL:HB	1.97	0.46
1:A:114:PHE:CE2	1:A:254:ALA:HB3	2.51	0.46
1:D:147:ASN:HD21	1:D:255:PHE:HZ	1.64	0.46
2:E:9:ALA:H	2:E:17:LEU:HD21	1.81	0.46
2:E:51:LEU:CD1	2:E:55:GLU:N	2.79	0.46
3:F:1:ILE:HD13	3:F:1:ILE:HA	1.74	0.46
3:F:202:LYS:HA	4:F:308:HOH:O	2.16	0.46
3:I:91:CYS:N	3:I:102:PHE:CE2	2.72	0.46
1:J:215:ALA:H	1:J:217:ARG:NH1	2.13	0.46
2:K:51:LEU:CD2	2:K:56:ARG:HB2	2.36	0.46
2:K:53:GLY:O	2:K:54:SER:HB2	2.16	0.46
2:K:82:MET:HG3	2:K:85:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:97:VAL:O	3:L:99:TYR:CD1	2.69	0.46
1:A:57:ILE:CG1	1:A:81:GLU:OE2	2.64	0.46
2:B:4:LEU:HB2	2:B:112:GLY:CA	2.46	0.46
3:C:9:SER:HA	3:C:106:LYS:H	1.80	0.46
3:C:97:VAL:CG1	3:C:98:PRO:N	2.79	0.46
1:D:84:SER:O	1:D:86:ASP:N	2.48	0.46
1:D:232:THR:C	1:D:233:LEU:HD13	2.41	0.46
3:F:3:MET:CG	3:F:5:GLN:HE21	2.21	0.46
1:G:200:PHE:HB3	1:G:243:GLU:HB2	1.97	0.46
2:H:117:VAL:O	2:H:117:VAL:HG13	2.15	0.46
2:H:156:GLU:OE2	2:H:175:PRO:HG3	2.16	0.46
3:I:20:ILE:HG21	3:I:105:THR:HG21	1.97	0.46
3:L:140:ASN:HB2	3:L:141:ASN:ND2	2.31	0.46
1:A:208:LYS:HG2	1:A:209:LYS:N	2.30	0.46
3:C:51:ILE:HD13	3:C:76:LEU:HD12	1.98	0.46
3:C:133:ALA:O	3:C:183:THR:HB	2.16	0.46
1:D:49:PRO:CB	1:D:76:TRP:HB2	2.38	0.46
1:D:145:TYR:CZ	1:D:229:TYR:OH	2.68	0.46
3:F:39:PHE:CD2	3:F:51:ILE:HB	2.50	0.46
3:F:78:ILE:HG22	3:F:79:ASN:O	2.16	0.46
1:G:151:LEU:HD12	1:G:250:VAL:CG1	2.46	0.46
3:I:1:ILE:O	3:I:2:GLN:HB3	2.16	0.46
3:I:89:TYR:N	3:I:89:TYR:CD2	2.83	0.46
3:I:96:GLU:O	3:I:97:VAL:HG23	2.16	0.46
1:J:161:LEU:C	1:J:161:LEU:CD2	2.88	0.46
3:C:132:GLY:HA2	3:C:184:LEU:C	2.41	0.45
2:E:51:LEU:HD13	2:E:52:GLY:O	2.17	0.45
2:E:86:ARG:N	2:E:119:VAL:HG11	2.31	0.45
1:G:77:SER:O	1:G:106:SER:O	2.34	0.45
1:G:172:GLU:O	1:G:256:ALA:HA	2.16	0.45
1:G:222:ASP:O	1:G:222:ASP:OD1	2.33	0.45
3:I:42:LYS:HE2	3:I:42:LYS:HB3	1.82	0.45
3:I:144:PRO:O	3:I:201:HIS:HE1	1.99	0.45
1:J:54:LYS:HE3	1:J:67:CYS:CA	2.46	0.45
1:J:200:PHE:CE2	1:J:201:VAL:O	2.70	0.45
2:K:18:ARG:HD2	2:K:81:GLU:HB2	1.96	0.45
3:L:123:PRO:CB	3:L:133:ALA:HB1	2.42	0.45
1:A:126:HIS:ND1	1:A:126:HIS:N	2.64	0.45
1:A:258:GLU:HG3	1:A:259:ARG:N	2.32	0.45
2:B:203:ILE:HD11	2:B:216:ASP:CB	2.35	0.45
3:C:92:GLN:CA	3:C:101:THR:HG23	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:LEU:HD23	1:D:251:PRO:N	2.31	0.45
2:E:215:VAL:HG22	2:E:216:ASP:N	2.30	0.45
1:G:75:SER:OG	1:G:110:SER:HA	2.16	0.45
1:G:133:THR:C	1:G:142:LYS:HB2	2.41	0.45
2:H:54:SER:O	2:H:55:GLU:C	2.60	0.45
2:H:171:VAL:HB	2:H:189:VAL:HG13	1.98	0.45
2:K:69:ILE:CG1	2:K:70:SER:N	2.79	0.45
3:L:36:ILE:O	3:L:36:ILE:HG23	2.16	0.45
1:D:177:TRP:CE2	1:D:230:TYR:HB2	2.52	0.45
1:D:200:PHE:CG	1:D:201:VAL:N	2.84	0.45
1:D:231:TRP:HZ3	1:D:233:LEU:HD22	1.80	0.45
2:E:6:GLU:HG3	2:E:35:TRP:CZ3	2.51	0.45
2:E:180:SER:O	2:E:181:SER:C	2.58	0.45
1:G:116:ILE:HG23	1:G:117:PHE:N	2.31	0.45
1:G:219:LYS:CG	1:G:222:ASP:HA	2.46	0.45
2:H:83:ASN:O	2:H:84:SER:C	2.58	0.45
1:J:48:ALA:HB1	1:J:78:TYR:CE1	2.51	0.45
3:L:34:ASN:O	3:L:95:LYS:HD3	2.15	0.45
3:L:193:ASN:O	3:L:211:SER:CB	2.64	0.45
1:A:84:SER:OG	1:A:87:ASN:HB2	2.16	0.45
2:B:30:ASP:O	2:B:52:GLY:HA3	2.17	0.45
3:C:14:PRO:O	3:C:81:VAL:O	2.33	0.45
1:D:182:PRO:HG2	1:D:188:GLN:HA	1.99	0.45
3:F:120:ILE:HB	3:F:197:CYS:SG	2.57	0.45
3:F:139:LEU:O	3:F:176:TYR:HA	2.17	0.45
3:F:167:THR:CG2	3:F:168:ASP:N	2.79	0.45
1:G:65:PRO:C	1:G:67:CYS:H	2.24	0.45
1:G:100:GLU:HG2	1:G:231:TRP:HZ2	1.82	0.45
1:J:211:LYS:HB2	1:J:211:LYS:HZ1	1.77	0.45
2:K:90:THR:HG23	2:K:118:THR:HA	1.99	0.45
2:K:127:PRO:HB3	2:K:150:VAL:HG13	1.97	0.45
2:B:33:MET:HE1	2:B:97:ARG:HB2	1.99	0.45
2:B:47:VAL:O	2:B:48:SER:HB3	2.16	0.45
1:D:61:ILE:HD13	1:D:61:ILE:O	2.15	0.45
1:D:147:ASN:ND2	1:D:255:PHE:HZ	2.14	0.45
1:D:160:LYS:H	1:D:160:LYS:CD	2.25	0.45
2:E:45:GLU:CB	2:E:60:ARG:NH2	2.76	0.45
1:G:199:VAL:CG1	1:G:248:LEU:HD22	2.46	0.45
3:I:143:TYR:CE1	3:I:144:PRO:HB3	2.52	0.45
1:J:253:TYR:OH	3:L:97:VAL:HG23	2.17	0.45
3:L:97:VAL:HG13	3:L:98:PRO:CD	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:108:GLU:OE1	3:L:108:GLU:CA	2.58	0.45
3:L:195:TYR:C	3:L:210:LYS:HA	2.39	0.45
1:A:64:ASN:OD1	1:A:66:GLU:HG2	2.17	0.45
1:A:122:SER:HB2	1:A:123:TRP:CE2	2.52	0.45
2:B:146:LEU:HD13	2:B:146:LEU:HA	1.77	0.45
3:C:113:ASP:CG	3:C:142:PHE:HA	2.42	0.45
2:E:50:ILE:CG2	2:E:69:ILE:HG23	2.47	0.45
3:F:38:TRP:CA	3:F:49:LEU:HD23	2.46	0.45
3:F:191:ARG:NE	3:F:192:HIS:CE1	2.85	0.45
1:G:73:ALA:HB3	4:G:608:HOH:O	2.16	0.45
1:G:91:TYR:CD1	1:G:91:TYR:C	2.95	0.45
2:H:98:HIS:CD2	2:H:98:HIS:H	2.34	0.45
2:H:201:THR:HG23	2:H:218:LYS:HD3	1.99	0.45
3:I:7:PRO:HG3	3:I:21:THR:H	1.78	0.45
1:J:54:LYS:HE3	1:J:67:CYS:C	2.42	0.45
1:J:235:GLU:CG	1:J:236:PRO:CD	2.92	0.45
2:K:92:VAL:HG11	2:K:94:TYR:CE2	2.52	0.45
3:L:42:LYS:HE3	3:L:85:ASP:O	2.16	0.45
1:A:174:LEU:HD12	1:A:231:TRP:CE3	2.51	0.45
3:C:114:ALA:O	3:C:116:PRO:HD3	2.17	0.45
3:C:151:TRP:CZ3	3:C:197:CYS:HB3	2.52	0.45
3:C:207:PRO:O	3:C:208:ILE:HD12	2.17	0.45
1:D:217:ARG:HB3	1:D:218:PRO:HD2	1.97	0.45
1:G:101:LEU:HD23	1:G:101:LEU:HA	1.73	0.45
2:H:37:ARG:HD3	2:H:93:TYR:CZ	2.52	0.45
3:I:34:ASN:O	3:I:95:LYS:HG3	2.17	0.45
3:I:111:ARG:NE	3:I:173:ASP:HA	2.24	0.45
3:I:150:LYS:HE2	3:I:150:LYS:HB2	1.70	0.45
3:I:203:THR:O	3:I:204:SER:C	2.59	0.45
2:K:63:VAL:HG12	2:K:64:LYS:N	2.31	0.45
3:L:40:GLN:HE21	3:L:50:LEU:HD21	1.81	0.45
3:L:114:ALA:HA	3:L:201:HIS:CD2	2.52	0.45
1:A:138:HIS:HB2	1:A:143:SER:HB2	1.99	0.45
1:A:258:GLU:C	1:A:259:ARG:HG2	2.38	0.45
2:B:27:THR:HG22	2:B:31:TYR:CB	2.47	0.45
1:D:56:ASN:OD1	1:D:56:ASN:N	2.43	0.45
1:D:151:LEU:HD12	1:D:250:VAL:CG1	2.47	0.45
1:D:212:PRO:HB3	1:D:247:ASN:ND2	2.31	0.45
2:E:45:GLU:HB3	2:E:60:ARG:HH12	1.78	0.45
3:F:8:ALA:HB1	3:F:105:THR:OG1	2.17	0.45
2:H:113:GLN:O	3:I:45:GLN:NE2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:91:CYS:SG	3:I:102:PHE:CD2	3.10	0.45
1:J:76:TRP:CD2	1:J:108:VAL:HG22	2.52	0.45
1:J:132:VAL:HG23	1:J:142:LYS:HG3	1.98	0.45
3:L:34:ASN:N	3:L:34:ASN:OD1	2.49	0.45
3:L:140:ASN:HA	3:L:176:TYR:CB	2.24	0.45
3:L:140:ASN:HB3	3:L:176:TYR:CD1	2.51	0.45
2:B:35:TRP:CH2	2:B:95:CYS:HB2	2.52	0.45
2:B:54:SER:O	2:B:56:ARG:HD2	2.17	0.45
3:C:210:LYS:HD2	3:C:211:SER:N	2.18	0.45
1:D:125:ASN:C	1:D:154:LYS:HD3	2.42	0.45
2:E:31:TYR:O	2:E:71:ARG:NH2	2.50	0.45
2:E:97:ARG:HG2	2:E:98:HIS:H	1.82	0.45
2:E:179:GLN:CB	3:I:60:GLY:HA2	2.29	0.45
1:G:177:TRP:CZ2	1:G:206:TYR:CZ	3.05	0.45
2:H:72:ASP:CB	2:H:79:TYR:CE2	2.93	0.45
2:K:33:MET:C	2:K:98:HIS:CE1	2.95	0.45
2:K:211:SER:O	2:K:213:THR:N	2.50	0.45
1:A:114:PHE:CE1	1:A:116:ILE:HA	2.52	0.45
1:A:118:PRO:HB2	1:A:120:THR:OG1	2.17	0.45
1:A:216:ILE:N	1:D:96:ILE:HG23	2.32	0.45
2:B:189:VAL:HG23	3:C:138:PHE:CE2	2.52	0.45
3:C:120:ILE:CG2	3:C:121:PHE:N	2.80	0.45
3:F:174:SER:C	3:F:175:THR:OG1	2.59	0.45
2:H:27:THR:HB	2:H:31:TYR:CD2	2.52	0.45
1:J:70:LEU:O	1:J:71:SER:OG	2.32	0.45
2:K:51:LEU:HD21	2:K:56:ARG:CB	2.35	0.45
2:E:50:ILE:HG22	2:E:57:SER:OG	2.17	0.44
3:F:26:GLU:O	3:F:27:SER:OG	2.33	0.44
2:H:162:TRP:HA	2:H:203:ILE:O	2.17	0.44
1:J:216:ILE:O	1:J:216:ILE:HG22	2.16	0.44
2:K:43:GLY:O	2:K:44:LEU:CD2	2.65	0.44
2:K:209:LYS:HB2	2:K:210:PRO:CD	2.47	0.44
2:K:215:VAL:C	2:K:216:ASP:OD1	2.60	0.44
3:L:195:TYR:H	3:L:210:LYS:HA	1.81	0.44
3:C:166:TRP:HA	3:C:166:TRP:CE3	2.51	0.44
1:D:127:ASP:N	1:D:154:LYS:HB3	2.31	0.44
1:D:220:VAL:O	1:D:223:GLN:HB2	2.17	0.44
3:F:135:VAL:CG1	3:F:151:TRP:CZ3	3.00	0.44
3:F:172:LYS:O	3:F:173:ASP:CB	2.65	0.44
1:G:164:SER:H	2:H:56:ARG:NH2	2.15	0.44
2:H:194:SER:C	2:H:196:SER:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:128:LEU:O	3:I:128:LEU:HD23	2.17	0.44
3:L:209:VAL:HG23	3:L:210:LYS:CG	2.47	0.44
2:B:45:GLU:HG2	2:B:60:ARG:CZ	2.47	0.44
2:B:196:SER:O	2:B:202:TYR:HE2	1.99	0.44
2:E:66:ARG:CZ	2:E:86:ARG:HD3	2.46	0.44
3:F:54:ALA:O	3:F:67:GLY:HA3	2.18	0.44
3:F:97:VAL:HG13	3:F:98:PRO:HD2	1.99	0.44
1:G:54:LYS:CB	1:G:66:GLU:O	2.65	0.44
1:G:180:HIS:N	1:G:247:ASN:O	2.48	0.44
2:H:218:LYS:HB2	2:H:218:LYS:HZ2	1.81	0.44
3:I:136:VAL:HG13	3:I:180:SER:OG	2.17	0.44
1:J:89:THR:HB	1:J:145:TYR:OH	2.17	0.44
1:J:97:ASP:HB3	1:J:231:TRP:HE1	1.80	0.44
2:K:37:ARG:HG2	2:K:47:VAL:HG13	1.97	0.44
3:L:16:GLN:HG3	3:L:17:ARG:H	1.82	0.44
3:L:86:THR:H	3:L:109:ILE:HD11	1.83	0.44
1:A:57:ILE:HD12	1:A:102:ARG:HE	1.83	0.44
2:B:38:GLN:HA	2:B:44:LEU:N	2.14	0.44
2:B:56:ARG:N	2:B:56:ARG:CD	2.79	0.44
2:B:97:ARG:HG2	2:B:98:HIS:N	2.32	0.44
