Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 02:57 am BST

PDB ID	:	6CUX
Title	:	Escherichia coli RpoB S531L mutant RNA polymerase holoenzyme in complex with Kanglemycin A
Authors	:	Molodtsov, V.; Murakami, K.S.
Deposited on	:	2018-03-26
Resolution	:	4.10 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 ⓘ) were used in the production of this report:

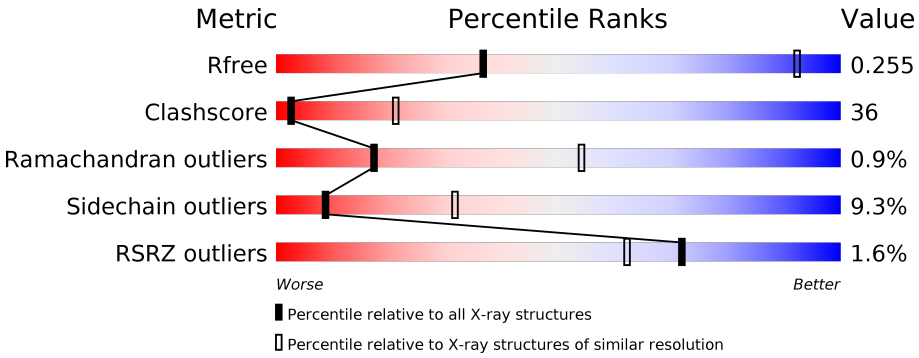
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 4.10 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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	329	33% 29% 7% 31%
1	B	329	% 23% 39% • • 35%
1	G	329	% 29% 34% 6% 32%
1	H	329	2% 28% 34% • 35%
2	C	1342	% 44% 49% 6%
2	I	1342	2% 46% 47% 5% ••

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Mol	Chain	Length	Quality of chain
3	D	1407	35% 40% 8% 17%
3	J	1407	% 37% 39% 6% 18%
4	E	91	56% 34% 8%
4	K	91	11% 36% 47% 13%
5	F	613	2% 39% 32% 5% 24%
5	L	613	% 38% 35% 23%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ZN	J	1502	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55005 atoms, of which 62 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1753	1091	311	345	6			
1	B	214	Total	C	N	O	S	0	0	0
			1649	1029	290	324	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	215	Total	C	N	O	S	0	0	0
			1659	1037	291	325	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1339	Total	C	N	O	S	0	0	0
			10548	6620	1834	2050	44			
2	I	1328	Total	C	N	O	S	0	0	0
			10486	6583	1822	2038	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	531	LEU	SER	conflict	UNP P0A8V2
I	531	LEU	SER	conflict	UNP P0A8V2

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9089	5714	1627	1702	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

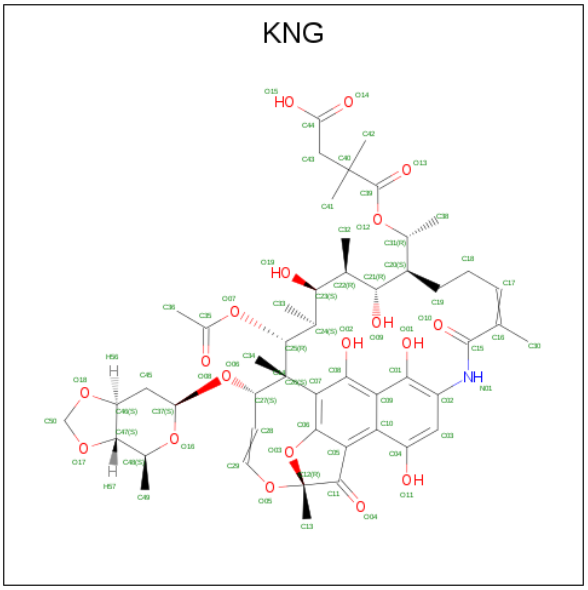
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is Kanglemycin A (three-letter code: KNG) (formula: $C_{50}H_{67}NO_{19}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			132	50	62	1	19		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

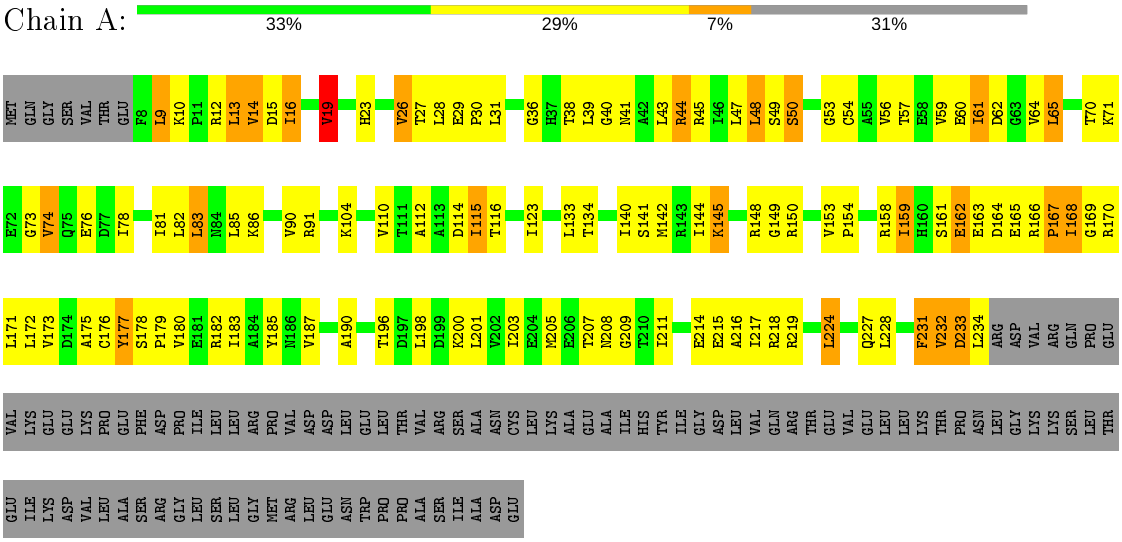
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	J	2	Total Zn 2 2	0	0
8	D	2	Total Zn 2 2	0	0

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.

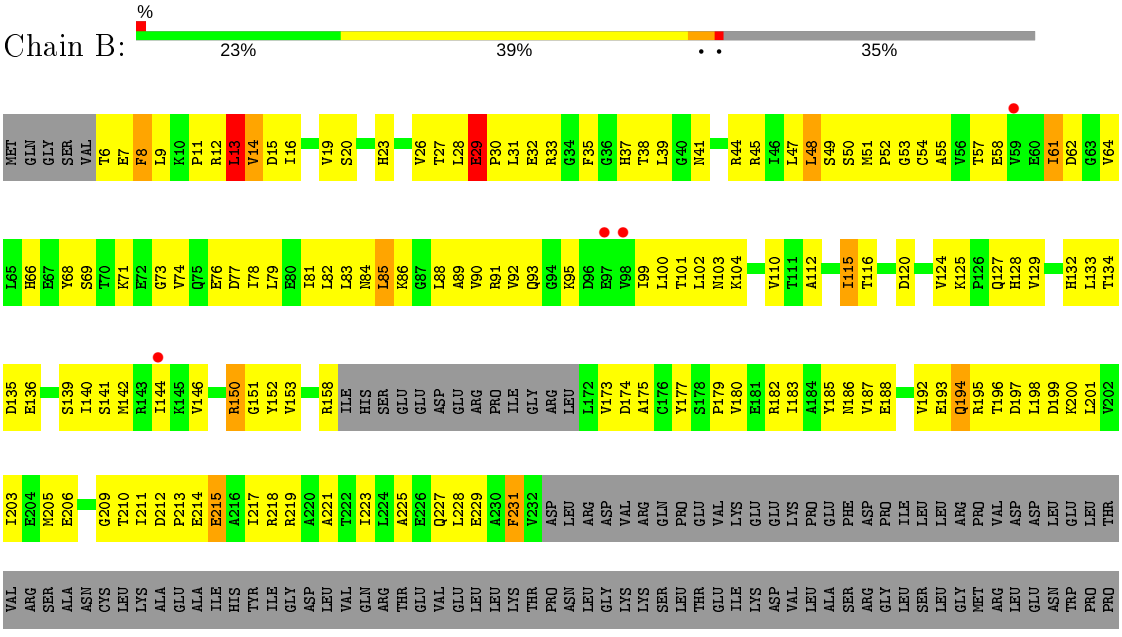
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



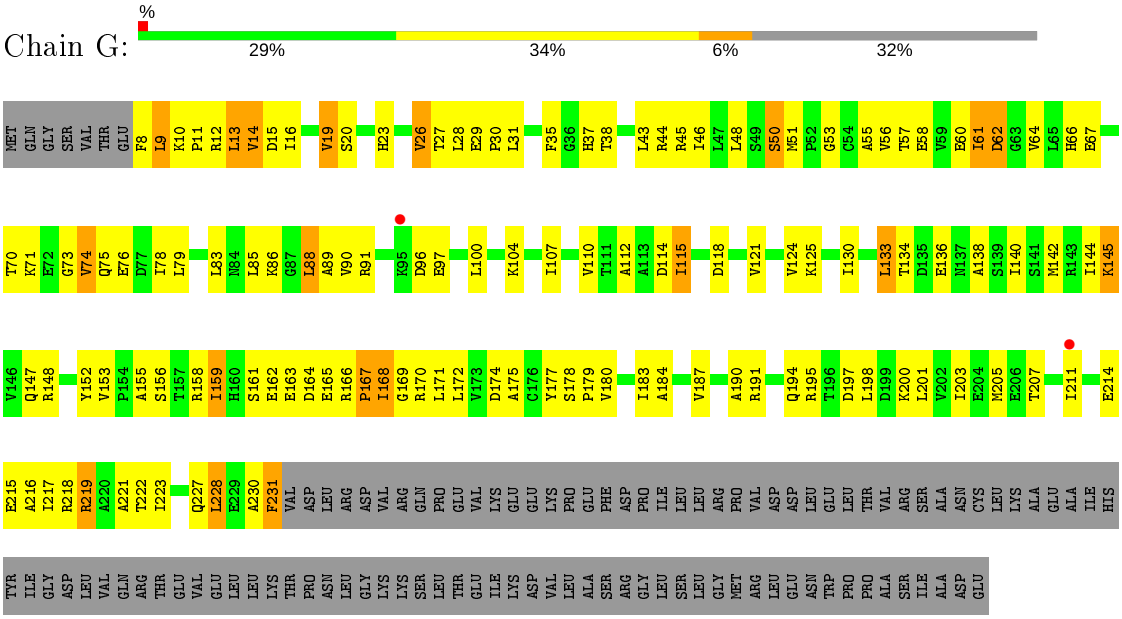
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



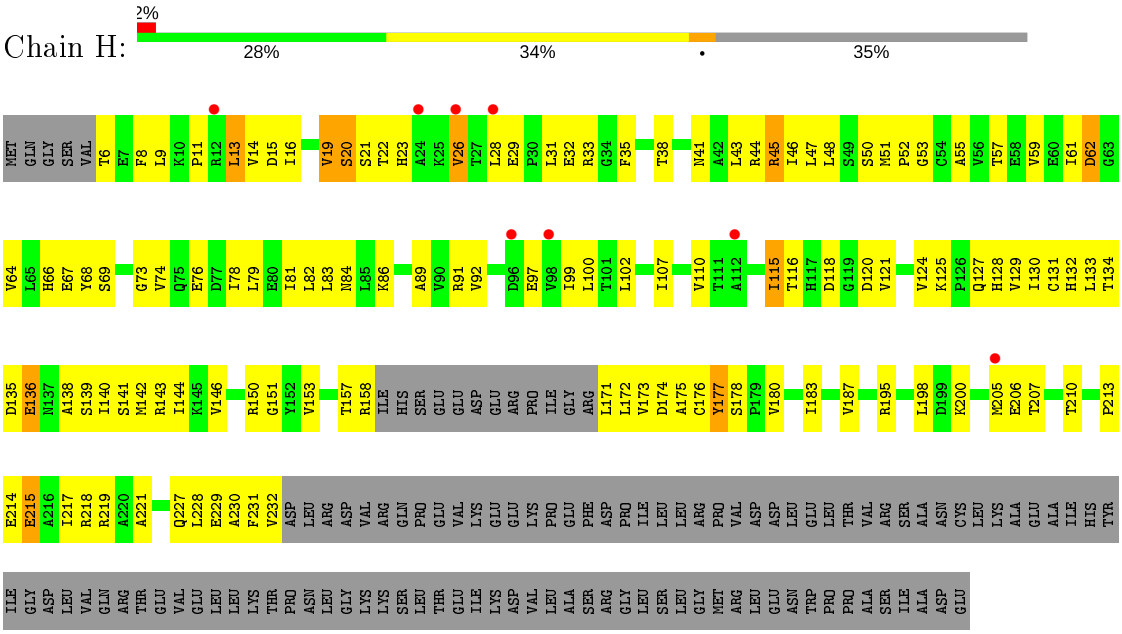
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



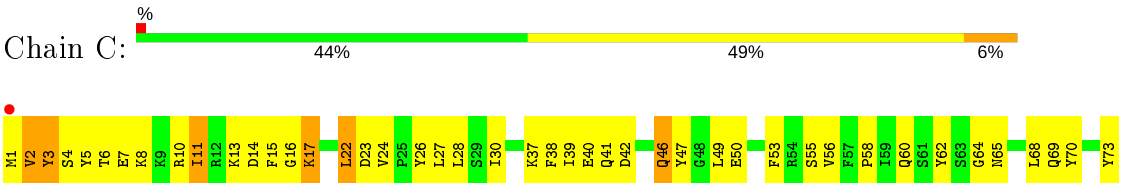
- Molecule 1: DNA-directed RNA polymerase subunit alpha

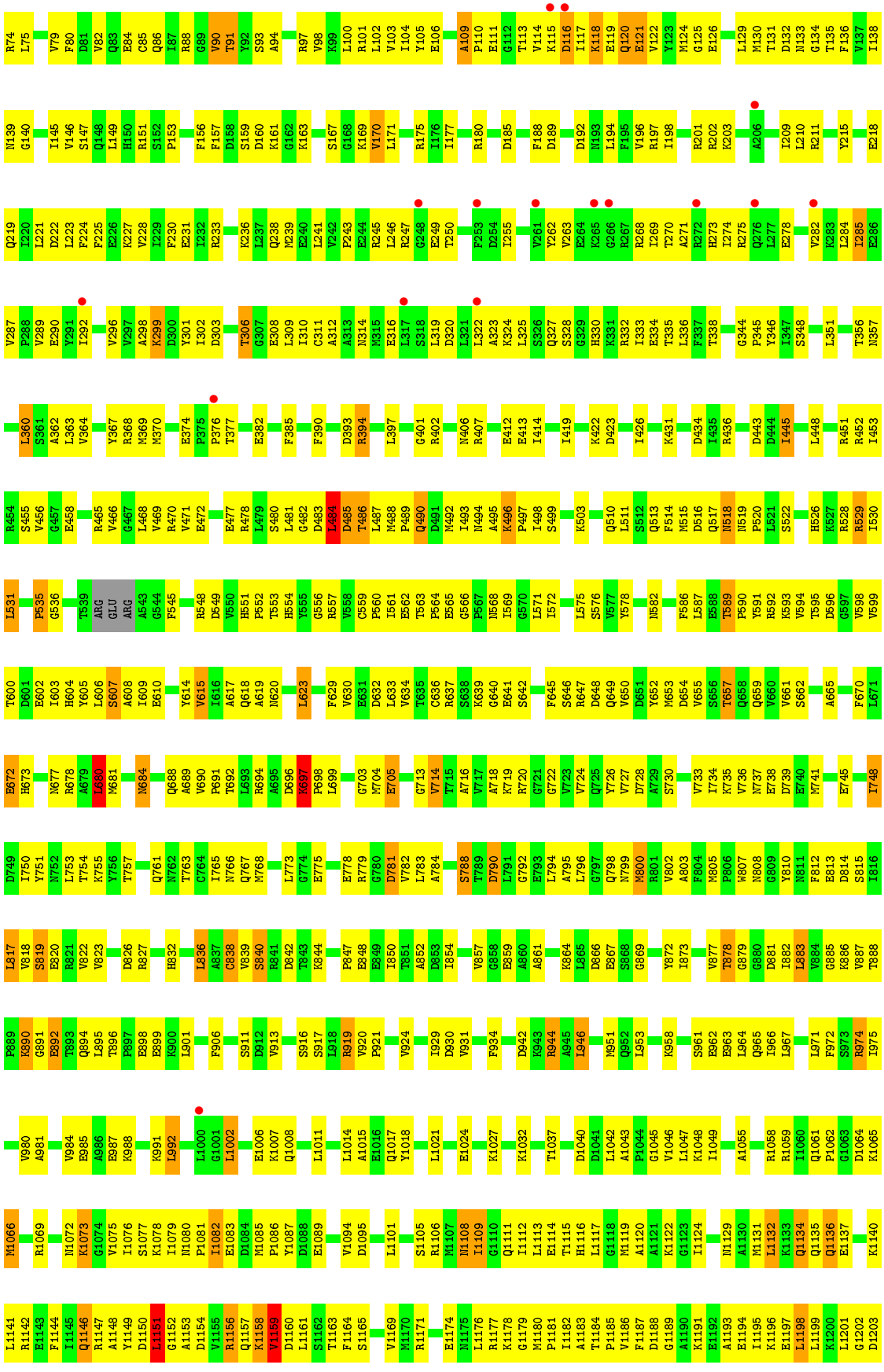
Chain H:



- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:

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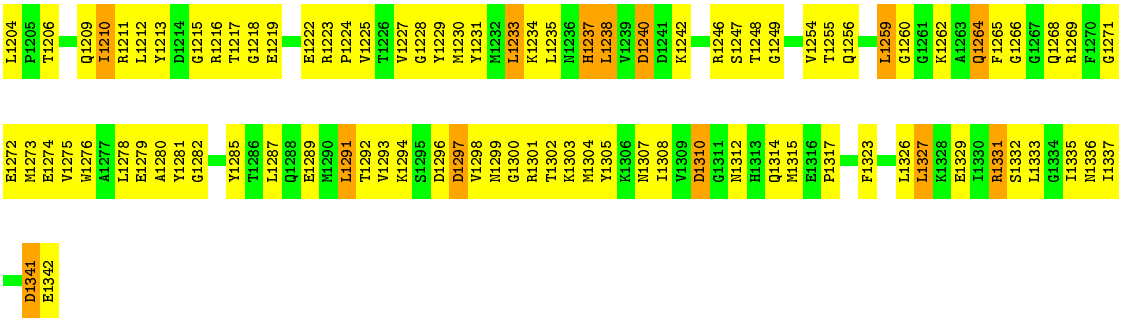
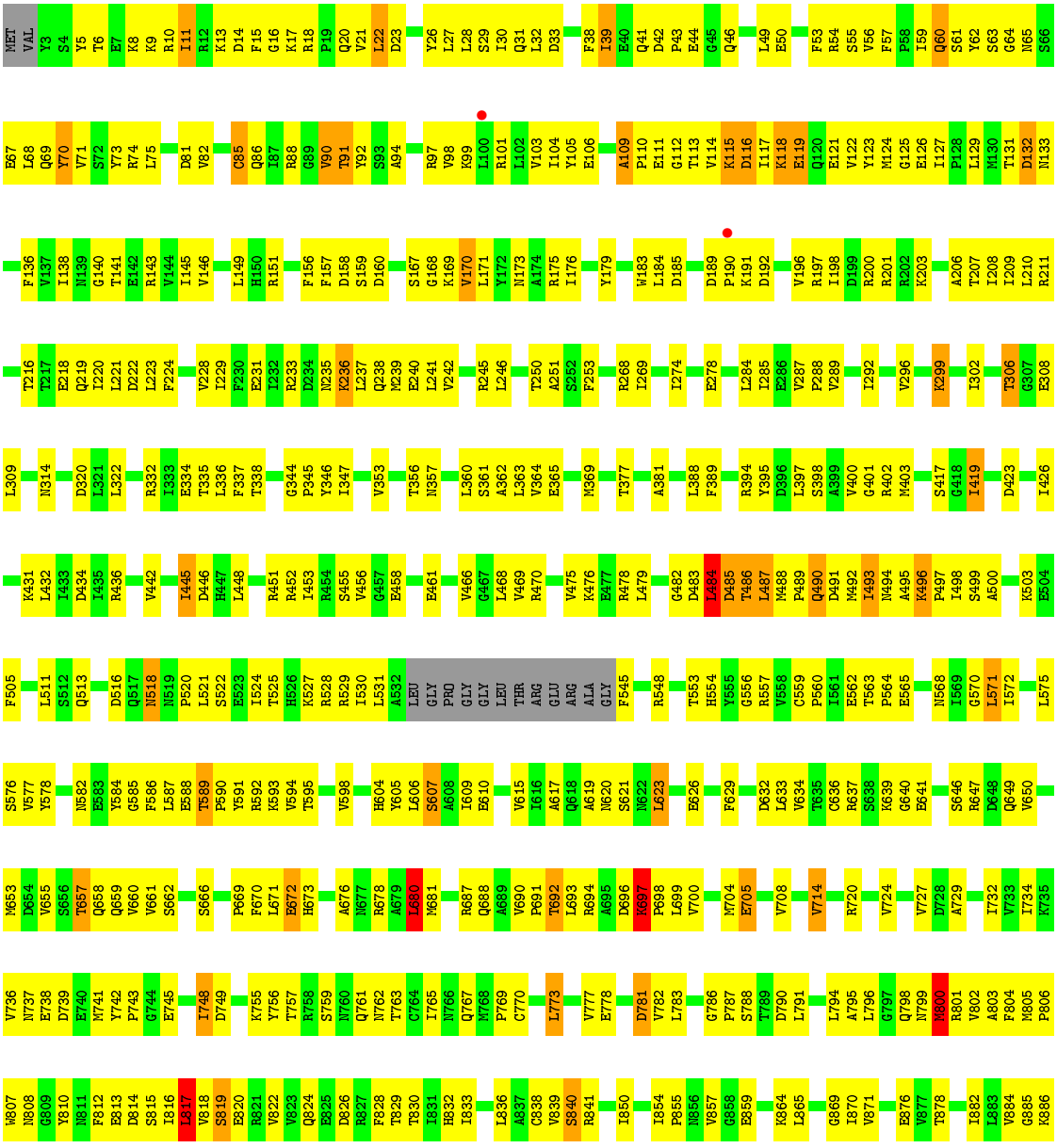
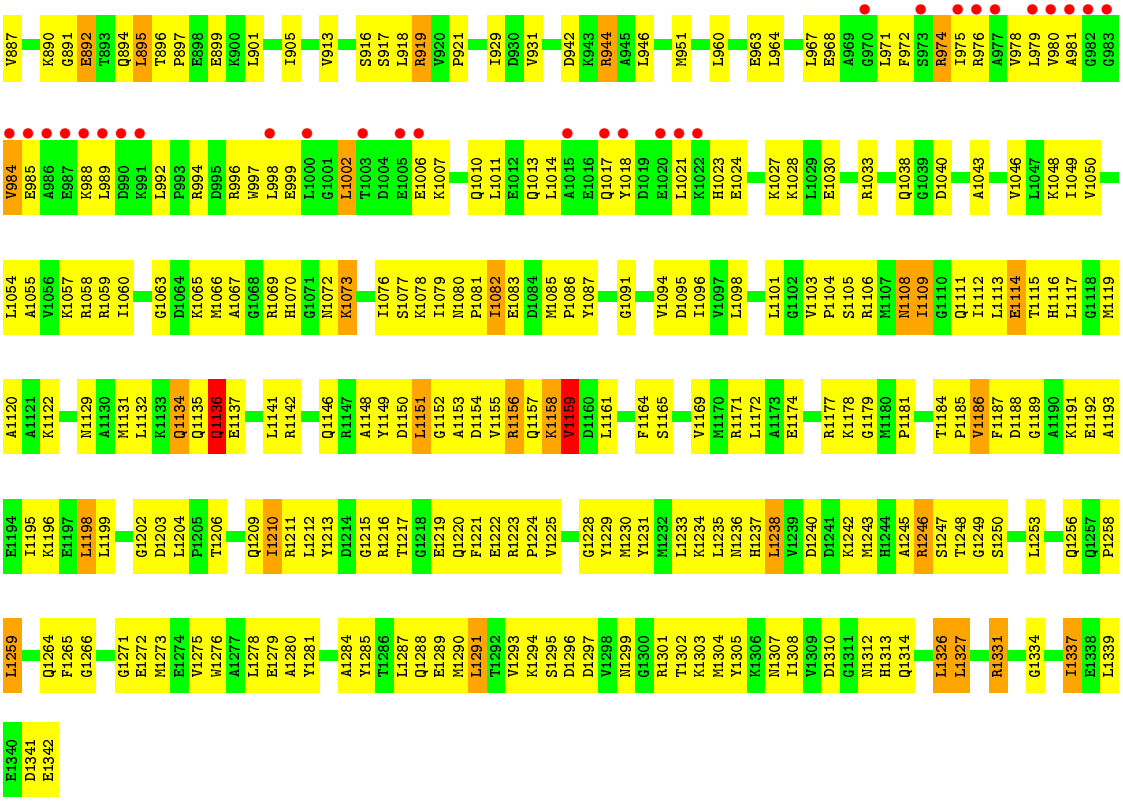
N139 G140 I145 V146 S147 Q148 L149 H150 R151 S152 P153 F156 F157 D158 S159 D160 K161 G162 K163 S167 G168 K169 V170 L171 R175 I176 I177 R180 D185 F188 D189 D192 N193 L194 F195 V196 R197 I198 R201 R202 K203 A206 I209 L210 R211 Y215 E218
Q219 I220 L221 D222 L223 F224 F225 E226 K227 V228 I229 F230 E231 I232 R233 K236 L237 Q238 M239 E240 L241 V242 P243 E244 R245 L246 R247 G248 E249 T250 F253 D254 I255 V261 Y262 V263 E264 K265 G266 R267 R268 I269 T270 A271 R272 H273 I274 R275 Q276 L277 E278 V282 K283 L284 I285 E286
V287 P288 V289 E290 Y291 I292 V296 V297 A298 K299 D300 Y301 I302 D303 T306 G307 E308 L309 I310 C311 A312 A313 N314 M315 E316 L317 S318 L319 D320 L321 L322 A323 K324 L325 S326 Q327 S328 G329 H330 K331 R332 I333 E334 T335 L336 F337 T338 G344 P345 Y346 I347 S348 L351 T356 N357
L360 S361 A362 L363 V364 Y367 R368 M369 M370 E374 P375 P376 T377 E382 F385 F390 D393 R394 L397 G401 R402 N406 R407 E412 E413 I414 I419 K422 D423 I426 K431 D434 I435 R436 D443 D444 I445 L448 R451 R452 I453
R454 S455 V456 G457 E458 R465 V466 G467 L468 M469 R470 V471 E472 E477 R478 L479 S480 L481 G482 D483 L484 D485 T486 L487 M488 P489 Q490 D491 M492 I493 N494 A495 K496 P497 I498 S499 K503 Q510 L511 S512 Q513 F514 M515 D516 Q517 N518 N519 P520 L521 S522 H526 K527 R528 R529 I530
L531 P535 G536 T539 ARG GLU ARG A543 G544 F545 R548 D549 V550 H551 P552 T553 H554 Y555 G556 R557 V558 C559 P560 I561 E562 T563 P564 E565 G566 P567 N568 I569 G570 L571 I572 L575 S576 V577 Y578 N582 P586 L587 E588 T589 P590 Y591 R592 K593 V594 T595 D596 G597 V598 V599
T600 D601 E602 I603 H604 Y605 L606 S607 A608 I609 E610 Y614 V615 I616 A617 Q618 A619 N620 L623 F629 V630 E631 D632 L633 V634 T635 C636 R637 S638 K639 G640 E641 S642 F645 S646 R647 D648 Q649 Y650 D651 Y652 M653 D654 V655 S656 T657 D658 Q659 V660 V661 S662 A665 F670 L671
E672 H673 N677 R678 A679 L680 V681 N684 Q688 A689 V690 P691 T692 L693 R694 A695 D696 K697 P698 L699 G703 M704 E705 G713 V714 T715 A716 V717 A718 K719 R720 G721 G722 V723 V724 Q725 V726 V727 D728 A729 S730 V733 I734 K735 V736 N737 E738 D739 E740 M741 E745 I748
D749 I750 Y751 N752 L753 T754 K755 Y756 T757 Q761 N762 T763 G764 I765 N766 Q767 M768 L773 G774 E775 E778 R779 G780 D781 V782 L783 A784 S788 T789 D790 L791 G792 E793 L794 A795 L796 G797 Q798 N799 M800 R801 V802 A803 F804 M805 P806 W807 N808 G809 Y810 N811 F812 E813 D814 S815 I816
L817 V818 S819 E820 R821 V822 V823 D826 R827 H832 L836 A837 C838 V839 S840 R841 D842 T843 K844 P847 E848 E849 I850 T851 A852 D853 I854 V857 G858 E859 A860 A861 K864 L865 D866 E867 S868 G869 Y872 I873 V877 T878 G879 G880 D881 I882 L883 V884 G885 K886 T888
P889 K890 G891 E892 T893 Q894 L895 T896 F897 E898 E899 K900 L901 F906 S911 D912 V913 S916 S917 L918 R919 V920 P921 V924 I929 D930 V931 F934 D942 K943 R944 A945 L946 N951 Q952 L953 K958 S961 E962 E963 L964 Q965 I966 L967 I971 F972 S973 R974 I975
V980 A981 V984 E985 A986 E987 K988 K991 L992 L1000 G1001 L1002 E1006 K1007 Q1008 L1011 L1014 A1015 E1016 Q1017 Y1018 L1021 E1024 K1027 K1032 T1037 D1040 D1041 L1042 A1043 P1044 G1045 V1046 L1047 K1048 I1049 A1055 R1058 R1059 I1060 Q1061 P1062 G1063 D1064 K1065
M1066 R1069 N1072 K1073 G1074 Y1075 I1076 S1077 K1078 I1079 N1080 P1081 I1082 E1083 D1084 M1085 P1086 Y1087 D1088 E1089 V1094 D1095 L1101 S1105 R1106 M1107 N1108 I1109 G1110 Q1111 I1112 L1113 E1114 T1115 H1116 L1117 G1118 M1119 A1120 A1121 K1122 G1123 I1124 N1129 A1130 M1131 L1132 K1133 Q1134 Q1135 Q1136 E1137 K1140
L1141 R1142 E1143 F1144 I1145 Q1146 R1147 A1148 Y1149 D1150 L1151 G1152 A1153 D1154 V1155 R1156 Q1157 K1158 V1159 D1160 L1161 S1162 T1163 F1164 S1165 V1169 M1170 R1171 E1174 N1175 L1176 R1177 K1178 G1179 M1180 P1181 I1182 A1183 T1184 P1185 V1186 F1187 D1188 G1189 A1190 K1191 E1192 A1193 E1194 I1195 K1196 E1197 L1198 L1199 K1200 L1201 G1202 D1203



