



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 11:40 PM GMT

PDB ID : 4F15
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

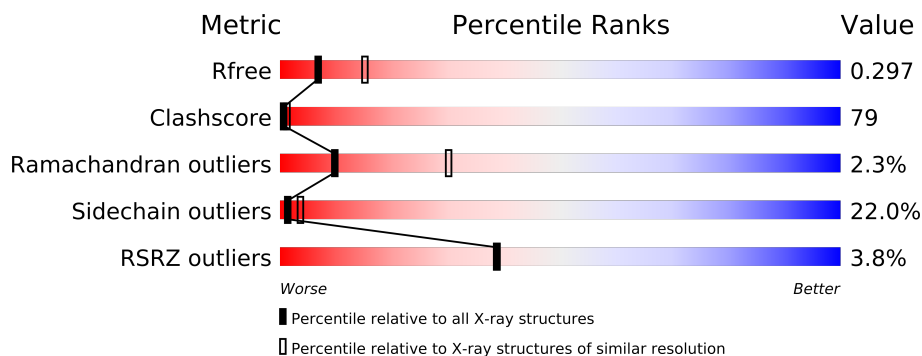
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	518	
1	D	518	
1	G	518	
1	J	518	
2	B	219	
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 hydrogen and 0 are deuterium.

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	O	0	0
			6	6		
4	L	15	Total	O	0	0
			15	15		

VAL	LYS	VAL	K244	H181	F114
LYS	LYS	T245	T245	P182	E115
THR	THR	G246	G246	S183	I116
GLN	THR	N247	N247	T184	F117
ASN	THR	LYS	LYS	S185	P118
ALA	THR	ALA	ALA	S186	K119
GLU	LEU	V248	V248	K187	K119
ARG	ARG	V250	V250	D187	T120
THR	LEU	P251	P251	Q188	S121
ALA	ALA	R252	R252		
LYS	THR	Y253	Y253	L191	H126
ASN	THR	A254	A254	Y192	D127
ARG	GLY	F255	F255	Q193	S128
GLU	LEU	N194	N194	M194	N129
GLU	ASN	A195	A195	A195	K130
ILE	ASN	D196	D196	D196	G131
VAL	VAL	V199	V199	V199	V132
K383	LYS	F200	F200	F200	T133
V385	VAL	G264	G264	G261	C136
I386	ILE	ILE	ILE	G202	P137
E387	ILE	ILE	ILE	S203	H138
K388	SER	ILE	ILE	S204	A139
K389	ARG	SER	SER	R205	G140
T391	GLY	THR	THR	A141	A141
Q392	LEU	ASP	ASP	K208	K142
PHE	THR	THR	THR	K209	S143
ALA	ALA	VAL	VAL	F144	F144
THR	ILE	HIS	HIS	K210	Y145
VAL	GLY	ALA	ALA	P212	K146
LYS	GLY	LYS	LYS	E213	N147
VAL	ASN	ASN	ASN	T214	E213
ARG	PHE	THR	THR	A215	L148
THR	ILE	GLU	GLU	L216	I149
VAL	GLY	CYS	CYS	L217	W150
LYS	GLY	GLN	GLN	R218	L151
ASN	THR	THR	THR	P218	V152
ASN	LYS	PRO	PRO	K219	K153
GLY	ARG	LYS	LYS	V220	K154
CYS	ILE	GLY	GLY	R221	G155
PHE	GLU	ALA	ALA	D222	N156
GLU	ASN	ASP	ASP	Q223	S157
LEU	LEU	ASN	ASN	E224	
TYR	TYR	THR	THR	G225	
LYS	LYS	SER	SER	R226	L161
		LEU	LEU	M227	S162
V414	TYR	PRO	PRO	N228	K163
D415	HIS	PHE	PHE	Y229	S164
D416	HIS	GLN	GLN	Y230	Y165
G417	GLN	ASN	ASN	W231	I166
F418	ASN	ILE	ILE	T232	I166
L419	GLU	HIS	HIS	D233	N167
D420	GLN	PRO	PRO	V234	D168
I421	GLY	ILE	ILE		K169
W422	SER	THR	THR		
T423	LYS	GLY	GLY	V173	V173
Y424	ASN	TYR	TYR	L174	L174
W425	ALA	ALA	ALA	V175	V175
A426	THR	THR	THR	L176	L176
E427	ASP	ASP	ASP	W177	W177
LEU	LEU	LYS	LYS	G178	G178
TYR	TYR	TYR	TYR	I179	I179
TYR	TYR	TYR	TYR	E243	E243

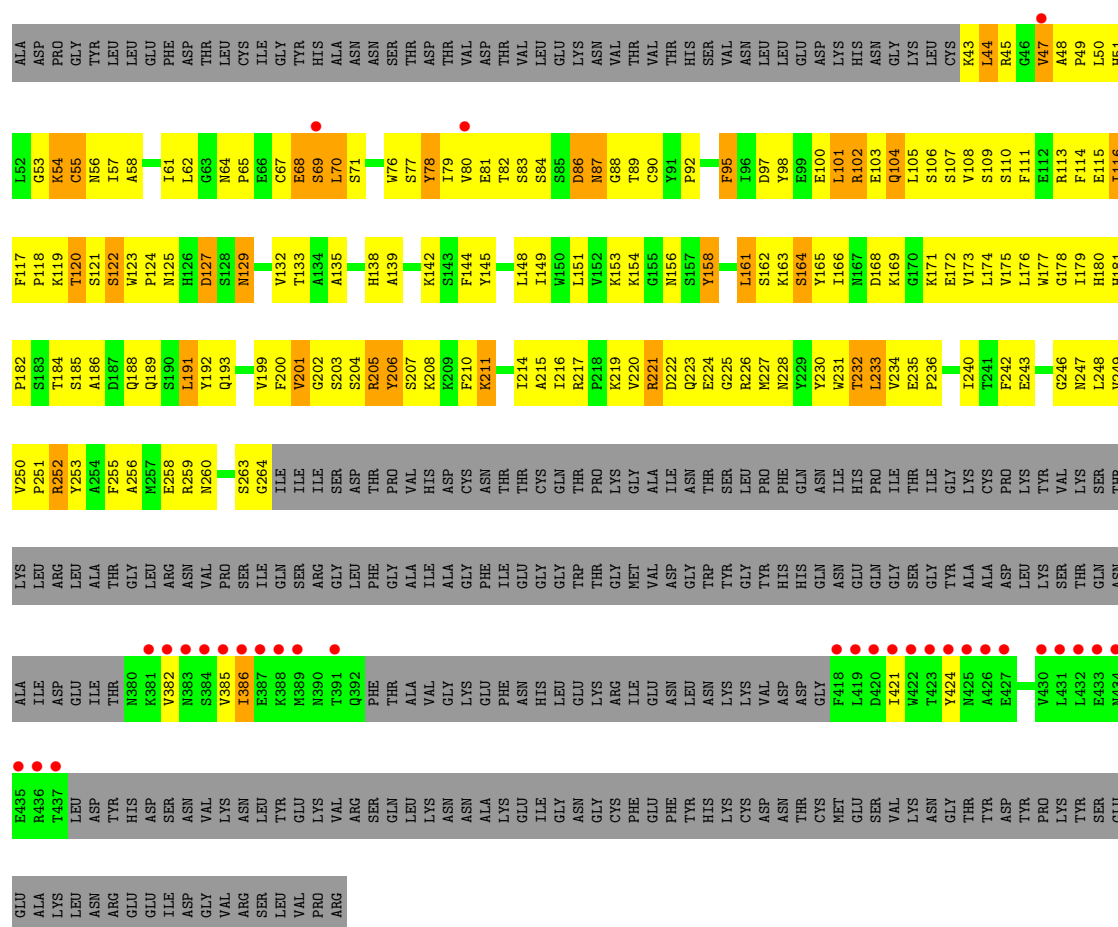
● Molecule 1: Hemagglutinin

Chain G: 

ALA	ASP	ALA	K54	F117	S183	G246	LYS	THR	LEU
PRO	GLY	ASP	C55	P118	T184	N247	SER	GLN	LEU
TYR	THR	PRO	N56	T119	A186	L248	THR	ASN	GLU
GLU	GLU	TYR	I57	T120	S185	V249	LYS	ALA	ASN
LEU	LEU	TYR	A58	S121	D187	V250	ILE	ILE	GLU
LEU	LEU	LEU	G59	S122	Q188	P251	ARG	ASP	ARG
LEU	LEU	LEU	W60		Q189	R252	LEU	GLU	THR
LEU	LEU	LEU	I61		S190		ALA	ILE	LYS
PHE	THR	PHE	N64	D127	L191	F255	THR	THR	LEU
ASP	ASP	ASP	P65	S128	Y192	A256	GLY	ASN	ASP
THR	THR	THR	E66	K130	Q193	M257	LEU	LYS	THR
LEU	LEU	LEU	C67	K131	A197	E258	ARG	VAL	GLU
CYS	CYS	CYS	E68	V132	Y198	R259	ASN	SER	THR
ILE	ILE	ILE	S69	T133	Y199	A261	VAL	SER	LEU
GLY	GLY	GLY	L70	A134	F200	G264	PRO	VAL	ASP
TYR	TYR	TYR	S71	A135	V201		ILE	ILE	VAL
HIS	HIS	HIS	T72	C136	G202		GLN	GLN	LYS
ALA	ALA	ALA	A73	P137	S203		THR	THR	GLU
ASN	ASN	ASN	S74	H138	Y206		SER	SER	TYR
SER	SER	SER	S75		S207		GLY	GLY	GLU
THR	THR	THR	W76	K142	K208		THR	PHE	VAL
ASP	ASP	ASP	T77	S143	F144		PRO	THR	ARG
VAL	VAL	VAL	Y78	F144	Y145		GLY	GLY	GLN
VAL	VAL	VAL	T79	K146	E81		ALA	ALA	LEU
ASP	ASP	ASP	V80	N147	K211		ILE	ILE	LEU
THR	THR	THR	T82	L148	E212		ALA	ALA	LYS
LEU	LEU	LEU	S83	I214	E213		GLY	GLY	ASN
GLU	GLU	GLU	S84	W150	I215		PHE	PHE	ASN
LYS	LYS	LYS	S85	L151	I216		ILE	ILE	ALA
ASN	ASN	ASN	D86	V152	R217		GLU	GLU	LYS
VAL	VAL	VAL	N87	K153	P218		GLY	GLY	GLU
THR	THR	THR	T88	G154	K219		THR	THR	ILE
VAL	VAL	VAL	T89	G155	V220		LYS	LYS	GLY
THR	THR	THR	C90	N156	R221		GLY	GLY	ASN
HIS	HIS	HIS	Y91	S157	D222		MET	MET	CYS
SER	SER	SER	P92	Y158	Q223		VAL	VAL	PHE
VAL	VAL	VAL	G93	P159	E224		ASP	ASP	GLU
ASN	ASN	ASN	D94	K160	G225		GLY	GLY	GLU
LEU	LEU	LEU	F95	L161	R226		THR	THR	PHE
GLU	GLU	GLU	I96	S162	M227		SER	SER	TYR
ASP	ASP	ASP	Y97	K163	N228		GLY	GLY	LYS
LYS	LYS	LYS	X98	S164	Y229		TYR	TYR	CYS
HIS	HIS	HIS	E99	Y165	Z230		PRO	PRO	ASP
GLN	GLN	GLN	E100	I166	W231		PHE	PHE	ASN
ASN	ASN	ASN	L101	N167	T232		GLN	GLN	THR
ILE	ILE	ILE	R102	D168	L233		ASN	ASN	THR
GLY	GLY	GLY	E103	K169	V234		GLU	GLU	CYS
LYS	LYS	LYS	Q104	G170	E235		PRO	PRO	MET
LEU	LEU	LEU	L105	K171	P236		ILE	ILE	GLU
K43	L44	K43	S106	E172	G237		THR	THR	SER
L44	L44	L44	S107	V173	D238		GLY	GLY	VAL
A45	P49	A45	V108		K239		TYR	TYR	LYS
P49	L50	P49	S109	W177	T240		ALA	ALA	GLY
L50	H51	L50	S110	G178	T241		LYS	LYS	THR
H51	L52	H51	F114	I179	F242		ASP	ASP	TYR
L52	E115	L52	H180	H180	E243		LEU	LEU	ASP
G53	P182	G53	P182	P182	A244		LYS	LYS	TYR
					T245		VAL	VAL	PRO

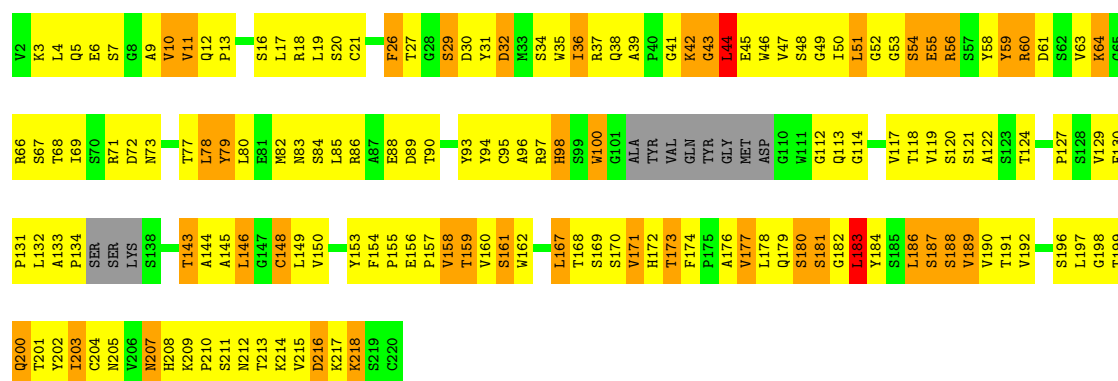
- Molecule 1: Hemagglutinin

Chain J:



- Molecule 2: Fab fragment, heavy chain

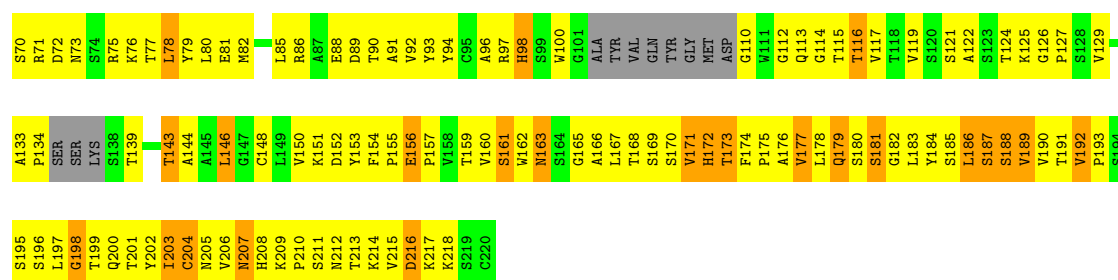
Chain B:



- Molecule 2: Fab fragment, heavy chain

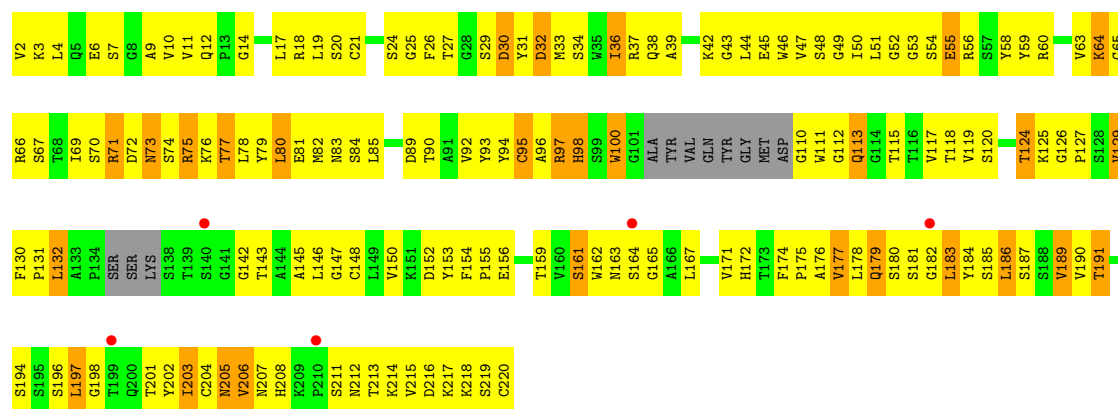
Chain E:





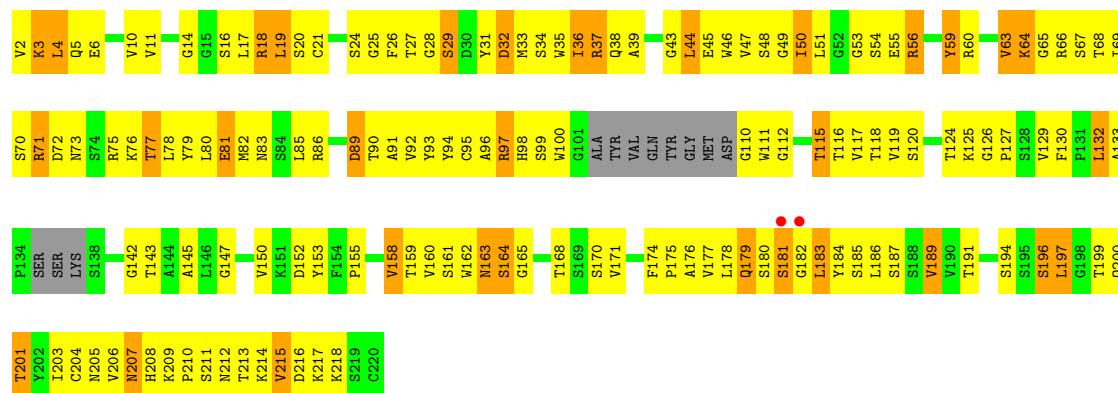
• Molecule 2: Fab fragment, heavy chain

Chain H:



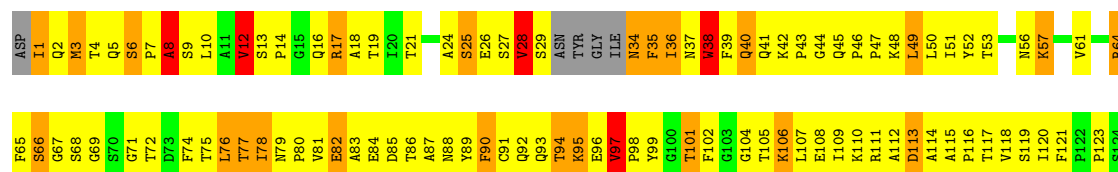
• Molecule 2: Fab fragment, heavy chain

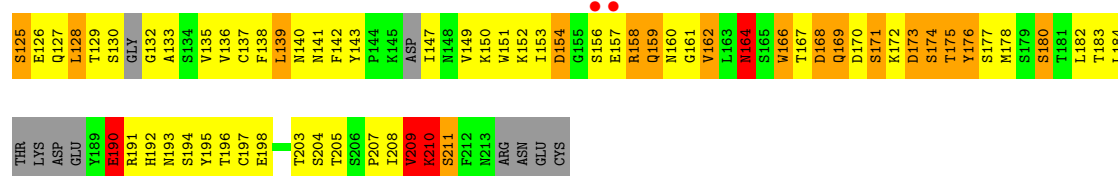
Chain K:



• Molecule 3: Fab fragment, light chain

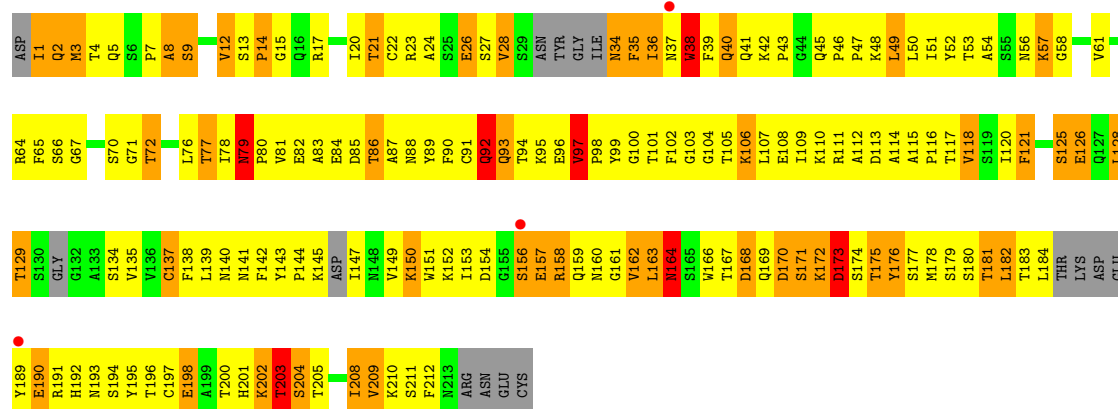
Chain C:





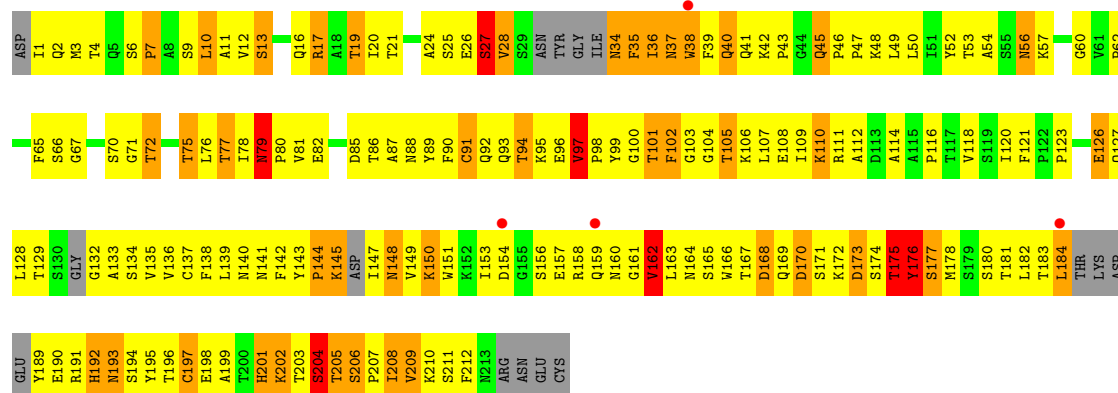
• Molecule 3: Fab fragment, light chain

Chain F:



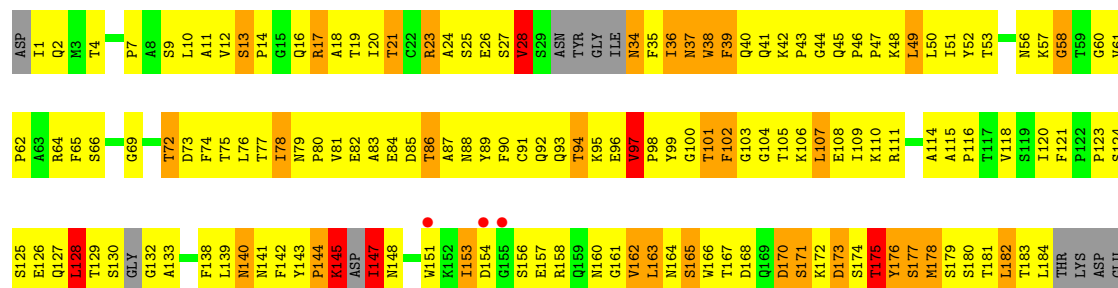
• Molecule 3: Fab fragment, light chain

Chain I:



• Molecule 3: Fab fragment, light chain

Chain L:



Y189	E190	R191	H192	N193	S194	Y195	T196	C197	E198	A199	T200	H201	K202	T203	S204	T205	S206	P207	T208	V209	K210	S211	F212	N213	ARG	ASN	GLU	CYS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

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	2.91 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.233 , 0.289 0.236 , 0.297	Depositor DCC
R_{free} test set	3266 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 20.9	EDS
Estimated twinning fraction	0.492 for h,-k,-l 0.457 for h,-k,-l	Xtriage
Reported twinning fraction	0.492 for h,-k,-l	Depositor
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 66880 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	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 50.53 % 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 6.3850e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.39	0/1861	0.63	0/2523
1	D	0.41	0/1919	0.67	0/2602
1	G	0.42	0/1826	0.69	0/2474
1	J	0.41	0/1965	0.67	1/2667 (0.0%)
2	B	0.45	0/1577	0.76	3/2141 (0.1%)
2	E	0.42	0/1577	0.74	3/2141 (0.1%)
2	H	0.43	0/1577	0.73	0/2141
2	K	0.43	0/1577	0.72	0/2141
3	C	0.50	0/1590	0.86	4/2157 (0.2%)
3	F	0.51	0/1590	0.79	1/2157 (0.0%)
3	I	0.78	1/1591 (0.1%)	0.85	5/2160 (0.2%)
3	L	0.84	1/1591 (0.1%)	0.90	7/2160 (0.3%)
All	All	0.52	2/20241 (0.0%)	0.75	24/27464 (0.1%)

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	27.80	1.98	1.34
3	I	145	LYS	C-N	24.11	1.89	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	145	LYS	O-C-N	-12.89	102.07	122.70
3	L	145	LYS	C-N-CA	9.08	144.39	121.70
2	E	43	GLY	N-CA-C	-6.80	96.09	113.10
2	B	43	GLY	N-CA-C	-6.76	96.19	113.10
3	C	94	THR	N-CA-C	-6.63	93.11	111.00
3	I	175	THR	N-CA-C	6.30	128.00	111.00
3	L	94	THR	N-CA-C	-6.24	94.16	111.00
3	L	58	GLY	N-CA-C	-6.00	98.10	113.10
3	C	38	TRP	N-CA-C	-5.91	95.04	111.00
3	F	94	THR	N-CA-C	-5.84	95.24	111.00
2	E	51	LEU	CA-CB-CG	5.79	128.61	115.30
3	I	176	TYR	N-CA-C	5.70	126.40	111.00
3	I	94	THR	N-CA-C	-5.66	95.71	111.00
3	C	210	LYS	N-CA-C	5.43	125.66	111.00
2	B	183	LEU	N-CA-C	-5.42	96.36	111.00
3	C	88	ASN	N-CA-C	-5.41	96.38	111.00
2	B	44	LEU	N-CA-C	5.38	125.52	111.00
3	L	175	THR	N-CA-C	5.37	125.48	111.00
3	L	37	ASN	N-CA-C	5.35	125.44	111.00
3	I	27	SER	N-CA-C	5.33	125.40	111.00
3	L	209	VAL	N-CA-C	5.29	125.30	111.00
2	E	198	GLY	N-CA-C	-5.26	99.96	113.10
3	I	209	VAL	N-CA-C	5.19	125.02	111.00
1	J	70	LEU	N-CA-C	5.09	124.74	111.00

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
3	C	175	THR	Peptide
3	C	190	GLU	Peptide

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Mol	Chain	Res	Type	Group
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 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1813	0	1716	191	0
1	D	1872	0	1743	214	0
1	G	1778	0	1702	239	0
1	J	1918	0	1760	219	0
2	B	1544	0	1505	262	0
2	E	1544	0	1505	254	0
2	H	1544	0	1505	274	0
2	K	1544	0	1505	247	0
3	C	1557	0	1503	343	0
3	F	1557	0	1503	355	0
3	I	1557	0	1503	317	0
3	L	1557	0	1503	332	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	3059	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 79.