2:B:131:PRO:HD3	2:B:217:LYS:HD2	2.00	0.44
2:B:171:VAL:HG23	2:B:189:VAL:HG12	2.00	0.44
2:B:180:SER:HA	3:L:60:GLY:O	2.18	0.44
3:C:159:GLN:HG3	3:C:160:ASN:N	2.33	0.44
3:C:173:ASP:HB2	3:C:174:SER:H	1.72	0.44
3:F:79:ASN:O	3:F:80:PRO:O	2.35	0.44
3:F:115:ALA:HA	3:F:116:PRO:HD2	1.87	0.44
1:G:64:ASN:OD1	1:G:65:PRO:HD2	2.17	0.44
1:G:86:ASP:OD1	1:G:86:ASP:N	2.50	0.44
1:G:200:PHE:CG	1:G:201:VAL:N	2.85	0.44
3:I:7:PRO:CG	3:I:21:THR:H	2.30	0.44
1:J:172:GLU:O	1:J:256:ALA:HA	2.17	0.44
2:K:17:LEU:N	2:K:82:MET:O	2.43	0.44
2:K:51:LEU:H	2:K:51:LEU:HG	1.62	0.44
2:K:194:SER:O	2:K:197:LEU:HG	2.16	0.44
3:L:142:PHE:HE2	3:L:177:SER:N	2.15	0.44
1:A:176:LEU:HD12	1:A:176:LEU:N	2.33	0.44
1:D:101:LEU:O	1:D:103:GLU:N	2.51	0.44
2:E:4:LEU:HD12	2:E:111:TRP:C	2.42	0.44
1:G:192:TYR:HB3	1:G:246:GLY:HA3	1.99	0.44
2:H:98:HIS:HA	3:I:36:ILE:HG22	1.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1:ILE:HD11	3:I:98:PRO:CB	2.42	0.44
3:I:40:GLN:HB2	3:I:89:TYR:CE1	2.53	0.44
3:L:142:PHE:CE2	3:L:177:SER:N	2.85	0.44
3:L:170:ASP:OD2	3:L:172:LYS:N	2.50	0.44
3:C:41:GLN:HG3	3:C:45:GLN:O	2.17	0.44
1:D:127:ASP:OD2	1:D:130:LYS:HG2	2.18	0.44
2:E:206:VAL:C	2:E:207:ASN:OD1	2.61	0.44
3:F:70:SER:OG	3:F:71:GLY:N	2.50	0.44
3:F:81:VAL:HG13	3:F:85:ASP:HB2	2.00	0.44
2:H:34:SER:HA	2:H:49:GLY:HA2	1.98	0.44
3:I:86:THR:O	3:I:89:TYR:HE2	2.00	0.44
1:J:84:SER:O	1:J:85:SER:C	2.60	0.44
1:J:101:LEU:HD22	1:J:105:LEU:HD11	1.98	0.44
1:J:153:LYS:HZ1	1:J:190:SER:HA	1.81	0.44
1:A:65:PRO:C	1:A:67:CYS:H	2.24	0.44
3:C:42:LYS:O	3:C:44:GLY:N	2.50	0.44
3:C:128:LEU:CD1	3:C:129:THR:H	2.19	0.44
2:E:192:VAL:HG12	2:E:193:PRO:HD2	1.99	0.44
3:F:51:ILE:HD11	3:F:66:SER:HA	2.00	0.44
3:F:162:VAL:O	3:F:162:VAL:HG23	2.17	0.44
1:G:177:TRP:HZ2	1:G:206:TYR:CZ	2.35	0.44
1:G:239:LYS:O	1:G:239:LYS:HD2	2.18	0.44
2:H:34:SER:HB2	2:H:98:HIS:NE2	2.33	0.44
1:J:114:PHE:N	1:J:114:PHE:CD2	2.85	0.44
1:J:217:ARG:O	1:J:218:PRO:C	2.60	0.44
2:K:51:LEU:HD11	2:K:56:ARG:HB2	1.99	0.44
2:K:68:THR:N	2:K:81:GLU:O	2.44	0.44
3:L:53:THR:HG22	3:L:53:THR:O	2.17	0.44
3:L:64:ARG:NH2	3:L:85:ASP:OD1	2.51	0.44
3:C:12:VAL:HG11	3:C:81:VAL:HG21	2.00	0.44
3:C:152:LYS:O	3:C:195:TYR:HA	2.18	0.44
1:D:137:PRO:HA	1:D:143:SER:N	2.28	0.44
2:E:4:LEU:HB2	2:E:112:GLY:HA3	2.00	0.44
3:F:8:ALA:O	3:F:9:SER:CB	2.64	0.44
1:G:56:ASN:O	1:G:57:ILE:C	2.61	0.44
1:G:161:LEU:C	1:G:161:LEU:CD2	2.91	0.44
1:G:173:VAL:O	1:G:234:VAL:N	2.42	0.44
2:H:163:ASN:C	2:H:164:SER:HG	2.23	0.44
2:H:176:ALA:HB2	3:I:166:TRP:NE1	2.31	0.44
3:I:37:ASN:HD22	3:I:38:TRP:C	2.26	0.44
3:I:161:GLY:C	3:I:162:VAL:HG13	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:190:GLU:HB3	3:I:191:ARG:H	1.57	0.44
1:J:48:ALA:HB2	1:J:78:TYR:HE1	1.78	0.44
1:J:56:ASN:ND2	1:J:88:GLY:HA2	2.33	0.44
2:K:98:HIS:CD2	3:L:36:ILE:HG21	2.52	0.44
3:L:189:TYR:HB3	3:L:190:GLU:H	1.59	0.44
1:A:117:PHE:HB2	1:A:122:SER:OG	2.17	0.44
1:A:137:PRO:HA	1:A:143:SER:N	2.28	0.44
1:A:147:ASN:ND2	1:A:253:TYR:HB2	2.33	0.44
1:A:153:LYS:HD2	1:A:156:ASN:HA	2.00	0.44
2:E:161:SER:HG	2:E:163:ASN:HD22	1.63	0.44
3:F:120:ILE:HG12	3:F:121:PHE:N	2.32	0.44
2:K:69:ILE:HG13	2:K:70:SER:H	1.83	0.44
2:K:163:ASN:O	2:K:164:SER:HB2	2.18	0.44
3:L:38:TRP:C	3:L:38:TRP:HD1	2.26	0.44
3:L:115:ALA:HA	3:L:116:PRO:HD3	1.78	0.44
1:A:165:TYR:C	1:A:165:TYR:CD2	2.95	0.43
2:B:37:ARG:O	2:B:45:GLU:N	2.33	0.43
2:B:186:LEU:HD12	2:B:187:SER:C	2.42	0.43
3:C:158:ARG:NH2	2:K:97:ARG:HD2	2.29	0.43
1:D:79:ILE:H	1:D:79:ILE:CD1	2.24	0.43
2:E:32:ASP:C	2:E:98:HIS:NE2	2.76	0.43
2:E:168:THR:O	2:E:169:SER:CB	2.66	0.43
2:E:174:PHE:O	3:F:166:TRP:CD1	2.70	0.43
3:F:211:SER:O	3:F:212:PHE:CB	2.66	0.43
2:H:111:TRP:CH2	3:I:38:TRP:CE3	3.06	0.43
2:H:178:LEU:N	2:H:183:LEU:O	2.49	0.43
2:K:59:TYR:HE1	2:K:69:ILE:HG22	1.80	0.43
2:K:99:SER:HB3	3:L:35:PHE:CD1	2.53	0.43
2:B:26:PHE:O	2:B:27:THR:C	2.61	0.43
2:B:36:ILE:HA	2:B:47:VAL:HG22	2.00	0.43
2:B:50:ILE:HD12	2:B:55:GLU:HG3	2.00	0.43
2:B:157:PRO:O	2:B:208:HIS:CD2	2.68	0.43
3:C:54:ALA:O	3:C:67:GLY:C	2.61	0.43
3:C:64:ARG:HB3	3:C:80:PRO:HD2	1.99	0.43
3:F:189:TYR:HB3	3:F:190:GLU:H	1.57	0.43
3:I:7:PRO:HD2	3:I:21:THR:O	2.17	0.43
2:K:170:SER:HB2	2:K:189:VAL:O	2.18	0.43
3:L:209:VAL:HG23	3:L:210:LYS:HB2	2.00	0.43
1:A:82:THR:O	1:A:82:THR:OG1	2.32	0.43
1:A:121:SER:HB3	2:B:58:TYR:HA	2.00	0.43
1:D:184:THR:C	1:D:214:ILE:HG21	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:CYS:HB2	1:G:60:TRP:HB2	2.00	0.43
1:G:200:PHE:O	1:G:201:VAL:HG23	2.18	0.43
2:H:34:SER:HB3	2:H:48:SER:O	2.18	0.43
2:H:124:THR:OG1	2:H:155:PRO:HD3	2.19	0.43
2:H:130:PHE:CD1	3:I:126:GLU:HB2	2.54	0.43
3:I:195:TYR:H	3:I:210:LYS:HA	1.83	0.43
1:J:123:TRP:CZ3	1:J:163:LYS:HG3	2.50	0.43
2:K:215:VAL:HG23	2:K:216:ASP:N	2.32	0.43
3:L:108:GLU:CD	3:L:109:ILE:N	2.71	0.43
3:L:143:TYR:CD2	3:L:144:PRO:CD	3.01	0.43
3:L:156:SER:OG	3:L:157:GLU:N	2.50	0.43
2:B:51:LEU:CD1	2:B:56:ARG:HG2	2.48	0.43
3:C:97:VAL:O	3:C:98:PRO:C	2.59	0.43
3:C:139:LEU:O	3:C:142:PHE:CE2	2.72	0.43
3:C:140:ASN:ND2	3:C:176:TYR:CD1	2.86	0.43
1:D:99:GLU:CG	1:D:100:GLU:N	2.81	0.43
1:D:127:ASP:OD2	1:D:127:ASP:C	2.60	0.43
1:D:183:SER:HB2	1:D:184:THR:HG23	1.99	0.43
2:E:211:SER:O	2:E:212:ASN:HB3	2.18	0.43
3:F:49:LEU:HD11	3:F:52:TYR:HB3	2.01	0.43
3:F:152:LYS:O	3:F:195:TYR:HA	2.18	0.43
2:H:150:VAL:O	2:H:185:SER:HA	2.18	0.43
2:H:174:PHE:CD2	3:I:166:TRP:CE3	3.04	0.43
1:J:165:TYR:OH	1:J:169:LYS:HD2	2.18	0.43
2:K:197:LEU:O	2:K:197:LEU:CD1	2.62	0.43
2:B:130:PHE:CE1	3:C:127:GLN:HG3	2.53	0.43
3:C:46:PRO:HA	3:C:47:PRO:HD3	1.61	0.43
3:C:183:THR:HG22	3:C:184:LEU:N	2.34	0.43
2:E:97:ARG:HG2	2:E:98:HIS:N	2.34	0.43
2:E:177:VAL:HG22	2:E:184:TYR:HE2	1.84	0.43
3:F:85:ASP:O	3:F:86:THR:C	2.61	0.43
3:F:163:LEU:HD23	3:F:163:LEU:O	2.19	0.43
1:G:79:ILE:HG22	1:G:80:VAL:H	1.81	0.43
1:G:83:SER:C	1:G:85:SER:H	2.26	0.43
1:G:100:GLU:HG2	1:G:231:TRP:CZ2	2.53	0.43
1:J:158:TYR:C	1:J:158:TYR:CD1	2.96	0.43
1:J:169:LYS:HZ1	1:J:256:ALA:HB1	1.84	0.43
2:K:82:MET:HB2	2:K:85:LEU:HD21	2.00	0.43
1:A:91:TYR:OH	1:A:180:HIS:NE2	2.32	0.43
1:A:101:LEU:O	1:A:102:ARG:C	2.61	0.43
1:A:101:LEU:CD2	1:A:105:LEU:HG	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LEU:O	2:B:79:TYR:HA	2.18	0.43
3:C:81:VAL:HG11	3:C:109:ILE:HG13	1.99	0.43
1:D:107:SER:OG	1:D:259:ARG:HG2	2.19	0.43
1:D:167:ASN:OD1	1:D:167:ASN:C	2.60	0.43
2:E:177:VAL:O	2:E:178:LEU:C	2.59	0.43
3:F:102:PHE:CG	3:F:103:GLY:N	2.86	0.43
3:F:189:TYR:O	3:F:190:GLU:HB2	2.19	0.43
2:H:46:TRP:HE3	2:H:60:ARG:NH2	2.16	0.43
3:L:24:ALA:O	3:L:72:THR:OG1	2.32	0.43
3:L:37:ASN:O	3:L:49:LEU:HA	2.19	0.43
1:A:181:HIS:HB3	1:A:213:GLU:O	2.19	0.43
1:A:220:VAL:O	1:A:221:ARG:HB2	2.19	0.43
2:E:13:PRO:C	2:E:15:GLY:H	2.27	0.43
2:E:90:THR:O	2:E:91:ALA:HB2	2.18	0.43
2:E:178:LEU:HB3	2:E:180:SER:HB2	2.01	0.43
1:J:118:PRO:O	1:J:122:SER:CB	2.66	0.43
1:J:188:GLN:NE2	1:J:247:ASN:OD1	2.51	0.43
3:L:57:LYS:HD3	3:L:61:VAL:O	2.19	0.43
2:B:38:GLN:O	2:B:38:GLN:CG	2.66	0.43
2:B:211:SER:O	2:B:212:ASN:CB	2.66	0.43
3:C:26:GLU:HG2	3:C:27:SER:H	1.84	0.43
3:C:39:PHE:HB3	3:C:50:LEU:CD1	2.41	0.43
3:C:48:LYS:HG2	3:C:49:LEU:N	2.34	0.43
3:C:50:LEU:HD22	3:C:65:PHE:CG	2.53	0.43
1:D:64:ASN:O	1:D:67:CYS:HB2	2.18	0.43
1:D:113:ARG:HA	1:D:254:ALA:O	2.19	0.43
3:F:13:SER:CB	3:F:110:LYS:HB3	2.49	0.43
3:F:52:TYR:HE2	3:F:58:GLY:HA2	1.82	0.43
2:H:11:VAL:HG22	2:H:12:GLN:N	2.33	0.43
3:I:56:ASN:OD1	3:I:56:ASN:N	2.51	0.43
3:I:116:PRO:CB	3:I:139:LEU:HB3	2.41	0.43
1:J:219:LYS:CD	1:J:222:ASP:HA	2.36	0.43
2:K:183:LEU:HD13	2:K:183:LEU:HA	1.85	0.43
3:C:177:SER:O	3:C:178:MET:HG3	2.18	0.43
1:D:192:TYR:CD1	1:D:192:TYR:N	2.87	0.43
2:E:208:HIS:O	2:E:209:LYS:C	2.61	0.43
2:E:208:HIS:NE2	2:E:210:PRO:CG	2.81	0.43
3:F:66:SER:O	3:F:77:THR:HG22	2.18	0.43
3:F:173:ASP:OD1	3:F:174:SER:C	2.62	0.43
1:G:199:VAL:CG1	1:G:200:PHE:N	2.78	0.43
2:H:63:VAL:HG13	2:H:66:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:90:PHE:HA	3:I:102:PHE:CE2	2.53	0.43
1:J:79:ILE:HG22	1:J:80:VAL:N	2.33	0.43
1:J:116:ILE:HG12	1:J:117:PHE:CG	2.54	0.43
2:K:110:GLY:C	2:K:111:TRP:CD1	2.97	0.43
2:K:133:ALA:C	3:L:121:PHE:CE1	2.90	0.43
2:K:162:TRP:CE3	2:K:204:CYS:HB3	2.53	0.43
2:K:176:ALA:HB2	3:L:166:TRP:NE1	2.31	0.43
2:K:207:ASN:CA	2:K:213:THR:O	2.67	0.43
3:L:145:LYS:CD	3:L:167:THR:HG21	2.47	0.43
2:B:100:TRP:CD2	3:C:34:ASN:HA	2.54	0.43
2:B:122:ALA:HB3	2:B:154:PHE:CZ	2.54	0.43
