Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:47 am BST

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

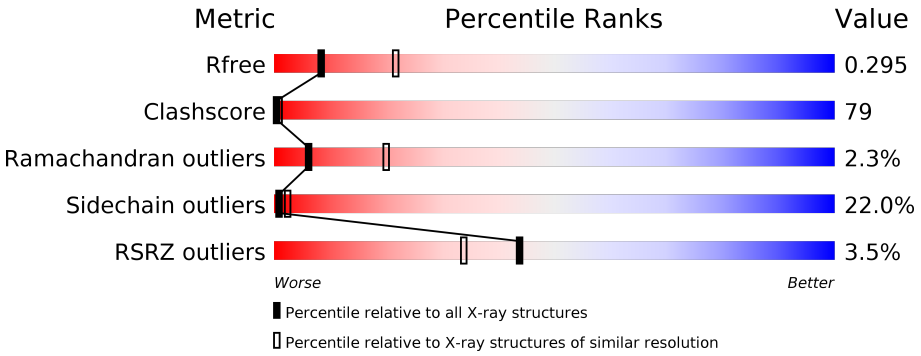
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	518	3% 16% 24% 5% 55%
1	D	518	5% 15% 26% 6% 53%
1	G	518	% 12% 25% 6% 56%
1	J	518	6% 17% 26% 6% 51%
2	B	219	24% 52% 18% • 5%
2	E	219	20% 57% 18% 5%

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Mol	Chain	Length	Quality of chain
2	H	219	2% 24% 58% 13% 5%
2	K	219	% 26% 54% 15% 5%
3	C	218	16% 55% 18% 7%
3	F	218	% 16% 52% 22% 7%
3	I	218	16% 55% 19% 7%
3	L	218	% 14% 57% 18% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19900 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

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

There are 60 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

- Molecule 4 is water.

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

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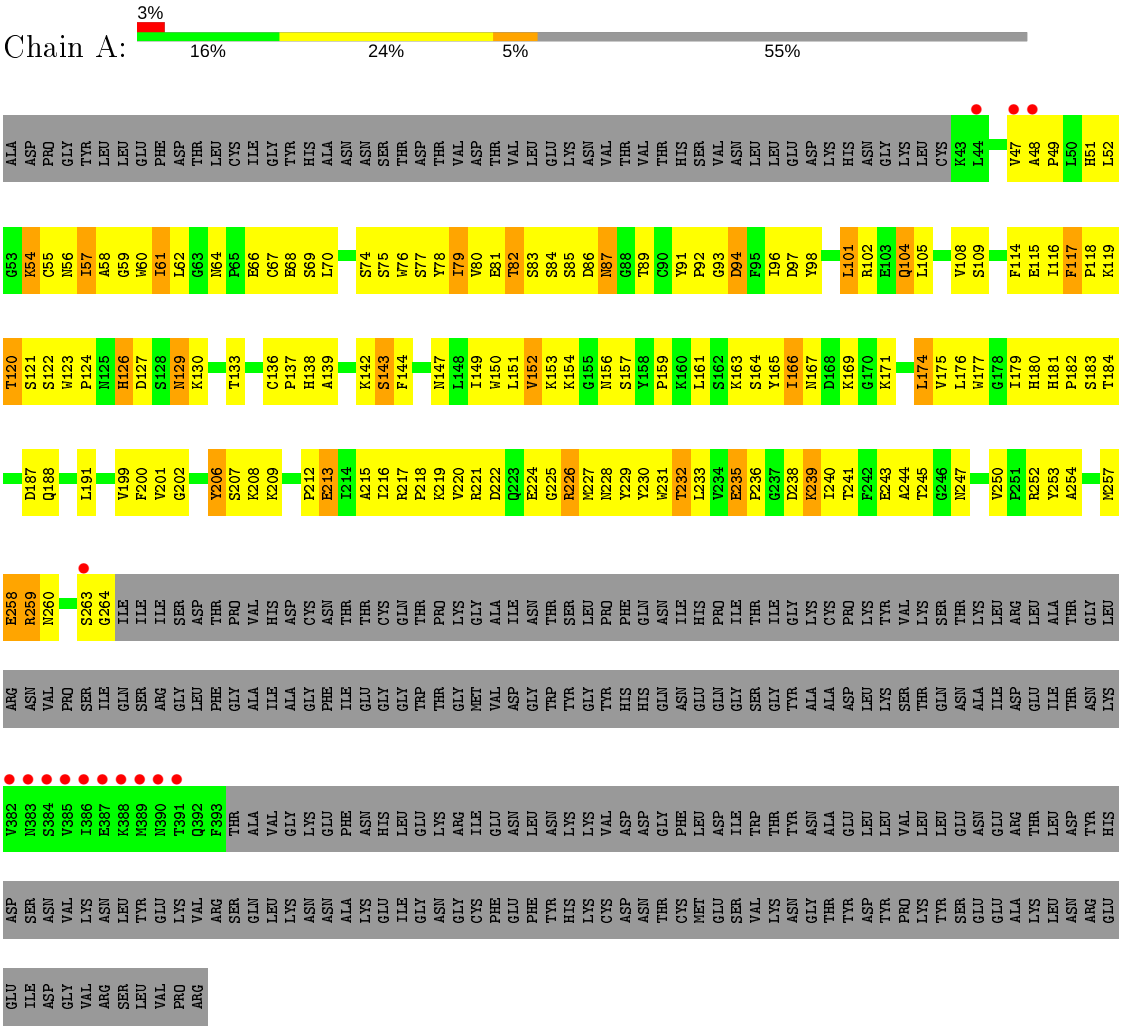
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	6	Total O 6 6	0	0
4	L	15	Total O 15 15	0	0

3 Residue-property plots (i)

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

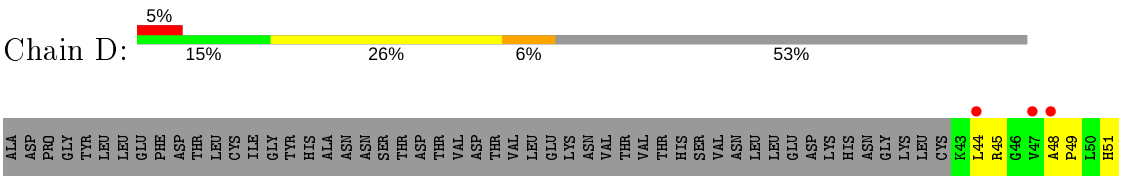
- Molecule 1: Hemagglutinin

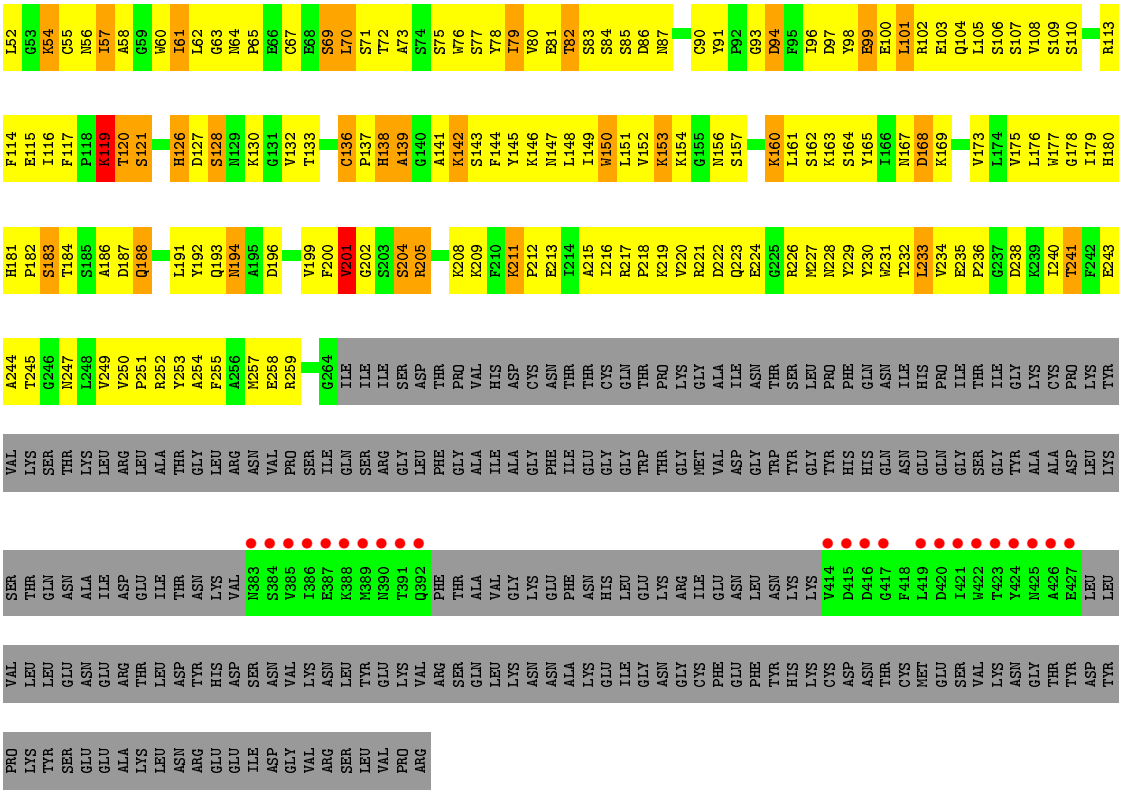
Chain A:



- Molecule 1: Hemagglutinin

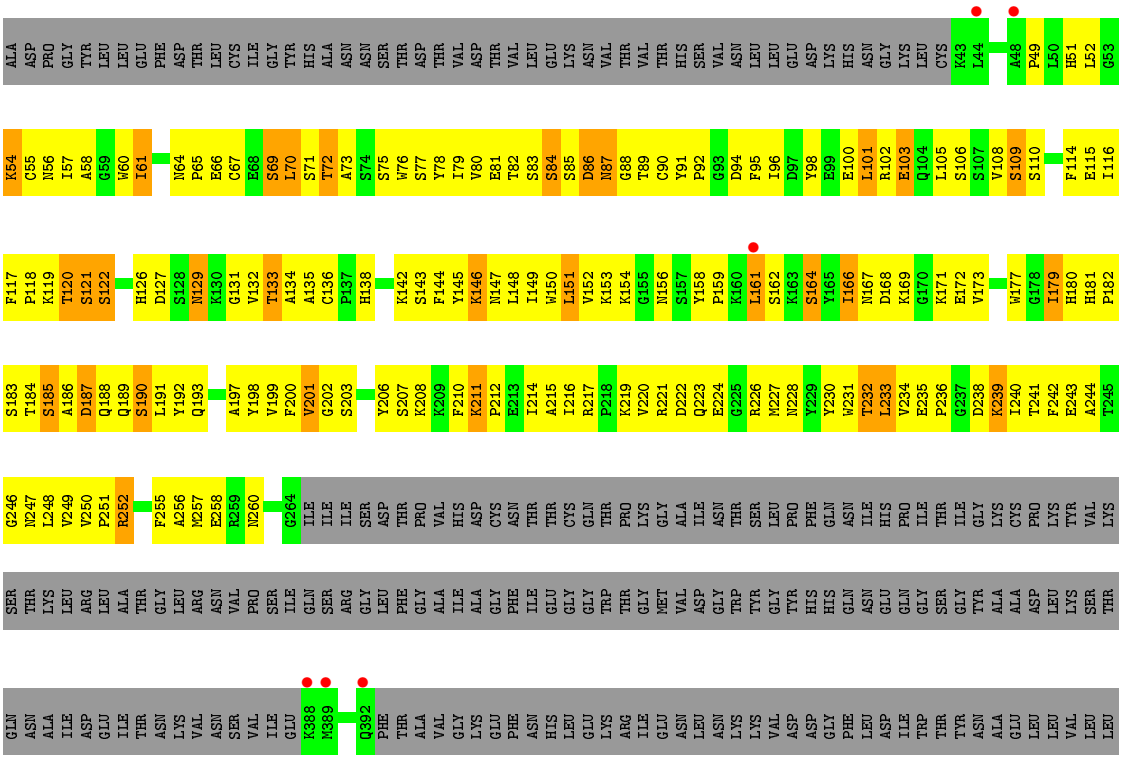
Chain D:

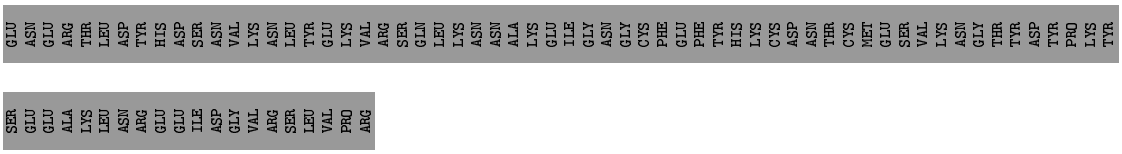




• Molecule 1: Hemagglutinin

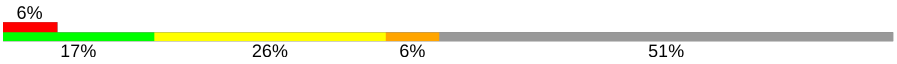
Chain G:

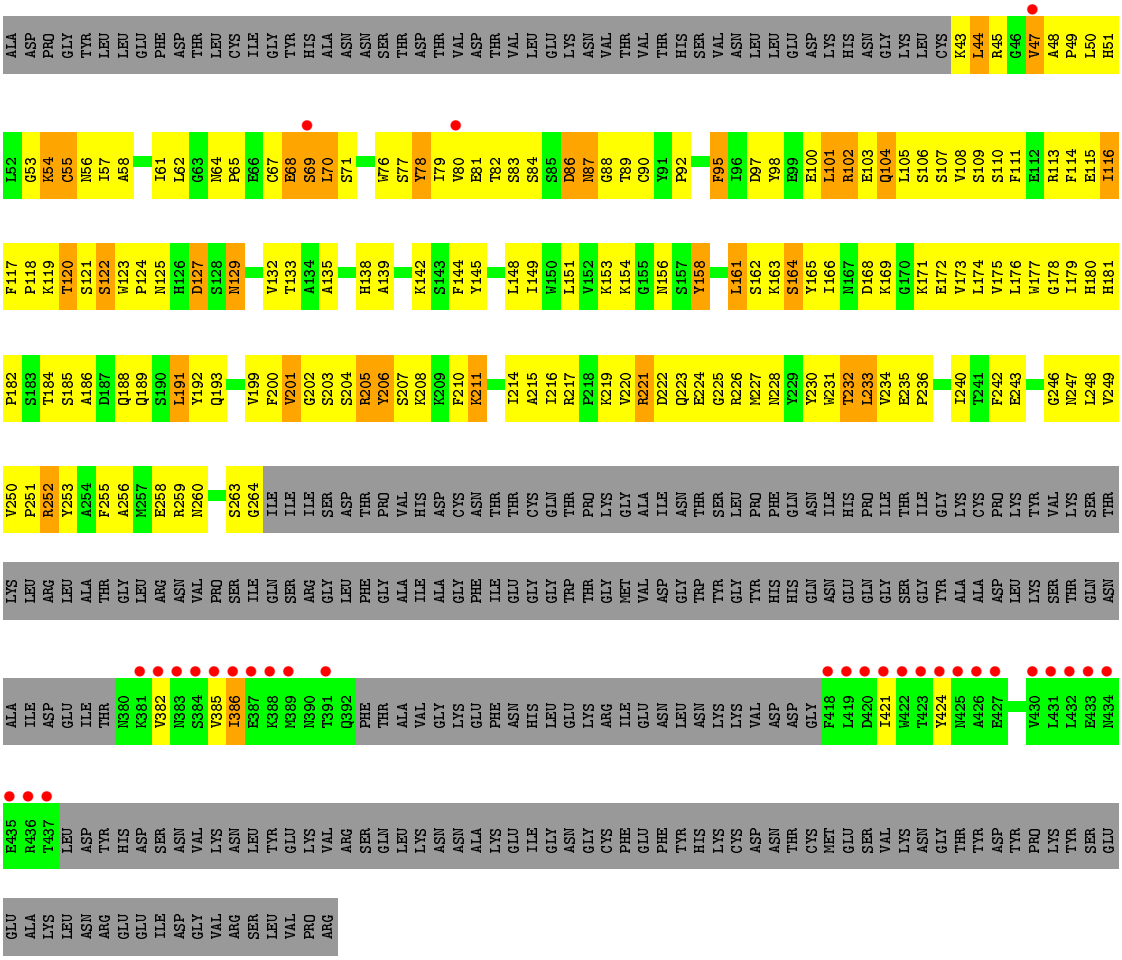




• Molecule 1: Hemagglutinin

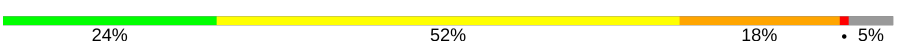
Chain J:

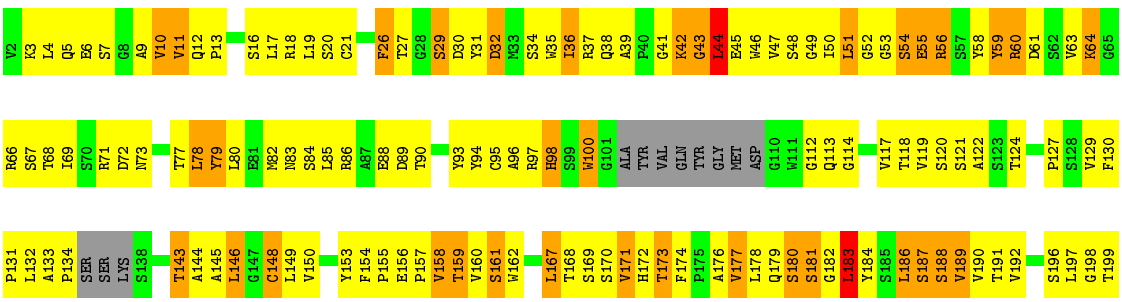


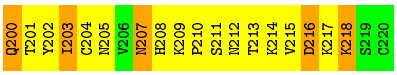


• Molecule 2: Fab fragment, heavy chain

Chain B:

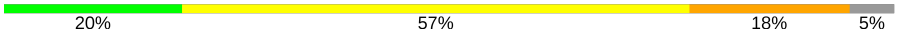


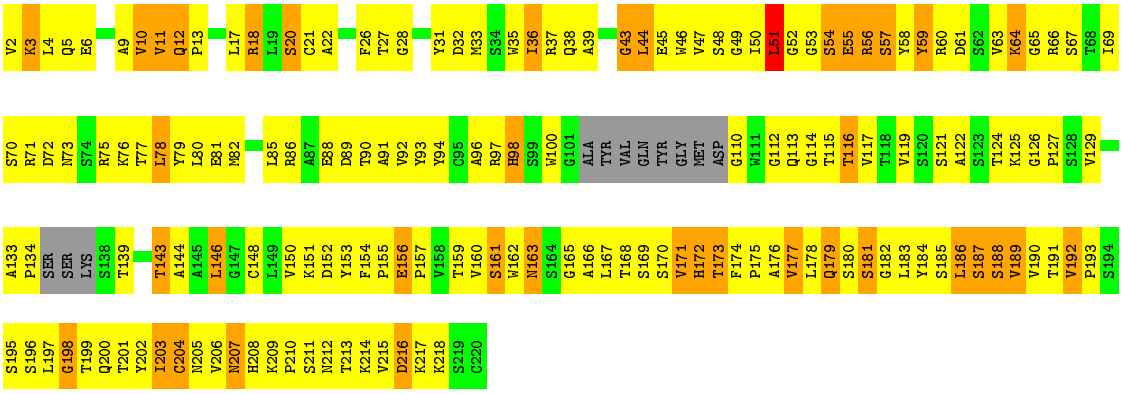




• Molecule 2: Fab fragment, heavy chain

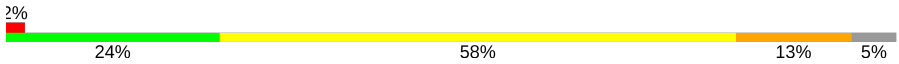
Chain E:

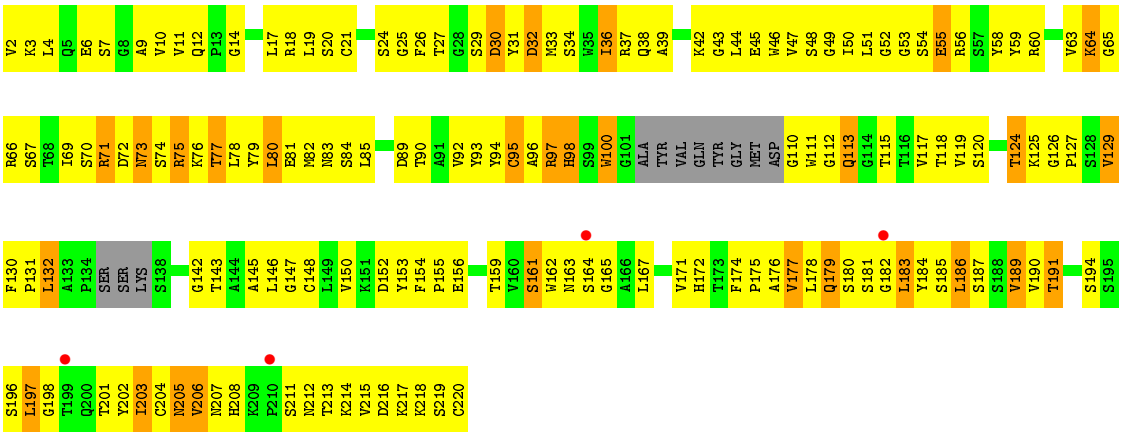




• Molecule 2: Fab fragment, heavy chain

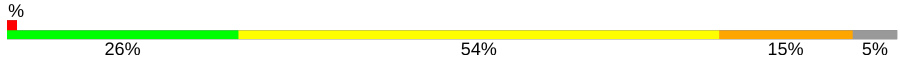
Chain H:

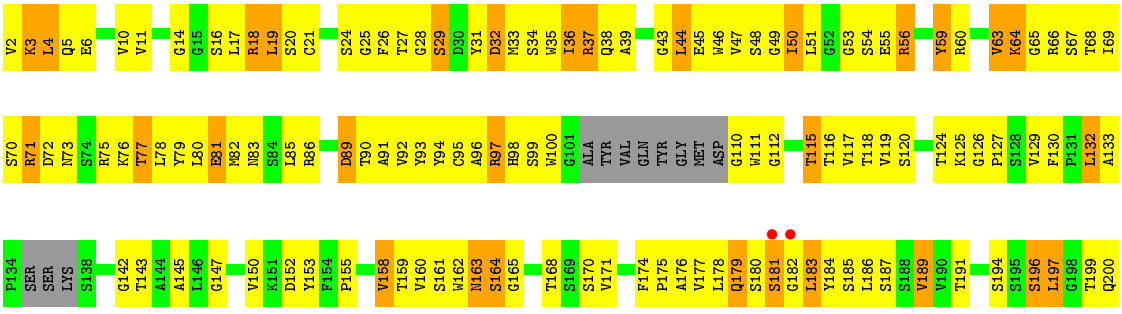


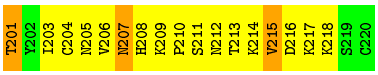


• Molecule 2: Fab fragment, heavy chain

Chain K:

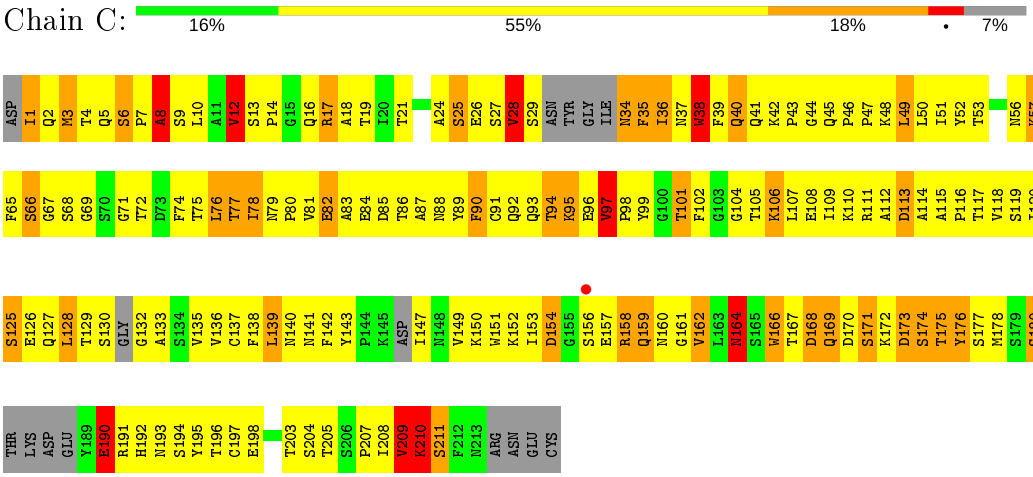






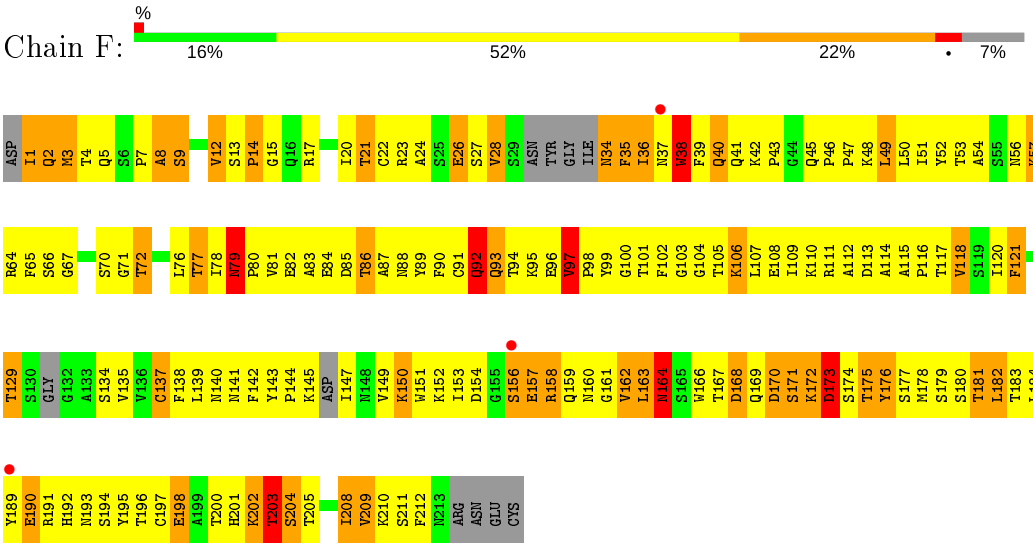
• Molecule 3: Fab fragment, light chain

Chain C:



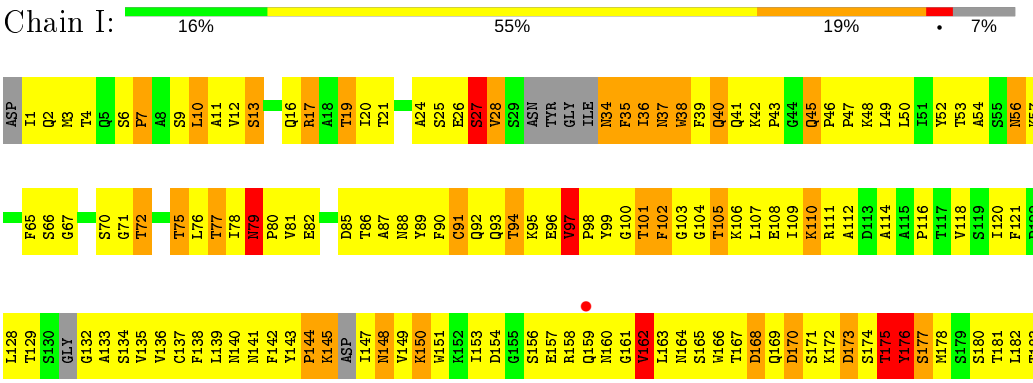
• Molecule 3: Fab fragment, light chain

Chain F:



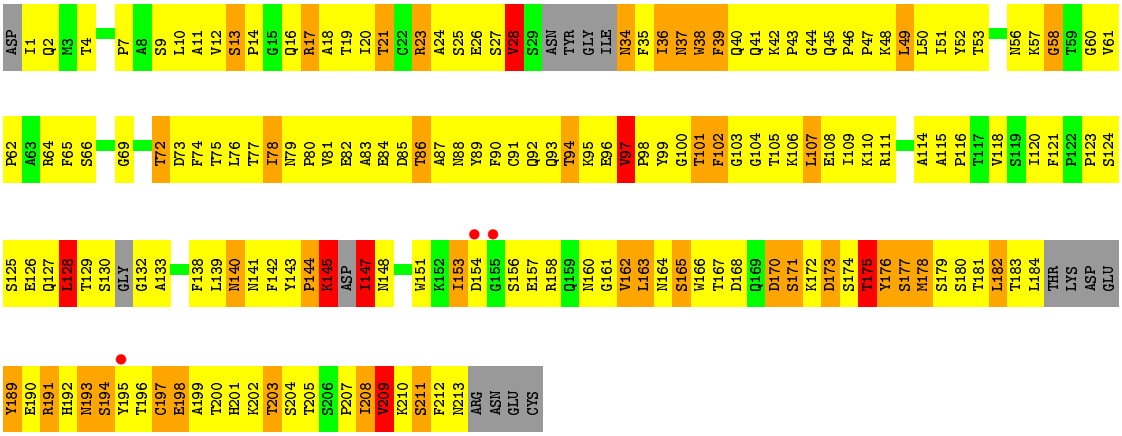
• Molecule 3: Fab fragment, light chain

Chain I:



- Molecule 3: Fab fragment, light chain

Chain L:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.46 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.233 , 0.289 0.236 , 0.295	Depositor DCC
R_{free} test set	3381 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	36.2	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 21.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
Reported twinning fraction	0.492 for h,-k,-l	Depositor
Outliers	2 of 66880 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	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 50.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1107e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 79.