- Molecule 2: DNA-directed RNA polymerase subunit beta

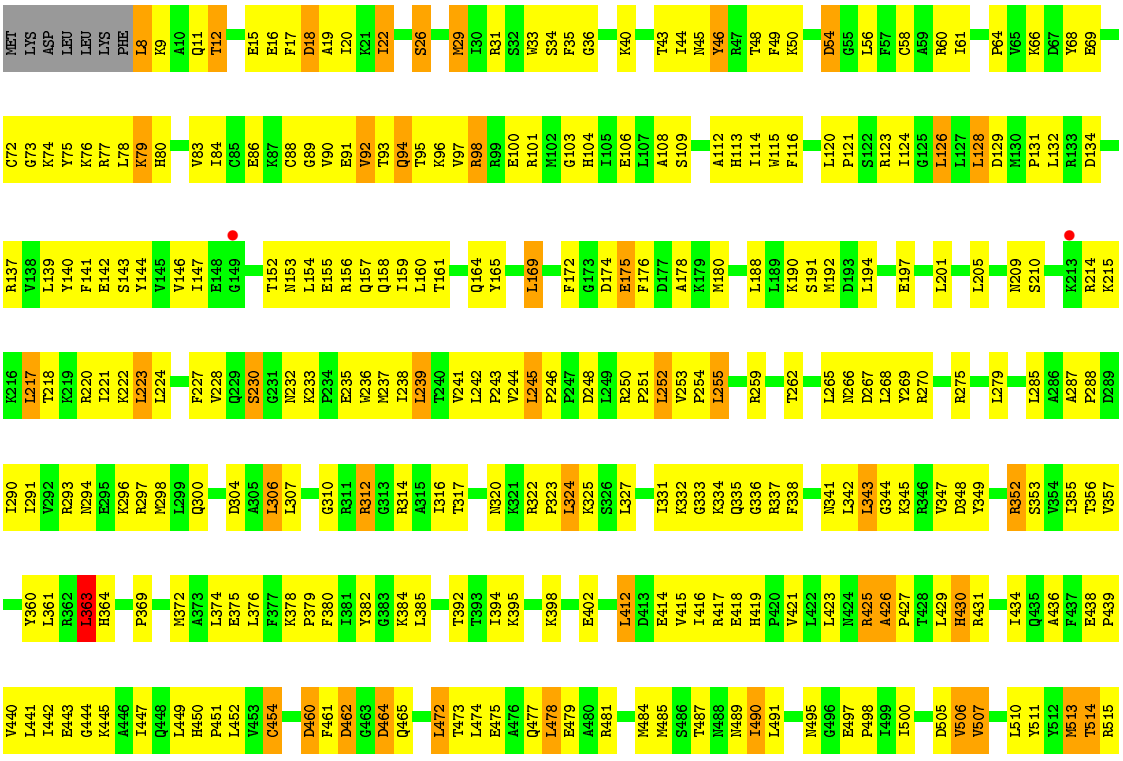
Chain I:

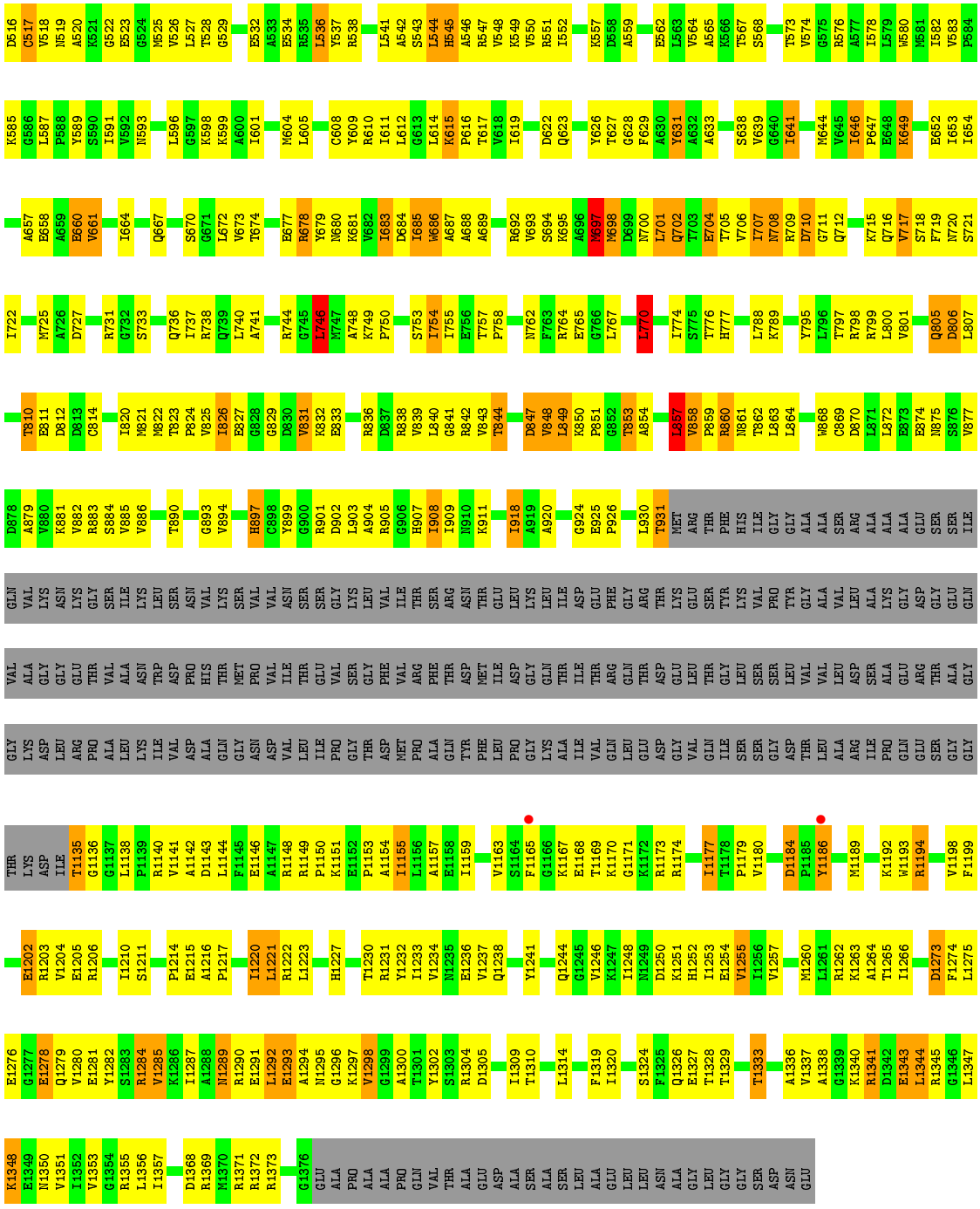




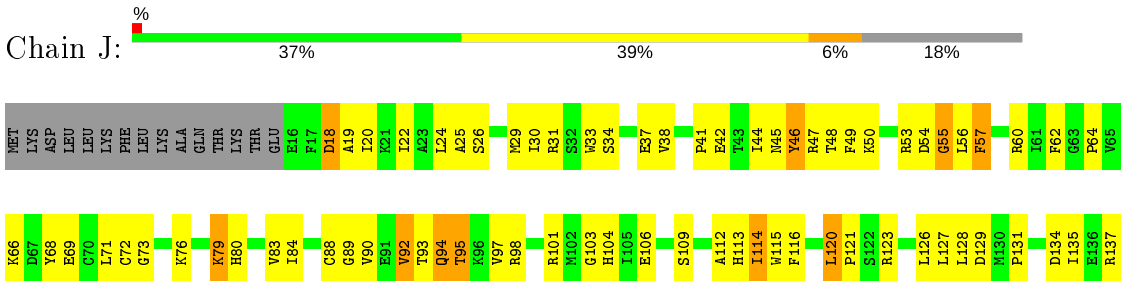
- Molecule 3: DNA-directed RNA polymerase subunit beta'

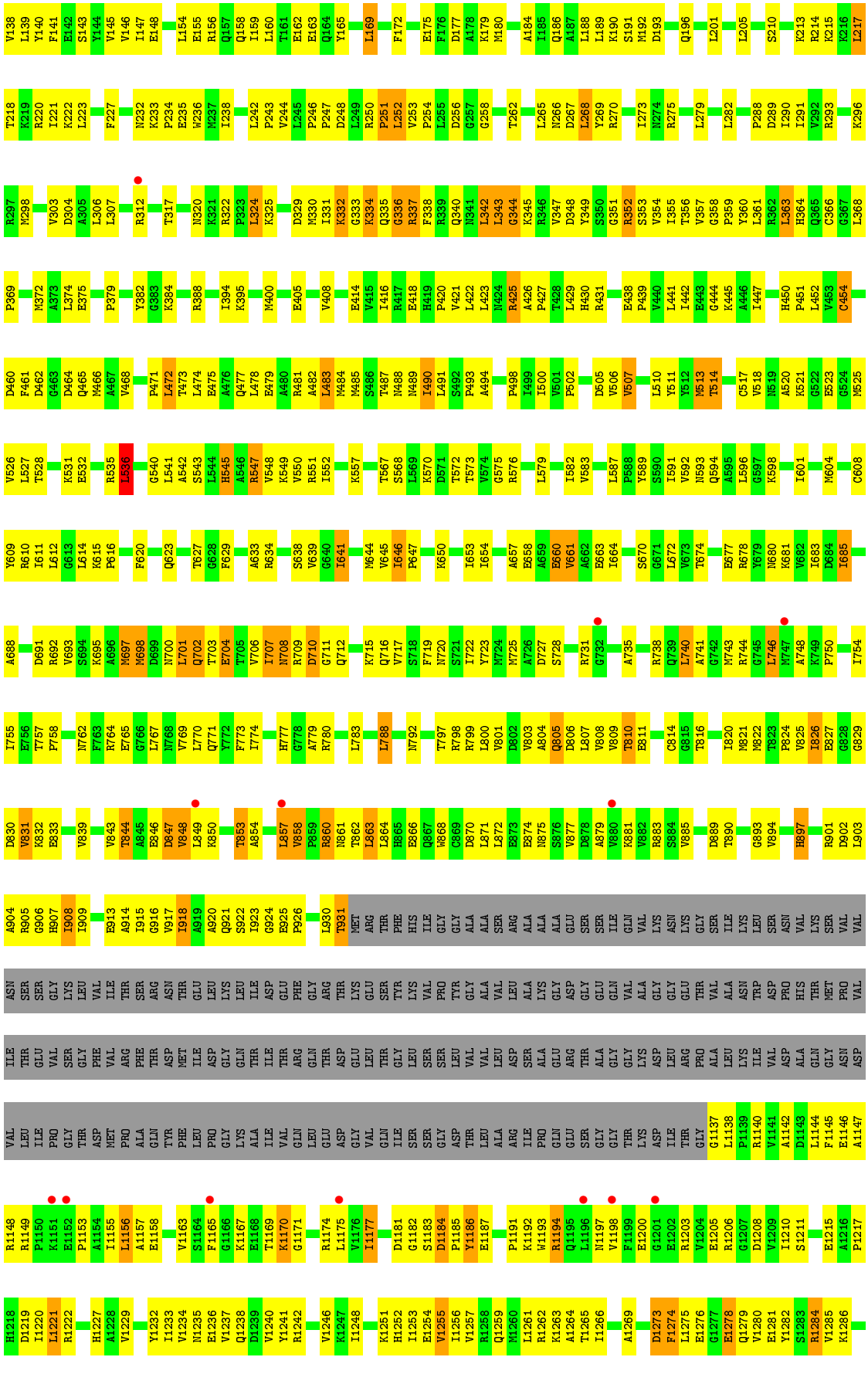
Chain D:

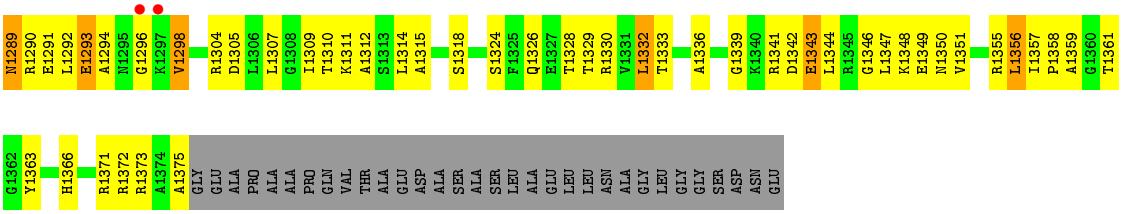




• Molecule 3: DNA-directed RNA polymerase subunit beta'

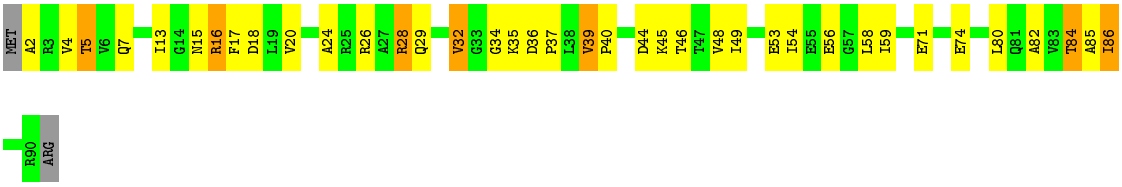






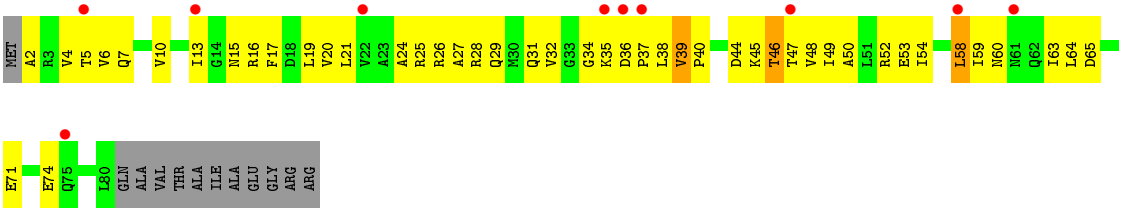
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



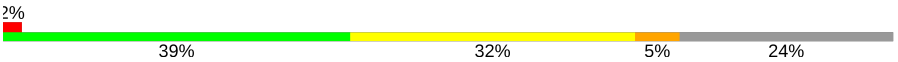
• Molecule 4: DNA-directed RNA polymerase subunit omega

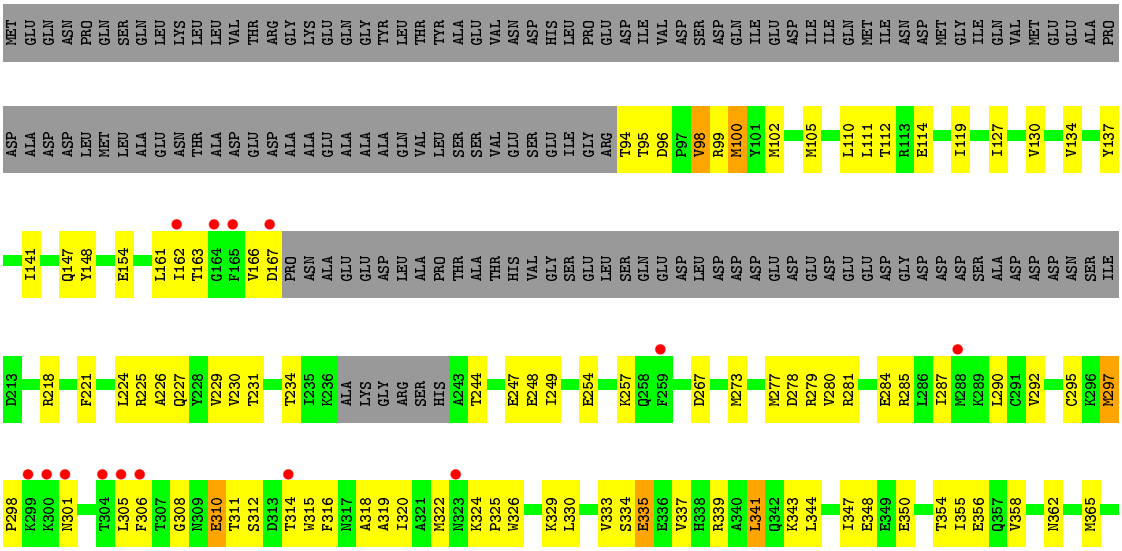
Chain K:

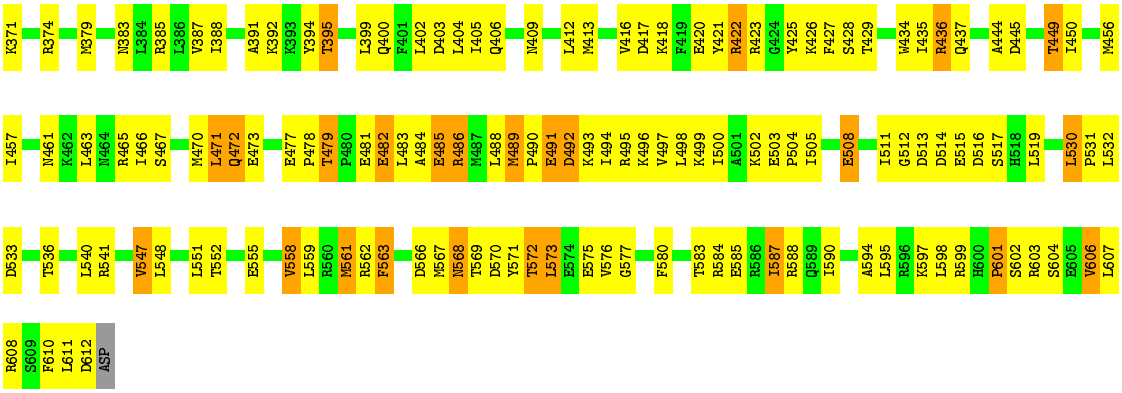


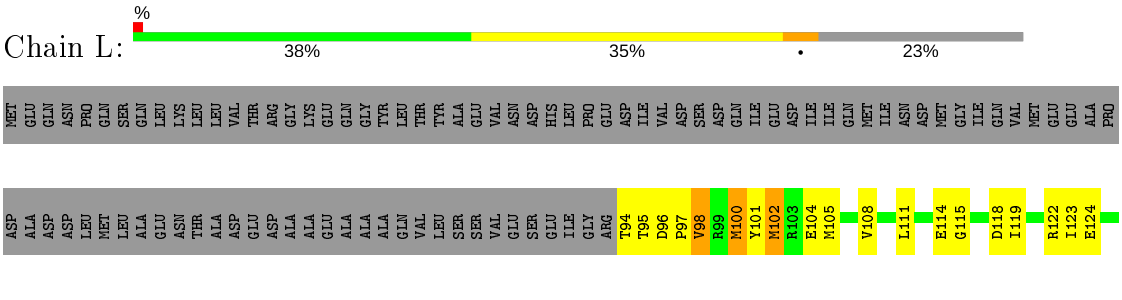
• Molecule 5: RNA polymerase sigma factor RpoD

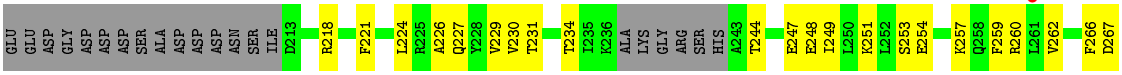
Chain F:

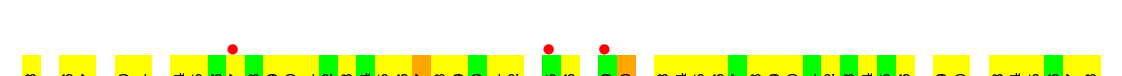


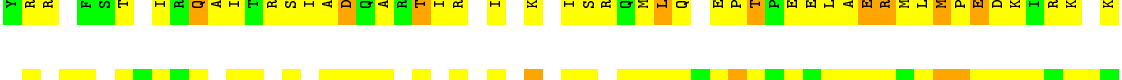


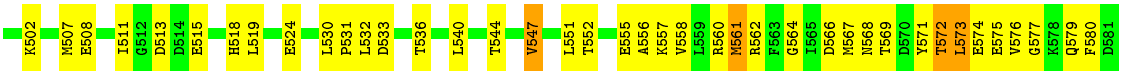












• Molecule 5: RNA polymerase sigma factor RpoD

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	188.17Å 204.69Å 311.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.03 – 4.10 45.03 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (45.03-4.10) 99.0 (45.03-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 4.13Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.210 , 0.255 0.210 , 0.255	Depositor DCC
R_{free} test set	2001 reflections (2.14%)	wwPDB-VP
Wilson B-factor (Å^2)	190.5	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 182.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	55005	wwPDB-VP
Average B, all atoms (Å^2)	241.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: KNG, ZN, MG

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	0.67	1/1774 (0.1%)	1.07	9/2405 (0.4%)
1	B	0.63	0/1668	1.07	7/2260 (0.3%)
1	G	0.50	0/1751	0.82	2/2373 (0.1%)
1	H	0.47	0/1678	0.79	0/2274
2	C	0.67	6/10716 (0.1%)	0.98	24/14458 (0.2%)
2	I	0.56	2/10653 (0.0%)	0.85	14/14373 (0.1%)
3	D	0.71	8/9229 (0.1%)	1.08	42/12459 (0.3%)
3	J	0.60	1/9140 (0.0%)	0.92	16/12341 (0.1%)
4	E	0.62	0/693	0.85	0/935
4	K	0.30	0/629	0.50	0/847
5	F	0.51	0/3864	0.79	2/5194 (0.0%)
5	L	0.48	0/3872	0.76	0/5205
All	All	0.61	18/55667 (0.0%)	0.93	116/75124 (0.2%)

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	B	0	1
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	2
4	E	0	1
5	F	0	1
5	L	0	1
All	All	0	12

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	517	CYS	CB-SG	-9.59	1.66	1.82
2	C	1274	GLU	CG-CD	7.89	1.63	1.51
3	D	426	ALA	C-N	-6.92	1.21	1.34
3	D	727	ASP	CB-CG	5.86	1.64	1.51
2	C	838	CYS	CB-SG	-5.63	1.72	1.81
2	C	1329	GLU	CB-CG	-5.61	1.41	1.52
2	C	807	TRP	CB-CG	-5.60	1.40	1.50
3	D	511	TYR	CB-CG	-5.44	1.43	1.51
2	I	562	GLU	CB-CG	5.42	1.62	1.52
3	D	686	TRP	CB-CG	-5.36	1.40	1.50
2	C	1064	ASP	CB-CG	5.26	1.62	1.51
3	D	464	ASP	CB-CG	5.21	1.62	1.51
3	J	57	PHE	CB-CG	-5.17	1.42	1.51
1	A	19	VAL	CB-CG1	-5.13	1.42	1.52
3	D	511	TYR	CD1-CE1	-5.13	1.31	1.39
2	C	1329	GLU	CG-CD	-5.06	1.44	1.51
2	I	505	PHE	CB-CG	-5.05	1.42	1.51
3	D	144	TYR	CD2-CE2	-5.04	1.31	1.39