All (3059) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:145:LYS:C	3:I:147:ILE:N	1.89	1.25
3:C:38:TRP:CD2	3:C:39:PHE:HA	1.74	1.21
2:B:171:VAL:HG21	3:C:176:TYR:CE1	1.76	1.19
3:L:145:LYS:C	3:L:147:ILE:N	1.98	1.16
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:I:184:LEU:C	3:I:189:TYR:N	2.02	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
1:J:177:TRP:HB3	4:J:601:HOH:O	1.51	1.10
3:C:1:ILE:HD11	3:C:98:PRO:HB2	1.31	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
3:F:141:ASN:CA	3:F:175:THR:HG22	1.89	1.02
1:A:202:GLY:HA3	1:A:241:THR:H	1.18	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
1:A:91:TYR:CD1	1:A:227:MET:HB2	1.97	0.99
2:E:179:GLN:HB3	3:I:60:GLY:HA2	1.40	0.99
3:C:203:THR:HG23	3:C:205:THR:H	1.28	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:142:PHE:HZ	3:L:177:SER:HB3	1.25	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:38:TRP:HB2	3:L:47:PRO:CB	1.93	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
3:I:100:GLY:HA3	4:I:306:HOH:O	1.62	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: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
2:E:162:TRP:H	2:E:167:LEU:HG	1.28	0.97
1:A:149:ILE:HB	1:A:250:VAL:HG23	1.43	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
3:F:92:GLN:HG2	3:F:101:THR:CG2	1.94	0.97
1:D:84:SER:O	1:D:87:ASN:N	1.97	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:HE3	1:D:160:LYS:H	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:382:VAL:O	1:J:386:ILE:N	2.00	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
3:I:194:SER:HB2	3:I:210:LYS:CD	1.97	0.94
1:D:119:LYS:NZ	1:D:128:SER:O	2.01	0.94
2:B:171:VAL:HG21	3:C:176:TYR:CZ	2.02	0.94
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
2:B:162:TRP:H	2:B:167:LEU:HD11	1.32	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
3:L:91:CYS:SG	3:L:102:PHE:HD2	1.90	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:235:GLU:HG3	1:J:236:PRO:HD2	1.48	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:I:38:TRP:HB2	3:I:47:PRO:HB2	1.50	0.92
3:F:153:ILE:HG13	3:F:154:ASP:H	1.34	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
3:I:38:TRP:HZ3	3:I:92:GLN:HE21	1.10	0.91
2:E:6:GLU:HA	2:E:20:SER:O	1.70	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
2:H:44:LEU:O	4:H:305:HOH:O	1.89	0.91
1:A:201:VAL:CG1	1:A:202:GLY:H	1.82	0.91
1:J:84:SER:O	1:J:87:ASN:N	2.02	0.91
3:F:38:TRP:HA	3:F:49:LEU:HA	1.51	0.91
3:F:4:THR:HG22	3:F:24:ALA:HA	1.53	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
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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:8:ALA:HB1	3:F:105:THR:HG23	1.54	0.89
1:J:78:TYR:HB3	1:J:264:GLY:HA3	1.54	0.89
3:F:24:ALA:HB3	3:F:72:THR:HA	1.52	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
2:K:28:GLY:H	2:K:76:LYS:HZ2	1.16	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
3:F:86:THR:OG1	3:F:87:ALA:N	2.05	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
2:E:46:TRP:H	2:E:60:ARG:HH22	0.89	0.88
1:A:259:ARG:HB3	1:A:259:ARG:NH1	1.86	0.88
3:F:108:GLU:HG3	3:F:109:ILE:H	1.38	0.88
1:D:93:GLY:HA3	1:D:227:MET:O	1.74	0.88
3:C:38:TRP:O	3:C:38:TRP:CD1	2.26	0.88
3:I:38:TRP:HZ3	3:I:92:GLN:NE2	1.70	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:L:162:VAL:HG23	3:L:182:LEU:HG	1.57	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
2:E:45:GLU:HB3	2:E:60:ARG:CZ	2.03	0.87
1:A:49:PRO:HG2	1:A:77:SER:H	1.38	0.87
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:J:201:VAL:CG1	1:J:202:GLY:H	1.86	0.87
2:H:14:GLY:N	2:H:85:LEU:O	2.08	0.87
1:D:49:PRO:HB2	1:D:76:TRP:HB2	1.55	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
3:C:128:LEU:HD13	3:C:129:THR:H	1.37	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:E:38:GLN:HG3	2:E:43:GLY:HA2	1.57	0.86
1:A:49:PRO:HB2	1:A:76:TRP:HB2	1.58	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:L:102:PHE:HD1	3:L:104:GLY:H	1.20	0.85
3:C:194:SER:HA	3:C:210:LYS:HB2	1.57	0.85
3:F:173:ASP:CG	3:F:175:THR:HG23	1.96	0.85
3:C:170:ASP:OD2	3:C:172:LYS:N	2.10	0.85
1:A:149:ILE:HB	1:A:250:VAL:CG2	2.05	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
3:I:6:SER:HB3	3:I:7:PRO:HD2	1.55	0.85
3:I:196:THR:HA	3:I:209:VAL:HA	1.55	0.85
2:H:176:ALA:HB2	3:I:166:TRP:CE2	2.11	0.85
2:K:150:VAL:HB	2:K:186:LEU:HB3	1.58	0.85
3:I:173:ASP:OD1	3:I:173:ASP:N	2.05	0.85
2:E:173:THR:HG23	2:E:187:SER:O	1.76	0.85
2:E:46:TRP:N	2:E:60:ARG:NH2	2.21	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
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
3:I:10:LEU:O	3:I:107:LEU:HA	1.78	0.84
1:A:93:GLY:HA3	1:A:227:MET:O	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:K:37:ARG:HB3	2:K:93:TYR:CE2	2.13	0.84
2:E:32:ASP:CB	2:E:51:LEU:HA	2.05	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.60	0.84
3:F:9:SER:N	3:F:105:THR:HG23	1.93	0.84
2:E:181:SER:HB3	3:I:62:PRO:HG3	1.60	0.84
3:F:110:LYS:HB3	3:F:110:LYS:HZ2	1.42	0.83
1:J:54:LYS:HZ2	1:J:54:LYS:HB3	1.41	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
3:F:182:LEU:C	3:F:182:LEU:HD12	1.99	0.83
3:C:35:PHE:CE1	3:C:49:LEU:HD11	2.14	0.83
2:K:11:VAL:O	2:K:120:SER:N	2.11	0.83
2:H:129:VAL:HG11	2:H:206:VAL:HG21	1.59	0.83
2:E:10:VAL:HG22	2:E:155:PRO:HG3	1.60	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
1:J:201:VAL:HG12	1:J:202:GLY:N	1.94	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
3:I:38:TRP:HA	3:I:48:LYS:O	1.78	0.82
1:D:148:LEU:HD23	1:D:251:PRO:HA	1.60	0.82
1:D:153:LYS:HE3	1:D:156:ASN:HA	1.61	0.82
2:K:171:VAL:HG22	3:L:176:TYR:CZ	2.14	0.82
2:B:180:SER:HB3	3:L:62:PRO:HA	1.61	0.82
2:H:59:TYR:CE1	2:H:69:ILE:HG22	2.14	0.82
2:E:168:THR:O	2:E:169:SER:OG	1.97	0.82
2:H:146:LEU:HD11	2:H:219:SER:OG	1.78	0.82
3:L:162:VAL:O	3:L:164:ASN:ND2	2.12	0.82
2:K:27:THR:C	2:K:29:SER:H	1.82	0.82
1:D:144:PHE:CE2	1:D:150:TRP:HB2	2.15	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
1:D:258:GLU:HG2	1:D:259:ARG:H	1.44	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
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
1:A:104:GLN:HE22	1:A:233:LEU:HD22	1.45	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:193:ASN:O	3:I:211:SER:HB3	1.80	0.81
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.12	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
3:L:128:LEU:HD12	3:L:129:THR:H	1.46	0.81
1:J:204:SER:HB3	4:J:603:HOH:O	1.79	0.81
3:L:42:LYS:HD3	3:L:87:ALA:HB2	1.62	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:F:3:MET:HG3	3:F:5:GLN:HE21	1.43	0.81
1:D:116:ILE:HG13	1:D:165:TYR:CD1	2.15	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:K:63:VAL:C	2:K:65:GLY:H	1.84	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
3:C:176:TYR:HD2	3:C:176:TYR:H	1.29	0.80
2:E:45:GLU:HB3	2:E:60:ARG:NH2	1.97	0.80
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:I:116:PRO:HB2	3:I:139:LEU:HB3	1.64	0.80
2:E:178:LEU:N	2:E:183:LEU:O	2.15	0.80
2:E:51:LEU:HG	2:E:56:ARG:HB2	1.63	0.80
2:K:171:VAL:HB	2:K:189:VAL:HG22	1.62	0.80
2:H:207:ASN:HB3	2:H:214:LYS:HG3	1.64	0.80
1:D:148:LEU:HD21	1:D:176:LEU:O	1.82	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:HD2	3:L:191:ARG:O	1.82	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
1:A:51:HIS:CE1	1:A:80:VAL:HG21	2.16	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
3:L:98:PRO:HB2	4:L:309:HOH:O	1.82	0.79
1:G:235:GLU:HG3	1:G:236:PRO:HD2	1.62	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:34:SER:OG	2:H:49:GLY:HA3	1.81	0.79
2:K:111:TRP:CZ2	3:L:38:TRP:HB3	2.17	0.79
2:H:67:SER:HA	2:H:81:GLU:O	1.83	0.79
3:L:2:GLN:O	3:L:2:GLN:HG2	1.80	0.79
2:H:197:LEU:HD12	2:H:198:GLY:N	1.98	0.79
1:A:167:ASN:ND2	1:A:236:PRO:HA	1.97	0.79
3:L:141:ASN:HA	3:L:175:THR:HB	1.65	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
2:H:45:GLU:HB3	2:H:60:ARG:HH11	1.48	0.79
2:K:97:ARG:O	3:L:36:ILE:HB	1.82	0.79
2:K:5:GLN:O	2:K:21:CYS:HA	1.83	0.79
3:C:116:PRO:O	3:C:140:ASN:N	2.16	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
2:K:178:LEU:O	2:K:180:SER:N	2.16	0.78
1:G:138:HIS:HB2	1:G:143:SER:HB2	1.65	0.78
2:E:45:GLU:HB3	2:E:60:ARG:NH1	1.98	0.78
3:F:45:GLN:HB3	3:F:46:PRO:CD	2.12	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
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
2:H:2:VAL:HG22	2:H:25:GLY:HA3	1.64	0.78
1:A:57:ILE:O	1:A:61:ILE:HG22	1.83	0.78
2:K:111:TRP:CH2	3:L:38:TRP:HB3	2.18	0.78
1:J:49:PRO:HB2	1:J:76:TRP:HB2	1.66	0.78
1:G:49:PRO:HD2	1:G:77:SER:OG	1.83	0.78
1:A:55:CYS:SG	1:A:66:GLU:HG3	2.24	0.78
2:B:173:THR:HB	3:C:178:MET:HE3	1.64	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
3:I:1:ILE:HD11	3:I:98:PRO:HB2	1.66	0.78
1:G:118:PRO:HG2	2:H:58:TYR:CE1	2.17	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
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
1:G:91:TYR:HH	1:G:180:HIS:HE2	1.33	0.77
3:C:57:LYS:HD3	3:C:61:VAL:O	1.83	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:24:ALA:HB3	3:C:72:THR:HA	1.65	0.77
3:C:16:GLN:HG3	3:C:17:ARG:H	1.48	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:156:SER:OG	3:F:158:ARG:O	2.02	0.77
3:F:27:SER:O	3:F:28:VAL:HG22	1.84	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
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
1:J:57:ILE:N	1:J:81:GLU:OE2	2.15	0.77
2:K:18:ARG:HG3	2:K:81:GLU:HA	1.66	0.77
3:L:195:TYR:O	3:L:210:LYS:N	2.18	0.77
3:L:123:PRO:HB3	3:L:133:ALA:HB1	1.67	0.77
2:B:171:VAL:HG11	3:C:176:TYR:CD2	2.20	0.77
1:G:54:LYS:CD	1:G:54:LYS:H	1.92	0.77
3:I:49:LEU:HD23	3:I:50:LEU:N	2.00	0.77
1:G:119:LYS:HZ1	1:G:129:ASN:ND2	1.81	0.77
2:E:32:ASP:HB3	2:E:51:LEU:CA	2.11	0.76
2:E:32:ASP:HA	2:E:71:ARG:HH22	1.48	0.76
1:D:133:THR:HB	1:D:150:TRP:HZ3	1.48	0.76
1:A:144:PHE:CE2	1:A:150:TRP:HB2	2.20	0.76
3:F:108:GLU:HG3	3:F:109:ILE:N	1.99	0.76
1:J:199:VAL:HG12	1:J:200:PHE:N	2.00	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:D:101:LEU:O	1:D:104:GLN:N	2.19	0.76
3:F:183:THR:HG22	3:F:184:LEU:H	1.50	0.76
3:F:137:CYS:HB2	3:F:151:TRP:CZ2	2.20	0.76
2:K:178:LEU:HD23	2:K:179:GLN:HB2	1.66	0.76
1:J:182:PRO:HD2	1:J:214:ILE:HG13	1.68	0.76
1:D:51:HIS:HA	1:D:80:VAL:HB	1.67	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
2:K:10:VAL:HG21	2:K:155:PRO:HG3	1.66	0.76
3:I:162:VAL:HG23	3:I:164:ASN:OD1	1.85	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:G:120:THR:OG1	1:G:121:SER:N	2.16	0.76
3:F:182:LEU:O	3:F:182:LEU:HD12	1.86	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: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:75:ARG:O	2:K:77:THR:HG23	1.87	0.75
3:L:163:LEU:HD12	3:L:163:LEU:C	2.06	0.75
3:I:123:PRO:HB3	3:I:133:ALA:HB1	1.68	0.75
3:L:203:THR:HG23	3:L:203:THR:O	1.86	0.75
3:L:7:PRO:HG2	3:L:21:THR:HG23	1.69	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
3:C:38:TRP:CZ2	3:C:39:PHE:CD1	2.75	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
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
3:C:166:TRP:HE3	3:C:167:THR:H	1.33	0.75
1:A:201:VAL:HG12	1:A:202:GLY:N	2.01	0.75
1:A:259:ARG:CZ	1:A:259:ARG:HB3	2.17	0.75
2:K:16:SER:OG	2:K:83:ASN:OD1	2.04	0.75
1:G:135:ALA:HB2	1:G:223:GLN:HE21	1.52	0.75
3:F:38:TRP:O	3:F:38:TRP:CE3	2.39	0.75
1:G:171:LYS:CD	1:G:258:GLU:HG3	2.16	0.75
3:L:162:VAL:HG21	3:L:182:LEU:N	2.00	0.75
2:B:11:VAL:HG11	2:B:85:LEU:HD12	1.68	0.75
3:I:17:ARG:HB3	3:I:79:ASN:OD1	1.87	0.75
2:E:196:SER:HB3	2:E:202:TYR:CE2	2.22	0.75
3:F:38:TRP:C	3:F:38:TRP:CE3	2.60	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
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
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:F:9:SER:HB3	3:F:106:LYS:HZ2	1.51	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:F:210:LYS:HG2	3:F:211:SER:H	1.51	0.74
2:E:198:GLY:HA3	4:E:305:HOH:O	1.86	0.74
1:J:50:LEU:HD23	1:J:79:ILE:HG12	1.68	0.74
2:B:100:TRP:HA	3:C:34:ASN:N	2.02	0.74
3:L:42:LYS:O	3:L:44:GLY:N	2.21	0.74
3:F:182:LEU:HD23	4:F:302:HOH:O	1.86	0.74
3:F:93:GLN:HA	3:F:100:GLY:O	1.86	0.74
1:J:182:PRO:HG2	1:J:188:GLN:HB2	1.70	0.74
3:I:111:ARG:HE	3:I:173:ASP:HA	1.51	0.74
3:C:86:THR:HA	3:C:107:LEU:O	1.88	0.73
3:L:167:THR:HG22	3:L:168:ASP:H	1.53	0.73
1:A:137:PRO:HA	1:A:143:SER:H	1.52	0.73
1:G:201:VAL:HG12	1:G:202:GLY:H	1.52	0.73
2:K:163:ASN:C	2:K:165:GLY:H	1.90	0.73
2:B:196:SER:HB3	2:B:202:TYR:OH	1.89	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
2:B:36:ILE:HB	2:B:46:TRP:HA	1.69	0.73
2:B:180:SER:C	2:B:182:GLY:H	1.83	0.73
3:L:45:GLN:HB3	3:L:46:PRO:CD	2.16	0.73
2:H:50:ILE:HG23	2:H:69:ILE:HD13	1.69	0.73
3:C:153:ILE:HG13	3:C:154:ASP:H	1.51	0.73
3:F:92:GLN:CG	3:F:101:THR:HG23	2.11	0.73
1:A:202:GLY:HA3	1:A:241:THR:N	1.99	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
2:K:45:GLU:CD	2:K:46:TRP:H	1.92	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
2:B:160:VAL:HG21	2:B:186:LEU:HD11	1.71	0.73
3:C:110:LYS:HZ2	3:C:110:LYS:HB3	1.51	0.73
3:L:108:GLU:HA	3:L:108:GLU:OE1	1.85	0.73
1:D:137:PRO:CA	1:D:142:LYS:HA	2.17	0.73
1:A:201:VAL:CG1	1:A:202:GLY:N	2.51	0.73
1:A:120:THR:OG1	1:A:121:SER:N	2.20	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:169:LYS:HB3	1:A:171:LYS:H	1.53	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
1:J:251:PRO:HG3	4:J:601:HOH:O	1.88	0.73
1:J:199:VAL:CG1	1:J:200:PHE:H	2.01	0.73
2:H:10:VAL:HG22	2:H:118:THR:HB	1.69	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
3:C:38:TRP:HH2	3:C:89:TYR:HB3	1.54	0.72
1:G:54:LYS:N	1:G:54:LYS:HD3	2.00	0.72
1:J:102:ARG:NH1	1:J:102:ARG:HG3	2.03	0.72
3:L:162:VAL:CG2	3:L:182:LEU:H	2.02	0.72
1:A:54:LYS:HG2	1:A:55:CYS:H	1.53	0.72
2:K:197:LEU:HD13	2:K:197:LEU:O	1.89	0.72
3:L:170:ASP:HB3	3:L:174:SER:O	1.88	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: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
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
1:D:109:SER:HB3	1:D:258:GLU:HB3	1.72	0.72
3:C:92:GLN:HG3	3:C:93:GLN:N	2.04	0.72
2:B:144:ALA:N	2:B:192:VAL:O	2.23	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
2:K:171:VAL:HG22	3:L:176:TYR:CE2	2.26	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
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:168:ASP:N	3:I:168:ASP:OD1	2.21	0.71
2:B:162:TRP:N	2:B:167:LEU:HD11	2.05	0.71
2:K:178:LEU:HD11	3:L:182:LEU:HD13	1.72	0.71
3:L:17:ARG:HG2	3:L:17:ARG:O	1.90	0.71
3:F:168:ASP:N	3:F:168:ASP:OD1	2.21	0.71
2:H:93:TYR:HE1	2:H:117:VAL:HG12	1.56	0.71
2:E:63:VAL:CG1	2:E:67:SER:H	2.04	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:167:ASN:OD1	1:A:169:LYS:N	2.23	0.71
2:E:156:GLU:HB2	2:E:157:PRO:HA	1.71	0.71
2:H:72:ASP:HB3	2:H:79:TYR:CE2	2.26	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
3:I:17:ARG:HA	3:I:78:ILE:O	1.91	0.71
3:F:140:ASN:HB3	3:F:141:ASN:ND2	2.05	0.71
2:H:3:LYS:N	2:H:24:SER:HB2	2.06	0.71
1:G:79:ILE:HG22	1:G:80:VAL:N	2.05	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:209:VAL:HG23	3:L:210:LYS:N	2.05	0.71
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
1:D:148:LEU:HD23	1:D:251:PRO:CA	2.21	0.70
2:K:50:ILE:HD11	2:K:71:ARG:HG2	1.73	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
3:L:102:PHE:HD1	3:L:103:GLY:N	1.89	0.70
1:J:54:LYS:NZ	1:J:69:SER:HB3	2.06	0.70
3:C:123:PRO:HD3	3:C:135:VAL:HG22	1.73	0.70
2:B:173:THR:HG22	3:C:178:MET:SD	2.32	0.70
3:F:175:THR:HB	3:F:176:TYR:CD2	2.27	0.70
3:I:109:ILE:HG22	3:I:110:LYS:N	2.06	0.70
1:A:115:GLU:HB2	3:C:96:GLU:HG2	1.73	0.70
3:I:141:ASN:HA	3:I:175:THR:CB	2.20	0.70
2:H:153:TYR:OH	2:H:156:GLU:OE2	2.08	0.70
2:E:63:VAL:HG13	2:E:66:ARG:HB2	1.73	0.70
3:F:39:PHE:HB3	3:F:76:LEU:HD22	1.74	0.70
3:C:158:ARG:HH22	2:K:97:ARG:CD	2.03	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:I:161:GLY:O	3:I:162:VAL:HG22	1.91	0.70
2:H:33:MET:HB3	2:H:78:LEU:HD13	1.71	0.70
3:L:108:GLU:CD	3:L:109:ILE:H	1.93	0.70
3:I:120:ILE:HD11	3:I:151:TRP:CH2	2.27	0.70
2:B:203:ILE:HG13	2:B:204:CYS:N	2.07	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:J:201:VAL:HG13	1:J:240:ILE:HD11	1.72	0.70
2:H:6:GLU:OE2	2:H:112:GLY:HA3	1.92	0.70
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
1:A:55:CYS:HB2	1:A:60:TRP:HB2	1.73	0.69
2:K:34:SER:OG	2:K:49:GLY:HA3	1.92	0.69
1:G:201:VAL:HG12	1:G:202:GLY:N	2.07	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:E:51:LEU:CD1	2:E:56:ARG:H	2.05	0.69
3:C:97:VAL:HG13	3:C:98:PRO:HD2	1.74	0.69
3:F:153:ILE:HA	3:F:194:SER:O	1.92	0.69
3:F:34:ASN:HD22	3:F:34:ASN:N	1.89	0.69
3:L:11:ALA:CB	3:L:108:GLU:HB3	2.21	0.69
2:E:6:GLU:OE1	2:E:6:GLU:N	2.26	0.69
3:F:23:ARG:HG3	3:F:72:THR:O	1.92	0.69
2:E:53:GLY:O	2:E:54:SER:HB2	1.90	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
2:H:98:HIS:HA	3:I:36:ILE:CG2	2.22	0.69
1:G:201:VAL:CG1	1:G:202:GLY:N	2.53	0.69
2:H:63:VAL:C	2:H:65:GLY:H	1.95	0.69
2:B:127:PRO:CA	2:B:153:TYR:HB3	2.23	0.69
1:J:248:LEU:HD12	1:J:249:VAL:N	2.08	0.69
3:C:207:PRO:C	3:C:208:ILE:HD12	2.13	0.69
3:L:173:ASP:OD2	3:L:173:ASP:N	2.26	0.69
3:F:101:THR:HG22	3:F:102:PHE:H	1.57	0.69
3:F:38:TRP:CE3	3:F:39:PHE:HA	2.28	0.69
2:H:171:VAL:HG22	3:I:176:TYR:CZ	2.28	0.69
1:A:91:TYR:HH	1:A:180:HIS:HE2	1.38	0.69
1:G:199:VAL:HG12	1:G:200:PHE:N	2.07	0.69
1:G:121:SER:OG	2:H:64:LYS:HD2	1.92	0.69
2:H:83:ASN:OD1	2:H:84:SER:N	2.25	0.69
3:C:195:TYR:H	3:C:210:LYS:CB	2.05	0.69
2:K:2:VAL:HA	2:K:24:SER:O	1.93	0.69
1:G:58:ALA:HB2	1:G:98:TYR:CE1	2.28	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:L:170:ASP:OD2	3:L:171:SER:N	2.26	0.69
3:I:1:ILE:HG12	3:I:1:ILE:O	1.93	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:162:VAL:O	3:I:164:ASN:ND2	2.26	0.69
2:B:27:THR:HG23	2:B:30:ASP:OD1	1.93	0.68
2:E:45:GLU:C	2:E:60:ARG:HH12	1.95	0.68
3:C:2:GLN:OE1	3:C:97:VAL:HG21	1.93	0.68
1:J:69:SER:OG	1:J:70:LEU:N	2.26	0.68
3:F:210:LYS:HE2	3:F:212:PHE:CZ	2.28	0.68
3:F:26:GLU:CD	3:F:27:SER:HB2	2.14	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
2:H:44:LEU:HG	2:H:45:GLU:N	2.07	0.68
1:A:123:TRP:CZ3	1:A:163:LYS:HG3	2.28	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
3:F:170:ASP:OD2	3:F:172:LYS:N	2.26	0.68
3:F:41:GLN:NE2	4:F:307:HOH:O	1.97	0.68
3:F:7:PRO:HG2	3:F:21:THR:HG23	1.75	0.68
3:L:36:ILE:HD13	3:L:36:ILE:O	1.93	0.68
2:E:208:HIS:O	2:E:212:ASN:O	2.11	0.68
1:G:235:GLU:HG3	1:G:236:PRO:CD	2.22	0.68
2:B:186:LEU:HD12	2:B:187:SER:N	2.09	0.68
3:C:109:ILE:HD12	3:C:109:ILE: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
1:J:49:PRO:HG2	1:J:77:SER:HB3	1.74	0.68
1:G:92:PRO:HG3	1:G:223:GLN:HB2	1.75	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
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
2:K:51:LEU:CD1	2:K:56:ARG:H	2.07	0.68
3:C:125:SER:O	3:C:128:LEU:HD12	1.92	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:10:VAL:HG22	2:K:155:PRO:HG3	1.75	0.68
2:K:34:SER:HG	2:K:98:HIS:CE1	2.12	0.68
3:I:170:ASP:HB3	3:I:175:THR:OG1	1.95	0.67
2:H:203:ILE:HG12	2:H:204:CYS:N	2.09	0.67
3:C:39:PHE:N	3:C:48:LYS:O	2.27	0.67