3:C:39:PHE:CD1	3:C:76:LEU:HD13	2.53	0.43
3:F:8:ALA:CB	3:F:105:THR:HG23	2.38	0.43
3:F:97:VAL:O	3:F:99:TYR:CE1	2.72	0.43
3:F:192:HIS:O	3:F:195:TYR:CZ	2.72	0.43
3:F:202:LYS:O	3:F:203:THR:CG2	2.59	0.43
2:H:27:THR:HG22	2:H:31:TYR:HD2	1.82	0.43
1:J:227:MET:HB3	1:J:227:MET:HE2	1.72	0.43
3:L:45:GLN:HA	3:L:45:GLN:OE1	2.18	0.43
1:A:179:ILE:HD11	1:A:199:VAL:CG1	2.45	0.42
2:B:36:ILE:HG13	2:B:45:GLU:O	2.19	0.42
2:B:86:ARG:N	2:B:119:VAL:HG11	2.34	0.42
3:C:38:TRP:HH2	3:C:89:TYR:CB	2.25	0.42
1:D:115:GLU:HB2	3:F:96:GLU:CD	2.43	0.42
3:F:45:GLN:CB	3:F:46:PRO:HD2	2.48	0.42
3:F:150:LYS:HB3	3:F:198:GLU:HG2	2.01	0.42
1:G:116:ILE:N	1:G:252:ARG:O	2.52	0.42
1:G:167:ASN:OD1	1:G:169:LYS:HB2	2.19	0.42
1:G:215:ALA:H	1:G:217:ARG:NH1	2.17	0.42
2:H:33:MET:C	2:H:98:HIS:NE2	2.77	0.42
2:H:203:ILE:HG13	2:H:217:LYS:O	2.19	0.42
1:J:158:TYR:C	1:J:158:TYR:HD1	2.27	0.42
3:L:42:LYS:CD	3:L:87:ALA:HB2	2.41	0.42
3:L:164:ASN:HB3	4:L:302:HOH:O	2.17	0.42
3:L:175:THR:HB	3:L:176:TYR:CD1	2.54	0.42
1:A:55:CYS:SG	1:A:66:GLU:CG	3.04	0.42
2:B:9:ALA:O	2:B:117:VAL:HA	2.19	0.42
2:B:85:LEU:HD23	2:B:85:LEU:HA	1.85	0.42
2:E:4:LEU:HD11	2:E:110:GLY:O	2.20	0.42
2:E:88:GLU:HG3	2:E:89:ASP:N	2.33	0.42
3:F:126:GLU:CD	3:F:126:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:LEU:HB3	2:H:82:MET:HE2	2.02	0.42
2:H:66:ARG:NH2	2:H:84:SER:O	2.52	0.42
2:H:174:PHE:CG	2:H:175:PRO:HD2	2.50	0.42
2:H:178:LEU:O	2:H:178:LEU:HD23	2.20	0.42
2:H:218:LYS:NZ	2:H:218:LYS:CB	2.82	0.42
3:I:145:LYS:CA	3:I:147:ILE:N	2.77	0.42
1:J:67:CYS:C	1:J:68:GLU:CG	2.89	0.42
2:K:34:SER:HB2	2:K:98:HIS:NE2	2.34	0.42
3:L:142:PHE:CE1	3:L:144:PRO:O	2.73	0.42
1:A:85:SER:OG	1:A:86:ASP:N	2.53	0.42
1:A:239:LYS:NZ	1:A:241:THR:OG1	2.47	0.42
3:C:97:VAL:O	3:C:99:TYR:CD1	2.71	0.42
3:C:167:THR:HG22	3:C:168:ASP:N	2.23	0.42
1:D:77:SER:OG	1:D:78:TYR:N	2.51	0.42
2:E:180:SER:H	3:I:60:GLY:HA2	1.85	0.42
3:F:13:SER:HB3	3:F:110:LYS:HZ2	1.83	0.42
3:F:42:LYS:NZ	3:F:84:GLU:OE1	2.38	0.42
1:G:133:THR:CG2	1:G:144:PHE:HD1	2.31	0.42
1:G:219:LYS:HD3	1:G:224:GLU:HG3	2.02	0.42
2:H:125:LYS:CE	2:H:126:GLY:O	2.67	0.42
2:H:161:SER:HB3	2:H:205:ASN:ND2	2.34	0.42
3:I:141:ASN:CA	3:I:175:THR:HG22	2.29	0.42
3:I:162:VAL:O	3:I:164:ASN:OD1	2.37	0.42
3:L:40:GLN:HB2	3:L:50:LEU:HD11	2.01	0.42
2:B:75:ARG:C	2:B:77:THR:H	2.28	0.42
3:C:38:TRP:NE1	3:C:90:PHE:O	2.52	0.42
3:C:139:LEU:O	3:C:142:PHE:HE2	2.02	0.42
2:E:146:LEU:HD13	2:E:146:LEU:HA	1.77	0.42
2:E:203:ILE:HG13	2:E:217:LYS:O	2.20	0.42
3:F:13:SER:HB3	3:F:110:LYS:CB	2.48	0.42
3:F:191:ARG:HG3	3:F:192:HIS:CE1	2.54	0.42
2:H:39:ALA:H	2:H:44:LEU:HB2	1.85	0.42
2:H:153:TYR:CD1	2:H:153:TYR:C	2.97	0.42
3:I:7:PRO:HG2	3:I:7:PRO:O	2.19	0.42
3:I:202:LYS:C	3:I:203:THR:HG1	2.23	0.42
1:J:117:PHE:HB2	1:J:251:PRO:O	2.18	0.42
1:J:179:ILE:O	1:J:179:ILE:HG13	2.19	0.42
3:L:147:ILE:HG12	3:L:200:THR:O	2.19	0.42
2:B:150:VAL:O	2:B:186:LEU:N	2.47	0.42
2:B:196:SER:HB3	2:B:202:TYR:CE2	2.54	0.42
3:C:110:LYS:HZ2	3:C:110:LYS:CB	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:CYS:C	1:D:68:GLU:HG3	2.44	0.42
1:D:117:PHE:O	1:D:118:PRO:C	2.58	0.42
2:E:69:ILE:HG12	2:E:70:SER:N	2.33	0.42
2:E:143:THR:CG2	2:E:191:THR:HG23	2.48	0.42
2:E:166:ALA:C	2:E:168:THR:N	2.77	0.42
3:F:150:LYS:HB3	3:F:198:GLU:CG	2.49	0.42
1:G:76:TRP:CZ3	1:G:108:VAL:HG21	2.54	0.42
1:G:199:VAL:CG1	1:G:200:PHE:H	2.14	0.42
1:G:240:ILE:HG23	1:G:240:ILE:O	2.18	0.42
2:H:163:ASN:C	2:H:164:SER:OG	2.62	0.42
2:H:183:LEU:HA	2:H:183:LEU:HD13	1.75	0.42
1:J:76:TRP:CD1	1:J:76:TRP:C	2.97	0.42
2:K:100:TRP:HE1	3:L:34:ASN:HA	1.85	0.42
3:L:37:ASN:OD1	3:L:38:TRP:N	2.52	0.42
2:B:45:GLU:HA	2:B:45:GLU:OE2	2.19	0.42
3:C:6:SER:HA	3:C:21:THR:O	2.19	0.42
3:C:42:LYS:HA	3:C:42:LYS:HE2	2.01	0.42
1:D:184:THR:H	1:D:187:ASP:HB2	1.84	0.42
1:D:208:LYS:CG	1:D:209:LYS:N	2.82	0.42
1:D:220:VAL:O	1:D:221:ARG:HB2	2.18	0.42
2:E:50:ILE:CD1	2:E:71:ARG:HB2	2.37	0.42
2:E:141:GLY:C	2:E:143:THR:H	2.28	0.42
3:F:128:LEU:HG	3:F:129:THR:N	2.35	0.42
3:F:162:VAL:O	3:F:164:ASN:OD1	2.37	0.42
1:G:102:ARG:HG3	1:G:103:GLU:N	2.35	0.42
2:H:9:ALA:C	2:H:10:VAL:HG23	2.45	0.42
2:H:27:THR:CG2	2:H:30:ASP:H	2.33	0.42
3:I:62:PRO:HD2	3:I:65:PHE:CE2	2.55	0.42
3:I:165:SER:HA	3:I:178:MET:O	2.19	0.42
3:I:168:ASP:O	3:I:169:GLN:HB2	2.19	0.42
3:I:204:SER:C	3:I:205:THR:HG22	2.45	0.42
1:J:92:PRO:HG3	1:J:223:GLN:HB2	2.01	0.42
1:J:215:ALA:O	1:J:217:ARG:HD2	2.20	0.42
2:K:161:SER:O	2:K:204:CYS:HA	2.19	0.42
3:L:129:THR:O	3:L:130:SER:OG	2.36	0.42
3:C:192:HIS:CE1	3:C:194:SER:CB	3.02	0.42
1:D:91:TYR:O	1:D:229:TYR:OH	2.29	0.42
1:D:127:ASP:HB2	1:D:154:LYS:CB	2.49	0.42
1:D:217:ARG:HD2	1:D:226:ARG:HG2	2.00	0.42
3:F:57:LYS:CB	3:F:57:LYS:HZ3	2.32	0.42
1:G:71:SER:O	1:G:73:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:127:ASP:N	1:J:154:LYS:HB2	2.34	0.42
2:K:76:LYS:C	2:K:77:THR:CG2	2.92	0.42
2:K:214:LYS:C	2:K:215:VAL:HG12	2.44	0.42
3:L:13:SER:N	3:L:110:LYS:HD2	2.34	0.42
3:L:42:LYS:C	3:L:44:GLY:N	2.68	0.42
3:L:95:LYS:C	3:L:99:TYR:HE1	2.26	0.42
2:B:72:ASP:C	2:B:72:ASP:OD1	2.61	0.42
1:D:52:LEU:HD12	1:D:81:GLU:HG2	2.00	0.42
1:D:149:ILE:CD1	1:D:252:ARG:HB2	2.50	0.42
2:E:76:LYS:HD3	2:E:76:LYS:HA	1.91	0.42
3:F:192:HIS:O	3:F:195:TYR:CE1	2.73	0.42
1:G:57:ILE:HD11	1:G:79:ILE:HD12	2.01	0.42
2:H:127:PRO:HB3	2:H:150:VAL:HG13	1.99	0.42
2:H:186:LEU:HD12	2:H:186:LEU:O	2.19	0.42
2:K:196:SER:O	2:K:200:GLN:HB2	2.20	0.42
3:L:108:GLU:C	3:L:109:ILE:HD12	2.44	0.42
3:L:143:TYR:HA	3:L:144:PRO:HA	1.61	0.42
2:B:35:TRP:HA	2:B:94:TYR:O	2.20	0.42
3:C:86:THR:H	3:C:107:LEU:HD22	1.84	0.42
1:D:69:SER:OG	1:D:70:LEU:HB2	2.20	0.42
2:E:59:TYR:CD2	2:E:59:TYR:N	2.88	0.42
2:E:215:VAL:CG2	2:E:216:ASP:N	2.82	0.42
3:F:2:GLN:NE2	3:F:97:VAL:HG21	2.35	0.42
3:F:159:GLN:CG	3:F:160:ASN:H	2.33	0.42
2:H:42:LYS:HE2	2:H:42:LYS:HB2	1.86	0.42
2:H:94:TYR:OH	3:I:45:GLN:OE1	2.33	0.42
3:I:35:PHE:O	3:I:35:PHE:CD1	2.73	0.42
3:I:140:ASN:HB3	3:I:176:TYR:CD1	2.55	0.42
2:K:19:LEU:N	2:K:19:LEU:CD1	2.83	0.42
3:L:97:VAL:HG13	3:L:98:PRO:N	2.35	0.42
1:A:96:ILE:N	1:A:96:ILE:HD13	2.35	0.42
2:B:173:THR:CG2	2:B:187:SER:O	2.67	0.42
3:C:82:GLU:N	3:C:85:ASP:OD2	2.47	0.42
3:C:118:VAL:HG13	3:C:139:LEU:HD23	2.01	0.42
1:D:240:ILE:O	1:D:240:ILE:HG23	2.19	0.42
2:E:85:LEU:HD23	2:E:85:LEU:HA	1.83	0.42
3:F:109:ILE:CG2	3:F:110:LYS:H	2.32	0.42
3:F:207:PRO:C	3:F:208:ILE:HD12	2.44	0.42
1:G:76:TRP:CZ2	1:G:105:LEU:O	2.73	0.42
3:L:52:TYR:CD1	3:L:56:ASN:HB2	2.55	0.42
3:L:95:LYS:C	3:L:99:TYR:CE1	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLN:NE2	1:A:231:TRP:CH2	2.88	0.41
1:A:133:THR:O	1:A:142:LYS:HB2	2.20	0.41
2:B:132:LEU:HD13	3:C:136:VAL:HB	2.02	0.41
3:C:38:TRP:HH2	3:C:89:TYR:CD1	2.33	0.41
3:C:136:VAL:HG22	3:C:180:SER:HB3	2.02	0.41
1:D:72:THR:O	1:D:73:ALA:HB2	2.20	0.41
2:E:127:PRO:HA	2:E:153:TYR:HB3	2.02	0.41
2:E:162:TRP:HB2	2:E:167:LEU:HD23	2.02	0.41
3:F:164:ASN:HB3	3:F:180:SER:N	2.35	0.41
1:G:90:CYS:O	1:G:221:ARG:NH1	2.53	0.41
2:H:130:PHE:HA	2:H:131:PRO:HD2	1.92	0.41
1:J:76:TRP:CE2	1:J:108:VAL:HG22	2.55	0.41
2:K:94:TYR:CE1	3:L:46:PRO:HB3	2.55	0.41
3:L:13:SER:CA	3:L:110:LYS:HD2	2.50	0.41
3:L:133:ALA:O	3:L:183:THR:O	2.38	0.41
1:A:219:LYS:HB2	1:A:219:LYS:HE3	1.84	0.41
1:D:116:ILE:CG2	1:D:117:PHE:H	2.33	0.41
1:D:119:LYS:HG2	1:D:120:THR:N	2.35	0.41
2:E:177:VAL:HA	2:E:184:TYR:HD2	1.84	0.41
3:F:38:TRP:HA	3:F:49:LEU:HD23	2.02	0.41
1:G:79:ILE:CG2	1:G:80:VAL:H	2.32	0.41
1:G:157:SER:C	1:G:159:PRO:HD3	2.45	0.41
1:G:173:VAL:HA	1:G:256:ALA:HA	2.02	0.41
2:H:63:VAL:HG13	2:H:66:ARG:H	1.85	0.41
1:J:51:HIS:CD2	1:J:80:VAL:CB	3.02	0.41
1:J:86:ASP:OD1	1:J:86:ASP:N	2.38	0.41
1:J:114:PHE:O	1:J:253:TYR:HA	2.19	0.41
2:K:39:ALA:HB3	2:K:44:LEU:HG	2.01	0.41
3:L:69:GLY:HA3	3:L:74:PHE:CD1	2.55	0.41
1:A:54:LYS:HD2	1:A:69:SER:HB2	2.02	0.41
2:B:85:LEU:HB3	2:B:119:VAL:CG1	2.50	0.41
3:C:35:PHE:HB3	3:C:95:LYS:CD	2.41	0.41
2:E:28:GLY:N	2:E:76:LYS:NZ	2.66	0.41
2:E:47:VAL:O	2:E:48:SER:CB	2.68	0.41
2:E:133:ALA:HA	2:E:134:PRO:HD3	1.87	0.41
2:E:177:VAL:HA	2:E:184:TYR:HA	2.02	0.41
1:G:79:ILE:HD11	1:G:105:LEU:CB	2.50	0.41
1:G:164:SER:C	2:H:56:ARG:HH22	2.29	0.41
2:H:48:SER:OG	2:H:49:GLY:N	2.53	0.41
3:I:165:SER:C	3:I:166:TRP:CD1	2.98	0.41
3:L:128:LEU:HG	3:L:129:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:HD2	1:A:253:TYR:CD2	2.55	0.41
2:B:133:ALA:HA	2:B:134:PRO:HD3	1.94	0.41
2:B:134:PRO:HD3	2:B:146:LEU:CD1	2.50	0.41