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1296	ASP	CB-CG-OD2	-10.40	108.94	118.30
2	C	1233	LEU	CA-CB-CG	9.43	137.00	115.30
2	C	1291	LEU	CA-CB-CG	9.27	136.63	115.30
2	C	1151	LEU	CA-CB-CG	-9.11	94.34	115.30
3	D	605	LEU	CB-CG-CD2	-8.72	96.18	111.00
3	D	727	ASP	CB-CG-OD1	8.36	125.83	118.30
3	J	472	LEU	CA-CB-CG	8.21	134.17	115.30
3	D	770	LEU	CB-CG-CD2	-8.00	97.41	111.00
3	D	807	LEU	CB-CG-CD2	-7.90	97.58	111.00
2	C	1259	LEU	CA-CB-CG	-7.74	97.50	115.30
5	F	563	PHE	C-N-CA	-7.72	106.09	122.30
1	B	85	LEU	CA-CB-CG	-7.55	97.93	115.30
3	J	42	GLU	CA-CB-CG	7.53	129.96	113.40
3	D	1344	LEU	CB-CG-CD2	7.52	123.78	111.00
1	A	177	TYR	CA-CB-CG	7.19	127.06	113.40
3	J	343	LEU	CA-CB-CG	7.13	131.69	115.30
3	D	297	ARG	NE-CZ-NH1	-7.11	116.75	120.30
2	I	1259	LEU	CA-CB-CG	-7.01	99.17	115.30
3	J	114	ILE	CG1-CB-CG2	-6.99	96.01	111.40
2	C	529	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	A	177	TYR	CB-CG-CD1	6.85	125.11	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	126	LEU	CB-CG-CD1	-6.79	99.46	111.00
2	C	1278	LEU	CB-CG-CD1	-6.76	99.51	111.00
3	D	128	LEU	CA-CB-CG	6.66	130.62	115.30
3	D	857	LEU	CA-CB-CG	6.57	130.41	115.30
2	I	1253	LEU	CA-CB-CG	6.56	130.40	115.30
1	B	150	ARG	NE-CZ-NH1	6.55	123.58	120.30
3	D	412	LEU	CB-CG-CD2	-6.55	99.87	111.00
3	D	307	LEU	CB-CG-CD2	-6.52	99.91	111.00
3	J	483	LEU	CB-CG-CD2	-6.52	99.92	111.00
3	J	1156	LEU	CA-CB-CG	6.47	130.19	115.30
3	D	478	LEU	CB-CG-CD2	-6.44	100.05	111.00
3	D	1344	LEU	CA-CB-CG	-6.42	100.54	115.30
3	D	361	LEU	CB-CG-CD1	-6.41	100.11	111.00
3	D	306	LEU	CA-CB-CG	6.39	130.00	115.30
5	F	436	ARG	NE-CZ-NH1	-6.27	117.17	120.30
2	I	1326	LEU	CB-CG-CD1	-6.23	100.41	111.00
3	D	631	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	B	100	LEU	CA-CB-CG	6.10	129.34	115.30
3	D	746	LEU	CA-CB-CG	6.10	129.34	115.30
2	I	432	LEU	CB-CG-CD1	-6.09	100.65	111.00
3	J	727	ASP	CB-CG-OD1	6.08	123.77	118.30
3	D	245	LEU	CB-CG-CD1	-6.08	100.67	111.00
2	I	1291	LEU	CA-CB-CG	6.01	129.13	115.30
2	C	883	LEU	CA-CB-CG	-5.98	101.54	115.30
1	B	79	LEU	CA-CB-CG	5.96	129.00	115.30
2	C	17	LYS	CD-CE-NZ	5.94	125.36	111.70
1	A	48	LEU	CA-CB-CG	5.92	128.92	115.30
2	C	790	ASP	CB-CG-OD1	5.89	123.60	118.30
3	D	460	ASP	CB-CA-C	-5.82	98.76	110.40
3	J	120	LEU	CA-CB-CG	5.76	128.55	115.30
1	B	88	LEU	CB-CG-CD2	-5.73	101.26	111.00
1	G	88	LEU	CA-CB-CG	5.73	128.48	115.30
3	J	1332	LEU	CA-CB-CG	5.73	128.47	115.30
3	D	363	LEU	CA-CB-CG	-5.72	102.15	115.30
2	I	1054	LEU	CB-CG-CD2	-5.69	101.33	111.00
3	D	343	LEU	CB-CG-CD1	-5.66	101.37	111.00
3	D	239	LEU	CB-CG-CD2	-5.66	101.38	111.00
1	G	228	LEU	CA-CB-CG	-5.65	102.30	115.30
2	I	571	LEU	CB-CG-CD2	-5.62	101.45	111.00
3	J	268	LEU	CB-CG-CD1	-5.60	101.48	111.00
2	C	1297	ASP	CB-CG-OD1	-5.58	113.28	118.30
2	C	529	ARG	CG-CD-NE	-5.57	100.11	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1348	LYS	CA-CB-CG	5.56	125.63	113.40
3	D	1341	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	C	1326	LEU	CB-CG-CD2	5.55	120.43	111.00
1	A	224	LEU	CA-CB-CG	-5.51	102.63	115.30
3	D	223	LEU	CB-CG-CD2	5.50	120.35	111.00
2	C	1240	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	177	TYR	CB-CG-CD2	-5.48	117.71	121.00
3	D	447	ILE	CG1-CB-CG2	-5.48	99.35	111.40
1	A	16	ILE	CG1-CB-CG2	5.43	123.34	111.40
3	D	194	LEU	CB-CG-CD2	-5.40	101.83	111.00
1	B	48	LEU	CB-CG-CD2	-5.39	101.83	111.00
2	C	1066	MET	CG-SD-CE	5.38	108.81	100.20
3	J	536	LEU	CA-CB-CG	5.35	127.61	115.30
3	D	615	LYS	CD-CE-NZ	5.33	123.95	111.70
3	D	22	ILE	CG1-CB-CG2	-5.30	99.73	111.40
2	C	680	LEU	CB-CG-CD1	-5.30	102.00	111.00
2	I	680	LEU	CB-CG-CD1	-5.29	102.00	111.00
2	I	1337	ILE	CG1-CB-CG2	-5.28	99.79	111.40
3	J	863	LEU	CA-CB-CG	5.26	127.41	115.30
2	I	697	LYS	N-CA-C	-5.26	96.81	111.00
2	C	1274	GLU	OE1-CD-OE2	-5.25	117.00	123.30
3	J	368	LEU	CB-CG-CD2	-5.24	102.08	111.00
2	I	1296	ASP	CB-CG-OD2	-5.24	113.58	118.30
2	C	1132	LEU	CA-CB-CG	5.24	127.34	115.30
3	D	649	LYS	CD-CE-NZ	5.24	123.74	111.70
3	D	472	LEU	CA-CB-CG	5.21	127.27	115.30
2	C	1179	GLY	N-CA-C	-5.19	100.11	113.10
3	D	544	LEU	CB-CG-CD2	-5.18	102.19	111.00
2	C	1069	ARG	NE-CZ-NH1	-5.17	117.71	120.30
2	C	836	LEU	CB-CG-CD2	-5.17	102.22	111.00
3	D	126	LEU	CA-CB-CG	5.16	127.16	115.30
3	J	830	ASP	CB-CG-OD1	5.16	122.94	118.30
1	B	54	CYS	CA-CB-SG	5.15	123.27	114.00
3	D	449	LEU	CB-CG-CD2	-5.14	102.27	111.00
2	I	817	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	44	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	D	255	LEU	CB-CG-CD2	-5.12	102.29	111.00
3	D	1168	GLU	CA-CB-CG	5.12	124.68	113.40
2	C	1273	MET	CG-SD-CE	-5.12	92.01	100.20
3	D	631	TYR	CB-CG-CD1	5.11	124.07	121.00
3	D	1220	ILE	CG1-CB-CG2	-5.11	100.16	111.40
2	I	800	MET	CB-CG-SD	-5.10	97.10	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	462	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	83	LEU	CB-CG-CD2	5.09	119.65	111.00
2	C	1326	LEU	CB-CG-CD1	-5.09	102.35	111.00
3	J	55	GLY	N-CA-C	-5.08	100.39	113.10
2	I	484	LEU	CA-CB-CG	5.08	126.98	115.30
3	D	1292	LEU	CA-CB-CG	5.07	126.97	115.30
3	D	697	MET	CB-CG-SD	5.05	127.56	112.40
3	D	464	ASP	CB-CG-OD2	5.04	122.83	118.30
3	J	1356	LEU	CB-CG-CD2	-5.01	102.48	111.00
2	C	1291	LEU	CB-CG-CD2	-5.00	102.49	111.00
1	A	65	LEU	CB-CG-CD1	-5.00	102.50	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	GLU	Peptide
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
4	E	32	VAL	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
2	I	236	LYS	Peptide
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
5	L	601	PRO	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	1753	0	1780	152	0
1	B	1649	0	1674	184	0
1	G	1730	0	1756	191	0
1	H	1659	0	1692	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	10548	0	10553	852	0
2	I	10486	0	10496	746	0
3	D	9089	0	9265	765	0
3	J	9001	0	9169	751	0
4	E	691	0	695	36	0
4	K	627	0	634	59	0
5	F	3813	0	3880	264	0
5	L	3821	0	3884	246	0
6	C	70	62	0	10	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	2	0
All	All	54943	62	55478	4003	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 36.