2:H:171:VAL:C	2:H:172:HIS:HD1	1.97	0.67
1:J:97:ASP:CB	1:J:231:TRP:HE1	2.07	0.67
2:H:17:LEU:HB3	2:H:82:MET:HE2	1.76	0.67
2:K:33:MET:HB2	2:K:78:LEU:HD13	1.76	0.67
3:C:190:GLU:OE2	3:C:191:ARG:NE	2.27	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
1:J:133:THR:HG23	1:J:135:ALA:H	1.57	0.67
3:F:64:ARG:NH2	3:F:85:ASP:OD1	2.21	0.67
3:C:120:ILE:HG13	3:C:197:CYS:SG	2.35	0.67
3:F:89:TYR:O	3:F:104:GLY:HA2	1.93	0.67
3:L:208:ILE:C	3:L:209:VAL:HG12	2.14	0.67
2:E:156:GLU:CB	2:E:157:PRO:HA	2.25	0.67
1:J:220:VAL:HG12	1:J:221:ARG:HD2	1.77	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:N	3:C:176:TYR:CD2	2.61	0.67
2:K:178:LEU:C	2:K:180:SER:H	1.96	0.67
3:L:194:SER:HB3	3:L:210:LYS:CD	2.24	0.67
1:A:54:LYS:H	1:A:54:LYS:HD3	1.59	0.67
2:H:93:TYR:HE1	2:H:117:VAL:CG1	2.08	0.67
1:G:180:HIS:O	1:G:247:ASN:ND2	2.27	0.67
1:J:174:LEU:N	1:J:255:PHE:O	2.26	0.67
2:H:154:PHE:O	2:H:208:HIS:HE1	1.78	0.67
1:D:169:LYS:HB2	4:D:604:HOH:O	1.95	0.67
3:L:138:PHE:C	3:L:139:LEU:HD12	2.16	0.67
3:F:53:THR:HG22	3:F:53:THR:O	1.95	0.67
2:B:203:ILE:HD12	2:B:217:LYS:C	2.15	0.67
1:A:60:TRP:HA	1:A:67:CYS:SG	2.34	0.67
3:C:168:ASP:N	3:C:168:ASP:OD1	2.26	0.67
3:F:140:ASN:HB3	3:F:141:ASN:HD22	1.57	0.67
3:I:194:SER:HB2	3:I:210:LYS:CG	2.25	0.67
3:L:125:SER:O	3:L:128:LEU:HD23	1.94	0.67
2:H:111:TRP:CE3	3:I:47:PRO:HG2	2.30	0.66
1:G:119:LYS:HZ1	1:G:129:ASN:HB3	1.57	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:57:ILE:O	1:G:61:ILE:HG22	1.95	0.66
1:D:219:LYS:HG3	1:D:224:GLU:HG3	1.77	0.66
1:A:179:ILE:HD11	1:A:199:VAL:HG11	1.76	0.66
1:D:162:SER:C	1:D:163:LYS:HD2	2.14	0.66
2:B:181:SER:OG	3:L:84:GLU:OE2	2.14	0.66
1:J:115:GLU:H	3:L:96:GLU:HG2	1.59	0.66
3:I:116:PRO:CG	3:I:139:LEU:HD23	2.24	0.66
2:B:49:GLY:HA3	4:B:306:HOH:O	1.93	0.66
3:C:64:ARG:HH22	3:C:85:ASP:CG	1.98	0.66
2:E:32:ASP:HB2	2:E:50:ILE:O	1.94	0.66
1:D:121:SER:HB2	2:E:58:TYR:HA	1.78	0.66
3:I:6:SER:HB2	3:I:102:PHE:CE1	2.30	0.66
2:H:63:VAL:O	2:H:65:GLY:N	2.29	0.66
2:H:82:MET:HB3	2:H:85:LEU:HD21	1.76	0.66
1:A:54:LYS:N	1:A:54:LYS:HD3	2.10	0.66
2:E:196:SER:HB3	2:E:202:TYR:HE2	1.59	0.66
3:C:150:LYS:HB3	3:C:198:GLU:CG	2.25	0.66
2:H:71:ARG:HA	2:H:78:LEU:HA	1.76	0.66
2:H:213:THR:HG22	2:H:213:THR:O	1.95	0.66
3:C:39:PHE:HB2	3:C:50:LEU:CB	2.25	0.66
3:I:140:ASN:HB2	3:I:141:ASN:HD22	1.61	0.66
3:F:194:SER:HA	3:F:210:LYS:HG3	1.78	0.66
2:H:159:THR:HB	2:H:207:ASN:OD1	1.95	0.66
1:G:76:TRP:NE1	1:G:105:LEU:O	2.29	0.66
1:A:54:LYS:HD2	1:A:69:SER:OG	1.95	0.66
1:D:97:ASP:HA	1:D:99:GLU:OE2	1.95	0.66
3:C:39:PHE:N	3:C:49:LEU:HA	2.10	0.66
3:I:7:PRO:HD3	3:I:21:THR:O	1.95	0.66
2:K:66:ARG:HH21	2:K:85:LEU:HA	1.61	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: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:158:ARG:HD3	2:H:31:TYR:CE2	2.31	0.66
3:F:9:SER:HA	3:F:106:LYS:HB2	1.75	0.66
2:E:28:GLY:O	2:E:71:ARG:NH1	2.29	0.66
2:E:171:VAL:HG23	2:E:189:VAL:HG22	1.77	0.66
2:K:27:THR:C	2:K:29:SER:N	2.48	0.66
3:F:210:LYS:CG	3:F:211:SER:H	2.07	0.66
3:L:202:LYS:O	3:L:203:THR:HG22	1.96	0.66
2:E:72:ASP:OD1	2:E:75:ARG:N	2.19	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:91:CYS:SG	3:L:102:PHE:CD2	2.82	0.66
2:K:178:LEU:HA	3:L:163:LEU:HD21	1.78	0.66
1:D:149:ILE:HB	1:D:250:VAL:HG23	1.78	0.66
1:J:51:HIS:CD2	1:J:80:VAL:HB	2.30	0.66
2:E:127:PRO:CA	2:E:153:TYR:HB3	2.26	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:L:92:GLN:HA	3:L:101:THR:HA	1.77	0.65
3:I:116:PRO:HB3	3:I:142:PHE:CD2	2.31	0.65
3:C:79:ASN:HB3	3:C:80:PRO:HD3	1.76	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:B:203:ILE:HB	2:B:218:LYS:HA	1.77	0.65
2:H:146:LEU:HD11	2:H:219:SER:CB	2.27	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
1:A:182:PRO:HG2	1:A:188:GLN:HA	1.78	0.65
3:C:36:ILE:HD12	3:C:93:GLN:NE2	2.11	0.65
3:F:170:ASP:OD2	3:F:170:ASP:C	2.33	0.65
2:H:9:ALA:H	2:H:17:LEU:HD21	1.60	0.65
3:L:110:LYS:O	3:L:111:ARG:HD3	1.97	0.65
2:K:3:LYS:N	2:K:24:SER:HB2	2.08	0.65
1:G:219:LYS:HG3	1:G:223:GLN:N	2.10	0.65
3:C:110:LYS:NZ	3:C:110:LYS:HB3	2.12	0.65
3:C:196:THR:HG23	3:C:208:ILE:O	1.97	0.65
3:I:102:PHE:CE1	3:I:104:GLY:N	2.65	0.65
3:F:164:ASN:OD1	3:F:164:ASN:N	2.28	0.65
2:K:207:ASN:N	2:K:207:ASN:OD1	2.29	0.65
1:G:70:LEU:O	1:G:71:SER:OG	2.14	0.65
2:B:56:ARG:HD2	2:B:56:ARG:N	2.12	0.65
3:C:38:TRP:CH2	3:C:89:TYR:CD1	2.83	0.65
3:L:111:ARG:NH2	4:L:311:HOH:O	2.29	0.65
3:F:79:ASN:O	3:F:80:PRO:C	2.34	0.65
2:K:67:SER:HA	2:K:81:GLU:O	1.97	0.65
3:L:92:GLN:CG	3:L:101:THR:HB	2.27	0.65
3:L:37:ASN:ND2	3:L:93:GLN:HB2	2.12	0.65
1:J:84:SER:O	1:J:88:GLY:N	2.30	0.65
1:G:241:THR:HG22	1:G:242:PHE:N	2.10	0.65
3:L:145:LYS:HD3	3:L:167:THR:HG21	1.79	0.65
3:L:62:PRO:HG2	3:L:65:PHE:CE2	2.32	0.65
1:D:91:TYR:CD1	1:D:227:MET:HE2	2.32	0.65
1:G:171:LYS:HB3	1:G:257:MET:O	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:140:ASN:CG	3:C:176:TYR:CD1	2.70	0.65
3:L:109:ILE:HG22	3:L:110:LYS:N	2.12	0.65
3:L:102:PHE:CE1	3:L:104:GLY:CA	2.80	0.65
1:D:101:LEU:HA	1:D:104:GLN:HB3	1.77	0.65
3:I:198:GLU:HB3	3:I:207:PRO:HA	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
1:A:126:HIS:HA	1:A:154:LYS:HG2	1.79	0.65
3:I:202:LYS:O	3:I:203:THR:OG1	2.11	0.65
3:C:108:GLU:HG3	3:C:109:ILE:H	1.61	0.65
3:L:195:TYR:O	3:L:210:LYS:CA	2.45	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
1:A:84:SER:O	1:A:87:ASN:N	2.22	0.65
2:B:27:THR:HG22	2:B:31:TYR:HB2	1.79	0.65
2:E:32:ASP:CG	2:E:98:HIS:CE1	2.70	0.65
3:I:120:ILE:HD11	3:I:151:TRP:CZ3	2.32	0.65
1:J:54:LYS:HZ1	1:J:69:SER:HB3	1.62	0.65
1:A:57:ILE:HG13	1:A:81:GLU:OE2	1.97	0.65
1:G:153:LYS:HG3	1:G:191:LEU:O	1.97	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:A:206:TYR:CD2	1:A:206:TYR:C	2.71	0.65
3:L:102:PHE:CD1	3:L:102:PHE:C	2.70	0.64
1:G:169:LYS:HE2	1:G:256:ALA:HB2	1.79	0.64
1:G:206:TYR:CE2	1:G:208:LYS:HB2	2.31	0.64
2:E:169:SER:N	4:E:308:HOH:O	2.29	0.64
1:A:101:LEU:HA	1:A:104:GLN:HB3	1.78	0.64
3:F:3:MET:HG2	3:F:3:MET:O	1.96	0.64
1:G:193:GLN:NE2	1:G:193:GLN:HA	2.12	0.64
3:L:142:PHE:H	3:L:175:THR:HA	1.61	0.64
3:F:140:ASN:CG	3:F:176:TYR:HD1	1.99	0.64
3:L:92:GLN:CD	3:L:101:THR:HB	2.17	0.64
1:D:60:TRP:HA	1:D:67:CYS:SG	2.37	0.64
1:D:137:PRO:HA	1:D:143:SER:H	1.61	0.64
1:A:118:PRO:O	1:A:122:SER:OG	2.08	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
1:A:166:ILE:N	1:A:166:ILE:HD12	2.13	0.64
3:C:7:PRO:O	3:C:105:THR:OG1	2.14	0.64
2:E:51:LEU:HD12	2:E:56:ARG:H	1.60	0.64
1:D:54:LYS:HD2	1:D:67:CYS:HA	1.80	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:173:VAL:HA	1:G:255:PHE:O	1.98	0.64
1:D:153:LYS:HD2	1:D:193:GLN:HB2	1.78	0.64
2:B:156:GLU:HB3	2:B:157:PRO:HA	1.79	0.64
2:B:197:LEU:C	2:B:199:THR:H	2.01	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:I:2:GLN:HG2	3:I:2:GLN:O	1.98	0.64
3:F:152:LYS:O	3:F:196:THR:N	2.26	0.64
2:K:59:TYR:CE1	2:K:69:ILE:HG22	2.32	0.64
2:E:82:MET:HE1	2:E:117:VAL:HG21	1.79	0.64
1:G:211:LYS:HB2	1:G:211:LYS:NZ	2.12	0.64
3:C:38:TRP:CE2	3:C:39:PHE:HA	2.32	0.64
3:C:38:TRP:CD1	3:C:90:PHE:O	2.50	0.64
2:B:3:LYS:C	2:B:4:LEU:HD12	2.18	0.64
1:D:79:ILE:HD12	1:D:79:ILE:H	1.61	0.64
3:I:92:GLN:NE2	3:I:101:THR:HG22	2.12	0.64
3:L:34:ASN:O	3:L:95:LYS:HB3	1.98	0.64
2:E:180:SER:O	2:E:182:GLY:N	2.30	0.64
2:K:97:ARG:NE	2:K:110:GLY:HA3	2.13	0.64
2:B:181:SER:CB	3:L:62:PRO:HG3	2.21	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
3:I:16:GLN:HA	3:I:80:PRO:HA	1.79	0.64
2:H:45:GLU:HB3	2:H:60:ARG:NH1	2.13	0.64
2:E:181:SER:HB3	3:I:62:PRO:CG	2.28	0.64
2:B:34:SER:O	2:B:96:ALA:N	2.30	0.64
3:F:38:TRP:CH2	3:F:91:CYS:HA	2.32	0.64
2:K:45:GLU:OE2	3:L:99:TYR:O	2.15	0.64
1:D:91:TYR:HH	1:D:180:HIS:CD2	2.15	0.64
3:I:120:ILE:HD13	3:I:197:CYS:SG	2.38	0.64
3:C:158:ARG:HH22	2:K:97:ARG:HD2	1.63	0.64
1:G:166:ILE:HA	1:G:239:LYS:HB2	1.80	0.64
3:L:162:VAL:O	3:L:164:ASN:CG	2.34	0.64
3:L:153:ILE:HG22	3:L:192:HIS:CD2	2.33	0.64
2:E:146:LEU:O	2:E:190:VAL:N	2.27	0.64
2:B:51:LEU:HD11	2:B:56:ARG:H	1.61	0.63
3:C:111:ARG:NH1	3:C:172:LYS:O	2.31	0.63
1:A:115:GLU:HB2	3:C:96:GLU:CG	2.28	0.63
3:I:208:ILE:HG23	3:I:209:VAL:N	2.12	0.63
2:B:201:THR:CG2	2:B:218:LYS:HE3	2.29	0.63
2:H:11:VAL:O	2:H:120:SER:N	2.29	0.63
3:C:195:TYR:H	3:C:210:LYS:HB2	1.63	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:49:GLY:HA3	4:E:304:HOH:O	1.98	0.63
2:K:203:ILE:HD11	2:K:216:ASP:C	2.17	0.63
3:C:38:TRP:CZ3	3:C:89:TYR:CD1	2.86	0.63
1:A:76:TRP:CH2	1:A:108:VAL:HG21	2.33	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
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
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
1:D:91:TYR:OH	1:D:180:HIS:NE2	2.32	0.63
2:H:178:LEU:C	2:H:180:SER:H	2.01	0.63
1:D:116:ILE:HG13	1:D:165:TYR:HD1	1.61	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:I:66:SER:O	3:I:76:LEU:HD12	1.98	0.63
3:C:7:PRO:HG2	4:C:309:HOH:O	1.99	0.63
3:L:141:ASN:HA	3:L:175:THR:CG2	2.27	0.63
1:J:201:VAL:CG1	1:J:202:GLY:N	2.54	0.63
1:G:186:ALA:O	1:G:190:SER:OG	2.17	0.63
3:C:92:GLN:HA	3:C:101:THR:HG23	1.81	0.63
3:C:85:ASP:O	3:C:86:THR:C	2.37	0.63
1:J:153:LYS:HG2	1:J:191:LEU:O	1.99	0.63
3:F:182:LEU:CD1	3:F:182:LEU:C	2.67	0.63
2:E:82:MET:HE3	2:E:117:VAL:HG11	1.79	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:J:49:PRO:HD2	1:J:77:SER:OG	1.99	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
2:K:18:ARG:HG3	2:K:81:GLU:CA	2.28	0.63
1:D:144:PHE:CZ	1:D:227:MET:HE1	2.34	0.63
2:K:55:GLU:HG3	2:K:71:ARG:HD2	1.80	0.63
2:E:89:ASP:O	2:E:93:TYR:OH	2.10	0.63
2:K:152:ASP:C	2:K:183:LEU:HD12	2.19	0.63
1:G:153:LYS:HZ1	1:G:156:ASN:HA	1.63	0.63
3:I:17:ARG:O	3:I:17:ARG:HG3	1.99	0.63
2:B:178:LEU:HD12	2:B:179:GLN:N	2.13	0.63
2:E:21:CYS:HB3	2:E:78:LEU:HD23	1.80	0.63
2:K:133:ALA:C	3:L:121:PHE:HE1	2.02	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:162:TRP:CZ3	2:B:204:CYS:HB3	2.34	0.62
2:K:163:ASN:N	2:K:163:ASN:ND2	2.43	0.62
2:B:161:SER:O	2:B:205:ASN:N	2.30	0.62
1:D:121:SER:CB	2:E:58:TYR:HA	2.29	0.62
3:F:38:TRP:C	3:F:38:TRP:CD2	2.72	0.62
1:D:127:ASP:HB2	1:D:154:LYS:HB3	1.81	0.62
1:D:164:SER:OG	1:D:241:THR:HG23	1.98	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:G:188:GLN:HE22	1:G:197:ALA:CB	2.12	0.62
3:I:147:ILE:HG12	3:I:148:ASN:H	1.63	0.62
1:A:48:ALA:HB2	1:A:78:TYR:CZ	2.34	0.62
3:I:132:GLY:N	3:I:184:LEU:O	2.32	0.62
3:I:91:CYS:SG	3:I:102:PHE:HB3	2.40	0.62
2:K:86:ARG:O	2:K:89:ASP:HB2	1.99	0.62
3:I:196:THR:HG1	3:I:209:VAL:HG23	1.64	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
2:H:27:THR:C	2:H:29:SER:H	2.01	0.62
1:G:161:LEU:O	1:G:243:GLU:HA	2.00	0.62
1:G:57:ILE:N	1:G:81:GLU:OE2	2.23	0.62
2:K:132:LEU:HD12	2:K:147:GLY:HA3	1.82	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: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: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
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
3:F:45:GLN:HB3	3:F:46:PRO:HD3	1.81	0.62
3:I:108:GLU:C	3:I:109:ILE:HD12	2.20	0.62
3:I:92:GLN:NE2	3:I:101:THR:CG2	2.63	0.62
1:G:202:GLY:O	1:G:203:SER:OG	2.16	0.62
1:D:168:ASP:N	1:D:168:ASP:OD1	2.33	0.62
3:L:147:ILE:HG13	3:L:201:HIS:CG	2.35	0.62
3:F:35:PHE:HB3	3:F:95:LYS:HD3	1.81	0.62
1:J:118:PRO:HB2	1:J:120:THR:HG23	1.80	0.62
1:D:56:ASN:O	1:D:57:ILE:C	2.38	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:67:CYS:C	1:J:68:GLU:HG3	2.20	0.62
2:E:162:TRP:HB3	2:E:166:ALA:CB	2.29	0.62
1:J:95:PHE:HB3	1:J:98:TYR:HB2	1.82	0.62
2:E:98:HIS:CD2	2:E:98:HIS:N	2.67	0.61
1:D:55:CYS:HB2	1:D:60:TRP:HB2	1.82	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:258:GLU:O	1:D:259:ARG:HG3	1.99	0.61
1:D:215:ALA:O	1:D:217:ARG:NH1	2.32	0.61
3:I:10:LEU:HD23	3:I:11:ALA:H	1.64	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:34:ASN:N	3:I:34:ASN:OD1	2.32	0.61
2:E:93:TYR:O	2:E:114:GLY:HA2	2.00	0.61
3:F:150:LYS:O	3:F:198:GLU:N	2.17	0.61
1:D:219:LYS:HG2	1:D:222:ASP:HA	1.80	0.61
1:D:187:ASP:O	1:D:191:LEU:HD13	2.00	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:L:17:ARG:NE	4:L:308:HOH:O	2.23	0.61
3:F:38:TRP:CZ3	3:F:91:CYS:HA	2.36	0.61
1:D:146:LYS:HD2	1:D:252:ARG:NH2	2.14	0.61
3:L:151:TRP:CZ2	3:L:180:SER:HA	2.36	0.61
3:C:13:SER:HB3	3:C:110:LYS:HZ2	1.64	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
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
1:J:119:LYS:HZ3	1:J:129:ASN:HB3	1.65	0.61
1:G:153:LYS:HZ3	1:G:156:ASN:HA	1.66	0.61
1:A:127:ASP:N	1:A:154:LYS:HB3	2.15	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
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
1:J:57:ILE:O	1:J:61:ILE:HG22	2.01	0.61
1:A:104:GLN:HE22	1:A:233:LEU:CD2	2.13	0.61
2:K:147:GLY:C	2:K:162:TRP:HH2	2.03	0.61
2:K:38:GLN:HG3	2:K:43:GLY:HA2	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:142:PHE:CD1	3:L:144:PRO:O	2.53	0.61
2:H:50:ILE:HB	2:H:56:ARG:O	2.01	0.61
3:I:170:ASP:C	3:I:170:ASP:OD2	2.39	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:OD1	1:G:87:ASN:N	2.34	0.61
2:K:177:VAL:HG22	2:K:184:TYR:CE2	2.36	0.61
3:C:78:ILE:O	3:C:78:ILE:HG12	2.00	0.61
3:I:20:ILE:HG22	3:I:21:THR:N	2.16	0.61
2:K:63:VAL:C	2:K:65:GLY:N	2.54	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:C:153:ILE:HG13	3:C:154:ASP:N	2.16	0.61
1:A:235:GLU:HG3	1:A:236:PRO:HD2	1.82	0.61
2:E:122:ALA:HB3	2:E:154:PHE:CZ	2.35	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
1:J:184:THR:C	1:J:214:ILE:HG21	2.21	0.61
2:E:10:VAL:CG2	2:E:155:PRO:HG3	2.30	0.61
2:K:197:LEU:C	2:K:199:THR:H	2.02	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
3:L:38:TRP:NE1	3:L:90:PHE:CD2	2.67	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
1:G:91:TYR:OH	1:G:180:HIS:NE2	2.24	0.60
3:F:173:ASP:OD2	3:F:175:THR:HG23	2.00	0.60
3:I:39:PHE:O	3:I:89:TYR:HA	2.01	0.60
2:E:113:GLN:HG3	2:E:114:GLY:O	2.01	0.60
2:H:153:TYR:N	2:H:183:LEU:HD12	2.16	0.60
2:H:6:GLU:N	2:H:6:GLU:OE1	2.34	0.60
3:I:164:ASN:HB3	3:I:180:SER:H	1.66	0.60
3:I:107:LEU:HG	3:I:107:LEU:O	2.01	0.60
2:E:212:ASN:CG	2:E:213:THR:H	2.05	0.60
1:G:101:LEU:HG	1:G:231:TRP:CE2	2.37	0.60
3:F:107:LEU:HD23	3:F:107:LEU:O	2.02	0.60
3:F:41:GLN:HB2	3:F:47:PRO:HB3	1.83	0.60
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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: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
2:H:9:ALA:O	2:H:10:VAL:HG23	2.01	0.60
2:B:127:PRO:HB3	2:B:153:TYR:CB	2.30	0.60
2:H:69:ILE:CG1	2:H:70:SER:H	2.15	0.60
3:C:53:THR:HG22	3:C:53:THR:O	2.01	0.60
3:I:175:THR:HB	3:I:176:TYR:CD1	2.37	0.60
3:C:45:GLN:OE1	3:C:45:GLN:HA	2.01	0.60
2:B:148:CYS:HB2	2:B:162:TRP:CH2	2.37	0.60
1:A:183:SER:HA	1:A:215:ALA:O	2.01	0.60
1:A:169:LYS:CB	1:A:171:LYS:H	2.14	0.60
2:H:72:ASP:CB	2:H:79:TYR:HE2	2.15	0.60
3:F:149:VAL:HG21	3:F:179:SER:OG	2.02	0.60
2:E:207:ASN:N	2:E:207:ASN:OD1	2.34	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
2:B:27:THR:HG23	2:B:30:ASP:CG	2.22	0.60
3:L:42:LYS:C	3:L:44:GLY:H	2.06	0.60
3:F:38:TRP:CZ2	3:F:89:TYR:HB3	2.36	0.60
1:J:77:SER:O	1:J:106:SER:O	2.20	0.60
2:E:6:GLU:OE1	2:E:113:GLN:HG2	2.02	0.60
1:D:167:ASN:ND2	1:D:236:PRO:HA	2.16	0.60
1:D:149:ILE:HB	1:D:250:VAL:CG2	2.31	0.60
3:F:96:GLU:N	4:F:309:HOH:O	2.22	0.59
3:I:37:ASN:OD1	3:I:92:GLN:HB3	2.02	0.59
1:G:201:VAL:HG13	1:G:240:ILE:HD11	1.84	0.59
1:D:75:SER:OG	1:D:108:VAL:O	2.20	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
1:D:108:VAL:HG12	1:D:257:MET:CE	2.32	0.59
1:G:92:PRO:CG	1:G:223:GLN:HB2	2.31	0.59
3:C:169:GLN:HA	3:C:169:GLN:OE1	2.02	0.59
2:B:180:SER:C	2:B:182:GLY:N	2.50	0.59
3:L:141:ASN:HA	3:L:175:THR:HG22	1.82	0.59
3:I:102:PHE:CE1	3:I:104:GLY:CA	2.86	0.59
3:I:20:ILE:HG22	3:I:21:THR:H	1.66	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:J:97:ASP:HB2	1:J:231:TRP:HE1	1.66	0.59
1:J:84:SER:HB3	1:J:87:ASN:HB2	1.84	0.59
1:G:72:THR:HG21	3:I:70:SER:OG	2.03	0.59
3:F:39:PHE:H	3:F:50:LEU:H	1.47	0.59
2:H:100:TRP:CD1	3:I:34:ASN:CA	2.85	0.59
2:E:178:LEU:O	2:E:180:SER:HB2	2.02	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
2:E:127:PRO:HB3	2:E:153:TYR:CD2	2.38	0.59
1:A:48:ALA:HB2	1:A:78:TYR:CE2	2.38	0.59
1:D:58:ALA:O	1:D:62:LEU:HB2	2.01	0.59
2:H:38:GLN:HG3	2:H:43:GLY:HA2	1.84	0.59
2:E:152:ASP:HB3	2:E:183:LEU:HD23	1.84	0.59
3:C:204:SER:O	3:C:205:THR:CG2	2.50	0.59
2:K:4:LEU:HD23	2:K:95:CYS:O	2.03	0.59
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.82	0.59
2:B:168:THR:O	2:B:169:SER:OG	2.14	0.59
3:F:36:ILE:H	3:F:93:GLN:NE2	2.00	0.59
3:L:89:TYR:O	3:L:102:PHE:CZ	2.55	0.59
3:C:210:LYS:CG	3:C:211:SER:N	2.65	0.59
1:G:132:VAL:HB	1:G:142:LYS:O	2.02	0.59
1:A:58:ALA:HB2	1:A:98:TYR:CE1	2.38	0.59
1:G:179:ILE:HG12	1:G:180:HIS:N	2.18	0.59
3:C:108:GLU:HG3	3:C:109:ILE:N	2.18	0.59
2:E:171:VAL:HG21	3:F:176:TYR:CE1	2.38	0.59
3:F:86:THR:HA	3:F:107:LEU:HD23	1.85	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
3:L:96:GLU:O	3:L:97:VAL:HB	2.02	0.59
1:D:153:LYS:HG2	1:D:153:LYS:O	1.99	0.59
1:G:69:SER:OG	1:G:70:LEU:HB2	2.02	0.59
2:B:161:SER:OG	2:B:205:ASN:HB2	2.02	0.59
2:B:53:GLY:O	2:B:54:SER:HB2	2.03	0.59
3:F:110:LYS:O	3:F:111:ARG:HG3	2.03	0.59
3:C:97:VAL:HG12	3:C:98:PRO:O	2.03	0.59
3:C:45:GLN:HB3	3:C:46:PRO:CD	2.30	0.59
1:A:49:PRO:HB2	1:A:76:TRP:CB	2.32	0.59
2:E:21:CYS:O	2:E:77:THR:HA	2.03	0.59
1:J:153:LYS:HB3	1:J:158:TYR:HB2	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:10:VAL:HG22	2:B:155:PRO:HG3	1.85	0.59
1:G:193:GLN:HE21	1:G:193:GLN:HA	1.68	0.59
1:D:228:ASN:HB3	1:D:230:TYR:CE1	2.37	0.59
3:I:149:VAL:HG23	3:I:150:LYS:N	2.17	0.59
3:C:39:PHE:HB3	3:C:50:LEU:HB2	1.82	0.59
1:J:54:LYS:HE3	1:J:67:CYS:HA	1.84	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: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
3:L:167:THR:HG22	3:L:168:ASP:N	2.18	0.59
1:G:134:ALA:N	1:G:142:LYS:HD2	2.18	0.59
2:B:10:VAL:CG2	2:B:155:PRO:HG3	2.33	0.59
2:K:203:ILE:HG13	2:K:217:LYS:O	2.02	0.59
2:H:163:ASN:O	2:H:164:SER:OG	2.20	0.59
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:G:118:PRO:HB3	1:G:120:THR:HG23	1.84	0.58
1:J:221:ARG:O	1:J:223:GLN:HG2	2.03	0.58
1:D:219:LYS:HD2	1:D:222:ASP:OD1	2.03	0.58
1:A:94:ASP:OD1	1:A:94:ASP:N	2.34	0.58
3:F:158:ARG:HG3	3:F:159:GLN:H	1.68	0.58
1:J:120:THR:O	1:J:122:SER:N	2.35	0.58
1:G:201:VAL:HG13	1:G:202:GLY:H	1.67	0.58
3:L:162:VAL:CG2	3:L:182:LEU:HG	2.32	0.58
1:D:51:HIS:ND1	1:D:80:VAL:HG11	2.17	0.58
2:B:86:ARG:HG3	2:B:88:GLU:OE1	2.03	0.58
1:J:171:LYS:HZ2	1:J:258:GLU:HG3	1.68	0.58
2:K:163:ASN:C	2:K:165:GLY:N	2.56	0.58
3:F:34:ASN:N	3:F:34:ASN:ND2	2.51	0.58
1:D:181:HIS:ND1	1:D:212:PRO:HA	2.18	0.58
3:F:39:PHE:O	3:F:40:GLN:HB2	2.03	0.58
2:H:92:VAL:HA	2:H:115:THR:O	2.03	0.58
3:F:192:HIS:O	3:F:195:TYR:OH	2.13	0.58
3:C:193:ASN:O	3:C:211:SER:HB3	2.04	0.58
1:G:131:GLY:HA3	1:G:150:TRP:HB3	1.85	0.58
3:F:114:ALA:HA	3:F:201:HIS:CD2	2.39	0.58
1:G:180:HIS:O	1:G:182:PRO:HD3	2.03	0.58
2:H:132:LEU:HB3	3:I:121:PHE:CD1	2.39	0.58
3:I:162:VAL:O	3:I:164:ASN:CG	2.41	0.58
2:E:129:VAL:HG13	2:E:150:VAL:HG22	1.83	0.58
2:H:33:MET:CB	2:H:78:LEU:HD13	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:94:ASP:HB2	1:D:228:ASN:OD1	2.04	0.58