1:D:65:PRO:C	1:D:67:CYS:N	2.78	0.41
1:D:205:ARG:HA	1:D:205:ARG:HD2	1.48	0.41
1:G:61:ILE:O	1:G:61:ILE:HG13	2.19	0.41
2:H:97:ARG:HB3	2:H:110:GLY:CA	2.32	0.41
1:J:169:LYS:NZ	1:J:256:ALA:HB1	2.35	0.41
1:J:171:LYS:NZ	1:J:258:GLU:HG3	2.34	0.41
2:K:99:SER:O	2:K:100:TRP:CG	2.73	0.41
3:L:83:ALA:O	3:L:171:SER:O	2.38	0.41
1:A:119:LYS:O	1:A:123:TRP:CD1	2.73	0.41
1:A:161:LEU:HD22	1:A:244:ALA:HB3	2.03	0.41
2:B:27:THR:HG21	2:B:31:TYR:CG	2.55	0.41
2:B:64:LYS:HD3	2:B:64:LYS:HA	1.32	0.41
2:B:171:VAL:O	2:B:188:SER:HA	2.20	0.41
2:B:174:PHE:N	2:B:174:PHE:HD1	2.19	0.41
3:C:34:ASN:N	3:C:34:ASN:HD22	2.18	0.41
3:C:78:ILE:CD1	3:C:85:ASP:CG	2.93	0.41
2:H:36:ILE:HD13	2:H:111:TRP:CH2	2.55	0.41
2:H:50:ILE:HG23	2:H:69:ILE:CD1	2.47	0.41
2:H:94:TYR:CE1	2:H:113:GLN:C	2.99	0.41
1:J:115:GLU:HG2	3:L:96:GLU:HG2	2.02	0.41
2:K:26:PHE:HB3	2:K:27:THR:H	1.47	0.41
3:C:118:VAL:HB	3:C:208:ILE:CD1	2.50	0.41
2:E:39:ALA:HA	2:E:91:ALA:CB	2.51	0.41
3:F:42:LYS:NZ	3:F:84:GLU:O	2.54	0.41
3:F:147:ILE:HG23	3:F:147:ILE:O	2.21	0.41
1:G:166:ILE:HD13	1:G:166:ILE:H	1.83	0.41
2:H:51:LEU:CD1	2:H:56:ARG:H	2.33	0.41
2:H:60:ARG:NH2	3:I:99:TYR:O	2.45	0.41
2:H:94:TYR:CE1	3:I:47:PRO:HD2	2.56	0.41
2:H:205:ASN:HB3	2:H:216:ASP:OD1	2.20	0.41
3:I:4:THR:O	3:I:102:PHE:HB2	2.20	0.41
2:K:10:VAL:HG12	2:K:118:THR:O	2.21	0.41
3:L:16:GLN:OE1	3:L:16:GLN:HA	2.21	0.41
1:A:84:SER:O	1:A:85:SER:C	2.64	0.41
1:A:123:TRP:HZ3	1:A:163:LYS:HG3	1.84	0.41
2:B:35:TRP:HB2	2:B:48:SER:OG	2.20	0.41
3:C:3:MET:O	3:C:25:SER:HB3	2.21	0.41
3:C:17:ARG:CZ	3:C:17:ARG:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:109:ILE:N	3:C:109:ILE:CD1	2.79	0.41
3:C:142:PHE:O	3:C:174:SER:HB3	2.21	0.41
3:C:168:ASP:OD1	3:C:176:TYR:O	2.38	0.41
1:D:54:LYS:CD	1:D:67:CYS:HA	2.50	0.41
1:D:165:TYR:CE2	1:D:167:ASN:HB2	2.54	0.41
3:F:38:TRP:CZ3	3:F:39:PHE:CG	3.08	0.41
1:G:58:ALA:HB2	1:G:98:TYR:HE1	1.82	0.41
1:G:116:ILE:HG22	1:G:252:ARG:O	2.21	0.41
1:G:136:CYS:HB3	1:G:144:PHE:HA	2.01	0.41
2:H:27:THR:CG2	2:H:30:ASP:HB3	2.50	0.41
3:I:20:ILE:CG2	3:I:21:THR:N	2.83	0.41
3:I:21:THR:HG22	3:I:75:THR:OG1	2.21	0.41
3:I:121:PHE:N	3:I:136:VAL:O	2.47	0.41
3:I:135:VAL:HG22	3:I:151:TRP:CH2	2.55	0.41
1:J:56:ASN:HB3	1:J:83:SER:HA	2.02	0.41
1:A:60:TRP:C	1:A:62:LEU:N	2.78	0.41
1:A:263:SER:OG	1:A:264:GLY:N	2.52	0.41
2:B:27:THR:HG22	2:B:31:TYR:CG	2.55	0.41
2:B:178:LEU:HB3	2:B:183:LEU:HB3	2.01	0.41
3:C:92:GLN:OE1	3:C:101:THR:HG21	2.21	0.41
3:C:135:VAL:HG12	3:C:151:TRP:CH2	2.52	0.41
1:D:149:ILE:HG13	1:D:252:ARG:HB2	2.02	0.41
1:D:184:THR:OG1	1:D:186:ALA:HB3	2.21	0.41
2:E:161:SER:OG	2:E:163:ASN:ND2	2.45	0.41
1:G:180:HIS:HD2	1:G:227:MET:HG3	1.86	0.41
1:G:187:ASP:HA	1:G:190:SER:OG	2.20	0.41
2:H:17:LEU:HD23	2:H:117:VAL:HG23	2.03	0.41
2:H:63:VAL:HG12	2:H:64:LYS:N	2.35	0.41
1:J:49:PRO:O	1:J:78:TYR:O	2.39	0.41
1:J:101:LEU:O	1:J:102:ARG:C	2.62	0.41
3:L:210:LYS:HB3	3:L:211:SER:H	1.39	0.41
1:A:58:ALA:O	1:A:62:LEU:HB2	2.21	0.41
1:A:157:SER:OG	1:A:159:PRO:HD3	2.20	0.41
1:A:217:ARG:HB3	1:A:218:PRO:HD2	2.01	0.41
2:B:45:GLU:HG2	2:B:60:ARG:NH1	2.36	0.41
3:C:153:ILE:CG1	3:C:154:ASP:N	2.81	0.41
3:C:167:THR:CG2	3:C:168:ASP:H	2.27	0.41
1:D:137:PRO:CB	1:D:142:LYS:HA	2.50	0.41
2:E:26:PHE:HB3	2:E:27:THR:H	1.64	0.41
2:E:156:GLU:CB	2:E:157:PRO:CA	2.98	0.41
3:F:166:TRP:CE3	3:F:166:TRP:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:SER:C	1:G:191:LEU:HD12	2.46	0.41
2:H:96:ALA:HB1	3:I:36:ILE:HD12	2.03	0.41
2:H:97:ARG:NH2	2:H:110:GLY:N	2.68	0.41
3:I:7:PRO:HD3	3:I:21:THR:OG1	2.21	0.41
3:I:143:TYR:HA	3:I:144:PRO:HA	1.76	0.41
1:J:151:LEU:HD23	1:J:151:LEU:HA	1.94	0.41
2:K:36:ILE:CB	2:K:46:TRP:HA	2.48	0.41
2:K:82:MET:HE2	2:K:82:MET:HB3	1.60	0.41
3:L:41:GLN:HB2	3:L:47:PRO:HB3	2.02	0.41
3:L:120:ILE:HD12	3:L:120:ILE:HA	1.97	0.41
1:A:84:SER:OG	1:A:87:ASN:OD1	2.32	0.41
1:A:109:SER:HB3	1:A:258:GLU:CG	2.50	0.41
1:A:206:TYR:CD2	1:A:207:SER:N	2.88	0.41
2:B:200:GLN:O	2:B:202:TYR:CD2	2.74	0.41
2:B:209:LYS:N	2:B:210:PRO:CD	2.84	0.41
3:C:8:ALA:HB1	3:C:10:LEU:HG	2.03	0.41
3:C:92:GLN:CD	3:C:101:THR:CG2	2.94	0.41
3:C:196:THR:OG1	3:C:209:VAL:HB	2.21	0.41
1:D:138:HIS:N	1:D:141:ALA:O	2.43	0.41
1:D:200:PHE:CE2	1:D:201:VAL:O	2.74	0.41
3:F:153:ILE:CA	3:F:194:SER:O	2.67	0.41
2:H:100:TRP:HD1	3:I:34:ASN:N	2.19	0.41
3:I:70:SER:OG	3:I:71:GLY:N	2.54	0.41
3:I:184:LEU:O	3:I:189:TYR:HB2	2.21	0.41
1:J:126:HIS:C	1:J:154:LYS:HB2	2.46	0.41
3:L:91:CYS:N	3:L:102:PHE:CD2	2.82	0.41
1:A:116:ILE:HG23	1:A:117:PHE:H	1.87	0.40
2:B:10:VAL:HG22	2:B:155:PRO:CG	2.50	0.40
2:B:26:PHE:HD1	2:B:27:THR:H	1.69	0.40
3:C:39:PHE:HB2	3:C:50:LEU:CA	2.51	0.40
1:D:217:ARG:HB3	1:D:218:PRO:CD	2.51	0.40
3:F:38:TRP:CE2	3:F:39:PHE:CA	2.91	0.40
1:G:72:THR:H	1:G:72:THR:HG23	1.49	0.40
2:H:176:ALA:HB2	3:I:166:TRP:CZ2	2.51	0.40
2:H:178:LEU:CG	3:I:182:LEU:HD13	2.51	0.40
1:J:71:SER:OG	1:J:71:SER:O	2.34	0.40
1:J:92:PRO:HD2	1:J:223:GLN:HG3	2.03	0.40
3:L:44:GLY:O	3:L:45:GLN:HG2	2.21	0.40
1:A:96:ILE:HG21	1:D:215:ALA:HB1	2.03	0.40
2:B:21:CYS:O	2:B:77:THR:CA	2.68	0.40
3:C:35:PHE:HD1	3:C:37:ASN:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:17:LEU:HD23	2:E:117:VAL:HG13	2.01	0.40
2:E:75:ARG:C	2:E:77:THR:H	2.30	0.40
2:E:173:THR:O	2:E:173:THR:OG1	2.38	0.40
3:F:141:ASN:HD21	3:F:176:TYR:HE1	1.69	0.40
1:G:57:ILE:HG21	1:G:105:LEU:HD12	2.03	0.40
1:G:220:VAL:O	1:G:221:ARG:C	2.62	0.40
3:I:91:CYS:SG	3:I:102:PHE:HD2	2.44	0.40
1:J:95:PHE:HB3	1:J:98:TYR:CB	2.49	0.40
1:J:148:LEU:HD23	1:J:251:PRO:HA	2.03	0.40
2:K:55:GLU:HG2	2:K:71:ARG:HD2	2.03	0.40
1:A:79:ILE:H	1:A:79:ILE:HD12	1.85	0.40
1:A:174:LEU:HD21	1:A:176:LEU:HD11	2.02	0.40
2:B:47:VAL:O	2:B:48:SER:CB	2.69	0.40
2:B:177:VAL:HG13	2:B:184:TYR:CE2	2.56	0.40
1:D:57:ILE:O	1:D:58:ALA:C	2.65	0.40
1:D:227:MET:SD	1:D:249:VAL:HG21	2.61	0.40
1:G:95:PHE:HE2	1:G:231:TRP:HD1	1.70	0.40
1:G:115:GLU:O	1:G:115:GLU:HG3	2.21	0.40
2:H:94:TYR:HE1	3:I:46:PRO:HB3	1.86	0.40
3:I:20:ILE:CG2	3:I:21:THR:H	2.33	0.40
3:I:102:PHE:CD1	3:I:102:PHE:C	2.99	0.40
3:I:102:PHE:CD1	3:I:104:GLY:N	2.78	0.40
3:I:114:ALA:HA	3:I:201:HIS:HD2	1.85	0.40
3:I:138:PHE:HE1	3:I:178:MET:HG3	1.87	0.40
1:J:56:ASN:O	1:J:57:ILE:C	2.63	0.40
1:J:78:TYR:HA	1:J:106:SER:HA	2.04	0.40
1:J:102:ARG:NH1	1:J:102:ARG:CG	2.77	0.40
2:K:99:SER:HB3	3:L:35:PHE:CE1	2.56	0.40
2:K:177:VAL:HA	2:K:184:TYR:HA	2.04	0.40
3:L:132:GLY:HA2	3:L:184:LEU:HB3	2.03	0.40
1:A:56:ASN:HB2	1:A:81:GLU:OE1	2.21	0.40
2:B:10:VAL:HG13	2:B:118:THR:HB	2.02	0.40
2:B:51:LEU:HD11	2:B:55:GLU:N	2.36	0.40
2:B:86:ARG:NE	2:B:88:GLU:OE2	2.54	0.40
3:C:86:THR:N	3:C:107:LEU:HD22	2.37	0.40
3:C:108:GLU:CG	3:C:109:ILE:N	2.82	0.40
1:D:99:GLU:O	1:D:100:GLU:C	2.64	0.40
1:D:136:CYS:O	1:D:143:SER:O	2.38	0.40
2:E:22:ALA:HA	2:E:77:THR:HG22	2.03	0.40
3:F:65:PHE:CD1	3:F:78:ILE:HG12	2.56	0.40
3:F:129:THR:O	3:F:129:THR:OG1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:145:LYS:CD	3:F:167:THR:HG21	2.51	0.40
1:G:169:LYS:CE	1:G:256:ALA:CB	2.99	0.40
3:I:116:PRO:O	3:I:117:THR:C	2.64	0.40
1:J:48:ALA:HA	1:J:49:PRO:HD3	1.95	0.40
1:J:202:GLY:O	1:J:206:TYR:O	2.39	0.40
2:K:158:VAL:CG1	2:K:159:THR:N	2.84	0.40
2:K:174:PHE:HA	2:K:175:PRO:HD2	1.78	0.40
2:B:174:PHE:O	3:C:166:TRP:CD2	2.75	0.40
3:C:37:ASN:ND2	3:C:39:PHE:HE2	2.14	0.40
3:C:210:LYS:HG3	3:C:211:SER:N	2.37	0.40
1:D:52:LEU:HD21	1:D:60:TRP:CE3	2.57	0.40
1:D:184:THR:O	1:D:187:ASP:N	2.54	0.40
1:D:208:LYS:CG	1:D:209:LYS:H	2.35	0.40
3:F:57:LYS:CB	3:F:57:LYS:NZ	2.81	0.40
1:G:188:GLN:HE22	1:G:197:ALA:HB3	1.84	0.40
3:I:40:GLN:HA	3:I:88:ASN:O	2.22	0.40
1:J:78:TYR:HA	1:J:106:SER:CA	2.52	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	230/518 (44%)	198 (86%)	29 (13%)	3 (1%)	9	29
1	D	240/518 (46%)	199 (83%)	35 (15%)	6 (2%)	4	15
1	G	223/518 (43%)	193 (86%)	27 (12%)	3 (1%)	9	29
1	J	249/518 (48%)	211 (85%)	35 (14%)	3 (1%)	10	31
2	B	202/219 (92%)	175 (87%)	25 (12%)	2 (1%)	12	36
2	E	202/219 (92%)	172 (85%)	29 (14%)	1 (0%)	24	53
2	H	202/219 (92%)	174 (86%)	26 (13%)	2 (1%)	12	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	202/219 (92%)	177 (88%)	21 (10%)	4 (2%)	6	19
3	C	193/218 (88%)	150 (78%)	37 (19%)	6 (3%)	3	11
3	F	193/218 (88%)	142 (74%)	38 (20%)	13 (7%)	1	2
3	I	195/218 (89%)	141 (72%)	45 (23%)	9 (5%)	2	6
3	L	195/218 (89%)	145 (74%)	44 (23%)	6 (3%)	3	11
All	All	2526/3820 (66%)	2077 (82%)	391 (16%)	58 (2%)	5	16