All (4003) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.21	1.21
5:L:561:MET:HA	5:L:567:MET:HE1	1.27	1.17
2:C:1271:GLY:HA2	3:D:343:LEU:HD11	1.22	1.16
2:I:942:ASP:OD2	2:I:1048:LYS:NZ	1.78	1.16
1:B:183:ILE:HD11	1:B:205:MET:HG3	1.21	1.15
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.30	1.14
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.28	1.14
1:H:79:LEU:HD11	3:J:526:VAL:HG21	1.24	1.13
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.31	1.13
1:G:45:ARG:HG2	1:H:38:THR:HB	1.17	1.12
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.16	1.11
3:D:342:LEU:HA	3:D:343:LEU:HD13	1.20	1.11
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.32	1.10
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.10	1.10
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.14	1.10
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.11	1.09
2:C:1271:GLY:CA	3:D:343:LEU:HD11	1.80	1.09
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.31	1.08
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.35	1.08
3:D:342:LEU:HA	3:D:343:LEU:CD1	1.84	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.36	1.07
3:D:1289:ASN:OD1	3:D:1290:ARG:NH1	1.86	1.07
1:B:23:HIS:HB2	1:B:205:MET:O	1.51	1.07
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.15	1.06
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.33	1.06
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.36	1.06
2:C:1289:GLU:OE2	3:D:473:THR:HG22	1.57	1.05
2:C:1291:LEU:HD21	3:D:1351:VAL:HG13	1.33	1.05
2:C:1131:MET:CE	2:C:1141:LEU:HD12	1.85	1.05
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.37	1.05
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.34	1.04
1:B:35:PHE:HA	1:B:38:THR:HG22	1.39	1.04
3:D:848:VAL:HG23	3:D:858:VAL:HG13	1.39	1.04
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.34	1.04
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.36	1.03
2:I:1234:LYS:HE2	2:I:1238:LEU:HD23	1.40	1.02
5:L:470:MET:CE	5:L:478:PRO:HB3	1.89	1.02
1:H:57:THR:HG21	1:H:158:ARG:HE	1.22	1.02
2:I:1289:GLU:OE2	3:J:473:THR:HG22	1.58	1.02
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.41	1.02
3:J:384:LYS:NZ	3:J:414:GLU:OE1	1.93	1.02
1:B:29:GLU:HB3	1:B:30:PRO:HD3	1.37	1.02
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.39	1.02
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.41	1.02
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.38	1.01
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.43	1.01
2:I:1291:LEU:HD21	3:J:1351:VAL:HG13	1.42	1.01
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.43	1.01
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.40	1.00
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.43	1.00
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	1.77	1.00
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.43	1.00
2:C:109:ALA:HB1	2:C:110:PRO:C	1.82	1.00
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.41	0.99
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.38	0.99
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.24	0.99
1:G:45:ARG:HG2	1:H:38:THR:CB	1.92	0.99
2:C:1269:ARG:HD3	3:D:343:LEU:HB3	1.43	0.99
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.40	0.99
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.42	0.99
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.43	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.42	0.98
1:H:83:LEU:HD11	3:J:526:VAL:CG2	1.94	0.98
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.46	0.98
5:L:470:MET:HE2	5:L:478:PRO:HB3	1.42	0.98
2:I:972:PHE:CE2	2:I:998:LEU:HD11	1.99	0.97
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.44	0.97
2:C:490:GLN:HG3	5:F:472:GLN:HE21	1.29	0.97
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	1.80	0.97
3:J:1266:ILE:HB	3:J:1274:PHE:O	1.65	0.97
3:J:186:GLN:HG3	3:J:238:ILE:HB	1.46	0.97
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.44	0.96
1:A:13:LEU:H	1:A:13:LEU:HD23	1.31	0.96
1:H:91:ARG:NH1	1:H:210:THR:O	1.97	0.96
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	1.47	0.96
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.45	0.96
2:I:109:ALA:HB1	2:I:110:PRO:C	1.85	0.96
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	1.47	0.95
1:H:23:HIS:HB2	1:H:205:MET:O	1.66	0.95
1:B:29:GLU:OE1	1:B:200:LYS:HE2	1.64	0.95
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.48	0.95
2:C:529:ARG:HH12	6:C:2001:KNG:C18	1.80	0.95
1:A:45:ARG:HG2	1:B:38:THR:HB	1.47	0.95
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.28	0.95
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.48	0.95
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.48	0.95
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.46	0.95
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.46	0.94
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.48	0.94
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.46	0.94
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.49	0.94
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.47	0.94
1:G:23:HIS:HB2	1:G:205:MET:O	1.66	0.94
1:A:211:ILE:HG21	1:A:216:ALA:HB2	1.48	0.94
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.01	0.94
1:H:62:ASP:HB2	1:H:141:SER:O	1.67	0.94
2:C:510:GLN:HA	6:C:2001:KNG:C49	1.98	0.93
3:D:576:ARG:NH1	3:D:593:ASN:O	2.02	0.93
5:F:484:ALA:HB1	5:F:491:GLU:CB	1.98	0.93
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.50	0.93
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	1.97	0.93
3:D:18:ASP:HB2	3:D:1373:ARG:NH2	1.83	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:ALA:O	1:H:146:VAL:HG13	1.68	0.93
2:C:145:ILE:CG2	2:C:456:VAL:HG22	1.99	0.93
2:C:1248:THR:HG21	5:F:531:PRO:CG	1.98	0.93
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.51	0.93
2:I:125:GLY:CA	2:I:499:SER:HB2	1.99	0.93
2:C:745:GLU:CG	2:C:1017:GLN:HB3	1.99	0.93
2:C:818:VAL:CG2	2:C:1076:ILE:HD13	1.98	0.93
2:C:1271:GLY:HA2	3:D:343:LEU:CD1	1.98	0.93
2:C:151:ARG:NE	2:C:445:ILE:HD11	1.84	0.92
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.50	0.92
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.33	0.92
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	1.83	0.92
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	1.85	0.92
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.49	0.92
3:D:1273:ASP:HB3	3:D:1276:GLU:HG3	1.52	0.91
3:D:460:ASP:HB2	3:D:464:ASP:OD2	1.71	0.91
3:J:45:ASN:HB3	3:J:48:THR:O	1.71	0.91
2:I:1158:LYS:O	2:I:1159:VAL:HG13	1.70	0.91
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.52	0.91
1:A:23:HIS:HB2	1:A:205:MET:O	1.71	0.91
1:B:183:ILE:CD1	1:B:205:MET:HG3	2.01	0.91
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.52	0.91
3:J:507:VAL:HG11	3:J:598:LYS:HG3	1.52	0.91
2:I:1131:MET:HE1	2:I:1141:LEU:HD12	1.53	0.90
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.00	0.90
3:D:536:LEU:HD13	3:D:541:LEU:HB2	1.52	0.90
3:J:186:GLN:HB2	3:J:238:ILE:HG21	1.53	0.90
3:J:418:GLU:HG3	4:K:44:ASP:HA	1.53	0.90
1:B:104:LYS:HG2	1:B:110:VAL:HG22	1.52	0.90
3:J:126:LEU:HD13	3:J:223:LEU:CD2	2.01	0.90
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.53	0.90
3:D:74:LYS:NZ	3:D:86:GLU:OE1	2.05	0.90
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.50	0.90
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.52	0.89
2:C:5:TYR:HD1	2:C:8:LYS:HD3	1.38	0.89
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.54	0.89
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.08	0.89
5:L:316:PHE:CZ	5:L:334:SER:HA	2.08	0.89
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.08	0.89
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.07	0.89
3:J:98:ARG:HB3	3:J:248:ASP:OD2	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ILE:CG2	1:A:216:ALA:HB2	2.03	0.89
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.55	0.89
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.54	0.89
5:F:316:PHE:HZ	5:F:334:SER:HA	1.38	0.89
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.54	0.89
2:C:483:ASP:HB2	2:C:486:THR:HG21	1.51	0.89
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.38	0.89
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.36	0.89
2:C:818:VAL:HG23	2:C:1076:ILE:HD13	1.55	0.89
1:H:51:MET:HG3	1:H:52:PRO:HD2	1.55	0.89
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.54	0.88
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.07	0.88
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.55	0.88
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.54	0.88
2:C:1248:THR:HG21	5:F:531:PRO:HG2	1.54	0.88
1:G:70:THR:CG2	2:I:755:LYS:HE2	2.02	0.88
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.03	0.88
1:B:53:GLY:HA3	1:B:177:TYR:O	1.73	0.88
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.03	0.88
3:D:363:LEU:HG	3:D:363:LEU:O	1.72	0.88
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.56	0.88
3:D:859:PRO:HG2	3:D:862:THR:HG21	1.55	0.88
2:I:593:LYS:HE3	2:I:595:THR:CG2	2.04	0.88
2:C:697:LYS:HA	2:C:795:ALA:HB2	1.55	0.87
3:D:336:GLY:HA3	3:D:1324:SER:O	1.74	0.87
3:D:56:LEU:HD12	3:D:56:LEU:H	1.38	0.87
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.03	0.87
2:I:1077:SER:HA	3:J:356:THR:OG1	1.73	0.87
3:J:94:GLN:O	3:J:97:VAL:HG23	1.75	0.87
2:C:302:ILE:HG22	2:C:309:LEU:CA	2.04	0.87
2:C:1066:MET:CE	2:C:1076:ILE:HB	2.03	0.87
2:C:296:VAL:HB	2:C:336:LEU:HD12	1.54	0.87
2:C:887:VAL:HB	2:C:913:VAL:HG21	1.55	0.87
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.57	0.87
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.10	0.87
3:D:857:LEU:HD23	3:D:875:ASN:ND2	1.90	0.86
1:G:12:ARG:H	1:G:30:PRO:HD2	1.39	0.86
2:I:891:GLY:O	2:I:892:GLU:HG3	1.74	0.86
3:J:510:LEU:HD22	3:J:601:ILE:CD1	2.05	0.86
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.08	0.86
2:I:819:SER:HB2	2:I:1085:MET:SD	2.14	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:ILE:HB	1:A:64:VAL:HG21	1.58	0.86
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.57	0.86
3:D:905:ARG:HH21	3:D:907:HIS:CB	1.87	0.86
3:D:799:ARG:NH1	3:D:1146:GLU:OE1	2.09	0.86
1:B:86:LYS:NZ	1:B:174:ASP:OD2	2.08	0.86
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.57	0.86
3:J:1280:VAL:CG2	3:J:1304:ARG:HE	1.89	0.86
1:H:110:VAL:HG21	1:H:140:ILE:HD11	1.58	0.86
2:C:145:ILE:CB	2:C:456:VAL:HG22	2.05	0.86
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.05	0.86
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.56	0.86
2:C:490:GLN:HG3	5:F:472:GLN:NE2	1.91	0.86
3:J:722:ILE:HD11	3:J:740:LEU:HD23	1.58	0.85
5:F:343:LYS:H	5:F:343:LYS:HD2	1.40	0.85
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.04	0.85
2:I:30:ILE:HD12	2:I:30:ILE:H	1.39	0.85
3:D:97:VAL:HG11	3:D:101:ARG:CZ	2.06	0.85
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.41	0.85
2:I:887:VAL:HB	2:I:913:VAL:HG21	1.58	0.85
2:I:963:GLU:O	2:I:967:LEU:HB2	1.77	0.85
5:L:470:MET:SD	5:L:486:ARG:NH1	2.49	0.85
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.58	0.85
1:H:53:GLY:HA3	1:H:177:TYR:O	1.76	0.85
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.56	0.85
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.41	0.85
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.07	0.85
1:B:125:LYS:HE2	1:B:128:HIS:CD2	2.11	0.85
2:C:698:PRO:HG3	2:C:1231:TYR:CE2	2.11	0.85
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.57	0.85
3:J:653:ILE:HD13	3:J:692:ARG:HB3	1.57	0.85
2:C:593:LYS:HB3	2:C:602:GLU:HG3	1.58	0.85
5:F:540:LEU:HD12	5:F:610:PHE:CD1	2.11	0.85
2:I:223:LEU:HD13	2:I:426:ILE:HD13	1.59	0.84
1:G:83:LEU:HD23	2:I:694:ARG:NH2	1.92	0.84
5:L:148:TYR:OH	5:L:218:ARG:HA	1.77	0.84
5:L:119:ILE:HG23	5:L:375:ALA:HB1	1.58	0.84
3:D:700:ASN:O	3:D:704:GLU:HB2	1.77	0.84
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.24	0.84
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.11	0.84
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.58	0.84
5:L:316:PHE:HZ	5:L:334:SER:HA	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.57	0.84
3:J:425:ARG:NH1	3:J:464:ASP:OD1	2.11	0.84
2:C:890:LYS:HE2	2:C:891:GLY:H	1.41	0.84
3:J:1167:LYS:HD3	3:J:1174:ARG:HD2	1.60	0.84
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.13	0.84
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.13	0.84
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.13	0.84
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.41	0.84
1:G:231:PHE:HB3	1:H:218:ARG:HH11	1.42	0.84
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.59	0.83
1:H:29:GLU:OE2	1:H:200:LYS:HE3	1.77	0.83
2:C:2:VAL:O	2:C:3:TYR:HB2	1.79	0.83
2:C:561:ILE:HD11	2:C:665:ALA:HB1	1.58	0.83
3:J:363:LEU:HG	3:J:363:LEU:O	1.77	0.83
1:B:62:ASP:HB2	1:B:141:SER:O	1.77	0.83
1:B:6:THR:HG23	1:B:6:THR:O	1.79	0.83
2:I:1024:GLU:HG2	2:I:1028:LYS:HD3	1.60	0.83
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.60	0.83
3:J:843:VAL:HG13	3:J:883:ARG:HD3	1.59	0.83
2:I:972:PHE:HD1	2:I:994:ARG:HH21	1.21	0.83
2:C:745:GLU:HG3	2:C:1017:GLN:CB	2.06	0.83
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.61	0.83
5:L:281:ARG:O	5:L:285:ARG:HG3	1.78	0.83
6:C:2001:KNG:O07	6:C:2001:KNG:O19	1.90	0.83
5:F:573:LEU:H	5:F:573:LEU:HD23	1.44	0.82
3:J:479:GLU:HG3	4:K:20:VAL:HG11	1.59	0.82
3:J:700:ASN:O	3:J:704:GLU:HB2	1.80	0.82
1:A:166:ARG:O	1:A:168:ILE:N	2.11	0.82
1:H:57:THR:O	1:H:173:VAL:HG22	1.79	0.82
2:I:1248:THR:HG21	5:L:531:PRO:HG3	1.61	0.82
3:D:35:PHE:HD1	3:D:101:ARG:HB3	1.45	0.82
1:G:14:VAL:HG22	1:G:15:ASP:H	1.45	0.82
3:J:1198:VAL:HB	3:J:1210:ILE:HA	1.61	0.82
1:B:11:PRO:HB2	1:B:28:LEU:HD11	1.62	0.82
1:A:228:LEU:HD22	1:B:221:ALA:HB1	1.61	0.82
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.60	0.82
3:J:1263:LYS:HE2	3:J:1279:GLN:HE21	1.43	0.82
1:A:14:VAL:HG22	1:A:15:ASP:H	1.43	0.82
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.60	0.81
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.61	0.81
2:C:453:ILE:HD12	2:C:587:LEU:HD21	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.62	0.81
3:D:140:TYR:CE2	5:F:95:THR:HG22	2.15	0.81
1:G:191:ARG:NH1	1:G:197:ASP:HA	1.95	0.81
2:I:1142:ARG:HD3	2:I:1161:LEU:CD1	2.10	0.81
2:C:133:ASN:ND2	2:C:713:GLY:HA3	1.94	0.81
3:D:1290:ARG:HD3	3:D:1294:ALA:HB1	1.63	0.81
1:A:233:ASP:C	1:A:234:LEU:HD22	2.00	0.81
2:C:890:LYS:HE2	2:C:891:GLY:N	1.96	0.81
3:J:1140:ARG:NH2	3:J:1236:GLU:HG2	1.92	0.81
2:I:145:ILE:HB	2:I:456:VAL:HG22	1.61	0.81
3:J:138:VAL:HG21	3:J:145:VAL:HB	1.63	0.81
1:G:118:ASP:HB3	1:G:121:VAL:CG2	2.09	0.81
1:H:32:GLU:HA	1:H:198:LEU:HD22	1.61	0.81
3:J:210:SER:O	3:J:214:ARG:HG2	1.79	0.81
3:J:901:ARG:HD2	3:J:906:GLY:O	1.80	0.81
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.63	0.81
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.62	0.81
5:F:354:THR:O	5:F:358:VAL:HG23	1.80	0.81
2:I:1247:SER:HB3	3:J:375:GLU:O	1.80	0.81
2:C:145:ILE:HB	2:C:456:VAL:CG2	2.11	0.80
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.46	0.80
3:J:363:LEU:CD2	3:J:487:THR:HG22	2.10	0.80
3:J:97:VAL:HG11	3:J:101:ARG:NH2	1.96	0.80
5:F:284:GLU:HG2	5:F:310:GLU:OE1	1.81	0.80
2:C:1158:LYS:O	2:C:1159:VAL:HG13	1.81	0.80
2:C:883:LEU:HD11	2:C:920:VAL:HG22	1.63	0.80
5:F:399:LEU:HB3	5:F:404:LEU:HD21	1.61	0.80
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.45	0.80
1:H:35:PHE:HA	1:H:38:THR:HG22	1.63	0.80
3:D:342:LEU:CA	3:D:343:LEU:HD13	2.08	0.80
1:H:64:VAL:HG11	1:H:69:SER:OG	1.81	0.80
2:I:237:LEU:HD23	2:I:289:VAL:HG23	1.64	0.80
2:C:1131:MET:HE2	2:C:1141:LEU:HA	1.61	0.80
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.64	0.80
3:D:343:LEU:HD12	3:D:344:GLY:HA3	1.61	0.80
2:I:133:ASN:O	2:I:527:LYS:NZ	2.14	0.80
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.64	0.80
2:C:40:GLU:O	2:C:73:TYR:OH	1.99	0.80
1:H:99:ILE:HD11	1:H:143:ARG:HB3	1.63	0.80
2:I:452:ARG:NH1	2:I:585:GLY:HA3	1.97	0.80
2:I:901:LEU:HD11	2:I:905:ILE:HD11	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:597:LYS:O	5:F:603:ARG:HG3	1.82	0.79
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.64	0.79
3:J:517:CYS:HA	3:J:716:GLN:NE2	1.98	0.79
5:L:289:LYS:HA	5:L:293:GLU:OE1	1.82	0.79
5:L:489:MET:CE	5:L:493:LYS:HD2	2.12	0.79
3:J:290:ILE:HD12	3:J:290:ILE:H	1.48	0.79
2:C:1142:ARG:HD3	2:C:1161:LEU:HD11	1.62	0.79
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.63	0.79
3:D:694:SER:OG	3:D:738:ARG:NE	2.13	0.79
2:I:56:VAL:HG11	2:I:468:LEU:HD13	1.64	0.79
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.44	0.79
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.46	0.79
3:D:418:GLU:O	3:D:481:ARG:NH2	2.16	0.79
3:D:848:VAL:CG2	3:D:858:VAL:HG13	2.12	0.79
1:B:29:GLU:HB3	1:B:30:PRO:CD	2.12	0.79
2:C:1157:GLN:O	2:C:1158:LYS:HG2	1.83	0.79
2:C:890:LYS:NZ	2:C:891:GLY:O	2.14	0.79
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.65	0.79
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.63	0.79
1:B:212:ASP:OD1	1:B:214:GLU:HB3	1.83	0.79
2:C:269:ILE:HG22	2:C:274:ILE:HG13	1.65	0.79
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.65	0.79
1:B:125:LYS:HE2	1:B:128:HIS:HD2	1.47	0.79
2:C:302:ILE:CG2	2:C:309:LEU:HA	2.12	0.79
2:C:156:PHE:CE1	2:C:443:ASP:HB2	2.17	0.79
5:L:132:CYS:SG	5:L:257:LYS:NZ	2.54	0.79
2:I:192:ASP:OD2	2:I:436:ARG:NH2	2.16	0.79
1:B:89:ALA:HB3	1:B:124:VAL:CG1	2.12	0.78
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.12	0.78
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.65	0.78
1:B:205:MET:HE1	1:B:213:PRO:HA	1.65	0.78
3:D:1280:VAL:O	3:D:1284:ARG:HB3	1.82	0.78
5:F:148:TYR:OH	5:F:218:ARG:HA	1.84	0.78
2:C:1242:LYS:HD2	3:D:465:GLN:OE1	1.83	0.78
2:C:1276:TRP:CE2	3:D:801:VAL:HG21	2.19	0.78
2:C:1196:LYS:CD	2:C:1206:THR:HG23	2.13	0.78
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.66	0.78
2:C:748:ILE:HD11	2:C:967:LEU:HD12	1.64	0.78
2:C:93:SER:OG	2:C:126:GLU:OE1	2.00	0.78
2:C:3:TYR:CE1	2:C:11:ILE:HD11	2.18	0.78
1:G:227:GLN:HE21	1:H:35:PHE:HD2	1.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:425:ARG:HG2	3:J:426:ALA:H	1.49	0.78
3:J:814:CYS:HB3	3:J:890:THR:OG1	1.84	0.78
3:D:1280:VAL:HG11	3:D:1304:ARG:NH2	1.98	0.78
1:H:13:LEU:HD12	1:H:16:ILE:HD11	1.65	0.78
3:J:1280:VAL:CG1	3:J:1304:ARG:HH21	1.97	0.78
2:I:985:GLU:CG	2:I:988:LYS:HD2	2.14	0.78
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.64	0.78
1:B:64:VAL:HG11	1:B:69:SER:CB	2.14	0.78
3:J:647:PRO:CG	3:J:697:MET:HB3	2.13	0.78
1:A:38:THR:OG1	1:B:45:ARG:HG2	1.83	0.77
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.65	0.77
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.17	0.77
3:D:333:GLY:HA3	3:D:338:PHE:CE1	2.19	0.77
3:J:827:GLU:O	3:J:829:GLY:N	2.14	0.77
3:J:872:LEU:CD2	3:J:877:VAL:HG11	2.14	0.77
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.16	0.77
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.65	0.77
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.49	0.77
3:J:97:VAL:HG11	3:J:101:ARG:CZ	2.14	0.77
5:F:314:THR:O	5:F:318:ALA:HB3	1.84	0.77
5:F:371:LYS:HA	5:F:374:ARG:NH1	1.99	0.77
3:J:1269:ALA:HB2	3:J:1274:PHE:CE1	2.19	0.77
3:J:870:ASP:O	3:J:874:GLU:HG2	1.84	0.77
5:L:470:MET:HE1	5:L:482:GLU:HG2	1.65	0.77
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.19	0.77
3:D:518:VAL:CG1	3:D:707:ILE:HD13	2.14	0.77
2:I:122:VAL:HG11	2:I:493:ILE:HD13	1.64	0.77
1:A:10:LYS:HE2	1:B:229:GLU:OE1	1.85	0.77
1:B:47:LEU:HD13	1:B:183:ILE:HG12	1.65	0.77
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.25	0.77
1:H:51:MET:O	1:H:150:ARG:HA	1.85	0.77
2:I:1234:LYS:CE	2:I:1238:LEU:HD23	2.13	0.77
2:I:175:ARG:HD3	2:I:183:TRP:CE3	2.19	0.77
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.67	0.76
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.67	0.76
1:G:13:LEU:H	1:G:13:LEU:HD23	1.49	0.76
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.18	0.76
3:D:45:ASN:HB3	3:D:48:THR:O	1.85	0.76
5:F:426:LYS:HE2	5:F:428:SER:OG	1.85	0.76
3:J:698:MET:O	3:J:702:GLN:HB3	1.85	0.76
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:738:GLU:HG2	2:I:741:MET:CE	2.15	0.76
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.66	0.76
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.18	0.76
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.19	0.76
2:I:698:PRO:HG3	2:I:1231:TYR:CE2	2.20	0.76
3:J:1140:ARG:HH21	3:J:1236:GLU:CG	1.97	0.76
3:D:259:ARG:NH1	5:F:505:ILE:HD11	2.01	0.76
2:I:1038:GLN:HG3	2:I:1038:GLN:O	1.84	0.76
2:I:62:TYR:CZ	2:I:476:LYS:HB3	2.21	0.76
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.67	0.76
2:C:1142:ARG:NH2	2:C:1165:SER:HB2	1.99	0.76
2:C:453:ILE:HD11	2:C:587:LEU:HD11	1.68	0.76
2:C:703:GLY:N	2:C:705:GLU:OE2	2.18	0.76
2:I:666:SER:OG	2:I:704:MET:HG3	1.85	0.76
3:J:488:ASN:HD21	4:K:6:VAL:HG22	1.51	0.76
3:D:79:LYS:HG3	3:D:80:HIS:N	1.98	0.76
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.19	0.76
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.49	0.76
2:C:726:TYR:OH	2:C:728:ASP:OD2	2.03	0.76
2:C:724:VAL:HG23	2:C:775:GLU:O	1.86	0.76
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.67	0.75
2:C:1217:THR:OG1	2:C:1219:GLU:HG2	1.85	0.75
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.16	0.75
3:D:843:VAL:HG11	3:D:897:HIS:O	1.85	0.75
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.68	0.75
5:F:470:MET:CE	5:F:478:PRO:HB3	2.16	0.75
3:J:1156:LEU:HD23	3:J:1219:ASP:HB3	1.68	0.75
2:C:561:ILE:HD11	2:C:665:ALA:CB	2.15	0.75
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.67	0.75
1:G:43:LEU:HD13	1:G:217:ILE:HD11	1.67	0.75
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.68	0.75
1:B:183:ILE:HD11	1:B:205:MET:CG	2.12	0.75
2:C:1299:ASN:HD22	2:C:1303:LYS:HE2	1.49	0.75
3:D:1371:ARG:HH21	3:J:854:ALA:HA	1.51	0.75
5:F:444:ALA:HB1	5:F:457:ILE:CD1	2.17	0.75
2:I:896:THR:HB	2:I:897:PRO:HD2	1.68	0.75
3:J:1221:LEU:HD22	3:J:1221:LEU:O	1.86	0.75
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	1.69	0.75
2:C:323:ALA:O	2:C:327:GLN:HG3	1.87	0.75
2:I:250:THR:HA	2:I:268:ARG:HA	1.68	0.75
3:J:903:LEU:HD23	3:J:905:ARG:CG	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.51	0.75