All (3059) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3: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	Interatomic distance (Å)	Clash overlap (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
3:C:1:ILE:HD11	3:C:98:PRO:HB2	1.31	1.10
1:J:177:TRP:HB3	4:J:601:HOH:O	1.51	1.10
2:B:181:SER:HB2	3:L:62:PRO:HG3	1.33	1.09
3:L:38:TRP:HB2	3:L:47:PRO:HB2	1.09	1.07
3:L:45:GLN:HB3	3:L:46:PRO:HD2	1.36	1.07
3:L:140:ASN:HA	3:L:176:TYR:HB3	1.33	1.07
1:G:54:LYS:HD3	1:G:54:LYS:H	1.19	1.06
2:B:59:TYR:HE1	2:B:69:ILE:HG22	1.18	1.04
2:E:46:TRP:H	2:E:60:ARG:NH2	1.54	1.04
3:I:140:ASN:HA	3:I:176:TYR:HB3	1.35	1.04
1:D:91:TYR:HD1	1:D:227:MET:HB2	1.18	1.03
1:G:171:LYS:HD3	1:G:258:GLU:HG3	1.36	1.03
3:L:142:PHE:CZ	3:L:177:SER:HB3	1.94	1.02
1:A:202:GLY:HA3	1:A:241:THR:H	1.18	1.02
3:F:141:ASN:CA	3:F:175:THR:HG22	1.89	1.02
3:I:141:ASN:HA	3:I:175:THR:HG22	1.41	1.02
1:J:201:VAL:HG12	1:J:202:GLY:H	1.23	1.01
3:C:39:PHE:O	3:C:50:LEU:HG	1.60	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
3:C:203:THR:HG23	3:C:205:THR:H	1.28	0.99
2:E:179:GLN:HB3	3:I:60:GLY:HA2	1.40	0.99
2:K:14:GLY:N	2:K:85:LEU:O	1.94	0.99
2:H:97:ARG:HB3	2:H:110:GLY:HA3	1.44	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:142:PHE:HZ	3:L:177:SER:HB3	1.25	0.98
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
1:A:91:TYR:HD1	1:A:227:MET:HB2	1.25	0.97
1:G:119:LYS:NZ	1:G:129:ASN:HD22	1.61	0.97
3:I:100:GLY:HA3	4:I:306:HOH:O	1.62	0.97
3:C:113:ASP:OD1	3:C:115:ALA:N	1.96	0.97
2:K:32:ASP:HB2	2:K:98:HIS:HD1	1.29	0.97
1:A:149:ILE:HB	1:A:250:VAL:HG23	1.43	0.97
2:E:162:TRP:H	2:E:167:LEU:HG	1.28	0.97
1:G:217:ARG:HD3	1:G:226:ARG:HG2	1.45	0.97
3:L:145:LYS:NZ	3:L:167:THR:OG1	1.98	0.97
3:C:42:LYS:NZ	3:C:84:GLU:OE2	1.97	0.97
1:D:84:SER:O	1:D:87:ASN:N	1.97	0.97
3:F:92:GLN:HG2	3:F:101:THR:CG2	1.94	0.97
3:C:4:THR:HG22	3:C:24:ALA:HA	1.46	0.96
1:D:137:PRO:HA	1:D:142:LYS:HA	1.48	0.96
3:C:35:PHE:HE1	3:C:49:LEU:HD11	1.30	0.96
1:D:160:LYS: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
1:D:119:LYS:NZ	1:D:128:SER:O	2.01	0.94
3:I:194:SER:HB2	3:I:210:LYS:CD	1.97	0.94
2:B:162:TRP:H	2:B:167:LEU:HD11	1.32	0.94
2:B:171:VAL:HG21	3:C:176:TYR:CZ	2.02	0.94
1:G:199:VAL:HG12	1:G:200:PHE:H	1.32	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
3:F:39:PHE:O	3:F:50:LEU:HG	1.66	0.93