3:I:167:THR:HG22	3:I:168:ASP:H	1.67	0.58
3:C:113:ASP:O	3:C:143:TYR:O	2.21	0.58
3:L:140:ASN:HB2	3:L:141:ASN:HD22	1.69	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:F:20:ILE:HG12	3:F:105:THR:HG21	1.85	0.58
3:C:158:ARG:HG3	2:K:31:TYR:CZ	2.38	0.58
1:J:48:ALA:CB	1:J:78:TYR:CE1	2.86	0.58
2:B:127:PRO:HA	2:B:153:TYR:HB3	1.85	0.58
2:E:160:VAL:HG22	2:E:206:VAL:HG22	1.85	0.58
2:B:176:ALA:HB2	3:C:166:TRP:CZ2	2.38	0.58
3:F:169:GLN:OE1	3:F:169:GLN:HA	2.03	0.58
3:F:108:GLU:OE2	3:F:173:ASP:O	2.21	0.58
2:H:171:VAL:HG22	3:I:176:TYR:CE2	2.37	0.58
1:G:199:VAL:HG13	1:G:244:ALA:HB2	1.86	0.58
2:E:67:SER:HA	2:E:81:GLU:O	2.03	0.58
3:F:150:LYS:HE3	3:F:150:LYS:HA	1.85	0.58
3:C:159:GLN:HG3	3:C:160:ASN:H	1.67	0.58
3:L:193:ASN:O	3:L:211:SER:OG	2.19	0.58
1:G:187:ASP:O	1:G:191:LEU:HD13	2.03	0.58
2:B:197:LEU:HG	2:B:198:GLY:N	2.19	0.58
2:B:171:VAL:CG2	3:C:176:TYR:CZ	2.83	0.58
2:E:59:TYR:HE1	2:E:69:ILE:HG22	1.67	0.58
2:E:59:TYR:CE1	2:E:69:ILE:HG22	2.38	0.58
1:J:199:VAL:CG1	1:J:200:PHE:N	2.64	0.58
1:A:76:TRP:CZ3	1:A:108:VAL:HG21	2.39	0.58
1:D:51:HIS:CE1	1:D:80:VAL:HG21	2.39	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
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:145:LYS:HD2	3:F:167:THR:HG21	1.84	0.58
3:L:102:PHE:HD1	3:L:102:PHE:C	2.06	0.58
1:A:177:TRP:CE2	1:A:230:TYR:HB2	2.39	0.58
1:J:100:GLU:HG2	1:J:231:TRP:HZ2	1.68	0.58
3:F:71:GLY:O	3:F:72:THR:HG22	2.04	0.58
2:B:157:PRO:O	2:B:208:HIS:HD2	1.87	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:I:102:PHE:CD1	3:I:103:GLY:N	2.71	0.58
2:K:36:ILE:HG13	2:K:36:ILE:O	2.03	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:119:LYS:HZ2	1:J:129:ASN:HB3	1.68	0.58
3:F:151:TRP:CZ3	3:F:197:CYS:HB3	2.38	0.58
2:K:209:LYS:O	2:K:212:ASN:N	2.26	0.58
1:D:138:HIS:O	1:D:139:ALA:C	2.41	0.58
2:B:160:VAL:O	2:B:172:HIS:NE2	2.36	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
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
2:B:63:VAL:HG13	2:B:67:SER:H	1.69	0.58
1:A:104:GLN:HG3	1:A:104:GLN:O	2.04	0.58
2:E:200:GLN:HG2	2:E:202:TYR:CE2	2.39	0.58
1:J:114:PHE:HA	3:L:96:GLU:OE1	2.04	0.57
1:A:165:TYR:O	1:A:239:LYS:HA	2.04	0.57
1:J:158:TYR:CZ	1:J:246:GLY:HA2	2.39	0.57
1:G:231:TRP:HZ3	1:G:233:LEU:HD13	1.68	0.57
2:E:11:VAL:HG22	2:E:12:GLN:O	2.03	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: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
3:L:49:LEU:O	3:L:50:LEU:HD23	2.04	0.57
1:J:48:ALA:HB2	1:J:78:TYR:CE1	2.38	0.57
2:B:29:SER:HA	2:B:73:ASN:HD22	1.69	0.57
3:I:37:ASN:O	3:I:49:LEU:HB2	2.04	0.57
3:C:157:GLU:O	2:K:27:THR:HG21	2.03	0.57
1:G:242:PHE:CE1	1:G:251:PRO:HG2	2.39	0.57
1:D:126:HIS:HA	1:D:154:LYS:HG2	1.85	0.57
3:F:126:GLU:N	3:F:126:GLU:OE1	2.38	0.57
3:F:108:GLU:C	3:F:109:ILE:HD12	2.25	0.57
3:L:94:THR:O	3:L:99:TYR:CD1	2.58	0.57
1:J:123:TRP:HZ3	1:J:163:LYS:HG3	1.70	0.57
2:B:45:GLU:CD	2:B:46:TRP:N	2.58	0.57
3:F:45:GLN:CB	3:F:46:PRO:CD	2.82	0.57
1:A:121:SER:HB2	2:B:58:TYR:HD1	1.68	0.57
2:H:208:HIS:ND1	2:H:211:SER:OG	2.35	0.57
3:C:38:TRP:CH2	3:C:89:TYR:CB	2.87	0.57
2:H:98:HIS:N	2:H:98:HIS:CD2	2.72	0.57
2:K:17:LEU:HD23	2:K:82:MET:SD	2.44	0.57
1:D:57:ILE:CD1	1:D:102:ARG:HG3	2.34	0.57
3:C:203:THR:HG23	3:C:205:THR:N	2.10	0.57
1:G:119:LYS:NZ	1:G:129:ASN:ND2	2.40	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:63:VAL:CG1	2:B:67:SER:HB2	2.30	0.57
2:H:145:ALA:HB2	2:H:191:THR:HG23	1.85	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
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:233:LEU:HD12	1:J:233:LEU:N	2.20	0.57
1:J:56:ASN:HB3	1:J:84:SER:H	1.69	0.57
3:L:130:SER:HB3	3:L:132:GLY:N	2.20	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
2:B:35:TRP:HE1	2:B:78:LEU:HD13	1.69	0.57
3:C:64:ARG:NH2	3:C:85:ASP:CG	2.56	0.57
3:L:141:ASN:HA	3:L:175:THR:CA	2.35	0.57
3:F:116:PRO:CA	3:F:142:PHE:HB3	2.31	0.57
3:F:113:ASP:O	3:F:143:TYR:O	2.22	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
2:B:190:VAL:HG22	2:B:192:VAL:HG23	1.84	0.57
1:J:227:MET:SD	1:J:249:VAL:HG21	2.44	0.57
3:L:28:VAL:HG23	3:L:74:PHE:CE2	2.40	0.57
3:C:52:TYR:O	3:C:56:ASN:HB2	2.05	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
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
3:C:4:THR:O	3:C:102:PHE:HB2	2.05	0.57
3:C:90:PHE:CD2	3:C:90:PHE:N	2.72	0.57
2:B:174:PHE:O	3:C:166:TRP:NE1	2.38	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
2:H:49:GLY:HA3	4:H:302:HOH:O	2.03	0.57
3:F:2:GLN:CD	3:F:97:VAL:HG21	2.24	0.57
3:I:6:SER:CB	3:I:7:PRO:HD2	2.25	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
3:L:20:ILE:HG22	3:L:21:THR:H	1.70	0.57
2:B:61:ASP:HB3	2:K:142:GLY:O	2.04	0.57
2:B:45:GLU:CD	2:B:46:TRP:H	2.08	0.56
3:C:38:TRP:NE1	3:C:91:CYS:HA	2.19	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:173:THR:CB	3:C:178:MET:HE3	2.32	0.56
3:F:45:GLN:HB3	3:F:46:PRO:HD2	1.85	0.56
3:F:4:THR:HG22	3:F:24:ALA:CA	2.31	0.56
1:A:52:LEU:HD12	1:A:81:GLU:HG3	1.86	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:162:VAL:HG23	3:I:162:VAL:O	2.04	0.56
2:B:134:PRO:HD3	2:B:146:LEU:HD11	1.87	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
2:H:34:SER:N	2:H:98:HIS:NE2	2.53	0.56
3:I:170:ASP:CG	3:I:171:SER:N	2.59	0.56
2:E:178:LEU:O	2:E:179:GLN:C	2.42	0.56
1:A:147:ASN:HD22	1:A:253:TYR:HB2	1.70	0.56
2:H:178:LEU:O	2:H:180:SER:N	2.38	0.56
1:G:144:PHE:CG	1:G:145:TYR:N	2.73	0.56
3:I:159:GLN:CG	3:I:160:ASN:N	2.64	0.56
2:B:10:VAL:CG1	2:B:155:PRO:HG3	2.35	0.56
3:F:183:THR:CG2	3:F:184:LEU:H	2.17	0.56
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.35	0.56
2:E:122:ALA:HB3	2:E:154:PHE:CE2	2.40	0.56
2:B:122:ALA:HB3	2:B:154:PHE:CE2	2.41	0.56
2:E:173:THR:HG21	3:F:178:MET:HG2	1.86	0.56
1:A:239:LYS:O	1:A:239:LYS:HG3	2.06	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:161:LEU:HD23	1:A:161:LEU:C	2.25	0.56
2:B:207:ASN:OD1	2:B:207:ASN:N	2.38	0.56
3:C:140:ASN:HA	3:C:176:TYR:HA	1.88	0.56
3:L:45:GLN:CB	3:L:46:PRO:HD2	2.23	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
3:L:49:LEU:HD23	3:L:50:LEU:H	1.71	0.56
2:K:34:SER:OG	2:K:98:HIS:CE1	2.59	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: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
3:C:9:SER:HA	3:C:105:THR:HG23	1.86	0.56
3:L:142:PHE:N	3:L:175:THR:HA	2.20	0.56
3:I:6:SER:CB	3:I:102:PHE:CE1	2.89	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:50:LEU:O	3:L:58:GLY:N	2.30	0.56
3:I:195:TYR:N	3:I:210:LYS:HA	2.21	0.56
2:E:208:HIS:CE1	2:E:210:PRO:HG2	2.39	0.56
2:H:152:ASP:N	2:H:184:TYR:O	2.39	0.56
3:L:162:VAL:HG21	3:L:181:THR:CA	2.35	0.56
3:C:162:VAL:HG11	3:C:182:LEU:O	2.06	0.56
3:C:36:ILE:O	3:C:93:GLN:HG3	2.06	0.56
2:B:171:VAL:HG21	3:C:176:TYR:CD1	2.37	0.56
2:H:69:ILE:HG12	2:H:70:SER:H	1.70	0.56
3:I:195:TYR:O	3:I:210:LYS:N	2.39	0.56
2:B:162:TRP:CD1	2:B:170:SER:OG	2.56	0.56
3:L:198:GLU:HB3	3:L:207:PRO:HB3	1.88	0.56
2:E:203:ILE:HD11	2:E:216:ASP:HB2	1.88	0.56
3:L:120:ILE:HD13	3:L:197:CYS:CB	2.36	0.56
3:L:178:MET:C	3:L:178:MET:SD	2.85	0.56
3:C:64:ARG:NH2	3:C:82:GLU:H	2.03	0.56
2:B:178:LEU:O	2:B:180:SER:N	2.39	0.56
3:F:109:ILE:HG22	3:F:110:LYS:N	2.21	0.56
1:G:54:LYS:HZ1	1:G:60:TRP:HD1	1.52	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
3:F:118:VAL:HB	3:F:208:ILE:HD13	1.87	0.56
2:E:36:ILE:HD12	2:E:45:GLU:C	2.26	0.56
3:C:128:LEU:HD13	3:C:129:THR:HG23	1.87	0.56
2:B:11:VAL:O	2:B:120:SER:N	2.37	0.56
3:I:118:VAL:HG22	3:I:139:LEU:HG	1.88	0.56
2:B:12:GLN:HG3	2:B:121:SER:HA	1.88	0.56
2:B:32:ASP:CB	2:B:50:ILE:O	2.54	0.55
2:E:46:TRP:N	2:E:60:ARG:NH1	2.54	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:G:84:SER:O	1:G:87:ASN:N	2.37	0.55
2:B:182:GLY:O	2:B:183:LEU:HB2	2.06	0.55
1:A:216:ILE:H	1:D:96:ILE:HG23	1.71	0.55
1:G:79:ILE:CG2	1:G:80:VAL:N	2.69	0.55
3:C:150:LYS:O	3:C:198:GLU:HG2	2.07	0.55
3:C:166:TRP:O	3:C:177:SER:HA	2.07	0.55
2:H:34:SER:OG	2:H:98:HIS:NE2	2.39	0.55
1:D:48:ALA:HB3	1:D:51:HIS:CE1	2.42	0.55
2:B:63:VAL:CG1	2:B:67:SER:H	2.19	0.55
1:G:52:LEU:HD12	1:G:81:GLU:HB3	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:207:ASN:HA	2:K:213:THR:O	2.06	0.55
3:L:116:PRO:O	3:L:140:ASN:N	2.36	0.55
3:L:12:VAL:HG12	3:L:13:SER:N	2.21	0.55
3:L:172:LYS:HG2	3:L:172:LYS:O	2.06	0.55
2:E:186:LEU:HG	2:E:187:SER:N	2.20	0.55
3:L:102:PHE:CE1	3:L:104:GLY:N	2.73	0.55
3:L:102:PHE:HE1	3:L:104:GLY:C	2.09	0.55
1:D:101:LEU:CD2	1:D:105:LEU:HG	2.37	0.55
1:A:144:PHE:CZ	1:A:227:MET:HE1	2.42	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:205:THR:O	3:L:207:PRO:HD3	2.06	0.55
1:A:56:ASN:O	1:A:57:ILE:C	2.43	0.55
2:E:18:ARG:HD2	2:E:79:TYR:HB3	1.89	0.55
3:C:110:LYS:C	3:C:111:ARG:HD3	2.27	0.55
2:H:97:ARG:O	3:I:36:ILE:CB	2.55	0.55
3:L:102:PHE:CD1	3:L:103:GLY:N	2.74	0.55
1:J:200:PHE:O	1:J:201:VAL:HG23	2.07	0.55
3:C:153:ILE:CG1	3:C:154:ASP:H	2.20	0.55
2:K:176:ALA:CB	3:L:166:TRP:CE2	2.88	0.55
3:I:79:ASN:HB3	3:I:80:PRO:CD	2.36	0.55
3:C:113:ASP:OD1	3:C:113:ASP:C	2.45	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
2:E:179:GLN:O	2:E:180:SER:C	2.45	0.55
2:H:186:LEU:HD12	2:H:186:LEU:C	2.26	0.55
2:H:207:ASN:HB3	2:H:214:LYS:CG	2.36	0.55
1:J:84:SER:CB	1:J:88:GLY:H	2.16	0.55
2:E:129:VAL:HG11	2:E:206:VAL:HG21	1.89	0.55
2:B:3:LYS:O	2:B:4:LEU:HD12	2.07	0.55
3:C:38:TRP:CD2	3:C:90:PHE:O	2.60	0.55
2:B:129:VAL:HG22	2:B:150:VAL:HG22	1.89	0.55
3:F:86:THR:HG22	3:F:109:ILE:CD1	2.31	0.55
1:G:54:LYS:HG2	1:G:55:CYS:N	2.22	0.55
2:K:97:ARG:N	2:K:110:GLY:O	2.35	0.55
2:K:32:ASP:CB	2:K:98:HIS:HD1	2.13	0.55
1:J:106:SER:HG	1:J:263:SER:HG	1.47	0.55
1:G:166:ILE:N	1:G:166:ILE:HD13	2.21	0.55
1:G:200:PHE:CE2	1:G:201:VAL:O	2.60	0.55
3:F:193:ASN:O	3:F:211:SER:HB3	2.06	0.55
3:I:81:VAL:O	3:I:82:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:207:ASN:ND2	2:K:214:LYS:HD2	2.22	0.55
1:J:107:SER:HB2	1:J:260:ASN:OD1	2.06	0.55
3:I:42:LYS:HG2	3:I:87:ALA:HB2	1.87	0.55
1:A:59:GLY:HA2	1:A:89:THR:HG22	1.88	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
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: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
1:G:149:ILE:HD11	1:G:252:ARG:HG3	1.87	0.55
3:L:109:ILE:HG22	3:L:110:LYS:H	1.72	0.55
3:F:39:PHE:C	3:F:50:LEU:HG	2.27	0.55
3:F:38:TRP:CZ2	3:F:90:PHE:N	2.75	0.55
2:H:152:ASP:C	2:H:183:LEU:HD12	2.27	0.55
1:D:76:TRP:CZ3	1:D:108:VAL:HG21	2.41	0.55
3:F:203:THR:O	3:F:205:THR:N	2.39	0.55
2:K:125:LYS:HD2	2:K:126:GLY:H	1.71	0.55
2:H:130:PHE:CD2	3:I:127:GLN:HB2	2.42	0.55
2:E:124:THR:HA	2:E:154:PHE:O	2.07	0.55
3:L:142:PHE:CD1	3:L:142:PHE:O	2.59	0.55
2:E:173:THR:CG2	3:F:178:MET:SD	2.95	0.55
3:L:34:ASN:ND2	3:L:96:GLU:OE2	2.34	0.55
1:G:203:SER:HB3	1:G:239:LYS:O	2.06	0.55
3:F:209:VAL:HG22	3:F:210:LYS:HB3	1.87	0.55
2:H:202:TYR:HE1	2:H:219:SER:HB2	1.70	0.55
3:L:27:SER:C	3:L:28:VAL:HG22	2.27	0.55
1:J:178:GLY:HA2	1:J:228:ASN:O	2.07	0.55
2:E:28:GLY:H	2:E:76:LYS:HZ3	1.55	0.54
1:G:54:LYS:HB2	1:G:66:GLU:O	2.06	0.54
3:I:10:LEU:HD23	3:I:11:ALA:N	2.22	0.54
3:L:38:TRP:HE1	3:L:90:PHE:CB	2.19	0.54
2:K:34:SER:HA	2:K:49:GLY:HA2	1.89	0.54
1:A:121:SER:CB	2:B:58:TYR:HA	2.37	0.54
3:F:153:ILE:HG22	3:F:195:TYR:CE2	2.42	0.54
1:D:252:ARG:HD2	1:D:253:TYR:N	2.22	0.54
1:A:167:ASN:CG	1:A:236:PRO:HA	2.28	0.54
1:G:219:LYS:HG2	1:G:222:ASP:HA	1.89	0.54
2:K:48:SER:OG	2:K:59:TYR:HD1	1.90	0.54
2:B:122:ALA:O	2:B:154:PHE:HE2	1.90	0.54
3:C:24:ALA:HB1	3:C:26:GLU:O	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:35:PHE:CD1	3:C:36:ILE:HA	2.43	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
3:F:42:LYS:HD2	3:F:87:ALA:HB2	1.89	0.54
3:I:38:TRP:HB3	3:I:47:PRO:HB2	1.86	0.54
1:J:54:LYS:NZ	1:J:54:LYS:HB3	2.06	0.54
1:G:132:VAL:O	1:G:132:VAL:HG23	2.07	0.54
3:C:128:LEU:CD1	3:C:129:THR:HG23	2.37	0.54
1:G:188:GLN:NE2	1:G:197:ALA:CB	2.70	0.54
2:H:78:LEU:HD23	2:H:78:LEU:H	1.73	0.54
2:H:75:ARG:O	2:H:76:LYS:HB2	2.07	0.54
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
1:G:127:ASP:N	1:G:154:LYS:HB2	2.22	0.54
2:B:54:SER:CB	2:B:56:ARG:HH11	2.21	0.54
3:L:143:TYR:CD2	3:L:144:PRO:HD3	2.41	0.54
2:E:46:TRP:N	2:E:60:ARG:HH12	2.05	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
3:L:209:VAL:HG23	3:L:210:LYS:CB	2.37	0.54
1:D:63:GLY:O	1:D:146:LYS:N	2.25	0.54
2:E:196:SER:O	2:E:200:GLN:N	2.40	0.54
3:L:28:VAL:HG23	3:L:72:THR:H	1.72	0.54
2:K:38:GLN:HG3	2:K:43:GLY:CA	2.37	0.54
2:H:164:SER:HA	2:H:167:LEU:HB2	1.89	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
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
2:K:211:SER:C	2:K:213:THR:H	2.11	0.54
1:D:228:ASN:HB3	1:D:230:TYR:HE1	1.73	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
3:I:20:ILE:CG2	3:I:105:THR:HG21	2.38	0.54
1:G:119:LYS:HZ3	1:G:129:ASN:HB3	1.67	0.54
1:D:48:ALA:HB1	1:D:80:VAL:CG2	2.37	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: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:I:170:ASP:HB3	3:I:175:THR:HG1	1.71	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:205:ASN:HD22	2:E:214:LYS:CE	2.21	0.54
1:J:161:LEU:HD23	1:J:161:LEU:C	2.27	0.54
3:L:69:GLY:HA2	3:L:73:ASP:O	2.08	0.54
2:E:144:ALA:N	2:E:192:VAL:O	2.39	0.54
2:K:37:ARG:HB3	2:K:93:TYR:CD2	2.43	0.54
3:F:166:TRP:O	3:F:177:SER:CA	2.55	0.54
2:H:32:ASP:HB2	2:H:98:HIS:ND1	2.22	0.54
3:I:38:TRP:CG	3:I:47:PRO:HB3	2.39	0.54
1:A:252:ARG:HD2	1:A:253:TYR:N	2.23	0.54
3:I:27:SER:O	3:I:28:VAL:CG2	2.54	0.54
2:B:10:VAL:HG13	2:B:155:PRO:HG3	1.88	0.54
1:G:101:LEU:HD22	1:G:105:LEU:HD11	1.90	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:B:203:ILE:HD12	2:B:218:LYS:N	2.23	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:J:138:HIS:O	1:J:139:ALA:C	2.47	0.54
3:I:167:THR:HG23	3:I:177:SER:HB2	1.90	0.54
3:C:8:ALA:HB3	4:C:309:HOH:O	2.06	0.54
3:L:109:ILE:CG2	3:L:110:LYS:H	2.21	0.54
3:I:109:ILE:CG2	3:I:110:LYS:N	2.70	0.54
3:F:9:SER:HB3	3:F:106:LYS:HZ1	1.71	0.54
2:K:98:HIS:HD2	3:L:36:ILE:HG21	1.73	0.54
1:A:216:ILE:O	1:D:96:ILE:HA	2.08	0.54
2:E:143:THR:HG23	2:E:191:THR:HG23	1.90	0.54
2:B:78:LEU:O	2:B:78:LEU:HD12	2.08	0.53
2:B:177:VAL:HG12	2:B:183:LEU:H	1.73	0.53
3:F:38:TRP:CZ2	3:F:89:TYR:C	2.81	0.53
3:I:170:ASP:OD2	3:I:172:LYS:N	2.41	0.53
3:F:152:LYS:N	3:F:196:THR:O	2.41	0.53
3:L:209:VAL:HG23	3:L:210:LYS:HG3	1.90	0.53
3:F:164:ASN:HB3	3:F:180:SER:O	2.08	0.53
1:J:98:TYR:CG	1:J:98:TYR:O	2.60	0.53
3:I:143:TYR:CZ	3:I:144:PRO:HB3	2.43	0.53
3:C:38:TRP:CE2	3:C:39:PHE:CD1	2.97	0.53
3:C:135:VAL:HG12	3:C:151:TRP:HH2	1.74	0.53
3:C:83:ALA:O	3:C:171:SER:O	2.26	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
2:B:43:GLY:O	2:B:44:LEU:HG	2.07	0.53
2:B:21:CYS:O	2:B:77:THR:HA	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:D:94:ASP:OD1	1:D:94:ASP:N	2.38	0.53
2:H:218:LYS:HB2	2:H:218:LYS:NZ	2.23	0.53
2:B:83:ASN:OD1	2:B:84:SER:N	2.41	0.53
3:I:147:ILE:HG23	3:I:148:ASN:N	2.22	0.53
3:C:108:GLU:HG2	3:C:169:GLN:NE2	2.24	0.53
3:F:172:LYS:N	3:F:172:LYS:HD3	2.23	0.53
3:I:92:GLN:HG2	3:I:101:THR:HB	1.90	0.53
2:K:99:SER:HB3	3:L:35:PHE:O	2.09	0.53
1:D:133:THR:CB	1:D:150:TRP:HZ3	2.21	0.53
1:J:64:ASN:OD1	1:J:65:PRO:HD2	2.08	0.53
3:L:151:TRP:HZ2	3:L:180:SER:HA	1.71	0.53
3:I:144:PRO:O	3:I:201:HIS:CE1	2.61	0.53
3:F:57:LYS:HD3	3:F:61:VAL:O	2.07	0.53
1:G:83:SER:O	1:G:85:SER:N	2.42	0.53
2:B:97:ARG:O	3:C:36:ILE:HG12	2.09	0.53
1:J:48:ALA:CB	1:J:78:TYR:HE1	2.20	0.53
2:H:82:MET:HE1	2:H:117:VAL:HG21	1.89	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
2:K:90:THR:HG23	2:K:117:VAL:O	2.09	0.53
2:B:208:HIS:C	2:B:210:PRO:HD2	2.29	0.53
1:J:149:ILE:O	1:J:250:VAL:HG22	2.09	0.53
3:L:10:LEU:O	3:L:107:LEU:HA	2.08	0.53
3:L:81:VAL:HG12	3:L:82:GLU:N	2.24	0.53
3:I:1:ILE:HG22	3:I:3:MET:CE	2.39	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:L:161:GLY:O	3:L:162:VAL:HG12	2.09	0.53
3:F:114:ALA:HB1	3:F:202:LYS:O	2.08	0.53
3:L:118:VAL:O	3:L:208:ILE:HD12	2.08	0.53
3:I:24:ALA:HB3	3:I:72:THR:OG1	2.08	0.53
3:F:36:ILE:H	3:F:93:GLN:HE22	1.57	0.53
3:F:159:GLN:NE2	2:H:26:PHE:HE2	2.07	0.53
1:J:118:PRO:O	1:J:122:SER:OG	2.23	0.53
1:G:169:LYS:HE2	1:G:256:ALA:CB	2.39	0.53
2:E:162:TRP:HB3	2:E:166:ALA:HB1	1.90	0.53
2:E:4:LEU:HB2	2:E:112:GLY:CA	2.39	0.53
3:F:134:SER:HB2	3:F:181:THR:O	2.09	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:53:GLY:O	2:H:54:SER:HB2	2.09	0.53
3:I:102:PHE:CE1	3:I:104:GLY:C	2.81	0.53
2:K:100:TRP:NE1	3:L:34:ASN:HA	2.22	0.53
2:H:176:ALA:CB	3:I:166:TRP:CZ2	2.91	0.53
1:G:57:ILE:HD13	1:G:102:ARG:HB2	1.89	0.53
1:D:99:GLU:CD	1:D:99:GLU:H	2.12	0.53
1:D:178:GLY:O	1:D:179:ILE:HD12	2.09	0.53
3:C:17:ARG:HA	3:C:79:ASN:O	2.08	0.53
3:L:17:ARG:HA	3:L:79:ASN:HA	1.90	0.53
2:E:213:THR:O	2:E:213:THR:HG22	2.07	0.53
2:H:2:VAL:HG13	2:H:24:SER:O	2.08	0.53
2:E:13:PRO:CD	2:E:121:SER:HB2	2.38	0.53
2:B:98:HIS:CD2	2:B:98:HIS:H	2.27	0.53
1:J:115:GLU:HG3	1:J:115:GLU:O	2.09	0.53
1:A:259:ARG:HB3	1:A:259:ARG:HH11	1.70	0.53
2:E:161:SER:HA	2:E:167:LEU:HD11	1.90	0.53
1:J:203:SER:OG	1:J:204:SER:N	2.39	0.53
3:L:205:THR:O	3:L:205:THR:HG23	2.09	0.53
1:D:231:TRP:HZ3	1:D:233:LEU:CD2	2.22	0.53
3:I:202:LYS:HG2	3:I:202:LYS:O	2.09	0.53
2:E:12:GLN:HG3	2:E:121:SER:OG	2.09	0.53
3:C:7:PRO:HG3	3:C:21:THR:OG1	2.08	0.53
3:L:170:ASP:HB3	3:L:175:THR:OG1	2.09	0.53
3:F:38:TRP:HZ2	3:F:89:TYR:C	2.12	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
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
2:B:86:ARG:H	2:B:89:ASP:HB2	1.74	0.53
1:G:221:ARG:O	1:G:223:GLN:HG2	2.08	0.53
2:B:51:LEU:HD12	2:B:56:ARG:N	2.21	0.52
3:C:108:GLU:C	3:C:109:ILE:HD12	2.28	0.52
2:K:174:PHE:CD1	2:K:175:PRO:HD2	2.43	0.52
2:K:94:TYR:HE1	3:L:46:PRO:HB3	1.75	0.52
2:H:51:LEU:HD11	2:H:56:ARG:HD3	1.90	0.52
1:A:49:PRO:HD3	1:A:77:SER:OG	2.09	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:B:50:ILE:HG23	2:B:69:ILE:HG12	1.90	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:118:PRO:HG2	2:H:58:TYR:CZ	2.45	0.52
3:L:163:LEU:HD12	3:L:163:LEU:O	2.09	0.52
3:I:111:ARG:HH21	3:I:173:ASP:HA	1.74	0.52
3:L:127:GLN:HG2	3:L:132:GLY:O	2.08	0.52
3:L:1:ILE:HG22	3:L:1:ILE:O	2.10	0.52
3:I:167:THR:HG22	3:I:168:ASP:N	2.24	0.52
3:I:140:ASN:HB3	3:I:141:ASN:ND2	2.24	0.52
1:G:172:GLU:OE2	1:G:258:GLU:HA	2.09	0.52
1:A:201:VAL:HG13	1:A:202:GLY:H	1.68	0.52
2:K:20:SER:OG	2:K:21:CYS:N	2.42	0.52
2:B:35:TRP:CD1	2:B:80:LEU:HB2	2.44	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
3:F:105:THR:HG22	3:F:106:LYS:N	2.24	0.52
2:H:90:THR:HG23	2:H:117:VAL:O	2.09	0.52
2:H:129:VAL:O	2:H:217:LYS:HE3	2.10	0.52
3:C:190:GLU:CD	3:C:191:ARG:HG3	2.30	0.52
2:K:153:TYR:N	2:K:183:LEU:HD12	2.25	0.52
2:B:13:PRO:HD3	2:B:120:SER:C	2.30	0.52
3:F:3:MET:HG3	3:F:5:GLN:NE2	2.20	0.52
2:H:132:LEU:HB3	3:I:121:PHE:CG	2.45	0.52
3:L:26:GLU:O	3:L:27:SER:HB2	2.09	0.52
3:I:19:THR:CG2	3:I:77:THR:HG22	2.39	0.52
2:H:125:LYS:HD2	2:H:126:GLY:N	2.24	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:57:LYS:HZ1	3:C:65:PHE:HB2	1.73	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
2:K:97:ARG:N	3:L:36:ILE:HG13	2.25	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