3:D:491:LEU:CD2	3:D:498:PRO:HA	2.17	0.75
2:I:1211:ARG:HD3	2:I:1213:TYR:OH	1.86	0.75
3:J:1205:GLU:O	3:J:1208:ASP:HB2	1.87	0.75
1:A:218:ARG:HG3	1:B:231:PHE:O	1.86	0.75
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.51	0.75
2:C:720:ARG:NH2	2:C:736:VAL:HG21	2.02	0.75
3:D:1174:ARG:HG2	3:D:1189:MET:SD	2.27	0.75
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.68	0.75
3:J:805:GLN:OE1	3:J:1348:LYS:HD3	1.87	0.75
3:J:517:CYS:CA	3:J:716:GLN:HE22	1.98	0.75
3:J:514:THR:CG2	3:J:596:LEU:HB2	2.17	0.75
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.52	0.75
1:A:179:PRO:HA	1:A:208:ASN:OD1	1.87	0.75
2:C:1080:ASN:HB3	2:C:1085:MET:HE2	1.68	0.75
2:I:1024:GLU:HG2	2:I:1028:LYS:CD	2.16	0.75
2:I:607:SER:HB3	2:I:610:GLU:OE1	1.87	0.75
5:L:341:LEU:HD23	5:L:344:LEU:HD23	1.66	0.75
1:A:104:LYS:NZ	1:A:114:ASP:OD2	2.14	0.75
3:D:222:LYS:NZ	3:D:1276:GLU:OE1	2.17	0.75
1:H:51:MET:HG3	1:H:52:PRO:CD	2.17	0.75
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.17	0.74
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.20	0.74
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.67	0.74
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.15	0.74
2:I:13:LYS:NZ	2:I:1148:ALA:O	2.20	0.74
5:L:576:VAL:HG12	5:L:587:ILE:HD11	1.69	0.74
2:C:1219:GLU:OE2	3:D:538:ARG:NH1	2.16	0.74
5:F:379:MET:HG2	5:F:416:VAL:CG2	2.17	0.74
1:H:41:ASN:OD1	1:H:44:ARG:NH1	2.19	0.74
2:I:122:VAL:CG1	2:I:493:ILE:HD13	2.17	0.74
5:L:280:VAL:HG22	5:L:347:ILE:CD1	2.17	0.74
1:B:152:TYR:CE2	3:D:536:LEU:HD21	2.22	0.74
3:D:16:GLU:HG3	3:D:1369:ARG:NH2	2.01	0.74
3:D:709:ARG:C	3:D:711:GLY:H	1.88	0.74
2:I:829:THR:HG23	2:I:1059:ARG:HA	1.68	0.74
3:J:844:THR:HG23	3:J:864:LEU:HD11	1.68	0.74
5:L:322:MET:HE2	5:L:324:LYS:CG	2.17	0.74
2:C:519:ASN:HB3	2:C:522:SER:CB	2.16	0.74
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.26	0.74
3:D:210:SER:O	3:D:214:ARG:HG2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:418:GLU:H	4:E:45:LYS:NZ	1.85	0.74
2:I:1086:PRO:O	2:I:1094:VAL:HG12	1.87	0.74
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.70	0.74
3:J:154:LEU:HD22	3:J:160:LEU:HD11	1.70	0.74
1:A:27:THR:C	1:A:28:LEU:HD12	2.07	0.74
1:B:103:ASN:OD1	1:B:141:SER:OG	2.03	0.74
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.67	0.74
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.70	0.74
5:F:461:ASN:O	5:F:465:ARG:HG2	1.88	0.74
1:G:161:SER:O	1:G:163:GLU:HG3	1.86	0.74
2:I:1114:GLU:OE1	2:I:1230:MET:HA	1.87	0.74
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.69	0.74
1:B:35:PHE:HA	1:B:38:THR:CG2	2.16	0.74
2:I:175:ARG:NH2	2:I:200:ARG:HH12	1.86	0.74
5:F:316:PHE:CZ	5:F:334:SER:HA	2.20	0.74
2:I:594:VAL:HG11	2:I:650:VAL:HG23	1.69	0.74
2:I:86:GLN:HA	2:I:140:GLY:HA2	1.69	0.74
2:C:24:VAL:HG21	2:C:704:MET:SD	2.28	0.74
2:C:74:ARG:NH2	2:C:97:ARG:HG3	2.02	0.74
3:D:252:LEU:HD23	3:D:262:THR:HB	1.68	0.74
3:D:810:THR:HG21	3:D:893:GLY:HA3	1.68	0.74
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.50	0.74
3:J:647:PRO:HG3	3:J:697:MET:CB	2.16	0.74
5:L:470:MET:HE3	5:L:478:PRO:HB3	1.69	0.74
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.69	0.74
2:C:778:GLU:O	2:C:781:ASP:HB2	1.88	0.74
3:D:97:VAL:HG11	3:D:101:ARG:NH2	2.03	0.74
3:D:709:ARG:O	3:D:711:GLY:N	2.21	0.74
1:G:58:GLU:OE2	1:G:170:ARG:NH1	2.21	0.74
2:I:886:LYS:H	2:I:917:SER:HB3	1.51	0.74
5:L:598:LEU:O	5:L:604:SER:OG	2.06	0.74
3:D:215:LYS:O	3:D:218:THR:HG22	1.88	0.73
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.03	0.73
1:A:36:GLY:HA3	1:A:187:VAL:HG11	1.70	0.73
2:C:1142:ARG:CD	2:C:1161:LEU:HD11	2.17	0.73
2:C:593:LYS:HE3	2:C:595:THR:CG2	2.18	0.73
2:C:730:SER:O	2:C:753:LEU:HB2	1.88	0.73
2:C:1196:LYS:HD2	2:C:1206:THR:CG2	2.16	0.73
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.70	0.73
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.20	0.73
1:H:102:LEU:O	1:H:141:SER:HA	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.52	0.73
3:J:1241:TYR:HD2	3:J:1246:VAL:HG11	1.53	0.73
2:C:980:VAL:O	2:C:984:VAL:HB	1.89	0.73
3:D:647:PRO:CG	3:D:697:MET:HB3	2.19	0.73
2:I:1151:LEU:HD11	2:I:1198:LEU:HD23	1.70	0.73
2:I:1288:GLN:HE21	3:J:1355:ARG:HA	1.54	0.73
2:C:1131:MET:HE3	2:C:1141:LEU:HD12	1.70	0.73
3:D:1290:ARG:HD3	3:D:1294:ALA:CB	2.18	0.73
5:F:470:MET:HE2	5:F:478:PRO:HB3	1.68	0.73
1:G:51:MET:HE1	1:G:216:ALA:HA	1.71	0.73
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.70	0.73
1:A:47:LEU:O	1:A:180:VAL:HG21	1.89	0.73
2:C:930:ASP:OD2	2:C:931:VAL:N	2.20	0.73
3:D:930:LEU:HD12	3:D:1138:LEU:CD1	2.18	0.73
3:D:797:THR:CG2	3:D:924:GLY:HA3	2.15	0.73
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.70	0.73
5:L:162:ILE:HD13	5:L:221:PHE:HE2	1.54	0.73
1:B:57:THR:O	1:B:173:VAL:HG22	1.89	0.73
2:C:169:LYS:O	2:C:170:VAL:HG22	1.89	0.73
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.22	0.73
3:D:622:ASP:HB3	3:D:626:TYR:HE2	1.54	0.73
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.70	0.73
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.70	0.73
3:D:884:SER:OG	3:D:1254:GLU:OE1	2.07	0.73
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	1.71	0.73
1:G:13:LEU:HD22	1:H:231:PHE:CZ	2.23	0.72
2:I:136:PHE:CZ	2:I:456:VAL:HG11	2.24	0.72
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.71	0.72
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.69	0.72
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.69	0.72
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.71	0.72
1:A:57:THR:HG22	1:A:158:ARG:NH2	2.04	0.72
1:A:62:ASP:OD1	1:A:141:SER:OG	2.06	0.72
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.03	0.72
3:D:1198:VAL:HB	3:D:1210:ILE:HA	1.70	0.72
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.20	0.72
1:G:191:ARG:HH12	1:G:197:ASP:HA	1.55	0.72
3:J:232:ASN:HA	3:J:236:TRP:HZ3	1.53	0.72
1:H:79:LEU:CD1	3:J:526:VAL:HG21	2.12	0.72
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.22	0.72
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:CG1	1:A:27:THR:HB	2.19	0.72
2:C:1291:LEU:HD21	3:D:1351:VAL:CG1	2.17	0.72
1:H:16:ILE:HD13	1:H:214:GLU:OE2	1.90	0.72
5:L:289:LYS:HE3	5:L:293:GLU:HG2	1.72	0.72
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.72	0.72
2:I:149:LEU:HD12	2:I:452:ARG:O	1.88	0.72
3:J:848:VAL:HG23	3:J:858:VAL:HG13	1.72	0.72
1:B:102:LEU:HD11	1:B:110:VAL:HG11	1.70	0.72
2:C:136:PHE:CZ	2:C:456:VAL:HG11	2.25	0.72
1:H:6:THR:O	1:H:6:THR:HG22	1.89	0.72
1:B:51:MET:HG3	1:B:52:PRO:HD2	1.72	0.72
2:C:514:PHE:O	6:C:2001:KNG:C32	2.38	0.72
3:D:267:ASP:HA	3:D:270:ARG:HH21	1.55	0.72
2:I:1023:HIS:O	2:I:1027:LYS:HG2	1.90	0.72
2:I:1065:LYS:CD	2:I:1235:LEU:HD12	2.20	0.72
2:I:119:GLU:CG	2:I:489:PRO:HD2	2.20	0.72
3:J:479:GLU:CG	4:K:20:VAL:HG11	2.19	0.72
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	1.71	0.72
2:C:1305:TYR:OH	5:F:532:LEU:HG	1.90	0.72
1:G:38:THR:OG1	1:H:45:ARG:HD3	1.89	0.72
1:H:142:MET:HG3	1:H:144:ILE:HG13	1.72	0.72
2:I:1234:LYS:HE2	2:I:1238:LEU:CD2	2.18	0.72
3:J:1137:GLY:O	3:J:1140:ARG:HB3	1.90	0.72
2:C:722:GLY:HA2	2:C:737:ASN:OD1	1.90	0.72
5:L:314:THR:O	5:L:318:ALA:HB3	1.90	0.72
5:L:489:MET:HE3	5:L:493:LYS:HD2	1.70	0.72
3:D:520:ALA:HB3	3:D:546:ALA:HB2	1.72	0.71
5:F:234:THR:HG21	5:F:248:GLU:OE2	1.89	0.71
2:I:1238:LEU:H	2:I:1238:LEU:HD12	1.53	0.71
5:L:341:LEU:CD2	5:L:344:LEU:HD23	2.19	0.71
2:C:582:ASN:HB3	2:C:586:PHE:H	1.54	0.71
3:D:137:ARG:HD3	3:D:143:SER:HB2	1.72	0.71
3:D:418:GLU:H	4:E:45:LYS:HZ3	1.38	0.71
1:G:46:ILE:HD12	1:H:35:PHE:CZ	2.25	0.71
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.71	0.71
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.54	0.71
3:J:1280:VAL:O	3:J:1284:ARG:HB3	1.90	0.71
3:J:71:LEU:O	3:J:71:LEU:HD22	1.90	0.71
2:C:496:LYS:HB3	2:C:497:PRO:HD3	1.72	0.71
2:C:1271:GLY:HA3	3:D:343:LEU:HD21	1.70	0.71
2:I:817:LEU:HD11	2:I:1080:ASN:HD22	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1131:MET:CE	2:I:1141:LEU:HD12	2.21	0.71
3:D:270:ARG:NH2	5:F:449:THR:HG23	2.05	0.71
3:J:810:THR:HG21	3:J:893:GLY:HA3	1.72	0.71
3:J:903:LEU:HD23	3:J:905:ARG:HG3	1.73	0.71
5:L:94:THR:OG1	5:L:95:THR:N	2.24	0.71
5:F:466:ILE:HG22	5:F:470:MET:HG3	1.71	0.71
2:I:237:LEU:CD1	2:I:292:ILE:HD11	2.21	0.71
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.26	0.71
2:I:557:ARG:NH2	2:I:607:SER:O	2.23	0.71
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.20	0.71
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.71	0.71
3:D:479:GLU:HG3	4:E:20:VAL:HG11	1.72	0.71
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.53	0.71
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.73	0.71
2:I:696:ASP:HB2	2:I:798:GLN:CG	2.20	0.71
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.21	0.71
3:J:799:ARG:NH1	3:J:1146:GLU:OE1	2.24	0.71
5:L:492:ASP:CB	5:L:495:ARG:HH12	2.02	0.71
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.70	0.71
2:I:466:VAL:O	2:I:469:VAL:HG22	1.90	0.71
2:I:1285:TYR:CZ	3:J:1356:LEU:HD11	2.26	0.71
3:J:279:LEU:HD23	3:J:279:LEU:O	1.89	0.71
3:J:647:PRO:HG3	3:J:697:MET:CA	2.20	0.71
2:C:589:THR:OG1	2:C:659:GLN:NE2	2.23	0.71
3:D:1241:TYR:HD2	3:D:1246:VAL:HG11	1.54	0.71
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.71	0.71
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.56	0.70
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.23	0.70
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.73	0.70
2:C:1308:ILE:HD12	3:D:380:PHE:CZ	2.26	0.70
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.55	0.70
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.25	0.70
2:I:1247:SER:OG	3:J:375:GLU:OE2	2.09	0.70
5:L:384:LEU:HD22	5:L:409:ASN:HD21	1.56	0.70
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.54	0.70
2:C:109:ALA:HB1	2:C:111:GLU:N	2.04	0.70
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.73	0.70
1:B:83:LEU:HD11	3:D:526:VAL:HG23	1.74	0.70
2:C:1101:LEU:O	3:D:731:ARG:HD3	1.91	0.70
3:J:30:ILE:HD13	3:J:243:PRO:HD3	1.71	0.70
2:C:41:GLN:NE2	2:C:73:TYR:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:116:PHE:CE1	3:D:1333:THR:HG22	2.27	0.70
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.27	0.70
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.72	0.70
2:C:1285:TYR:CE2	3:D:1356:LEU:HD11	2.26	0.70
2:C:980:VAL:HA	2:C:984:VAL:HA	1.74	0.70
3:J:126:LEU:HD13	3:J:223:LEU:HD22	1.74	0.70
3:J:658:GLU:O	3:J:661:VAL:HG13	1.92	0.70
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.27	0.70
2:C:593:LYS:HB3	2:C:602:GLU:CG	2.22	0.70
1:G:57:THR:HG22	1:G:158:ARG:NH2	2.06	0.70
3:J:1252:HIS:O	3:J:1255:VAL:HG13	1.91	0.70
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.74	0.70
1:A:218:ARG:NH1	1:B:231:PHE:HA	2.06	0.70
2:C:1144:PHE:O	2:C:1147:ARG:HB2	1.92	0.70
2:C:197:ARG:NH1	2:C:201:ARG:O	2.24	0.70
2:I:1285:TYR:CE2	3:J:1356:LEU:HD11	2.27	0.70
3:J:513:MET:O	3:J:575:GLY:HA3	1.91	0.70
3:D:658:GLU:O	3:D:661:VAL:HG13	1.91	0.70
2:C:818:VAL:HB	2:C:1076:ILE:HD11	1.73	0.70
3:D:121:PRO:HG2	3:D:123:ARG:NH2	2.07	0.70
3:J:460:ASP:HB2	3:J:464:ASP:OD2	1.92	0.70
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.74	0.70
2:C:1248:THR:HB	5:F:532:LEU:HD11	1.74	0.70
3:D:115:TRP:CZ2	3:D:1329:THR:HG23	2.26	0.70
3:D:507:VAL:HG11	3:D:598:LYS:HG3	1.74	0.70
1:G:228:LEU:HD22	1:H:221:ALA:HB1	1.73	0.70
2:I:1272:GLU:H	3:J:343:LEU:HD12	1.56	0.70
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.06	0.69
5:F:281:ARG:O	5:F:285:ARG:HG3	1.92	0.69
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.74	0.69
5:F:362:ASN:HB2	5:F:365:MET:CE	2.23	0.69
1:H:57:THR:HG21	1:H:158:ARG:NE	2.04	0.69
1:A:164:ASP:OD1	1:A:166:ARG:HB2	1.92	0.69
1:B:23:HIS:HB3	1:B:206:GLU:HG2	1.74	0.69
2:C:30:ILE:HD12	2:C:30:ILE:H	1.58	0.69
3:D:11:GLN:HG3	3:D:12:THR:H	1.57	0.69
3:D:18:ASP:HB2	3:D:1373:ARG:HH22	1.57	0.69
5:F:281:ARG:HG2	5:F:285:ARG:HD2	1.74	0.69
2:I:1105:SER:HB2	3:J:731:ARG:CG	2.21	0.69
1:B:205:MET:CE	1:B:213:PRO:HB3	2.23	0.69
2:C:619:ALA:CA	2:C:654:ASP:HB2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.74	0.69
3:D:1290:ARG:HD2	3:D:1295:ASN:HD22	1.58	0.69
3:D:56:LEU:N	3:D:56:LEU:HD12	2.07	0.69
2:C:618:GLN:OE1	3:D:770:LEU:HD13	1.93	0.69
5:F:548:LEU:HD23	5:F:551:LEU:HD12	1.75	0.69
1:H:176:CYS:O	1:H:178:SER:N	2.25	0.69
2:I:564:PRO:HG3	2:I:572:ILE:HG13	1.73	0.69
2:I:680:LEU:HD22	3:J:783:LEU:CD1	2.22	0.69
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.74	0.69
3:D:19:ALA:HA	3:D:1344:LEU:CD1	2.22	0.69
2:C:1281:TYR:HD1	3:D:484:MET:HG2	1.55	0.69
1:H:79:LEU:HD11	3:J:526:VAL:CG2	2.14	0.69
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.74	0.69
3:D:872:LEU:O	3:D:877:VAL:HG12	1.93	0.69
5:F:297:MET:HG3	5:F:326:TRP:HB2	1.75	0.69
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.08	0.69
2:C:1304:MET:HE2	3:D:472:LEU:HD12	1.73	0.69
2:C:101:ARG:HH21	2:C:118:LYS:HE3	1.57	0.69
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.74	0.69
3:J:1236:GLU:HA	3:J:1236:GLU:OE2	1.91	0.69
1:B:74:VAL:HG13	1:B:132:HIS:O	1.93	0.69
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.74	0.69
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.26	0.69
2:I:98:VAL:HG21	2:I:124:MET:HE3	1.75	0.69
3:J:526:VAL:CG1	3:J:549:LYS:HB2	2.22	0.69
6:C:2001:KNG:C34	6:C:2001:KNG:C33	2.71	0.69
2:C:545:PHE:HD1	2:C:548:ARG:HD3	1.57	0.69
3:D:528:THR:O	3:D:551:ARG:HB3	1.93	0.69
3:D:98:ARG:HB3	3:D:248:ASP:OD2	1.93	0.69
1:G:231:PHE:HB3	1:H:218:ARG:HG2	1.74	0.69
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.75	0.69
2:C:812:PHE:CE2	3:D:451:PRO:HB3	2.27	0.69
1:B:83:LEU:HD11	3:D:526:VAL:CG2	2.23	0.69
3:D:623:GLN:O	3:D:627:THR:HG22	1.93	0.69
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.75	0.69
2:I:1065:LYS:HD3	2:I:1235:LEU:HD12	1.75	0.69
2:I:528:ARG:NH2	2:I:576:SER:O	2.26	0.69
2:I:617:ALA:HB3	2:I:653:MET:HG3	1.73	0.69
3:J:179:LYS:HB2	3:J:184:ALA:HB2	1.74	0.69
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.10	0.69
5:L:576:VAL:HG12	5:L:587:ILE:CD1	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1280:VAL:CG1	3:D:1304:ARG:HH21	2.02	0.68
3:D:427:PRO:O	3:D:429:LEU:HD22	1.93	0.68
3:J:526:VAL:HA	3:J:549:LYS:O	1.94	0.68
2:C:156:PHE:CD1	2:C:443:ASP:HB2	2.26	0.68
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.74	0.68
2:C:582:ASN:HB3	2:C:586:PHE:N	2.07	0.68
1:A:70:THR:CG2	2:C:755:LYS:HE2	2.23	0.68
1:B:35:PHE:CA	1:B:38:THR:HG22	2.20	0.68
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.33	0.68
2:C:299:LYS:HG2	2:C:334:GLU:OE1	1.93	0.68
3:D:161:THR:HG23	3:D:164:GLN:H	1.58	0.68
5:F:137:TYR:CE2	5:F:273:MET:HG2	2.27	0.68
1:G:9:LEU:HD21	1:G:195:ARG:HH21	1.58	0.68
3:J:30:ILE:CG2	3:J:243:PRO:HG3	2.24	0.68
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.57	0.68
1:G:43:LEU:HD12	1:G:203:ILE:HD11	1.76	0.68
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.29	0.68
3:D:1290:ARG:CG	3:D:1298:VAL:HG12	2.23	0.68
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.08	0.68
2:C:564:PRO:HA	2:C:684:ASN:HD21	1.59	0.68
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.75	0.68
3:D:514:THR:CG2	3:D:596:LEU:HB2	2.23	0.68
3:J:1290:ARG:CG	3:J:1298:VAL:HG12	2.23	0.68
3:J:514:THR:HG21	3:J:596:LEU:HB2	1.75	0.68
3:J:748:ALA:O	3:J:777:HIS:HD2	1.76	0.68
1:B:182:ARG:O	1:B:183:ILE:HD12	1.93	0.68
2:C:109:ALA:HB1	2:C:111:GLU:HA	1.75	0.68
2:C:1146:GLN:HG2	2:C:1160:ASP:OD1	1.93	0.68
2:C:748:ILE:CD1	2:C:967:LEU:HD12	2.22	0.68
2:C:866:ASP:HA	2:C:872:TYR:OH	1.94	0.68
3:D:647:PRO:HG3	3:D:697:MET:CB	2.23	0.68
3:D:518:VAL:HG11	3:D:707:ILE:HD13	1.74	0.68
1:H:84:ASN:ND2	1:H:129:VAL:O	2.27	0.68
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.75	0.68
3:J:1263:LYS:HE2	3:J:1279:GLN:NE2	2.09	0.68
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.76	0.68
3:J:843:VAL:CG1	3:J:883:ARG:HD3	2.22	0.68
4:K:10:VAL:HG13	4:K:16:ARG:HB2	1.76	0.68
3:J:332:LYS:HE2	3:J:1329:THR:OG1	1.94	0.68
2:I:1242:LYS:HD2	3:J:465:GLN:OE1	1.93	0.68
3:D:681:LYS:O	3:D:685:ILE:HG23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1263:LYS:HE2	3:D:1279:GLN:HE21	1.58	0.68
3:D:259:ARG:HG2	5:F:502:LYS:HE3	1.76	0.68
1:G:166:ARG:O	1:G:168:ILE:N	2.27	0.68
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.76	0.67
3:D:259:ARG:CZ	5:F:505:ILE:HD11	2.24	0.67
5:F:387:VAL:HG22	5:F:435:ILE:HD13	1.76	0.67
2:I:960:LEU:CD1	2:I:1028:LYS:HE2	2.24	0.67
2:I:971:LEU:HD21	2:I:1014:LEU:O	1.94	0.67
3:J:825:VAL:C	3:J:826:ILE:HG13	2.14	0.67
5:L:137:TYR:CE2	5:L:273:MET:HG2	2.28	0.67
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.76	0.67
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.76	0.67
2:I:8:LYS:HE3	2:I:1171:ARG:HH21	1.57	0.67
2:I:452:ARG:NH1	2:I:584:TYR:O	2.26	0.67
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.76	0.67
3:J:156:ARG:NH2	3:J:191:SER:OG	2.25	0.67
5:L:280:VAL:CG2	5:L:347:ILE:HD13	2.24	0.67
2:I:794:LEU:HG	2:I:796:LEU:HD11	1.77	0.67
3:J:1252:HIS:HA	3:J:1255:VAL:CG1	2.23	0.67
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.76	0.67
5:L:601:PRO:HA	5:L:604:SER:HB2	1.77	0.67
1:A:224:LEU:O	1:A:224:LEU:HD23	1.94	0.67
2:C:100:LEU:HD12	2:C:122:VAL:HG11	1.76	0.67
2:C:477:GLU:O	2:C:480:SER:HB3	1.94	0.67
3:D:649:LYS:HD2	3:D:652:GLU:OE1	1.95	0.67
1:H:205:MET:HG2	1:H:206:GLU:H	1.59	0.67
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.25	0.67
2:I:1284:ALA:HB1	3:J:1356:LEU:HD22	1.74	0.67
1:A:50:SER:HB2	1:B:8:PHE:HZ	1.58	0.67
2:C:1202:GLY:O	2:C:1203:ASP:HB2	1.94	0.67
1:G:90:VAL:HG22	1:G:91:ARG:H	1.60	0.67
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.29	0.67
2:C:549:ASP:OD1	3:D:750:PRO:HB3	1.94	0.67
3:D:126:LEU:HD11	3:D:223:LEU:HD22	1.77	0.67
2:I:980:VAL:O	2:I:984:VAL:HB	1.94	0.67
3:J:1177:ILE:HD12	3:J:1186:TYR:HB3	1.77	0.67
2:I:1314:GLN:HG2	4:K:28:ARG:NE	2.10	0.67
5:L:484:ALA:HB1	5:L:491:GLU:CG	2.25	0.67
3:D:789:LYS:NZ	3:D:931:THR:O	2.17	0.67
2:I:218:GLU:O	2:I:222:ASP:HB2	1.95	0.67
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:872:LEU:HD22	3:J:877:VAL:CG1	2.22	0.67
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.09	0.67
2:C:1148:ALA:HB1	2:C:1180:MET:HE2	1.75	0.67
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.77	0.67
3:J:1165:PHE:HE1	3:J:1200:GLU:HB3	1.59	0.67
1:B:90:VAL:HG22	1:B:91:ARG:H	1.58	0.67
1:G:50:SER:CB	1:H:8:PHE:HE1	2.07	0.67
2:I:123:TYR:OH	2:I:126:GLU:HG3	1.95	0.67
2:I:770:CYS:HB2	2:I:791:LEU:HD23	1.77	0.67
2:C:1291:LEU:CD2	3:D:1351:VAL:HG13	2.20	0.67
2:I:979:LEU:CD1	2:I:1011:LEU:HD11	2.25	0.67
3:J:336:GLY:O	3:J:337:ARG:HB2	1.94	0.67
2:I:170:VAL:HG23	2:I:171:LEU:N	2.08	0.66
2:I:338:THR:CG2	2:I:345:PRO:HB3	2.25	0.66
2:I:146:VAL:HG21	2:I:513:GLN:NE2	2.09	0.66
2:I:738:GLU:HG2	2:I:741:MET:HE2	1.77	0.66
5:L:127:ILE:O	5:L:130:VAL:HG22	1.93	0.66
5:L:483:LEU:H	5:L:483:LEU:HD12	1.59	0.66
1:A:61:ILE:HB	1:A:64:VAL:HG23	1.77	0.66
3:D:1206:ARG:NH2	3:D:1223:LEU:O	2.28	0.66
3:D:161:THR:CG2	3:D:164:GLN:H	2.07	0.66
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.77	0.66
3:J:833:GLU:OE1	3:J:1242:ARG:HD3	1.95	0.66
2:I:1272:GLU:H	3:J:343:LEU:CD1	2.08	0.66
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.76	0.66
5:F:127:ILE:O	5:F:130:VAL:HG22	1.96	0.66
5:F:110:LEU:HD21	5:F:385:ARG:HD3	1.76	0.66
1:H:82:LEU:HD22	1:H:173:VAL:CG1	2.24	0.66
2:I:115:LYS:HG3	2:I:485:ASP:OD2	1.95	0.66
3:J:1169:THR:CG2	3:J:1192:LYS:HD3	2.24	0.66
3:J:1197:ASN:HB2	3:J:1211:SER:HA	1.78	0.66
2:I:138:ILE:HB	2:I:143:ARG:HD3	1.78	0.66
2:I:975:ILE:HG23	2:I:1011:LEU:HD22	1.77	0.66
3:J:1252:HIS:HA	3:J:1255:VAL:HG13	1.77	0.66
5:L:322:MET:HE2	5:L:324:LYS:HG3	1.76	0.66
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.76	0.66
3:D:75:TYR:CE2	3:D:83:VAL:HG21	2.31	0.66
5:F:572:THR:HG23	5:F:575:GLU:HB2	1.78	0.66
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.76	0.66
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.10	0.66
2:I:56:VAL:CG1	2:I:468:LEU:HD13	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1269:ALA:HB2	3:J:1274:PHE:CD1	2.30	0.66
1:A:154:PRO:HB2	2:C:1059:ARG:HH21	1.60	0.66
2:C:1248:THR:HG21	5:F:531:PRO:HG3	1.76	0.66
2:C:471:VAL:HG21	2:C:498:ILE:HD11	1.78	0.66
2:C:145:ILE:HA	2:C:511:LEU:O	1.95	0.66
2:I:1078:LYS:HG2	2:I:1079:ILE:N	2.10	0.66
2:I:1202:GLY:O	2:I:1203:ASP:HB2	1.96	0.66
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.09	0.66
2:C:2:VAL:O	2:C:2:VAL:HG12	1.96	0.66
3:D:11:GLN:O	3:D:12:THR:HG23	1.96	0.66
2:I:1157:GLN:O	2:I:1158:LYS:HG2	1.96	0.66
3:J:767:LEU:HD23	3:J:771:GLN:HB3	1.78	0.66
5:L:166:VAL:O	5:L:167:ASP:HB2	1.96	0.66
5:L:573:LEU:H	5:L:573:LEU:HD23	1.61	0.66
2:C:1132:LEU:HD22	2:C:1177:ARG:NH1	2.11	0.66
2:C:1298:VAL:HG11	3:D:96:LYS:HE3	1.77	0.66
1:H:74:VAL:HG22	1:H:133:LEU:HD12	1.77	0.66
1:H:153:VAL:HB	1:H:175:ALA:HB3	1.76	0.66
3:J:126:LEU:HD13	3:J:223:LEU:HD21	1.78	0.66
5:L:544:THR:HG22	5:L:607:LEU:HD21	1.78	0.66
5:L:96:ASP:O	5:L:98:VAL:N	2.28	0.66
2:C:832:HIS:HD1	2:C:1058:ARG:HD2	1.61	0.65
5:F:391:ALA:HB3	5:F:405:ILE:HG22	1.78	0.65
3:J:494:ALA:CB	3:J:922:SER:HB3	2.25	0.65
2:C:819:SER:HB2	2:C:1085:MET:SD	2.36	0.65
2:C:1131:MET:HB3	2:C:1141:LEU:CD1	2.26	0.65
2:C:1131:MET:HE2	2:C:1141:LEU:CD1	2.21	0.65
2:C:1158:LYS:O	2:C:1159:VAL:HG22	1.96	0.65
2:C:17:LYS:HE3	2:C:1154:ASP:CB	2.23	0.65
5:F:280:VAL:CG2	5:F:347:ILE:HD13	2.19	0.65
1:H:13:LEU:CD1	1:H:16:ILE:HD11	2.26	0.65
2:I:145:ILE:CG2	2:I:456:VAL:HG22	2.26	0.65
1:A:159:ILE:HG12	1:A:159:ILE:O	1.96	0.65
1:A:45:ARG:HG2	1:B:38:THR:CB	2.22	0.65
1:G:167:PRO:HB2	1:G:170:ARG:HB2	1.76	0.65
1:G:86:LYS:HZ3	1:G:174:ASP:HB2	1.59	0.65
2:I:237:LEU:CD2	2:I:289:VAL:HG23	2.27	0.65
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.61	0.65
5:L:466:ILE:CD1	5:L:487:MET:HG2	2.26	0.65
3:D:129:ASP:HB2	3:D:220:ARG:CZ	2.26	0.65
3:D:646:ILE:HG23	3:D:741:ALA:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.78	0.65
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.77	0.65
2:I:802:VAL:CG2	2:I:1098:LEU:HD13	2.26	0.65
3:D:290:ILE:HD12	3:D:290:ILE:H	1.61	0.65
2:I:274:ILE:HG22	2:I:278:GLU:OE1	1.97	0.65
2:I:69:GLN:NE2	2:I:101:ARG:HD2	2.10	0.65
5:L:287:ILE:HG21	5:L:315:TRP:CH2	2.31	0.65