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:109:ILE:HG22	3:C:110:LYS:H	1.36	0.89
3:C:92:GLN:NE2	3:C:101:THR:OG1	2.05	0.89
3:C:38:TRP:CE3	3:C:40:GLN:N	2.41	0.89
3:F:8:ALA:HB1	3:F:105:THR:HG23	1.54	0.89
3:F:24:ALA:HB3	3:F:72:THR:HA	1.52	0.89
1:J:78:TYR:HB3	1:J:264:GLY:HA3	1.54	0.89
1:D:202:GLY:HA3	1:D:241:THR:H	1.37	0.89
2:H:174:PHE:CD1	2:H:175:PRO:HD2	2.06	0.89
3:L:141:ASN:HA	3:L:175:THR:CB	2.03	0.89
2:H:54:SER:HB3	2:H:56:ARG:HE	1.37	0.89
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
1:A:259:ARG:HB3	1:A:259:ARG:NH1	1.86	0.88
2:E:46:TRP:H	2:E:60:ARG:HH22	0.89	0.88
1:D:93:GLY:HA3	1:D:227:MET:O	1.74	0.88
3:F:108:GLU:HG3	3:F:109:ILE:H	1.38	0.88
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:I:159:GLN:HG3	3:I:160:ASN:H	1.39	0.87
2:K:3:LYS:H	2:K:24:SER:HB2	1.40	0.87
3:L:162:VAL:HG23	3:L:182:LEU:HG	1.57	0.87
1:A:49:PRO:HG2	1:A:77:SER:H	1.38	0.87
2:E:45:GLU:HB3	2:E:60:ARG:CZ	2.03	0.87
3:F:9:SER:HB3	3:F:106:LYS:NZ	1.89	0.87
2:H:4:LEU:HD23	2:H:95:CYS:HB3	1.53	0.87
3:L:86:THR:OG1	3:L:87:ALA:N	2.02	0.87
3:C:106:LYS:HG3	3:C:107:LEU:N	1.86	0.87
1:D:49:PRO:HB2	1:D:76:TRP:HB2	1.55	0.87
2:H:14:GLY:N	2:H:85:LEU:O	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:201:VAL:CG1	1:J:202:GLY:H	1.86	0.87
3:L:64:ARG:NH1	3:L:82:GLU:OE1	2.08	0.87
1:A:201:VAL:HG12	1:A:202:GLY:H	1.39	0.86
3:C:128:LEU:HD13	3:C:129:THR:H	1.37	0.86
3:I:27:SER:O	3:I:28:VAL:HG22	1.76	0.86
2:H:44:LEU:HG	2:H:45:GLU:H	1.37	0.86
2:E:50:ILE:HD11	2:E:71:ARG:HB2	1.56	0.86
2:K:96:ALA:HB1	3:L:36:ILE:HD12	1.57	0.86
1:A:49:PRO:HB2	1:A:76:TRP:HB2	1.58	0.86
2:E:38:GLN:HG3	2:E:43:GLY:HA2	1.57	0.86
1:D:145:TYR:OH	1:D:229:TYR:OH	1.91	0.86
3:F:8:ALA:HB1	3:F:105:THR:CG2	2.05	0.85
3:C:194:SER:HA	3:C:210:LYS:HB2	1.57	0.85
3:L:102:PHE:HD1	3:L:104:GLY:H	1.20	0.85
3:F:173:ASP:CG	3:F:175:THR:HG23	1.96	0.85
1:A:149:ILE:HB	1:A:250:VAL:CG2	2.05	0.85
3:C:170:ASP:OD2	3:C:172:LYS:N	2.10	0.85
3:C:1:ILE:HD11	3:C:98:PRO:CB	2.05	0.85
3:C:86:THR:OG1	3:C:87:ALA:N	2.05	0.85
2:E:174:PHE:O	3:F:166:TRP:CE2	2.30	0.85
2:H:176:ALA:HB2	3:I:166:TRP:CE2	2.11	0.85
3:I:173:ASP:N	3:I:173:ASP:OD1	2.05	0.85
3:I:196:THR:HA	3:I:209:VAL:HA	1.55	0.85
3:I:6:SER:HB3	3:I:7:PRO:HD2	1.55	0.85
2:K:150:VAL:HB	2:K:186:LEU:HB3	1.58	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:162:VAL:O	3:C:164:ASN:ND2	2.10	0.84
3:C:45:GLN:HB3	3:C:46:PRO:HD2	1.55	0.84
2:B:63:VAL:HG11	2:B:67:SER:HB2	1.56	0.84
3:F:170:ASP:OD2	3:F:171:SER:N	2.11	0.84
3:F:202:LYS:O	3:F:203:THR:HG23	1.76	0.84
1:A:93:GLY:HA3	1:A:227:MET:O	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:10:LEU:O	3:I:107:LEU:HA	1.78	0.84
3:C:64:ARG:NH2	3:C:85:ASP:OD1	2.09	0.84
3:C:43:PRO:HD3	3:C:87:ALA:HA	1.57	0.84
2:E:32:ASP:CB	2:E:51:LEU:HA	2.05	0.84
2:K:37:ARG:HB3	2:K:93:TYR:CE2	2.13	0.84
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.60	0.84
2:E:181:SER:HB3	3:I:62:PRO:HG3	1.60	0.84
3:F:9:SER:N	3:F:105:THR:HG23	1.93	0.84
3:F:110:LYS:HB3	3:F:110:LYS:HZ2	1.42	0.83
1:J:133:THR:O	1:J:142:LYS:HB2	1.78	0.83
1:J:54:LYS:HZ2	1:J:54:LYS:HB3	1.41	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:HD12	3:F:182:LEU:C	1.99	0.83
3:C:35:PHE:CE1	3:C:49:LEU:HD11	2.14	0.83
2:E:10:VAL:HG22	2:E:155:PRO:HG3	1.60	0.83
2:H:129:VAL:HG11	2:H:206:VAL:HG21	1.59	0.83
2:K:11:VAL:O	2:K:120:SER:N	2.11	0.83
3:C:71:GLY:O	3:C:72:THR:HG22	1.78	0.83
1:J:206:TYR:HE2	1:J:208:LYS:HB2	1.43	0.83
3:C:141:ASN:HA	3:C:175:THR:HG22	1.57	0.83
3:L:195:TYR:O	3:L:210:LYS:HA	1.77	0.83
1:J:180:HIS:O	1:J:247:ASN:ND2	2.11	0.83
3:L:184:LEU:O	3:L:189:TYR:HB2	1.78	0.82
2:B:86:ARG:HG2	2:B:89:ASP:OD2	1.79	0.82
1:J:201:VAL:HG12	1:J:202:GLY:N	1.94	0.82
1:J:58:ALA:HB2	1:J:98:TYR:CE1	2.13	0.82
1:D:148:LEU:HD23	1:D:251:PRO:HA	1.60	0.82
3:I:38:TRP:HA	3:I:48:LYS:O	1.78	0.82
1:D:153:LYS:HE3	1:D:156:ASN:HA	1.61	0.82
2:B:180:SER:HB3	3:L:62:PRO:HA	1.61	0.82
2:E:168:THR:O	2:E:169:SER:OG	1.97	0.82
2:H:146:LEU:HD11	2:H:219:SER:OG	1.78	0.82
2:H:59:TYR:CE1	2:H:69:ILE:HG22	2.14	0.82
2:K:171:VAL:HG22	3:L:176:TYR:CZ	2.14	0.82
3:L:162:VAL:O	3:L:164:ASN:ND2	2.12	0.82
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
1:D:258:GLU:HG2	1:D:259:ARG:H	1.44	0.82
2:E:45:GLU:OE1	2:E:60:ARG:NH2	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:9:SER:HA	3:F:106:LYS:H	1.45	0.82
3:C:39:PHE:HB2	3:C:50:LEU:HB2	1.62	0.82
2:K:32:ASP:HB2	2:K:98:HIS:ND1	1.95	0.82
1:A:104:GLN:HE22	1:A:233:LEU:HD22	1.45	0.81
2:K:95:CYS:O	2:K:112:GLY:N	2.12	0.81
2:K:46:TRP:O	2:K:60:ARG:HG3	1.80	0.81
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.12	0.81
3:I:193:ASN:O	3:I:211:SER:HB3	1.80	0.81
2:B:51:LEU:CD1	2:B:56:ARG:H	1.93	0.81
1:G:119:LYS:NZ	1:G:129:ASN:HB3	1.93	0.81
2:E:66:ARG:NH2	2:E:86:ARG:HD3	1.95	0.81
1:J:204:SER:HB3	4:J:603:HOH:O	1.79	0.81
3:L:128:LEU:HD12	3:L:129:THR:H	1.46	0.81
1:D:116:ILE:HG13	1:D:165:TYR:CD1	2.15	0.81
3:F:3:MET:HG3	3:F:5:GLN:HE21	1.43	0.81
2:H:203:ILE:HD11	2:H:216:ASP:HB3	1.63	0.81
3:F:158:ARG:NH2	2:H:97:ARG:HD2	1.94	0.81
3:L:42:LYS:HD3	3:L:87:ALA:HB2	1.62	0.81
3:F:158:ARG:HH22	2:H:97:ARG:CD	1.92	0.81
3:L:198:GLU:HA	3:L:207:PRO:HA	1.63	0.81
2:B:178:LEU:N	2:B:183:LEU:O	2.12	0.81
2:E:151:LYS:HG2	2:E:185:SER:OG	1.81	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
3:F:96:GLU:O	3:F:97:VAL:HG23	1.81	0.81
2:K:176:ALA:HB2	3:L:166:TRP:CE2	2.15	0.81
2:B:155:PRO:O	2:B:208:HIS:NE2	2.14	0.80
2:B:82:MET:HB3	2:B:85:LEU:HD21	1.63	0.80
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:E:178:LEU:N	2:E:183:LEU:O	2.15	0.80
3:I:116:PRO:HB2	3:I:139:LEU:HB3	1.64	0.80
2:E:51:LEU:HG	2:E:56:ARG:HB2	1.63	0.80
2:K:171:VAL:HB	2:K:189:VAL:HG22	1.62	0.80
1:D:148:LEU:HD21	1:D:176:LEU:O	1.82	0.80
2:H:207:ASN:HB3	2:H:214:LYS:HG3	1.64	0.80
3:F:116:PRO:O	3:F:140:ASN:N	2.15	0.80
2:H:100:TRP:CD1	3:I:34:ASN:HA	2.16	0.80
3:L:191:ARG:O	3:L:191:ARG:HD2	1.82	0.80
1:A:51:HIS:CE1	1:A:80:VAL:HG21	2.16	0.80
2:B:50:ILE:HD11	2:B:71:ARG:CB	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:SER:O	3:C:205:THR:HG22	1.82	0.80
2:E:60:ARG:O	2:E:64:LYS:HB2	1.82	0.79
3:C:167:THR:HG22	3:C:168:ASP:H	1.47	0.79
1:G:235:GLU:HG3	1:G:236:PRO:HD2	1.62	0.79
3:L:98:PRO:HB2	4:L:309:HOH:O	1.82	0.79
2:E:32:ASP:HA	2:E:71:ARG:NH2	1.98	0.79
3:F:166:TRP:O	3:F:177:SER:HA	1.82	0.79
2:H:34:SER:OG	2:H:49:GLY:HA3	1.81	0.79
2:H:67:SER:HA	2:H:81:GLU:O	1.83	0.79
2:K:111:TRP:CZ2	3:L:38:TRP:HB3	2.17	0.79
3:L:2:GLN:O	3:L:2:GLN:HG2	1.80	0.79
1:A:167:ASN:ND2	1:A:236:PRO:HA	1.97	0.79
2:H:197:LEU:HD12	2:H:198:GLY:N	1.98	0.79
3:F:38:TRP:NE1	3:F:40:GLN:N	2.30	0.79
3:I:170:ASP:OD2	3:I:171:SER:N	2.15	0.79
3:L:141:ASN:HA	3:L:175:THR:HB	1.65	0.79
2:H:45:GLU:HB3	2:H:60:ARG:HH11	1.48	0.79
2:K:5:GLN:O	2:K:21:CYS:HA	1.83	0.79
2:K:97:ARG:O	3:L:36:ILE:HB	1.82	0.79
3:C:116:PRO:O	3:C:140:ASN:N	2.16	0.79
1:J:120:THR:OG1	1:J:121:SER:N	2.14	0.79
3:L:162:VAL:HG21	3:L:181:THR:HA	1.65	0.79
3:C:38:TRP:CZ3	3:C:89:TYR:HA	2.18	0.78
2:E:174:PHE:O	3:F:166:TRP:NE1	2.15	0.78
1:G:138:HIS:HB2	1:G:143:SER:HB2	1.65	0.78
2:K:178:LEU:O	2:K:180:SER:N	2.16	0.78
1:A:116:ILE:HG22	1:A:252:ARG:O	1.82	0.78
1:D:160:LYS:H	1:D:160:LYS:CE	1.96	0.78
2:E:45:GLU:HB3	2:E:60:ARG:NH1	1.98	0.78
3:F:45:GLN:HB3	3:F:46:PRO:CD	2.12	0.78
1:J:84:SER:HB3	1:J:88:GLY:H	1.48	0.78
3:C:210:LYS:CD	3:C:211:SER:H	1.95	0.78
1:A:57:ILE:O	1:A:61:ILE:HG22	1.83	0.78
2:H:2:VAL:HG22	2:H:25:GLY:HA3	1.64	0.78
1:A:55:CYS:SG	1:A:66:GLU:HG3	2.24	0.78
1:G:49:PRO:HD2	1:G:77:SER:OG	1.83	0.78
1:J:49:PRO:HB2	1:J:76:TRP:HB2	1.66	0.78
2:K:111:TRP:CH2	3:L:38:TRP:HB3	2.18	0.78
2:B: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:PRO:HG2	2:H:58:TYR:CE1	2.17	0.78
3:I:1:ILE:HD11	3:I:98:PRO:HB2	1.66	0.78
1:J:119:LYS:NZ	1:J:129:ASN:HB3	1.99	0.78
3:I:37:ASN:ND2	3:I:38:TRP:N	2.32	0.78
1:D:133:THR:O	1:D:142:LYS:HB2	1.84	0.77
1:G:91:TYR:HH	1:G:180:HIS:HE2	1.33	0.77
1:G:206:TYR:HE2	1:G:208:LYS:HB2	1.49	0.77
3:C:16:GLN:HG3	3:C:17:ARG:H	1.48	0.77
3:C:24:ALA:HB3	3:C:72:THR:HA	1.65	0.77
3:C:57:LYS:HD3	3:C:61:VAL:O	1.83	0.77
1:G:153:LYS:NZ	1:G:156:ASN:HA	1.98	0.77
1:J:211:LYS:HB2	1:J:211:LYS:NZ	1.98	0.77
3:F: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
1:J:57:ILE:N	1:J:81:GLU:OE2	2.15	0.77
2:K:63:VAL:O	2:K:65:GLY:N	2.17	0.77
3:L:102:PHE:HE1	3:L:104:GLY:CA	1.98	0.77
2:K:18:ARG:HG3	2:K:81:GLU:HA	1.66	0.77
3:L:123:PRO:HB3	3:L:133:ALA:HB1	1.67	0.77
3:L:195:TYR:O	3:L:210:LYS:N	2.18	0.77
2:B:171:VAL:HG11	3:C:176:TYR:CD2	2.20	0.77
1:G:119:LYS:HZ1	1:G:129:ASN:ND2	1.81	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
2:E:32:ASP:HB3	2:E:51:LEU:CA	2.11	0.76
1:A:144:PHE:CE2	1:A:150:TRP:HB2	2.20	0.76
1:D:133:THR:HB	1:D:150:TRP:HZ3	1.48	0.76
2:E:32:ASP:HA	2:E:71:ARG:HH22	1.48	0.76
3:F:108:GLU:HG3	3:F:109:ILE:N	1.99	0.76
1:G:199:VAL:HG11	1:G:248:LEU:HD13	1.66	0.76
2:H:21:CYS:O	2:H:77:THR:HB	1.84	0.76
1:J:199:VAL:HG12	1:J:200:PHE:N	2.00	0.76
1:D:101:LEU:O	1:D:104:GLN:N	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:137:CYS:HB2	3:F:151:TRP:CZ2	2.20	0.76
3:F:183:THR:HG22	3:F:184:LEU:H	1.50	0.76
1:D:51:HIS:HA	1:D:80:VAL:HB	1.67	0.76
1:J:182:PRO:HD2	1:J:214:ILE:HG13	1.68	0.76
2:K:178:LEU:HD23	2:K:179:GLN:HB2	1.66	0.76
1:A:75:SER:HB2	1:A:109:SER:O	1.86	0.76
3:C:129:THR:O	3:C:130:SER:OG	2.04	0.76
3:I:162:VAL:HG23	3:I:164:ASN:OD1	1.85	0.76
2:K:10:VAL:HG21	2:K:155:PRO:HG3	1.66	0.76
3:C:39:PHE:HB3	3:C:50:LEU:HD12	1.67	0.76
3:I:45:GLN:NE2	3:I:46:PRO:HD3	2.00	0.76
2:K:96:ALA:HB1	3:L:36:ILE:HD11	1.68	0.76
1:A:127:ASP:OD2	1:A:130:LYS:HG2	1.86	0.76
1:D:204:SER:OG	1:D:238:ASP:OD2	2.04	0.76
3:F:182:LEU:HD12	3:F:182:LEU:O	1.86	0.76
1:G:120:THR:OG1	1:G:121:SER:N	2.16	0.76
3:F:183:THR:HG22	3:F:184:LEU:N	2.01	0.75
1:G:126:HIS:CE1	1:G:159:PRO:HD2	2.21	0.75
3:I:123:PRO:HB3	3:I:133:ALA:HB1	1.68	0.75
2:K:75:ARG:O	2:K:77:THR:HG23	1.87	0.75
3:L:163:LEU:HD12	3:L:163:LEU:C	2.06	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
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:C:38:TRP:CZ2	3:C:39:PHE:CD1	2.75	0.75
3:F:198:GLU:HG3	3:F:198:GLU:O	1.87	0.75
3:F:41:GLN:N	3:F:88:ASN:O	2.19	0.75
1:A:201:VAL:HG12	1:A:202:GLY:N	2.01	0.75
1:A:259:ARG:HB3	1:A:259:ARG:CZ	2.17	0.75
3:C:166:TRP:HE3	3:C:167:THR:H	1.33	0.75
1:G:135:ALA:HB2	1:G:223:GLN:HE21	1.52	0.75
2:K:16:SER:OG	2:K:83:ASN:OD1	2.04	0.75
2:B:11:VAL:HG11	2:B:85:LEU:HD12	1.68	0.75
2:E:196:SER:HB3	2:E:202:TYR:CE2	2.22	0.75
3:F:38:TRP: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:I:17:ARG:HB3	3:I:79:ASN:OD1	1.87	0.75
3:L:162:VAL:HG21	3:L:182:LEU:N	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:THR:HG23	2:B:155:PRO:HD2	1.67	0.75
3:F:38:TRP:C	3:F:38:TRP:CE3	2.60	0.75
1:G:49:PRO:HB2	1:G:76:TRP:HB2	1.69	0.75
2:K:11:VAL:HG21	2:K:85:LEU:HD12	1.68	0.75
3:L:39:PHE:O	3:L:89:TYR:HA	1.87	0.75
3:L:18:ALA:HB3	3:L:78:ILE:HG23	1.68	0.74
3:F:174:SER:O	3:F:175:THR:OG1	2.04	0.74
3:I:95:LYS:O	3:I:99:TYR:HE1	1.70	0.74
1:A:96:ILE:HG22	1:A:97:ASP:OD2	1.87	0.74
3:C:150:LYS:HB3	3:C:198:GLU:HG3	1.70	0.74
3:F:9:SER:HB3	3:F:106:LYS:HZ2	1.51	0.74
1:G:84:SER:O	1:G:88:GLY:N	2.19	0.74
1:J:171:LYS:NZ	1:J:258:GLU:OE2	2.20	0.74
2:B:100:TRP:HA	3:C:34:ASN:N	2.02	0.74
2:E:198:GLY:HA3	4:E:305:HOH:O	1.86	0.74
3:F:210:LYS:HG2	3:F:211:SER:H	1.51	0.74
1:J:50:LEU:HD23	1:J:79:ILE:HG12	1.68	0.74
3:F:182:LEU:HD23	4:F:302:HOH:O	1.86	0.74
3:L:42:LYS:O	3:L:44:GLY:N	2.21	0.74
3:F:93:GLN:HA	3:F:100:GLY:O	1.86	0.74
3:I:111:ARG:HE	3:I:173:ASP:HA	1.51	0.74
1:J:182:PRO:HG2	1:J:188:GLN:HB2	1.70	0.74
1:A:137:PRO:HA	1:A:143:SER:H	1.52	0.73
2:B:196:SER:HB3	2:B:202:TYR:OH	1.89	0.73
3:C:86:THR:HA	3:C:107:LEU:O	1.88	0.73
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
3:L:167:THR:HG22	3:L:168:ASP:H	1.53	0.73
3:C:38:TRP:O	3:C:39:PHE:HD2	1.69	0.73
2:E:160:VAL:O	2:E:172:HIS:NE2	2.17	0.73
3:C:18:ALA:HB3	3:C:78:ILE:HG23	1.70	0.73
3:I:116:PRO:HG3	3:I:139:LEU:HD23	1.71	0.73
3:I:37:ASN:ND2	3:I:38:TRP:H	1.86	0.73
2:E:203:ILE:HB	2:E:218:LYS:HA	1.71	0.73
2:B:180:SER:C	2:B:182:GLY:H	1.83	0.73
2:B:36:ILE:HB	2:B:46:TRP:HA	1.69	0.73
3:C:153:ILE:HG13	3:C:154:ASP:H	1.51	0.73
2:H:50:ILE:HG23	2:H:69:ILE:HD13	1.69	0.73
3:L:45:GLN:HB3	3:L:46:PRO:CD	2.16	0.73
1:A:202:GLY:HA3	1:A:241:THR:N	1.99	0.73
3:F:92:GLN:CG	3:F:101:THR:HG23	2.11	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:156:SER:O	3:L:157:GLU:HB2	1.89	0.73
2:E:46:TRP:O	2:E:60:ARG:CZ	2.36	0.73
1:J:111:PHE:CZ	1:J:255:PHE:CD1	2.76	0.73
2:K:45:GLU:CD	2:K:46:TRP:H	1.92	0.73
3:L:52:TYR:N	3:L:56:ASN:O	2.20	0.73
1:A:120:THR:OG1	1:A:121:SER:N	2.20	0.73
1:A:169:LYS:HB3	1:A:171:LYS:H	1.53	0.73
1:A:201:VAL:CG1	1:A:202:GLY:N	2.51	0.73
2:B:160:VAL:HG21	2:B:186:LEU:HD11	1.71	0.73
3:C:110:LYS:HZ2	3:C:110:LYS:HB3	1.51	0.73
1:D:137:PRO:CA	1:D:142:LYS:HA	2.17	0.73
3:L:108:GLU:HA	3:L:108:GLU:OE1	1.85	0.73
2:H:10:VAL:HG22	2:H:118:THR:HB	1.69	0.73
1:J:199:VAL:CG1	1:J:200:PHE:H	2.01	0.73
1:J:251:PRO:HG3	4:J:601:HOH:O	1.88	0.73
3:L:79:ASN:HB3	3:L:80:PRO:HD3	1.70	0.73
3:L:81:VAL:O	3:L:82:GLU:HG3	1.89	0.73
2:B:6:GLU:OE1	2:B:113:GLN:HG2	1.89	0.72
3:F:39:PHE:CD1	3:F:76:LEU:HB2	2.23	0.72
1:G:179:ILE:HD11	1:G:212:PRO:HB3	1.71	0.72
1:A:137:PRO:HA	1:A:142:LYS:HA	1.70	0.72
2:B:178:LEU:HD12	2:B:179:GLN:H	1.54	0.72
1:A:54:LYS:HG2	1:A:55:CYS:H	1.53	0.72
3:C:38:TRP:HH2	3:C:89:TYR:HB3	1.54	0.72
1:G:54:LYS:HD3	1:G:54:LYS:N	2.00	0.72
1:J:102:ARG:HG3	1:J:102:ARG:NH1	2.03	0.72
2:K:197:LEU:O	2:K:197:LEU:HD13	1.89	0.72
3:L:162:VAL:CG2	3:L:182:LEU:H	2.02	0.72
3:I:9:SER:HB3	3:I:106:LYS:HG3	1.70	0.72
3:L:170:ASP:HB3	3:L:174:SER:O	1.88	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:208:HIS:O	2:H:212:ASN:N	2.22	0.72
2:H:3:LYS:H	2:H:24:SER:HB2	1.51	0.72
1:D:109:SER:HB3	1:D:258:GLU:HB3	1.72	0.72
3:F:108:GLU:CG	3:F:109:ILE:H	2.02	0.72
2:H:97:ARG:O	3:I:36:ILE:HB	1.89	0.72
2:B:144:ALA:N	2:B:192:VAL:O	2.23	0.72
3:C:92:GLN:HG3	3:C:93:GLN:N	2.04	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:156:SER:O	3:C:157:GLU:HB2	1.87	0.71
1:J:57:ILE:HG13	1:J:81:GLU:OE2	1.89	0.71
2:K:171:VAL:HG22	3:L:176:TYR:CE2	2.26	0.71
1:A:227:MET:HG2	1:A:229:TYR:CE2	2.25	0.71
2:H:176:ALA:O	2:H:184:TYR:HA	1.89	0.71
2:B:162:TRP:N	2:B:167:LEU:HD11	2.05	0.71
3:I:168:ASP:N	3:I:168:ASP:OD1	2.21	0.71
2:K:178:LEU:HD11	3:L:182:LEU:HD13	1.72	0.71
1:A:167:ASN:OD1	1:A:169:LYS:N	2.23	0.71
2:E:156:GLU:HB2	2:E:157:PRO:HA	1.71	0.71
2:E:63:VAL:CG1	2:E:67:SER:H	2.04	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:H:72:ASP:HB3	2:H:79:TYR:CE2	2.26	0.71
3:L:17:ARG:HG2	3:L:17:ARG:O	1.90	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
1:G:79:ILE:HG22	1:G:80:VAL:N	2.05	0.71
2:H:3:LYS:N	2:H:24:SER:HB2	2.06	0.71
3: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:D:148:LEU:HD23	1:D:251:PRO:CA	2.21	0.70
1:G:115:GLU:HG2	3:I:96:GLU:HG2	1.71	0.70
3:I:142:PHE:H	3:I:175:THR:HA	1.55	0.70
2:B:127:PRO:CB	2:B:153:TYR:HB3	2.19	0.70
1:G:96:ILE:HG13	1:G:230:TYR:CE2	2.25	0.70
2:K:50:ILE:HD11	2:K:71:ARG:HG2	1.73	0.70
1:J:54:LYS:NZ	1:J:69:SER:HB3	2.06	0.70
3:L:102:PHE:HD1	3:L:103:GLY:N	1.89	0.70
1:A:115:GLU:HB2	3:C:96:GLU:HG2	1.73	0.70
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
2:E:63:VAL:HG13	2:E:66:ARG:HB2	1.73	0.70
3:F:175:THR:HB	3:F:176:TYR:CD2	2.27	0.70
2:H:153:TYR:OH	2:H:156:GLU:OE2	2.08	0.70
3:I:109:ILE:HG22	3:I:110:LYS:N	2.06	0.70
3:I:141:ASN:HA	3:I:175:THR:CB	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:33:MET:HB3	2:H:78:LEU:HD13	1.71	0.70
3:I:161:GLY:O	3:I:162:VAL:HG22	1.91	0.70
2:B:203:ILE:HG13	2:B:204:CYS:N	2.07	0.70
3:I:120:ILE:HD11	3:I:151:TRP:CH2	2.27	0.70
1:J:162:SER:HA	1:J:242:PHE:O	1.92	0.70
3:L:108:GLU:CD	3:L:109:ILE:H	1.93	0.70
2:B:6:GLU:HA	2:B:20:SER:O	1.91	0.70
3:C:210:LYS:CG	3:C:211:SER:H	2.02	0.70
3:I:111:ARG:HE	3:I:173:ASP:CA	2.05	0.70
3:L:126:GLU:N	3:L:126:GLU:OE1	2.25	0.70
3:C:35:PHE:HE1	3:C:49:LEU:CD1	2.04	0.70
2:H:6:GLU:OE2	2:H:112:GLY:HA3	1.92	0.70
1:J:201:VAL:HG13	1:J:240:ILE:HD11	1.72	0.70
1:A:55:CYS:HB2	1:A:60:TRP:HB2	1.73	0.69
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: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:K:34:SER:OG	2:K:49:GLY:HA3	1.92	0.69
3:C:97:VAL:HG13	3:C:98:PRO:HD2	1.74	0.69
2:E:51:LEU:CD1	2:E:56:ARG:H	2.05	0.69
3:F:153:ILE:HA	3:F:194:SER:O	1.92	0.69
3:F:34:ASN:N	3:F:34:ASN:HD22	1.89	0.69
2:E:53:GLY:O	2:E:54:SER:HB2	1.90	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
3:L:11:ALA:CB	3:L:108:GLU:HB3	2.21	0.69
2:B:127:PRO:CA	2:B:153:TYR:HB3	2.23	0.69
3:C:109:ILE:HG22	3:C:110:LYS:N	2.07	0.69
3:C:110:LYS:O	3:C:111:ARG:HD3	1.92	0.69
1:G:201:VAL:CG1	1:G:202:GLY:N	2.53	0.69
1:G:54:LYS:HG3	1:G:67:CYS:CA	2.11	0.69
2:H:63:VAL:C	2:H:65:GLY:H	1.95	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:HIS:HA	3:I:36:ILE:CG2	2.22	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
1:G:199:VAL:HG12	1:G:200:PHE:N	2.07	0.69
2:H:171:VAL:HG22	3:I:176:TYR:CZ	2.28	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
2:K:2:VAL:HA	2:K:24:SER:O	1.93	0.69
1:A:91:TYR:HH	1:A:180:HIS:HE2	1.38	0.69
3:C:195:TYR:H	3:C:210:LYS:CB	2.05	0.69
3:F:38:TRP:CE3	3:F:39:PHE:HA	2.28	0.69
1:G:58:ALA:HB2	1:G:98:TYR:CE1	2.28	0.69
3:C:120:ILE:HD12	3:C:208:ILE:HG22	1.73	0.69
2:K:160:VAL:HG22	2:K:206:VAL:HG22	1.75	0.69
3:C:158:ARG:HG3	2:K:31:TYR:OH	1.92	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
3:I:1:ILE:HG12	3:I:1:ILE:O	1.93	0.69
3:L:170:ASP:OD2	3:L:171:SER:N	2.26	0.69
2:B:27:THR:HG23	2:B:30:ASP:OD1	1.93	0.68
3:C:2:GLN:OE1	3:C:97:VAL:HG21	1.93	0.68
2:E:45:GLU:C	2:E:60:ARG:HH12	1.95	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:J:69:SER:OG	1:J:70:LEU:N	2.26	0.68
1:D:49:PRO:HG2	1:D:77:SER:H	1.57	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:H:44:LEU:HG	2:H:45:GLU:N	2.07	0.68
2:K:125:LYS:HD2	2:K:126:GLY:N	2.07	0.68
2:E:208:HIS:O	2:E:212:ASN:O	2.11	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
1:G:235:GLU:HG3	1:G:236:PRO:CD	2.22	0.68
3:L:36:ILE:HD13	3:L:36:ILE:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:92:PRO:HG3	1:G:223:GLN:HB2	1.75	0.68
1:J:49:PRO:HG2	1:J:77:SER:HB3	1.74	0.68
1:A:219:LYS:HG3	1:A:224:GLU:CG	2.23	0.68
2:H:162:TRP:CE3	2:H:190:VAL:HG11	2.28	0.68
3:I:38:TRP:HB2	3:I:47:PRO:CB	2.24	0.68
2:K:67:SER:HB3	2:K:80:LEU:HD11	1.76	0.68
3:C:125:SER:O	3:C:128:LEU:HD12	1.92	0.68
2:K:51:LEU:CD1	2:K:56:ARG:H	2.07	0.68
3:C:128:LEU:HD22	3:C:129:THR:N	2.09	0.68
3:C:64:ARG:O	3:C:78:ILE:HA	1.94	0.68
2:E:66:ARG:HH22	2:E:86:ARG:HD3	1.58	0.68
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:190:GLU:OE2	3:C:191:ARG:NE	2.27	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
2:H:17:LEU:HB3	2:H:82:MET:HE2	1.76	0.67
1:J:97:ASP:CB	1:J:231:TRP:HE1	2.07	0.67
2:K:33:MET:HB2	2:K:78:LEU:HD13	1.76	0.67
3:C:38:TRP:CD2	3:C:39:PHE:CA	2.68	0.67
3:C:39:PHE:HB2	3:C:50:LEU:N	2.07	0.67
3:F:64:ARG:NH2	3:F:85:ASP:OD1	2.21	0.67
1:J:133:THR:HG23	1:J:135:ALA:H	1.57	0.67
3:C:120:ILE:HG13	3:C:197:CYS:SG	2.35	0.67
2:E:156:GLU:CB	2:E:157:PRO:HA	2.25	0.67
3:F:89:TYR:O	3:F:104:GLY:HA2	1.93	0.67
1:J:220:VAL:HG12	1:J:221:ARG:HD2	1.77	0.67
3:L:208:ILE:C	3:L:209:VAL:HG12	2.14	0.67
1:A:54:LYS:H	1:A:54:LYS:HD3	1.59	0.67
2:B:174:PHE:O	3:C:166:TRP:CE2	2.47	0.67
2:B:98:HIS:HB3	3:C:36:ILE:HG13	1.75	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:G:180:HIS:O	1:G:247:ASN:ND2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:TYR:HE1	2:H:117:VAL:CG1	2.08	0.67
1:J:174:LEU:N	1:J:255:PHE:O	2.26	0.67
1:D:169:LYS:HB2	4:D:604:HOH:O	1.95	0.67
3:F:53:THR:HG22	3:F:53:THR:O	1.95	0.67
2:H:154:PHE:O	2:H:208:HIS:HE1	1.78	0.67
3:L:138:PHE:C	3:L:139:LEU:HD12	2.16	0.67
1:A:60:TRP:HA	1:A:67:CYS:SG	2.34	0.67
2:B:203:ILE:HD12	2:B:217:LYS:C	2.15	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
1:G:119:LYS:HZ1	1:G:129:ASN:HB3	1.57	0.66
1:G:57:ILE:O	1:G:61:ILE:HG22	1.95	0.66
2:H:111:TRP:CE3	3:I:47:PRO:HG2	2.30	0.66
1:J:78:TYR:HB3	1:J:264:GLY:CA	2.25	0.66
3:L:196:THR:OG1	3:L:210:LYS:HG3	1.95	0.66
1:A:179:ILE:HD11	1:A:199:VAL:HG11	1.76	0.66
1:D:162:SER:C	1:D:163:LYS:HD2	2.14	0.66
1:D:219:LYS:HG3	1:D:224:GLU:HG3	1.77	0.66
2:B:49:GLY:HA3	4:B:306:HOH:O	1.93	0.66
3:I:116:PRO:CG	3:I:139:LEU:HD23	2.24	0.66
1:J:115:GLU:H	3:L:96:GLU:HG2	1.59	0.66
2:B:181:SER:OG	3:L:84:GLU:OE2	2.14	0.66
1:A:54:LYS:HD3	1:A:54:LYS:N	2.10	0.66
3:C:150:LYS:HB3	3:C:198:GLU:CG	2.25	0.66
3:C:64:ARG:HH22	3:C:85:ASP:CG	1.98	0.66
2:E:196:SER:HB3	2:E:202:TYR:HE2	1.59	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
2:H:213:THR:HG22	2:H:213:THR:O	1.95	0.66
2:H:63:VAL:O	2:H:65:GLY:N	2.29	0.66
2:H:71:ARG:HA	2:H:78:LEU:HA	1.76	0.66
2:H:82:MET:HB3	2:H:85:LEU:HD21	1.76	0.66
3:I:6:SER:HB2	3:I:102:PHE:CE1	2.30	0.66
1:A:54:LYS:HD2	1:A:69:SER:OG	1.95	0.66
3:C:39:PHE:HB2	3:C:50:LEU:CB	2.25	0.66
1:D:97:ASP:HA	1:D:99:GLU:OE2	1.95	0.66
3:F:194:SER:HA	3:F:210:LYS:HG3	1.78	0.66
1:G:76:TRP:NE1	1:G:105:LEU:O	2.29	0.66
2:H:159:THR:HB	2:H:207:ASN:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:140:ASN:HB2	3:I:141:ASN:HD22	1.61	0.66
3:C:39:PHE:N	3:C:49:LEU:HA	2.10	0.66
1:D:258:GLU:HG2	1:D:259:ARG:N	2.10	0.66
2:H:131:PRO:HD2	3:I:126:GLU:HG3	1.77	0.66
3:I:7:PRO:HD3	3:I:21:THR:O	1.95	0.66
2:K:66:ARG:HH21	2:K:85:LEU:HA	1.61	0.66
3:I:38:TRP:CG	3:I:47:PRO:HB2	2.31	0.66
2:K:28:GLY:H	2:K:76:LYS:NZ	1.91	0.66
2:B:54:SER:HB3	2:B:56:ARG:HH11	1.59	0.66
3:F:9:SER:HA	3:F:106:LYS:HB2	1.75	0.66
3:F:158:ARG:HD3	2:H:31:TYR:CE2	2.31	0.66
2:E:171:VAL:HG23	2:E:189:VAL:HG22	1.77	0.66
2:E:28:GLY:O	2:E:71:ARG:NH1	2.29	0.66
2:E:72:ASP:OD1	2:E:75:ARG:N	2.19	0.66
3:F:210:LYS:CG	3:F:211:SER:H	2.07	0.66
2:K:27:THR:C	2:K:29:SER:N	2.48	0.66
3:L:202:LYS:O	3:L:203:THR:HG22	1.96	0.66
1:D:149:ILE:HB	1:D:250:VAL:HG23	1.78	0.66
2:E:127:PRO:CA	2:E:153:TYR:HB3	2.26	0.66
1:J:51:HIS:CD2	1:J:80:VAL:HB	2.30	0.66
2:K:178:LEU:HA	3:L:163:LEU:HD21	1.78	0.66
3:L:91:CYS:SG	3:L:102:PHE:CD2	2.82	0.66
3:F:168:ASP:OD1	3:F:176:TYR:O	2.14	0.65
3:I:116:PRO:HB3	3:I:142:PHE:CD2	2.31	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
1:A:182:PRO:HG2	1:A:188:GLN:HA	1.78	0.65
2:B:203:ILE:HB	2:B:218:LYS:HA	1.77	0.65
3:C:79:ASN:HB3	3:C:80:PRO:HD3	1.76	0.65
2:H:146:LEU:HD11	2:H:219:SER:CB	2.27	0.65
3:I:38:TRP:CG	3:I:47:PRO:CB	2.79	0.65
2:K:163:ASN:HD22	2:K:163:ASN:N	1.92	0.65
2:K:36:ILE:HB	2:K:46:TRP:HA	1.79	0.65
3:L:120:ILE:HD13	3:L:197:CYS:HB3	1.79	0.65
3:C:36:ILE:HD12	3:C:93:GLN:NE2	2.11	0.65
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
1:G:219:LYS:HG3	1:G:223:GLN:N	2.10	0.65
2:K:3:LYS:N	2:K:24:SER:HB2	2.08	0.65
3:L:110:LYS:O	3:L:111:ARG:HD3	1.97	0.65
3:C:110:LYS:NZ	3:C:110:LYS:HB3	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:196:THR:HG23	3:C:208:ILE:O	1.97	0.65
3:F:164:ASN:OD1	3:F:164:ASN:N	2.28	0.65
1:G:70:LEU:O	1:G:71:SER:OG	2.14	0.65
3:I:102:PHE:CE1	3:I:104:GLY:N	2.65	0.65
2:K:207:ASN:OD1	2:K:207:ASN:N	2.29	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:F:79:ASN:O	3:F:80:PRO:C	2.34	0.65