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	8	ALA
3	F	173	ASP
3	L	144	PRO
3	L	147	ILE
1	A	120	THR
2	B	181	SER
3	C	40	GLN
3	F	8	ALA
3	F	28	VAL
3	F	190	GLU
3	F	203	THR
3	F	204	SER
1	G	84	SER
3	I	28	VAL
3	I	204	SER
2	K	64	LYS
3	L	28	VAL
3	C	12	VAL
3	C	28	VAL
1	D	119	LYS
2	E	64	LYS
3	F	9	SER
3	F	40	GLN
3	F	86	THR
2	H	179	GLN
2	K	179	GLN
3	L	128	LEU
1	D	70	LEU
1	D	120	THR
1	G	72	THR

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Mol	Chain	Res	Type
2	H	64	LYS
1	J	201	VAL
2	B	183	LEU
1	D	188	GLN
1	G	201	VAL
3	I	85	ASP
2	K	164	SER
3	L	97	VAL
3	C	97	VAL
3	F	162	VAL
3	I	27	SER
3	I	79	ASN
3	I	97	VAL
3	I	162	VAL
3	L	162	VAL
3	C	162	VAL
3	F	79	ASN
3	F	97	VAL
1	J	386	ILE
1	A	57	ILE
1	D	201	VAL
3	F	12	VAL
3	I	12	VAL
1	J	47	VAL
2	K	63	VAL
1	A	47	VAL
1	D	57	ILE
3	I	144	PRO