1:A:175:ALA:HB1	1:A:177:TYR:CE1	2.32	0.65
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.59	0.65
2:I:197:ARG:NH1	2:I:201:ARG:O	2.29	0.65
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.60	0.65
4:K:27:ALA:HB2	4:K:50:ALA:HB2	1.78	0.65
3:D:1262:ARG:HD2	3:D:1279:GLN:OE1	1.96	0.65
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.79	0.65
5:F:230:VAL:O	5:F:234:THR:HG23	1.96	0.65
3:J:248:ASP:O	3:J:251:PRO:HG3	1.97	0.65
1:A:177:TYR:O	1:A:178:SER:HB2	1.95	0.65
2:C:1331:ARG:HG2	3:D:33:TRP:CH2	2.31	0.65
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.78	0.65
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.77	0.65
2:C:545:PHE:CD1	2:C:548:ARG:HD3	2.31	0.65
2:C:873:ILE:HG13	2:C:944:ARG:HH22	1.62	0.65
3:D:797:THR:HG22	3:D:924:GLY:CA	2.17	0.65
3:D:839:VAL:HG12	3:D:839:VAL:O	1.97	0.65
2:I:169:LYS:O	2:I:170:VAL:HG22	1.97	0.65
3:J:518:VAL:HG11	3:J:707:ILE:HD13	1.79	0.65
3:D:1265:THR:HG23	3:D:1305:ASP:OD2	1.97	0.65
3:D:744:ARG:HG3	3:D:744:ARG:O	1.96	0.65
5:F:110:LEU:HD21	5:F:385:ARG:CD	2.27	0.65
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.78	0.65
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.78	0.64
2:I:865:LEU:HD22	2:I:869:GLY:O	1.98	0.64
2:C:338:THR:HB	2:C:345:PRO:HB3	1.79	0.64
3:D:1327:GLU:OE2	3:D:1329:THR:HB	1.97	0.64
2:I:979:LEU:HD13	2:I:1011:LEU:HD21	1.78	0.64
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.78	0.64
5:L:105:MET:CE	5:L:385:ARG:HG2	2.26	0.64
1:B:112:ALA:O	1:B:115:ILE:HG13	1.98	0.64
5:F:418:LYS:HD2	5:F:434:TRP:CZ2	2.32	0.64
1:H:74:VAL:HG13	1:H:132:HIS:O	1.97	0.64
2:I:145:ILE:CB	2:I:456:VAL:HG22	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLU:OE2	1:A:172:LEU:HD11	1.97	0.64
2:C:1136:GLN:O	2:C:1137:GLU:HB3	1.96	0.64
3:D:1149:ARG:NH2	3:D:1153:PRO:HG2	2.12	0.64
3:D:140:TYR:HE2	5:F:95:THR:CG2	2.09	0.64
3:D:248:ASP:O	3:D:251:PRO:HG3	1.97	0.64
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.78	0.64
1:A:78:ILE:HD13	1:A:81:ILE:HD12	1.79	0.64
2:C:1164:PHE:O	2:C:1169:VAL:HG23	1.98	0.64
2:I:836:LEU:HD21	2:I:921:PRO:HD3	1.78	0.64
3:J:421:VAL:HG22	3:J:439:PRO:HG3	1.80	0.64
1:A:224:LEU:HB3	1:B:228:LEU:HD11	1.79	0.64
1:A:41:ASN:CG	2:C:1218:GLY:HA3	2.17	0.64
2:C:53:PHE:CD1	2:C:468:LEU:HD11	2.32	0.64
2:C:815:SER:HB3	2:C:1077:SER:HB3	1.79	0.64
3:D:94:GLN:O	3:D:97:VAL:HG23	1.97	0.64
1:H:110:VAL:HG21	1:H:140:ILE:CD1	2.27	0.64
1:H:76:GLU:HB3	1:H:81:ILE:CG1	2.27	0.64
1:H:82:LEU:HD22	1:H:173:VAL:HG12	1.77	0.64
2:I:10:ARG:CZ	2:I:697:LYS:HD3	2.28	0.64
3:J:227:PHE:HE1	3:J:234:PRO:HD3	1.61	0.64
5:F:484:ALA:CB	5:F:491:GLU:HB2	2.20	0.64
1:H:118:ASP:HB2	1:H:121:VAL:HG23	1.79	0.64
2:I:671:LEU:HD23	2:I:1186:VAL:CG1	2.27	0.64
2:I:1248:THR:HG21	5:L:531:PRO:CG	2.26	0.64
2:I:1299:ASN:HD22	2:I:1303:LYS:HE2	1.62	0.64
2:I:231:GLU:HG2	2:I:332:ARG:HD3	1.80	0.64
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.62	0.64
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.13	0.64
3:J:210:SER:OG	3:J:213:LYS:HD2	1.98	0.64
3:J:405:GLU:O	3:J:408:VAL:HG22	1.98	0.64
3:J:653:ILE:HD13	3:J:692:ARG:CB	2.26	0.64
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	1.79	0.64
1:B:182:ARG:C	1:B:183:ILE:HD12	2.17	0.64
2:C:296:VAL:HB	2:C:336:LEU:CD1	2.25	0.64
2:I:1272:GLU:HB2	3:J:342:LEU:CB	2.28	0.64
3:J:857:LEU:HD12	3:J:858:VAL:H	1.62	0.64
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.80	0.64
5:F:601:PRO:HA	5:F:604:SER:HB2	1.80	0.64
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.80	0.64
2:I:819:SER:HB2	2:I:1085:MET:CG	2.27	0.64
3:J:56:LEU:HD21	3:J:269:TYR:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1131:MET:HB3	2:C:1141:LEU:HD11	1.80	0.63
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.61	0.63
2:C:301:TYR:O	2:C:309:LEU:HD12	1.98	0.63
2:C:832:HIS:ND1	2:C:1058:ARG:HD2	2.13	0.63
3:D:1238:GLN:HG2	3:D:1253:ILE:CD1	2.29	0.63
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.79	0.63
2:I:1136:GLN:O	2:I:1137:GLU:HB3	1.97	0.63
2:I:494:ASN:HD22	2:I:497:PRO:CD	2.11	0.63
3:J:1266:ILE:HD12	3:J:1273:ASP:O	1.99	0.63
3:J:320:ASN:OD1	3:J:322:ARG:HB3	1.97	0.63
3:J:502:PRO:HB3	3:J:506:VAL:HG21	1.79	0.63
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.33	0.63
2:C:133:ASN:HD21	2:C:713:GLY:HA3	1.60	0.63
1:G:11:PRO:HB3	1:G:31:LEU:CD2	2.27	0.63
2:I:119:GLU:HB2	2:I:489:PRO:CG	2.29	0.63
5:L:316:PHE:O	5:L:320:ILE:HG13	1.97	0.63
5:L:470:MET:HE1	5:L:482:GLU:CG	2.28	0.63
2:C:1112:ILE:HD11	3:D:639:VAL:HG13	1.81	0.63
2:C:27:LEU:O	2:C:528:ARG:NH1	2.31	0.63
2:C:296:VAL:CB	2:C:336:LEU:HD12	2.27	0.63
2:C:980:VAL:HG13	2:C:984:VAL:HG23	1.81	0.63
3:D:1198:VAL:HG11	3:D:1210:ILE:HG23	1.80	0.63
5:F:555:GLU:HG2	5:F:590:ILE:CG2	2.27	0.63
3:J:658:GLU:HA	3:J:661:VAL:CG1	2.27	0.63
5:L:315:TRP:CZ2	5:L:341:LEU:HD11	2.32	0.63
2:C:223:LEU:HD13	2:C:426:ILE:HD13	1.81	0.63
2:C:268:ARG:HH21	2:C:270:THR:CG2	2.12	0.63
2:C:878:THR:OG1	2:C:879:GLY:N	2.26	0.63
5:F:134:VAL:HG13	5:F:273:MET:HE3	1.79	0.63
5:F:166:VAL:O	5:F:167:ASP:HB2	1.98	0.63
5:F:399:LEU:HB3	5:F:404:LEU:CD2	2.29	0.63
1:H:22:THR:OG1	1:H:207:THR:O	2.16	0.63
2:I:170:VAL:O	2:I:171:LEU:HG	1.98	0.63
2:I:697:LYS:HA	2:I:795:ALA:HB2	1.79	0.63
5:L:114:GLU:HG3	5:L:115:GLY:N	2.14	0.63
3:J:270:ARG:NH2	5:L:449:THR:HG23	2.12	0.63
1:B:33:ARG:HD2	2:C:1081:PRO:HG3	1.81	0.63
2:C:138:ILE:HG22	2:C:139:ASN:N	2.13	0.63
2:C:290:GLU:HG2	2:C:319:LEU:CD1	2.29	0.63
2:C:896:THR:OG1	2:C:899:GLU:HG3	1.99	0.63
3:D:849:LEU:HB3	3:D:853:THR:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:812:ASP:HB2	3:D:911:LYS:NZ	2.14	0.63
1:G:16:ILE:HG23	1:G:26:VAL:HG12	1.80	0.63
2:I:17:LYS:NZ	2:I:1154:ASP:HB3	2.13	0.63
3:D:708:ASN:OD1	3:D:708:ASN:N	2.30	0.63
2:I:1291:LEU:HD21	3:J:1351:VAL:CG1	2.25	0.63
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.81	0.63
1:A:185:TYR:HE1	2:C:1087:TYR:OH	1.82	0.63
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.13	0.63
3:D:1287:ILE:HG21	3:D:1300:ALA:O	1.98	0.63
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.47	0.63
5:F:490:PRO:CG	5:F:493:LYS:HE3	2.21	0.63
3:J:1361:THR:HG23	4:K:21:LEU:HD13	1.79	0.63
3:J:905:ARG:HH21	3:J:907:HIS:CB	2.11	0.63
5:L:97:PRO:HA	5:L:100:MET:HG3	1.80	0.63
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.64	0.63
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.81	0.63
3:D:73:GLY:O	3:D:76:LYS:HG3	1.99	0.63
2:I:42:ASP:OD2	2:I:46:GLN:HB3	1.97	0.63
2:I:119:GLU:HB2	2:I:489:PRO:HG2	1.80	0.63
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.79	0.63
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.58	0.63
3:J:490:ILE:O	3:J:490:ILE:HG13	1.99	0.63
3:J:488:ASN:ND2	4:K:6:VAL:HG22	2.13	0.63
2:C:818:VAL:HB	2:C:1076:ILE:CD1	2.28	0.63
3:D:1290:ARG:CD	3:D:1294:ALA:HB1	2.29	0.63
3:D:514:THR:HG21	3:D:596:LEU:HB2	1.80	0.63
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.79	0.63
2:I:557:ARG:HH21	2:I:607:SER:C	2.02	0.63
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.14	0.63
1:B:73:GLY:O	1:B:134:THR:HG22	1.99	0.62
3:D:146:VAL:HG23	3:D:158:GLN:O	1.99	0.62
3:D:205:LEU:O	3:D:205:LEU:HD13	1.99	0.62
5:F:337:VAL:HG12	5:F:341:LEU:HD12	1.79	0.62
1:G:169:GLY:O	1:G:171:LEU:HD22	1.99	0.62
3:J:349:TYR:CD1	3:J:472:LEU:HD21	2.34	0.62
3:J:722:ILE:CD1	3:J:740:LEU:HD23	2.29	0.62
2:C:1292:THR:HG21	2:C:1317:PRO:CB	2.29	0.62
2:C:153:PRO:HB3	2:C:177:ILE:O	1.98	0.62
2:C:285:ILE:HD11	2:C:287:VAL:HG12	1.81	0.62
3:D:232:ASN:ND2	3:D:1337:VAL:O	2.32	0.62
3:D:161:THR:HG22	3:D:164:GLN:CG	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:8:LEU:HD23	3:D:9:LYS:H	1.64	0.62
2:I:65:ASN:HB3	2:I:105:TYR:HD2	1.63	0.62
3:J:576:ARG:NH1	3:J:593:ASN:O	2.32	0.62
2:C:886:LYS:H	2:C:917:SER:HB3	1.63	0.62
3:D:19:ALA:HA	3:D:1344:LEU:HD12	1.81	0.62
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.47	0.62
2:I:175:ARG:HD3	2:I:183:TRP:HZ3	1.61	0.62
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.81	0.62
3:J:56:LEU:H	3:J:56:LEU:HD12	1.62	0.62
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.34	0.62
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.31	0.62
2:C:338:THR:CG2	2:C:345:PRO:HB3	2.29	0.62
3:D:825:VAL:HG13	3:D:833:GLU:HB3	1.81	0.62
3:D:872:LEU:CD2	3:D:877:VAL:HG11	2.30	0.62
3:J:1263:LYS:NZ	3:J:1315:ALA:HB1	2.15	0.62
3:J:56:LEU:HD11	3:J:273:ILE:HD12	1.80	0.62
5:L:395:THR:OG1	5:L:396:ASN:N	2.30	0.62
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.30	0.62
2:C:1080:ASN:HB3	2:C:1085:MET:CE	2.28	0.62
2:C:309:LEU:HD11	2:C:311:CYS:O	1.99	0.62
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.80	0.62
1:H:59:VAL:HG22	1:H:144:ILE:HG23	1.81	0.62
2:I:211:ARG:HD3	2:I:357:ASN:O	2.00	0.62
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.82	0.62
2:I:832:HIS:ND1	2:I:1058:ARG:HD2	2.14	0.62
3:J:808:VAL:HG13	3:J:913:GLU:O	1.99	0.62
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.13	0.62
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.81	0.62
2:I:296:VAL:HB	2:I:336:LEU:HD12	1.80	0.62
2:I:770:CYS:HB2	2:I:791:LEU:CD2	2.30	0.62
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.80	0.62
5:L:363:ARG:CZ	5:L:367:ILE:HD11	2.30	0.62
2:C:13:LYS:NZ	2:C:1148:ALA:O	2.32	0.62
3:D:18:ASP:HB2	3:D:1373:ARG:CZ	2.29	0.62
5:F:423:ARG:HD2	5:F:425:TYR:CE2	2.34	0.62
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.07	0.62
1:G:66:HIS:CA	1:G:171:LEU:HD11	2.22	0.62
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.39	0.62
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.34	0.62
2:I:494:ASN:HB3	2:I:497:PRO:CD	2.30	0.62
2:I:839:VAL:HG12	2:I:1049:ILE:CG1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:53:ARG:HH22	3:J:60:ARG:HD2	1.65	0.62
3:J:71:LEU:C	3:J:71:LEU:HD13	2.20	0.62
3:J:807:LEU:HD23	3:J:915:ILE:HG13	1.82	0.62
2:C:109:ALA:HB1	2:C:111:GLU:CA	2.29	0.62
2:C:478:ARG:HG2	2:C:492:MET:HG2	1.80	0.62
3:D:1344:LEU:N	3:D:1344:LEU:HD12	2.15	0.62
3:D:849:LEU:HD22	3:D:849:LEU:H	1.65	0.62
1:G:230:ALA:HB3	1:G:231:PHE:CE2	2.35	0.62
1:H:59:VAL:HG13	1:H:144:ILE:HG12	1.82	0.62
2:I:658:GLN:O	2:I:661:VAL:HG22	1.98	0.62
3:J:1265:THR:HG23	3:J:1305:ASP:OD2	1.99	0.62
3:J:222:LYS:HE2	3:J:1276:GLU:OE1	2.00	0.62
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.80	0.62
5:L:111:LEU:HD11	5:L:119:ILE:HD12	1.82	0.62
2:C:696:ASP:O	2:C:697:LYS:HB3	2.00	0.62
2:C:810:TYR:CE1	2:C:1078:LYS:HD2	2.35	0.62
3:D:825:VAL:C	3:D:826:ILE:HG13	2.20	0.62
1:G:195:ARG:HG2	1:G:198:LEU:HG	1.82	0.62
2:I:389:PHE:O	2:I:419:ILE:HG22	2.00	0.62
3:J:902:ASP:HB2	3:J:1251:LYS:HE3	1.82	0.62
5:L:354:THR:O	5:L:358:VAL:HG23	2.00	0.62
5:L:384:LEU:HD22	5:L:409:ASN:ND2	2.13	0.62
1:A:74:VAL:HG22	1:A:76:GLU:H	1.64	0.62
1:B:214:GLU:O	1:B:218:ARG:HG3	2.00	0.62
2:C:101:ARG:NH2	2:C:118:LYS:HE3	2.13	0.62
2:C:218:GLU:HG3	2:C:299:LYS:HA	1.81	0.62
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	1.82	0.62
3:D:224:LEU:O	3:D:228:VAL:HG23	2.00	0.62
2:C:42:ASP:OD2	2:C:46:GLN:HB3	2.00	0.61
3:D:800:LEU:HB3	3:D:920:ALA:CB	2.31	0.61
3:D:859:PRO:HG2	3:D:862:THR:CG2	2.30	0.61
2:I:820:GLU:HG2	2:I:824:GLN:HG3	1.80	0.61
3:J:824:PRO:HB2	3:J:826:ILE:HG23	1.81	0.61
3:J:905:ARG:HH21	3:J:907:HIS:HB2	1.65	0.61
4:K:26:ARG:HG2	4:K:59:ILE:HG21	1.81	0.61
5:L:486:ARG:CZ	5:L:486:ARG:HB2	2.29	0.61
1:B:101:THR:HG22	1:B:103:ASN:ND2	2.15	0.61
2:C:157:PHE:CE2	2:C:431:LYS:HG2	2.35	0.61
2:C:563:THR:OG1	2:C:564:PRO:HD2	1.99	0.61
3:D:16:GLU:HG3	3:D:1369:ARG:HH22	1.63	0.61
3:D:697:MET:SD	3:D:741:ALA:HB3	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.65	0.61
2:I:109:ALA:HB1	2:I:111:GLU:N	2.15	0.61
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.82	0.61
2:I:344:GLY:HA3	2:I:346:TYR:CE2	2.35	0.61
1:B:73:GLY:C	1:B:134:THR:HG22	2.20	0.61
5:F:341:LEU:HD23	5:F:344:LEU:HD23	1.82	0.61
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.30	0.61
2:I:50:GLU:OE1	2:I:54:ARG:NE	2.34	0.61
2:I:452:ARG:HH12	2:I:585:GLY:HA3	1.63	0.61
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.83	0.61
3:J:709:ARG:O	3:J:711:GLY:N	2.32	0.61
3:J:488:ASN:HD21	4:K:6:VAL:CG2	2.13	0.61
2:C:1289:GLU:OE2	3:D:473:THR:CG2	2.43	0.61
2:C:720:ARG:NE	2:C:736:VAL:HG11	2.14	0.61
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.24	0.61
3:D:156:ARG:NH2	3:D:191:SER:OG	2.33	0.61
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.35	0.61
4:E:26:ARG:NH1	4:E:29:GLN:OE1	2.32	0.61
5:F:348:GLU:HG2	5:F:354:THR:HA	1.81	0.61
2:I:103:VAL:HG12	2:I:116:ASP:CB	2.25	0.61
2:I:1101:LEU:O	3:J:731:ARG:HD3	2.00	0.61
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.36	0.61
2:I:49:LEU:HD12	2:I:73:TYR:CE2	2.36	0.61
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.82	0.61
3:J:800:LEU:HD11	3:J:1309:ILE:HD13	1.81	0.61
3:J:702:GLN:HA	3:J:723:TYR:CE2	2.34	0.61
3:J:72:CYS:SG	8:J:1502:ZN:ZN	1.87	0.61
2:C:289:VAL:HG13	2:C:319:LEU:HD11	1.82	0.61
2:C:553:THR:O	2:C:557:ARG:HD2	2.01	0.61
5:F:585:GLU:HA	5:F:588:ARG:HD3	1.82	0.61
1:G:71:LYS:HB2	1:G:78:ILE:HD11	1.82	0.61
2:I:98:VAL:HG21	2:I:124:MET:CE	2.29	0.61
3:J:1253:ILE:O	3:J:1257:VAL:HG23	2.00	0.61
3:J:664:ILE:HD12	3:J:681:LYS:HG2	1.83	0.61
2:C:726:TYR:CZ	2:C:728:ASP:HB2	2.34	0.61
3:J:709:ARG:C	3:J:711:GLY:H	2.02	0.61
5:L:492:ASP:O	5:L:495:ARG:NH1	2.33	0.61
2:C:484:LEU:CD1	2:C:485:ASP:H	2.14	0.61
2:C:30:ILE:HD11	2:C:575:LEU:HD22	1.82	0.61
5:F:105:MET:CE	5:F:385:ARG:HG2	2.31	0.61
3:J:325:LYS:HE2	3:J:330:MET:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:98:VAL:HA	5:L:402:LEU:HD21	1.83	0.61
1:A:10:LYS:HA	1:B:227:GLN:HE22	1.66	0.61
2:C:1002:LEU:N	2:C:1008:GLN:OE1	2.33	0.61
2:C:15:PHE:CE1	2:C:1194:GLU:HB3	2.36	0.61
3:D:355:ILE:HG12	3:D:464:ASP:O	2.01	0.61
2:C:1308:ILE:CG2	3:D:379:PRO:HB2	2.30	0.61
3:D:425:ARG:HG2	3:D:426:ALA:H	1.63	0.61
3:D:582:ILE:CD1	3:D:627:THR:HG21	2.30	0.61
3:D:647:PRO:HG3	3:D:697:MET:CA	2.31	0.61
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.35	0.61
3:J:1146:GLU:OE2	3:J:1310:THR:HG22	1.99	0.61
5:L:383:ASN:HB2	5:L:412:LEU:HD21	1.82	0.61
5:L:582:VAL:CG1	5:L:586:ARG:HG2	2.31	0.61
2:C:1142:ARG:HD3	2:C:1161:LEU:CD1	2.29	0.61
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.81	0.61
2:C:225:PHE:HZ	2:C:348:SER:H	1.49	0.61
3:D:697:MET:CE	3:D:737:ILE:HG22	2.30	0.61
5:F:519:LEU:C	5:F:519:LEU:HD23	2.20	0.61
1:G:118:ASP:H	1:G:121:VAL:HB	1.65	0.61
2:I:1220:GLN:HG2	2:I:1221:PHE:H	1.65	0.61
3:J:1241:TYR:CD2	3:J:1246:VAL:HG11	2.35	0.61
2:C:453:ILE:CD1	2:C:587:LEU:HD11	2.30	0.61
2:C:46:GLN:OE1	2:C:47:TYR:N	2.33	0.61
5:F:280:VAL:HG11	5:F:355:ILE:HG23	1.83	0.61
3:J:902:ASP:CB	3:J:1251:LYS:HE3	2.30	0.61
3:J:64:PRO:HG3	3:J:90:VAL:HG12	1.83	0.61
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.81	0.61
2:C:1152:GLY:O	2:C:1153:ALA:HB2	2.01	0.60
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.82	0.60
3:D:93:THR:HG22	3:D:94:GLN:N	2.16	0.60
2:I:206:ALA:O	2:I:209:ILE:HG22	2.01	0.60
3:J:131:PRO:O	3:J:135:ILE:HG13	2.00	0.60
1:A:43:LEU:HD12	1:A:203:ILE:HD11	1.82	0.60
1:A:228:LEU:O	1:A:232:VAL:HG23	2.01	0.60
2:C:91:THR:HG21	2:C:503:LYS:NZ	2.15	0.60
1:H:171:LEU:HB2	1:H:172:LEU:HD12	1.84	0.60
2:I:146:VAL:CG2	2:I:513:GLN:NE2	2.64	0.60
3:J:364:HIS:HB3	4:K:4:VAL:HG23	1.82	0.60
5:L:134:VAL:HG22	5:L:273:MET:HE3	1.83	0.60
2:C:169:LYS:HG2	2:C:169:LYS:O	2.02	0.60
3:D:495:ASN:ND2	3:D:497:GLU:HB2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.82	0.60
1:G:44:ARG:HG3	1:G:183:ILE:CG2	2.31	0.60
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.83	0.60
1:H:48:LEU:HD22	3:J:535:ARG:HG3	1.83	0.60
4:K:27:ALA:HB1	4:K:46:THR:OG1	2.01	0.60
1:B:19:VAL:HB	1:B:23:HIS:NE2	2.17	0.60
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.36	0.60
2:C:303:ASP:OD2	2:C:328:SER:HB3	2.02	0.60
2:C:58:PRO:HB3	2:C:69:GLN:HB3	1.83	0.60
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.82	0.60
1:G:50:SER:HB2	1:H:8:PHE:CE1	2.35	0.60
2:I:119:GLU:HG3	2:I:489:PRO:N	2.16	0.60
3:J:883:ARG:NH1	3:J:897:HIS:HD2	2.00	0.60
2:C:832:HIS:CE1	2:C:1058:ARG:HD2	2.37	0.60
3:D:9:LYS:HE2	3:D:11:GLN:C	2.22	0.60
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.14	0.60
3:D:259:ARG:CZ	5:F:505:ILE:CD1	2.79	0.60
5:F:555:GLU:HG2	5:F:590:ILE:HG22	1.82	0.60
2:I:1279:GLU:HG2	3:J:1357:ILE:HD13	1.83	0.60
2:I:237:LEU:HD11	2:I:292:ILE:HD11	1.83	0.60
3:J:22:ILE:HG23	3:J:1336:ALA:HA	1.82	0.60
2:C:688:GLN:OE1	2:C:1237:HIS:CE1	2.54	0.60
2:C:1247:SER:HB3	3:D:375:GLU:O	2.01	0.60
5:F:287:ILE:HD11	5:F:341:LEU:HG	1.84	0.60
1:G:57:THR:OG1	1:G:147:GLN:HG2	2.02	0.60
1:G:83:LEU:HD23	2:I:694:ARG:HH21	1.62	0.60
2:I:65:ASN:HB3	2:I:105:TYR:CD2	2.36	0.60
2:I:1150:ASP:O	2:I:1155:VAL:HG21	2.02	0.60
3:J:232:ASN:HA	3:J:236:TRP:CZ3	2.34	0.60
3:J:494:ALA:HB2	3:J:922:SER:HB3	1.83	0.60
2:C:646:SER:HB3	2:C:649:GLN:CG	2.24	0.60
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.66	0.60
1:H:118:ASP:H	1:H:121:VAL:HB	1.66	0.60
1:H:206:GLU:OE1	3:J:531:LYS:NZ	2.22	0.60
2:I:619:ALA:CB	2:I:657:THR:HA	2.31	0.60
3:J:1280:VAL:HG21	3:J:1304:ARG:CD	2.31	0.60
3:J:154:LEU:HD23	3:J:160:LEU:HD21	1.83	0.60
3:J:215:LYS:O	3:J:218:THR:HG22	2.02	0.60
5:L:484:ALA:CB	5:L:491:GLU:HB2	2.23	0.60
5:L:561:MET:HA	5:L:567:MET:CE	2.16	0.60
1:B:49:SER:O	1:B:151:GLY:HA2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:MET:SD	2:C:134:GLY:HA2	2.42	0.60
2:C:161:LYS:HA	2:C:170:VAL:HA	1.83	0.60
2:C:221:LEU:HD21	2:C:351:LEU:HD12	1.84	0.60
2:C:596:ASP:OD2	2:C:598:VAL:HG23	2.01	0.60
3:D:93:THR:HG22	3:D:94:GLN:H	1.66	0.60
1:G:231:PHE:CB	1:H:218:ARG:HH11	2.14	0.60
3:J:1158:GLU:O	3:J:1206:ARG:NH1	2.35	0.60
3:J:1233:ILE:HG21	3:J:1257:VAL:HG22	1.82	0.60
5:L:147:GLN:HE22	5:L:150:ARG:HH11	1.48	0.60
1:A:50:SER:CB	1:B:8:PHE:HZ	2.15	0.60
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.34	0.60
5:L:277:MET:HE3	5:L:281:ARG:HH21	1.66	0.60
1:B:90:VAL:HG22	1:B:91:ARG:N	2.17	0.60
2:C:1248:THR:HB	5:F:532:LEU:CD1	2.31	0.60
2:C:705:GLU:HB2	2:C:794:LEU:H	1.67	0.60
3:D:1347:LEU:HG	3:D:1357:ILE:CG2	2.32	0.60
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.37	0.60
3:D:77:ARG:HG3	3:D:79:LYS:H	1.66	0.60
5:F:137:TYR:CD2	5:F:273:MET:HG2	2.37	0.60
1:G:48:LEU:CA	1:G:180:VAL:HG21	2.25	0.60
2:I:1080:ASN:HB3	2:I:1085:MET:HE2	1.82	0.60
3:J:126:LEU:HD12	3:J:127:LEU:N	2.17	0.60
2:C:30:ILE:HD11	2:C:575:LEU:CD2	2.32	0.59
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.66	0.59
3:D:154:LEU:CD2	3:D:160:LEU:HD11	2.32	0.59
3:D:515:ARG:O	3:D:545:HIS:HB3	2.02	0.59
1:H:158:ARG:CG	1:H:172:LEU:HD23	2.31	0.59
2:I:55:SER:OG	2:I:56:VAL:N	2.35	0.59
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.83	0.59
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.17	0.59
3:J:416:ILE:HG12	3:J:441:LEU:CD2	2.31	0.59
3:J:426:ALA:CB	3:J:427:PRO:HD3	2.29	0.59
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.37	0.59
2:I:1280:ALA:CB	3:J:918:ILE:HG22	2.32	0.59
2:C:170:VAL:HG23	2:C:171:LEU:N	2.15	0.59
2:C:698:PRO:HD3	2:C:795:ALA:HA	1.84	0.59
3:D:11:GLN:HG2	3:D:15:GLU:CG	2.31	0.59
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.20	0.59
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.35	0.59
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.37	0.59
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:492:ASP:HB2	5:L:495:ARG:NH1	2.08	0.59
1:A:182:ARG:O	1:A:183:ILE:HD12	2.03	0.59
2:C:243:PRO:HB2	2:C:278:GLU:CG	2.32	0.59
2:C:30:ILE:CD1	2:C:575:LEU:HD22	2.32	0.59
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.35	0.59
3:D:140:TYR:HB3	5:F:100:MET:SD	2.42	0.59
3:D:552:ILE:HG21	3:D:589:TYR:CE1	2.38	0.59
5:F:298:PRO:HD2	5:F:326:TRP:HB3	1.83	0.59
5:F:463:LEU:HD22	5:F:483:LEU:CD2	2.32	0.59
1:G:56:VAL:CG1	1:G:86:LYS:HA	2.32	0.59
2:I:1063:GLY:O	3:J:354:VAL:HG11	2.02	0.59
2:I:119:GLU:HG3	2:I:489:PRO:CD	2.31	0.59
2:I:1288:GLN:NE2	3:J:1355:ARG:HA	2.16	0.59
2:I:802:VAL:HG23	2:I:1098:LEU:HD13	1.84	0.59
2:I:886:LYS:CE	2:I:916:SER:HB3	2.31	0.59
3:J:1347:LEU:HG	3:J:1357:ILE:CG2	2.32	0.59
1:A:10:LYS:HA	1:B:227:GLN:NE2	2.17	0.59
2:C:149:LEU:HD12	2:C:452:ARG:O	2.02	0.59
2:C:269:ILE:HG23	2:C:273:HIS:CB	2.31	0.59
2:C:901:LEU:HD13	5:F:563:PHE:CE2	2.38	0.59
1:H:43:LEU:HD12	1:H:43:LEU:N	2.17	0.59
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.83	0.59
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.84	0.59
1:A:57:THR:O	1:A:173:VAL:HG22	2.02	0.59
2:C:1292:THR:HG21	2:C:1317:PRO:HB2	1.84	0.59
2:C:519:ASN:O	2:C:522:SER:HB3	2.01	0.59
3:D:36:GLY:HA3	3:D:61:ILE:HG23	1.83	0.59
3:D:518:VAL:HG11	3:D:707:ILE:HB	1.84	0.59
2:I:1080:ASN:HB3	2:I:1085:MET:CE	2.32	0.59
2:I:1287:LEU:HD22	3:J:1357:ILE:CD1	2.33	0.59
1:H:83:LEU:HD21	3:J:526:VAL:HB	1.85	0.59
1:A:169:GLY:O	1:A:171:LEU:HD22	2.03	0.59
1:B:77:ASP:O	1:B:81:ILE:HG13	2.02	0.59
2:C:109:ALA:CB	2:C:111:GLU:HA	2.33	0.59
2:C:241:LEU:HD11	2:C:246:LEU:CD1	2.30	0.59
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.35	0.59
3:D:1280:VAL:CG2	3:D:1304:ARG:HE	2.01	0.59
2:C:1285:TYR:CD2	3:D:1356:LEU:HD21	2.37	0.59
3:D:205:LEU:C	3:D:205:LEU:HD13	2.22	0.59
3:D:510:LEU:HG	3:D:513:MET:CE	2.31	0.59
3:D:536:LEU:HD13	3:D:541:LEU:CB	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ILE:HG12	1:G:159:ILE:O	2.02	0.59
2:I:1284:ALA:CB	3:J:1356:LEU:HD22	2.31	0.59
5:L:348:GLU:HA	5:L:353:LEU:O	2.02	0.59
2:C:1281:TYR:CE2	3:D:431:ARG:HG3	2.37	0.59
2:C:1299:ASN:ND2	2:C:1303:LYS:HE2	2.15	0.59
4:K:27:ALA:HB2	4:K:50:ALA:CB	2.32	0.59
1:A:59:VAL:HG21	1:A:85:LEU:CD1	2.33	0.59
2:C:125:GLY:HA2	2:C:499:SER:HB2	1.85	0.59
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.38	0.59
1:H:64:VAL:HG11	1:H:69:SER:HG	1.66	0.59
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.85	0.59
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.33	0.59
2:I:806:PRO:HB3	3:J:505:ASP:OD1	2.03	0.59
3:J:797:THR:CG2	3:J:924:GLY:HA3	2.30	0.59
5:L:362:ASN:HB2	5:L:365:MET:CE	2.32	0.59
1:A:28:LEU:N	1:A:28:LEU:HD12	2.18	0.59
1:B:37:HIS:NE2	2:C:1216:ARG:HD2	2.17	0.59
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.84	0.59
4:E:44:ASP:HB3	4:E:48:VAL:HB	1.85	0.59
2:I:607:SER:N	2:I:610:GLU:OE1	2.33	0.59
1:A:187:VAL:HG12	1:A:201:LEU:HD13	1.85	0.59
1:A:9:LEU:HD11	1:A:198:LEU:HD11	1.84	0.59