1:G:241:THR:HG22	1:G:242:PHE:N	2.10	0.65
1:J:84:SER:O	1:J:88:GLY:N	2.30	0.65
2:K:67:SER:HA	2:K:81:GLU:O	1.97	0.65
3:L:92:GLN:CG	3:L:101:THR:HB	2.27	0.65
3:L:111:ARG:NH2	4:L:311:HOH:O	2.29	0.65
3:L:37:ASN:ND2	3:L:93:GLN:HB2	2.12	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
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:A:126:HIS:HA	1:A:154:LYS:HG2	1.79	0.65
3:C:140:ASN:CG	3:C:176:TYR:CD1	2.70	0.65
1:D:101:LEU:HA	1:D:104:GLN:HB3	1.77	0.65
2:E:162:TRP:N	2:E:167:LEU:HG	2.08	0.65
2:H:127:PRO:HB2	2:H:150:VAL:HG13	1.76	0.65
3:I:198:GLU:HB3	3:I:207:PRO:HA	1.77	0.65
3:I:202:LYS:O	3:I:203:THR:OG1	2.11	0.65
3:L:102:PHE:CE1	3:L:104:GLY:CA	2.80	0.65
3:L:109:ILE:HG22	3:L:110:LYS:N	2.12	0.65
1:A:84:SER:O	1:A:87:ASN:N	2.22	0.65
3:C:108:GLU:HG3	3:C:109:ILE:H	1.61	0.65
2:E:63:VAL:O	2:E:65:GLY:N	2.28	0.65
2:K:210:PRO:HD2	4:K:306:HOH:O	1.97	0.65
3:L:195:TYR:O	3:L:210:LYS:CA	2.45	0.65
1:A:206:TYR:CD2	1:A:206:TYR:C	2.71	0.65
1:A:57:ILE:HG13	1:A:81:GLU:OE2	1.97	0.65
2:B:27:THR:HG22	2:B:31:TYR:HB2	1.79	0.65
1:D:162:SER:O	1:D:163:LYS:HD2	1.97	0.65
2:E:4:LEU:HD12	2:E:112:GLY:N	2.11	0.65
2:E:32:ASP:CG	2:E:98:HIS:CE1	2.70	0.65
1:G:153:LYS:HG3	1:G:191:LEU:O	1.97	0.65
3:I:120:ILE:HD11	3:I:151:TRP:CZ3	2.32	0.65
1:J:54:LYS:HZ1	1:J:69:SER:HB3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HA	1:A:104:GLN:HB3	1.78	0.64
2:E:169:SER:N	4:E:308:HOH:O	2.29	0.64
3:F:3:MET:HG2	3:F:3:MET:O	1.96	0.64
1:G:193:GLN:NE2	1:G:193:GLN:HA	2.12	0.64
1:G:206:TYR:CE2	1:G:208:LYS:HB2	2.31	0.64
1:G:169:LYS:HE2	1:G:256:ALA:HB2	1.79	0.64
3:L:102:PHE:CD1	3:L:102:PHE:C	2.70	0.64
1:D:60:TRP:HA	1:D:67:CYS:SG	2.37	0.64
3:F:140:ASN:CG	3:F:176:TYR:HD1	1.99	0.64
3:L:142:PHE:H	3:L:175:THR:HA	1.61	0.64
3:L:92:GLN:CD	3:L:101:THR:HB	2.17	0.64
1:A:118:PRO:O	1:A:122:SER:OG	2.08	0.64
1:A:166:ILE:N	1:A:166:ILE:HD12	2.13	0.64
1:D:137:PRO:HA	1:D:143:SER:H	1.61	0.64
1:G:121:SER:H	2:H:64:LYS:HE3	1.62	0.64
3:L:52:TYR:O	3:L:56:ASN:HB2	1.97	0.64
2:B:156:GLU:HB3	2:B:157:PRO:HA	1.79	0.64
2:B:197:LEU:C	2:B:199:THR:H	2.01	0.64
3:C:7:PRO:O	3:C:105:THR:OG1	2.14	0.64
1:D:153:LYS:HD2	1:D:193:GLN:HB2	1.78	0.64
1:D:54:LYS:HD2	1:D:67:CYS:HA	1.80	0.64
2:E:51:LEU:HD12	2:E:56:ARG:H	1.60	0.64
1:G:173:VAL:HA	1:G:255:PHE:O	1.98	0.64
2:B:51:LEU:HG	2:B:56:ARG:HG2	1.80	0.64
2:E:82:MET:HE1	2:E:117:VAL:HG21	1.79	0.64
3:F:152:LYS:O	3:F:196:THR:N	2.26	0.64
3:F:38:TRP:HZ2	3:F:89:TYR:HB3	1.62	0.64
1:G:211:LYS:HB2	1:G:211:LYS:NZ	2.12	0.64
3:I:2:GLN:HG2	3:I:2:GLN:O	1.98	0.64
2:K:59:TYR:CE1	2:K:69:ILE:HG22	2.32	0.64
2:B:3:LYS:C	2:B:4:LEU:HD12	2.18	0.64
3:C:38:TRP:CD1	3:C:90:PHE:O	2.50	0.64
3:C:38:TRP:CE2	3:C:39:PHE:HA	2.32	0.64
1:D:79:ILE:HD12	1:D:79:ILE:H	1.61	0.64
2:E:180:SER:O	2:E:182:GLY:N	2.30	0.64
3:I:92:GLN:NE2	3:I:101:THR:HG22	2.12	0.64
2:K:97:ARG:NE	2:K:110:GLY:HA3	2.13	0.64
3:L:34:ASN:O	3:L:95:LYS:HB3	1.98	0.64
3:I:163:LEU:O	3:I:182:LEU:HD11	1.97	0.64
3:I:16:GLN:HA	3:I:80:PRO:HA	1.79	0.64
2:K:6:GLU:OE2	2:K:112:GLY:HA3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:SER:CB	3:L:62:PRO:HG3	2.21	0.64
2:B:34:SER:O	2:B:96:ALA:N	2.30	0.64
2:E:181:SER:HB3	3:I:62:PRO:CG	2.28	0.64
2:H:45:GLU:HB3	2:H:60:ARG:NH1	2.13	0.64
1:D:91:TYR:HH	1:D:180:HIS:CD2	2.15	0.64
2:E:146:LEU:O	2:E:190:VAL:N	2.27	0.64
3:F:38:TRP:CH2	3:F:91:CYS:HA	2.32	0.64
1:G:166:ILE:HA	1:G:239:LYS:HB2	1.80	0.64
3:I:120:ILE:HD13	3:I:197:CYS:SG	2.38	0.64
3:C:158:ARG:HH22	2:K:97:ARG:HD2	1.63	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:K:45:GLU:OE2	3:L:99:TYR:O	2.15	0.64
2:B:201:THR:CG2	2:B:218:LYS:HE3	2.29	0.63
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
3:C:195:TYR:H	3:C:210:LYS:HB2	1.63	0.63
1:A:115:GLU:HB2	3:C:96:GLU:CG	2.28	0.63
2:E:49:GLY:HA3	4:E:304:HOH:O	1.98	0.63
2:H:11:VAL:O	2:H:120:SER:N	2.29	0.63
3:I:208:ILE:HG23	3:I:209:VAL:N	2.12	0.63
2:K:203:ILE:HD11	2:K:216:ASP:C	2.17	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
3:C:38:TRP:CZ3	3:C:89:TYR:CD1	2.86	0.63
2:H:18:ARG:HG3	2:H:81:GLU:HA	1.80	0.63
2:K:2:VAL:HG22	2:K:25:GLY:HA3	1.80	0.63
1:D:116:ILE:HG13	1:D:165:TYR:HD1	1.61	0.63
1:D:91:TYR:OH	1:D:180:HIS:NE2	2.32	0.63
2:E:28:GLY:H	2:E:76:LYS:NZ	1.97	0.63
2:H:178:LEU:C	2:H:180:SER:H	2.01	0.63
3:I:2:GLN:HA	3:I:25:SER:OG	1.99	0.63
3:I:66:SER:O	3:I:76:LEU:HD12	1.98	0.63
1:J:165:TYR:HE2	1:J:173:VAL:HG21	1.63	0.63
1:J:149:ILE:HB	1:J:250:VAL:HG23	1.79	0.63
3:L:141:ASN:CA	3:L:175:THR:HB	2.28	0.63
3:L:87:ALA:O	3:L:106:LYS:O	2.17	0.63
3:C:7:PRO:HG2	4:C:309:HOH:O	1.99	0.63
1:G:186:ALA:O	1:G:190:SER:OG	2.17	0.63
1:J:201:VAL:CG1	1:J:202:GLY:N	2.54	0.63
3:L:141:ASN:HA	3:L:175:THR:CG2	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:85:ASP:O	3:C:86:THR:C	2.37	0.63
3:C:92:GLN:HA	3:C:101:THR:HG23	1.81	0.63
2:E:82:MET:HE3	2:E:117:VAL:HG11	1.79	0.63
3:F:182:LEU:CD1	3:F:182:LEU:C	2.67	0.63
1:J:153:LYS:HG2	1:J:191:LEU:O	1.99	0.63
2:K:203:ILE:HD12	2:K:218:LYS:HG3	1.81	0.63
2:B:32:ASP:HA	2:B:71:ARG:NH2	2.11	0.63
3:F:41:GLN:HG2	3:F:42:LYS:N	2.14	0.63
1:G:153:LYS:CG	1:G:193:GLN:HB2	2.28	0.63
3:I:203:THR:O	3:I:205:THR:N	2.32	0.63
1:J:49:PRO:HD2	1:J:77:SER:OG	1.99	0.63
1:D:144:PHE:CZ	1:D:227:MET:HE1	2.34	0.63
2:E:89:ASP:O	2:E:93:TYR:OH	2.10	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:K:152:ASP:C	2:K:183:LEU:HD12	2.19	0.63
2:K:18:ARG:HG3	2:K:81:GLU:CA	2.28	0.63
2:K:55:GLU:HG3	2:K:71:ARG:HD2	1.80	0.63
2:B:178:LEU:HD12	2:B:179:GLN:N	2.13	0.63
2: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
2:B:161:SER:O	2:B:205:ASN:N	2.30	0.62
2:B:181:SER:HB2	3:L:62:PRO:CG	2.18	0.62
2:B:162:TRP:CZ3	2:B:204:CYS:HB3	2.34	0.62
3:F:7:PRO:O	3:F:8:ALA:HB2	1.99	0.62
2:K:97:ARG:HE	2:K:110:GLY:HA3	1.63	0.62
2:K:163:ASN:ND2	2:K:163:ASN:N	2.43	0.62
1:D:127:ASP:HB2	1:D:154:LYS:HB3	1.81	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:164:SER:OG	1:D:241:THR:HG23	1.98	0.62
1:G:188:GLN:HE22	1:G:197:ALA:CB	2.12	0.62
3:I:91:CYS:H	3:I:102:PHE:HE2	1.45	0.62
3:I:109:ILE:CG2	3:I:110:LYS:H	2.11	0.62
1:A:48:ALA:HB2	1:A:78:TYR:CZ	2.34	0.62
3:I:147:ILE:HG12	3:I:148:ASN:H	1.63	0.62
3:I:91:CYS:SG	3:I:102:PHE:HB3	2.40	0.62
3:I:132:GLY:N	3:I:184:LEU:O	2.32	0.62
3:I:196:THR:HG1	3:I:209:VAL:HG23	1.64	0.62
2:K:86:ARG:O	2:K:89:ASP:HB2	1.99	0.62
3:F:39:PHE:CE1	3:F:76:LEU:HB2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:ILE:HB	2:H:46:TRP:HA	1.81	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:H:27:THR:C	2:H:29:SER:H	2.01	0.62
3:I:156:SER:O	3:I:157:GLU:HB2	2.00	0.62
1:J:43:LYS:HB3	1:J:43:LYS:NZ	2.14	0.62
2:K:132:LEU:HD12	2:K:147:GLY:HA3	1.82	0.62
3:C:153:ILE:HG22	3:C:195:TYR:CD1	2.34	0.62
1:G:131:GLY:O	1:G:144:PHE:HB2	1.99	0.62
2:H:194:SER:O	2:H:197:LEU:N	2.19	0.62
1:J:102:ARG:HG2	1:J:103:GLU:N	2.15	0.62
3:L:28:VAL:HG23	3:L:74:PHE:HE2	1.65	0.62
3:C:86:THR:HG22	3:C:109:ILE:CD1	2.30	0.62
1:D:168:ASP:N	1:D:168:ASP:OD1	2.33	0.62
3:F:45:GLN:HB3	3:F:46:PRO:HD3	1.81	0.62
1:G:202:GLY:O	1:G:203:SER:OG	2.16	0.62
3:I: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:D:56:ASN:O	1:D:57:ILE:C	2.38	0.62
2:E:162:TRP:HB3	2:E:166:ALA:CB	2.29	0.62
3:F:35:PHE:HB3	3:F:95:LYS:HD3	1.81	0.62
1:J:118:PRO:HB2	1:J:120:THR:HG23	1.80	0.62
1:J:67:CYS:C	1:J:68:GLU:HG3	2.20	0.62
1:J:95:PHE:HB3	1:J:98:TYR:HB2	1.82	0.62
3:L:147:ILE:HG13	3:L:201:HIS:CG	2.35	0.62
1:D:215:ALA:O	1:D:217:ARG:NH1	2.32	0.61
1:D:258:GLU:O	1:D:259:ARG:HG3	1.99	0.61
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:E:98:HIS:N	2:E:98:HIS:CD2	2.67	0.61
2:H:37:ARG:NH1	2:H:93:TYR:OH	2.31	0.61
1:D:187:ASP:O	1:D:191:LEU:HD13	2.00	0.61
1:D:219:LYS:HG2	1:D:222:ASP:HA	1.80	0.61
2:E:93:TYR:O	2:E:114:GLY:HA2	2.00	0.61
3:F:150:LYS:O	3:F:198:GLU:N	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LYS:HD2	1:D:252:ARG:NH2	2.14	0.61
3:F:38:TRP:CZ3	3:F:91:CYS:HA	2.36	0.61
3:L:151:TRP:CZ2	3:L:180:SER:HA	2.36	0.61
3:L:17:ARG:NE	4:L:308:HOH:O	2.23	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
1:A:127:ASP:N	1:A:154:LYS:HB3	2.15	0.61
3:C:37:ASN:HD22	3:C:39:PHE:HE2	1.47	0.61
3:F:38:TRP:HE1	3:F:89:TYR:HA	1.66	0.61
1:G:121:SER:N	2:H:64:LYS:HE3	2.15	0.61
1:G:153:LYS:HZ3	1:G:156:ASN:HA	1.66	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:A:123:TRP:HE1	1:A:149:ILE:HD13	1.65	0.61
1:A:104:GLN:HE22	1:A:233:LEU:CD2	2.13	0.61
1:D:160:LYS:HE3	1:D:160:LYS:N	2.09	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:J:57:ILE:O	1:J:61:ILE:HG22	2.01	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
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: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
2:K:177:VAL:HG22	2:K:184:TYR:CE2	2.36	0.61
3:L:142:PHE:CD1	3:L:144:PRO:O	2.53	0.61
1:A:235:GLU:HG3	1:A:236:PRO:HD2	1.82	0.61
3:C:153:ILE:HG13	3:C:154:ASP:N	2.16	0.61
3:C:78:ILE:O	3:C:78:ILE:HG12	2.00	0.61
2:E:122:ALA:HB3	2:E:154:PHE:CZ	2.35	0.61
2:E:162:TRP:O	2:E:166:ALA:HB3	2.00	0.61
3:F:153:ILE:HG13	3:F:154:ASP:N	2.12	0.61
3:I:20:ILE:HG22	3:I:21:THR:N	2.16	0.61
2:K:63:VAL:C	2:K:65:GLY:N	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:10:VAL:CG2	2:E:155:PRO:HG3	2.30	0.61
1:G:51:HIS:HB3	4:G:604:HOH:O	1.99	0.61
1:J:184:THR:C	1:J:214:ILE:HG21	2.21	0.61
2:K:197:LEU:C	2:K:199:THR:H	2.02	0.61
3:C:109:ILE:O	3:C:143:TYR:OH	2.15	0.60
1:G:91:TYR:OH	1:G:180:HIS:NE2	2.24	0.60
2:H:51:LEU:HD11	2:H:56:ARG:CD	2.31	0.60
2:H:93:TYR:N	2:H:115:THR:O	2.32	0.60
2:K:127:PRO:CB	2:K:150:VAL:HG13	2.31	0.60
2:K:33:MET:CB	2:K:78:LEU:HD13	2.30	0.60
3:L:38:TRP:NE1	3:L:90:PHE:CD2	2.67	0.60
2:E:113:GLN:HG3	2:E:114:GLY:O	2.01	0.60
3:F:173:ASP:OD2	3:F:175:THR:HG23	2.00	0.60
2:H: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:39:PHE:O	3:I:89:TYR:HA	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:I:107:LEU:HG	3:I:107:LEU:O	2.01	0.60
3:F:107:LEU:O	3:F:107:LEU:HD23	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
3:I:164:ASN:OD1	3:I:180:SER:O	2.19	0.60
3:L:9:SER:HA	3:L:105:THR:HG23	1.82	0.60
2:B:127:PRO:HB3	2:B:153:TYR:CB	2.30	0.60
3:C:38:TRP:CE3	3:C:39:PHE:CA	2.82	0.60
3:F:38:TRP:O	3:F:39:PHE:CD2	2.53	0.60
3:F:38:TRP:HD1	3:F:40:GLN:O	1.84	0.60
2:H:51:LEU:HD11	2:H:56:ARG:H	1.66	0.60
2:H:9:ALA:O	2:H:10:VAL:HG23	2.01	0.60
3:I:193:ASN:OD1	3:I:194:SER:HB3	2.01	0.60
3:C:53:THR:HG22	3:C:53:THR:O	2.01	0.60
2:H:69:ILE:CG1	2:H:70:SER:H	2.15	0.60
1:A:169:LYS:CB	1:A:171:LYS:H	2.14	0.60
1:A:183:SER:HA	1:A:215:ALA:O	2.01	0.60
2:B:148:CYS:HB2	2:B:162:TRP:CH2	2.37	0.60
3:C:45:GLN:OE1	3:C:45:GLN:HA	2.01	0.60
2:E:207:ASN:OD1	2:E:207:ASN:N	2.34	0.60
3:F:149:VAL:HG21	3:F:179:SER:OG	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:ASP:CB	2:H:79:TYR:HE2	2.15	0.60
3:I:175:THR:HB	3:I:176:TYR:CD1	2.37	0.60
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
1:D:149:ILE:HB	1:D:250:VAL:CG2	2.31	0.60
1:D:167:ASN:ND2	1:D:236:PRO:HA	2.16	0.60
2:E:6:GLU:OE1	2:E:113:GLN:HG2	2.02	0.60
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
3:L:42:LYS:C	3:L:44:GLY:H	2.06	0.60
1:D:75:SER:OG	1:D:108:VAL:O	2.20	0.59
3:F:96:GLU:N	4:F:309:HOH:O	2.22	0.59
1:G:201:VAL:HG13	1:G:240:ILE:HD11	1.84	0.59
3:I:37:ASN:OD1	3:I:92:GLN:HB3	2.02	0.59
1:D:108:VAL:HG12	1:D:257:MET:CE	2.32	0.59
1:G:92:PRO:CG	1:G:223:GLN:HB2	2.31	0.59
3:I:199:ALA:HB3	3:I:206:SER:HB3	1.84	0.59
1:J:97:ASP:HB2	1:J:231:TRP:NE1	2.18	0.59
2:B:180:SER:C	2:B:182:GLY:N	2.50	0.59
3:C:169:GLN:HA	3:C:169:GLN:OE1	2.02	0.59
3:I:93:GLN:HA	3:I:100:GLY:O	2.02	0.59
3:I:102:PHE:CE1	3:I:104:GLY:CA	2.86	0.59
3:I:20:ILE:HG22	3:I:21:THR:H	1.66	0.59
3:I:38:TRP:CB	3:I:47:PRO:CB	2.75	0.59
1:G:72:THR:HG21	3:I:70:SER:OG	2.03	0.59
1:J:84:SER:HB3	1:J:87:ASN:HB2	1.84	0.59
1:J:97:ASP:HB2	1:J:231:TRP:HE1	1.66	0.59
3:L:141:ASN:HA	3:L:175:THR:HG22	1.82	0.59
1:A:48:ALA:HB2	1:A:78:TYR:CE2	2.38	0.59
1:D:58:ALA:O	1:D:62:LEU:HB2	2.01	0.59
2:E:127:PRO:HB3	2:E:153:TYR:CD2	2.38	0.59
2:E:178:LEU:O	2:E:180:SER:HB2	2.02	0.59
3:F:39:PHE:H	3:F:50:LEU:H	1.47	0.59
2:H:100:TRP:CD1	3:I:34:ASN:CA	2.85	0.59
2:H:38:GLN:HG3	2:H:43:GLY:HA2	1.84	0.59
1:J:235:GLU:CG	1:J:236:PRO:HD2	2.27	0.59
2:K:125:LYS:HE3	2:K:126:GLY:O	2.03	0.59
2:K:55:GLU:CG	2:K:71:ARG:HD2	2.32	0.59
2:B:168:THR:O	2:B:169:SER:OG	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:SER:O	3:C:205:THR:CG2	2.50	0.59
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.82	0.59
2:E:152:ASP:HB3	2:E:183:LEU:HD23	1.84	0.59
2:K:4:LEU:HD23	2:K:95:CYS:O	2.03	0.59
1:A:58:ALA:HB2	1:A:98:TYR:CE1	2.38	0.59
3:C:210:LYS:CG	3:C:211:SER:N	2.65	0.59
3:F:36:ILE:H	3:F:93:GLN:NE2	2.00	0.59
1:G:132:VAL:HB	1:G:142:LYS:O	2.02	0.59
1:G:179:ILE:HG12	1:G:180:HIS:N	2.18	0.59
3:L:89:TYR:O	3:L:102:PHE:CZ	2.55	0.59
2:B:161:SER:OG	2:B:205:ASN:HB2	2.02	0.59
3:C:108:GLU:HG3	3:C:109:ILE:N	2.18	0.59
1:D:153:LYS:HG2	1:D:153:LYS:O	1.99	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
1:G:69:SER:OG	1:G:70:LEU:HB2	2.02	0.59
2:H:27:THR:CG2	2:H:31:TYR:HD2	2.15	0.59
3:I:2:GLN:OE1	3:I:94:THR:HG21	2.03	0.59
3:L:96:GLU:O	3:L:97:VAL:HB	2.02	0.59
1:A:49:PRO:HB2	1:A:76:TRP:CB	2.32	0.59
2:B:10:VAL:HG22	2:B:155:PRO:HG3	1.85	0.59
2:B:53:GLY:O	2:B:54:SER:HB2	2.03	0.59
3:C:45:GLN:HB3	3:C:46:PRO:CD	2.30	0.59
3:C:97:VAL:HG12	3:C:98:PRO:O	2.03	0.59
1:D:228:ASN:HB3	1:D:230:TYR:CE1	2.37	0.59
2:E:21:CYS:O	2:E:77:THR:HA	2.03	0.59
3:F:110:LYS:O	3:F:111:ARG:HG3	2.03	0.59
1:G:193:GLN:HE21	1:G:193:GLN:HA	1.68	0.59
1:J:153:LYS:HB3	1:J:158:TYR:HB2	1.85	0.59
3:C:39:PHE:HB3	3:C:50:LEU:HB2	1.82	0.59
3:F:23:ARG:CG	3:F:72:THR:O	2.50	0.59
1:G:182:PRO:HG2	1:G:188:GLN:HB2	1.85	0.59
3:I:149:VAL:HG23	3:I:150:LYS:N	2.17	0.59
1:J:54:LYS:HE3	1:J:67:CYS:HA	1.84	0.59
2:B:10:VAL:CG2	2:B:155:PRO:HG3	2.33	0.59
3:C:140:ASN:OD1	3:C:176:TYR:HB3	2.02	0.59
3:C:38:TRP:CG	3:C:90:PHE:O	2.56	0.59
1:G:134:ALA:N	1:G:142:LYS:HD2	2.18	0.59
2:H:163:ASN:O	2:H:164:SER:OG	2.20	0.59
2:K:203:ILE:HG13	2:K:217:LYS:O	2.02	0.59
3:L:167:THR:HG22	3:L:168:ASP:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ASP:N	1:A:94:ASP:OD1	2.34	0.58
1:D:219:LYS:HD2	1:D:222:ASP:OD1	2.03	0.58
1:G:118:PRO:HB3	1:G:120:THR:HG23	1.84	0.58
2:H:34:SER:CB	2:H:98:HIS:NE2	2.65	0.58
3:I:208:ILE:HG23	3:I:209:VAL:H	1.68	0.58
1:J:221:ARG:O	1:J:223:GLN:HG2	2.03	0.58
2:B:86:ARG:HG3	2:B:88:GLU:OE1	2.03	0.58
1:D:181:HIS:ND1	1:D:212:PRO:HA	2.18	0.58
1:D:51:HIS:ND1	1:D:80:VAL:HG11	2.17	0.58
3:F:158:ARG:HG3	3:F:159:GLN:H	1.68	0.58
3:F:34:ASN:N	3:F:34:ASN:ND2	2.51	0.58
1:G:201:VAL:HG13	1:G:202:GLY:H	1.67	0.58
1:J:120:THR:O	1:J:122:SER:N	2.35	0.58
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:L:162:VAL:CG2	3:L:182:LEU:HG	2.32	0.58
3:C:193:ASN:O	3:C:211:SER:HB3	2.04	0.58
1:D:94:ASP:HB2	1:D:228:ASN:OD1	2.04	0.58
2:E:129:VAL:HG13	2:E:150:VAL:HG22	1.83	0.58
3:F:114:ALA:HA	3:F:201:HIS:CD2	2.39	0.58
3:F:192:HIS:O	3:F:195:TYR:OH	2.13	0.58
3:F:39:PHE:O	3:F:40:GLN:HB2	2.03	0.58
1:G:131:GLY:HA3	1:G:150:TRP:HB3	1.85	0.58
1:G:180:HIS:O	1:G:182:PRO:HD3	2.03	0.58
2:H:33:MET:CB	2:H:78:LEU:HD13	2.33	0.58
2:H:92:VAL:HA	2:H:115:THR:O	2.03	0.58
2:H:132:LEU:HB3	3:I:121:PHE:CD1	2.39	0.58
3:I:162:VAL:O	3:I:164:ASN:CG	2.41	0.58
2:B:127:PRO:HA	2:B:153:TYR:HB3	1.85	0.58
3:C:113:ASP:O	3:C:143:TYR:O	2.21	0.58
2:E:160:VAL:HG22	2:E:206:VAL:HG22	1.85	0.58
3:F:20:ILE:HG12	3:F:105:THR:HG21	1.85	0.58
3:I:167:THR:HG22	3:I:168:ASP:H	1.67	0.58
1:J:48:ALA:CB	1:J:78:TYR:CE1	2.86	0.58
3:C:158:ARG:HG3	2:K:31:TYR:CZ	2.38	0.58
2:K:66:ARG:NH2	2:K:85:LEU:HA	2.18	0.58
3:L:140:ASN:HB2	3:L:141:ASN:HD22	1.69	0.58
3:L:94:THR:O	3:L:99:TYR:HD1	1.86	0.58
3:C:159:GLN:HG3	3:C:160:ASN:H	1.67	0.58
2:B:176:ALA:HB2	3:C:166:TRP:CZ2	2.38	0.58
2:E:67:SER:HA	2:E:81:GLU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:150:LYS:HE3	3:F:150:LYS:HA	1.85	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
1:G:199:VAL:HG13	1:G:244:ALA:HB2	1.86	0.58
2:H:171:VAL:HG22	3:I:176:TYR:CE2	2.37	0.58
2:B:197:LEU:HG	2:B:198:GLY:N	2.19	0.58
1:G:187:ASP:O	1:G:191:LEU:HD13	2.03	0.58
3:L:193:ASN:O	3:L:211:SER:OG	2.19	0.58
1:A:76:TRP:CZ3	1:A:108:VAL:HG21	2.39	0.58
2:B:171:VAL:CG2	3:C:176:TYR:CZ	2.83	0.58
1:D:51:HIS:CE1	1:D:80:VAL:HG21	2.39	0.58
2:E:59:TYR:CE1	2:E:69:ILE:HG22	2.38	0.58
2:E:59:TYR:HE1	2:E:69:ILE:HG22	1.67	0.58
2:H:208:HIS:N	2:H:212:ASN:O	2.36	0.58
3:I:72:THR:O	3:I:72:THR:HG23	2.04	0.58
1:J:199:VAL:CG1	1:J:200:PHE:N	2.64	0.58
1:A:177:TRP:CE2	1:A:230:TYR:HB2	2.39	0.58
2:B:157:PRO:O	2:B:208:HIS:HD2	1.87	0.58
3:C:106:LYS:CG	3:C:107:LEU:N	2.65	0.58
3:C:38:TRP:CZ3	3:C:89:TYR:CA	2.87	0.58
3:F:145:LYS:HD2	3:F:167:THR:HG21	1.84	0.58
3:F:71:GLY:O	3:F:72:THR:HG22	2.04	0.58
1:J:100:GLU:HG2	1:J:231:TRP:HZ2	1.68	0.58
3:L:102:PHE:HD1	3:L:102:PHE:C	2.06	0.58
3:L:20:ILE:HG22	3:L:21:THR:N	2.17	0.58
1:D:138:HIS:O	1:D:139:ALA:C	2.41	0.58
2:E:171:VAL:HG11	3:F:176:TYR:CD2	2.39	0.58
3:F:151:TRP:CZ3	3:F:197:CYS:HB3	2.38	0.58
3:I:102:PHE:CD1	3:I:103:GLY:N	2.71	0.58
1:J:119:LYS:HZ2	1:J:129:ASN:HB3	1.68	0.58
2:K:209:LYS:O	2:K:212:ASN:N	2.26	0.58
2:K:36:ILE:O	2:K:36:ILE:HG13	2.03	0.58
1:A:104:GLN:O	1:A:104:GLN:HG3	2.04	0.58
2:B:160:VAL:O	2:B:172:HIS:NE2	2.36	0.58
2:B:63:VAL:HG13	2:B:67:SER:H	1.69	0.58
2:E:200:GLN:HG2	2:E:202:TYR:CE2	2.39	0.58
2:H:34:SER:OG	2:H:98:HIS:CE1	2.56	0.58
2:K:28:GLY:HA2	4:K:301:HOH:O	2.04	0.58
3:L:14:PRO:HG3	3:L:111:ARG:NH1	2.19	0.58
3:L:62:PRO:HG2	3:L:65:PHE:CD2	2.38	0.58
1:A:165:TYR:O	1:A:239:LYS:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:VAL:HG22	2:E:12:GLN:O	2.03	0.57
1:G:231:TRP:HZ3	1:G:233:LEU:HD13	1.68	0.57
1:J:114:PHE:HA	3:L:96:GLU:OE1	2.04	0.57
1:J:158:TYR:CZ	1:J:246:GLY:HA2	2.39	0.57
2:B:29:SER:HA	2:B:73:ASN:HD22	1.69	0.57
1:D:202:GLY:HA3	1:D:241:THR:N	2.16	0.57
3:F:13:SER:HB3	3:F:110:LYS:HD3	1.84	0.57
1:J:118:PRO:HB2	1:J:120:THR:CG2	2.34	0.57
1:J:48:ALA:HB2	1:J:78:TYR:CE1	2.38	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
3:C:157:GLU:O	2:K:27:THR:HG21	2.03	0.57
1:D:126:HIS:HA	1:D:154:LYS:HG2	1.85	0.57
3:F:126:GLU:N	3:F:126:GLU:OE1	2.38	0.57
1:G:242:PHE:CE1	1:G:251:PRO:HG2	2.39	0.57
3:I:37:ASN:O	3:I:49:LEU:HB2	2.04	0.57
3:F:108:GLU:C	3:F:109:ILE:HD12	2.25	0.57
1:J:123:TRP:HZ3	1:J:163:LYS:HG3	1.70	0.57
3:L:94:THR:O	3:L:99:TYR:CD1	2.58	0.57
2:B:45:GLU:CD	2:B:46:TRP:N	2.58	0.57
1:A:121:SER:HB2	2:B:58:TYR:HD1	1.68	0.57
3:F:45:GLN:CB	3:F:46:PRO:CD	2.82	0.57
2:H:208:HIS:ND1	2:H:211:SER:OG	2.35	0.57
2:B:63:VAL:CG1	2:B:67:SER:HB2	2.30	0.57
3:C:203:THR:HG23	3:C:205:THR:N	2.10	0.57
3:C:38:TRP:CH2	3:C:89:TYR:CB	2.87	0.57
1:D:57:ILE:CD1	1:D:102:ARG:HG3	2.34	0.57
1:G:119:LYS:NZ	1:G:129:ASN:ND2	2.40	0.57
2:H:145:ALA:HB2	2:H:191:THR:HG23	1.85	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
3:C:138:PHE:CE1	3:C:178:MET:HG2	2.38	0.57
3:C:38:TRP:CE2	3:C:90:PHE:O	2.58	0.57
1:G:219:LYS:HA	1:G:223:GLN:O	2.05	0.57
2:H:177:VAL:HG12	2:H:182:GLY:HA2	1.87	0.57
3:I:106:LYS:O	3:I:107:LEU:HB3	2.05	0.57
3:I:209:VAL:HG22	3:I:210:LYS:CG	2.35	0.57
1:J: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
2:B:190:VAL:HG22	2:B:192:VAL:HG23	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:TRP:HE1	2:B:78:LEU:HD13	1.69	0.57
3:C:52:TYR:O	3:C:56:ASN:HB2	2.05	0.57
3:C:64:ARG:NH2	3:C:85:ASP:CG	2.56	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:227:MET:SD	1:J:249:VAL:HG21	2.44	0.57
1:J:51:HIS:HD2	1:J:80:VAL:HB	1.70	0.57
3:L:141:ASN:HA	3:L:175:THR:CA	2.35	0.57
3:L:28:VAL:HG23	3:L:74:PHE:CE2	2.40	0.57
2:B:32:ASP:HB3	2:B:51:LEU:CA	2.18	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:177:VAL:HG12	2:H:182:GLY:CA	2.35	0.57
2:H:69:ILE:HG12	2:H:70:SER:N	2.19	0.57
2:B:180:SER:HB3	3:L:62:PRO:CA	2.33	0.57
2:B:174:PHE:O	3:C:166:TRP:NE1	2.38	0.57
3:C:4:THR:O	3:C:102:PHE:HB2	2.05	0.57
3:C:90:PHE:N	3:C:90:PHE:CD2	2.72	0.57
1:D:57:ILE:O	1:D:61:ILE:HG22	2.04	0.57
3:F:2:GLN:CD	3:F:97:VAL:HG21	2.24	0.57
1:G:89:THR:HB	1:G:145:TYR:OH	2.05	0.57
2:H:49:GLY:HA3	4:H:302:HOH:O	2.03	0.57
3:I:6:SER:CB	3:I:7:PRO:HD2	2.25	0.57
2:B:61:ASP:HB3	2:K:142:GLY:O	2.04	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
3:L:20:ILE:HG22	3:L:21:THR:H	1.70	0.57
1:A:52:LEU:HD12	1:A:81:GLU:HG3	1.86	0.56
2:B:45:GLU:CD	2:B:46:TRP:H	2.08	0.56
2:B:173:THR:CB	3:C:178:MET:HE3	2.32	0.56
3:C:38:TRP:NE1	3:C:91:CYS:HA	2.19	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
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:O	3:I:162:VAL:HG23	2.04	0.56
1:A:147:ASN:HD22	1:A:253:TYR:HB2	1.70	0.56
2:B:10:VAL:CG1	2:B:155:PRO:HG3	2.35	0.56
2:B:134:PRO:HD3	2:B:146:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:142:PHE:H	3:F:175:THR:HA	1.70	0.56
3:F:167:THR:HG22	3:F:168:ASP:N	2.20	0.56
3:F:183:THR:CG2	3:F:184:LEU:H	2.17	0.56
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:B:122:ALA:HB3	2:B:154:PHE:CE2	2.41	0.56
2:E:178:LEU:O	2:E:179:GLN:C	2.42	0.56
1:G:144:PHE:CG	1:G:145:TYR:N	2.73	0.56
2:H:178:LEU:O	2:H:180:SER:N	2.38	0.56
3:I:159:GLN:CG	3:I:160:ASN:N	2.64	0.56
1:A:161:LEU:HD23	1:A:161:LEU:C	2.25	0.56
1:A:239:LYS:O	1:A:239:LYS:HG3	2.06	0.56
2:B:207:ASN:N	2:B:207:ASN:OD1	2.38	0.56
2:E:173:THR:HG21	3:F:178:MET:HG2	1.86	0.56
2:K:110:GLY:N	4:K:304:HOH:O	2.37	0.56
2:K:150:VAL:O	2:K:186:LEU:N	2.28	0.56
1:A:225:GLY:O	1:A:226:ARG:HD3	2.06	0.56
2:B:211:SER:O	2:B:212:ASN:HB3	2.05	0.56
3:C:140:ASN:HA	3:C:176:TYR:HA	1.88	0.56
3:F:151:TRP:CH2	3:F:197:CYS:HB3	2.40	0.56
1:G:92:PRO:HD2	1:G:223:GLN:HG3	1.88	0.56
2:H:98:HIS:HA	3:I:36:ILE:HG21	1.87	0.56
1:J:116:ILE:HG23	1:J:252:ARG:O	2.05	0.56
2:K:34:SER:OG	2:K:98:HIS:CE1	2.59	0.56
3:L:45:GLN:CB	3:L:46:PRO:HD2	2.23	0.56
3:L:49:LEU:HD23	3:L:50:LEU:H	1.71	0.56
3:C:162:VAL:HG11	3:C:182:LEU:O	2.06	0.56
3:C:9:SER:HA	3:C:105:THR:HG23	1.86	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:I:195:TYR:N	3:I:210:LYS:HA	2.21	0.56
3:I:6:SER:CB	3:I:102:PHE:CE1	2.89	0.56
3:L:162:VAL:HG21	3:L:181:THR:CA	2.35	0.56
3:L:142:PHE:N	3:L:175:THR:HA	2.20	0.56
3:L:50:LEU:O	3:L:58:GLY:N	2.30	0.56
2:B:162:TRP:CD1	2:B:170:SER:OG	2.56	0.56
2:B:171:VAL:HG21	3:C:176:TYR:CD1	2.37	0.56
3:C:36:ILE:O	3:C:93:GLN:HG3	2.06	0.56
2:E:203:ILE:HD11	2:E:216:ASP:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:L:198:GLU:HB3	3:L:207:PRO:HB3	1.88	0.56
2:B:178:LEU:O	2:B:180:SER:N	2.39	0.56
3:C:64:ARG:NH2	3:C:82:GLU:H	2.03	0.56
3:F:109:ILE:HG22	3:F:110:LYS:N	2.21	0.56
3:F:118:VAL:HB	3:F:208:ILE:HD13	1.87	0.56
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
2:B:11:VAL:O	2:B:120:SER:N	2.37	0.56
3:C:128:LEU:HD13	3:C:129:THR:HG23	1.87	0.56
2:E:36:ILE:HD12	2:E:45:GLU:C	2.26	0.56
2:B:12:GLN:HG3	2:B:121:SER:HA	1.88	0.56
3:I:118:VAL:HG22	3:I:139:LEU:HG	1.88	0.56
2:B:32:ASP:CB	2:B:50:ILE:O	2.54	0.55
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
1:G:84:SER:O	1:G:87:ASN:N	2.37	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
2:B:182:GLY:O	2:B:183:LEU:HB2	2.06	0.55
3:C:150:LYS:O	3:C:198:GLU:HG2	2.07	0.55