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	190/451 (42%)	158 (83%)	32 (17%)	2	7
1	D	190/451 (42%)	151 (80%)	39 (20%)	1	4
1	G	190/451 (42%)	156 (82%)	34 (18%)	2	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	190/451 (42%)	154 (81%)	36 (19%)	1	5
2	B	173/182 (95%)	130 (75%)	43 (25%)	0	2
2	E	173/182 (95%)	125 (72%)	48 (28%)	0	1
2	H	173/182 (95%)	133 (77%)	40 (23%)	1	2
2	K	173/182 (95%)	133 (77%)	40 (23%)	1	2
3	C	177/190 (93%)	124 (70%)	53 (30%)	0	1
3	F	177/190 (93%)	127 (72%)	50 (28%)	0	1
3	I	177/190 (93%)	124 (70%)	53 (30%)	0	1
3	L	177/190 (93%)	123 (70%)	54 (30%)	0	1
All	All	2160/3292 (66%)	1638 (76%)	522 (24%)	1	2

All (522) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	61	ILE
1	A	68	GLU
1	A	70	LEU
1	A	79	ILE
1	A	82	THR
1	A	83	SER
1	A	87	ASN
1	A	94	ASP
1	A	101	LEU
1	A	104	GLN
1	A	117	PHE
1	A	126	HIS
1	A	132	VAL
1	A	136	CYS
1	A	138	HIS
1	A	143	SER
1	A	152	VAL
1	A	161	LEU
1	A	164	SER
1	A	166	ILE
1	A	174	LEU
1	A	191	LEU
1	A	206	TYR
1	A	226	ARG