3:L:138:PHE:O	3:L:139:LEU:HD12	2.09	0.52
3:L:143:TYR:CD2	3:L:143:TYR:C	2.83	0.52
3:I:97:VAL:HG13	3:I:98:PRO:HD2	1.91	0.52
1:D:227:MET:HG2	1:D:229:TYR:CE2	2.45	0.52
1:D:91:TYR:OH	1:D:180:HIS:CD2	2.63	0.52
3:I:197:CYS:O	3:I:208:ILE:N	2.35	0.52
1:A:91:TYR:HD1	1:A:227:MET:CB	2.11	0.52
1:G:202:GLY:O	1:G:206:TYR:O	2.27	0.52
1:J:182:PRO:HG2	1:J:188:GLN:CB	2.39	0.52
2:B:196:SER:HB3	2:B:202:TYR:CZ	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:139:LEU:HD21	3:L:199:ALA:HB1	1.91	0.52
3:C:9:SER:O	3:C:10:LEU:HD23	2.09	0.52
3:L:168:ASP:OD2	3:L:176:TYR:HD2	1.93	0.52
2:K:17:LEU:HB3	2:K:82:MET:CG	2.40	0.52
3:I:139:LEU:HD21	3:I:199:ALA:HB2	1.92	0.52
1:D:90:CYS:SG	1:D:145:TYR:CZ	3.03	0.52
2:E:162:TRP:HB3	2:E:166:ALA:HB3	1.91	0.52
2:H:66:ARG:HH22	2:H:89:ASP:CG	2.12	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
1:D:116:ILE:HG23	1:D:117:PHE:N	2.25	0.52
1:A:56:ASN:HA	1:A:81:GLU:HG2	1.92	0.52
3:F:125:SER:O	3:F:128:LEU:HD23	2.10	0.52
1:J:144:PHE:CG	1:J:145:TYR:N	2.78	0.52
3:C:140:ASN:CG	3:C:176:TYR:HD1	2.14	0.52
3:F:111:ARG:HB2	3:F:143:TYR:CD1	2.45	0.52
3:F:86:THR:HA	3:F:107:LEU:CD2	2.40	0.52
1:J:201:VAL:CG1	1:J:240:ILE:HD11	2.39	0.52
1:J:76:TRP:CD1	1:J:106:SER:O	2.63	0.52
1:G:248:LEU:HD12	1:G:249:VAL:N	2.25	0.52
1:J:92:PRO:CG	1:J:223:GLN:HB2	2.39	0.52
3:C:38:TRP:HE1	3:C:91:CYS:HA	1.74	0.52
2:B:134:PRO:HB3	3:C:121:PHE:HE1	1.74	0.52
3:L:43:PRO:HD3	3:L:87:ALA:HA	1.91	0.52
3:I:45:GLN:CD	3:I:46:PRO:HD3	2.29	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
2:E:152:ASP:CB	2:E:183:LEU:HD23	2.40	0.52
2:H:174:PHE:HD2	3:I:166:TRP:HE3	1.58	0.52
1:D:77:SER:O	1:D:106:SER:O	2.28	0.52
1:G:232:THR:HG23	1:G:233:LEU:N	2.24	0.52
1:G:127:ASP:HB2	1:G:153:LYS:O	2.10	0.52
2:B:4:LEU:HB2	2:B:112:GLY:HA2	1.91	0.52
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
3:I:196:THR:HG23	3:I:208:ILE:O	2.09	0.51
1:A:133:THR:CG2	1:A:150:TRP:HZ3	2.23	0.51
1:A:228:ASN:HB3	1:A:230:TYR:CE1	2.45	0.51
3:L:161:GLY:O	3:L:162:VAL:CG1	2.58	0.51
1:G:188:GLN:NE2	1:G:197:ALA:HB2	2.25	0.51
3:F:110:LYS:HG2	3:F:111:ARG:H	1.74	0.51
2:K:63:VAL:HG13	2:K:67:SER:H	1.74	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:118:PRO:O	1:G:122:SER:OG	2.28	0.51
3:F:153:ILE:CG1	3:F:154:ASP:H	2.15	0.51
2:K:178:LEU:HD23	2:K:178:LEU:C	2.31	0.51
2:K:6:GLU:HB3	2:K:115:THR:HB	1.92	0.51
1:D:165:TYR:HE2	1:D:167:ASN:HB2	1.74	0.51
3:F:183:THR:CG2	3:F:184:LEU:N	2.70	0.51
1:J:260:ASN:OD1	1:J:260:ASN:C	2.49	0.51
1:A:129:ASN:HB2	4:A:604:HOH:O	2.09	0.51
1:J:181:HIS:O	1:J:225:GLY:HA3	2.10	0.51
1:G:146:LYS:HG2	1:G:147:ASN:OD1	2.10	0.51
2:B:50:ILE:HB	2:B:56:ARG:O	2.11	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
2:B:44:LEU:N	4:B:302:HOH:O	2.42	0.51
1:A:206:TYR:C	1:A:206:TYR:HD2	2.14	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
3:I:27:SER:C	3:I:28:VAL:HG22	2.30	0.51
3:F:172:LYS:CD	3:F:172:LYS:N	2.73	0.51
2:K:97:ARG:H	3:L:36:ILE:HG13	1.76	0.51
3:F:164:ASN:HB3	3:F:180:SER:H	1.75	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
3:F:151:TRP:N	4:F:305:HOH:O	2.38	0.51
3:L:203:THR:CG2	3:L:203:THR:O	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
3:I:41:GLN:HB2	3:I:47:PRO:HA	1.93	0.51
2:H:147:GLY:O	2:H:148:CYS:SG	2.68	0.51
1:G:134:ALA:HA	1:G:142:LYS:HB3	1.92	0.51
3:C:37:ASN:OD1	3:C:95:LYS:NZ	2.30	0.51
2:K:171:VAL:HB	2:K:189:VAL:CG2	2.38	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
3:I:11:ALA:HA	3:I:108:GLU:O	2.09	0.51
3:L:92:GLN:HG3	3:L:100:GLY:O	2.11	0.51
2:H:93:TYR:CE1	2:H:117:VAL:CG1	2.92	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
2:B:85:LEU:HB3	2:B:119:VAL:HG13	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:96:ILE:HA	1:D:216:ILE:O	2.11	0.51
2:H:164:SER:HA	2:H:167:LEU:HD12	1.92	0.51
1:J:44:LEU:HD11	1:J:47:VAL:HG23	1.92	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:L:17:ARG:HB2	3:L:79:ASN:OD1	2.11	0.51
3:F:35:PHE:CE1	3:F:49:LEU:HD11	2.46	0.51
3:I:9:SER:HB2	3:I:106:LYS:NZ	2.25	0.51
1:J:115:GLU:OE1	3:L:99:TYR:OH	2.22	0.51
3:L:38:TRP:CD1	3:L:38:TRP:C	2.84	0.51
1:A:259:ARG:CZ	1:A:259:ARG:CB	2.89	0.51
2:H:10:VAL:HG13	2:H:118:THR:O	2.11	0.51
2:E:208:HIS:NE2	2:E:210:PRO:HG2	2.26	0.51
1:J:153:LYS:CB	1:J:158:TYR:HB2	2.41	0.51
1:A:232:THR:HG21	1:A:240:ILE:HD12	1.93	0.51
3:L:1:ILE:O	3:L:2:GLN:HB3	2.10	0.51
3:I:16:GLN:O	3:I:81:VAL:HG23	2.10	0.51
1:D:173:VAL:O	1:D:233:LEU:HA	2.11	0.51
3:C:29:SER:HB3	4:C:310:HOH:O	2.10	0.51
1:J:166:ILE:N	1:J:166:ILE:HD13	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
2:H:27:THR:C	2:H:29:SER:N	2.64	0.51
3:F:38:TRP:HE3	3:F:38:TRP:O	1.88	0.51
1:J:54:LYS:HZ2	1:J:54:LYS:CB	2.14	0.51
3:I:26:GLU:O	3:I:27:SER:HB2	2.10	0.51
3:F:121:PHE:N	3:F:121:PHE:CD2	2.79	0.51
2:H:72:ASP:HB3	2:H:79:TYR:CZ	2.46	0.51
1:D:211:LYS:NZ	1:D:211:LYS:HB2	2.26	0.51
2:H:125:LYS:HE3	2:H:126:GLY:O	2.11	0.51
1:J:144:PHE:CZ	1:J:145:TYR:HD2	2.28	0.51
1:D:175:VAL:O	1:D:231:TRP:HA	2.11	0.51
1:A:48:ALA:CB	1:A:78:TYR:CZ	2.93	0.51
3:F:149:VAL:HG22	3:F:149:VAL:O	2.11	0.51
3:C:13:SER:HB3	3:C:110:LYS:NZ	2.25	0.50
2:E:173:THR:HG22	3:F:178:MET:CE	2.40	0.50
2:H:32:ASP:HB2	2:H:98:HIS:HD1	1.76	0.50
1:J:62:LEU:HD22	1:J:148:LEU:HD11	1.92	0.50
3:L:102:PHE:HE1	3:L:104:GLY:HA2	1.75	0.50
1:D:91:TYR:HD1	1:D:227:MET:CB	2.08	0.50
2:B:38:GLN:OE1	3:C:41:GLN:NE2	2.44	0.50
1:A:138:HIS:O	1:A:139:ALA:C	2.49	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:100:GLU:HG2	1:J:231:TRP:CZ2	2.46	0.50
1:G:199:VAL:HA	1:G:243:GLU:O	2.11	0.50
3:C:154:ASP:OD1	3:C:191:ARG:NH1	2.45	0.50
1:G:144:PHE:CZ	1:G:145:TYR:HD2	2.28	0.50
1:D:165:TYR:C	1:D:165:TYR:CD2	2.85	0.50
2:K:207:ASN:HA	2:K:214:LYS:HA	1.92	0.50
2:K:162:TRP:CE2	2:K:204:CYS:HB3	2.45	0.50
2:K:145:ALA:HA	2:K:191:THR:HA	1.93	0.50
2:B:93:TYR:O	2:B:114:GLY:HA2	2.11	0.50
1:A:184:THR:O	1:A:187:ASP:N	2.45	0.50
1:J:53:GLY:HA2	1:J:82:THR:HG23	1.93	0.50
3:I:148:ASN:C	3:I:148:ASN:OD1	2.49	0.50
3:L:141:ASN:H	3:L:175:THR:HB	1.75	0.50
2:K:97:ARG:O	2:K:97:ARG:NE	2.45	0.50
2:H:17:LEU:HB3	2:H:82:MET:CE	2.40	0.50
3:L:208:ILE:C	3:L:209:VAL:CG1	2.78	0.50
3:I:79:ASN:O	3:I:80:PRO:C	2.48	0.50
3:C:175:THR:HB	3:C:176:TYR:CD2	2.47	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
3:L:102:PHE:CE1	3:L:104:GLY:HA2	2.45	0.50
3:F:189:TYR:O	3:F:190:GLU:CB	2.59	0.50
1:D:178:GLY:C	1:D:179:ILE:HD12	2.30	0.50
2:B:69:ILE:HD11	2:B:78:LEU:HD22	1.94	0.50
2:B:98:HIS:HD2	2:B:98:HIS:H	1.59	0.50
3:C:108:GLU:CG	3:C:109:ILE:H	2.23	0.50
2:K:92:VAL:HG12	2:K:93:TYR:N	2.26	0.50
3:F:13:SER:CB	3:F:110:LYS:HZ2	2.24	0.50
3:F:172:LYS:O	3:F:173:ASP:HB3	2.11	0.50
3:F:159:GLN:NE2	2:H:26:PHE:CE2	2.80	0.50
3:I:89:TYR:O	3:I:102:PHE:CZ	2.64	0.50
3:L:40:GLN:HA	3:L:88:ASN:O	2.11	0.50
1:D:54:LYS:HZ3	1:D:54:LYS:H	1.59	0.50
2:K:50:ILE:HD11	2:K:71:ARG:CG	2.41	0.50
2:B:4:LEU:HD22	2:B:112:GLY:N	2.26	0.50
2:K:218:LYS:NZ	2:K:218:LYS:HB2	2.27	0.50
2:B:98:HIS:CB	3:C:36:ILE:HG13	2.40	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
3:L:37:ASN:HD21	3:L:93:GLN:H	1.59	0.50
1:D:132:VAL:HA	1:D:144:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:204:SER:OG	1:J:205:ARG:N	2.44	0.50
2:B:200:GLN:HB3	2:B:202:TYR:CZ	2.46	0.50
2:K:125:LYS:HG3	2:K:126:GLY:O	2.12	0.50
3:C:3:MET:O	3:C:25:SER:N	2.44	0.50
2:B:50:ILE:HG23	2:B:69:ILE:CG1	2.42	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: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
3:F:173:ASP:OD2	3:F:175:THR:CG2	2.59	0.50
3:F:52:TYR:CE2	3:F:58:GLY:HA2	2.47	0.50
3:I:91:CYS:N	3:I:102:PHE:HD2	2.07	0.50
2:H:18:ARG:HA	2:H:80:LEU:O	2.12	0.50
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
2:K:127:PRO:HB2	2:K:150:VAL:HG13	1.93	0.50
3:I:111:ARG:O	3:I:112:ALA:HB3	2.12	0.50
3:F:162:VAL:HB	3:F:182:LEU:HG	1.94	0.50
1:G:101:LEU:HG	1:G:231:TRP:CD2	2.46	0.50
2:E:13:PRO:HD3	2:E:121:SER:HB2	1.94	0.50
3:C:69:GLY:HA3	3:C:74:PHE:HA	1.93	0.50
3:I:53:THR:O	3:I:53:THR:HG22	2.12	0.50
3:C:50:LEU:CD1	3:C:89:TYR:HE1	2.16	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
3:F:38:TRP:CE2	3:F:90:PHE:O	2.65	0.50
2:K:60:ARG:O	2:K:64:LYS:NZ	2.44	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
2:B:167:LEU:HA	2:B:170:SER:HB2	1.93	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
1:J:186:ALA:O	1:J:189:GLN:HG2	2.11	0.50
2:H:95:CYS:O	2:H:112:GLY:N	2.39	0.50
1:D:49:PRO:HD2	1:D:78:TYR:O	2.11	0.50
2:B:208:HIS:CD2	2:B:210:PRO:HD2	2.47	0.50
3:I:54:ALA:O	3:I:67:GLY:HA3	2.12	0.50
3:C:92:GLN:CG	3:C:93:GLN:N	2.74	0.50
2:B:174:PHE:O	3:C:166:TRP:CD1	2.64	0.50
3:L:78:ILE:HD11	3:L:80:PRO:O	2.12	0.50
3:F:138:PHE:CD1	3:F:178:MET:HG3	2.47	0.50
3:F:38:TRP:CZ2	3:F:90:PHE:C	2.85	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:63:VAL:HG12	2:B:64:LYS:N	2.26	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
1:G:198:TYR:HB2	1:G:210:PHE:O	2.12	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
2:H:27:THR:CG2	2:H:31:TYR:CD2	2.95	0.50
1:A:101:LEU:O	1:A:104:GLN:N	2.44	0.50
2:E:200:GLN:HG2	2:E:202:TYR:CZ	2.46	0.50
2:E:197:LEU:HG	2:E:198:GLY:N	2.26	0.50
1:G:162:SER:HA	1:G:242:PHE:O	2.12	0.50
2:K:116:THR:HG21	4:K:302:HOH:O	2.11	0.50
2:B:27:THR:HG23	2:B:30:ASP:OD2	2.11	0.49
3:L:143:TYR:HD1	3:L:174:SER:OG	1.94	0.49
3:L:81:VAL:HG12	3:L:82:GLU:H	1.74	0.49
3:I:40:GLN:HB3	3:I:50:LEU:HD11	1.94	0.49
3:I:209:VAL:HG22	3:I:210:LYS:N	2.27	0.49
2:E:35:TRP:CD1	2:E:80:LEU:HB2	2.47	0.49
3:L:196:THR:HA	3:L:209:VAL:HB	1.94	0.49
3:F:162:VAL:CG2	3:F:162:VAL:O	2.59	0.49
2:B:100:TRP:NE1	3:C:34:ASN:OD1	2.44	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:D:149:ILE:HD11	1:D:252:ARG:HB2	1.94	0.49
2:K:211:SER:C	2:K:213:THR:N	2.65	0.49
2:E:125:LYS:HD2	2:E:126:GLY:N	2.27	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
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:I:138:PHE:C	3:I:139:LEU:HD12	2.32	0.49
2:E:205:ASN:ND2	2:E:214:LYS:HE3	2.27	0.49
2:B:127:PRO:HD2	2:B:213:THR:HG21	1.93	0.49
1:A:104:GLN:NE2	1:A:233:LEU:HD22	2.22	0.49
2:B:196:SER:C	2:B:202:TYR:HE2	2.15	0.49
2:H:194:SER:O	2:H:196:SER:N	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:159:GLN:HG3	3:F:160:ASN:H	1.77	0.49
2:K:45:GLU:OE1	2:K:46:TRP:N	2.46	0.49
3:I:120:ILE:HB	3:I:208:ILE:CG2	2.42	0.49
1:A:109:SER:HB3	1:A:258:GLU:HG2	1.93	0.49
2:E:209:LYS:N	2:E:210:PRO:CD	2.75	0.49
2:E:203:ILE:HG13	2:E:204:CYS:N	2.25	0.49
3:C:35:PHE:HB2	3:C:95:LYS:HE2	1.94	0.49
3:F:138:PHE:C	3:F:139:LEU:HD12	2.33	0.49
2:H:96:ALA:HB1	3:I:36:ILE:HD11	1.95	0.49
3:F:26:GLU:O	3:F:72:THR:HB	2.13	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
2:B:30:ASP:OD1	2:B:30:ASP:N	2.44	0.49
3:L:108:GLU:CG	3:L:109:ILE:N	2.75	0.49
2:E:61:ASP:OD1	2:H:142:GLY:HA2	2.13	0.49
2:H:97:ARG:NE	2:H:110:GLY:HA3	2.27	0.49
1:A:115:GLU:CB	3:C:96:GLU:HG2	2.39	0.49
1:D:144:PHE:HZ	1:D:227:MET:HE1	1.74	0.49
3:I:209:VAL:HG22	3:I:210:LYS:CB	2.43	0.49
1:G:206:TYR:OH	1:G:208:LYS:HD2	2.12	0.49
1:D:108:VAL:HG12	1:D:257:MET:HE1	1.95	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
1:A:200:PHE:HB3	1:A:243:GLU:HB3	1.95	0.49
2:E:186:LEU:HD12	2:E:187:SER:H	1.78	0.49
3:I:141:ASN:N	3:I:176:TYR:HD1	2.10	0.49
2:H:162:TRP:CE2	2:H:204:CYS:HB3	2.47	0.49
1:G:231:TRP:CE3	1:G:232:THR:HA	2.47	0.49
1:D:179:ILE:HG22	1:D:181:HIS:CE1	2.48	0.49
3:C:64:ARG:NH2	3:C:82:GLU:HB2	2.28	0.49
3:L:141:ASN:N	3:L:175:THR:HB	2.27	0.49
3:I:9:SER:HB2	3:I:106:LYS:HZ3	1.78	0.49
3:I:141:ASN:HA	3:I:175:THR:HB	1.92	0.49
1:D:103:GLU:OE1	1:D:104:GLN:N	2.46	0.49
1:A:144:PHE:CE1	1:A:227:MET:HE1	2.48	0.49
2:K:54:SER:HB3	2:K:56:ARG:NE	2.28	0.49
1:J:56:ASN:HD21	1:J:88:GLY:HA2	1.77	0.49
2:H:176:ALA:CB	3:I:166:TRP:CE2	2.90	0.49
2:K:176:ALA:O	2:K:185:SER:N	2.45	0.49
1:G:101:LEU:HD22	1:G:105:LEU:CD1	2.42	0.49
1:G:56:ASN:HB3	1:G:82:THR:O	2.11	0.49
1:D:221:ARG:O	1:D:223:GLN:HG2	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:183:THR:CG2	3:C:184:LEU:N	2.75	0.49
3:L:88:ASN:ND2	3:L:90:PHE:CE2	2.80	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
1:A:151:LEU:HD12	1:A:250:VAL:HG13	1.94	0.49
2:K:201:THR:CG2	2:K:218:LYS:HD3	2.42	0.49
2:K:39:ALA:CB	2:K:44:LEU:HG	2.43	0.49
3:C:78:ILE:HD11	3:C:81:VAL:HA	1.94	0.49
3:L:62:PRO:HB2	3:L:64:ARG:HG3	1.94	0.49
2:H:46:TRP:O	2:H:60:ARG:NH1	2.46	0.49
3:I:209:VAL:HG23	3:I:210:LYS:HD3	1.94	0.49
2:H:90:THR:CG2	2:H:118:THR:HA	2.36	0.49
2:K:162:TRP:CZ2	2:K:204:CYS:HB3	2.48	0.49
2:E:173:THR:HG21	3:F:178:MET:CG	2.43	0.48
2:K:34:SER:CB	2:K:98:HIS:NE2	2.76	0.48
2:K:34:SER:OG	2:K:49:GLY:CA	2.61	0.48
2:H:37:ARG:HB3	2:H:93:TYR:CE2	2.48	0.48
1:A:183:SER:OG	1:A:224:GLU:HB2	2.13	0.48
2:K:178:LEU:C	2:K:180:SER:N	2.65	0.48
1:D:151:LEU:HD12	1:D:250:VAL:HG13	1.94	0.48
2:E:72:ASP:OD1	2:E:75:ARG:HB2	2.12	0.48
2:K:162:TRP:CH2	2:K:204:CYS:HB3	2.47	0.48
1:D:179:ILE:HG22	1:D:181:HIS:NE2	2.27	0.48
2:B:32:ASP:HB2	2:B:98:HIS:NE2	2.28	0.48
2:B:78:LEU:HD12	2:B:78:LEU:C	2.33	0.48
3:C:39:PHE:O	3:C:40:GLN:HB2	2.12	0.48
3:C:12:VAL:HG13	3:C:13:SER:N	2.27	0.48
3:I:197:CYS:O	3:I:208:ILE:O	2.31	0.48
1:A:226:ARG:HD3	1:A:226:ARG:HA	1.46	0.48
1:G:56:ASN:HA	1:G:81:GLU:HB2	1.95	0.48
2:E:172:HIS:ND1	2:E:188:SER:HB2	2.28	0.48
1:J:113:ARG:HB2	1:J:255:PHE:CE1	2.47	0.48
1:D:97:ASP:HB2	1:D:231:TRP:HE1	1.79	0.48
3:C:66:SER:N	3:C:77:THR:O	2.45	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
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
3:I:102:PHE:HE1	3:I:104:GLY:C	2.17	0.48
3:L:90:PHE:HA	3:L:102:PHE:CZ	2.49	0.48
1:D:119:LYS:HG2	1:D:120:THR:H	1.77	0.48
1:J:184:THR:O	1:J:186:ALA:N	2.46	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:192:TYR:HB3	1:J:246:GLY:HA3	1.95	0.48
1:G:57:ILE:CD1	1:G:102:ARG:HB2	2.43	0.48
3:L:170:ASP:CB	3:L:175:THR:OG1	2.61	0.48
2:H:97:ARG:HE	2:H:110:GLY:HA3	1.79	0.48
3:F:38:TRP:HB2	3:F:48:LYS:O	2.14	0.48
1:D:57:ILE:HG13	1:D:81:GLU:OE2	2.14	0.48
3:L:36:ILE:HD13	3:L:36:ILE:C	2.33	0.48
1:A:122:SER:O	1:A:124:PRO:HD3	2.13	0.48
3:F:193:ASN:ND2	3:F:211:SER:OG	2.46	0.48
1:D:51:HIS:ND1	1:D:80:VAL:HG21	2.27	0.48
1:A:57:ILE:HG22	1:A:58:ALA:N	2.29	0.48
2:K:163:ASN:H	2:K:163:ASN:HD22	1.61	0.48
1:J:165:TYR:CE2	1:J:173:VAL:HG21	2.48	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:F:140:ASN:OD1	3:F:176:TYR:HD1	1.96	0.48
1:D:227:MET:HB3	1:D:229:TYR:CZ	2.48	0.48
3:C:205:THR:HG23	3:C:205:THR:O	2.13	0.48
3:C:194:SER:HA	3:C:210:LYS:CB	2.36	0.48
3:L:127:GLN:O	3:L:130:SER:OG	2.32	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:F:149:VAL:CG2	3:F:149:VAL:O	2.60	0.48
2:B:51:LEU:HD13	2:B:52:GLY:O	2.13	0.48
2:B:171:VAL:HG11	3:C:176:TYR:CE2	2.48	0.48
2:E:173:THR:HG22	3:F:178:MET:HE2	1.95	0.48
2:E:38:GLN:OE1	3:F:41:GLN:NE2	2.42	0.48
3:F:170:ASP:CG	3:F:171:SER:N	2.67	0.48
3:L:102:PHE:CD1	3:L:104:GLY:N	2.63	0.48
1:D:90:CYS:SG	1:D:145:TYR:CE1	3.07	0.48
3:I:209:VAL:CG2	3:I:210:LYS:N	2.76	0.48
3:C:164:ASN:N	3:C:164:ASN:ND2	2.61	0.48
1:J:133:THR:HG23	1:J:135:ALA:N	2.25	0.48
1:A:54:LYS:HG2	1:A:55:CYS:N	2.23	0.48
3:I:162:VAL:O	3:I:162:VAL:CG2	2.61	0.48
2:E:125:LYS:HD2	2:E:126:GLY:H	1.78	0.48
2:B:145:ALA:HA	2:B:191:THR:HA	1.96	0.48
3:C:38:TRP:CG	3:C:39:PHE:HA	2.41	0.48
2:B:180:SER:O	2:B:182:GLY:O	2.32	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:C:45:GLN:CB	3:C:46:PRO:HD2	2.35	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:186:LEU:C	2:H:186:LEU:CD1	2.82	0.48
3:L:163:LEU:C	3:L:163:LEU:CD1	2.77	0.48
1:J:185:SER:N	1:J:214:ILE:HG21	2.29	0.48
2:E:10:VAL:HG13	2:E:155:PRO:HB3	1.96	0.48
1:A:105:LEU:HD23	1:A:257:MET:SD	2.54	0.48
2:E:92:VAL:HA	2:E:115:THR:O	2.12	0.48
3:I:52:TYR:O	3:I:56:ASN:HB2	2.14	0.48
3:C:93:GLN:O	3:C:94:THR:C	2.46	0.48
3:C:140:ASN:ND2	3:C:176:TYR:HD1	2.12	0.48
1:A:219:LYS:HG2	1:A:222:ASP:C	2.34	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:J:151:LEU:HD12	1:J:250:VAL:CG1	2.43	0.48
2:H:163:ASN:C	2:H:165:GLY:H	2.16	0.48
2:B:36:ILE:CB	2:B:46:TRP:HA	2.41	0.48
2:B:173:THR:HB	3:C:178:MET:CE	2.38	0.48
2:E:46:TRP:C	2:E:60:ARG:NH1	2.67	0.48
3:I:92:GLN:O	3:I:93:GLN:C	2.52	0.48
1:A:232:THR:HG23	1:A:233:LEU:N	2.28	0.48
2:H:2:VAL:HA	2:H:24:SER:C	2.34	0.48
1:J:110:SER:HB2	1:J:171:LYS:NZ	2.29	0.48
1:J:92:PRO:HB2	1:J:226:ARG:HD2	1.94	0.48
2:E:2:VAL:N	2:E:3:LYS:HE2	2.29	0.48
3:C:9:SER:C	3:C:106:LYS:HG2	2.34	0.48
3:L:79:ASN:HB3	3:L:80:PRO:CD	2.41	0.48
2:H:197:LEU:HD12	2:H:198:GLY:H	1.75	0.48
3:I:1:ILE:HG22	3:I:3:MET:HE1	1.96	0.48
1:J:122:SER:C	1:J:124:PRO:HD3	2.33	0.48
1:A:215:ALA:HB1	1:D:96:ILE:HG21	1.95	0.48
1:G:188:GLN:O	1:G:192:TYR:N	2.41	0.48
1:J:217:ARG:N	1:J:224:GLU:O	2.38	0.48
2:K:205:ASN:HA	2:K:215:VAL:O	2.14	0.48
2:K:38:GLN:O	2:K:91:ALA:HB1	2.13	0.48
1:J:125:ASN:O	1:J:154:LYS:HB3	2.14	0.48
1:G:114:PHE:N	1:G:114:PHE:CD2	2.79	0.48
3:C:39:PHE:CB	3:C:50:LEU:H	2.19	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
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
3:F:37:ASN:OD1	3:F:95:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:137:PRO:CA	1:A:142:LYS:HA	2.41	0.47
3:C:157:GLU:O	3:C:158:ARG:HG2	2.14	0.47
2:E:205:ASN:HD22	2:E:214:LYS:HE3	1.79	0.47
2:K:50:ILE:HB	2:K:56:ARG:O	2.14	0.47
2:H:6:GLU:HA	2:H:20:SER:O	2.14	0.47
1:D:153:LYS:HE3	1:D:156:ASN:CA	2.40	0.47
2:E:146:LEU:N	2:E:190:VAL:O	2.48	0.47
1:D:82:THR:OG1	1:D:82:THR:O	2.31	0.47
2:E:116:THR:HG22	2:E:116:THR:O	2.14	0.47
2:B:177:VAL:HG12	2:B:182:GLY:HA2	1.97	0.47
3:F:97:VAL:CG1	3:F:98:PRO:N	2.76	0.47
2:H:52:GLY:O	2:H:53:GLY:C	2.52	0.47
1:J:114:PHE:HA	3:L:96:GLU:CD	2.35	0.47
1:D:64:ASN:OD1	1:D:65:PRO:HD2	2.14	0.47
3:I:209:VAL:CG2	3:I:210:LYS:HG2	2.43	0.47
1:A:133:THR:HG21	1:A:150:TRP:HZ3	1.77	0.47
1:A:49:PRO:CD	1:A:77:SER:OG	2.62	0.47
2:H:117:VAL:CG1	2:H:117:VAL:O	2.60	0.47
3:F:209:VAL:HG22	3:F:210:LYS:CB	2.44	0.47
2:E:86:ARG:O	2:E:119:VAL:HG21	2.14	0.47
2:K:175:PRO:O	3:L:166:TRP:CE3	2.66	0.47
3:I:123:PRO:CB	3:I:133:ALA:HB1	2.41	0.47
1:J:176:LEU:HA	1:J:230:TYR:O	2.15	0.47
3:C:7:PRO:CD	3:C:21:THR:O	2.53	0.47
2:E:56:ARG:HA	2:E:56:ARG:HD2	1.46	0.47
2:E:48:SER:CB	2:E:59:TYR:HD1	2.27	0.47
3:F:38:TRP:CD2	3:F:90:PHE:O	2.66	0.47
1:J:120:THR:O	1:J:121:SER:C	2.51	0.47
2:K:11:VAL:O	2:K:119:VAL:HA	2.15	0.47
2:H:93:TYR:CE1	2:H:117:VAL:HG12	2.45	0.47
2:H:63:VAL:CG1	2:H:66:ARG:H	2.26	0.47
2:H:162:TRP:CZ2	2:H:204:CYS:HB3	2.50	0.47
1:A:175:VAL:C	1:A:176:LEU:HD12	2.34	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
3:L:23:ARG:HD2	3:L:72:THR:HG23	1.96	0.47
1:D:211:LYS:HG3	1:D:212:PRO:HD2	1.96	0.47
2:B:150:VAL:HB	2:B:186:LEU:HG	1.95	0.47
3:L:86:THR:HG22	3:L:109:ILE:HD13	1.97	0.47
1:D:164:SER:H	2:E:56:ARG:HH22	1.60	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:F:38:TRP:CE2	3:F:90:PHE:N	2.82	0.47
3:I:9:SER:HB3	3:I:106:LYS:CG	2.42	0.47
1:J:200:PHE:CG	1:J:201:VAL:N	2.82	0.47
1:J:101:LEU:HG	1:J:231:TRP:CE2	2.48	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
1:J:182:PRO:O	1:J:214:ILE:HG23	2.13	0.47
1:G:151:LEU:HD12	1:G:250:VAL:HG11	1.97	0.47
2:B:143:THR:HG22	2:B:143:THR:O	2.13	0.47
3:L:12:VAL:O	3:L:109:ILE:HA	2.15	0.47