1: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
2:B:63:VAL:CG1	2:B:67:SER:H	2.19	0.55
3:C:166:TRP:O	3:C:177:SER:HA	2.07	0.55
1:D:48:ALA:HB3	1:D:51:HIS:CE1	2.42	0.55
1:G:52:LEU:HD12	1:G:81:GLU:HB3	1.87	0.55
2:H:34:SER:OG	2:H:98:HIS:NE2	2.39	0.55
2:K:207:ASN:HA	2:K:213:THR:O	2.06	0.55
1:A:144:PHE:CZ	1:A:227:MET:HE1	2.42	0.55
1:A:56:ASN:O	1:A:57:ILE:C	2.43	0.55
1:D:101:LEU:CD2	1:D:105:LEU:HG	2.37	0.55
2:E:186:LEU:HG	2:E:187:SER:N	2.20	0.55
2:E:18:ARG:HD2	2:E:79:TYR:HB3	1.89	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:102:PHE:HE1	3:L:104:GLY:C	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:102:PHE:CE1	3:L:104:GLY:N	2.73	0.55
3:L:116:PRO:O	3:L:140:ASN:N	2.36	0.55
3:L: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
3:L:205:THR:O	3:L:207:PRO:HD3	2.06	0.55
3:C:110:LYS:C	3:C:111:ARG:HD3	2.27	0.55
3:C:153:ILE:CG1	3:C:154:ASP:H	2.20	0.55
2:H:97:ARG:O	3:I:36:ILE:CB	2.55	0.55
3:I:79:ASN:HB3	3:I:80:PRO:CD	2.36	0.55
1:J:200:PHE:O	1:J:201:VAL:HG23	2.07	0.55
3:L:102:PHE:CD1	3:L:103:GLY:N	2.74	0.55
2:K:176:ALA:CB	3:L:166:TRP:CE2	2.88	0.55
2:B:3:LYS:O	2:B:4:LEU:HD12	2.07	0.55
3:C:113:ASP:OD1	3:C:113:ASP:C	2.45	0.55
2:E:129:VAL:HG11	2:E:206:VAL:HG21	1.89	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
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
3:I:95:LYS:O	3:I:99:TYR:CE1	2.56	0.55
1:J:84:SER:CB	1:J:88:GLY:H	2.16	0.55
1:A:59:GLY:HA2	1:A:89:THR:HG22	1.88	0.55
2:B:129:VAL:HG22	2:B:150:VAL:HG22	1.89	0.55
3:C:38:TRP:CD2	3:C:90:PHE:O	2.60	0.55
3:F:193:ASN:O	3:F:211:SER:HB3	2.06	0.55
3:F:86:THR:HG22	3:F:109:ILE:CD1	2.31	0.55
1:G:166:ILE:HD13	1:G:166:ILE:N	2.21	0.55
1:G:200:PHE:CE2	1:G:201:VAL:O	2.60	0.55
1:G:54:LYS:HG2	1:G:55:CYS:N	2.22	0.55
3:I:81:VAL:O	3:I:82:GLU:HG3	2.07	0.55
3:I:42:LYS:HG2	3:I:87:ALA:HB2	1.87	0.55
1:J:106:SER:HG	1:J:263:SER:HG	1.47	0.55
1:J:107:SER:HB2	1:J:260:ASN:OD1	2.06	0.55
2:K:97:ARG:N	2:K:110:GLY:O	2.35	0.55
2:K:207:ASN:ND2	2:K:214:LYS:HD2	2.22	0.55
2:K:32:ASP:CB	2:K:98:HIS:HD1	2.13	0.55
2:E:32:ASP:CB	2:E:50:ILE:O	2.55	0.55
3:F:78:ILE:HD12	3:F:107:LEU:HD11	1.89	0.55
1:G:149:ILE:HD11	1:G:252:ARG:HG3	1.87	0.55
2:H:146:LEU:HD13	2:H:147:GLY:N	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:76:TRP:CZ3	1:D:108:VAL:HG21	2.41	0.55
2:E:124:THR:HA	2:E:154:PHE:O	2.07	0.55
3:F:203:THR:O	3:F:205:THR:N	2.39	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
2:H:130:PHE:CD2	3:I:127:GLN:HB2	2.42	0.55
2:K:125:LYS:HD2	2:K:126:GLY:H	1.71	0.55
3:L:109:ILE:HG22	3:L:110:LYS:H	1.72	0.55
2:E:173:THR:CG2	3:F:178:MET:SD	2.95	0.55
3:F:209:VAL:HG22	3:F:210:LYS:HB3	1.87	0.55
1:G:203:SER:HB3	1:G:239:LYS:O	2.06	0.55
2:H:202:TYR:HE1	2:H:219:SER:HB2	1.70	0.55
1:J:178:GLY:HA2	1:J:228:ASN:O	2.07	0.55
3:L:142:PHE:CD1	3:L:142:PHE:O	2.59	0.55
3:L:27:SER:C	3:L:28:VAL:HG22	2.27	0.55
3:L:34:ASN:ND2	3:L:96:GLU:OE2	2.34	0.55
1:A:167:ASN:CG	1:A:236:PRO:HA	2.28	0.54
2:B:122:ALA:O	2:B:154:PHE:HE2	1.90	0.54
1:A:121:SER:CB	2:B:58:TYR:HA	2.37	0.54
1:D:252:ARG:HD2	1:D:253:TYR:N	2.22	0.54
2:E:28:GLY:H	2:E:76:LYS:HZ3	1.55	0.54
3:F:153:ILE:HG22	3:F:195:TYR:CE2	2.42	0.54
1:G:219:LYS:HG2	1:G:222:ASP:HA	1.89	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
2:K:34:SER:HA	2:K:49:GLY:HA2	1.89	0.54
2:K:48:SER:OG	2:K:59:TYR:HD1	1.90	0.54
3:L:38:TRP:HE1	3:L:90:PHE:CB	2.19	0.54
3:C:128:LEU:CD1	3:C:129:THR:HG23	2.37	0.54
3:C:24:ALA:HB1	3:C:26:GLU:O	2.07	0.54
3:C:35:PHE:CD1	3:C:36:ILE:HA	2.43	0.54
3:F:42:LYS:HD2	3:F:87:ALA:HB2	1.89	0.54
1:G:132:VAL:O	1:G:132:VAL:HG23	2.07	0.54
1:G:188:GLN:NE2	1:G:197:ALA:CB	2.70	0.54
2:H:75:ARG:O	2:H:76:LYS:HB2	2.07	0.54
2:H:78:LEU:HD23	2:H:78:LEU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:L:108:GLU:CG	3:L:109:ILE:H	2.20	0.54
3:L:109:ILE:CG2	3:L:110:LYS:N	2.70	0.54
1:G:127:ASP:N	1:G:154:LYS:HB2	2.22	0.54
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
2:B:54:SER:CB	2:B:56:ARG:HH11	2.21	0.54
1:D:63:GLY:O	1:D:146:LYS:N	2.25	0.54
2:E:196:SER:O	2:E:200:GLN:N	2.40	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:164:SER:HA	2:H:167:LEU:HB2	1.89	0.54
2:H:54:SER:CB	2:H:56:ARG:HE	2.16	0.54
2:K:38:GLN:HG3	2:K:43:GLY:CA	2.37	0.54
3:L:143:TYR:CD2	3:L:144:PRO:HD3	2.41	0.54
3:L:209:VAL:HG23	3:L:210:LYS:CB	2.37	0.54
3:L:28:VAL:HG23	3:L:72:THR:H	1.72	0.54
1:D:228:ASN:HB3	1:D:230:TYR:HE1	1.73	0.54
1:G:182:PRO:HD2	1:G:214:ILE:HG13	1.90	0.54
2:H:72:ASP:HB3	2:H:79:TYR:OH	2.08	0.54
3:I:86:THR:HG22	3:I:109:ILE:HD13	1.90	0.54
2:K:211:SER:C	2:K:213:THR:H	2.11	0.54
2:K:18:ARG:HA	2:K:80:LEU:O	2.07	0.54
2:B:32:ASP:OD2	2:B:32:ASP:N	2.25	0.54
3:C:111:ARG:O	3:C:112:ALA:HB3	2.07	0.54
1:D:48:ALA:HB1	1:D:80:VAL:CG2	2.37	0.54
1:G:119:LYS:HZ3	1:G:129:ASN:HB3	1.67	0.54
3:I:20:ILE:CG2	3:I:105:THR:HG21	2.38	0.54
2:B:20:SER:O	2:B:35:TRP:HH2	1.90	0.54
3:C:51:ILE:HG12	3:C:67:GLY:N	2.23	0.54
2:E:144:ALA:N	2:E:192:VAL:O	2.39	0.54
2:E:205:ASN:HD22	2:E:214:LYS:CE	2.21	0.54
2:H:69:ILE:CG1	2:H:70:SER:N	2.71	0.54
3:I:170:ASP:HB3	3:I:175:THR:HG1	1.71	0.54
1:J:121:SER:N	2:K:64:LYS:HE3	2.23	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
1:A:252:ARG:HD2	1:A:253:TYR:N	2.23	0.54
2:B:10:VAL:HG13	2:B:155:PRO:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:166:TRP:O	3:F:177:SER:CA	2.55	0.54
1:G:101:LEU:HD22	1:G:105:LEU:HD11	1.90	0.54
2:H:32:ASP:HB2	2:H:98:HIS:ND1	2.22	0.54
3:I:27:SER:O	3:I:28:VAL:CG2	2.54	0.54
3:I:38:TRP:CG	3:I:47:PRO:HB3	2.39	0.54
2:K:37:ARG:HB3	2:K:93:TYR:CD2	2.43	0.54
2:B:203:ILE:HD12	2:B:218:LYS:N	2.23	0.54
3:F:84:GLU:O	3:F:86:THR:N	2.41	0.54
2:H:72:ASP:HB3	2:H:79:TYR:HE2	1.68	0.54
1:J:138:HIS:O	1:J:139:ALA:C	2.47	0.54
2:K:201:THR:HG22	2:K:218:LYS:HD3	1.89	0.54
4:B:307:HOH:O	3:L:172:LYS:HD2	2.07	0.54
1:A:216:ILE:O	1:D:96:ILE:HA	2.08	0.54
3:C:8:ALA:HB3	4:C:309:HOH:O	2.06	0.54
2:E:143:THR:HG23	2:E:191:THR:HG23	1.90	0.54
3:F:9:SER:HB3	3:F:106:LYS:HZ1	1.71	0.54
3:I:109:ILE:CG2	3:I:110:LYS:N	2.70	0.54
3:I:167:THR:HG23	3:I:177:SER:HB2	1.90	0.54
3:L:109:ILE:CG2	3:L:110:LYS:H	2.21	0.54
2:K:98:HIS:HD2	3:L:36:ILE:HG21	1.73	0.54
2:B:177:VAL:HG12	2:B:183:LEU:H	1.73	0.53
2:B:78:LEU:O	2:B:78:LEU:HD12	2.08	0.53
3:F:164:ASN:HB3	3:F:180:SER:O	2.08	0.53
3:F:152:LYS:N	3:F:196:THR:O	2.41	0.53
3:F:38:TRP:CZ2	3:F:89:TYR:C	2.81	0.53
3:I:143:TYR:CZ	3:I:144:PRO:HB3	2.43	0.53
3:I:170:ASP:OD2	3:I:172:LYS:N	2.41	0.53
1:J:98:TYR:O	1:J:98:TYR:CG	2.60	0.53
3:L:209:VAL:HG23	3:L:210:LYS:HG3	1.90	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
2:B:83:ASN:OD1	2:B:84:SER:N	2.41	0.53
3:C:135:VAL:HG12	3:C:151:TRP:HH2	1.74	0.53
3:C:38:TRP:CE2	3:C:39:PHE:CD1	2.97	0.53
3:C:83:ALA:O	3:C:171:SER:O	2.26	0.53
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
3:I:89:TYR:O	3:I:102:PHE:CE2	2.61	0.53
3:I:140:ASN:CB	3:I:141:ASN:ND2	2.72	0.53
1:J:149:ILE:HB	1:J:250:VAL:CG2	2.38	0.53
3:L:27:SER:O	3:L:28:VAL:HG13	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:GLU:HG2	3:C:169:GLN:NE2	2.24	0.53
1:D:133:THR:CB	1:D:150:TRP:HZ3	2.21	0.53
3:F:172:LYS:N	3:F:172:LYS:HD3	2.23	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
3:I:147:ILE:HG23	3:I:148:ASN:N	2.22	0.53
3:I:144:PRO:O	3:I:201:HIS:CE1	2.61	0.53
3:I:92:GLN:HG2	3:I:101:THR:HB	1.90	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
2:K:99:SER:HB3	3:L:35:PHE:O	2.09	0.53
2:B:208:HIS:C	2:B:210:PRO:HD2	2.29	0.53
2:B:97:ARG:O	3:C:36:ILE:HG12	2.09	0.53
2:H:162:TRP:CD2	2:H:190:VAL:HG11	2.43	0.53
2:H:82:MET:HE1	2:H:117:VAL:HG21	1.89	0.53
2:H:174:PHE:CD2	3:I:166:TRP:HE3	2.26	0.53
1:J:149:ILE:O	1:J:250:VAL:HG22	2.09	0.53
1:J:48:ALA:CB	1:J:78:TYR:HE1	2.20	0.53
2:K:90:THR:HG23	2:K:117:VAL:O	2.09	0.53
3:L:10:LEU:O	3:L:107:LEU:HA	2.08	0.53
3:F:114:ALA:HB1	3:F:202:LYS:O	2.08	0.53
3:F:26:GLU:OE2	3:F:27:SER:HB2	2.08	0.53
3:F:9:SER:CA	3:F:106:LYS:HB2	2.39	0.53
3:I:1:ILE:HG22	3:I:3:MET:CE	2.39	0.53
3:I:24:ALA:HB3	3:I:72:THR:OG1	2.08	0.53
3:L:118:VAL:O	3:L:208:ILE:HD12	2.08	0.53
3:L:161:GLY:O	3:L:162:VAL:HG12	2.09	0.53
3:L:81:VAL:HG12	3:L:82:GLU:N	2.24	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:F:159:GLN:NE2	2:H:26:PHE:HE2	2.07	0.53
3:F:36:ILE:H	3:F:93:GLN:HE22	1.57	0.53
1:G:169:LYS:HE2	1:G:256:ALA:CB	2.39	0.53
1:J:118:PRO:O	1:J:122:SER:OG	2.23	0.53
3:C:38:TRP:CZ3	3:C:89:TYR:HD1	2.24	0.53
3:C:81:VAL:HG13	3:C:85:ASP:OD2	2.09	0.53
1:D:178:GLY:O	1:D:179:ILE:HD12	2.09	0.53
1:D:99:GLU:CD	1:D:99:GLU:H	2.12	0.53
1:G:57:ILE:HD13	1:G:102:ARG:HB2	1.89	0.53
2:H:176:ALA:CB	3:I:166:TRP:CZ2	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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
3:C:17:ARG:HA	3:C:79:ASN:O	2.08	0.53
2:E:13:PRO:CD	2:E:121:SER:HB2	2.38	0.53
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
3:L:17:ARG:HA	3:L:79:ASN:HA	1.90	0.53
1:A:259:ARG:HH11	1:A:259:ARG:HB3	1.70	0.53
2:B:98:HIS:CD2	2:B:98:HIS:H	2.27	0.53
1:D:231:TRP:HZ3	1:D:233:LEU:CD2	2.22	0.53
2:E:12:GLN:HG3	2:E:121:SER:OG	2.09	0.53
2:E:161:SER:HA	2:E:167:LEU:HD11	1.90	0.53
3:I:202:LYS:HG2	3:I:202:LYS:O	2.09	0.53
1:J:115:GLU:O	1:J:115:GLU:HG3	2.09	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
2:B:86:ARG:H	2:B:89:ASP:HB2	1.74	0.53
3:C:7:PRO:HG3	3:C:21:THR:OG1	2.08	0.53
2:E:209:LYS:N	2:E:210:PRO:HD2	2.23	0.53
2:E:208:HIS:CD2	2:E:210:PRO:HD2	2.44	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
1:G:221:ARG:O	1:G:223:GLN:HG2	2.08	0.53
3:L:170:ASP:HB3	3:L:175:THR:OG1	2.09	0.53
2:B:51:LEU:HD12	2:B:56:ARG:N	2.21	0.52
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
1:A:49:PRO:HD3	1:A:77:SER:OG	2.09	0.52
2:H:51:LEU:HD11	2:H:56:ARG:HD3	1.90	0.52
1:J:76:TRP:NE1	1:J:105:LEU:O	2.42	0.52
2:K:72:ASP:HB2	2:K:79:TYR:HE2	1.74	0.52
2:K:94:TYR:HE1	3:L:46:PRO:HB3	1.75	0.52
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
1:G:118:PRO:HG2	2:H:58:TYR:CZ	2.45	0.52
3:I:111:ARG:HH21	3:I:173:ASP:HA	1.74	0.52
3:L:127:GLN:HG2	3:L:132:GLY:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:163:LEU:HD12	3:L:163:LEU:O	2.09	0.52
3:L:1:ILE:HG22	3:L:1:ILE:O	2.10	0.52
1:A:201:VAL:HG13	1:A:202:GLY:H	1.68	0.52
1:G:172:GLU:OE2	1:G:258:GLU:HA	2.09	0.52
3:I:140:ASN:HB3	3:I:141:ASN:ND2	2.24	0.52
3:I:167:THR:HG22	3:I:168:ASP:N	2.24	0.52
2:K:20:SER:OG	2:K:21:CYS:N	2.42	0.52
2:B:13:PRO:HD3	2:B:120:SER:C	2.30	0.52
2:B:35:TRP:CD1	2:B:80:LEU:HB2	2.44	0.52
3:C:190:GLU:CD	3:C:191:ARG:HG3	2.30	0.52
3:F:105:THR:HG22	3:F:106:LYS:N	2.24	0.52
3:F:110:LYS:HG2	3:F:111:ARG:N	2.24	0.52
3:F:3:MET:HG3	3:F:5:GLN:NE2	2.20	0.52
2:H:90:THR:HG23	2:H:117:VAL:O	2.09	0.52
2:H:125:LYS:HD2	2:H:126:GLY:N	2.24	0.52
2:H:129:VAL:O	2:H:217:LYS:HE3	2.10	0.52
2:H:132:LEU:HB3	3:I:121:PHE:CG	2.45	0.52
2:H:34:SER:HG	2:H:49:GLY:HA3	1.74	0.52
3:I:19:THR:CG2	3:I:77:THR:HG22	2.39	0.52
2:K:153:TYR:N	2:K:183:LEU:HD12	2.25	0.52
3:L:26:GLU:O	3:L:27:SER:HB2	2.09	0.52
2:B:51:LEU:CG	2:B:56:ARG:HG2	2.39	0.52
3:C:116:PRO:HA	3:C:142:PHE:HB3	1.92	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
2:E:32:ASP:OD2	2:E:98:HIS:CE1	2.62	0.52
3:F:27:SER:O	3:F:28:VAL:CG2	2.57	0.52
1:G:182:PRO:HG3	1:G:192:TYR:HE1	1.75	0.52
3:L:138:PHE:O	3:L:139:LEU:HD12	2.09	0.52
2:K:97:ARG:N	3:L:36:ILE:HG13	2.25	0.52
1:A:91:TYR:HD1	1:A:227:MET:CB	2.11	0.52
2:B:196:SER:HB3	2:B:202:TYR:CZ	2.45	0.52
1:D:91:TYR:OH	1:D:180:HIS:CD2	2.63	0.52
1:D:227:MET:HG2	1:D:229:TYR:CE2	2.45	0.52
1:G:202:GLY:O	1:G:206:TYR:O	2.27	0.52
3:I:197:CYS:O	3:I:208:ILE:N	2.35	0.52
3:I:97:VAL:HG13	3:I:98:PRO:HD2	1.91	0.52
1:J:182:PRO:HG2	1:J:188:GLN:CB	2.39	0.52
3:L:139:LEU:HD21	3:L:199:ALA:HB1	1.91	0.52
3:L:143:TYR:CD2	3:L:143:TYR:C	2.83	0.52
1:A:56:ASN:HA	1:A:81:GLU:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:SER:O	3:C:10:LEU:HD23	2.09	0.52
1:D:116:ILE:HG23	1:D:117:PHE:N	2.25	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
3:F:125:SER:O	3:F:128:LEU:HD23	2.10	0.52
2:H:66:ARG:HH22	2:H:89:ASP:CG	2.12	0.52
3:I:139:LEU:HD21	3:I:199:ALA:HB2	1.92	0.52
1:J:144:PHE:CG	1:J:145:TYR:N	2.78	0.52
2:K:17:LEU:HB3	2:K:82:MET:CG	2.40	0.52
2:K:180:SER:OG	2:K:183:LEU:N	2.42	0.52
2:K:21:CYS:O	2:K:77:THR:HB	2.10	0.52
3:L:168:ASP:OD2	3:L:176:TYR:HD2	1.93	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:G:248:LEU:HD12	1:G:249:VAL:N	2.25	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:J:92:PRO:CG	1:J:223:GLN:HB2	2.39	0.52
2:B:4:LEU:HB2	2:B:112:GLY:HA2	1.91	0.52
2:B:134:PRO:HB3	3:C:121:PHE:HE1	1.74	0.52
3:C:38:TRP:HE1	3:C:91:CYS:HA	1.74	0.52
1:D:77:SER:O	1:D:106:SER:O	2.28	0.52
2:E:152:ASP:CB	2:E:183:LEU:HD23	2.40	0.52
1:G:127:ASP:HB2	1:G:153:LYS:O	2.10	0.52
1:G:232:THR:HG23	1:G:233:LEU:N	2.24	0.52
2:H:174:PHE:HD2	3:I:166:TRP:HE3	1.58	0.52
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
3:L:43:PRO:HD3	3:L:87:ALA:HA	1.91	0.52
1:A:133:THR:CG2	1:A:150:TRP:HZ3	2.23	0.51
1:A:228:ASN:HB3	1:A:230:TYR:CE1	2.45	0.51
3:C:83:ALA:HB1	3:C:171:SER:O	2.10	0.51
3:C:39:PHE:CB	3:C:50:LEU:CB	2.83	0.51
1:G:188:GLN:NE2	1:G:197:ALA:HB2	2.25	0.51
3:I:196:THR:HG23	3:I:208:ILE:O	2.09	0.51
3:L:161:GLY:O	3:L:162:VAL:CG1	2.58	0.51
1:A:129:ASN:HB2	4:A:604:HOH:O	2.09	0.51
1:D:165:TYR:HE2	1:D:167:ASN:HB2	1.74	0.51
3:F:110:LYS:HG2	3:F:111:ARG:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:153:ILE:CG1	3:F:154:ASP:H	2.15	0.51
3:F:183:THR:CG2	3:F:184:LEU:N	2.70	0.51
1:G:118:PRO:O	1:G:122:SER:OG	2.28	0.51
1:G:146:LYS:HG2	1:G:147:ASN:OD1	2.10	0.51
1:J:181:HIS:O	1:J:225:GLY:HA3	2.10	0.51
1:J:260:ASN:OD1	1:J:260:ASN:C	2.49	0.51
2:K:178:LEU:HD23	2:K:178:LEU:C	2.31	0.51
2:K:63:VAL:HG13	2:K:67:SER:H	1.74	0.51
2:K:6:GLU:HB3	2:K:115:THR:HB	1.92	0.51
1:A:206:TYR:C	1:A:206:TYR:HD2	2.14	0.51
2:B:44:LEU:N	4:B:302:HOH:O	2.42	0.51
2:B:50:ILE:HB	2:B:56:ARG:O	2.11	0.51
3:F:39:PHE:HB2	3:F:50:LEU:HB2	1.93	0.51
2:K:100:TRP:CD1	3:L:34:ASN:N	2.78	0.51
3:C:48:LYS:HG2	3:C:49:LEU:H	1.75	0.51
3:C:50:LEU:HD11	3:C:89:TYR:CE1	2.28	0.51
3:C:83:ALA:O	3:C:86:THR:CG2	2.59	0.51
3:I:27:SER:C	3:I:28:VAL:HG22	2.30	0.51
2:K:11:VAL:HG11	2:K:85:LEU:HD13	1.92	0.51
1:A:51:HIS:ND1	1:A:80:VAL:HG11	2.26	0.51
1:A:54:LYS:HD2	1:A:69:SER:CB	2.40	0.51
3:F:151:TRP:N	4:F:305:HOH:O	2.38	0.51
3:F:172:LYS:CD	3:F:172:LYS:N	2.73	0.51
3:F:164:ASN:HB3	3:F:180:SER:H	1.75	0.51
3:L:203:THR:CG2	3:L:203:THR:O	2.57	0.51
2:K:97:ARG:H	3:L:36:ILE:HG13	1.76	0.51
3:C:141:ASN:HA	3:C:175:THR:CG2	2.36	0.51
3:F:42:LYS:HD3	3:F:84:GLU:OE2	2.10	0.51
1:G:134:ALA:HA	1:G:142:LYS:HB3	1.92	0.51
2:H:147:GLY:O	2:H:148:CYS:SG	2.68	0.51
3:I:41:GLN:HB2	3:I:47:PRO:HA	1.93	0.51
2:B:85:LEU:HB3	2:B:119:VAL:HG13	1.93	0.51
3:C:37:ASN:OD1	3:C:95:LYS:NZ	2.30	0.51
1:A:96:ILE:HA	1:D:216:ILE:O	2.11	0.51
3:F:13:SER:HB2	3:F:110:LYS:NZ	2.26	0.51
2:E:94:TYR:CE1	3:F:46:PRO:HB3	2.45	0.51
2:H:93:TYR:CE1	2:H:117:VAL:CG1	2.92	0.51
2:H:164:SER:HA	2:H:167:LEU:HD12	1.92	0.51
3:I:11:ALA:HA	3:I:108:GLU:O	2.09	0.51
1:J:44:LEU:HD11	1:J:47:VAL:HG23	1.92	0.51
2:K:171:VAL:HB	2:K:189:VAL:CG2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:L:92:GLN:HG3	3:L:100:GLY:O	2.11	0.51
1:A:232:THR:HG21	1:A:240:ILE:HD12	1.93	0.51
1:A:259:ARG:CB	1:A:259:ARG:CZ	2.89	0.51
2:B:98:HIS:CD2	2:B:98:HIS:N	2.78	0.51
3:C:9:SER:CB	3:C:106:LYS:HB3	2.07	0.51
3:C:29:SER:HB3	4:C:310:HOH:O	2.10	0.51
1:D:173:VAL:O	1:D:233:LEU:HA	2.11	0.51
2:E:208:HIS:NE2	2:E:210:PRO:HG2	2.26	0.51
3:F:35:PHE:CE1	3:F:49:LEU:HD11	2.46	0.51
2:H:10:VAL:HG13	2:H:118:THR:O	2.11	0.51
3:I:16:GLN:O	3:I:81:VAL:HG23	2.10	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
1:J:153:LYS:CB	1:J:158:TYR:HB2	2.41	0.51
1:J:166:ILE:N	1:J:166:ILE:HD13	2.26	0.51
3:L:1:ILE:O	3:L:2:GLN:HB3	2.10	0.51
3:L:38:TRP:CD1	3:L:38:TRP:C	2.84	0.51
3:L:17:ARG:HB2	3:L:79:ASN:OD1	2.11	0.51
1:D:211:LYS:NZ	1:D:211:LYS:HB2	2.26	0.51
2:E:47:VAL:O	2:E:48:SER:HB3	2.11	0.51
2:E:50:ILE:HG23	2:E:69:ILE:HD13	1.92	0.51
3:F:121:PHE:N	3:F:121:PHE:CD2	2.79	0.51
3:F:38:TRP:HE3	3:F:38:TRP:O	1.88	0.51
2:H:125:LYS:HE3	2:H:126:GLY:O	2.11	0.51
2:H:27:THR:C	2:H:29:SER:N	2.64	0.51
2:H:72:ASP:HB3	2:H:79:TYR:CZ	2.46	0.51
3:I:26:GLU:O	3:I:27:SER:HB2	2.10	0.51
1:J:144:PHE:CZ	1:J:145:TYR:HD2	2.28	0.51
1:J:54:LYS:HZ2	1:J:54:LYS:CB	2.14	0.51
1:A:48:ALA:CB	1:A:78:TYR:CZ	2.93	0.51
1:D:175:VAL:O	1:D:231:TRP:HA	2.11	0.51
3:F:149:VAL:HG22	3:F:149:VAL:O	2.11	0.51
1:A:138:HIS:O	1:A:139:ALA:C	2.49	0.50
1:A:184:THR:O	1:A:187:ASP:N	2.45	0.50
2:B:38:GLN:OE1	3:C:41:GLN:NE2	2.44	0.50
2:B:93:TYR:O	2:B:114:GLY:HA2	2.11	0.50
3:C:13:SER:HB3	3:C:110:LYS:NZ	2.25	0.50
3:C:154:ASP:OD1	3:C:191:ARG:NH1	2.45	0.50
1:D:165:TYR:CD2	1:D:165:TYR:C	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:TYR:HD1	1:D:227:MET:CB	2.08	0.50
2:E:173:THR:HG22	3:F:178:MET:CE	2.40	0.50
1:G:144:PHE:CZ	1:G:145:TYR:HD2	2.28	0.50
1:G:199:VAL:HA	1:G:243:GLU:O	2.11	0.50
2:H:32:ASP:HB2	2:H:98:HIS:HD1	1.76	0.50
1:J:62:LEU:HD22	1:J:148:LEU:HD11	1.92	0.50
1:J:100:GLU:HG2	1:J:231:TRP:CZ2	2.46	0.50
1:J:53:GLY:HA2	1:J:82:THR:HG23	1.93	0.50
2:K:145:ALA:HA	2:K:191:THR:HA	1.93	0.50
2:K:162:TRP:CE2	2:K:204:CYS:HB3	2.45	0.50
2:K:207:ASN:HA	2:K:214:LYS:HA	1.92	0.50
3:L:102:PHE:HE1	3:L:104:GLY:HA2	1.75	0.50
2:H:17:LEU:HB3	2:H:82:MET:CE	2.40	0.50
3:I:148:ASN:C	3:I:148:ASN:OD1	2.49	0.50
3:I:79:ASN:O	3:I:80:PRO:C	2.48	0.50
2:K:97:ARG:O	2:K:97:ARG:NE	2.45	0.50
3:L:141:ASN:H	3:L:175:THR:HB	1.75	0.50
3:L:208:ILE:C	3:L:209:VAL:CG1	2.78	0.50
3:C:175:THR:HB	3:C:176:TYR:CD2	2.47	0.50
1:D:178:GLY:C	1:D:179:ILE:HD12	2.30	0.50
3:F:189:TYR:O	3:F:190:GLU:CB	2.59	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
2:B:4:LEU:HD22	2:B:112:GLY:N	2.26	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
1:D:54:LYS:HZ3	1:D:54:LYS:H	1.59	0.50
3:F:13:SER:CB	3:F:110:LYS:HZ2	2.24	0.50
3:F:159:GLN:NE2	2:H:26:PHE:CE2	2.80	0.50
3:F:172:LYS:O	3:F:173:ASP:HB3	2.11	0.50
3:I:89:TYR:O	3:I:102:PHE:CZ	2.64	0.50
2:K:218:LYS:NZ	2:K:218:LYS:HB2	2.27	0.50
2:K:50:ILE:HD11	2:K:71:ARG:CG	2.41	0.50
2:K:92:VAL:HG12	2:K:93:TYR:N	2.26	0.50
3:L:40:GLN:HA	3:L:88:ASN:O	2.11	0.50
2:B:200:GLN:HB3	2:B:202:TYR:CZ	2.46	0.50
2:B:98:HIS:CB	3:C:36:ILE:HG13	2.40	0.50
3:C:3:MET:O	3:C:25:SER:N	2.44	0.50
1:D:132:VAL:HA	1:D:144:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:109:ILE:CG2	3:F:110:LYS:N	2.74	0.50
2:H:51:LEU:HD11	2:H:56:ARG:HD2	1.92	0.50
3:I:13:SER:HB3	3:I:110:LYS:NZ	2.27	0.50
1:J:204:SER:OG	1:J:205:ARG:N	2.44	0.50
2:K:125:LYS:HG3	2:K:126:GLY:O	2.12	0.50
3:L:37:ASN:HD21	3:L:93:GLN:H	1.59	0.50
2:B:50:ILE:HG23	2:B:69:ILE:CG1	2.42	0.50
3:C:13:SER:OG	3:C:110:LYS:HD3	2.11	0.50
3:C:64:ARG:HH21	3:C:82:GLU:H	1.58	0.50
3:C:69:GLY:HA3	3:C:74:PHE:HA	1.93	0.50
3:C:83:ALA:O	3:C:86:THR:HG21	2.12	0.50
1:D:201:VAL:HG23	1:D:208:LYS:H	1.77	0.50
2:E:13:PRO:HD3	2:E:121:SER:HB2	1.94	0.50
3:F:173:ASP:OD2	3:F:175:THR:CG2	2.59	0.50
3:F:162:VAL:HB	3:F:182:LEU:HG	1.94	0.50
3:F:52:TYR:CE2	3:F:58:GLY:HA2	2.47	0.50
1:G:101:LEU:HG	1:G:231:TRP:CD2	2.46	0.50
2:H:18:ARG:HA	2:H:80:LEU:O	2.12	0.50
3:I:111:ARG:O	3:I:112:ALA:HB3	2.12	0.50
3:I:53:THR:O	3:I:53:THR:HG22	2.12	0.50
3:I:91:CYS:N	3:I:102:PHE:HD2	2.07	0.50
2:K:127:PRO:HB2	2:K:150:VAL:HG13	1.93	0.50
2:K:182:GLY:O	2:K:183:LEU:HD22	2.12	0.50
2:K:178:LEU:HA	3:L:163:LEU:CD2	2.42	0.50
2:B:167:LEU:HA	2:B:170:SER:HB2	1.93	0.50
2:B:208:HIS:CD2	2:B:210:PRO:HD2	2.47	0.50
3:C:50:LEU:CD1	3:C:89:TYR:HE1	2.16	0.50
1:D:49:PRO:HD2	1:D:78:TYR:O	2.11	0.50
3:F:38:TRP:CE2	3:F:90:PHE:O	2.65	0.50
2:H:95:CYS:O	2:H:112:GLY:N	2.39	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
3:I:120:ILE:CD1	3:I:137:CYS:HB2	2.42	0.50
3:I:54:ALA:O	3:I:67:GLY:HA3	2.12	0.50
1:J:186:ALA:O	1:J:189:GLN:HG2	2.11	0.50
1:J:54:LYS:HB2	1:J:55:CYS:SG	2.52	0.50
2:K:60:ARG:O	2:K:64:LYS:NZ	2.44	0.50
3:L:143:TYR:HD2	3:L:144:PRO:HD3	1.76	0.50
3:L:142:PHE:HD1	3:L:144:PRO:O	1.93	0.50
2:B:63:VAL:HG12	2:B:64:LYS:N	2.26	0.50
2:B:174:PHE:O	3:C:166:TRP:CD1	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:GLN:CG	3:C:93:GLN:N	2.74	0.50
3:F:138:PHE:CD1	3:F:178:MET:HG3	2.47	0.50
3:F:38:TRP:CZ2	3:F:90:PHE:C	2.85	0.50
1:G:198:TYR:HB2	1:G:210:PHE:O	2.12	0.50
1:G:201:VAL:HG11	1:G:206:TYR:CD2	2.47	0.50
2:H:150:VAL:HG21	2:H:206:VAL:HG11	1.94	0.50
2:K:162:TRP:HA	2:K:203:ILE:O	2.11	0.50
2:K:21:CYS:HB2	2:K:35:TRP:CZ2	2.46	0.50
3:L:28:VAL:CG2	3:L:74:PHE:CE2	2.94	0.50
3:L:78:ILE:HD11	3:L:80:PRO:O	2.12	0.50
1:A:101:LEU:O	1:A:104:GLN:N	2.44	0.50
2:E:197:LEU:HG	2:E:198:GLY:N	2.26	0.50
2:E:200:GLN:HG2	2:E:202:TYR:CZ	2.46	0.50
3:F:138:PHE:HD1	3:F:178:MET:HG3	1.77	0.50
3:F:156:SER:OG	3:F:157:GLU:N	2.44	0.50
1:G:162:SER:HA	1:G:242:PHE:O	2.12	0.50
2:H:27:THR:CG2	2:H:31:TYR:CD2	2.95	0.50
2:K:116:THR:HG21	4:K:302:HOH:O	2.11	0.50
2:B:100:TRP:NE1	3:C:34:ASN:OD1	2.44	0.49
2:B:27:THR:HG23	2:B:30:ASP:OD2	2.11	0.49
2:E:35:TRP:CD1	2:E:80:LEU:HB2	2.47	0.49
3:F:162:VAL:CG2	3:F:162:VAL:O	2.59	0.49
3:I:209:VAL:HG22	3:I:210:LYS:N	2.27	0.49
3:I:40:GLN:HB3	3:I:50:LEU:HD11	1.94	0.49
3:L:143:TYR:HD1	3:L:174:SER:OG	1.94	0.49
3:L:196:THR:HA	3:L:209:VAL:HB	1.94	0.49
3:L:81:VAL:HG12	3:L:82:GLU:H	1.74	0.49
1:D:149:ILE:HD11	1:D:252:ARG:HB2	1.94	0.49
2:E:125:LYS:HD2	2:E:126:GLY:N	2.27	0.49
1:G:248:LEU:HD12	1:G:249:VAL:H	1.76	0.49
2:K:211:SER:C	2:K:213:THR:N	2.65	0.49
2:K:72:ASP:N	2:K:77:THR:O	2.44	0.49
1:A:104:GLN:NE2	1:A:233:LEU:HD22	2.22	0.49
2:B:196:SER:C	2:B:202:TYR:HE2	2.15	0.49
2:B:127:PRO:HD2	2:B:213:THR:HG21	1.93	0.49
3:C:101:THR:HG22	3:C:102:PHE:H	1.76	0.49
3:C:109:ILE:CG2	3:C:110:LYS:H	2.16	0.49
2:E:205:ASN:ND2	2:E:214:LYS:HE3	2.27	0.49
3:F:12:VAL:HG22	3:F:13:SER:N	2.27	0.49
3:F:141:ASN:ND2	3:F:176:TYR:CE1	2.81	0.49
3:I:138:PHE:C	3:I:139:LEU:HD12	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:109:SER:HB3	1:A:258:GLU:HG2	1.93	0.49
2:E:203:ILE:HG13	2:E:204:CYS:N	2.25	0.49
2:E:209:LYS:N	2:E:210:PRO:CD	2.75	0.49
3:F:159:GLN:HG3	3:F:160:ASN:H	1.77	0.49
2:H:194:SER:O	2:H:196:SER:N	2.45	0.49
3:I:120:ILE:HB	3:I:208:ILE:CG2	2.42	0.49
2:K:45:GLU:OE1	2:K:46:TRP:N	2.46	0.49
3:C:35:PHE:HB2	3:C:95:LYS:HE2	1.94	0.49
1:D:153:LYS:HG3	1:D:157:SER:N	2.27	0.49
2:E:63:VAL:HG11	2:E:67:SER:H	1.76	0.49
3:F:138:PHE:C	3:F:139:LEU:HD12	2.33	0.49
3:F:26:GLU:O	3:F:72:THR:HB	2.13	0.49
2:H:96:ALA:HB1	3:I:36:ILE:HD11	1.95	0.49
1:A:115:GLU:CB	3:C:96:GLU:HG2	2.39	0.49
1:A:200:PHE:HB3	1:A:243:GLU:HB3	1.95	0.49
2:B:30:ASP:OD1	2:B:30:ASP:N	2.44	0.49
1:D:144:PHE:HZ	1:D:227:MET:HE1	1.74	0.49
1:D:108:VAL:HG12	1:D:257:MET:HE1	1.95	0.49
2:E:61:ASP:OD1	2:H:142:GLY:HA2	2.13	0.49
1:G:206:TYR:OH	1:G:208:LYS:HD2	2.12	0.49
1:G:219:LYS:HD3	1:G:224:GLU:CG	2.42	0.49
1:G:241:THR:CG2	1:G:242:PHE:N	2.76	0.49
2:H:97:ARG:NE	2:H:110:GLY:HA3	2.27	0.49
3:I:209:VAL:HG22	3:I:210:LYS:CB	2.43	0.49
3:L:108:GLU:CG	3:L:109:ILE:N	2.75	0.49
1:D:179:ILE:HG22	1:D:181:HIS:CE1	2.48	0.49
2:E:186:LEU:HD12	2:E:187:SER:H	1.78	0.49
1:G:231:TRP:CE3	1:G:232:THR:HA	2.47	0.49
2:H:162:TRP:CE2	2:H:204:CYS:HB3	2.47	0.49
3:I:141:ASN:N	3:I:176:TYR:HD1	2.10	0.49
1:A:144:PHE:CE1	1:A:227:MET:HE1	2.48	0.49