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Mol	Chain	Res	Type
1	A	232	THR
1	A	235	GLU
1	A	238	ASP
1	A	239	LYS
1	A	245	THR
1	A	258	GLU
1	A	259	ARG
2	B	7	SER
2	B	10	VAL
2	B	11	VAL
2	B	16	SER
2	B	19	LEU
2	B	26	PHE
2	B	29	SER
2	B	32	ASP
2	B	36	ILE
2	B	42	LYS
2	B	51	LEU
2	B	54	SER
2	B	55	GLU
2	B	59	TYR
2	B	60	ARG
2	B	64	LYS
2	B	68	THR
2	B	78	LEU
2	B	92	VAL
2	B	100	TRP
2	B	119	VAL
2	B	143	THR
2	B	146	LEU
2	B	148	CYS
2	B	158	VAL
2	B	159	THR
2	B	161	SER
2	B	167	LEU
2	B	171	VAL
2	B	173	THR
2	B	177	VAL
2	B	180	SER
2	B	186	LEU
2	B	187	SER
2	B	188	SER

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Mol	Chain	Res	Type
2	B	189	VAL
2	B	200	GLN
2	B	203	ILE
2	B	207	ASN
2	B	214	LYS
2	B	215	VAL
2	B	217	LYS
2	B	218	LYS
3	C	1	ILE
3	C	3	MET
3	C	6	SER
3	C	12	VAL
3	C	17	ARG
3	C	19	THR
3	C	25	SER
3	C	28	VAL
3	C	34	ASN
3	C	36	ILE
3	C	48	LYS
3	C	49	LEU
3	C	51	ILE
3	C	57	LYS
3	C	66	SER
3	C	75	THR
3	C	76	LEU
3	C	77	THR
3	C	78	ILE
3	C	82	GLU
3	C	90	PHE
3	C	95	LYS
3	C	97	VAL
3	C	101	THR
3	C	106	LYS
3	C	109	ILE
3	C	110	LYS
3	C	113	ASP
3	C	117	THR
3	C	118	VAL
3	C	119	SER
3	C	120	ILE
3	C	126	GLU
3	C	128	LEU

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Mol	Chain	Res	Type
3	C	129	THR
3	C	137	CYS
3	C	139	LEU
3	C	147	ILE
3	C	149	VAL
3	C	154	ASP
3	C	158	ARG
3	C	164	ASN
3	C	168	ASP
3	C	169	GLN
3	C	173	ASP
3	C	174	SER
3	C	176	TYR
3	C	180	SER
3	C	190	GLU
3	C	202	LYS
3	C	209	VAL
3	C	210	LYS
3	C	211	SER
1	D	44	LEU
1	D	45	ARG
1	D	54	LYS
1	D	61	ILE
1	D	79	ILE
1	D	82	THR
1	D	83	SER
1	D	85	SER
1	D	94	ASP
1	D	101	LEU
1	D	110	SER
1	D	121	SER
1	D	126	HIS
1	D	128	SER
1	D	129	ASN
1	D	132	VAL
1	D	136	CYS
1	D	138	HIS
1	D	142	LYS
1	D	152	VAL
1	D	153	LYS
1	D	160	LYS
1	D	168	ASP

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Mol	Chain	Res	Type
1	D	174	LEU
1	D	175	VAL
1	D	183	SER
1	D	196	ASP
1	D	201	VAL
1	D	204	SER
1	D	205	ARG
1	D	211	LYS
1	D	213	GLU
1	D	216	ILE
1	D	232	THR
1	D	233	LEU
1	D	234	VAL
1	D	235	GLU
1	D	241	THR
1	D	245	THR
2	E	3	LYS
2	E	10	VAL
2	E	11	VAL
2	E	12	GLN
2	E	18	ARG
2	E	20	SER
2	E	34	SER
2	E	36	ILE
2	E	44	LEU
2	E	47	VAL
2	E	51	LEU
2	E	55	GLU
2	E	56	ARG
2	E	57	SER
2	E	59	TYR
2	E	64	LYS
2	E	73	ASN
2	E	78	LEU
2	E	98	HIS
2	E	116	THR
2	E	139	THR
2	E	143	THR
2	E	146	LEU
2	E	148	CYS
2	E	156	GLU
2	E	158	VAL