3:F:173:ASP:OD1	3:F:175:THR:OG1	2.32	0.47
1:G:54:LYS:CG	1:G:67:CYS:HA	2.12	0.47
3:F:38:TRP:CH2	3:F:39:PHE:CD1	3.02	0.47
2:H:51:LEU:HD12	2:H:52:GLY:O	2.13	0.47
1:D:64:ASN:HD21	1:D:90:CYS:HB3	1.79	0.47
2:E:181:SER:CB	3:I:62:PRO:HG3	2.38	0.47
2:H:37:ARG:HB3	2:H:93:TYR:CD2	2.48	0.47
3:F:114:ALA:HA	3:F:201:HIS:HD2	1.79	0.47
3:C:34:ASN:N	3:C:34:ASN:ND2	2.62	0.47
2:B:196:SER:O	2:B:200:GLN:N	2.48	0.47
1:J:248:LEU:HD12	1:J:249:VAL:H	1.75	0.47
2:E:2:VAL:C	2:E:3:LYS:HE2	2.34	0.47
1:D:114:PHE:CE2	1:D:254:ALA:HB3	2.49	0.47
2:B:27:THR:CG2	2:B:31:TYR:CG	2.98	0.47
3:C:116:PRO:HB2	3:C:139:LEU:HB3	1.96	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
2:E:45:GLU:OE2	3:F:101:THR:N	2.43	0.47
2:E:46:TRP:CE3	2:E:46:TRP:O	2.67	0.47
3:F:95:LYS:O	3:F:96:GLU:HG3	2.15	0.47
2:H:46:TRP:HE3	2:H:60:ARG:CZ	2.27	0.47
2:K:63:VAL:HG13	2:K:66:ARG:HB2	1.96	0.47
2:H:202:TYR:CD1	2:H:219:SER:HB2	2.48	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
3:F:126:GLU:O	3:F:129:THR:HG23	2.15	0.47
3:C:68:SER:OG	3:C:75:THR:HB	2.14	0.47
3:I:148:ASN:OD1	3:I:149:VAL:N	2.47	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:43:PRO:HD3	3:F:87:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:F:52:TYR:O	3:F:56:ASN:HB2	2.14	0.47
3:I:6:SER:HB3	3:I:7:PRO:CD	2.38	0.47
3:C:97:VAL:HG13	3:C:98:PRO:CD	2.42	0.47
2:K:66:ARG:HH22	2:K:89:ASP:CG	2.18	0.47
1:A:177:TRP:CZ2	1:A:230:TYR:HB2	2.50	0.47
1:G:119:LYS:HZ2	1:G:129:ASN:HD22	1.53	0.47
1:J:382:VAL:O	1:J:385:VAL:N	2.48	0.47
2:H:63:VAL:HG11	2:H:67:SER:H	1.80	0.47
2:B:211:SER:CB	2:B:213:THR:HG1	2.28	0.47
2:B:17:LEU:HD21	2:B:19:LEU:HD13	1.95	0.47
3:L:204:SER:HA	4:L:310:HOH:O	2.15	0.47
1:G:235:GLU:CG	1:G:236:PRO:CD	2.91	0.47
3:L:2:GLN:HA	3:L:25:SER:OG	2.14	0.47
1:G:77:SER:OG	1:G:78:TYR:N	2.48	0.47
1:G:184:THR:C	1:G:214:ILE:HG21	2.35	0.47
3:I:81:VAL:HG12	3:I:82:GLU:H	1.78	0.47
2:H:208:HIS:O	2:H:212:ASN:CA	2.62	0.47
1:J:217:ARG:HD3	1:J:226:ARG:HG2	1.97	0.47
2:B:197:LEU:C	2:B:199:THR:N	2.66	0.47
2:E:82:MET:CE	2:E:117:VAL:HG21	2.45	0.47
1:D:184:THR:H	1:D:187:ASP:CB	2.28	0.47
1:A:212:PRO:HB3	1:A:247:ASN:ND2	2.29	0.47
1:D:161:LEU:O	1:D:243:GLU:HA	2.15	0.47
1:G:94:ASP:O	1:G:228:ASN:HA	2.15	0.47
2:B:6:GLU:HG2	2:B:35:TRP:HZ3	1.80	0.47
3:C:89:TYR:O	3:C:104:GLY:HA2	2.15	0.47
3:C:5:GLN:HB3	3:C:102:PHE:CD1	2.50	0.47
2:B:174:PHE:CD1	2:B:174:PHE:N	2.80	0.47
3:F:41:GLN:O	3:F:87:ALA:HB1	2.15	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
3:C:153:ILE:HA	3:C:194:SER:O	2.15	0.47
1:G:187:ASP:O	1:G:191:LEU:HB2	2.14	0.47
2:E:203:ILE:HD12	2:E:217:LYS:C	2.34	0.47
2:B:173:THR:CG2	3:C:178:MET:SD	3.02	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
2:E:36:ILE:O	2:E:94:TYR:HB2	2.15	0.47
3:F:158:ARG:HD3	2:H:31:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:17:LEU:HB3	2:K:82:MET:HG2	1.96	0.47
1:D:57:ILE:HD11	1:D:102:ARG:HG3	1.97	0.47
1:J:64:ASN:O	1:J:67:CYS:HB2	2.15	0.47
2:B:86:ARG:NE	2:B:88:GLU:OE1	2.45	0.47
2:K:162:TRP:CD1	2:K:162:TRP:N	2.82	0.47
1:A:161:LEU:HD23	1:A:161:LEU:O	2.15	0.47
2:E:37:ARG:O	2:E:37:ARG:HG3	2.14	0.47
3:C:89:TYR:O	3:C:104:GLY:CA	2.63	0.47
2:B:173:THR:HG23	2:B:187:SER:O	2.15	0.47
3:C:138:PHE:HD1	3:C:178:MET:CG	2.14	0.47
2:B:173:THR:CA	3:C:178:MET:HE3	2.45	0.47
3:L:42:LYS:C	3:L:44:GLY:N	2.68	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
1:D:115:GLU:HB2	3:F:96:GLU:CG	2.45	0.47
3:I:41:GLN:HA	4:I:305:HOH:O	2.14	0.47
2:K:17:LEU:O	2:K:82:MET:N	2.42	0.47
3:I:116:PRO:HA	3:I:140:ASN:O	2.15	0.47
1:D:98:TYR:HE2	1:D:102:ARG:HH21	1.54	0.47
3:C:161:GLY:C	3:C:162:VAL:HG22	2.36	0.47
1:A:57:ILE:HD11	1:A:79:ILE:HD13	1.97	0.47
3:L:156:SER:O	3:L:157:GLU:CB	2.61	0.47
1:D:188:GLN:NE2	1:D:194:ASN:O	2.48	0.47
3:C:50:LEU:HD13	3:C:65:PHE:CD1	2.50	0.46
3:L:16:GLN:O	3:L:81:VAL:HG23	2.15	0.46
2:E:38:GLN:HB3	2:E:94:TYR:HE2	1.80	0.46
2:E:64:LYS:O	2:E:64:LYS:HG3	2.15	0.46
3:F:167:THR:CG2	3:F:168:ASP:H	2.28	0.46
2:H:46:TRP:CH2	2:H:59:TYR:O	2.68	0.46
3:I:9:SER:CB	3:I:106:LYS:HG3	2.42	0.46
2:E:180:SER:C	2:E:182:GLY:N	2.68	0.46
1:A:123:TRP:NE1	1:A:149:ILE:HD13	2.29	0.46
2:H:146:LEU:HD12	2:H:162:TRP:CZ3	2.51	0.46
1:G:135:ALA:HB3	1:G:223:GLN:HE21	1.80	0.46
3:L:139:LEU:HD21	3:L:199:ALA:CB	2.45	0.46
1:D:99:GLU:HG2	1:D:100:GLU:N	2.29	0.46
2:K:162:TRP:CD2	2:K:204:CYS:HB3	2.50	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:J:177:TRP:N	1:J:177:TRP:CE3	2.83	0.46
1:G:186:ALA:O	1:G:189:GLN:HB3	2.15	0.46
1:A:152:VAL:HG11	1:A:191:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:132:LEU:HD11	2:B:149:LEU:HB2	1.98	0.46
3:L:111:ARG:HB2	3:L:143:TYR:CD1	2.51	0.46
2:K:78:LEU:HD23	2:K:78:LEU:H	1.80	0.46
1:G:132:VAL:CG2	1:G:132:VAL:O	2.63	0.46
1:J:182:PRO:HG2	1:J:188:GLN:CA	2.45	0.46
3:C:128:LEU:HD13	3:C:129:THR:N	2.18	0.46
1:J:90:CYS:HB2	1:J:135:ALA:O	2.15	0.46
2:K:176:ALA:CB	3:L:166:TRP:CZ2	2.98	0.46
2:H:132:LEU:HD13	2:H:132:LEU:N	2.31	0.46
2:K:171:VAL:HG22	3:L:176:TYR:CE1	2.50	0.46
2:H:44:LEU:N	4:H:305:HOH:O	2.48	0.46
3:L:92:GLN:O	3:L:93:GLN:C	2.54	0.46
3:F:196:THR:CG2	3:F:209:VAL:HG23	2.45	0.46
1:D:165:TYR:HB3	1:D:240:ILE:HG22	1.97	0.46
1:G:231:TRP:CZ3	1:G:233:LEU:HD13	2.49	0.46
1:G:197:ALA:O	1:G:212:PRO:HD2	2.15	0.46
1:G:149:ILE:HB	1:G:250:VAL:CG2	2.45	0.46
3:I:143:TYR:HB2	3:I:174:SER:HB2	1.97	0.46
1:G:75:SER:OG	1:G:109:SER:O	2.30	0.46
2:H:73:ASN:N	2:H:73:ASN:OD1	2.37	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:HD2	3:C:90:PHE:N	2.12	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
1:G:220:VAL:HG23	1:G:226:ARG:HH22	1.80	0.46
2:H:63:VAL:CG1	2:H:67:SER:H	2.28	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
3:L:179:SER:HB2	4:L:302:HOH:O	2.15	0.46
1:D:116:ILE:HG22	1:D:252:ARG:O	2.16	0.46
2:B:156:GLU:CB	2:B:157:PRO:HA	2.46	0.46
1:D:99:GLU:CG	1:D:100:GLU:H	2.29	0.46
2:K:162:TRP:CZ3	2:K:204:CYS:HB3	2.50	0.46
1:A:153:LYS:HB2	1:A:157:SER:O	2.16	0.46
2:K:158:VAL:HG23	2:K:208:HIS:HD2	1.80	0.46
1:G:216:ILE:O	1:G:216:ILE:HG22	2.16	0.46
2:E:171:VAL:HG21	3:F:176:TYR:CD1	2.50	0.46
1:J:231:TRP:HZ3	1:J:233:LEU:HD11	1.79	0.46
1:J:49:PRO:HG2	1:J:77:SER:CB	2.44	0.46
2:B:162:TRP:HD1	2:B:170:SER:OG	1.98	0.46
2:K:174:PHE:HD2	3:L:166:TRP:HE3	1.64	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:215:VAL:HG22	2:E:216:ASP:N	2.30	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:K:147:GLY:O	2:K:162:TRP:HH2	1.98	0.46
1:A:153:LYS:HG3	1:A:153:LYS:O	2.15	0.46
2:H:119:VAL:O	2:H:119:VAL:HG12	2.16	0.46
2:E:174:PHE:CD1	2:E:175:PRO:HD2	2.51	0.46
3:F:13:SER:HB3	3:F:110:LYS:CD	2.46	0.46
3:F:96:GLU:O	3:F:97:VAL:CG2	2.60	0.46
1:D:144:PHE:CZ	1:D:150:TRP:HB2	2.49	0.46
1:J:101:LEU:HG	1:J:231:TRP:CD2	2.50	0.46
3:F:24:ALA:N	3:F:72:THR:O	2.48	0.46
2:H:179:GLN:HG2	3:I:163:LEU:HB2	1.96	0.46
1:J:211:LYS:HB2	1:J:211:LYS:HZ2	1.79	0.46
3:I:164:ASN:CG	3:I:180:SER:O	2.54	0.46
3:I:191:ARG:HG2	3:I:192:HIS:H	1.79	0.46
1:D:199:VAL:HG13	1:D:244:ALA:HB2	1.98	0.46
2:E:51:LEU:CD1	2:E:55:GLU:N	2.79	0.46
3:I:91:CYS:N	3:I:102:PHE:CE2	2.72	0.46
2:K:82:MET:HG3	2:K:85:LEU:HD21	1.98	0.46
3:L:97:VAL:O	3:L:99:TYR:CD1	2.69	0.46
2:H:171:VAL:C	2:H:172:HIS:ND1	2.67	0.46
1:A:114:PHE:CE2	1:A:254:ALA:HB3	2.51	0.46
2:B:215:VAL:C	2:B:216:ASP:OD1	2.55	0.46
1:G:177:TRP:HZ2	1:G:206:TYR:HH	1.62	0.46
2:K:53:GLY:O	2:K:54:SER:HB2	2.16	0.46
2:K:51:LEU:CD2	2:K:56:ARG:HB2	2.36	0.46
3:L:161:GLY:C	3:L:162:VAL:HG12	2.36	0.46
3:F:202:LYS:HA	4:F:308:HOH:O	2.16	0.46
1:A:51:HIS:HA	1:A:80:VAL:HB	1.97	0.46
1:J:215:ALA:H	1:J:217:ARG:NH1	2.13	0.46
2:E:9:ALA:H	2:E:17:LEU:HD21	1.81	0.46
1:D:147:ASN:HD21	1:D:255:PHE:HZ	1.64	0.46
3:F:1:ILE:HD13	3:F:1:ILE:HA	1.74	0.46
3:C:9:SER:HA	3:C:106:LYS:H	1.80	0.46
3:L:140:ASN:HB2	3:L:141:ASN:ND2	2.31	0.46
3:I:20:ILE:HG21	3:I:105:THR:HG21	1.97	0.46
3:C:97:VAL:CG1	3:C:98:PRO:N	2.79	0.46
1:A:122:SER:C	1:A:124:PRO:HD3	2.36	0.46
1:D:84:SER:O	1:D:86:ASP:N	2.48	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:156:GLU:OE2	2:H:175:PRO:HG3	2.16	0.46
2:H:178:LEU:C	2:H:180:SER:N	2.69	0.46
3:F:3:MET:CG	3:F:5:GLN:HE21	2.21	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
1:J:43:LYS:HZ3	1:J:43:LYS:HB3	1.81	0.46
3:C:51:ILE:HD13	3:C:76:LEU:HD12	1.98	0.46
2:B:178:LEU:C	2:B:180:SER:H	2.20	0.46
3:F:78:ILE:HG22	3:F:79:ASN:O	2.16	0.46
3:F:39:PHE:CD2	3:F:51:ILE:HB	2.50	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:D:145:TYR:CZ	1:D:229:TYR:OH	2.68	0.46
1:D:49:PRO:CB	1:D:76:TRP:HB2	2.38	0.46
1:G:151:LEU:HD12	1:G:250:VAL:CG1	2.46	0.46
3:C:133:ALA:O	3:C:183:THR:HB	2.16	0.46
1:A:208:LYS:HG2	1:A:209:LYS:N	2.30	0.46
2:B:51:LEU:C	2:B:51:LEU:HD13	2.36	0.45
2:E:51:LEU:HD13	2:E:52:GLY:O	2.17	0.45
2:H:60:ARG:HH22	3:I:99:TYR:C	2.18	0.45
2:K:18:ARG:HD2	2:K:81:GLU:HB2	1.96	0.45
1:G:172:GLU:O	1:G:256:ALA:HA	2.16	0.45
1:J:200:PHE:CE2	1:J:201:VAL:O	2.70	0.45
1:J:54:LYS:HE3	1:J:67:CYS:CA	2.46	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:A:64:ASN:CG	1:A:66:GLU:HG2	2.37	0.45
3:L:123:PRO:CB	3:L:133:ALA:HB1	2.42	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
3:C:92:GLN:CA	3:C:101:THR:HG23	2.45	0.45
2:H:171:VAL:HB	2:H:189:VAL:HG13	1.98	0.45
1:A:258:GLU:HG3	1:A:259:ARG:N	2.32	0.45
3:L:36:ILE:HG23	3:L:36:ILE:O	2.16	0.45
2:B:203:ILE:HD11	2:B:216:ASP:CB	2.35	0.45
1:D:148:LEU:HD23	1:D:251:PRO:N	2.31	0.45
1:A:126:HIS:ND1	1:A:126:HIS:N	2.64	0.45
2:K:69:ILE:CG1	2:K:70:SER:N	2.79	0.45
1:G:75:SER:OG	1:G:110:SER:HA	2.16	0.45
1:D:200:PHE:CG	1:D:201:VAL:N	2.84	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:34:ASN:O	3:L:95:LYS:HD3	2.15	0.45
1:G:167:ASN:C	1:G:167:ASN:OD1	2.55	0.45
1:J:48:ALA:HB1	1:J:78:TYR:CE1	2.51	0.45
2:E:6:GLU:HG3	2:E:35:TRP:CZ3	2.51	0.45
3:L:193:ASN:O	3:L:211:SER:CB	2.64	0.45
1:G:219:LYS:CG	1:G:222:ASP:HA	2.46	0.45
1:D:231:TRP:HZ3	1:D:233:LEU:HD22	1.80	0.45
1:G:116:ILE:HG23	1:G:117:PHE:N	2.31	0.45
1:D:177:TRP:CE2	1:D:230:TYR:HB2	2.52	0.45
1:J:421:ILE:O	1:J:424:TYR:N	2.45	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
3:F:167:THR:CG2	3:F:168:ASP:N	2.79	0.45
3:F:139:LEU:O	3:F:176:TYR:HA	2.17	0.45
2:K:127:PRO:HB3	2:K:150:VAL:HG13	1.97	0.45
2:K:90:THR:HG23	2:K:118:THR:HA	1.99	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
3:F:120:ILE:HB	3:F:197:CYS:SG	2.57	0.45
1:A:84:SER:OG	1:A:87:ASN:HB2	2.16	0.45
1:D:182:PRO:HG2	1:D:188:GLN:HA	1.99	0.45
2:B:47:VAL:O	2:B:48:SER:HB3	2.16	0.45
3:L:108:GLU:OE1	3:L:108:GLU:CA	2.58	0.45
2:E:45:GLU:CB	2:E:60:ARG:NH2	2.76	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
1:D:61:ILE:HD13	1:D:61:ILE:O	2.15	0.45
1:A:150:TRP:C	1:A:150:TRP:CD1	2.90	0.45
1:D:160:LYS:CD	1:D:160:LYS:H	2.25	0.45
1:G:199:VAL:CG1	1:G:248:LEU:HD22	2.46	0.45
3:C:162:VAL:O	3:C:164:ASN:CG	2.55	0.45
1:A:167:ASN:OD1	1:A:167:ASN:C	2.54	0.45
3:I:143:TYR:CE1	3:I:144:PRO:HB3	2.52	0.45
1:D:147:ASN:ND2	1:D:255:PHE:HZ	2.14	0.45
2:B:146:LEU:HA	2:B:146:LEU:HD13	1.77	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
2:E:50:ILE:CG2	2:E:69:ILE:HG23	2.47	0.45
3:F:79:ASN:O	3:F:80:PRO:O	2.35	0.45
2:H:98:HIS:H	2:H:98:HIS:CD2	2.34	0.45
3:F:38:TRP:CA	3:F:49:LEU:HD23	2.46	0.45
3:I:7:PRO:HG3	3:I:21:THR:H	1.78	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:122:SER:HB2	1:A:123:TRP:CE2	2.52	0.45
2:H:63:VAL:C	2:H:65:GLY:N	2.64	0.45
1:J:235:GLU:CG	1:J:236:PRO:CD	2.92	0.45
3:F:191:ARG:NE	3:F:192:HIS:CE1	2.85	0.45
3:L:162:VAL:O	3:L:163:LEU:C	2.53	0.45
1:A:64:ASN:OD1	1:A:66:GLU:HG2	2.17	0.45
1:G:73:ALA:HB3	4:G:608:HOH:O	2.16	0.45
2:H:201:THR:HG23	2:H:218:LYS:HD3	1.99	0.45
3:L:213:ASN:C	3:L:213:ASN:OD1	2.55	0.45
3:I:150:LYS:HB2	3:I:150:LYS:HE2	1.70	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
3:L:114:ALA:HA	3:L:201:HIS:CD2	2.52	0.45
1:D:201:VAL:C	1:D:241:THR:O	2.55	0.45
3:I:34:ASN:O	3:I:95:LYS:HG3	2.17	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
2:H:37:ARG:HD3	2:H:93:TYR:CZ	2.52	0.45
3:I:111:ARG:NE	3:I:173:ASP:HA	2.24	0.45
1:A:174:LEU:HD12	1:A:231:TRP:CE3	2.51	0.45
1:G:101:LEU:HA	1:G:101:LEU:HD23	1.73	0.45
1:D:217:ARG:HB3	1:D:218:PRO:HD2	1.97	0.45
2:B:27:THR:HG22	2:B:31:TYR:CB	2.47	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:E:45:GLU:HB3	2:E:60:ARG:HH12	1.78	0.45
2:H:113:GLN:O	3:I:45:GLN:NE2	2.42	0.45
3:I:91:CYS:SG	3:I:102:PHE:CD2	3.10	0.45
3:L:34:ASN:N	3:L:34:ASN:OD1	2.49	0.45
1:D:150:TRP:CD1	1:D:150:TRP:C	2.90	0.45
1:D:56:ASN:OD1	1:D:56:ASN:N	2.43	0.45
3:F:8:ALA:HB1	3:F:105:THR:OG1	2.17	0.45
1:A:138:HIS:HB2	1:A:143:SER:HB2	1.99	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
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: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
2:B:78:LEU:CD1	2:B:78:LEU:C	2.85	0.45
2:E:31:TYR:O	2:E:71:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:97:ARG:HG2	2:E:98:HIS:H	1.82	0.45
1:A:229:TYR:C	1:A:230:TYR:CD1	2.90	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
3:C:210:LYS:HD2	3:C:211:SER:N	2.18	0.45
3:L:191:ARG:HD2	3:L:191:ARG:C	2.36	0.45
2:B:196:SER:O	2:B:202:TYR:HE2	1.99	0.45
2:H:72:ASP:CB	2:H:79:TYR:CE2	2.93	0.45
2:K:211:SER:O	2:K:213:THR:N	2.50	0.45
3:C:120:ILE:CG2	3:C:121:PHE:N	2.80	0.45
2:B:189:VAL:HG23	3:C:138:PHE:CE2	2.52	0.45
3:F:108:GLU:CG	3:F:109:ILE:N	2.65	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
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:K:51:LEU:HD21	2:K:56:ARG:CB	2.35	0.45
3:C:13:SER:CB	3:C:110:LYS:HZ2	2.30	0.44
2:E:50:ILE:HG22	2:E:57:SER:OG	2.17	0.44
2:H:162:TRP:HA	2:H:203:ILE:O	2.17	0.44
3:F:26:GLU:O	3:F:27:SER:OG	2.33	0.44
3:L:195:TYR:H	3:L:210:LYS:HA	1.81	0.44
2:K:209:LYS:HB2	2:K:210:PRO:CD	2.47	0.44
2:K:43:GLY:O	2:K:44:LEU:CD2	2.65	0.44
1:J:216:ILE:O	1:J:216:ILE:HG22	2.16	0.44
3:C:166:TRP:CE3	3:C:166:TRP:HA	2.51	0.44
3:F:140:ASN:CG	3:F:176:TYR:CD1	2.87	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
3:L:209:VAL:HG23	3:L:210:LYS:CG	2.47	0.44
3:F:135:VAL:CG1	3:F:151:TRP:CZ3	3.00	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
1:G:86:ASP:N	1:G:86:ASP:OD1	2.50	0.44
3:I:128:LEU:HD23	3:I:128:LEU:O	2.17	0.44
2:B:45:GLU:HG2	2:B:60:ARG:CZ	2.47	0.44
2:K:37:ARG:HG2	2:K:47:VAL:HG13	1.97	0.44
3:L:86:THR:H	3:L:109:ILE:HD11	1.83	0.44
3:L:16:GLN:HG3	3:L:17:ARG:H	1.82	0.44
1:G:54:LYS:CB	1:G:66:GLU:O	2.65	0.44
3:F:97:VAL:HG13	3:F:98:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:97:ASP:HB3	1:J:231:TRP:HE1	1.80	0.44
2:E:66:ARG:CZ	2:E:86:ARG:HD3	2.46	0.44
3:L:165:SER:C	3:L:166:TRP:CD1	2.90	0.44
1:G:180:HIS:N	1:G:247:ASN:O	2.48	0.44
3:I:136:VAL:HG13	3:I:180:SER:OG	2.17	0.44
2:K:215:VAL:HG23	2:K:216:ASP:N	2.32	0.44
2:H:218:LYS:HB2	2:H:218:LYS:HZ2	1.81	0.44
1:J:89:THR:HB	1:J:145:TYR:OH	2.17	0.44
3:F:54:ALA:O	3:F:67:GLY:HA3	2.18	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:171:VAL:HG23	2:B:189:VAL:HG12	2.00	0.44
3:C:173:ASP:HB2	3:C:174:SER:H	1.72	0.44
3:L:142:PHE:HE2	3:L:177:SER:N	2.15	0.44
2:B:180:SER:HA	3:L:60:GLY:O	2.18	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
3:I:7:PRO:CG	3:I:21:THR:H	2.30	0.44
2:K:17:LEU:N	2:K:82:MET:O	2.43	0.44
2:B:38:GLN:HA	2:B:44:LEU:N	2.14	0.44
2:B:131:PRO:HD3	2:B:217:LYS:HD2	2.00	0.44
1:G:200:PHE:CG	1:G:201:VAL:N	2.85	0.44
2:K:51:LEU:H	2:K:51:LEU:HG	1.62	0.44
2:H:178:LEU:C	2:H:178:LEU:HD23	2.38	0.44
1:A:57:ILE:HD12	1:A:102:ARG:HE	1.83	0.44
1:A:127:ASP:C	1:A:127:ASP:OD2	2.56	0.44
2:K:194:SER:O	2:K:197:LEU:HG	2.16	0.44
3:I:204:SER:C	3:I:205:THR:CG2	2.86	0.44
1:J:172:GLU:O	1:J:256:ALA:HA	2.17	0.44
3:C:159:GLN:HG3	3:C:160:ASN:N	2.33	0.44
2:B:36:ILE:HG13	2:B:45:GLU:C	2.36	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
2:H:98:HIS:HA	3:I:36:ILE:HG22	1.96	0.44
3:I:13:SER:HB3	3:I:110:LYS:HZ1	1.83	0.44
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
1:D:101:LEU:O	1:D:103:GLU:N	2.51	0.44
1:A:176:LEU:N	1:A:176:LEU:HD12	2.33	0.44
1:G:192:TYR:HB3	1:G:246:GLY:HA3	1.99	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:41:GLN:HG3	3:C:45:GLN:O	2.17	0.44
1:J:101:LEU:HD22	1:J:105:LEU:HD11	1.98	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
1:D:127:ASP:OD2	1:D:130:LYS:HG2	2.18	0.44
3:C:42:LYS:O	3:C:44:GLY:N	2.50	0.44
3:L:64:ARG:NH2	3:L:85:ASP:OD1	2.51	0.44
2:H:34:SER:HB2	2:H:98:HIS:NE2	2.33	0.44
3:F:51:ILE:HD11	3:F:66:SER:HA	2.00	0.44
1:J:114:PHE:N	1:J:114:PHE:CD2	2.85	0.44
2:K:68:THR:N	2:K:81:GLU:O	2.44	0.44
1:D:101:LEU:O	1:D:102:ARG:C	2.54	0.44
1:G:177:TRP:HZ2	1:G:206:TYR:CZ	2.35	0.44
1:G:239:LYS:HD2	1:G:239:LYS:O	2.18	0.44
2:K:51:LEU:HD11	2:K:56:ARG:HB2	1.99	0.44
3:C:128:LEU:CD1	3:C:129:THR:H	2.19	0.44
3:F:162:VAL:HG23	3:F:162:VAL:O	2.17	0.44
3:L:204:SER:C	3:L:205:THR:HG22	2.38	0.44
2:E:192:VAL:HG12	2:E:193:PRO:HD2	1.99	0.44
3:L:53:THR:HG22	3:L:53:THR:O	2.17	0.44
3:C:12:VAL:HG11	3:C:81:VAL:HG21	2.00	0.44
3:L:57:LYS:O	3:L:58:GLY:C	2.56	0.44
1:D:137:PRO:HA	1:D:143:SER:N	2.28	0.44
1:G:173:VAL:O	1:G:234:VAL:N	2.42	0.44
3:F:8:ALA:O	3:F:9:SER:CB	2.64	0.44
2:K:98:HIS:CD2	3:L:36:ILE:HG21	2.52	0.44
1:J:48:ALA:HB2	1:J:78:TYR:HE1	1.78	0.44
1:G:161:LEU:C	1:G:161:LEU:HD23	2.38	0.44
1:J:56:ASN:ND2	1:J:88:GLY:HA2	2.33	0.44
3:C:152:LYS:O	3:C:195:TYR:HA	2.18	0.44
2:H:176:ALA:HB2	3:I:166:TRP:NE1	2.31	0.44
3:L:189:TYR:HB3	3:L:190:GLU:H	1.59	0.44
3:I:190:GLU:HB3	3:I:191:ARG:H	1.57	0.44
2:E:4:LEU:HB2	2:E:112:GLY:HA3	2.00	0.44
3:L:115:ALA:HA	3:L:116:PRO:HD3	1.78	0.44
1:A:137:PRO:HA	1:A:143:SER:N	2.28	0.44
1:A:117:PHE:HB2	1:A:122:SER:OG	2.17	0.44
1:A:147:ASN:ND2	1:A:253:TYR:HB2	2.33	0.44
2:E:63:VAL:C	2:E:65:GLY:H	2.18	0.44
3:F:120:ILE:HG12	3:F:121:PHE:N	2.32	0.44
2:K:163:ASN:O	2:K:164:SER:HB2	2.18	0.44
2:K:69:ILE:HG13	2:K:70:SER:H	1.83	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:LYS:HD2	1:A:156:ASN:HA	2.00	0.44
2:B:37:ARG:O	2:B:45:GLU:N	2.33	0.43
2:E:174:PHE:O	3:F:166:TRP:CD1	2.70	0.43
2:H:111:TRP:CH2	3:I:38:TRP:CE3	3.06	0.43
2:K:99:SER:HB3	3:L:35:PHE:CD1	2.53	0.43
3:C:158:ARG:NH2	2:K:97:ARG:HD2	2.29	0.43
2:E:168:THR:O	2:E:169:SER:CB	2.66	0.43
3:F:211:SER:O	3:F:212:PHE:CB	2.66	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
1:D:79:ILE:CD1	1:D:79:ILE:H	2.24	0.43
1:D:70:LEU:O	1:D:71:SER:OG	2.22	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
3:C:64:ARG:HB3	3:C:80:PRO:HD2	1.99	0.43
2:K:170:SER:HB2	2:K:189:VAL:O	2.18	0.43
3:I:7:PRO:HD2	3:I:21:THR:O	2.17	0.43
3:I:178:MET:SD	3:I:178:MET:C	2.96	0.43
3:F:189:TYR:HB3	3:F:190:GLU:H	1.57	0.43
2:E:88:GLU:HG3	2:E:89:ASP:N	2.33	0.43
3:L:209:VAL:HG23	3:L:210:LYS:HB2	2.00	0.43
2:B:157:PRO:O	2:B:208:HIS:CD2	2.68	0.43
1:D:99:GLU:CG	1:D:100:GLU:N	2.81	0.43
3:L:143:TYR:CD2	3:L:144:PRO:CD	3.01	0.43
1:G:55:CYS:HB2	1:G:60:TRP:HB2	2.00	0.43
2:H:34:SER:HB3	2:H:48:SER:O	2.18	0.43
3:I:195:TYR:H	3:I:210:LYS:HA	1.83	0.43
1:A:121:SER:HB3	2:B:58:TYR:HA	2.00	0.43
1:G:200:PHE:O	1:G:201:VAL:HG23	2.18	0.43
2:H:124:THR:OG1	2:H:155:PRO:HD3	2.19	0.43
3:L:156:SER:OG	3:L:157:GLU:N	2.50	0.43
2:H:130:PHE:CD1	3:I:126:GLU:HB2	2.54	0.43
1:J:123:TRP:CZ3	1:J:163:LYS:HG3	2.50	0.43