1:B:19:VAL:O	1:B:20:SER:HB3	2.01	0.59
2:C:397:LEU:HB3	2:C:401:GLY:HA3	1.84	0.59
2:I:1331:ARG:HG2	3:J:33:TRP:CH2	2.37	0.59
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.03	0.58
2:C:640:GLY:O	2:C:641:GLU:HG3	2.03	0.58
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.33	0.58
2:C:819:SER:HB2	2:C:1085:MET:CG	2.33	0.58
3:D:161:THR:HG22	3:D:164:GLN:CB	2.33	0.58
3:D:426:ALA:CB	3:D:427:PRO:HD3	2.31	0.58
3:D:831:VAL:HG13	3:D:831:VAL:O	2.03	0.58
2:I:400:VAL:HG22	2:I:584:TYR:HD1	1.68	0.58
2:I:90:VAL:HG12	2:I:91:THR:H	1.67	0.58
1:A:36:GLY:HA3	1:A:187:VAL:CG1	2.33	0.58
2:C:1158:LYS:C	2:C:1159:VAL:HG22	2.23	0.58
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.02	0.58
3:D:418:GLU:HG3	4:E:45:LYS:H	1.68	0.58
3:D:840:LEU:HG	3:D:841:GLY:N	2.15	0.58
5:F:279:ARG:HH12	5:F:350:GLU:CD	2.06	0.58
2:I:724:VAL:CG1	2:I:727:VAL:HG22	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:514:THR:HG21	3:J:596:LEU:CB	2.31	0.58
3:J:850:LYS:HD3	3:J:875:ASN:HD21	1.68	0.58
1:A:150:ARG:HD2	1:B:8:PHE:CZ	2.38	0.58
3:D:416:ILE:HG12	3:D:441:LEU:HD21	1.85	0.58
3:D:518:VAL:N	3:D:716:GLN:HE22	2.01	0.58
3:D:842:ARG:HB3	3:D:882:VAL:CG1	2.33	0.58
2:I:223:LEU:CD1	2:I:426:ILE:HD13	2.31	0.58
3:J:1251:LYS:O	3:J:1254:GLU:HB2	2.02	0.58
5:L:123:ILE:HD13	5:L:376:LYS:HG2	1.85	0.58
5:F:343:LYS:O	5:F:347:ILE:HG13	2.04	0.58
1:G:164:ASP:OD1	1:G:166:ARG:HB2	2.02	0.58
1:H:158:ARG:HB3	1:H:172:LEU:CD2	2.33	0.58
3:J:1263:LYS:HZ1	3:J:1315:ALA:HB1	1.69	0.58
3:J:864:LEU:N	3:J:864:LEU:HD23	2.18	0.58
4:K:60:ASN:ND2	4:K:63:ILE:HD13	2.19	0.58
5:L:284:GLU:HG2	5:L:310:GLU:OE1	2.03	0.58
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.66	0.58
5:L:372:ALA:O	5:L:376:LYS:HG3	2.03	0.58
5:L:390:ILE:HD12	5:L:435:ILE:HG21	1.84	0.58
2:C:1165:SER:HA	2:C:1169:VAL:HG21	1.85	0.58
2:C:1209:GLN:HB3	2:C:1224:PRO:HB2	1.86	0.58
2:C:231:GLU:O	2:C:238:GLN:N	2.36	0.58
2:C:324:LYS:HA	2:C:327:GLN:HE21	1.69	0.58
5:F:298:PRO:CD	5:F:326:TRP:HB3	2.34	0.58
1:G:218:ARG:NH1	1:H:232:VAL:H	2.01	0.58
3:J:72:CYS:HG	8:J:1502:ZN:ZN	1.16	0.58
3:J:288:PRO:HG2	3:J:291:ILE:HG13	1.86	0.58
5:L:135:ALA:HB1	5:L:253:SER:HA	1.86	0.58
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.85	0.58
3:D:1150:PRO:HG3	3:D:1214:PRO:HB2	1.85	0.58
3:D:331:ILE:CG2	3:D:1328:THR:HG21	2.33	0.58
1:G:10:LYS:HE2	1:H:229:GLU:OE1	2.03	0.58
2:I:91:THR:HA	2:I:138:ILE:O	2.03	0.58
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.85	0.58
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.69	0.58
3:D:1165:PHE:HD2	3:D:1173:ARG:CD	2.17	0.58
3:D:698:MET:O	3:D:702:GLN:HB3	2.04	0.58
2:I:854:ILE:HD11	2:I:885:GLY:CA	2.34	0.58
3:J:1198:VAL:HG11	3:J:1210:ILE:HG23	1.85	0.58
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.68	0.58
3:J:179:LYS:HB2	3:J:184:ALA:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:653:ILE:HG21	3:J:692:ARG:HB2	1.86	0.58
5:L:470:MET:CE	5:L:482:GLU:HG2	2.31	0.58
1:B:205:MET:CE	1:B:213:PRO:HA	2.34	0.58
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.86	0.58
3:D:147:ILE:CG2	3:D:188:LEU:HG	2.32	0.58
3:D:697:MET:O	3:D:701:LEU:HB2	2.03	0.58
1:G:161:SER:O	1:G:163:GLU:N	2.36	0.58
2:I:556:GLY:HA2	2:I:659:GLN:O	2.04	0.58
3:J:863:LEU:CD1	3:J:901:ARG:HB3	2.26	0.58
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.86	0.58
2:C:156:PHE:HE1	2:C:443:ASP:HB2	1.65	0.58
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.85	0.58
1:H:20:SER:OG	1:H:21:SER:N	2.36	0.58
2:I:1304:MET:O	2:I:1307:ASN:N	2.37	0.58
3:J:502:PRO:HB3	3:J:506:VAL:CG2	2.33	0.58
3:J:744:ARG:HG3	3:J:744:ARG:O	2.03	0.58
2:C:619:ALA:HB2	2:C:654:ASP:CB	2.34	0.58
2:C:75:LEU:HD22	2:C:75:LEU:N	2.19	0.58
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.03	0.58
2:C:84:GLU:OE2	2:C:1032:LYS:HE3	2.04	0.58
2:C:980:VAL:HG13	2:C:984:VAL:CG2	2.34	0.58
3:D:11:GLN:HB2	3:D:15:GLU:OE2	2.03	0.58
3:D:1293:GLU:OE1	3:D:1294:ALA:N	2.34	0.58
3:D:342:LEU:HA	3:D:343:LEU:HD12	1.81	0.58
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.04	0.58
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.39	0.58
5:F:335:GLU:OE2	5:F:339:ARG:HG3	2.04	0.58
1:H:132:HIS:O	1:H:133:LEU:HD12	2.04	0.58
1:H:183:ILE:CD1	1:H:205:MET:HG3	2.34	0.58
1:H:213:PRO:O	1:H:217:ILE:HG13	2.03	0.58
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.67	0.58
2:I:996:ARG:HD2	2:I:999:GLU:OE1	2.04	0.58
3:J:30:ILE:HD13	3:J:243:PRO:CD	2.34	0.58
3:J:598:LYS:O	3:J:601:ILE:HG22	2.04	0.58
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.86	0.58
1:A:110:VAL:HG21	1:A:140:ILE:HD11	1.87	0.57
1:A:166:ARG:N	1:A:167:PRO:HD2	2.18	0.57
2:C:53:PHE:CE1	2:C:468:LEU:HD11	2.39	0.57
3:D:1309:ILE:HG13	3:D:1310:THR:H	1.69	0.57
3:D:514:THR:HG21	3:D:596:LEU:CB	2.34	0.57
2:C:1105:SER:HB2	3:D:731:ARG:CG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.85	0.57
5:F:324:LYS:HG3	5:F:326:TRP:CZ2	2.39	0.57
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.69	0.57
2:I:688:GLN:O	2:I:1235:LEU:HA	2.03	0.57
2:I:1295:SER:HB2	3:J:347:VAL:HG22	1.86	0.57
3:J:262:THR:C	5:L:507:MET:HB2	2.23	0.57
3:D:436:ALA:HB3	3:D:485:MET:HA	1.85	0.57
5:F:297:MET:CE	5:F:330:LEU:HD21	2.33	0.57
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.86	0.57
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.86	0.57
3:J:423:LEU:CD1	3:J:468:VAL:HG12	2.34	0.57
3:J:583:VAL:HG13	3:J:587:LEU:HD22	1.86	0.57
2:C:145:ILE:HG22	2:C:456:VAL:HG22	1.86	0.57
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.86	0.57
2:C:906:PHE:CE2	5:F:608:ARG:HG3	2.38	0.57
3:D:45:ASN:O	3:D:46:TYR:HD2	1.87	0.57
2:C:1305:TYR:CZ	5:F:532:LEU:HG	2.39	0.57
1:G:166:ARG:N	1:G:167:PRO:HD2	2.19	0.57
1:H:11:PRO:HB2	1:H:28:LEU:HD11	1.86	0.57
2:I:109:ALA:HB1	2:I:110:PRO:O	2.03	0.57
2:I:233:ARG:HH12	2:I:332:ARG:NH1	2.02	0.57
3:J:1144:LEU:HD11	3:J:1236:GLU:HB3	1.86	0.57
3:J:53:ARG:NH2	3:J:60:ARG:HD2	2.19	0.57
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.87	0.57
2:C:494:ASN:O	2:C:498:ILE:HD13	2.04	0.57
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.33	0.57
3:J:1278:GLU:OE2	3:J:1282:TYR:HD2	1.87	0.57
3:J:363:LEU:HD23	3:J:487:THR:CG2	2.27	0.57
2:C:239:MET:O	2:C:284:LEU:HD12	2.04	0.57
2:C:529:ARG:HH12	6:C:2001:KNG:C17	2.18	0.57
2:C:560:PRO:HB3	3:D:776:THR:HG21	1.87	0.57
3:D:870:ASP:O	3:D:874:GLU:HG2	2.04	0.57
1:G:133:LEU:HD11	1:G:138:ALA:O	2.04	0.57
1:G:231:PHE:HB3	1:H:218:ARG:HD3	1.86	0.57
2:I:1246:ARG:CZ	2:I:1258:PRO:HB3	2.35	0.57
3:J:141:PHE:HA	3:J:180:MET:HE2	1.85	0.57
5:L:147:GLN:HB3	5:L:161:LEU:CD1	2.35	0.57
3:D:142:GLU:CG	5:F:100:MET:HE1	2.35	0.57
3:D:364:HIS:HB3	3:D:487:THR:CG2	2.34	0.57
3:D:514:THR:HG21	3:D:596:LEU:HG	1.86	0.57
2:I:810:TYR:CE1	2:I:1078:LYS:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5:TYR:HB2	2:I:781:ASP:OD1	2.05	0.57
3:J:482:ALA:HB3	4:K:20:VAL:HG22	1.85	0.57
2:C:302:ILE:HG22	2:C:309:LEU:N	2.19	0.57
2:C:599:VAL:HG21	2:C:629:PHE:HE1	1.69	0.57
3:D:1165:PHE:HD2	3:D:1173:ARG:HD2	1.68	0.57
3:D:1234:VAL:O	3:D:1238:GLN:HB2	2.04	0.57
3:D:218:THR:HA	3:D:221:ILE:HG22	1.86	0.57
3:D:242:LEU:HD23	3:D:242:LEU:C	2.25	0.57
2:I:696:ASP:CB	2:I:798:GLN:HG2	2.31	0.57
5:L:322:MET:HE2	5:L:324:LYS:HG2	1.86	0.57
2:C:1017:GLN:O	2:C:1021:LEU:HG	2.05	0.57
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.87	0.57
2:C:55:SER:OG	2:C:56:VAL:N	2.36	0.57
3:D:11:GLN:HG2	3:D:15:GLU:HG2	1.85	0.57
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.87	0.57
3:D:689:ALA:O	3:D:693:VAL:HG23	2.04	0.57
5:F:547:VAL:HG23	5:F:603:ARG:HH11	1.70	0.57
2:I:62:TYR:CE1	2:I:476:LYS:HB3	2.39	0.57
3:J:623:GLN:O	3:J:627:THR:HG22	2.04	0.57
3:J:657:ALA:O	3:J:661:VAL:HG12	2.04	0.57
2:C:231:GLU:HG2	2:C:332:ARG:NH2	2.19	0.57
2:C:488:MET:O	2:C:490:GLN:N	2.35	0.57
2:C:599:VAL:CG2	2:C:629:PHE:HE1	2.18	0.57
2:C:617:ALA:HA	2:C:636:CYS:SG	2.44	0.57
3:D:825:VAL:CG1	3:D:833:GLU:HB3	2.34	0.57
5:F:483:LEU:HD12	5:F:483:LEU:H	1.70	0.57
2:I:169:LYS:O	2:I:169:LYS:HG2	2.05	0.57
3:J:127:LEU:HD21	3:J:234:PRO:HG3	1.87	0.57
3:J:147:ILE:O	3:J:177:ASP:HB3	2.05	0.57
3:D:1372:ARG:HH21	3:J:854:ALA:HB3	1.69	0.57
2:C:535:PRO:HG2	2:C:536:GLY:H	1.69	0.57
3:D:901:ARG:HA	3:D:908:ILE:HA	1.87	0.57
5:F:230:VAL:HG13	5:F:231:THR:H	1.70	0.57
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.86	0.57
5:F:569:THR:OG1	5:F:570:ASP:N	2.32	0.57
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	1.86	0.57
2:I:1299:ASN:HD22	2:I:1303:LYS:CE	2.17	0.57
2:I:870:ILE:HG21	2:I:931:VAL:HG11	1.86	0.57
3:J:1144:LEU:CD1	3:J:1236:GLU:HB3	2.35	0.57
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.05	0.57
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.05	0.56
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.01	0.56
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.70	0.56
5:F:315:TRP:O	5:F:319:ALA:HB3	2.05	0.56
3:D:392:THR:HG21	5:F:606:VAL:HA	1.87	0.56
2:I:101:ARG:HE	2:I:118:LYS:HD2	1.70	0.56
2:I:832:HIS:CE1	2:I:1058:ARG:HD2	2.40	0.56
2:I:208:ILE:HD11	2:I:365:GLU:HB3	1.86	0.56
2:I:30:ILE:HD11	2:I:575:LEU:HD22	1.86	0.56
2:I:696:ASP:O	2:I:697:LYS:HB3	2.05	0.56
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	1.86	0.56
3:J:1142:ALA:O	3:J:1146:GLU:HB2	2.05	0.56
3:J:165:TYR:O	3:J:169:LEU:HB2	2.05	0.56
3:J:583:VAL:HG21	3:J:592:VAL:HG11	1.87	0.56
2:C:1132:LEU:HD22	2:C:1177:ARG:CZ	2.35	0.56
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.40	0.56
3:D:849:LEU:CB	3:D:853:THR:HG23	2.35	0.56
1:G:231:PHE:HB3	1:H:218:ARG:CG	2.34	0.56
2:I:1122:LYS:HE2	2:I:1178:LYS:O	2.06	0.56
2:I:1238:LEU:CD1	2:I:1238:LEU:H	2.10	0.56
3:J:233:LYS:HB3	3:J:235:GLU:OE2	2.06	0.56
3:J:521:LYS:HE3	3:J:541:LEU:O	2.04	0.56
2:I:808:ASN:H	3:J:633:ALA:HB2	1.70	0.56
3:J:809:VAL:HA	3:J:894:VAL:O	2.05	0.56
4:K:53:GLU:OE1	4:K:59:ILE:HG13	2.05	0.56
2:C:211:ARG:HD3	2:C:357:ASN:O	2.05	0.56
2:C:469:VAL:O	2:C:472:GLU:HB3	2.04	0.56
3:D:19:ALA:O	3:D:20:ILE:HG13	2.05	0.56
3:D:267:ASP:HA	3:D:270:ARG:NH2	2.18	0.56
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.40	0.56
1:H:73:GLY:C	1:H:134:THR:HG22	2.26	0.56
1:H:215:GLU:OE1	1:H:219:ARG:NH1	2.38	0.56
1:G:50:SER:HB2	1:H:8:PHE:HE1	1.70	0.56
2:I:1308:ILE:CG2	3:J:379:PRO:HB2	2.35	0.56
1:A:218:ARG:HH12	1:B:231:PHE:HA	1.69	0.56
2:C:2:VAL:O	2:C:3:TYR:CB	2.53	0.56
2:C:309:LEU:HD21	2:C:312:ALA:CA	2.35	0.56
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.40	0.56
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.87	0.56
3:D:1142:ALA:O	3:D:1146:GLU:HB2	2.06	0.56
5:F:511:ILE:HG23	5:F:511:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:76:GLU:HB3	1:H:81:ILE:HG12	1.86	0.56
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.05	0.56
2:I:563:THR:HG22	2:I:680:LEU:HD11	1.88	0.56
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.86	0.56
3:J:69:GLU:HG3	3:J:76:LYS:HA	1.88	0.56
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.69	0.56
2:C:1238:LEU:HD12	2:C:1238:LEU:N	2.20	0.56
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	1.88	0.56
2:C:367:TYR:HD2	2:C:376:PRO:HB3	1.70	0.56
3:D:357:VAL:HG22	3:D:461:PHE:CD1	2.40	0.56
3:D:905:ARG:HH21	3:D:907:HIS:CG	2.23	0.56
1:G:140:ILE:HD12	1:G:142:MET:HE3	1.87	0.56
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.19	0.56
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.41	0.56
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.39	0.56
5:F:280:VAL:HG22	5:F:347:ILE:CD1	2.25	0.56
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.87	0.56
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.87	0.56
3:J:1264:ALA:HB2	3:J:1304:ARG:HA	1.88	0.56
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.87	0.56
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.37	0.56
5:L:119:ILE:CG2	5:L:375:ALA:HB1	2.32	0.56
1:B:11:PRO:CB	1:B:28:LEU:HD11	2.32	0.56
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.35	0.56
5:F:463:LEU:HD22	5:F:483:LEU:HD22	1.86	0.56
1:G:11:PRO:HB3	1:G:31:LEU:HD23	1.86	0.56
1:H:142:MET:SD	1:H:144:ILE:HD11	2.46	0.56
2:I:39:ILE:HD11	2:I:75:LEU:HG	1.87	0.56
3:J:289:ASP:HB3	3:J:293:ARG:NH2	2.20	0.56
3:J:825:VAL:HG13	3:J:833:GLU:HB3	1.87	0.56
1:B:210:THR:O	1:B:211:ILE:HD13	2.05	0.56
2:C:619:ALA:N	2:C:654:ASP:HB2	2.21	0.56
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.88	0.56
5:F:584:ARG:HA	5:F:584:ARG:HH11	1.71	0.56
2:I:109:ALA:HB1	2:I:111:GLU:CA	2.36	0.56
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.06	0.56
2:I:169:LYS:HE2	2:I:190:PRO:O	2.05	0.56
5:L:540:LEU:O	5:L:540:LEU:HD23	2.06	0.56
2:C:878:THR:HG23	2:C:881:ASP:OD2	2.05	0.56
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.40	0.56
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.03	0.56
2:I:495:ALA:HB3	5:L:471:LEU:HD22	1.87	0.56
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.87	0.56
3:D:709:ARG:C	3:D:711:GLY:N	2.58	0.56
1:G:112:ALA:O	1:G:115:ILE:HG13	2.05	0.56
1:H:127:GLN:O	1:H:127:GLN:HG2	2.05	0.56
2:I:17:LYS:HZ2	2:I:1154:ASP:HB3	1.70	0.56
2:I:1327:LEU:HD23	2:I:1331:ARG:HH21	1.69	0.56
5:L:412:LEU:HB2	5:L:435:ILE:HD11	1.88	0.56
2:C:1043:ALA:O	2:C:1046:VAL:HG12	2.06	0.56
2:C:1142:ARG:HH22	2:C:1165:SER:CB	2.17	0.56
2:C:722:GLY:HA3	2:C:735:LYS:O	2.06	0.56
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.21	0.56
1:H:97:GLU:HB2	1:H:146:VAL:O	2.06	0.56
3:J:1241:TYR:HD2	3:J:1246:VAL:CG1	2.19	0.56
1:A:231:PHE:HE2	1:B:39:LEU:HD13	1.72	0.55
1:A:12:ARG:H	1:A:30:PRO:HD2	1.71	0.55
2:C:1124:ILE:HB	2:C:1180:MET:HB2	1.88	0.55
1:G:104:LYS:CG	1:G:110:VAL:HG22	2.30	0.55
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.06	0.55
1:H:130:ILE:HG22	1:H:131:CYS:SG	2.47	0.55
1:H:89:ALA:HB3	1:H:124:VAL:CG1	2.36	0.55
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.71	0.55
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.89	0.55
3:J:1197:ASN:CB	3:J:1211:SER:HA	2.36	0.55
5:L:479:THR:HG23	5:L:481:GLU:H	1.71	0.55
1:A:214:GLU:O	1:A:217:ILE:HG22	2.06	0.55
1:B:23:HIS:CB	1:B:206:GLU:HG2	2.36	0.55
2:C:1131:MET:CE	2:C:1141:LEU:HA	2.33	0.55
2:C:215:TYR:HE2	2:C:422:LYS:HD2	1.71	0.55
3:D:1273:ASP:HB3	3:D:1276:GLU:CG	2.32	0.55
3:D:363:LEU:CG	3:D:363:LEU:O	2.47	0.55
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.70	0.55
5:F:551:LEU:HD21	5:F:598:LEU:HD21	1.87	0.55
5:F:552:THR:OG1	5:F:555:GLU:HG3	2.07	0.55
2:I:417:SER:OG	2:I:419:ILE:HG13	2.07	0.55
2:I:897:PRO:HB3	5:L:564:GLY:C	2.26	0.55
2:I:1291:LEU:CD2	3:J:1351:VAL:HG13	2.26	0.55
3:J:262:THR:O	5:L:507:MET:HB2	2.05	0.55
1:A:207:THR:HG22	1:A:208:ASN:N	2.21	0.55
2:C:90:VAL:HG12	2:C:91:THR:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.87	0.55
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.37	0.55
4:E:32:VAL:O	4:E:34:GLY:N	2.39	0.55
5:F:392:LYS:O	5:F:395:THR:HG22	2.06	0.55
1:H:158:ARG:HB3	1:H:172:LEU:HD22	1.88	0.55
2:I:1297:ASP:O	2:I:1301:ARG:HG2	2.07	0.55
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.88	0.55
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.42	0.55
1:B:29:GLU:CB	1:B:30:PRO:CD	2.82	0.55
2:C:11:ILE:HG21	2:C:1149:TYR:CE1	2.42	0.55
2:C:1238:LEU:H	2:C:1238:LEU:CD1	2.15	0.55
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.07	0.55
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.86	0.55
5:F:292:VAL:HG13	5:F:297:MET:O	2.07	0.55
3:J:244:VAL:HA	3:J:269:TYR:OH	2.07	0.55
3:J:848:VAL:CG2	3:J:858:VAL:HG13	2.36	0.55
1:B:104:LYS:CG	1:B:110:VAL:HG22	2.29	0.55
1:B:93:GLN:HB2	1:B:120:ASP:OD1	2.06	0.55
2:C:1137:GLU:HG2	2:C:1140:LYS:HG2	1.87	0.55
2:C:1246:ARG:HH11	2:C:1266:GLY:HA2	1.71	0.55
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.89	0.55
3:D:525:MET:O	3:D:548:VAL:HG13	2.07	0.55
4:E:80:LEU:O	4:E:84:THR:OG1	2.25	0.55
5:F:297:MET:HE3	5:F:330:LEU:HD21	1.87	0.55
5:F:606:VAL:HG13	5:F:607:LEU:HD12	1.87	0.55
2:I:1152:GLY:O	2:I:1153:ALA:HB2	2.07	0.55
2:I:1287:LEU:HD22	3:J:1357:ILE:CG1	2.37	0.55
5:L:316:PHE:CZ	5:L:337:VAL:HB	2.42	0.55
2:C:147:SER:OG	2:C:455:SER:HB3	2.07	0.55
3:D:141:PHE:O	3:D:180:MET:HE1	2.07	0.55
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.87	0.55
4:E:15:ASN:O	4:E:16:ARG:HB3	2.07	0.55
5:F:456:MET:SD	5:F:497:VAL:HG13	2.46	0.55
1:G:219:ARG:O	1:G:223:ILE:HG13	2.07	0.55
2:I:17:LYS:CE	2:I:1154:ASP:HB3	2.37	0.55
2:I:767:GLN:HG2	2:I:786:GLY:HA2	1.89	0.55
2:I:800:MET:O	2:I:1229:TYR:HA	2.07	0.55
2:I:960:LEU:HD12	2:I:1028:LYS:HE2	1.89	0.55
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.72	0.55
3:J:30:ILE:HD13	3:J:243:PRO:CG	2.36	0.55
3:J:489:ASN:HA	3:J:904:ALA:CB	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:227:LYS:HZ3	2:C:298:ALA:HB1	1.70	0.55
3:D:161:THR:N	3:D:164:GLN:OE1	2.39	0.55
3:D:317:THR:HB	3:D:324:LEU:HB3	1.88	0.55
3:D:398:LYS:O	3:D:402:GLU:HB2	2.06	0.55
2:I:1129:ASN:OD1	2:I:1177:ARG:NH2	2.39	0.55
2:I:887:VAL:HB	2:I:913:VAL:HG22	1.84	0.55
2:I:1243:MET:CE	3:J:445:LYS:HD3	2.37	0.55
5:L:277:MET:CE	5:L:281:ARG:HH21	2.19	0.55
5:L:582:VAL:HG12	5:L:586:ARG:HG2	1.89	0.55
1:B:205:MET:HG2	1:B:206:GLU:N	2.22	0.55
2:C:1119:MET:HB2	2:C:1228:GLY:CA	2.34	0.55
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.88	0.55
2:C:565:GLU:HB2	2:C:680:LEU:HD21	1.88	0.55
2:C:646:SER:CB	2:C:649:GLN:HG3	2.26	0.55
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.88	0.55
2:C:688:GLN:O	2:C:1235:LEU:HA	2.07	0.55
2:C:397:LEU:HD12	2:C:397:LEU:N	2.22	0.55
3:D:279:LEU:C	3:D:279:LEU:HD23	2.27	0.55
3:D:316:ILE:HA	3:D:323:PRO:HA	1.87	0.55
3:D:516:ASP:HA	3:D:545:HIS:HB2	1.88	0.55
1:G:218:ARG:NH1	1:H:232:VAL:N	2.55	0.55
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.36	0.55
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.41	0.55
2:I:891:GLY:C	2:I:892:GLU:HG3	2.28	0.55
4:K:15:ASN:O	4:K:16:ARG:HB3	2.07	0.55
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.89	0.55
3:D:137:ARG:HD3	3:D:143:SER:CB	2.37	0.55
3:D:291:ILE:HD13	5:F:409:ASN:HB3	1.89	0.55
5:F:513:ASP:OD2	5:F:515:GLU:HB2	2.07	0.55
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.89	0.55
3:J:1217:PRO:HG3	3:J:1232:TYR:HE2	1.71	0.55
3:J:186:GLN:CB	3:J:238:ILE:HG21	2.32	0.55
3:J:491:LEU:HD23	3:J:498:PRO:HA	1.89	0.55
5:L:445:ASP:OD2	5:L:451:ARG:HD2	2.06	0.55
1:A:14:VAL:HG13	1:A:27:THR:HB	1.88	0.54
2:C:1080:ASN:CB	2:C:1085:MET:CE	2.84	0.54
3:D:1273:ASP:HB2	3:D:1276:GLU:CD	2.27	0.54
2:C:1304:MET:CE	3:D:472:LEU:HD12	2.37	0.54
5:F:577:GLY:CA	5:F:583:THR:HG23	2.29	0.54
1:G:19:VAL:HG13	1:G:20:SER:H	1.72	0.54
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:884:VAL:O	2:I:917:SER:HB2	2.07	0.54
5:L:343:LYS:HD2	5:L:343:LYS:H	1.72	0.54
2:C:1142:ARG:NH2	2:C:1165:SER:CB	2.70	0.54
2:C:1144:PHE:CE1	2:C:1201:LEU:HD11	2.42	0.54
2:C:548:ARG:CZ	2:C:571:LEU:HD11	2.37	0.54
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.42	0.54
3:D:1193:TRP:HB2	3:D:1194:ARG:CZ	2.36	0.54
3:D:109:SER:HB2	3:D:296:LYS:HE2	1.88	0.54
3:D:451:PRO:O	3:D:454:CYS:HB2	2.07	0.54
3:D:697:MET:HE2	3:D:737:ILE:HG22	1.89	0.54
5:F:316:PHE:O	5:F:320:ILE:HG13	2.07	0.54
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.88	0.54
2:I:1115:THR:HG22	2:I:1228:GLY:HA3	1.89	0.54
2:I:1238:LEU:HD12	2:I:1238:LEU:N	2.20	0.54
3:J:591:ILE:HG23	3:J:604:MET:HE2	1.88	0.54
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.42	0.54
1:A:154:PRO:CB	2:C:1059:ARG:HH21	2.19	0.54
2:C:1089:GLU:OE2	2:C:1211:ARG:HD2	2.07	0.54
3:D:1227:HIS:O	3:D:1230:THR:HG22	2.07	0.54
3:D:1282:TYR:O	3:D:1285:VAL:HG12	2.07	0.54
1:B:196:THR:HG23	3:D:443:GLU:CG	2.38	0.54
3:D:92:VAL:O	3:D:92:VAL:HG22	2.07	0.54
2:I:840:SER:CB	2:I:850:ILE:HD11	2.37	0.54
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.38	0.54
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.73	0.54
2:C:3:TYR:CE1	2:C:11:ILE:CD1	2.90	0.54
2:C:484:LEU:HD12	2:C:485:ASP:H	1.72	0.54
2:C:599:VAL:CG2	2:C:629:PHE:CE1	2.90	0.54
5:F:111:LEU:HD11	5:F:119:ILE:HD12	1.90	0.54
5:F:486:ARG:HB2	5:F:486:ARG:CZ	2.37	0.54
1:H:32:GLU:OE2	1:H:195:ARG:NH2	2.41	0.54
2:I:1191:LYS:O	2:I:1195:ILE:HG13	2.08	0.54
3:J:1167:LYS:CD	3:J:1174:ARG:HD2	2.36	0.54
3:J:41:PRO:HB3	3:J:270:ARG:HG3	1.90	0.54
3:J:868:TRP:CZ3	3:J:871:LEU:HD13	2.42	0.54
3:J:483:LEU:HD21	4:K:17:PHE:CD1	2.43	0.54
5:L:315:TRP:CH2	5:L:341:LEU:HD11	2.43	0.54
1:B:101:THR:HG22	1:B:103:ASN:HD21	1.72	0.54
1:B:127:GLN:HG2	1:B:127:GLN:O	2.08	0.54
2:C:198:ILE:O	2:C:201:ARG:HB2	2.06	0.54
3:D:126:LEU:CD1	3:D:223:LEU:CD2	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:129:ASP:HB2	3:D:220:ARG:NH2	2.22	0.54
2:C:1113:LEU:CD1	3:D:641:ILE:HG13	2.37	0.54
4:E:36:ASP:HB2	4:E:37:PRO:HD2	1.89	0.54
5:F:505:ILE:HD12	5:F:505:ILE:N	2.23	0.54
1:B:140:ILE:O	1:B:140:ILE:HG23	2.07	0.54
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.08	0.54
2:C:233:ARG:HH12	2:C:332:ARG:HH12	1.56	0.54
2:I:1158:LYS:C	2:I:1159:VAL:HG22	2.28	0.54
2:I:818:VAL:HG13	2:I:822:VAL:HG21	1.90	0.54
5:L:114:GLU:HG3	5:L:115:GLY:H	1.72	0.54
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.07	0.54
2:C:518:ASN:O	2:C:691:PRO:HD3	2.08	0.54
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.22	0.54
3:D:384:LYS:NZ	3:D:414:GLU:OE1	2.36	0.54
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.22	0.54
1:H:231:PHE:N	1:H:231:PHE:CD2	2.76	0.54
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.23	0.54
3:J:418:GLU:HB3	4:K:48:VAL:HG23	1.89	0.54
3:J:843:VAL:HG11	3:J:897:HIS:O	2.08	0.54
5:L:571:TYR:HB3	5:L:575:GLU:HG2	1.88	0.54
2:C:1151:LEU:CD1	2:C:1198:LEU:HD23	2.38	0.54
2:C:221:LEU:HD21	2:C:351:LEU:CD1	2.38	0.54
2:C:325:LEU:CD1	2:C:333:ILE:HG12	2.38	0.54
2:C:38:PHE:CZ	2:C:49:LEU:HD21	2.43	0.54
5:F:320:ILE:HG12	5:F:330:LEU:HD12	1.89	0.54
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.27	0.54
2:I:219:GLN:HA	2:I:222:ASP:HB3	1.89	0.54
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.23	0.54
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.89	0.54
2:C:864:LYS:NZ	2:C:877:VAL:HA	2.23	0.54
3:D:56:LEU:H	3:D:56:LEU:CD1	2.17	0.54
3:D:872:LEU:O	3:D:877:VAL:CG1	2.56	0.54
2:I:60:GLN:O	2:I:476:LYS:HE2	2.07	0.54
2:I:864:LYS:NZ	2:I:876:GLU:O	2.40	0.54
3:J:210:SER:HB2	3:J:213:LYS:CG	2.38	0.54
5:L:353:LEU:HD13	5:L:361:ILE:HD12	1.90	0.54
1:B:201:LEU:HD21	1:B:203:ILE:HD11	1.89	0.54