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Mol	Chain	Res	Type
2	E	159	THR
2	E	161	SER
2	E	163	ASN
2	E	170	SER
2	E	171	VAL
2	E	173	THR
2	E	177	VAL
2	E	181	SER
2	E	183	LEU
2	E	186	LEU
2	E	187	SER
2	E	188	SER
2	E	189	VAL
2	E	191	THR
2	E	192	VAL
2	E	195	SER
2	E	199	THR
2	E	201	THR
2	E	203	ILE
2	E	207	ASN
2	E	209	LYS
2	E	216	ASP
3	F	1	ILE
3	F	2	GLN
3	F	3	MET
3	F	17	ARG
3	F	21	THR
3	F	22	CYS
3	F	26	GLU
3	F	34	ASN
3	F	36	ILE
3	F	38	TRP
3	F	49	LEU
3	F	57	LYS
3	F	59	THR
3	F	72	THR
3	F	77	THR
3	F	92	GLN
3	F	93	GLN
3	F	97	VAL
3	F	106	LYS
3	F	110	LYS

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Mol	Chain	Res	Type
3	F	117	THR
3	F	118	VAL
3	F	120	ILE
3	F	121	PHE
3	F	125	SER
3	F	126	GLU
3	F	128	LEU
3	F	129	THR
3	F	137	CYS
3	F	139	LEU
3	F	149	VAL
3	F	150	LYS
3	F	152	LYS
3	F	156	SER
3	F	157	GLU
3	F	158	ARG
3	F	162	VAL
3	F	163	LEU
3	F	164	ASN
3	F	168	ASP
3	F	170	ASP
3	F	171	SER
3	F	172	LYS
3	F	176	TYR
3	F	181	THR
3	F	182	LEU
3	F	198	GLU
3	F	200	THR
3	F	202	LYS
3	F	209	VAL
1	G	54	LYS
1	G	61	ILE
1	G	70	LEU
1	G	86	ASP
1	G	87	ASN
1	G	101	LEU
1	G	103	GLU
1	G	112	GLU
1	G	120	THR
1	G	122	SER
1	G	133	THR
1	G	146	LYS

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Mol	Chain	Res	Type
1	G	148	LEU
1	G	151	LEU
1	G	161	LEU
1	G	164	SER
1	G	166	ILE
1	G	168	ASP
1	G	174	LEU
1	G	179	ILE
1	G	181	HIS
1	G	183	SER
1	G	187	ASP
1	G	190	SER
1	G	201	VAL
1	G	209	LYS
1	G	211	LYS
1	G	216	ILE
1	G	227	MET
1	G	232	THR
1	G	233	LEU
1	G	239	LYS
1	G	252	ARG
1	G	260	ASN
2	H	7	SER
2	H	30	ASP
2	H	32	ASP
2	H	36	ILE
2	H	50	ILE
2	H	51	LEU
2	H	55	GLU
2	H	71	ARG
2	H	73	ASN
2	H	74	SER
2	H	75	ARG
2	H	77	THR
2	H	80	LEU
2	H	95	CYS
2	H	97	ARG
2	H	98	HIS
2	H	100	TRP
2	H	113	GLN
2	H	115	THR
2	H	124	THR

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Mol	Chain	Res	Type
2	H	129	VAL
2	H	132	LEU
2	H	143	THR
2	H	146	LEU
2	H	161	SER
2	H	173	THR
2	H	177	VAL
2	H	183	LEU
2	H	186	LEU
2	H	187	SER
2	H	189	VAL
2	H	190	VAL
2	H	191	THR
2	H	197	LEU
2	H	203	ILE
2	H	205	ASN
2	H	206	VAL
2	H	215	VAL
2	H	218	LYS
2	H	220	CYS
3	I	1	ILE
3	I	5	GLN
3	I	7	PRO
3	I	10	LEU
3	I	13	SER
3	I	19	THR
3	I	27	SER
3	I	34	ASN
3	I	36	ILE
3	I	37	ASN
3	I	38	TRP
3	I	40	GLN
3	I	45	GLN
3	I	72	THR
3	I	75	THR
3	I	77	THR
3	I	97	VAL
3	I	101	THR
3	I	102	PHE
3	I	105	THR
3	I	110	LYS
3	I	120	ILE

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Mol	Chain	Res	Type
3	I	126	GLU
3	I	128	LEU
3	I	129	THR
3	I	134	SER
3	I	136	VAL
3	I	148	ASN
3	I	149	VAL
3	I	150	LYS
3	I	153	ILE
3	I	158	ARG
3	I	162	VAL
3	I	163	LEU
3	I	168	ASP
3	I	170	ASP
3	I	173	ASP
3	I	176	TYR
3	I	177	SER
3	I	181	THR
3	I	182	LEU
3	I	183	THR
3	I	184	LEU
3	I	192	HIS
3	I	193	ASN
3	I	197	CYS
3	I	198	GLU
3	I	204	SER
3	I	205	THR
3	I	206	SER
3	I	208	ILE
3	I	210	LYS
3	I	212	PHE
1	J	43	LYS
1	J	45	ARG
1	J	54	LYS
1	J	55	CYS
1	J	68	GLU
1	J	69	SER
1	J	78	TYR
1	J	86	ASP
1	J	87	ASN
1	J	101	LEU
1	J	102	ARG

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Mol	Chain	Res	Type
1	J	104	GLN
1	J	108	VAL
1	J	109	SER
1	J	116	ILE
1	J	120	THR
1	J	122	SER
1	J	127	ASP
1	J	132	VAL
1	J	161	LEU
1	J	164	SER
1	J	166	ILE
1	J	168	ASP
1	J	175	VAL
1	J	191	LEU
1	J	207	SER
1	J	210	PHE
1	J	211	LYS
1	J	221	ARG
1	J	232	THR
1	J	233	LEU
1	J	234	VAL
1	J	239	LYS
1	J	252	ARG
1	J	259	ARG
1	J	260	ASN
2	K	4	LEU
2	K	10	VAL
2	K	18	ARG
2	K	19	LEU
2	K	29	SER
2	K	32	ASP
2	K	36	ILE
2	K	37	ARG
2	K	44	LEU
2	K	45	GLU
2	K	50	ILE
2	K	51	LEU
2	K	71	ARG
2	K	77	THR
2	K	81	GLU
2	K	86	ARG
2	K	89	ASP

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Mol	Chain	Res	Type
2	K	97	ARG
2	K	115	THR
2	K	124	THR
2	K	129	VAL
2	K	132	LEU
2	K	143	THR
2	K	158	VAL
2	K	163	ASN
2	K	167	LEU
2	K	168	THR
2	K	177	VAL
2	K	179	GLN
2	K	181	SER
2	K	183	LEU
2	K	187	SER
2	K	189	VAL
2	K	190	VAL
2	K	196	SER
2	K	197	LEU
2	K	201	THR
2	K	207	ASN
2	K	215	VAL
2	K	218	LYS
3	L	4	THR
3	L	5	GLN
3	L	13	SER
3	L	17	ARG
3	L	19	THR
3	L	21	THR
3	L	23	ARG
3	L	28	VAL
3	L	34	ASN
3	L	36	ILE
3	L	38	TRP
3	L	39	PHE
3	L	48	LYS
3	L	49	LEU
3	L	51	ILE
3	L	72	THR
3	L	75	THR
3	L	77	THR
3	L	78	ILE

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Mol	Chain	Res	Type
3	L	86	THR
3	L	88	ASN
3	L	97	VAL
3	L	101	THR
3	L	102	PHE
3	L	107	LEU
3	L	128	LEU
3	L	140	ASN
3	L	145	LYS
3	L	147	ILE
3	L	148	ASN
3	L	149	VAL
3	L	153	ILE
3	L	154	ASP
3	L	158	ARG
3	L	163	LEU
3	L	165	SER
3	L	170	ASP
3	L	171	SER
3	L	173	ASP
3	L	176	TYR
3	L	177	SER
3	L	182	LEU
3	L	183	THR
3	L	191	ARG
3	L	193	ASN
3	L	194	SER
3	L	197	CYS
3	L	198	GLU
3	L	202	LYS
3	L	203	THR
3	L	208	ILE
3	L	209	VAL
3	L	211	SER
3	L	212	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
1	A	188	GLN
1	A	247	ASN

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Mol	Chain	Res	Type
2	B	73	ASN
2	B	200	GLN
3	C	92	GLN
3	C	164	ASN
3	C	193	ASN
3	C	201	HIS
1	D	147	ASN
3	F	93	GLN
3	F	141	ASN
3	F	193	ASN
1	G	129	ASN
1	G	193	GLN
1	G	223	GLN
2	H	38	GLN
2	H	205	ASN
3	I	37	ASN
3	I	41	GLN
3	I	140	ASN
3	I	141	ASN
3	I	192	HIS
3	I	201	HIS
1	J	51	HIS
1	J	104	GLN
2	K	163	ASN
2	K	205	ASN
3	L	92	GLN
3	L	192	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	234/518 (45%)	-1.35	0 100 100	19, 34, 59, 76	8 (3%)
1	D	246/518 (47%)	-1.32	0 100 100	18, 30, 58, 95	21 (8%)
1	G	227/518 (43%)	-1.45	0 100 100	18, 32, 57, 70	2 (0%)
1	J	255/518 (49%)	-1.21	0 100 100	17, 31, 57, 71	30 (11%)
2	B	208/219 (94%)	-1.40	0 100 100	13, 29, 44, 58	0
2	E	208/219 (94%)	-1.41	0 100 100	19, 30, 42, 62	0
2	H	208/219 (94%)	-1.43	0 100 100	20, 29, 43, 53	0
2	K	208/219 (94%)	-1.36	0 100 100	21, 29, 41, 48	0
3	C	203/218 (93%)	-1.42	0 100 100	13, 28, 50, 68	0
3	F	203/218 (93%)	-1.36	0 100 100	20, 29, 49, 58	0
3	I	203/218 (93%)	-1.35	0 100 100	20, 30, 53, 71	0
3	L	203/218 (93%)	-1.38	0 100 100	18, 30, 57, 75	0
All	All	2606/3820 (68%)	-1.37	0 100 100	13, 30, 53, 95	61 (2%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.