1:A:82:THR:O	1:A:82:THR:OG1	2.32	0.43
2:B:51:LEU:CD1	2:B:56:ARG:HG2	2.48	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
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:E:211:SER:O	2:E:212:ASN:HB3	2.18	0.43
2:H:174:PHE:CD2	3:I:166:TRP:CE3	3.04	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:197:LEU:O	2:K:197:LEU:CD1	2.62	0.43
1:J:165:TYR:OH	1:J:169:LYS:HD2	2.18	0.43
1:D:183:SER:HB2	1:D:184:THR:HG23	1.99	0.43
2:E:97:ARG:HG2	2:E:98:HIS:N	2.34	0.43
2:H:30:ASP:O	2:H:30:ASP:CG	2.56	0.43
3:I:93:GLN:C	3:I:94:THR:O	2.54	0.43
2:K:82:MET:HB2	2:K:85:LEU:HD21	2.00	0.43
3:C:46:PRO:HA	3:C:47:PRO:HD3	1.61	0.43
1:A:57:ILE:H	1:A:81:GLU:CD	2.22	0.43
1:G:100:GLU:HG2	1:G:231:TRP:CZ2	2.53	0.43
1:G:79:ILE:HG22	1:G:80:VAL:H	1.81	0.43
3:C:183:THR:HG22	3:C:184:LEU:N	2.34	0.43
2:B:130:PHE:CE1	3:C:127:GLN:HG3	2.53	0.43
3:F:163:LEU:O	3:F:163:LEU:HD23	2.19	0.43
2:E:177:VAL:HG22	2:E:184:TYR:HE2	1.84	0.43
3:C:81:VAL:HG11	3:C:109:ILE:HG13	1.99	0.43
3:F:102:PHE:CG	3:F:103:GLY:N	2.86	0.43
2:H:46:TRP:HE3	2:H:60:ARG:NH2	2.16	0.43
3:L:37:ASN:O	3:L:49:LEU:HA	2.19	0.43
1:A:91:TYR:OH	1:A:180:HIS:NE2	2.32	0.43
3:F:189:TYR:O	3:F:190:GLU:HB2	2.19	0.43
1:D:107:SER:OG	1:D:259:ARG:HG2	2.19	0.43
1:D:108:VAL:HG12	1:D:257:MET:HE3	1.99	0.43
2:B:19:LEU:O	2:B:79:TYR:HA	2.18	0.43
1:A:101:LEU:CD2	1:A:105:LEU:HG	2.48	0.43
3:L:24:ALA:O	3:L:72:THR:OG1	2.32	0.43
3:F:84:GLU:C	3:F:86:THR:H	2.22	0.43
1:J:118:PRO:O	1:J:122:SER:CB	2.66	0.43
3:L:57:LYS:HD3	3:L:61:VAL:O	2.19	0.43
2:E:178:LEU:HB3	2:E:180:SER:HB2	2.01	0.43
1:A:92:PRO:C	1:A:226:ARG:HD2	2.39	0.43
1:J:188:GLN:NE2	1:J:247:ASN:OD1	2.51	0.43
3:F:162:VAL:O	3:F:164:ASN:CG	2.56	0.43
1:A:181:HIS:HB3	1:A:213:GLU:O	2.19	0.43
2:E:90:THR:O	2:E:91:ALA:HB2	2.18	0.43
1:A:220:VAL:O	1:A:221:ARG:HB2	2.19	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:116:PRO:CB	3:I:139:LEU:HB3	2.41	0.43
1:D:64:ASN:O	1:D:67:CYS:HB2	2.18	0.43
2:B:38:GLN:CG	2:B:38:GLN:O	2.66	0.43
1:J:71:SER:OG	1:J:71:SER:O	2.34	0.43
2:H:11:VAL:HG22	2:H:12:GLN:N	2.33	0.43
1:J:219:LYS:CD	1:J:222:ASP:HA	2.36	0.43
2:K:183:LEU:HA	2:K:183:LEU:HD13	1.85	0.43
2:B:211:SER:O	2:B:212:ASN:CB	2.66	0.43
3:I:56:ASN:N	3:I:56:ASN:OD1	2.51	0.43
1:D:113:ARG:HA	1:D:254:ALA:O	2.19	0.43
3:C:35:PHE:CD1	3:C:35:PHE:C	2.91	0.43
3:C:177:SER:O	3:C:178:MET:HG3	2.18	0.43
3:L:145:LYS:CD	3:L:167:THR:HG21	2.47	0.43
3:F:66:SER:O	3:F:77:THR:HG22	2.18	0.43
3:I:90:PHE:HA	3:I:102:PHE:CE2	2.53	0.43
1:J:116:ILE:HG12	1:J:117:PHE:CG	2.54	0.43
1:A:91:TYR:CD1	1:A:227:MET:HE2	2.53	0.43
3:C:204:SER:C	3:C:205:THR:HG22	2.38	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
2:E:208:HIS:NE2	2:E:210:PRO:CG	2.81	0.43
1:J:57:ILE:O	1:J:58:ALA:C	2.58	0.43
2:K:176:ALA:HB2	3:L:166:TRP:NE1	2.31	0.43
1:J:79:ILE:HG22	1:J:80:VAL:N	2.33	0.43
2:K:207:ASN:CA	2:K:213:THR:O	2.67	0.43
2:K:162:TRP:CE3	2:K:204:CYS:HB3	2.53	0.43
1:D:192:TYR:CD1	1:D:192:TYR:N	2.87	0.43
3:C:39:PHE:CD1	3:C:76:LEU:HD13	2.53	0.43
3:L:45:GLN:HA	3:L:45:GLN:OE1	2.18	0.43
2:E:69:ILE:HG12	2:E:70:SER:N	2.33	0.43
2:H:27:THR:HG22	2:H:31:TYR:HD2	1.82	0.43
3:F:97:VAL:O	3:F:99:TYR:CE1	2.72	0.43
3:F:8:ALA:CB	3:F:105:THR:HG23	2.38	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: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
2:B:36:ILE:HG13	2:B:45:GLU:O	2.19	0.42
3:C:38:TRP:HH2	3:C:89:TYR:CB	2.25	0.42
3:L:175:THR:HB	3:L:176:TYR:CD1	2.54	0.42
3:L:42:LYS:CD	3:L:87:ALA:HB2	2.41	0.42
3:F:45:GLN:CB	3:F:46:PRO:HD2	2.48	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:203:ILE:HG13	2:H:217:LYS:O	2.19	0.42
3:L:164:ASN:HB3	4:L:302:HOH:O	2.17	0.42
3:F:204:SER:C	3:F:205:THR:HG22	2.38	0.42
2:B:86:ARG:N	2:B:119:VAL:HG11	2.34	0.42
3:F:150:LYS:HB3	3:F:198:GLU:HG2	2.01	0.42
1:A:179:ILE:HD11	1:A:199:VAL:CG1	2.45	0.42
1:G:116:ILE:N	1:G:252:ARG:O	2.52	0.42
1:D:186:ALA:O	1:D:187:ASP:C	2.57	0.42
2:E:26:PHE:O	2:E:27:THR:C	2.57	0.42
3:I:145:LYS:CA	3:I:147:ILE:N	2.77	0.42
2:B:186:LEU:C	2:B:186:LEU:HD12	2.40	0.42
3:L:142:PHE:CE1	3:L:144:PRO:O	2.73	0.42
2:B:43:GLY:C	2:B:44:LEU:HD12	2.39	0.42
2:K:34:SER:HB2	2:K:98:HIS:NE2	2.34	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:B:85:LEU:HD23	2:B:85:LEU:HA	1.85	0.42
1:A:55:CYS:SG	1:A:66:GLU:CG	3.04	0.42
2:E:4:LEU:HD11	2:E:110:GLY:O	2.20	0.42
2:H:218:LYS:CB	2:H:218:LYS:NZ	2.82	0.42
2:B:9:ALA:O	2:B:117:VAL:HA	2.19	0.42
3:C:167:THR:HG22	3:C:168:ASP:N	2.23	0.42
3:C:84:GLU:C	3:C:86:THR:HG23	2.40	0.42
2:B:178:LEU:C	2:B:180:SER:N	2.72	0.42
2:E:32:ASP:HB3	2:E:51:LEU:C	2.39	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
3:C:97:VAL:O	3:C:99:TYR:CD1	2.71	0.42
3:L:40:GLN:HB2	3:L:50:LEU:HD11	2.01	0.42
3:I:141:ASN:CA	3:I:175:THR:HG22	2.29	0.42
1:A:239:LYS:NZ	1:A:241:THR:OG1	2.47	0.42
2:E:180:SER:H	3:I:60:GLY:HA2	1.85	0.42
2:H:161:SER:HB3	2:H:205:ASN:ND2	2.34	0.42
1:G:133:THR:CG2	1:G:144:PHE:HD1	2.31	0.42
1:D:77:SER:OG	1:D:78:TYR:N	2.51	0.42
3:I:162:VAL:O	3:I:164:ASN:OD1	2.37	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
1:D:192:TYR:C	1:D:194:ASN:H	2.23	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:SER:OG	1:A:86:ASP:N	2.53	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
3:L:147:ILE:HG12	3:L:200:THR:O	2.19	0.42
3:F:13:SER:HB3	3:F:110:LYS:CB	2.48	0.42
2:H:142:GLY:C	2:H:194:SER:OG	2.58	0.42
2:H:39:ALA:H	2:H:44:LEU:HB2	1.85	0.42
3:I:7:PRO:HG2	3:I:7:PRO:O	2.19	0.42
1:J:117:PHE:HB2	1:J:251:PRO:O	2.18	0.42
3:F:191:ARG:HG3	3:F:192:HIS:CE1	2.54	0.42
2:E:203:ILE:HG13	2:E:217:LYS:O	2.20	0.42
2:E:146:LEU:HA	2:E:146:LEU:HD13	1.77	0.42
3:F:128:LEU:HG	3:F:129:THR:N	2.35	0.42
1:J:179:ILE:O	1:J:179:ILE:HG13	2.19	0.42
2:B:150:VAL:O	2:B:186:LEU:N	2.47	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:E:178:LEU:C	2:E:180:SER:HB2	2.40	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:183:LEU:HD13	2:H:183:LEU:HA	1.75	0.42
1:G:76:TRP:CZ3	1:G:108:VAL:HG21	2.54	0.42
3:F:150:LYS:HB3	3:F:198:GLU:CG	2.49	0.42
2:B:196:SER:HB3	2:B:202:TYR:CE2	2.54	0.42
2:E:143:THR:CG2	2:E:191:THR:HG23	2.48	0.42
3:F:14:PRO:O	3:F:15:GLY:C	2.58	0.42
3:I:168:ASP:O	3:I:169:GLN:HB2	2.19	0.42
2:B:45:GLU:OE2	2:B:45:GLU:HA	2.19	0.42
3:C:42:LYS:HA	3:C:42:LYS:HE2	2.01	0.42
3:C:6:SER:HA	3:C:21:THR:O	2.19	0.42
3:L:170:ASP:C	3:L:170:ASP:OD2	2.58	0.42
1:D:208:LYS:CG	1:D:209:LYS:N	2.82	0.42
2:E:50:ILE:CD1	2:E:71:ARG:HB2	2.37	0.42
2:H:27:THR:CG2	2:H:30:ASP:H	2.33	0.42
3:I:165:SER:HA	3:I:178:MET:O	2.19	0.42
3:I:62:PRO:HD2	3:I:65:PHE:CE2	2.55	0.42
3:F:162:VAL:O	3:F:164:ASN:OD1	2.37	0.42
3:L:129:THR:O	3:L:130:SER:OG	2.36	0.42
1:G:102:ARG:HG3	1:G:103:GLU:N	2.35	0.42
1:G:184:THR:O	1:G:185:SER:C	2.58	0.42
1:J:215:ALA:O	1:J:217:ARG:HD2	2.20	0.42
1:J:92:PRO:HG3	1:J:223:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:161:SER:O	2:K:204:CYS:HA	2.19	0.42
1:D:184:THR:H	1:D:187:ASP:HB2	1.84	0.42
1:D:220:VAL:O	1:D:221:ARG:HB2	2.18	0.42
3:L:13:SER:N	3:L:110:LYS:HD2	2.34	0.42
2:B:181:SER:OG	3:L:84:GLU:CD	2.58	0.42
1:D:91:TYR:O	1:D:229:TYR:OH	2.29	0.42
3:C:192:HIS:CE1	3:C:194:SER:CB	3.02	0.42
1:D:217:ARG:HD2	1:D:226:ARG:HG2	2.00	0.42
1:G:71:SER:O	1:G:73:ALA:N	2.53	0.42
1:D:127:ASP:HB2	1:D:154:LYS:CB	2.49	0.42
3:F:57:LYS:CB	3:F:57:LYS:HZ3	2.32	0.42
1:J:127:ASP:N	1:J:154:LYS:HB2	2.34	0.42
3:L:143:TYR:HA	3:L:144:PRO:HA	1.61	0.42
2:E:76:LYS:HA	2:E:76:LYS:HD3	1.91	0.42
1:D:52:LEU:HD12	1:D:81:GLU:HG2	2.00	0.42
3:F:192:HIS:O	3:F:195:TYR:CE1	2.73	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
1:D:149:ILE:CD1	1:D:252:ARG:HB2	2.50	0.42
1:G:57:ILE:HD11	1:G:79:ILE:HD12	2.01	0.42
2:K:147:GLY:C	2:K:162:TRP:CH2	2.89	0.42
2:K:196:SER:O	2:K:200:GLN:HB2	2.20	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
2:E:59:TYR:N	2:E:59:TYR:CD2	2.88	0.42
3:F:159:GLN:CG	3:F:160:ASN:H	2.33	0.42
3:F:2:GLN:NE2	3:F:97:VAL:HG21	2.35	0.42
2:H:94:TYR:OH	3:I:45:GLN:OE1	2.33	0.42
3:L:97:VAL:HG13	3:L:98:PRO:N	2.35	0.42
3:I:140:ASN:HB3	3:I:176:TYR:CD1	2.55	0.42
3:F:27:SER:C	3:F:28:VAL:HG22	2.40	0.42
3:F:161:GLY:C	3:F:162:VAL:HG13	2.40	0.42
2:E:215:VAL:CG2	2:E:216:ASP:N	2.82	0.42
1:D:127:ASP:CG	1:D:130:LYS:HG2	2.39	0.42
1:D:69:SER:OG	1:D:70:LEU:HB2	2.20	0.42
2:K:19:LEU:CD1	2:K:19:LEU:N	2.83	0.42
2:H:42:LYS:HE2	2:H:42:LYS:HB2	1.86	0.42
3:I:35:PHE:O	3:I:35:PHE:CD1	2.73	0.42
2:B:173:THR:CG2	2:B:187:SER:O	2.67	0.42
3:C:118:VAL:HG13	3:C:139:LEU:HD23	2.01	0.42
3:C:82:GLU:N	3:C:85:ASP:OD2	2.47	0.42
3:F:109:ILE:CG2	3:F:110:LYS:H	2.32	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:240:ILE:O	1:D:240:ILE:HG23	2.19	0.42
1:G:76:TRP:CZ2	1:G:105:LEU:O	2.73	0.42
1:G:222:ASP:O	1:G:222:ASP:CG	2.57	0.42
1:A:96:ILE:HD13	1:A:96:ILE:N	2.35	0.42
3:L:52:TYR:CD1	3:L:56:ASN:HB2	2.55	0.42
2:E:85:LEU:HD23	2:E:85:LEU:HA	1.83	0.42
3:C:38:TRP:HH2	3:C:89:TYR:CD1	2.33	0.41
3:L:13:SER:CA	3:L:110:LYS:HD2	2.50	0.41
2:K:94:TYR:CE1	3:L:46:PRO:HB3	2.55	0.41
3:F:84:GLU:C	3:F:86:THR:N	2.72	0.41
1:A:133:THR:O	1:A:142:LYS:HB2	2.20	0.41
2:E:162:TRP:HB2	2:E:167:LEU:HD23	2.02	0.41
1:J:76:TRP:CE2	1:J:108:VAL:HG22	2.55	0.41
3:F:164:ASN:HB3	3:F:180:SER:N	2.35	0.41
1:A:104:GLN:NE2	1:A:231:TRP:CH2	2.88	0.41
3:L:133:ALA:O	3:L:183:THR:O	2.38	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
2:E:127:PRO:HA	2:E:153:TYR:HB3	2.02	0.41
2:B:132:LEU:HD13	3:C:136:VAL:HB	2.02	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
3:F:38:TRP:HA	3:F:49:LEU:HD23	2.02	0.41
1:J:114:PHE:O	1:J:253:TYR:HA	2.19	0.41
1:G:173:VAL:HA	1:G:256:ALA:HA	2.02	0.41
1:D:119:LYS:HG2	1:D:120:THR:N	2.35	0.41
2:H:63:VAL:HG13	2:H:66:ARG:H	1.85	0.41
1:A:219:LYS:HE3	1:A:219:LYS:HB2	1.84	0.41
1:D:116:ILE:CG2	1:D:117:PHE:H	2.33	0.41
1:G:79:ILE:CG2	1:G:80:VAL:H	2.32	0.41
1:J:51:HIS:CD2	1:J:80:VAL:CB	3.02	0.41
3:L:69:GLY:HA3	3:L:74:PHE:CD1	2.55	0.41
2:K:39:ALA:HB3	2:K:44:LEU:HG	2.01	0.41
2:E:177:VAL:HA	2:E:184:TYR:HD2	1.84	0.41
1:J:86:ASP:N	1:J:86:ASP:OD1	2.38	0.41
3:C:35:PHE:HB3	3:C:95:LYS:CD	2.41	0.41
2:E:47:VAL:O	2:E:48:SER:CB	2.68	0.41
2:E:28:GLY:N	2:E:76:LYS:NZ	2.66	0.41
2:E:173:THR:O	2:E:174:PHE:C	2.57	0.41
2:H:48:SER:OG	2:H:49:GLY:N	2.53	0.41
2:K:45:GLU:CD	2:K:46:TRP:N	2.68	0.41
2:E:208:HIS:C	2:E:210:PRO:HD2	2.40	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:L:128:LEU:HG	3:L:129:THR:OG1	2.20	0.41
2:B:85:LEU:HB3	2:B:119:VAL:CG1	2.50	0.41
2:B:19:LEU:HD22	2:B:82:MET:HE1	2.03	0.41
1:G:79:ILE:HD11	1:G:105:LEU:CB	2.50	0.41
1:A:54:LYS:HD2	1:A:69:SER:HB2	2.02	0.41
1:J:161:LEU:CD2	1:J:161:LEU:C	2.88	0.41
2:E:177:VAL:HA	2:E:184:TYR:HA	2.02	0.41
2:E:133:ALA:HA	2:E:134:PRO:HD3	1.87	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
3:L:83:ALA:O	3:L:171:SER:O	2.38	0.41
2:H:97:ARG:HB3	2:H:110:GLY:CA	2.32	0.41
2:K:99:SER:O	2:K:100:TRP:CG	2.73	0.41
3:F:7:PRO:O	3:F:8:ALA:CB	2.67	0.41
1:A:252:ARG:HD2	1:A:253:TYR:CD2	2.55	0.41
1:G:61:ILE:O	1:G:61:ILE:HG13	2.19	0.41
1:J:171:LYS:NZ	1:J:258:GLU:HG3	2.34	0.41
2:E:100:TRP:CD1	3:F:34:ASN:CG	2.93	0.41
1:A:206:TYR:CD2	1:A:207:SER:N	2.88	0.41
1:J:169:LYS:NZ	1:J:256:ALA:HB1	2.35	0.41
1:D:205:ARG:HA	1:D:205:ARG:HD2	1.48	0.41
2:B:27:THR:HG21	2:B:31:TYR:CG	2.55	0.41
2:B:171:VAL:O	2:B:188:SER:HA	2.20	0.41
2:B:174:PHE:HD1	2:B:174:PHE:N	2.19	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
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
2:E:161:SER:HG	2:E:163:ASN:HD22	1.66	0.41
1:A:119:LYS:O	1:A:123:TRP:CD1	2.73	0.41
2:H:83:ASN:O	2:H:84:SER:C	2.58	0.41
2:B:64:LYS:HD3	2:B:64:LYS:HA	1.32	0.41
3:C:34:ASN:N	3:C:34:ASN:HD22	2.18	0.41
1:A:161:LEU:HD22	1:A:244:ALA:HB3	2.03	0.41
3:C:118:VAL:HB	3:C:208:ILE:CD1	2.50	0.41
3:L:16:GLN:HA	3:L:16:GLN:OE1	2.21	0.41
3:F:42:LYS:NZ	3:F:84:GLU:O	2.54	0.41
2:H:51:LEU:CD1	2:H:56:ARG:H	2.33	0.41
2:H:94:TYR:CE1	3:I:47:PRO:HD2	2.56	0.41
3:I:4:THR:O	3:I:102:PHE:HB2	2.20	0.41
2:H:60:ARG:NH2	3:I:99:TYR:O	2.45	0.41
1:G:166:ILE:HD13	1:G:166:ILE:H	1.83	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:205:ASN:HB3	2:H:216:ASP:OD1	2.20	0.41
2:K:10:VAL:HG12	2:K:118:THR:O	2.21	0.41
3:L:196:THR:HG1	3:L:210:LYS:HZ2	1.58	0.41
2:B:19:LEU:HD22	2:B:82:MET:CE	2.50	0.41
2:E:39:ALA:HA	2:E:91:ALA:CB	2.51	0.41
3:F:147:ILE:HG23	3:F:147:ILE:O	2.21	0.41
2:B:35:TRP:HB2	2:B:48:SER:OG	2.20	0.41
3:C:109:ILE:CD1	3:C:109:ILE:N	2.79	0.41
3:C:168:ASP:OD1	3:C:176:TYR:O	2.38	0.41
3:C:142:PHE:O	3:C:174:SER:HB3	2.21	0.41
3:C:17:ARG:HB2	3:C:17:ARG:CZ	2.50	0.41
2:E:171:VAL:HB	3:F:178:MET:HE1	2.02	0.41
2:H:27:THR:CG2	2:H:30:ASP:HB3	2.50	0.41
3:F:38:TRP:CZ3	3:F:39:PHE:CG	3.08	0.41
3:I:1:ILE:HG22	3:I:3:MET:HE2	2.02	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
1:D:54:LYS:CD	1:D:67:CYS:HA	2.50	0.41
3:I:135:VAL:HG22	3:I:151:TRP:CH2	2.55	0.41
1:A:123:TRP:HZ3	1:A:163:LYS:HG3	1.84	0.41
1:J:56:ASN:HB3	1:J:83:SER:HA	2.02	0.41
1:G:136:CYS:HB3	1:G:144:PHE:HA	2.01	0.41
1:D:165:TYR:CE2	1:D:167:ASN:HB2	2.54	0.41
3:I:121:PHE:N	3:I:136:VAL:O	2.47	0.41
1:G:58:ALA:HB2	1:G:98:TYR:HE1	1.82	0.41
1:D:232:THR:C	1:D:233:LEU:HD13	2.41	0.41
1:G:116:ILE:HG22	1:G:252:ARG:O	2.21	0.41
3:I:203:THR:O	3:I:204:SER:C	2.59	0.41
3:C:3:MET:O	3:C:25:SER:HB3	2.21	0.41
2:B:27:THR:HG22	2:B:31:TYR:CG	2.55	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
2:B:178:LEU:HB3	2:B:183:LEU:HB3	2.01	0.41
2:E:161:SER:OG	2:E:163:ASN:ND2	2.45	0.41
1:J:49:PRO:O	1:J:78:TYR:O	2.39	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
3:L:210:LYS:HB3	3:L:211:SER:H	1.39	0.41
1:D:149:ILE:HG13	1:D:252:ARG:HB2	2.02	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
1:D:184:THR:OG1	1:D:186:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:263:SER:OG	1:A:264:GLY:N	2.52	0.41
1:J:104:GLN:O	1:J:104:GLN:HG3	2.18	0.41
2:B:45:GLU:HG2	2:B:60:ARG:NH1	2.36	0.41
3:C:167:THR:CG2	3:C:168:ASP:H	2.27	0.41
3:F:166:TRP:CE3	3:F:166:TRP:HA	2.56	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
2:K:36:ILE:CB	2:K:46:TRP:HA	2.48	0.41
3:L:41:GLN:HB2	3:L:47:PRO:HB3	2.02	0.41
1:D:137:PRO:CB	1:D:142:LYS:HA	2.50	0.41
3:C:153:ILE:CG1	3:C:154:ASP:N	2.81	0.41
1:G:133:THR:C	1:G:142:LYS:HB2	2.41	0.41
1:A:58:ALA:O	1:A:62:LEU:HB2	2.21	0.41
2:E:156:GLU:CB	2:E:157:PRO:CA	2.98	0.41
3:L:120:ILE:HA	3:L:120:ILE:HD12	1.97	0.41
1:J:151:LEU:HD23	1:J:151:LEU:HA	1.94	0.41
3:I:143:TYR:HA	3:I:144:PRO:HA	1.76	0.41
3:C:132:GLY:HA2	3:C:184:LEU:C	2.41	0.41
1:A:157:SER:OG	1:A:159:PRO:HD3	2.20	0.41
2:E:26:PHE:HB3	2:E:27:THR:H	1.64	0.41
1:A:217:ARG:HB3	1:A:218:PRO:HD2	2.01	0.41
3:C:196:THR:OG1	3:C:209:VAL:HB	2.21	0.41
3:C:8:ALA:HB1	3:C:10:LEU:HG	2.03	0.41
1:D:200:PHE:CE2	1:D:201:VAL:O	2.74	0.41
2:E:33:MET:HE3	2:E:97:ARG:HA	2.02	0.41
1:G:65:PRO:C	1:G:67:CYS:H	2.24	0.41
3:I:184:LEU:O	3:I:189:TYR:HB2	2.21	0.41
2:H:100:TRP:HD1	3:I:34:ASN:N	2.19	0.41
2:H:54:SER:O	2:H:55:GLU:C	2.60	0.41
3:L:91:CYS:N	3:L:102:PHE:CD2	2.82	0.41
2:E:180:SER:O	2:E:181:SER:C	2.58	0.41
1:A:109:SER:HB3	1:A:258:GLU:CG	2.50	0.41
3:F:153:ILE:CA	3:F:194:SER:O	2.67	0.41
2:B:209:LYS:N	2:B:210:PRO:CD	2.84	0.41
2:B:200:GLN:O	2:B:202:TYR:CD2	2.74	0.41
1:A:84:SER:OG	1:A:87:ASN:OD1	2.32	0.41
1:J:169:LYS:HZ1	1:J:256:ALA:HB1	1.86	0.41
3:I:70:SER:OG	3:I:71:GLY:N	2.54	0.41
1:D:138:HIS:N	1:D:141:ALA:O	2.43	0.41
2:B:158:VAL:CG1	2:B:159:THR:N	2.84	0.41
2:B:26:PHE:HD1	2:B:27:THR:H	1.69	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:39:PHE:HB2	3:C:50:LEU:CA	2.51	0.40
3:L:44:GLY:O	3:L:45:GLN:HG2	2.21	0.40
3:F:38:TRP:CE2	3:F:39:PHE:CA	2.91	0.40
1:A:258:GLU:C	1:A:259:ARG:HG2	2.38	0.40
1:A:116:ILE:HG23	1:A:117:PHE:H	1.87	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
2:B:10:VAL:HG22	2:B:155:PRO:CG	2.50	0.40
1:D:217:ARG:HB3	1:D:218:PRO:CD	2.51	0.40
1:J:92:PRO:HD2	1:J:223:GLN:HG3	2.03	0.40
1:G:72:THR:HG23	1:G:72:THR:H	1.49	0.40
3:C:35:PHE:HD1	3:C:37:ASN:H	1.69	0.40
3:F:141:ASN:HD21	3:F:176:TYR:HE1	1.69	0.40
3:I:91:CYS:SG	3:I:102:PHE:HD2	2.44	0.40
1:J:148:LEU:HD23	1:J:251:PRO:HA	2.03	0.40
2:B:21:CYS:O	2:B:77:THR:CA	2.68	0.40
2:K:55:GLU:HG2	2:K:71:ARG:HD2	2.03	0.40
3:L:195:TYR:C	3:L:210:LYS:HA	2.39	0.40
1:J:95:PHE:HB3	1:J:98:TYR:CB	2.49	0.40
1:G:57:ILE:HG21	1:G:105:LEU:HD12	2.03	0.40
1:A:96:ILE:HG21	1:D:215:ALA:HB1	2.03	0.40
2:E:17:LEU:HD23	2:E:117:VAL:HG13	2.01	0.40
2:B:47:VAL:O	2:B:48:SER:CB	2.69	0.40
3:C:113:ASP:CG	3:C:142:PHE:HA	2.42	0.40
2:B:177:VAL:HG13	2:B:184:TYR:CE2	2.56	0.40
1:G:115:GLU:HG3	1:G:115:GLU:O	2.21	0.40
3:I:102:PHE:CD1	3:I:104:GLY:N	2.78	0.40
3:I:20:ILE:CG2	3:I:21:THR:H	2.33	0.40
2:H:94:TYR:HE1	3:I:46:PRO:HB3	1.86	0.40
2:K:99:SER:HB3	3:L:35:PHE:CE1	2.56	0.40
3:I:138:PHE:HE1	3:I:178:MET:HG3	1.87	0.40
1:D:227:MET:SD	1:D:249:VAL:HG21	2.61	0.40
1:J:54:LYS:HE3	1:J:67:CYS:C	2.42	0.40
2:E:161:SER:OG	2:E:205:ASN:OD1	2.27	0.40
1:J:102:ARG:NH1	1:J:102:ARG:CG	2.77	0.40
1:J:78:TYR:HA	1:J:106:SER:HA	2.04	0.40
3:L:132:GLY:HA2	3:L:184:LEU:HB3	2.03	0.40
1:A:174:LEU:HD21	1:A:176:LEU:HD11	2.02	0.40
1:A:79:ILE:H	1:A:79:ILE:HD12	1.85	0.40
1:G:95:PHE:HE2	1:G:231:TRP:HD1	1.70	0.40
1:G:91:TYR:C	1:G:91:TYR:CD1	2.95	0.40
2:K:177:VAL:HA	2:K:184:TYR:HA	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:114:ALA:HA	3:I:201:HIS:HD2	1.85	0.40
2:B:51:LEU:HD11	2:B:55:GLU:N	2.36	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
2:E:173:THR:OG1	2:E:173:THR:O	2.38	0.40
3:F:145:LYS:CD	3:F:167:THR:HG21	2.51	0.40
3:F:65:PHE:CD1	3:F:78:ILE:HG12	2.56	0.40
1:D:136:CYS:O	1:D:143:SER:O	2.38	0.40
1:G:169:LYS:CE	1:G:256:ALA:CB	2.99	0.40
1:J:202:GLY:O	1:J:206:TYR:O	2.39	0.40
2:E:22:ALA:HA	2:E:77:THR:HG22	2.03	0.40
1:J:48:ALA:HA	1:J:49:PRO:HD3	1.95	0.40
2:B:86:ARG:NE	2:B:88:GLU:OE2	2.54	0.40
2:K:174:PHE:HA	2:K:175:PRO:HD2	1.78	0.40
2:B:10:VAL:HG13	2:B:118:THR:HB	2.02	0.40
1:A:56:ASN:HB2	1:A:81:GLU:OE1	2.21	0.40
3:F:129:THR:OG1	3:F:129:THR:O	2.40	0.40
2:K:158:VAL:CG1	2:K:159:THR:N	2.84	0.40
3:C:37:ASN:ND2	3:C:39:PHE:HE2	2.14	0.40
2:B:174:PHE:O	3:C:166:TRP:CD2	2.75	0.40
1:D:208:LYS:CG	1:D:209:LYS:H	2.35	0.40
3:I:40:GLN:HA	3:I:88:ASN:O	2.22	0.40
1:D:52:LEU:HD21	1:D:60:TRP:CE3	2.57	0.40
1:J:78:TYR:HA	1:J:106:SER:CA	2.52	0.40
3:C:210:LYS:HG3	3:C:211:SER:N	2.37	0.40
1:G:188:GLN:HE22	1:G:197:ALA:HB3	1.84	0.40
1:D:184:THR:O	1:D:187:ASP:N	2.54	0.40
3:F:57:LYS:CB	3:F:57:LYS:NZ	2.81	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%)	18 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	240/518 (46%)	199 (83%)	35 (15%)	6 (2%)	9	27
1	G	223/518 (43%)	193 (86%)	27 (12%)	3 (1%)	18	50
1	J	249/518 (48%)	211 (85%)	35 (14%)	3 (1%)	19	53
2	B	202/219 (92%)	175 (87%)	25 (12%)	2 (1%)	22	59
2	E	202/219 (92%)	172 (85%)	29 (14%)	1 (0%)	38	75
2	H	202/219 (92%)	174 (86%)	26 (13%)	2 (1%)	22	59
2	K	202/219 (92%)	177 (88%)	21 (10%)	4 (2%)	11	34
3	C	193/218 (88%)	150 (78%)	37 (19%)	6 (3%)	7	20
3	F	193/218 (88%)	142 (74%)	38 (20%)	13 (7%)	2	5
3	I	195/218 (89%)	141 (72%)	45 (23%)	9 (5%)	4	11
3	L	195/218 (89%)	145 (74%)	44 (23%)	6 (3%)	7	20
All	All	2526/3820 (66%)	2077 (82%)	391 (16%)	58 (2%)	10	30