3:C:183:THR:CG2	3:C:184:LEU:N	2.75	0.49
3:C:64:ARG:NH2	3:C:82:GLU:HB2	2.28	0.49
1:D:103:GLU:OE1	1:D:104:GLN:N	2.46	0.49
1:D:221:ARG:O	1:D:223:GLN:HG2	2.12	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
3:I:141:ASN:HA	3:I:175:THR:HB	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:176:ALA:CB	3:I:166:TRP:CE2	2.90	0.49
3:I:9:SER:HB2	3:I:106:LYS:HZ3	1.78	0.49
1:J:56:ASN:HD21	1:J:88:GLY:HA2	1.77	0.49
2:K:176:ALA:O	2:K:185:SER:N	2.45	0.49
2:K:54:SER:HB3	2:K:56:ARG:NE	2.28	0.49
3:L:141:ASN:N	3:L:175:THR:HB	2.27	0.49
1:A:151:LEU:HD12	1:A:250:VAL:HG13	1.94	0.49
2:E:152:ASP:OD1	2:E:178:LEU:HD22	2.13	0.49
2:K:201:THR:CG2	2:K:218:LYS:HD3	2.42	0.49
2:K:34:SER:OG	2:K:98:HIS:NE2	2.46	0.49
2:K:39:ALA:CB	2:K:44:LEU:HG	2.43	0.49
3:L:88:ASN:ND2	3:L:90:PHE:CE2	2.80	0.49
3:C:78:ILE:HD11	3:C:81:VAL:HA	1.94	0.49
2:H:90:THR:CG2	2:H:118:THR:HA	2.36	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:K:162:TRP:CZ2	2:K:204:CYS:HB3	2.48	0.49
3:L:62:PRO:HB2	3:L:64:ARG:HG3	1.94	0.49
1:A:183:SER:OG	1:A:224:GLU:HB2	2.13	0.48
1:D:179:ILE:HG22	1:D:181:HIS:NE2	2.27	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:E:173:THR:HG21	3:F:178:MET:CG	2.43	0.48
2:H:37:ARG:HB3	2:H:93:TYR:CE2	2.48	0.48
2:K:162:TRP:CH2	2:K:204:CYS:HB3	2.47	0.48
2:K:178:LEU:C	2:K:180:SER:N	2.65	0.48
2:K:34:SER:OG	2:K:49:GLY:CA	2.61	0.48
2:K:34:SER:CB	2:K:98:HIS:NE2	2.76	0.48
1:A:226:ARG:HD3	1:A:226:ARG:HA	1.46	0.48
2:B:32:ASP:HB2	2:B:98:HIS:NE2	2.28	0.48
2:B:78:LEU:C	2:B:78:LEU:HD12	2.33	0.48
3:C:12:VAL:HG13	3:C:13:SER:N	2.27	0.48
3:C:39:PHE:O	3:C:40:GLN:HB2	2.12	0.48
3:C:66:SER:N	3:C:77:THR:O	2.45	0.48
1:D:97:ASP:HB2	1:D:231:TRP:HE1	1.79	0.48
2:E:172:HIS:ND1	2:E:188:SER:HB2	2.28	0.48
1:G:56:ASN:HA	1:G:81:GLU:HB2	1.95	0.48
3:I:197:CYS:O	3:I:208:ILE:O	2.31	0.48
1:J:113:ARG:HB2	1:J:255:PHE:CE1	2.47	0.48
2:B:177:VAL:HA	2:B:184:TYR:CD2	2.48	0.48
2:B:35:TRP:CZ3	2:B:95:CYS:HB2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:LYS:HG2	1:D:120:THR:H	1.77	0.48
3:F:13:SER:CB	3:F:110:LYS:NZ	2.76	0.48
2:E:96:ALA:HB1	3:F:36:ILE:HG21	1.94	0.48
1:G:57:ILE:CD1	1:G:102:ARG:HB2	2.43	0.48
3:I:102:PHE:HE1	3:I:104:GLY:C	2.17	0.48
1:J:184:THR:O	1:J:186:ALA:N	2.46	0.48
1:J:192:TYR:HB3	1:J:246:GLY:HA3	1.95	0.48
3:L:90:PHE:HA	3:L:102:PHE:CZ	2.49	0.48
1:A:122:SER:O	1:A:124:PRO:HD3	2.13	0.48
1:A:57:ILE:HG22	1:A:58:ALA:N	2.29	0.48
1:D:51:HIS:ND1	1:D:80:VAL:HG21	2.27	0.48
1:D:57:ILE:HG13	1:D:81:GLU:OE2	2.14	0.48
3:F:193:ASN:ND2	3:F:211:SER:OG	2.46	0.48
3:F:38:TRP:HB2	3:F:48:LYS:O	2.14	0.48
2:H:97:ARG:HE	2:H:110:GLY:HA3	1.79	0.48
1:J:165:TYR:CE2	1:J:173:VAL:HG21	2.48	0.48
2:K:163:ASN:HD22	2:K:163:ASN:H	1.61	0.48
3:L:170:ASP:CB	3:L:175:THR:OG1	2.61	0.48
3:L:36:ILE:HD13	3:L:36:ILE:C	2.33	0.48
3:C:194:SER:HA	3:C:210:LYS:CB	2.36	0.48
3:C:205:THR:HG23	3:C:205:THR:O	2.13	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
1:D:227:MET:HB3	1:D:229:TYR:CZ	2.48	0.48
3:F:140:ASN:OD1	3:F:176:TYR:HD1	1.96	0.48
3:F:149:VAL:CG2	3:F:149:VAL:O	2.60	0.48
1:G:153:LYS:CD	1:G:193:GLN:HB2	2.43	0.48
1:G:219:LYS:HG3	1:G:223:GLN:H	1.78	0.48
3:L:127:GLN:O	3:L:130:SER:OG	2.32	0.48
1:A:54:LYS:HG2	1:A:55:CYS:N	2.23	0.48
2:B:145:ALA:HA	2:B:191:THR:HA	1.96	0.48
2:B:51:LEU:HD13	2:B:52:GLY:O	2.13	0.48
3:C:164:ASN:N	3:C:164:ASN:ND2	2.61	0.48
2:B:171:VAL:HG11	3:C:176:TYR:CE2	2.48	0.48
1:D:90:CYS:SG	1:D:145:TYR:CE1	3.07	0.48
2:E:125:LYS:HD2	2:E:126:GLY:H	1.78	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:I:162:VAL:O	3:I:162:VAL:CG2	2.61	0.48
3:I:209:VAL:CG2	3:I:210:LYS:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:133:THR:HG23	1:J:135:ALA:N	2.25	0.48
3:L:102:PHE:CD1	3:L:104:GLY:N	2.63	0.48
1:A:105:LEU:HD23	1:A:257:MET:SD	2.54	0.48
2:B:180:SER:O	2:B:182:GLY:O	2.32	0.48
3:C:38:TRP:CG	3:C:39:PHE:HA	2.41	0.48
3:C:45:GLN:CB	3:C:46:PRO:HD2	2.35	0.48
2:E:10:VAL:HG13	2:E:155:PRO:HB3	1.96	0.48
2:E:92:VAL:HA	2:E:115:THR:O	2.12	0.48
3:F:38:TRP:CD1	3:F:40:GLN:O	2.65	0.48
3:F:2:GLN:OE1	3:F:97:VAL:HG21	2.14	0.48
2:H:186:LEU:C	2:H:186:LEU:CD1	2.82	0.48
3:I:52:TYR:O	3:I:56:ASN:HB2	2.14	0.48
1:J:185:SER:N	1:J:214:ILE:HG21	2.29	0.48
3:L:163:LEU:C	3:L:163:LEU:CD1	2.77	0.48
1:A:219:LYS:HG2	1:A:222:ASP:C	2.34	0.48
3:C:140:ASN:ND2	3:C:176:TYR:HD1	2.12	0.48
3:C:93:GLN:O	3:C:94:THR:C	2.46	0.48
2:H:163:ASN:C	2:H:165:GLY:H	2.16	0.48
1:J:151:LEU:HD12	1:J:250:VAL:CG1	2.43	0.48
2:K:178:LEU:HD11	3:L:182:LEU:CD1	2.42	0.48
3:L:52:TYR:O	3:L:56:ASN:CB	2.62	0.48
3:L:56:ASN:ND2	4:L:303:HOH:O	2.46	0.48
1:A:232:THR:HG23	1:A:233:LEU:N	2.28	0.48
2:B:173:THR:HB	3:C:178:MET:CE	2.38	0.48
2:B:36:ILE:CB	2:B:46:TRP:HA	2.41	0.48
2:E:2:VAL:N	2:E:3:LYS:HE2	2.29	0.48
2:E:46:TRP:C	2:E:60:ARG:NH1	2.67	0.48
2:H:2:VAL:HA	2:H:24:SER:C	2.34	0.48
3:I:92:GLN:O	3:I:93:GLN:C	2.52	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
3:C:9:SER:C	3:C:106:LYS:HG2	2.34	0.48
1:A:215:ALA:HB1	1:D:96:ILE:HG21	1.95	0.48
1:G:114:PHE:N	1:G:114:PHE:CD2	2.79	0.48
1:G:188:GLN:O	1:G:192:TYR:N	2.41	0.48
2:H:197:LEU:HD12	2:H:198:GLY:H	1.75	0.48
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:J:125:ASN:O	1:J:154:LYS:HB3	2.14	0.48
1:J:217:ARG:N	1:J:224:GLU:O	2.38	0.48
2:K:205:ASN:HA	2:K:215:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:38:GLN:O	2:K:91:ALA:HB1	2.13	0.48
3:L:79:ASN:HB3	3:L:80:PRO:CD	2.41	0.48
1:A:137:PRO:CA	1:A:142:LYS:HA	2.41	0.47
3:C:157:GLU:O	3:C:158:ARG:HG2	2.14	0.47
3:C:39:PHE:CB	3:C:50:LEU:H	2.19	0.47
1:D:153:LYS:HE3	1:D:156:ASN:CA	2.40	0.47
1:D:82:THR:O	1:D:82:THR:OG1	2.31	0.47
2:E:116:THR:HG22	2:E:116:THR:O	2.14	0.47
2:E:146:LEU:N	2:E:190:VAL:O	2.48	0.47
2:E:205:ASN:HD22	2:E:214:LYS:HE3	1.79	0.47
2:E:56:ARG:HB3	2:E:58:TYR:CE1	2.49	0.47
2:E:28:GLY:O	2:E:71:ARG:CZ	2.62	0.47
3:F:158:ARG:HG3	3:F:159:GLN:N	2.29	0.47
3:F:83:ALA:O	3:F:171:SER:O	2.32	0.47
3:F:37:ASN:OD1	3:F:95:LYS:HE2	2.14	0.47
2:H:6:GLU:HA	2:H:20:SER:O	2.14	0.47
2:K:50:ILE:HB	2:K:56:ARG:O	2.14	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:B:177:VAL:HG12	2:B:182:GLY:HA2	1.97	0.47
1:D:64:ASN:OD1	1:D:65:PRO:HD2	2.14	0.47
2:E:86:ARG:O	2:E:119:VAL:HG21	2.14	0.47
3:F:209:VAL:HG22	3:F:210:LYS:CB	2.44	0.47
3:F:97:VAL:CG1	3:F:98:PRO:N	2.76	0.47
2:H:117:VAL:CG1	2:H:117:VAL:O	2.60	0.47
2:H:52:GLY:O	2:H:53:GLY:C	2.52	0.47
3:I:123:PRO:CB	3:I:133:ALA:HB1	2.41	0.47
3:I:209:VAL:CG2	3:I:210:LYS:HG2	2.43	0.47
1:J:114:PHE:HA	3:L:96:GLU:CD	2.35	0.47
1:J:176:LEU:HA	1:J:230:TYR:O	2.15	0.47
2:K:175:PRO:O	3:L:166:TRP:CE3	2.66	0.47
1:A:175:VAL:C	1:A:176:LEU:HD12	2.34	0.47
3:C:7:PRO:CD	3:C:21:THR:O	2.53	0.47
1:D:211:LYS:HG3	1:D:212:PRO:HD2	1.96	0.47
2:E:56:ARG:HD2	2:E:56:ARG:HA	1.46	0.47
2:E:48:SER:CB	2:E:59:TYR:HD1	2.27	0.47
3:F:135:VAL:HG12	3:F:151:TRP:CZ3	2.48	0.47
3:F:38:TRP:CD2	3:F:90:PHE:O	2.66	0.47
1:G:241:THR:HG22	1:G:242:PHE:H	1.76	0.47
2:H:93:TYR:CE1	2:H:117:VAL:HG12	2.45	0.47
2:H:162:TRP:CZ2	2:H:204:CYS:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:63:VAL:CG1	2:H:66:ARG:H	2.26	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
3:L:23:ARG:HD2	3:L:72:THR:HG23	1.96	0.47
2:B:143:THR:HG22	2:B:143:THR:O	2.13	0.47
2:B:150:VAL:HB	2:B:186:LEU:HG	1.95	0.47
1:D:164:SER:H	2:E:56:ARG:HH22	1.60	0.47
2:E:48:SER:HB3	2:E:59:TYR:HD1	1.78	0.47
3:F:13:SER:HB3	3:F:110:LYS:HB3	1.96	0.47
3:F:38:TRP:CE2	3:F:90:PHE:N	2.82	0.47
1:G:151:LEU:HD12	1:G:250:VAL:HG11	1.97	0.47
3:I:9:SER:HB3	3:I:106:LYS:CG	2.42	0.47
1:J:182:PRO:O	1:J:214:ILE:HG23	2.13	0.47
1:J:200:PHE:CG	1:J:201:VAL:N	2.82	0.47
1:J: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
3:L:86:THR:HG22	3:L:109:ILE:HD13	1.97	0.47
2:B:196:SER:O	2:B:200:GLN:N	2.48	0.47
3:C:34:ASN:N	3:C:34:ASN:ND2	2.62	0.47
1:D:114:PHE:CE2	1:D:254:ALA:HB3	2.49	0.47
1:D:64:ASN:HD21	1:D:90:CYS:HB3	1.79	0.47
2:E:2:VAL:C	2:E:3:LYS:HE2	2.34	0.47
3:F:114:ALA:HA	3:F:201:HIS:HD2	1.79	0.47
3:F:173:ASP:OD1	3:F:175:THR:OG1	2.32	0.47
3:F:38:TRP:CH2	3:F:39:PHE:CD1	3.02	0.47
1:G:54:LYS:CG	1:G:67:CYS:HA	2.12	0.47
2:H:37:ARG:HB3	2:H:93:TYR:CD2	2.48	0.47
2:H:51:LEU:HD12	2:H:52:GLY:O	2.13	0.47
2:E:181:SER:CB	3:I:62:PRO:HG3	2.38	0.47
1:J:248:LEU:HD12	1:J:249:VAL:H	1.75	0.47
3:L:12:VAL:O	3:L:109:ILE:HA	2.15	0.47
2:B:27:THR:CG2	2:B:31:TYR:CG	2.98	0.47
3:C:116:PRO:HB2	3:C:139:LEU:HB3	1.96	0.47
3:C:68:SER:OG	3:C:75:THR:HB	2.14	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
2:E:51:LEU:HD12	2:E:56:ARG:N	2.28	0.47
3:F:126:GLU:O	3:F:129:THR:HG23	2.15	0.47
2:E:173:THR:HG22	3:F:178:MET:SD	2.55	0.47
3:F:95:LYS:O	3:F:96:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:GLY:CA	1:G:150:TRP:HB3	2.44	0.47
1:G:153:LYS:HD2	1:G:193:GLN:HB2	1.95	0.47
2:H:202:TYR:CD1	2:H:219:SER:HB2	2.48	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
1:A:212:PRO:HB3	1:A:247:ASN:ND2	2.29	0.47
2:B:197:LEU:C	2:B:199:THR:N	2.66	0.47
3:C:97:VAL:HG13	3:C:98:PRO:CD	2.42	0.47
1:D:184:THR:H	1:D:187:ASP:CB	2.28	0.47
2:E:82:MET:CE	2:E:117:VAL:HG21	2.45	0.47
2:E:189:VAL:HG12	3:F:138:PHE:CE2	2.49	0.47
2:E:45:GLU:HB3	2:E:60:ARG:HH22	1.76	0.47
2:E:44:LEU:HD23	2:E:45:GLU:HG2	1.95	0.47
3:F:43:PRO:HD3	3:F:87:ALA:HA	1.97	0.47
1:G:119:LYS:HZ2	1:G:129:ASN:HD22	1.53	0.47
1:G:77:SER:OG	1:G:78:TYR:N	2.48	0.47
2:H:208:HIS:O	2:H:212:ASN:CA	2.62	0.47
2:H:63:VAL:HG11	2:H:67:SER:H	1.80	0.47
3:I:148:ASN:OD1	3:I:149:VAL:N	2.47	0.47
3:I:81:VAL:HG12	3:I:82:GLU:H	1.78	0.47
1:J:217:ARG:HD3	1:J:226:ARG:HG2	1.97	0.47
1:J:382:VAL:O	1:J:385:VAL:N	2.48	0.47
2:K:66:ARG:HH22	2:K:89:ASP:CG	2.18	0.47
3:L:204:SER:HA	4:L:310:HOH:O	2.15	0.47
3:L:2:GLN:HA	3:L:25:SER:OG	2.14	0.47
1:A:177:TRP:CZ2	1:A:230:TYR:HB2	2.50	0.47
2:B:17:LEU:HD21	2:B:19:LEU:HD13	1.95	0.47
2:B:211:SER:CB	2:B:213:THR:HG1	2.28	0.47
1:D:161:LEU:O	1:D:243:GLU:HA	2.15	0.47
3:F:143:TYR:CE2	3:F:144:PRO:HB3	2.49	0.47
3:F:167:THR:HG22	3:F:168:ASP:H	1.79	0.47
3:F:52:TYR:O	3:F:56:ASN:HB2	2.14	0.47
1:G:184:THR:C	1:G:214:ILE:HG21	2.35	0.47
1:G:235:GLU:CG	1:G:236:PRO:CD	2.91	0.47
1:G:94:ASP:O	1:G:228:ASN:HA	2.15	0.47
3:I:6:SER:HB3	3:I:7:PRO:CD	2.38	0.47
2:B:174:PHE:CD1	2:B:174:PHE:N	2.80	0.47
2:B:6:GLU:HG2	2:B:35:TRP:HZ3	1.80	0.47
3:C:5:GLN:HB3	3:C:102:PHE:CD1	2.50	0.47
3:C:153:ILE:HA	3:C:194:SER:O	2.15	0.47
3:C:89:TYR:O	3:C:104:GLY:HA2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:203:ILE:HD12	2:E:217:LYS:C	2.34	0.47
3:F:41:GLN:O	3:F:87:ALA:HB1	2.15	0.47
1:G:187:ASP:O	1:G:191:LEU:HB2	2.14	0.47
3:I:196:THR:OG1	3:I:210:LYS:CD	2.52	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
1:A:161:LEU:HD23	1:A:161:LEU:O	2.15	0.47
2:B:86:ARG:NE	2:B:88:GLU:OE1	2.45	0.47
2:B:173:THR:CG2	3:C:178:MET:SD	3.02	0.47
1:D:57:ILE:HD11	1:D:102:ARG:HG3	1.97	0.47
2:E:36:ILE:O	2:E:94:TYR:HB2	2.15	0.47
2:E:37:ARG:HG3	2:E:37:ARG:O	2.14	0.47
3:F:158:ARG:HD3	2:H:31:TYR:CZ	2.50	0.47
1:J:64:ASN:O	1:J:67:CYS:HB2	2.15	0.47
2:K:162:TRP:N	2:K:162:TRP:CD1	2.82	0.47
2:K:17:LEU:HB3	2:K:82:MET:HG2	1.96	0.47
3:L:14:PRO:HG3	3:L:111:ARG:HH12	1.79	0.47
3:L:173:ASP:HA	4:L:311:HOH:O	2.14	0.47
1:A:57:ILE:HD11	1:A:79:ILE:HD13	1.97	0.47
2:B:173:THR:HG23	2:B:187:SER:O	2.15	0.47
3:C:89:TYR:O	3:C:104:GLY:CA	2.63	0.47
3:C:138:PHE:HD1	3:C:178:MET:CG	2.14	0.47
3:C:161:GLY:C	3:C:162:VAL:HG22	2.36	0.47
2:B:173:THR:CA	3:C:178:MET:HE3	2.45	0.47
1:D:98:TYR:HE2	1:D:102:ARG:HH21	1.54	0.47
1:D:188:GLN:NE2	1:D:194:ASN:O	2.48	0.47
3:F:108:GLU:HG2	3:F:169:GLN:NE2	2.29	0.47
1:D:115:GLU:HB2	3:F:96:GLU:CG	2.45	0.47
2:H:47:VAL:O	2:H:48:SER:HB2	2.15	0.47
3:I:116:PRO:HA	3:I:140:ASN:O	2.15	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:L:156:SER:O	3:L:157:GLU:CB	2.61	0.47
3:L:42:LYS:C	3:L:44:GLY:N	2.68	0.47
1:A:123:TRP:NE1	1:A:149:ILE:HD13	2.29	0.46
3:C:50:LEU:HD13	3:C:65:PHE:CD1	2.50	0.46
1:D:99:GLU:HG2	1:D:100:GLU:N	2.29	0.46
2:E:180:SER:C	2:E:182:GLY:N	2.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:ALA:HB3	1:G:223:GLN:HE21	1.80	0.46
2:H:146:LEU:HD12	2:H:162:TRP:CZ3	2.51	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:K:162:TRP:CD2	2:K:204:CYS:HB3	2.50	0.46
3:L:16:GLN:O	3:L:81:VAL:HG23	2.15	0.46
3:L:139:LEU:HD21	3:L:199:ALA:CB	2.45	0.46
1:A:152:VAL:HG11	1:A:191:LEU:HD12	1.98	0.46
2:B:132:LEU:HD11	2:B:149:LEU:HB2	1.98	0.46
2:E:46:TRP:O	2:E:60:ARG:NH1	2.48	0.46
3:F:110:LYS:O	3:F:111:ARG:CG	2.64	0.46
1:G:186:ALA:O	1:G:189:GLN:HB3	2.15	0.46
1:J:177:TRP:N	1:J:177:TRP:CE3	2.83	0.46
3:C:128:LEU:HD13	3:C:129:THR:N	2.18	0.46
1:G:132:VAL:CG2	1:G:132:VAL:O	2.63	0.46
2:H:132:LEU:HD13	2:H:132:LEU:N	2.31	0.46
1:J:90:CYS:HB2	1:J:135:ALA:O	2.15	0.46
1:J:182:PRO:HG2	1:J:188:GLN:CA	2.45	0.46
2:K:78:LEU:HD23	2:K:78:LEU:H	1.80	0.46
3:L:111:ARG:HB2	3:L:143:TYR:CD1	2.51	0.46
2:K:176:ALA:CB	3:L:166:TRP:CZ2	2.98	0.46
1:D:165:TYR:HB3	1:D:240:ILE:HG22	1.97	0.46
3:F:196:THR:CG2	3:F:209:VAL:HG23	2.45	0.46
1:G:75:SER:OG	1:G:109:SER:O	2.30	0.46
1:G:149:ILE:HB	1:G:250:VAL:CG2	2.45	0.46
1:G:197:ALA:O	1:G:212:PRO:HD2	2.15	0.46
1:G:231:TRP:CZ3	1:G:233:LEU:HD13	2.49	0.46
2:H:44:LEU:N	4:H:305:HOH:O	2.48	0.46
2:H:73:ASN:OD1	2:H:73:ASN:N	2.37	0.46
3:I:143:TYR:HB2	3:I:174:SER:HB2	1.97	0.46
2:K:171:VAL:HG22	3:L:176:TYR:CE1	2.50	0.46
3:L:92:GLN:O	3:L:93:GLN:C	2.54	0.46
1:A:153:LYS:HB2	1:A:157:SER:O	2.16	0.46
2:B:156:GLU:CB	2:B:157:PRO:HA	2.46	0.46
3:C:37:ASN:HB3	3:C:38:TRP:O	2.15	0.46
3:C:38:TRP:CZ3	3:C:40:GLN:N	2.84	0.46
3:C:90:PHE:HD2	3:C:90:PHE:N	2.12	0.46
1:D:99:GLU:CG	1:D:100:GLU:H	2.29	0.46
1:D:116:ILE:HG22	1:D:252:ARG:O	2.16	0.46
2:E:186:LEU:CG	2:E:187:SER:N	2.78	0.46
3:F:193:ASN:HA	3:F:195:TYR:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:42:LYS:HD2	3:F:87:ALA:CB	2.45	0.46
1:G:133:THR:O	1:G:142:LYS:HB2	2.15	0.46
1:G:216:ILE:O	1:G:216:ILE:HG22	2.16	0.46
1:G:220:VAL:HG23	1:G:226:ARG:HH22	1.80	0.46
2:H:63:VAL:CG1	2:H:67:SER:H	2.28	0.46
2:K:158:VAL:HG23	2:K:208:HIS:HD2	1.80	0.46
2:K:162:TRP:CZ3	2:K:204:CYS:HB3	2.50	0.46
3:L:179:SER:HB2	4:L:302:HOH:O	2.15	0.46
1:A:153:LYS:HG3	1:A:153:LYS:O	2.15	0.46
2:B:162:TRP:HD1	2:B:170:SER:OG	1.98	0.46
2:E:215:VAL:HG22	2:E:216:ASP:N	2.30	0.46
2:E:171:VAL:HG21	3:F:176:TYR:CD1	2.50	0.46
1:G:117:PHE:HB2	1:G:251:PRO:O	2.16	0.46
1:G:149:ILE:CD1	1:G:252:ARG:HB2	2.45	0.46
2:H:119:VAL:O	2:H:119:VAL:HG12	2.16	0.46
1:J: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:K:147:GLY:O	2:K:162:TRP:HH2	1.98	0.46
2:K:174:PHE:HD2	3:L:166:TRP:HE3	1.64	0.46
1:D:144:PHE:CZ	1:D:150:TRP:HB2	2.49	0.46
1:D:199:VAL:HG13	1:D:244:ALA:HB2	1.98	0.46
2:E:174:PHE:CD1	2:E:175:PRO:HD2	2.51	0.46
3:F:13:SER:HB3	3:F:110:LYS:CD	2.46	0.46
3:F:24:ALA:N	3:F:72:THR:O	2.48	0.46
3:F:96:GLU:O	3:F:97:VAL:CG2	2.60	0.46
2:H:179:GLN:HG2	3:I:163:LEU:HB2	1.96	0.46
3:I: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:J:101:LEU:HG	1:J:231:TRP:CD2	2.50	0.46
1:J:211:LYS:HB2	1:J:211:LYS:HZ2	1.79	0.46
1:A:114:PHE:CE2	1:A:254:ALA:HB3	2.51	0.46
1:A:51:HIS:HA	1:A:80:VAL:HB	1.97	0.46
2:B:215:VAL:C	2:B:216:ASP:OD1	2.55	0.46
1:D:147:ASN:HD21	1:D:255:PHE:HZ	1.64	0.46
2:E:9:ALA:H	2:E:17:LEU:HD21	1.81	0.46
2:E:51:LEU:CD1	2:E:55:GLU:N	2.79	0.46
3:F:1:ILE:HD13	3:F:1:ILE:HA	1.74	0.46
3:F:202:LYS:HA	4:F:308:HOH:O	2.16	0.46
1:G:177:TRP:HZ2	1:G:206:TYR:HH	1.62	0.46
2:H:171:VAL:C	2:H:172:HIS:ND1	2.67	0.46
3:I:91:CYS:N	3:I:102:PHE:CE2	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:215:ALA:H	1:J:217:ARG:NH1	2.13	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
2:K:82:MET:HG3	2:K:85:LEU:HD21	1.98	0.46
3:L:161:GLY:C	3:L:162:VAL:HG12	2.36	0.46
3:L:97:VAL:O	3:L:99:TYR:CD1	2.69	0.46
1:A:122:SER:C	1:A:124:PRO:HD3	2.36	0.46
1:A:57:ILE:CG1	1:A:81:GLU:OE2	2.64	0.46
2:B:4:LEU:HB2	2:B:112:GLY:CA	2.46	0.46
3:C:9:SER:HA	3:C:106:LYS:H	1.80	0.46
3:C:97:VAL:CG1	3:C:98:PRO:N	2.79	0.46
1:D:84:SER:O	1:D:86:ASP:N	2.48	0.46
3:F:3:MET:CG	3:F:5:GLN:HE21	2.21	0.46
1:G:200:PHE:HB3	1:G:243:GLU:HB2	1.97	0.46
2:H:117:VAL:O	2:H:117:VAL:HG13	2.15	0.46
2:H:156:GLU:OE2	2:H:175:PRO:HG3	2.16	0.46
2:H:178:LEU:C	2:H:180:SER:N	2.69	0.46
3:I:20:ILE:HG21	3:I:105:THR:HG21	1.97	0.46
1:J:43:LYS:HZ3	1:J:43:LYS:HB3	1.81	0.46
3:L:140:ASN:HB2	3:L:141:ASN:ND2	2.31	0.46
1:A:208:LYS:HG2	1:A:209:LYS:N	2.30	0.46
2:B:178:LEU:C	2:B:180:SER:H	2.20	0.46
3:C:133:ALA:O	3:C:183:THR:HB	2.16	0.46
3:C:51:ILE:HD13	3:C:76:LEU:HD12	1.98	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
3:F:39:PHE:CD2	3:F:51:ILE:HB	2.50	0.46
3:F:78:ILE:HG22	3:F:79:ASN:O	2.16	0.46
1:G:151:LEU:HD12	1:G:250:VAL:CG1	2.46	0.46
3:I:1:ILE:O	3:I:2:GLN:HB3	2.16	0.46
3:I:89:TYR:CD2	3:I:89:TYR:N	2.83	0.46
3:I:96:GLU:O	3:I:97:VAL:HG23	2.16	0.46
1:A:64:ASN:CG	1:A:66:GLU:HG2	2.37	0.45
2:B:51:LEU:HD13	2:B:51:LEU:C	2.36	0.45
2:E:51:LEU:HD13	2:E:52:GLY:O	2.17	0.45
2:E:86:ARG:N	2:E:119:VAL:HG11	2.31	0.45
1:G:222:ASP:OD1	1:G:222:ASP:O	2.33	0.45
1:G:172:GLU:O	1:G:256:ALA:HA	2.16	0.45
1:G:77:SER:O	1:G:106:SER:O	2.34	0.45
2:H:60:ARG:HH22	3:I:99:TYR:C	2.18	0.45
3:I:144:PRO:O	3:I:201:HIS:HE1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:42:LYS:HE2	3:I:42:LYS:HB3	1.82	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:K:18:ARG:HD2	2:K:81:GLU:HB2	1.96	0.45
3:L:123:PRO:CB	3:L:133:ALA:HB1	2.42	0.45
1:A:126:HIS:ND1	1:A:126:HIS:N	2.64	0.45
1:A:258:GLU:HG3	1:A:259:ARG:N	2.32	0.45
2:B:203:ILE:HD11	2:B:216:ASP:CB	2.35	0.45
3:C:92:GLN:CA	3:C:101:THR:HG23	2.45	0.45
1:D:148:LEU:HD23	1:D:251:PRO:N	2.31	0.45
1:G:75:SER:OG	1:G:110:SER:HA	2.16	0.45
2:H:171:VAL:HB	2:H:189:VAL:HG13	1.98	0.45
2:K:69:ILE:CG1	2:K:70:SER:N	2.79	0.45
3:L:36:ILE:HG23	3:L:36:ILE:O	2.16	0.45
1:D:200:PHE:CG	1:D:201:VAL:N	2.84	0.45
1:D:177:TRP:CE2	1:D:230:TYR:HB2	2.52	0.45
1:D:231:TRP:HZ3	1:D:233:LEU:HD22	1.80	0.45
2:E:6:GLU:HG3	2:E:35:TRP:CZ3	2.51	0.45
1:G:116:ILE:HG23	1:G:117:PHE:N	2.31	0.45
1:G:167:ASN:C	1:G:167:ASN:OD1	2.55	0.45
1:G:219:LYS:CG	1:G:222:ASP:HA	2.46	0.45
1:J:421:ILE:O	1:J:424:TYR:N	2.45	0.45
1:J:48:ALA:HB1	1:J:78:TYR:CE1	2.51	0.45
3:L:193:ASN:O	3:L:211:SER:CB	2.64	0.45
3:L:34:ASN:O	3:L:95:LYS:HD3	2.15	0.45
1:A:84:SER:OG	1:A:87:ASN:HB2	2.16	0.45
2:B:30:ASP:O	2:B:52:GLY:HA3	2.17	0.45
3:C:14:PRO:O	3:C:81:VAL:O	2.33	0.45
1:D:182:PRO:HG2	1:D:188:GLN:HA	1.99	0.45
3:F:120:ILE:HB	3:F:197:CYS:SG	2.57	0.45
3:F: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
1:G:100:GLU:HG2	1:G:231:TRP:HZ2	1.82	0.45
1:J:211:LYS:HB2	1:J:211:LYS:HZ1	1.77	0.45
2:K: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:A:150:TRP:C	1:A:150:TRP:CD1	2.90	0.45
1:A:167:ASN:OD1	1:A:167:ASN:C	2.54	0.45
2:B:47:VAL:O	2:B:48:SER:HB3	2.16	0.45
3:C:162:VAL:O	3:C:164:ASN:CG	2.55	0.45
1:D:147:ASN:ND2	1:D:255:PHE:HZ	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:LYS:CD	1:D:160:LYS:H	2.25	0.45
1:D:61:ILE:HD13	1:D:61:ILE:O	2.15	0.45
2:E:45:GLU:CB	2:E:60:ARG:NH2	2.76	0.45
1:G:199:VAL:CG1	1:G:248:LEU:HD22	2.46	0.45
3:I:143:TYR:CE1	3:I:144:PRO:HB3	2.52	0.45
1:J:253:TYR:OH	3:L:97:VAL:HG23	2.17	0.45
3:L:108:GLU:OE1	3:L:108:GLU:CA	2.58	0.45
3:L:97:VAL:HG13	3:L:98:PRO:CD	2.47	0.45
1:A:122:SER:HB2	1:A:123:TRP:CE2	2.52	0.45
1:A:64:ASN:OD1	1:A:66:GLU:HG2	2.17	0.45
2:B:146:LEU:HA	2:B:146:LEU:HD13	1.77	0.45
2:E:50:ILE:CG2	2:E:69:ILE:HG23	2.47	0.45
3:F:191:ARG:NE	3:F:192:HIS:CE1	2.85	0.45
3:F:38:TRP:CA	3:F:49:LEU:HD23	2.46	0.45
3:F:79:ASN:O	3:F:80:PRO:O	2.35	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
2:H:63:VAL:C	2:H:65:GLY:N	2.64	0.45
2:H:98:HIS:H	2:H:98:HIS:CD2	2.34	0.45
3:I:7:PRO:HG3	3:I:21:THR:H	1.78	0.45
1:J:235:GLU:CG	1:J:236:PRO:CD	2.92	0.45
2:K:92:VAL:HG11	2:K:94:TYR:CE2	2.52	0.45
3:L:162:VAL:O	3:L:163:LEU:C	2.53	0.45
3:L:213:ASN:C	3:L:213:ASN:OD1	2.55	0.45
3:L:42:LYS:HE3	3:L:85:ASP:O	2.16	0.45
1:A:174:LEU:HD12	1:A:231:TRP:CE3	2.51	0.45
3:C:114:ALA:O	3:C:116:PRO:HD3	2.17	0.45
3:C:151:TRP:CZ3	3:C:197:CYS:HB3	2.52	0.45
3:C:207:PRO:O	3:C:208:ILE:HD12	2.17	0.45
1:D:201:VAL:C	1:D:241:THR:O	2.55	0.45
1:D:217:ARG:HB3	1:D:218:PRO:HD2	1.97	0.45
1:G:101:LEU:HA	1:G:101:LEU:HD23	1.73	0.45
2:H:37:ARG:HD3	2:H:93:TYR:CZ	2.52	0.45
3:I:150:LYS:HB2	3:I:150:LYS:HE2	1.70	0.45
3:I:111:ARG:NE	3:I:173:ASP:HA	2.24	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:114:ALA:HA	3:L:201:HIS:CD2	2.52	0.45
3:L:40:GLN:HE21	3:L:50:LEU:HD21	1.81	0.45
1:A:138:HIS:HB2	1:A:143:SER:HB2	1.99	0.45
2:B:27:THR:HG22	2:B:31:TYR:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:TRP:CD1	1:D:150:TRP:C	2.90	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
1:D:56:ASN:OD1	1:D:56:ASN:N	2.43	0.45
2:E:45:GLU:HB3	2:E:60:ARG:HH12	1.78	0.45
3:F:8:ALA:HB1	3:F:105:THR:OG1	2.17	0.45
2:H:113:GLN:O	3:I:45:GLN:NE2	2.42	0.45
3:I:91:CYS:SG	3:I:102:PHE:CD2	3.10	0.45
1:J:76:TRP:CD2	1:J:108:VAL:HG22	2.52	0.45
1:J:132:VAL:HG23	1:J:142:LYS:HG3	1.98	0.45
3:L: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
3:L:34:ASN:OD1	3:L:34:ASN:N	2.49	0.45
1:A:229:TYR:C	1:A:230:TYR:CD1	2.90	0.45
2:B:196:SER:O	2:B:202:TYR:HE2	1.99	0.45
2:B:54:SER:O	2:B:56:ARG:HD2	2.17	0.45
2:B:78:LEU:C	2:B:78:LEU:CD1	2.85	0.45
2:B:35:TRP:CH2	2:B:95:CYS:HB2	2.52	0.45
3:C:210:LYS:HD2	3:C:211:SER:N	2.18	0.45
2:E:31:TYR:O	2:E:71:ARG:NH2	2.50	0.45
2:E:97:ARG:HG2	2:E:98:HIS:H	1.82	0.45
1:G:177:TRP:CZ2	1:G:206:TYR:CZ	3.05	0.45
2:H:72:ASP:CB	2:H:79:TYR:CE2	2.93	0.45
2:E:179:GLN:CB	3:I:60:GLY:HA2	2.29	0.45
2:K:211:SER:O	2:K:213:THR:N	2.50	0.45
3:L:191:ARG:HD2	3:L:191:ARG:C	2.36	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
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
1:A:216:ILE:N	1:D:96:ILE:HG23	2.32	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
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
3:F:26:GLU:O	3:F:27:SER:OG	2.33	0.44
2:H:162:TRP:HA	2:H:203:ILE:O	2.17	0.44
1:J:216:ILE:O	1:J:216:ILE:HG22	2.16	0.44
2:K:209:LYS:HB2	2:K:210:PRO:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:43:GLY:O	2:K:44:LEU:CD2	2.65	0.44
3:L:195:TYR:H	3:L:210:LYS:HA	1.81	0.44
3:C:166:TRP:CE3	3:C:166:TRP:HA	2.51	0.44
1:D:127:ASP:N	1:D:154:LYS:HB3	2.31	0.44
1:D:220:VAL:O	1:D:223:GLN:HB2	2.17	0.44
3:F:140:ASN:CG	3:F:176:TYR:CD1	2.87	0.44
3:F:135:VAL:CG1	3:F:151:TRP:CZ3	3.00	0.44
3:F:172:LYS:O	3:F:173:ASP:CB	2.65	0.44
1:G:164:SER:H	2:H:56:ARG:NH2	2.15	0.44
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
3:L:209:VAL:HG23	3:L:210:LYS:CG	2.47	0.44
2:B:45:GLU:HG2	2:B:60:ARG:CZ	2.47	0.44
2:E:66:ARG:CZ	2:E:86:ARG:HD3	2.46	0.44
3:F:54:ALA:O	3:F:67:GLY:HA3	2.18	0.44
3:F:97:VAL:HG13	3:F:98:PRO:HD2	1.99	0.44
1:G:180:HIS:N	1:G:247:ASN:O	2.48	0.44
1:G:54:LYS:CB	1:G:66:GLU:O	2.65	0.44
2:H:218:LYS:HB2	2:H:218:LYS:HZ2	1.81	0.44
3:I:136:VAL:HG13	3:I:180:SER:OG	2.17	0.44
1:J:97:ASP:HB3	1:J:231:TRP:HE1	1.80	0.44
1:J:89:THR:HB	1:J:145:TYR:OH	2.17	0.44
2:K:215:VAL:HG23	2:K:216:ASP:N	2.32	0.44
2:K:37:ARG:HG2	2:K:47:VAL:HG13	1.97	0.44
3:L:165:SER:C	3:L:166:TRP:CD1	2.90	0.44
3:L:16:GLN:HG3	3:L:17:ARG:H	1.82	0.44
3:L:86:THR:H	3:L:109:ILE:HD11	1.83	0.44
1:A:127:ASP:C	1:A:127:ASP:OD2	2.56	0.44
1:A:57:ILE:HD12	1:A:102:ARG:HE	1.83	0.44
2:B:180:SER:HA	3:L:60:GLY:O	2.18	0.44
2:B:171:VAL:HG23	2:B:189:VAL:HG12	2.00	0.44
2:B:131:PRO:HD3	2:B:217:LYS:HD2	2.00	0.44
2:B:38:GLN:HA	2:B:44:LEU:N	2.14	0.44
2:B:56:ARG:N	2:B:56:ARG:CD	2.79	0.44
2:B:97:ARG:HG2	2:B:98:HIS:N	2.32	0.44
3:C:159:GLN:HG3	3:C:160:ASN:N	2.33	0.44
3:C:173:ASP:HB2	3:C:174:SER:H	1.72	0.44
3:F:115:ALA:HA	3:F:116:PRO:HD2	1.87	0.44
1:G:200:PHE:CG	1:G:201:VAL:N	2.85	0.44
1:G:64:ASN:OD1	1:G:65:PRO:HD2	2.17	0.44
2:H:178:LEU:C	2:H:178:LEU:HD23	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:204:SER:C	3:I:205:THR:CG2	2.86	0.44
3:I:7:PRO:CG	3:I:21:THR:H	2.30	0.44
1:J:172:GLU:O	1:J:256:ALA:HA	2.17	0.44
2:K:194:SER:O	2:K:197:LEU:HG	2.16	0.44
2:K:51:LEU:H	2:K:51:LEU:HG	1.62	0.44
2:K:17:LEU:N	2:K:82:MET:O	2.43	0.44
3:L:142:PHE:HE2	3:L:177:SER:N	2.15	0.44
1:A:176:LEU:N	1:A:176:LEU:HD12	2.33	0.44
2:B:36:ILE:HG13	2:B:45:GLU:C	2.36	0.44
1:D:101:LEU:O	1:D:103:GLU:N	2.51	0.44
1:G:192:TYR:HB3	1:G:246:GLY:HA3	1.99	0.44
2:H:98:HIS:HA	3:I:36:ILE:HG22	1.96	0.44
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
3:L:142:PHE:CE2	3:L:177:SER:N	2.85	0.44
3:L:170:ASP:OD2	3:L:172:LYS:N	2.50	0.44
3:C:41:GLN:HG3	3:C:45:GLN:O	2.17	0.44
1:D:127:ASP:OD2	1:D:130:LYS:HG2	2.18	0.44
3:F:70:SER:OG	3:F:71:GLY:N	2.50	0.44
3:F:81:VAL:HG13	3:F:85:ASP:HB2	2.00	0.44
2:H:34:SER:HA	2:H:49:GLY:HA2	1.98	0.44
3:I:86:THR:O	3:I:89:TYR:HE2	2.00	0.44
1:J:101:LEU:HD22	1:J:105:LEU:HD11	1.98	0.44
3:C:128:LEU:CD1	3:C:129:THR:H	2.19	0.44
3:C:42:LYS:O	3:C:44:GLY:N	2.50	0.44
1:D:101:LEU:O	1:D:102:ARG:C	2.54	0.44
2:E:192:VAL:HG12	2:E:193:PRO:HD2	1.99	0.44
3:F:162:VAL:O	3:F:162:VAL:HG23	2.17	0.44
3:F:51:ILE:HD11	3:F:66:SER:HA	2.00	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:H:34:SER:HB2	2:H:98:HIS:NE2	2.33	0.44
1:J:114:PHE:N	1:J:114:PHE:CD2	2.85	0.44
2:K:51:LEU:HD11	2:K:56:ARG:HB2	1.99	0.44
2:K:68:THR:N	2:K:81:GLU:O	2.44	0.44
3:L:204:SER:C	3:L:205:THR:HG22	2.38	0.44
3:L:53:THR:HG22	3:L:53:THR:O	2.17	0.44
3:L:64:ARG:NH2	3:L:85:ASP:OD1	2.51	0.44
3:C:12:VAL:HG11	3:C:81:VAL:HG21	2.00	0.44
3:C:152:LYS:O	3:C:195:TYR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:PRO:HA	1:D:143:SER:N	2.28	0.44
2:E:4:LEU:HB2	2:E:112:GLY:HA3	2.00	0.44
3:F:8:ALA:O	3:F:9:SER:CB	2.64	0.44
1:G:161:LEU:C	1:G:161:LEU:HD23	2.38	0.44
1:G:173:VAL:O	1:G:234:VAL:N	2.42	0.44
2:H:176:ALA:HB2	3:I:166:TRP:NE1	2.31	0.44
3:I:190:GLU:HB3	3:I:191:ARG:H	1.57	0.44
1:J:48:ALA:HB2	1:J:78:TYR:HE1	1.78	0.44
1:J:56:ASN:ND2	1:J:88:GLY:HA2	2.33	0.44
2:K:98:HIS:CD2	3:L:36:ILE:HG21	2.52	0.44
3:L:189:TYR:HB3	3:L:190:GLU:H	1.59	0.44
3:L:57:LYS:O	3:L:58:GLY:C	2.56	0.44
1:A:117:PHE:HB2	1:A:122:SER:OG	2.17	0.44
1:A:137:PRO:HA	1:A:143:SER:N	2.28	0.44
1:A:153:LYS:HD2	1:A:156:ASN:HA	2.00	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
3:L:115:ALA:HA	3:L:116:PRO:HD3	1.78	0.44
2:B:37:ARG:O	2:B:45:GLU:N	2.33	0.43
1:D:70:LEU:O	1:D:71:SER:OG	2.22	0.43
1:D:79:ILE:CD1	1:D:79:ILE:H	2.24	0.43
2:E:168:THR:O	2:E:169:SER:CB	2.66	0.43
2:E:174:PHE:O	3:F:166:TRP:CD1	2.70	0.43
3:F:211:SER:O	3:F:212:PHE:CB	2.66	0.43
2:H:178:LEU:N	2:H:183:LEU:O	2.49	0.43
2:H:111:TRP:CH2	3:I:38:TRP:CE3	3.06	0.43
2:K:59:TYR:HE1	2:K:69:ILE:HG22	1.80	0.43
3:C:158:ARG:NH2	2:K:97:ARG:HD2	2.29	0.43
2:K:99:SER:HB3	3:L:35:PHE:CD1	2.53	0.43
2:B:157:PRO:O	2:B:208:HIS:CD2	2.68	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
1:D:99:GLU:CG	1:D:100:GLU:N	2.81	0.43
2:E:88:GLU:HG3	2:E:89:ASP:N	2.33	0.43
3:F:189:TYR:HB3	3:F:190:GLU:H	1.57	0.43
3:I:178:MET:C	3:I:178:MET:SD	2.96	0.43
3:I:7:PRO:HD2	3:I:21:THR:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:170:SER:HB2	2:K:189:VAL:O	2.18	0.43
3:L:209:VAL:HG23	3:L:210:LYS:HB2	2.00	0.43
1:A:82:THR:O	1:A:82:THR:OG1	2.32	0.43
1:A:121:SER:HB3	2:B:58:TYR:HA	2.00	0.43
1:G:200:PHE:O	1:G:201:VAL:HG23	2.18	0.43
1:G:55:CYS:HB2	1:G:60:TRP:HB2	2.00	0.43
2:H:124:THR:OG1	2:H:155:PRO:HD3	2.19	0.43
2:H:34:SER:HB3	2:H:48:SER:O	2.18	0.43
2:H:130:PHE:CD1	3:I:126:GLU:HB2	2.54	0.43
3:I:195:TYR:H	3:I:210:LYS:HA	1.83	0.43
1:J:123:TRP:CZ3	1:J:163:LYS:HG3	2.50	0.43
3:L:143:TYR:CD2	3:L:144:PRO:CD	3.01	0.43
3:L:156:SER:OG	3:L:157:GLU:N	2.50	0.43
2:B:51:LEU:CD1	2:B:56:ARG:HG2	2.48	0.43
3:C:139:LEU:O	3:C:142:PHE:CE2	2.72	0.43
3:C:140:ASN:ND2	3:C:176:TYR:CD1	2.86	0.43
1:D:183:SER:HB2	1:D:184:THR:HG23	1.99	0.43
2:E:211:SER:O	2:E:212:ASN:HB3	2.18	0.43
3:F:152:LYS:O	3:F:195:TYR:HA	2.18	0.43
3:F:49:LEU:HD11	3:F:52:TYR:HB3	2.01	0.43
2:H:150:VAL:O	2:H:185:SER:HA	2.18	0.43
2:H:174:PHE:CD2	3:I:166:TRP:CE3	3.04	0.43
1:J:165:TYR:OH	1:J:169:LYS:HD2	2.18	0.43
2:K:197:LEU:O	2:K:197:LEU:CD1	2.62	0.43
1:A:57:ILE:H	1:A:81:GLU:CD	2.22	0.43
2:B:130:PHE:CE1	3:C:127:GLN:HG3	2.53	0.43
3:C:183:THR:HG22	3:C:184:LEU:N	2.34	0.43
3:C:46:PRO:HA	3:C:47:PRO:HD3	1.61	0.43
2:E:177:VAL:HG22	2:E:184:TYR:HE2	1.84	0.43
2:E:97:ARG:HG2	2:E:98:HIS:N	2.34	0.43
3:F:163:LEU:O	3:F:163:LEU:HD23	2.19	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
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
1:A:101:LEU:CD2	1:A:105:LEU:HG	2.48	0.43
1:A:91:TYR:OH	1:A:180:HIS:NE2	2.32	0.43
2:B:19:LEU:O	2:B:79:TYR:HA	2.18	0.43
3:C:81:VAL:HG11	3:C:109:ILE:HG13	1.99	0.43
1:D:107:SER:OG	1:D:259:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:VAL:HG12	1:D:257:MET:HE3	1.99	0.43
3:F:102:PHE:CG	3:F:103:GLY:N	2.86	0.43
3:F:189:TYR:O	3:F:190:GLU:HB2	2.19	0.43
2:H:46:TRP:HE3	2:H:60:ARG:NH2	2.16	0.43
3:L:24:ALA:O	3:L:72:THR:OG1	2.32	0.43
3:L:37:ASN:O	3:L:49:LEU:HA	2.19	0.43
1:A:181:HIS:HB3	1:A:213:GLU:O	2.19	0.43
1:A:220:VAL:O	1:A:221:ARG:HB2	2.19	0.43
1:A:92:PRO:C	1:A:226:ARG:HD2	2.39	0.43
2:E:178:LEU:HB3	2:E:180:SER:HB2	2.01	0.43
2:E:90:THR:O	2:E:91:ALA:HB2	2.18	0.43
3:F:162:VAL:O	3:F:164:ASN:CG	2.56	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
1:J:188:GLN:NE2	1:J:247:ASN:OD1	2.51	0.43
3:L:57:LYS:HD3	3:L:61:VAL:O	2.19	0.43
2:B:211:SER:O	2:B:212:ASN:CB	2.66	0.43
2:B:38:GLN:CG	2:B:38:GLN:O	2.66	0.43
3:C:26:GLU:HG2	3:C:27:SER:H	1.84	0.43
3:C:39:PHE:HB3	3:C:50:LEU:CD1	2.41	0.43
3:C:48:LYS:HG2	3:C:49:LEU:N	2.34	0.43
3:C:50:LEU:HD22	3:C:65:PHE:CG	2.53	0.43
1:D:113:ARG:HA	1:D:254:ALA:O	2.19	0.43
1:D:64:ASN:O	1:D:67:CYS:HB2	2.18	0.43
3:F:13:SER:CB	3:F:110:LYS:HB3	2.49	0.43
3:F:52:TYR:HE2	3:F:58:GLY:HA2	1.82	0.43
2:H:11:VAL:HG22	2:H:12:GLN:N	2.33	0.43
3:I:116:PRO:CB	3:I:139:LEU:HB3	2.41	0.43
3:I:56:ASN:N	3:I:56:ASN:OD1	2.51	0.43
1:J:219:LYS:CD	1:J:222:ASP:HA	2.36	0.43
1:J:71:SER:OG	1:J:71:SER:O	2.34	0.43
2:K:183:LEU:HA	2:K:183:LEU:HD13	1.85	0.43
1:A:91:TYR:CD1	1:A:227:MET:HE2	2.53	0.43
3:C:177:SER:O	3:C:178:MET:HG3	2.18	0.43
3:C:204:SER:C	3:C:205:THR:HG22	2.38	0.43
3:C:35:PHE:CD1	3:C:35:PHE:C	2.91	0.43
1:D:192:TYR:CD1	1:D:192:TYR:N	2.87	0.43
2:E:208:HIS:NE2	2:E:210:PRO:CG	2.81	0.43
3:F:66:SER:O	3:F:77:THR:HG22	2.18	0.43
1:G:199:VAL:CG1	1:G:200:PHE:N	2.78	0.43
2:H:63:VAL:HG13	2:H:66:ARG:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:90:PHE:HA	3:I:102:PHE:CE2	2.53	0.43
1:J:116:ILE:HG12	1:J:117:PHE:CG	2.54	0.43
1:J:57:ILE:O	1:J:58:ALA:C	2.58	0.43
1:J:79:ILE:HG22	1:J:80:VAL:N	2.33	0.43
2:K:162:TRP:CE3	2:K:204:CYS:HB3	2.53	0.43
2:K:176:ALA:HB2	3:L:166:TRP:NE1	2.31	0.43
2:K:207:ASN:CA	2:K:213:THR:O	2.67	0.43
3:L:145:LYS:CD	3:L:167:THR:HG21	2.47	0.43
2:B:100:TRP:CD2	3:C:34:ASN:HA	2.54	0.43
2:B:122:ALA:HB3	2:B:154:PHE:CZ	2.54	0.43
3:C:39:PHE:CD1	3:C:76:LEU:HD13	2.53	0.43
2:E:69:ILE:HG12	2:E:70:SER:N	2.33	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
3:F:97:VAL:O	3:F:99:TYR:CE1	2.72	0.43
2:H:27:THR:HG22	2:H:31:TYR:HD2	1.82	0.43
3:L:45:GLN:HA	3:L:45:GLN:OE1	2.18	0.43
1:A:179:ILE:HD11	1:A:199:VAL:CG1	2.45	0.42
2:B:86:ARG:N	2:B:119:VAL:HG11	2.34	0.42
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
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:F:150:LYS:HB3	3:F:198:GLU:HG2	2.01	0.42
3:F:204:SER:C	3:F:205:THR:HG22	2.38	0.42
3:F:45:GLN:CB	3:F:46:PRO:HD2	2.48	0.42
1:G:167:ASN:OD1	1:G:169:LYS:HB2	2.19	0.42
1:G:215:ALA:H	1:G:217:ARG:NH1	2.17	0.42
1:G:116:ILE:N	1:G:252:ARG:O	2.52	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: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
1:A:55:CYS:SG	1:A:66:GLU:CG	3.04	0.42
2:B:186:LEU:C	2:B:186:LEU:HD12	2.40	0.42
2:B:43:GLY:C	2:B:44:LEU:HD12	2.39	0.42
2:B:85:LEU:HD23	2:B:85:LEU:HA	1.85	0.42
2:B:9:ALA:O	2:B:117:VAL:HA	2.19	0.42
2:E:4:LEU:HD11	2:E:110:GLY:O	2.20	0.42
2:H:174:PHE:CG	2:H:175:PRO:HD2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:178:LEU:O	2:H:178:LEU:HD23	2.20	0.42
2:H:218:LYS:CB	2:H:218:LYS:NZ	2.82	0.42
2:H:66:ARG:NH2	2:H:84:SER:O	2.52	0.42
3:I:145:LYS:CA	3:I:147:ILE:N	2.77	0.42
2:K:34:SER:HB2	2:K:98:HIS:NE2	2.34	0.42
3:L:142:PHE:CE1	3:L:144:PRO:O	2.73	0.42
1:A:239:LYS:NZ	1:A:241:THR:OG1	2.47	0.42
1:A:85:SER:OG	1:A:86:ASP:N	2.53	0.42
2:B:178:LEU:C	2:B:180:SER:N	2.72	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
3:C:97:VAL:O	3:C:99:TYR:CD1	2.71	0.42
1:D:192:TYR:C	1:D:194:ASN:H	2.23	0.42
1:D:77:SER:OG	1:D:78:TYR:N	2.51	0.42
2:E:180:SER:H	3:I:60:GLY:HA2	1.85	0.42
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
1:G:133:THR:CG2	1:G:144:PHE:HD1	2.31	0.42
1:G:219:LYS:HD3	1:G:224:GLU:HG3	2.02	0.42
2:H:125:LYS:CE	2:H:126:GLY:O	2.67	0.42
2:H:161:SER:HB3	2:H:205:ASN:ND2	2.34	0.42
3:I:162:VAL:O	3:I:164:ASN:OD1	2.37	0.42
3:I:141:ASN:CA	3:I:175:THR:HG22	2.29	0.42
3:L:40:GLN:HB2	3:L:50:LEU:HD11	2.01	0.42
3:C:139:LEU:O	3:C:142:PHE:HE2	2.02	0.42
3:C:38:TRP:NE1	3:C:90:PHE:O	2.52	0.42
2:E:146:LEU:HA	2:E:146:LEU:HD13	1.77	0.42
2:E:203:ILE:HG13	2:E:217:LYS:O	2.20	0.42
3:F:13:SER:HB3	3:F:110:LYS:CB	2.48	0.42
3:F:128:LEU:HG	3:F:129:THR:N	2.35	0.42
3:F:191:ARG:HG3	3:F:192:HIS:CE1	2.54	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
1:J:179:ILE:O	1:J:179:ILE:HG13	2.19	0.42
3:L:147:ILE:HG12	3:L:200:THR:O	2.19	0.42
2:B:150:VAL:O	2:B:186:LEU:N	2.47	0.42
2:B:196:SER:HB3	2:B:202:TYR:CE2	2.54	0.42
2:E:143:THR:CG2	2:E:191:THR:HG23	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:178:LEU:C	2:E:180:SER:HB2	2.40	0.42
3:F:14:PRO:O	3:F:15:GLY:C	2.58	0.42
3:F:150:LYS:HB3	3:F:198:GLU:CG	2.49	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
1:G:76:TRP:CZ3	1:G:108:VAL:HG21	2.54	0.42
2:H:183:LEU:HD13	2:H:183:LEU:HA	1.75	0.42
2:K:100:TRP:HE1	3:L:34:ASN:HA	1.85	0.42
3:L:37:ASN:OD1	3:L:38:TRP:N	2.52	0.42
2:B:45:GLU:OE2	2:B:45:GLU:HA	2.19	0.42
3:C:42:LYS:HE2	3:C:42:LYS:HA	2.01	0.42
3:C:6:SER:HA	3:C:21:THR:O	2.19	0.42
1:D:184:THR:H	1:D:187:ASP:HB2	1.84	0.42
1:D:208:LYS:CG	1:D:209:LYS:N	2.82	0.42
1:D:220:VAL:O	1:D:221:ARG:HB2	2.18	0.42
2:E:50:ILE:CD1	2:E:71:ARG:HB2	2.37	0.42
3:F:162:VAL:O	3:F:164:ASN:OD1	2.37	0.42
1:G:102:ARG:HG3	1:G:103:GLU:N	2.35	0.42
1:G:184:THR:O	1:G:185:SER:C	2.58	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:168:ASP:O	3:I:169:GLN:HB2	2.19	0.42
3:I:62:PRO:HD2	3:I:65:PHE:CE2	2.55	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
2:K:161:SER:O	2:K:204:CYS:HA	2.19	0.42
3:L:129:THR:O	3:L:130:SER:OG	2.36	0.42
3:L:170:ASP:C	3:L:170:ASP:OD2	2.58	0.42
2:B:181:SER:OG	3:L:84:GLU:CD	2.58	0.42
3:C:192:HIS:CE1	3:C:194:SER:CB	3.02	0.42
1:D:127:ASP:HB2	1:D:154:LYS:CB	2.49	0.42
1:D:217:ARG:HD2	1:D:226:ARG:HG2	2.00	0.42
1:D:91:TYR:O	1:D:229:TYR:OH	2.29	0.42
3:F:57:LYS:CB	3:F:57:LYS:HZ3	2.32	0.42
1:G:71:SER:O	1:G:73:ALA:N	2.53	0.42
1:J:127:ASP:N	1:J:154:LYS:HB2	2.34	0.42
3:L:13:SER:N	3:L:110:LYS:HD2	2.34	0.42
1:D:149:ILE:CD1	1:D:252:ARG:HB2	2.50	0.42
1:D:52:LEU:HD12	1:D:81:GLU:HG2	2.00	0.42
2:E:76:LYS:HD3	2:E:76:LYS:HA	1.91	0.42
3:F:192:HIS:O	3:F:195:TYR:CE1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:ILE:HD11	1:G:79:ILE:HD12	2.01	0.42
2:H:127:PRO:HB3	2:H:150:VAL:HG13	1.99	0.42
2:H:186:LEU:HD12	2:H:186:LEU:O	2.19	0.42
2:K: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
3:L:143:TYR:HA	3:L:144:PRO:HA	1.61	0.42
2:B:35:TRP:HA	2:B:94:TYR:O	2.20	0.42
3:C:86:THR:H	3:C:107:LEU:HD22	1.84	0.42
1:D: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:E:215:VAL:CG2	2:E:216:ASP:N	2.82	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:161:GLY:C	3:F:162:VAL:HG13	2.40	0.42
3:F:27:SER:C	3:F:28:VAL:HG22	2.40	0.42
3:F:2:GLN:NE2	3:F:97:VAL:HG21	2.35	0.42
2:H:42:LYS:HE2	2:H:42:LYS:HB2	1.86	0.42
3:I:140:ASN:HB3	3:I:176:TYR:CD1	2.55	0.42
3:I:35:PHE:O	3:I:35:PHE:CD1	2.73	0.42
2:H:94:TYR:OH	3:I:45:GLN:OE1	2.33	0.42
2:K:19:LEU:CD1	2:K:19:LEU:N	2.83	0.42
3:L:97:VAL:HG13	3:L:98:PRO:N	2.35	0.42
1:A:96:ILE:HD13	1:A:96:ILE:N	2.35	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
1:D:240:ILE:O	1:D:240:ILE:HG23	2.19	0.42
2:E:85:LEU:HA	2:E:85:LEU:HD23	1.83	0.42
3:F:109:ILE:CG2	3:F:110:LYS:H	2.32	0.42
1:G:76:TRP:CZ2	1:G:105:LEU:O	2.73	0.42
1:G:222:ASP:CG	1:G:222:ASP:O	2.57	0.42
3:L:52:TYR:CD1	3:L:56:ASN:HB2	2.55	0.42
1:A:133:THR:O	1:A:142:LYS:HB2	2.20	0.41
1:A:104:GLN:NE2	1:A:231:TRP:CH2	2.88	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
3:C:38:TRP:HH2	3:C:89:TYR:CD1	2.33	0.41
1:D:72:THR:O	1:D:73:ALA:HB2	2.20	0.41
2:E:127:PRO:HA	2:E:153:TYR:HB3	2.02	0.41
2:E:162:TRP:HB2	2:E:167:LEU:HD23	2.02	0.41
3:F:164:ASN:HB3	3:F:180:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:84:GLU:C	3:F:86:THR:N	2.72	0.41
1:G:90:CYS:O	1:G:221:ARG:NH1	2.53	0.41
2:H:130:PHE:HA	2:H:131:PRO:HD2	1.92	0.41
1:J:76:TRP:CE2	1:J:108:VAL:HG22	2.55	0.41
3:L:133:ALA:O	3:L:183:THR:O	2.38	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
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:D:119:LYS:HG2	1:D:120:THR:N	2.35	0.41
2:E:177:VAL:HA	2:E:184:TYR:HD2	1.84	0.41
3:F:38:TRP:HA	3:F:49:LEU:HD23	2.02	0.41
1:G:173:VAL:HA	1:G:256:ALA:HA	2.02	0.41
1:G:79:ILE:CG2	1:G:80:VAL:H	2.32	0.41
2:H:63:VAL:HG13	2:H:66:ARG:H	1.85	0.41
1:J:114:PHE:O	1:J:253:TYR:HA	2.19	0.41
1:J:51:HIS:CD2	1:J:80:VAL:CB	3.02	0.41
1:J:86:ASP:N	1:J:86:ASP:OD1	2.38	0.41
2:K:39:ALA:HB3	2:K:44:LEU:HG	2.01	0.41
3:L:69:GLY:HA3	3:L:74:PHE:CD1	2.55	0.41
1:A:54:LYS:HD2	1:A:69:SER:HB2	2.02	0.41
2:B:19:LEU:HD22	2:B:82:MET:HE1	2.03	0.41
2:B:85:LEU:HB3	2:B:119:VAL:CG1	2.50	0.41
3:C:35:PHE:HB3	3:C:95:LYS:CD	2.41	0.41
2:E:133:ALA:HA	2:E:134:PRO:HD3	1.87	0.41
2:E:173:THR:O	2:E:174:PHE:C	2.57	0.41
2:E:177:VAL:HA	2:E:184:TYR:HA	2.02	0.41
2:E:208:HIS:C	2:E:210:PRO:HD2	2.40	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
1:G:79:ILE:HD11	1:G:105:LEU:CB	2.50	0.41
2:H:48:SER:OG	2:H:49:GLY:N	2.53	0.41
1:J:161:LEU:CD2	1:J:161:LEU:C	2.88	0.41
2:K:45:GLU:CD	2:K:46:TRP:N	2.68	0.41
3:L:128:LEU:HG	3:L:129:THR:OG1	2.20	0.41
1:A:206:TYR:CD2	1:A:207:SER:N	2.88	0.41
1:A:252:ARG:HD2	1:A:253:TYR:CD2	2.55	0.41
2:B:133:ALA:HA	2:B:134:PRO:HD3	1.94	0.41
2:B:134:PRO:HD3	2:B:146:LEU:CD1	2.50	0.41
1:D:205:ARG:HA	1:D:205:ARG:HD2	1.48	0.41
2:E:100:TRP:CD1	3:F:34:ASN:CG	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:7:PRO:O	3:F:8:ALA:CB	2.67	0.41
1:G:61:ILE:O	1:G:61:ILE:HG13	2.19	0.41
2:H:97:ARG:HB3	2:H:110:GLY:CA	2.32	0.41
1:J:169:LYS:NZ	1:J:256:ALA:HB1	2.35	0.41
1:J:171:LYS:NZ	1:J:258:GLU:HG3	2.34	0.41
2:K:99:SER:O	2:K:100:TRP:CG	2.73	0.41
3:L:83:ALA:O	3:L:171:SER:O	2.38	0.41
1:A:119:LYS:O	1:A:123:TRP:CD1	2.73	0.41
1:A:161:LEU:HD22	1:A:244:ALA:HB3	2.03	0.41
2:B:174:PHE:HD1	2:B:174:PHE:N	2.19	0.41
2:B:171:VAL:O	2:B:188:SER:HA	2.20	0.41
2:B:27:THR:HG21	2:B:31:TYR:CG	2.55	0.41
2:B:64:LYS:HA	2:B:64:LYS:HD3	1.32	0.41
3:C:34:ASN:N	3:C:34:ASN:HD22	2.18	0.41
2:E:161:SER:HG	2:E:163:ASN:HD22	1.66	0.41
2:H:36:ILE:HD13	2:H:111:TRP:CH2	2.55	0.41
2:H:50:ILE:HG23	2:H:69:ILE:CD1	2.47	0.41
2:H:83:ASN:O	2:H:84:SER:C	2.58	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:B:19:LEU:HD22	2:B:82:MET:CE	2.50	0.41
3:C:118:VAL:HB	3:C:208:ILE:CD1	2.50	0.41
2:E:39:ALA:HA	2:E:91:ALA:CB	2.51	0.41
3:F:147:ILE:HG23	3:F:147:ILE:O	2.21	0.41
3:F:42:LYS:NZ	3:F:84:GLU:O	2.54	0.41
1:G:166:ILE:HD13	1:G:166:ILE:H	1.83	0.41
2:H:205:ASN:HB3	2:H:216:ASP:OD1	2.20	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
2:K:10:VAL:HG12	2:K:118:THR:O	2.21	0.41
3:L:16:GLN:HA	3:L:16:GLN:OE1	2.21	0.41
3:L:196:THR:HG1	3:L:210:LYS:HZ2	1.58	0.41
1:A:123:TRP:HZ3	1:A:163:LYS:HG3	1.84	0.41
2:B:35:TRP:HB2	2:B:48:SER:OG	2.20	0.41
3:C:109:ILE:CD1	3:C:109:ILE:N	2.79	0.41
3:C:142:PHE:O	3:C:174:SER:HB3	2.21	0.41
3:C:168:ASP:OD1	3:C:176:TYR:O	2.38	0.41
3:C:17:ARG:HB2	3:C:17:ARG:CZ	2.50	0.41
3:C:3:MET:O	3:C:25:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:TYR:CE2	1:D:167:ASN:HB2	2.54	0.41
1:D:232:THR:C	1:D:233:LEU:HD13	2.41	0.41
1:D:54:LYS:CD	1:D:67:CYS:HA	2.50	0.41
2:E:171:VAL:HB	3:F:178:MET:HE1	2.02	0.41
3:F:38:TRP:CZ3	3:F:39:PHE:CG	3.08	0.41
1:G:136:CYS:HB3	1:G:144:PHE:HA	2.01	0.41
1:G:116:ILE:HG22	1:G:252:ARG:O	2.21	0.41
1:G:58:ALA:HB2	1:G:98:TYR:HE1	1.82	0.41
2:H:27:THR:CG2	2:H:30:ASP:HB3	2.50	0.41
3:I:121:PHE:N	3:I:136:VAL:O	2.47	0.41
3:I:135:VAL:HG22	3:I:151:TRP:CH2	2.55	0.41
3:I:1:ILE:HG22	3:I:3:MET:HE2	2.02	0.41
3:I:203:THR:O	3:I:204:SER:C	2.59	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:J:56:ASN:HB3	1:J:83:SER:HA	2.02	0.41
1:A:263:SER:OG	1:A:264:GLY:N	2.52	0.41
2:B:178:LEU:HB3	2:B:183:LEU:HB3	2.01	0.41
2:B:27:THR:HG22	2:B:31:TYR:CG	2.55	0.41
3:C:135:VAL:HG12	3:C:151:TRP:CH2	2.52	0.41
3:C:92:GLN:OE1	3:C:101:THR:HG21	2.21	0.41
1:D:184:THR:OG1	1:D:186:ALA:HB3	2.21	0.41
1:D:149:ILE:HG13	1:D:252:ARG:HB2	2.02	0.41
2:E:161:SER:OG	2:E:163:ASN:ND2	2.45	0.41
1:G:180:HIS:HD2	1:G:227:MET:HG3	1.86	0.41
1:G:187:ASP:HA	1:G:190:SER:OG	2.20	0.41
2:H:17:LEU:HD23	2:H:117:VAL:HG23	2.03	0.41
2:H:63:VAL:HG12	2:H:64:LYS:N	2.35	0.41
1:J:104:GLN:O	1:J:104:GLN:HG3	2.18	0.41
1:J:49:PRO:O	1:J:78:TYR:O	2.39	0.41
3:L:210:LYS:HB3	3:L:211:SER:H	1.39	0.41
1:A:58:ALA:O	1:A:62:LEU:HB2	2.21	0.41
2:B:45:GLU:HG2	2:B:60:ARG:NH1	2.36	0.41
3:C:132:GLY:HA2	3:C:184:LEU:C	2.41	0.41
3:C:167:THR:CG2	3:C:168:ASP:H	2.27	0.41
2:E:26:PHE:HB3	2:E:27:THR:H	1.64	0.41
2:H:97:ARG:NH2	2:H:110:GLY:N	2.68	0.41
2:H:96:ALA:HB1	3:I:36:ILE:HD12	2.03	0.41
3:I:143:TYR:HA	3:I:144:PRO:HA	1.76	0.41
1:J:151:LEU:HD23	1:J:151:LEU:HA	1.94	0.41
1:A:157:SER:OG	1:A:159:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HB3	1:A:218:PRO:HD2	2.01	0.41
3:C:153:ILE:CG1	3:C:154:ASP:N	2.81	0.41
1:D:137:PRO:CB	1:D:142:LYS:HA	2.50	0.41
2:E:156:GLU:CB	2:E:157:PRO:CA	2.98	0.41
3:F:166:TRP:CE3	3:F:166:TRP:HA	2.56	0.41
1:G:133:THR:C	1:G:142:LYS:HB2	2.41	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:120:ILE:HA	3:L:120:ILE:HD12	1.97	0.41
3:L:41:GLN:HB2	3:L:47:PRO:HB3	2.02	0.41
1:A:109:SER:HB3	1:A:258:GLU:CG	2.50	0.41
1:A:84:SER:OG	1:A:87:ASN:OD1	2.32	0.41
2:B:158:VAL:CG1	2:B:159:THR:N	2.84	0.41
2:B:200:GLN:O	2:B:202:TYR:CD2	2.74	0.41
2:B:209:LYS:N	2:B:210:PRO:CD	2.84	0.41
3:C: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:138:HIS:N	1:D:141:ALA:O	2.43	0.41
1:D:200:PHE:CE2	1:D:201:VAL:O	2.74	0.41
2:E:180:SER:O	2:E:181:SER:C	2.58	0.41
2:E:33:MET:HE3	2:E:97:ARG:HA	2.02	0.41
3:F:153:ILE:CA	3:F:194:SER:O	2.67	0.41
1:G:65:PRO:C	1:G:67:CYS:H	2.24	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:I:184:LEU:O	3:I:189:TYR:HB2	2.21	0.41
3:I:70:SER:OG	3:I:71:GLY:N	2.54	0.41
1:J:169:LYS:HZ1	1:J:256:ALA:HB1	1.86	0.41
3:L:91:CYS:N	3:L:102:PHE:CD2	2.82	0.41
1:A:116:ILE:HG23	1:A:117:PHE:H	1.87	0.40
1:A:258:GLU:C	1:A:259:ARG:HG2	2.38	0.40
2:B:10:VAL:HG22	2:B:155:PRO:CG	2.50	0.40
2:B:26:PHE:HD1	2:B:27:THR:H	1.69	0.40
3:C:39:PHE:HB2	3:C:50:LEU:CA	2.51	0.40
1:D:217:ARG:HB3	1:D:218:PRO:CD	2.51	0.40
3:F:38:TRP:CE2	3:F:39:PHE:CA	2.91	0.40
1:G:72:THR:H	1:G:72:THR:HG23	1.49	0.40
2:H:176:ALA:HB2	3:I:166:TRP:CZ2	2.51	0.40
2:H:178:LEU:CG	3:I:182:LEU:HD13	2.51	0.40
1:J:92:PRO:HD2	1:J:223:GLN:HG3	2.03	0.40
3:L:44:GLY:O	3:L:45:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:CYS:O	2:B:77:THR:CA	2.68	0.40
3:C:35:PHE:HD1	3:C:37:ASN:H	1.69	0.40
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
3:F:141:ASN:HD21	3:F:176:TYR:HE1	1.69	0.40
1:G:57:ILE:HG21	1:G:105:LEU:HD12	2.03	0.40
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
1:J:95:PHE:HB3	1:J:98:TYR:CB	2.49	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: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
2:B:177:VAL:HG13	2:B:184:TYR:CE2	2.56	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
1:D:227:MET:SD	1:D:249:VAL:HG21	2.61	0.40
2:E:161:SER:OG	2:E:205:ASN:OD1	2.27	0.40
1:G:115:GLU:O	1:G:115:GLU:HG3	2.21	0.40
1:G:91:TYR:CD1	1:G:91:TYR:C	2.95	0.40
1:G:95:PHE:HE2	1:G:231:TRP:HD1	1.70	0.40
3:I:102:PHE:CD1	3:I:104:GLY:N	2.78	0.40
3:I:114:ALA:HA	3:I:201:HIS:HD2	1.85	0.40
3:I:138:PHE:HE1	3:I:178:MET:HG3	1.87	0.40
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
1:J:102:ARG:CG	1:J:102:ARG:NH1	2.77	0.40
1:J:78:TYR:HA	1:J:106:SER:HA	2.04	0.40
1:J:54:LYS:HE3	1:J:67:CYS:C	2.42	0.40
2:K:177:VAL:HA	2:K:184:TYR:HA	2.04	0.40
2:K:99:SER:HB3	3:L:35:PHE:CE1	2.56	0.40
3:L:132:GLY:HA2	3:L:184:LEU:HB3	2.03	0.40
1:A:56:ASN:HB2	1:A:81:GLU:OE1	2.21	0.40
2:B:10:VAL:HG13	2:B:118:THR:HB	2.02	0.40
2:B:51:LEU:HD11	2:B:55:GLU:N	2.36	0.40
2:B:86:ARG:NE	2:B:88:GLU:OE2	2.54	0.40
3:C:86:THR:N	3:C:107:LEU:HD22	2.37	0.40
3:C:108:GLU:CG	3:C:109:ILE:N	2.82	0.40
1:D:136:CYS:O	1:D:143:SER:O	2.38	0.40
2:E:173:THR:OG1	2:E:173:THR:O	2.38	0.40
2:E:22:ALA:HA	2:E:77:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:129:THR:OG1	3:F:129:THR:O	2.40	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: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
1:J:48:ALA:HA	1:J:49:PRO:HD3	1.95	0.40
2:K:158:VAL:CG1	2:K:159:THR:N	2.84	0.40
2:K:174:PHE:HA	2:K:175:PRO:HD2	1.78	0.40
2:B:174:PHE:O	3:C:166:TRP:CD2	2.75	0.40
3:C:210:LYS:HG3	3:C:211:SER:N	2.37	0.40
3:C:37:ASN:ND2	3:C:39:PHE:HE2	2.14	0.40
1:D:184:THR:O	1:D:187:ASP:N	2.54	0.40
1:D:208:LYS:CG	1:D:209:LYS:H	2.35	0.40
1:D:52:LEU:HD21	1:D:60:TRP:CE3	2.57	0.40
3:F:57:LYS:CB	3:F:57:LYS:NZ	2.81	0.40
1:G:188:GLN:HE22	1:G:197:ALA:HB3	1.84	0.40
3:I:40:GLN:HA	3:I:88:ASN:O	2.22	0.40
1:J:78:TYR:HA	1:J:106:SER:CA	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	230/518 (44%)	198 (86%)	29 (13%)	3 (1%)	12 34
1	D	240/518 (46%)	199 (83%)	35 (15%)	6 (2%)	5 18
1	G	223/518 (43%)	193 (86%)	27 (12%)	3 (1%)	12 34
1	J	249/518 (48%)	211 (85%)	35 (14%)	3 (1%)	13 37
2	B	202/219 (92%)	175 (87%)	25 (12%)	2 (1%)	15 42
2	E	202/219 (92%)	172 (85%)	29 (14%)	1 (0%)	29 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	202/219 (92%)	174 (86%)	26 (13%)	2 (1%)	15 42
2	K	202/219 (92%)	177 (88%)	21 (10%)	4 (2%)	7 23
3	C	193/218 (88%)	150 (78%)	37 (19%)	6 (3%)	4 13
3	F	193/218 (88%)	142 (74%)	38 (20%)	13 (7%)	1 3
3	I	195/218 (89%)	141 (72%)	45 (23%)	9 (5%)	2 7
3	L	195/218 (89%)	145 (74%)	44 (23%)	6 (3%)	4 13
All	All	2526/3820 (66%)	2077 (82%)	391 (16%)	58 (2%)	6 20