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

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Mol	Chain	Res	Type
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
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%)	161 (85%)	29 (15%)	4	11
1	D	190/451 (42%)	154 (81%)	36 (19%)	2	6
1	G	190/451 (42%)	157 (83%)	33 (17%)	3	8
1	J	190/451 (42%)	156 (82%)	34 (18%)	2	7
2	B	173/182 (95%)	130 (75%)	43 (25%)	1	2
2	E	173/182 (95%)	129 (75%)	44 (25%)	1	2
2	H	173/182 (95%)	140 (81%)	33 (19%)	2	6
2	K	173/182 (95%)	139 (80%)	34 (20%)	2	5
3	C	177/190 (93%)	128 (72%)	49 (28%)	0	1
3	F	177/190 (93%)	135 (76%)	42 (24%)	1	3
3	I	177/190 (93%)	130 (73%)	47 (27%)	1	2
3	L	177/190 (93%)	125 (71%)	52 (29%)	0	1
All	All	2160/3292 (66%)	1684 (78%)	476 (22%)	1	3

All (476) 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	136	CYS
1	A	143	SER
1	A	152	VAL
1	A	164	SER
1	A	166	ILE
1	A	174	LEU
1	A	206	TYR
1	A	213	GLU
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	18	ARG
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	56	ARG
2	B	59	TYR
2	B	60	ARG
2	B	64	LYS
2	B	68	THR
2	B	78	LEU
2	B	79	TYR
2	B	98	HIS
2	B	100	TRP
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

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Mol	Chain	Res	Type
2	B	188	SER
2	B	189	VAL
2	B	200	GLN
2	B	203	ILE
2	B	207	ASN
2	B	214	LYS
2	B	216	ASP
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	49	LEU
3	C	57	LYS
3	C	64	ARG
3	C	66	SER
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	113	ASP
3	C	117	THR
3	C	119	SER
3	C	125	SER
3	C	126	GLU
3	C	128	LEU
3	C	137	CYS
3	C	139	LEU
3	C	147	ILE
3	C	149	VAL
3	C	154	ASP

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Mol	Chain	Res	Type
3	C	158	ARG
3	C	159	GLN
3	C	164	ASN
3	C	166	TRP
3	C	168	ASP
3	C	169	GLN
3	C	171	SER
3	C	173	ASP
3	C	174	SER
3	C	176	TYR
3	C	180	SER
3	C	190	GLU
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	99	GLU
1	D	101	LEU
1	D	110	SER
1	D	121	SER
1	D	126	HIS
1	D	128	SER
1	D	136	CYS
1	D	138	HIS
1	D	142	LYS
1	D	150	TRP
1	D	152	VAL
1	D	153	LYS
1	D	160	LYS
1	D	168	ASP
1	D	183	SER
1	D	194	ASN
1	D	196	ASP
1	D	201	VAL

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Mol	Chain	Res	Type
1	D	204	SER
1	D	205	ARG
1	D	211	LYS
1	D	213	GLU
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	36	ILE
2	E	44	LEU
2	E	51	LEU
2	E	54	SER
2	E	55	GLU
2	E	56	ARG
2	E	57	SER
2	E	59	TYR
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	159	THR
2	E	161	SER
2	E	163	ASN
2	E	170	SER
2	E	171	VAL
2	E	172	HIS
2	E	173	THR
2	E	177	VAL
2	E	181	SER
2	E	186	LEU

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Mol	Chain	Res	Type
2	E	187	SER
2	E	188	SER
2	E	189	VAL
2	E	192	VAL
2	E	195	SER
2	E	199	THR
2	E	201	THR
2	E	203	ILE
2	E	204	CYS
2	E	207	ASN
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	72	THR
3	F	77	THR
3	F	82	GLU
3	F	92	GLN
3	F	93	GLN
3	F	97	VAL
3	F	106	LYS
3	F	117	THR
3	F	118	VAL
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	150	LYS
3	F	156	SER
3	F	157	GLU
3	F	158	ARG

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Mol	Chain	Res	Type
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
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	109	SER
1	G	120	THR
1	G	122	SER
1	G	133	THR
1	G	146	LYS
1	G	148	LEU
1	G	151	LEU
1	G	158	TYR
1	G	161	LEU
1	G	164	SER
1	G	166	ILE
1	G	168	ASP
1	G	179	ILE
1	G	181	HIS
1	G	183	SER
1	G	185	SER
1	G	187	ASP
1	G	190	SER
1	G	207	SER
1	G	211	LYS
1	G	232	THR
1	G	233	LEU
1	G	238	ASP
1	G	239	LYS

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Mol	Chain	Res	Type
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	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	124	THR
2	H	129	VAL
2	H	132	LEU
2	H	143	THR
2	H	161	SER
2	H	177	VAL
2	H	183	LEU
2	H	186	LEU
2	H	187	SER
2	H	189	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	220	CYS
3	I	7	PRO
3	I	10	LEU
3	I	13	SER
3	I	17	ARG
3	I	19	THR
3	I	27	SER
3	I	34	ASN

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Mol	Chain	Res	Type
3	I	36	ILE
3	I	37	ASN
3	I	38	TRP
3	I	40	GLN
3	I	45	GLN
3	I	56	ASN
3	I	72	THR
3	I	75	THR
3	I	77	THR
3	I	91	CYS
3	I	97	VAL
3	I	101	THR
3	I	102	PHE
3	I	105	THR
3	I	110	LYS
3	I	126	GLU
3	I	129	THR
3	I	134	SER
3	I	148	ASN
3	I	150	LYS
3	I	153	ILE
3	I	154	ASP
3	I	158	ARG
3	I	162	VAL
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	183	THR
3	I	184	LEU
3	I	192	HIS
3	I	193	ASN
3	I	197	CYS
3	I	204	SER
3	I	205	THR
3	I	206	SER
3	I	208	ILE
3	I	212	PHE
1	J	45	ARG
1	J	54	LYS

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Mol	Chain	Res	Type
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	95	PHE
1	J	101	LEU
1	J	102	ARG
1	J	104	GLN
1	J	109	SER
1	J	116	ILE
1	J	120	THR
1	J	122	SER
1	J	127	ASP
1	J	158	TYR
1	J	161	LEU
1	J	164	SER
1	J	168	ASP
1	J	175	VAL
1	J	191	LEU
1	J	205	ARG
1	J	206	TYR
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	252	ARG
1	J	259	ARG
2	K	3	LYS
2	K	4	LEU
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	50	ILE

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Mol	Chain	Res	Type
2	K	56	ARG
2	K	59	TYR
2	K	71	ARG
2	K	77	THR
2	K	81	GLU
2	K	89	ASP
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	168	THR
2	K	181	SER
2	K	183	LEU
2	K	187	SER
2	K	189	VAL
2	K	196	SER
2	K	197	LEU
2	K	201	THR
2	K	207	ASN
2	K	215	VAL
3	L	4	THR
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	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	153	ILE
3	L	154	ASP
3	L	158	ARG
3	L	160	ASN
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	178	MET
3	L	182	LEU
3	L	189	TYR
3	L	191	ARG
3	L	193	ASN
3	L	194	SER
3	L	197	CYS
3	L	198	GLU
3	L	203	THR
3	L	208	ILE
3	L	209	VAL
3	L	211	SER
3	L	212	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
2	B	73	ASN
2	B	200	GLN
3	C	92	GLN

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Mol	Chain	Res	Type
3	C	127	GLN
3	C	164	ASN
3	C	193	ASN
3	C	201	HIS
3	F	5	GLN
3	F	93	GLN
3	F	141	ASN
3	F	193	ASN
1	G	129	ASN
1	G	193	GLN
1	G	223	GLN
3	I	34	ASN
3	I	37	ASN
3	I	141	ASN
3	I	201	HIS
1	J	51	HIS
2	K	163	ASN
3	L	92	GLN
3	L	192	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.11	15 (6%) 19 17	19, 35, 59, 76	8 (3%)
1	D	246/518 (47%)	0.34	26 (10%) 7 6	18, 32, 58, 95	21 (8%)
1	G	227/518 (43%)	-0.22	8 (3%) 42 42	18, 32, 57, 70	2 (0%)
1	J	255/518 (49%)	0.40	31 (12%) 5 4	21, 33, 57, 71	30 (11%)
2	B	208/219 (94%)	-0.32	0 100 100	13, 29, 44, 58	0
2	E	208/219 (94%)	-0.39	0 100 100	19, 30, 42, 62	0
2	H	208/219 (94%)	-0.36	5 (2%) 56 57	20, 29, 43, 53	0
2	K	208/219 (94%)	-0.30	2 (0%) 79 80	21, 29, 41, 48	0
3	C	203/218 (93%)	-0.23	2 (0%) 79 80	13, 28, 50, 68	0
3	F	203/218 (93%)	-0.19	3 (1%) 70 71	20, 29, 49, 58	0
3	I	203/218 (93%)	-0.17	4 (1%) 62 63	20, 30, 53, 71	0
3	L	203/218 (93%)	-0.16	4 (1%) 62 63	18, 30, 57, 75	0
All	All	2606/3820 (68%)	-0.11	100 (3%) 38 39	13, 31, 54, 95	61 (2%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	388	LYS	14.7
1	A	389	MET	13.4
1	J	387	GLU	12.3
1	D	389	MET	12.3
1	D	419	LEU	11.7
1	D	422	TRP	11.0
1	D	416	ASP	9.6
1	D	386	ILE	9.5
1	J	382	VAL	8.5
1	D	391	THR	8.5
1	J	383	ASN	8.5

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Mol	Chain	Res	Type	RSRZ
1	J	389	MET	7.9
1	D	387	GLU	7.9
1	A	387	GLU	7.8
1	D	415	ASP	7.3
1	A	385	VAL	7.2
1	D	390	ASN	7.1
1	J	386	ILE	6.8
1	J	426	ALA	6.7
1	D	383	ASN	6.6
1	J	420	ASP	6.5
1	A	47	VAL	6.3
1	D	420	ASP	6.3
1	A	386	ILE	6.2
1	G	389	MET	5.8
1	D	421	ILE	5.7
1	J	437	THR	5.5
1	J	423	THR	5.3
1	D	427	GLU	5.2
1	D	385	VAL	5.1
1	D	384	SER	5.0
1	D	417	GLY	5.0
1	J	425	ASN	4.9
1	D	414	VAL	4.9
1	A	48	ALA	4.8
1	D	423	THR	4.8
1	J	422	TRP	4.7
1	J	436	ARG	4.6
3	L	155	GLY	4.6
1	D	424	TYR	4.5
1	J	418	PHE	4.5
1	D	392	GLN	4.5
1	A	384	SER	4.5
3	I	159	GLN	4.2
1	J	432	LEU	4.2
1	D	44	LEU	4.0
1	A	388	LYS	4.0
1	D	47	VAL	3.9
1	D	388	LYS	3.8
2	K	181	SER	3.7
1	D	425	ASN	3.7
2	H	182	GLY	3.7
1	J	434	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	J	424	TYR	3.6
1	J	435	GLU	3.5
1	G	392	GLN	3.5
1	A	263	SER	3.5
1	J	419	LEU	3.4
1	J	431	LEU	3.4
1	J	384	SER	3.3
1	A	391	THR	3.3
1	G	388	LYS	3.2
1	J	421	ILE	3.2
1	D	48	ALA	3.2
1	G	44	LEU	3.2
1	A	383	ASN	3.1
1	J	385	VAL	3.0
3	F	189	TYR	3.0
2	H	199	THR	3.0
1	A	382	VAL	3.0
2	H	164	SER	2.9
1	G	48	ALA	2.9
2	K	182	GLY	2.9
1	J	433	GLU	2.9
1	J	381	LYS	2.9
3	C	156	SER	2.8
1	J	430	VAL	2.8
1	J	47	VAL	2.7
1	D	426	ALA	2.7
3	F	156	SER	2.7
1	A	390	ASN	2.6
1	A	44	LEU	2.6
1	J	427	GLU	2.6
3	F	37	ASN	2.5
1	J	391	THR	2.5
3	L	154	ASP	2.4
2	H	210	PRO	2.4
1	J	69	SER	2.4
1	J	80	VAL	2.3
1	G	261	ALA	2.3
1	G	161	LEU	2.2
3	I	184	LEU	2.2
3	I	154	ASP	2.1
3	L	195	TYR	2.1
3	C	157	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	I	38	TRP	2.1
1	G	391	THR	2.0
1	A	244	ALA	2.0
3	L	151	TRP	2.0
2	H	140	SER	2.0

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 carbohydrates 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.