All (58) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	2 8
1	D	190/451 (42%)	154 (81%)	36 (19%)	1 4

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

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
1	A	232	THR

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Mol	Chain	Res	Type
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
2	B	188	SER

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Mol	Chain	Res	Type
2	B	189	VAL
2	B	200	GLN
2	B	203	ILE
2	B	207	ASN
2	B	214	LYS
2	B	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
3	C	158	ARG

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Mol	Chain	Res	Type
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
1	D	204	SER

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Mol	Chain	Res	Type
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
2	E	187	SER

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Mol	Chain	Res	Type
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
3	F	163	LEU

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Mol	Chain	Res	Type
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
1	G	252	ARG

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Mol	Chain	Res	Type
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
3	I	36	ILE

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Mol	Chain	Res	Type
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
1	J	55	CYS

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Mol	Chain	Res	Type
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
2	K	56	ARG

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Mol	Chain	Res	Type
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
3	L	86	THR

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Mol	Chain	Res	Type
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
3	C	127	GLN

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Mol	Chain	Res	Type
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 molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	234/518 (45%)	0.03	14 (5%) 21 14	19, 35, 59, 76	8 (3%)
1	D	246/518 (47%)	0.25	26 (10%) 6 3	18, 32, 58, 95	21 (8%)
1	G	227/518 (43%)	-0.27	6 (2%) 56 46	18, 32, 57, 70	2 (0%)
1	J	255/518 (49%)	0.30	31 (12%) 4 2	21, 33, 57, 71	30 (11%)
2	B	208/219 (94%)	-0.37	0 100 100	13, 29, 44, 58	0
2	E	208/219 (94%)	-0.44	0 100 100	19, 30, 42, 62	0
2	H	208/219 (94%)	-0.40	4 (1%) 66 59	20, 29, 43, 53	0
2	K	208/219 (94%)	-0.35	2 (0%) 82 77	21, 29, 41, 48	0
3	C	203/218 (93%)	-0.29	1 (0%) 91 88	13, 28, 50, 68	0
3	F	203/218 (93%)	-0.24	3 (1%) 73 67	20, 29, 49, 58	0
3	I	203/218 (93%)	-0.23	1 (0%) 91 88	20, 30, 53, 71	0
3	L	203/218 (93%)	-0.22	3 (1%) 73 67	18, 30, 57, 75	0
All	All	2606/3820 (68%)	-0.17	91 (3%) 44 34	13, 31, 54, 95	61 (2%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	388	LYS	13.4
1	J	387	GLU	12.2
1	A	389	MET	12.2
1	D	419	LEU	11.1
1	D	389	MET	10.8
1	D	422	TRP	9.9
1	D	416	ASP	8.9
1	D	386	ILE	8.7
1	D	391	THR	8.0
1	J	382	VAL	7.9
1	J	383	ASN	7.9

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Mol	Chain	Res	Type	RSRZ
1	D	387	GLU	7.8
1	A	387	GLU	7.1
1	D	415	ASP	7.0
1	A	385	VAL	7.0
1	J	389	MET	6.9
1	D	390	ASN	6.6
1	J	386	ILE	6.3
1	D	383	ASN	6.3
1	J	420	ASP	5.9
1	J	426	ALA	5.8
1	A	47	VAL	5.8
1	D	420	ASP	5.8
1	A	386	ILE	5.5
1	G	389	MET	5.4
1	D	421	ILE	5.2
1	D	427	GLU	5.2
1	J	423	THR	5.0
1	D	384	SER	4.9
1	J	437	THR	4.9
1	A	384	SER	4.6
1	J	425	ASN	4.5
1	D	385	VAL	4.5
1	D	417	GLY	4.5
1	D	392	GLN	4.4
1	A	48	ALA	4.3
1	D	424	TYR	4.3
3	L	155	GLY	4.3
1	J	422	TRP	4.3
1	D	414	VAL	4.2
1	D	423	THR	4.2
1	J	436	ARG	4.1
1	J	418	PHE	4.0
3	I	159	GLN	3.8
1	D	47	VAL	3.8
1	A	388	LYS	3.7
1	J	432	LEU	3.7
1	D	44	LEU	3.6
1	J	434	ASN	3.6
1	D	425	ASN	3.5
1	D	388	LYS	3.5
1	J	384	SER	3.4
2	K	181	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	435	GLU	3.3
2	H	182	GLY	3.3
1	A	263	SER	3.3
1	G	392	GLN	3.2
1	J	431	LEU	3.1
1	J	424	TYR	3.1
1	J	419	LEU	3.1
1	G	388	LYS	3.0
1	A	391	THR	3.0
2	H	164	SER	2.9
1	D	48	ALA	2.9
1	G	44	LEU	2.9
1	A	383	ASN	2.9
2	H	199	THR	2.9
1	A	382	VAL	2.9
3	F	189	TYR	2.8
1	J	385	VAL	2.8
3	C	156	SER	2.7
1	J	381	LYS	2.7
1	J	421	ILE	2.6
2	K	182	GLY	2.6
3	F	156	SER	2.6
1	J	430	VAL	2.6
1	J	47	VAL	2.6
1	J	433	GLU	2.5
1	G	48	ALA	2.5
3	L	154	ASP	2.4
1	A	390	ASN	2.3
1	A	44	LEU	2.3
1	J	391	THR	2.3
3	F	37	ASN	2.3
1	J	427	GLU	2.3
1	D	426	ALA	2.3
1	J	69	SER	2.2
2	H	210	PRO	2.2
1	J	80	VAL	2.1
3	L	195	TYR	2.1
1	G	161	LEU	2.0

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

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

6.3 Carbohydrates

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.