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.22	0.54
2:C:231:GLU:HG2	2:C:332:ARG:CZ	2.38	0.54
3:D:1344:LEU:O	3:D:1345:ARG:HB2	2.08	0.54
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:598:LEU:HA	5:F:603:ARG:HB2	1.90	0.54
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.90	0.54
1:H:187:VAL:O	1:H:187:VAL:HG23	2.07	0.54
2:I:1129:ASN:OD1	2:I:1177:ARG:NE	2.39	0.54
1:A:73:GLY:O	1:A:134:THR:HG22	2.08	0.53
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.90	0.53
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.40	0.53
2:C:1271:GLY:CA	3:D:343:LEU:CD1	2.68	0.53
2:C:228:VAL:HB	2:C:335:THR:OG1	2.08	0.53
3:D:1314:LEU:HD12	3:D:1326:GLN:CD	2.28	0.53
1:G:70:THR:HG21	2:I:755:LYS:CE	2.26	0.53
1:G:11:PRO:HD3	1:H:227:GLN:CD	2.27	0.53
3:J:30:ILE:HD13	3:J:243:PRO:HG3	1.90	0.53
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.90	0.53
1:A:61:ILE:HG23	1:A:142:MET:HB3	1.89	0.53
1:A:159:ILE:HG12	1:A:162:GLU:OE2	2.08	0.53
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.90	0.53
2:C:1269:ARG:HD3	3:D:343:LEU:CB	2.28	0.53
2:C:782:VAL:HG11	2:C:792:GLY:HA3	1.90	0.53
3:D:670:SER:HB2	3:D:672:LEU:HD13	1.90	0.53
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.41	0.53
2:I:91:THR:HG21	2:I:503:LYS:NZ	2.24	0.53
2:I:796:LEU:H	2:I:796:LEU:HD12	1.71	0.53
3:J:1291:GLU:C	3:J:1292:LEU:HD12	2.29	0.53
3:J:129:ASP:HB2	3:J:220:ARG:CZ	2.38	0.53
3:J:526:VAL:HG12	3:J:549:LYS:CB	2.31	0.53
3:J:592:VAL:HA	3:J:596:LEU:HD21	1.89	0.53
2:C:1212:LEU:HD22	2:C:1225:VAL:CG2	2.39	0.53
2:C:782:VAL:HG11	2:C:792:GLY:CA	2.39	0.53
3:D:1350:ASN:OD1	3:D:1355:ARG:HD2	2.08	0.53
3:D:372:MET:O	3:D:376:LEU:HD12	2.08	0.53
1:H:205:MET:HG2	1:H:206:GLU:N	2.23	0.53
2:I:185:ASP:O	2:I:196:VAL:HG23	2.09	0.53
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.08	0.53
3:J:103:GLY:CA	3:J:244:VAL:HG22	2.39	0.53
3:J:325:LYS:HG3	3:J:329:ASP:HB2	1.90	0.53
3:J:357:VAL:HG22	3:J:461:PHE:CD1	2.44	0.53
3:J:615:LYS:HZ3	4:K:7:GLN:HG2	1.73	0.53
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.74	0.53
1:A:36:GLY:CA	1:A:187:VAL:HG11	2.36	0.53
2:C:696:ASP:HB2	2:C:798:GLN:CG	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.89	0.53
1:G:71:LYS:HZ2	1:G:140:ILE:HG22	1.73	0.53
1:H:67:GLU:N	1:H:67:GLU:OE1	2.42	0.53
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.42	0.53
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.08	0.53
2:I:21:VAL:HG11	2:I:592:ARG:CD	2.38	0.53
2:I:729:ALA:O	2:I:755:LYS:NZ	2.19	0.53
2:I:798:GLN:HB2	2:I:828:PHE:HE1	1.72	0.53
2:I:854:ILE:HD11	2:I:885:GLY:HA3	1.90	0.53
3:J:514:THR:OG1	3:J:594:GLN:O	2.27	0.53
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.90	0.53
5:L:315:TRP:HZ2	5:L:341:LEU:HD21	1.72	0.53
1:B:187:VAL:HG13	1:B:199:ASP:HB3	1.90	0.53
2:C:1134:GLN:C	2:C:1135:GLN:HG2	2.28	0.53
2:C:1307:ASN:HA	2:C:1310:ASP:HB2	1.89	0.53
2:C:219:GLN:HA	2:C:222:ASP:HB3	1.90	0.53
3:D:17:PHE:CE2	3:D:1355:ARG:NH2	2.76	0.53
1:G:231:PHE:HB3	1:H:218:ARG:CD	2.38	0.53
3:J:369:PRO:HB3	3:J:444:GLY:O	2.08	0.53
3:J:418:GLU:HB3	4:K:48:VAL:CG2	2.39	0.53
3:J:646:ILE:HG23	3:J:741:ALA:O	2.07	0.53
2:C:1075:VAL:HG23	3:D:461:PHE:O	2.09	0.53
2:C:102:LEU:O	2:C:116:ASP:HA	2.08	0.53
2:C:185:ASP:O	2:C:196:VAL:HG23	2.08	0.53
2:C:1:MET:O	2:C:2:VAL:HG23	2.07	0.53
2:C:338:THR:CB	2:C:345:PRO:HB3	2.38	0.53
2:C:516:ASP:O	2:C:522:SER:OG	2.17	0.53
2:C:557:ARG:HH21	2:C:607:SER:C	2.12	0.53
2:C:942:ASP:O	2:C:946:LEU:HB2	2.08	0.53
1:G:11:PRO:HG3	1:G:31:LEU:HD21	1.90	0.53
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.89	0.53
2:I:896:THR:H	2:I:899:GLU:HB2	1.73	0.53
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.43	0.53
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.90	0.53
3:J:44:ILE:HB	3:J:49:PHE:O	2.08	0.53
3:J:525:MET:O	3:J:548:VAL:HG13	2.08	0.53
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.74	0.53
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.08	0.53
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.73	0.53
2:I:224:PHE:CD2	2:I:347:ILE:HG13	2.44	0.53
2:I:985:GLU:HB3	2:I:988:LYS:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.90	0.53
3:D:141:PHE:HA	3:D:180:MET:HE2	1.90	0.53
3:D:333:GLY:HA3	3:D:338:PHE:CZ	2.43	0.53
1:G:37:HIS:NE2	1:G:187:VAL:HG21	2.23	0.53
2:I:151:ARG:NH2	2:I:156:PHE:CD2	2.75	0.53
3:J:210:SER:HB2	3:J:213:LYS:HG3	1.91	0.53
3:J:56:LEU:N	3:J:56:LEU:HD12	2.24	0.53
5:L:606:VAL:HG13	5:L:607:LEU:HD12	1.90	0.53
1:A:59:VAL:HG21	1:A:85:LEU:HD13	1.91	0.53
2:C:810:TYR:CD1	2:C:1078:LYS:HB2	2.44	0.53
2:C:992:LEU:H	2:C:992:LEU:HD23	1.73	0.53
3:D:152:THR:OG1	3:D:153:ASN:N	2.42	0.53
3:D:619:ILE:O	3:D:623:GLN:HG2	2.09	0.53
1:G:35:PHE:CE1	1:H:46:ILE:HG23	2.44	0.53
1:H:74:VAL:HG12	1:H:76:GLU:H	1.74	0.53
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.90	0.53
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.91	0.53
2:I:640:GLY:O	2:I:641:GLU:HG3	2.09	0.53
2:I:817:LEU:HD11	2:I:1080:ASN:ND2	2.24	0.53
5:L:552:THR:OG1	5:L:555:GLU:HG3	2.08	0.53
2:C:448:LEU:HA	2:C:451:ARG:HB2	1.90	0.53
2:C:629:PHE:CE2	2:C:634:VAL:HG11	2.43	0.53
3:D:1273:ASP:CB	3:D:1276:GLU:HG3	2.35	0.53
3:D:126:LEU:CD1	3:D:223:LEU:HD22	2.39	0.53
3:D:679:TYR:CE2	3:D:683:ILE:HD12	2.44	0.53
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.39	0.53
1:H:116:THR:HG23	1:H:116:THR:O	2.09	0.53
2:I:929:ILE:CD1	2:I:1055:ALA:HB2	2.31	0.53
2:I:132:ASP:N	2:I:132:ASP:OD1	2.28	0.53
3:J:41:PRO:CB	3:J:270:ARG:HG3	2.39	0.53
3:J:674:THR:OG1	3:J:677:GLU:HB2	2.09	0.53
2:I:560:PRO:HG3	3:J:773:PHE:CE2	2.44	0.53
5:L:108:VAL:HG11	5:L:381:GLU:C	2.29	0.53
1:B:197:ASP:C	1:B:198:LEU:HD22	2.29	0.52
2:C:1080:ASN:CB	2:C:1085:MET:HE3	2.38	0.52
2:C:1124:ILE:CG2	2:C:1180:MET:HG3	2.39	0.52
3:D:325:LYS:HB3	5:F:508:GLU:HG2	1.91	0.52
5:F:559:LEU:HD22	5:F:594:ALA:HB1	1.91	0.52
1:G:89:ALA:HB3	1:G:125:LYS:CD	2.39	0.52
1:G:10:LYS:HA	1:H:227:GLN:NE2	2.24	0.52
3:J:19:ALA:O	3:J:20:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:45:ASN:O	3:J:46:TYR:HD2	1.91	0.52
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.08	0.52
5:L:444:ALA:HB1	5:L:457:ILE:HD12	1.91	0.52
1:B:47:LEU:HD22	1:B:180:VAL:HG11	1.90	0.52
1:B:194:GLN:HA	1:B:194:GLN:OE1	2.09	0.52
2:C:1285:TYR:CE1	3:D:475:GLU:HG2	2.44	0.52
2:C:486:THR:HG23	2:C:487:LEU:H	1.74	0.52
5:F:383:ASN:ND2	5:F:427:PHE:HE2	2.06	0.52
5:F:598:LEU:HA	5:F:603:ARG:CB	2.39	0.52
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.91	0.52
3:J:342:LEU:N	3:J:344:GLY:HA2	2.24	0.52
3:J:431:ARG:NH2	3:J:489:ASN:OD1	2.42	0.52
3:J:79:LYS:HG3	3:J:80:HIS:N	2.22	0.52
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.92	0.52
2:C:325:LEU:HD13	2:C:333:ILE:HG12	1.91	0.52
4:E:82:ALA:O	4:E:85:ALA:HB3	2.09	0.52
5:F:479:THR:HG22	5:F:482:GLU:CB	2.39	0.52
2:I:38:PHE:CZ	2:I:49:LEU:HD21	2.45	0.52
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.44	0.52
3:J:502:PRO:HB3	3:J:506:VAL:HG11	1.91	0.52
1:B:205:MET:HE1	1:B:213:PRO:CA	2.35	0.52
2:C:94:ALA:HB2	2:C:129:LEU:CD1	2.37	0.52
3:D:106:GLU:OE2	3:D:241:VAL:HG22	2.10	0.52
3:D:748:ALA:O	3:D:777:HIS:HD2	1.91	0.52
2:I:871:VAL:O	2:I:944:ARG:NH1	2.40	0.52
3:J:24:LEU:HD11	3:J:116:PHE:CZ	2.44	0.52
2:I:1271:GLY:HA3	3:J:343:LEU:HD12	1.91	0.52
2:C:192:ASP:OD2	2:C:436:ARG:NH2	2.43	0.52
2:C:929:ILE:HD13	2:C:1055:ALA:HB2	1.92	0.52
3:D:227:PHE:O	3:D:230:SER:HB3	2.09	0.52
3:D:514:THR:HG21	3:D:596:LEU:CG	2.40	0.52
3:D:842:ARG:CB	3:D:882:VAL:HG11	2.39	0.52
5:F:551:LEU:HD21	5:F:598:LEU:CD2	2.39	0.52
1:G:9:LEU:HD21	1:G:195:ARG:NH2	2.22	0.52
1:H:125:LYS:HB3	1:H:128:HIS:HB2	1.92	0.52
2:I:65:ASN:CB	2:I:105:TYR:HD2	2.23	0.52
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.44	0.52
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.25	0.52
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.92	0.52
2:C:619:ALA:HB2	2:C:654:ASP:HB3	1.90	0.52
2:C:817:LEU:HD11	2:C:1080:ASN:ND2	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:97:VAL:HG12	3:D:101:ARG:CG	2.40	0.52
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	1.92	0.52
3:D:847:ASP:HA	3:D:860:ARG:H	1.75	0.52
1:H:158:ARG:HG3	1:H:172:LEU:HD23	1.92	0.52
2:I:816:ILE:O	2:I:1076:ILE:HD12	2.10	0.52
2:I:568:ASN:HB2	2:I:571:LEU:HB2	1.92	0.52
2:I:895:LEU:HB2	2:I:899:GLU:HB2	1.91	0.52
3:J:114:ILE:O	3:J:114:ILE:HG13	2.08	0.52
3:J:1269:ALA:HB2	3:J:1274:PHE:HE1	1.73	0.52
3:J:510:LEU:HG	3:J:513:MET:CE	2.40	0.52
5:L:409:ASN:O	5:L:413:MET:HG3	2.10	0.52
1:A:115:ILE:HG22	1:A:116:THR:H	1.74	0.52
1:A:166:ARG:O	1:A:167:PRO:C	2.48	0.52
1:B:47:LEU:CD1	1:B:183:ILE:HG12	2.35	0.52
1:B:66:HIS:CD2	1:B:68:TYR:OH	2.63	0.52
2:C:202:ARG:HH22	2:C:368:ARG:HH22	1.57	0.52
2:C:324:LYS:O	2:C:327:GLN:NE2	2.43	0.52
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.91	0.52
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.91	0.52
3:D:490:ILE:HB	3:D:500:ILE:HG13	1.91	0.52
3:D:79:LYS:HE3	3:D:80:HIS:HA	1.91	0.52
5:F:379:MET:HG2	5:F:416:VAL:HG21	1.90	0.52
5:F:547:VAL:HG22	5:F:598:LEU:HD22	1.91	0.52
2:I:619:ALA:HB1	2:I:657:THR:HA	1.90	0.52
3:J:1145:PHE:HB3	3:J:1309:ILE:CG2	2.40	0.52
5:L:147:GLN:HE22	5:L:150:ARG:NH1	2.07	0.52
1:B:64:VAL:HG11	1:B:69:SER:HB2	1.91	0.52
2:C:768:MET:O	2:C:784:ALA:HB1	2.10	0.52
2:C:796:LEU:HD12	2:C:796:LEU:H	1.75	0.52
3:D:161:THR:H	3:D:164:GLN:HB2	1.74	0.52
5:F:311:THR:HG21	5:F:348:GLU:CD	2.30	0.52
1:G:133:LEU:CD1	1:G:138:ALA:HB3	2.39	0.52
1:G:219:ARG:HG2	1:G:223:ILE:HD11	1.90	0.52
1:G:89:ALA:HB3	1:G:125:LYS:HD2	1.91	0.52
1:G:90:VAL:HG22	1:G:91:ARG:N	2.22	0.52
2:I:62:TYR:C	2:I:64:GLY:H	2.12	0.52
2:I:839:VAL:HG12	2:I:1049:ILE:CD1	2.40	0.52
2:I:1272:GLU:N	3:J:343:LEU:HD12	2.25	0.52
3:J:363:LEU:CG	3:J:363:LEU:O	2.56	0.52
3:J:827:GLU:HG2	3:J:832:LYS:HD2	1.91	0.52
1:B:55:ALA:O	1:B:146:VAL:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1113:LEU:HD11	3:D:641:ILE:HG13	1.90	0.52
3:D:97:VAL:CG1	3:D:101:ARG:CZ	2.85	0.52
1:G:231:PHE:N	1:G:231:PHE:CD2	2.76	0.52
1:G:64:VAL:HG11	1:G:78:ILE:HG13	1.92	0.52
2:I:1142:ARG:HH12	2:I:1169:VAL:HG21	1.75	0.52
2:I:680:LEU:HD22	3:J:783:LEU:HD11	1.92	0.52
3:J:1233:ILE:HG21	3:J:1257:VAL:CG2	2.40	0.52
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.91	0.52
5:L:290:LEU:HD12	5:L:337:VAL:HG22	1.92	0.52
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.92	0.52
2:C:958:LYS:O	2:C:962:GLU:HG2	2.10	0.52
3:D:1154:ALA:N	3:D:1214:PRO:O	2.33	0.52
3:D:1241:TYR:CD2	3:D:1246:VAL:HG11	2.41	0.52
3:D:287:ALA:HB1	3:D:288:PRO:HD2	1.92	0.52
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.45	0.52
5:F:513:ASP:C	5:F:515:GLU:H	2.13	0.52
2:I:197:ARG:NH2	2:I:203:LYS:HB2	2.25	0.52
2:I:778:GLU:O	2:I:781:ASP:HB2	2.10	0.52
2:I:836:LEU:CD2	2:I:921:PRO:HD3	2.40	0.52
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.45	0.52
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.92	0.52
3:J:825:VAL:O	3:J:826:ILE:HG13	2.10	0.52
2:C:864:LYS:HZ1	2:C:877:VAL:HA	1.75	0.51
3:D:658:GLU:HA	3:D:661:VAL:CG1	2.40	0.51
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.92	0.51
5:F:337:VAL:HG12	5:F:341:LEU:CD1	2.40	0.51
2:C:490:GLN:CG	5:F:472:GLN:NE2	2.71	0.51
5:F:547:VAL:HG23	5:F:603:ARG:NH1	2.25	0.51
3:D:392:THR:CG2	5:F:606:VAL:HA	2.40	0.51
2:I:568:ASN:CB	2:I:571:LEU:HD12	2.40	0.51
2:I:836:LEU:N	2:I:836:LEU:HD12	2.24	0.51
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.92	0.51
3:J:92:VAL:HG22	3:J:92:VAL:O	2.11	0.51
1:B:66:HIS:HB3	1:B:68:TYR:CE2	2.45	0.51
6:C:2001:KNG:C34	6:C:2001:KNG:C29	2.88	0.51
3:D:115:TRP:NE1	3:D:1329:THR:HG23	2.24	0.51
3:D:823:THR:HB	3:D:824:PRO:HD2	1.92	0.51
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.92	0.51
3:D:843:VAL:CG1	3:D:883:ARG:HD3	2.39	0.51
5:L:513:ASP:OD2	5:L:515:GLU:OE1	2.29	0.51
1:A:49:SER:OG	1:A:50:SER:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:17:LYS:CE	2:C:1154:ASP:HB3	2.32	0.51
2:C:255:ILE:HG23	2:C:285:ILE:HD13	1.92	0.51
2:C:309:LEU:HD21	2:C:312:ALA:HA	1.92	0.51
2:C:678:ARG:NE	2:C:1106:ARG:HG2	2.26	0.51
2:C:696:ASP:O	2:C:697:LYS:CB	2.59	0.51
3:D:1314:LEU:CD1	3:D:1326:GLN:OE1	2.58	0.51
3:D:317:THR:HG22	3:D:322:ARG:O	2.10	0.51
3:D:500:ILE:HG22	3:D:500:ILE:O	2.09	0.51
5:F:230:VAL:HG13	5:F:231:THR:N	2.25	0.51
5:F:470:MET:HE3	5:F:478:PRO:HB3	1.92	0.51
1:G:48:LEU:HA	1:G:180:VAL:CG2	2.27	0.51
2:I:810:TYR:CD1	2:I:1078:LYS:HB2	2.45	0.51
2:I:1132:LEU:HD11	2:I:1174:GLU:HG2	1.92	0.51
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.92	0.51
2:I:1273:MET:HA	2:I:1276:TRP:CE3	2.45	0.51
3:J:361:LEU:CD1	3:J:366:CYS:HA	2.41	0.51
3:J:521:LYS:NZ	3:J:540:GLY:O	2.33	0.51
1:B:74:VAL:HG22	1:B:133:LEU:HD12	1.92	0.51
2:C:1299:ASN:HD22	2:C:1303:LYS:CE	2.22	0.51
2:C:241:LEU:CD1	2:C:246:LEU:HD11	2.38	0.51
3:D:103:GLY:CA	3:D:244:VAL:HG22	2.40	0.51
3:D:108:ALA:HB1	3:D:279:LEU:HD22	1.92	0.51
3:D:129:ASP:HB2	3:D:220:ARG:NE	2.25	0.51
3:D:56:LEU:HD21	3:D:269:TYR:HB3	1.91	0.51
3:D:48:THR:HB	3:D:50:LYS:HG3	1.92	0.51
5:F:540:LEU:HA	5:F:610:PHE:CZ	2.46	0.51
2:I:598:VAL:HG13	2:I:626:GLU:O	2.10	0.51
2:I:62:TYR:O	2:I:64:GLY:N	2.43	0.51
2:I:975:ILE:HG13	2:I:1014:LEU:HD22	1.92	0.51
3:J:493:PRO:HB2	3:J:918:ILE:HD12	1.92	0.51
5:L:132:CYS:SG	5:L:257:LYS:CE	2.99	0.51
1:A:14:VAL:HG12	1:A:27:THR:HB	1.91	0.51
1:A:154:PRO:HB2	2:C:1059:ARG:NH2	2.25	0.51
2:C:1281:TYR:HE2	3:D:431:ARG:HG3	1.75	0.51
3:D:165:TYR:O	3:D:169:LEU:HB2	2.09	0.51
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.93	0.51
5:F:573:LEU:H	5:F:573:LEU:CD2	2.19	0.51
1:H:9:LEU:HB3	1:H:32:GLU:HG3	1.93	0.51
3:J:1263:LYS:CE	3:J:1279:GLN:HE21	2.20	0.51
3:J:821:MET:CE	3:J:879:ALA:HB1	2.40	0.51
3:J:863:LEU:C	3:J:864:LEU:HD23	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:382:TYR:HE2	5:L:532:LEU:HD23	1.75	0.51
1:A:231:PHE:HZ	1:B:201:LEU:HD23	1.76	0.51
1:B:58:GLU:OE1	1:B:158:ARG:NH2	2.43	0.51
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.73	0.51
5:F:310:GLU:O	5:F:344:LEU:HD21	2.11	0.51
2:I:518:ASN:O	2:I:691:PRO:HD3	2.11	0.51
2:I:978:VAL:CG1	2:I:1007:LYS:HB3	2.40	0.51
2:I:815:SER:CB	3:J:357:VAL:CG2	2.88	0.51
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.93	0.51
3:J:697:MET:SD	3:J:741:ALA:HB3	2.50	0.51
3:J:843:VAL:HG13	3:J:883:ARG:CD	2.37	0.51
1:B:197:ASP:OD1	1:B:197:ASP:N	2.42	0.51
2:C:1043:ALA:O	2:C:1046:VAL:CG1	2.58	0.51
2:C:1149:TYR:HB3	2:C:1159:VAL:HG11	1.93	0.51
2:C:557:ARG:NH2	2:C:608:ALA:HA	2.26	0.51
2:C:634:VAL:HG13	2:C:636:CYS:HG	1.75	0.51
3:D:160:LEU:HA	3:D:164:GLN:OE1	2.10	0.51
3:D:859:PRO:CG	3:D:862:THR:HG21	2.35	0.51
1:H:57:THR:CG2	1:H:158:ARG:HE	2.10	0.51
2:I:1158:LYS:O	2:I:1159:VAL:CG1	2.52	0.51
1:H:41:ASN:ND2	2:I:1217:THR:HA	2.26	0.51
2:I:159:SER:HB2	2:I:442:VAL:HG21	1.92	0.51
3:J:129:ASP:HB2	3:J:220:ARG:NH2	2.25	0.51
3:J:614:LEU:HB3	4:K:7:GLN:HG2	1.93	0.51
2:I:1109:ILE:HG12	3:J:644:MET:SD	2.51	0.51
3:J:660:GLU:O	3:J:664:ILE:HG12	2.11	0.51
4:K:60:ASN:H	4:K:63:ILE:HB	1.76	0.51
2:C:356:THR:HG21	2:C:362:ALA:HA	1.93	0.51
3:D:1221:LEU:O	3:D:1221:LEU:HD22	2.10	0.51
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.93	0.51
1:H:133:LEU:HD11	1:H:140:ILE:HD13	1.93	0.51
2:I:146:VAL:HG11	2:I:531:LEU:HD11	1.93	0.51
2:I:646:SER:HB3	2:I:649:GLN:CG	2.34	0.51
3:J:1293:GLU:O	3:J:1294:ALA:C	2.49	0.51
3:J:1328:THR:HG22	3:J:1332:LEU:HD23	1.93	0.51
3:J:19:ALA:HA	3:J:1344:LEU:CD1	2.40	0.51
2:C:1331:ARG:HA	2:C:1335:ILE:O	2.11	0.51
3:D:108:ALA:CB	3:D:279:LEU:HD22	2.40	0.51
3:D:1298:VAL:HG22	3:D:1298:VAL:O	2.11	0.51
3:D:858:VAL:HA	3:D:868:TRP:CZ3	2.46	0.51
4:E:15:ASN:HB3	4:E:18:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:165:GLU:C	1:G:167:PRO:HD2	2.31	0.51
2:I:119:GLU:CB	2:I:489:PRO:HB2	2.40	0.51
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.92	0.51
1:A:73:GLY:C	1:A:134:THR:HG22	2.31	0.51
2:C:1062:PRO:HA	2:C:1076:ILE:O	2.10	0.51
2:C:26:TYR:OH	2:C:28:LEU:HD12	2.10	0.51
2:C:802:VAL:HG12	2:C:1228:GLY:O	2.10	0.51
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.91	0.51
3:D:805:GLN:OE1	3:D:1348:LYS:HD3	2.11	0.51
1:G:73:GLY:O	1:G:134:THR:HG22	2.10	0.51
1:G:50:SER:CB	1:H:8:PHE:CE1	2.91	0.51
1:G:9:LEU:HD11	1:G:198:LEU:HD21	1.93	0.51
2:I:1174:GLU:OE2	2:I:1177:ARG:HD2	2.11	0.51
2:I:68:LEU:HD23	2:I:475:VAL:HG11	1.93	0.51
3:J:140:TYR:HB3	5:L:100:MET:SD	2.51	0.51
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.46	0.51
3:J:850:LYS:HG2	3:J:857:LEU:HD23	1.93	0.51
5:L:123:ILE:CD1	5:L:376:LYS:HG2	2.40	0.51
5:L:492:ASP:HA	5:L:495:ARG:NH2	2.26	0.51
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.10	0.50
2:C:529:ARG:NH1	6:C:2001:KNG:C17	2.74	0.50
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.92	0.50
3:D:495:ASN:HD21	3:D:497:GLU:HB2	1.75	0.50
3:D:40:LYS:HB2	3:D:54:ASP:O	2.11	0.50
1:G:211:ILE:HG21	1:G:216:ALA:HB2	1.93	0.50
1:H:13:LEU:HD23	1:H:13:LEU:H	1.76	0.50
2:I:1134:GLN:C	2:I:1135:GLN:HG2	2.31	0.50
2:I:151:ARG:HH21	2:I:156:PHE:HD2	1.54	0.50
2:I:216:THR:HG23	2:I:219:GLN:OE1	2.11	0.50
2:I:26:TYR:OH	2:I:28:LEU:HD12	2.10	0.50
2:I:974:ARG:HB3	2:I:1014:LEU:CD2	2.40	0.50
2:I:985:GLU:CB	2:I:988:LYS:HD2	2.41	0.50
2:I:994:ARG:HD2	2:I:997:TRP:CH2	2.46	0.50
3:J:1177:ILE:HG13	3:J:1186:TYR:O	2.10	0.50
3:J:902:ASP:HB2	3:J:1251:LYS:CE	2.40	0.50
3:J:233:LYS:N	3:J:236:TRP:CZ3	2.76	0.50
3:J:288:PRO:HG2	3:J:291:ILE:CG1	2.41	0.50
3:J:514:THR:HG23	3:J:596:LEU:HB2	1.90	0.50
3:J:797:THR:O	3:J:801:VAL:HG13	2.12	0.50
3:J:810:THR:HG23	3:J:811:GLU:H	1.76	0.50
1:B:86:LYS:HD3	1:B:174:ASP:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:ILE:HG22	2:C:1149:TYR:OH	2.11	0.50
2:C:689:ALA:HB2	2:C:1233:LEU:HG	1.93	0.50
2:C:1077:SER:HA	3:D:356:THR:OG1	2.11	0.50
2:I:796:LEU:N	2:I:796:LEU:HD12	2.25	0.50
3:J:1221:LEU:HD22	3:J:1221:LEU:C	2.31	0.50
3:J:115:TRP:CZ2	3:J:1329:THR:HG23	2.46	0.50
3:J:227:PHE:HE1	3:J:234:PRO:CD	2.23	0.50
2:I:841:ARG:CZ	3:J:256:ASP:HB3	2.41	0.50
2:I:1280:ALA:CB	3:J:431:ARG:HB3	2.42	0.50
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.92	0.50
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.93	0.50
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.77	0.50
2:C:1333:LEU:HD21	3:D:327:LEU:HB3	1.93	0.50
2:C:310:ILE:HD13	2:C:325:LEU:HA	1.93	0.50
3:D:1155:ILE:HD11	3:D:1211:SER:HB3	1.94	0.50
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.26	0.50
3:D:364:HIS:HB3	3:D:487:THR:HG23	1.92	0.50
2:C:1109:ILE:HD11	3:D:644:MET:SD	2.50	0.50
3:D:686:TRP:HA	3:D:686:TRP:CE3	2.45	0.50
3:D:770:LEU:O	3:D:774:ILE:HG13	2.11	0.50
1:G:221:ALA:HB1	1:H:228:LEU:HD22	1.92	0.50
2:I:229:ILE:HG21	2:I:240:GLU:OE2	2.11	0.50
2:I:478:ARG:HG2	2:I:492:MET:HG2	1.92	0.50
2:I:815:SER:OG	3:J:357:VAL:CG2	2.59	0.50
3:J:908:ILE:HD13	3:J:909:ILE:O	2.11	0.50
4:K:19:LEU:HD13	4:K:54:ILE:HG21	1.93	0.50
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.93	0.50
1:A:187:VAL:O	1:A:187:VAL:HG23	2.11	0.50
2:C:402:ARG:HD2	2:C:406:ASN:ND2	2.26	0.50
1:A:83:LEU:HD23	2:C:694:ARG:HH21	1.77	0.50
3:D:349:TYR:CD1	3:D:472:LEU:HD21	2.46	0.50
3:D:45:ASN:O	3:D:46:TYR:HB3	2.10	0.50
3:D:491:LEU:CD2	3:D:498:PRO:CA	2.88	0.50
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.92	0.50
1:G:214:GLU:HA	1:G:217:ILE:HG22	1.94	0.50
1:G:219:ARG:HA	1:G:222:THR:HB	1.92	0.50
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.92	0.50
3:J:146:VAL:HG23	3:J:158:GLN:O	2.11	0.50
3:J:205:LEU:C	3:J:205:LEU:HD13	2.32	0.50
5:L:147:GLN:CB	5:L:161:LEU:HD11	2.41	0.50
1:A:39:LEU:O	1:A:43:LEU:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.45	0.50
2:C:1191:LYS:O	2:C:1195:ILE:HG13	2.12	0.50
2:C:619:ALA:HA	2:C:654:ASP:HB2	1.90	0.50
2:C:1280:ALA:HB3	3:D:431:ARG:HB3	1.94	0.50
1:G:55:ALA:HB3	1:G:177:TYR:CD1	2.47	0.50
2:I:20:GLN:HG3	2:I:20:GLN:O	2.11	0.50
3:J:193:ASP:CG	3:J:196:GLN:HG2	2.31	0.50
3:J:483:LEU:HD21	4:K:17:PHE:HD1	1.76	0.50
5:L:462:LYS:O	5:L:466:ILE:HG13	2.12	0.50
5:L:467:SER:HB2	5:L:483:LEU:HD21	1.93	0.50
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.46	0.50
2:C:1323:PHE:CZ	2:C:1327:LEU:CD1	2.95	0.50
2:C:1323:PHE:CE1	2:C:1327:LEU:HD13	2.47	0.50
2:C:306:THR:OG1	2:C:308:GLU:HB2	2.12	0.50
2:C:215:TYR:CE2	2:C:422:LYS:HD2	2.47	0.50
3:D:812:ASP:HB2	3:D:911:LYS:HZ2	1.77	0.50
5:F:297:MET:CE	5:F:330:LEU:HD11	2.42	0.50
3:J:431:ARG:HH21	3:J:489:ASN:CG	2.14	0.50
3:J:903:LEU:HD23	3:J:905:ARG:CD	2.40	0.50
3:J:418:GLU:CG	4:K:44:ASP:HA	2.32	0.50
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.94	0.50
1:A:224:LEU:C	1:A:224:LEU:HD23	2.32	0.50
1:A:65:LEU:N	1:A:65:LEU:HD22	2.25	0.50
2:C:1315:MET:CE	2:C:1317:PRO:HB3	2.42	0.50
3:D:45:ASN:O	3:D:46:TYR:CD2	2.65	0.50
3:D:801:VAL:HG12	3:D:920:ALA:HB3	1.94	0.50
3:D:438:GLU:OE1	4:E:2:ALA:HB2	2.10	0.50
1:G:187:VAL:O	1:G:187:VAL:HG23	2.12	0.50
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.42	0.50
2:I:836:LEU:HD21	2:I:921:PRO:CD	2.41	0.50
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.75	0.50
3:J:388:ARG:CZ	3:J:414:GLU:OE2	2.59	0.50
3:J:735:ALA:O	3:J:738:ARG:HB3	2.12	0.50
5:L:441:ARG:HH12	5:L:445:ASP:CG	2.15	0.50
2:C:1210:ILE:HG13	2:C:1227:VAL:HG22	1.93	0.50
2:C:231:GLU:HG2	2:C:332:ARG:HD3	1.94	0.50
3:D:1278:GLU:HA	3:D:1278:GLU:OE1	2.11	0.50
3:D:132:LEU:HD13	3:D:132:LEU:C	2.32	0.50
3:D:141:PHE:CD1	3:D:293:ARG:HD3	2.47	0.50
3:D:165:TYR:CE2	3:D:178:ALA:HB3	2.47	0.50
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:398:LYS:HG2	3:D:402:GLU:OE2	2.11	0.50
5:F:392:LYS:O	5:F:395:THR:CG2	2.60	0.50
1:G:38:THR:HA	1:H:45:ARG:HD3	1.94	0.50
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.41	0.50
2:I:998:LEU:HD12	2:I:998:LEU:N	2.27	0.50
3:J:425:ARG:HG2	3:J:426:ALA:N	2.20	0.50
3:J:45:ASN:O	3:J:46:TYR:HB3	2.11	0.50
3:J:708:ASN:OD1	3:J:708:ASN:N	2.45	0.50
3:J:848:VAL:HG23	3:J:857:LEU:CD1	2.41	0.50
5:L:287:ILE:HD11	5:L:341:LEU:HG	1.94	0.50
5:L:392:LYS:O	5:L:395:THR:HG22	2.11	0.50
1:A:86:LYS:HD3	1:A:176:CYS:HB2	1.94	0.50
2:C:5:TYR:HD1	2:C:8:LYS:CD	2.19	0.50
3:D:810:THR:HG23	3:D:811:GLU:H	1.77	0.50
5:F:226:ALA:O	5:F:229:VAL:HG22	2.12	0.50
2:I:1220:GLN:HG2	2:I:1221:PHE:N	2.26	0.50
3:J:19:ALA:HA	3:J:1344:LEU:HD12	1.92	0.50
3:J:500:ILE:HG22	3:J:500:ILE:O	2.12	0.50
3:J:511:TYR:CD2	3:J:728:SER:HB3	2.47	0.50
3:J:903:LEU:HD13	3:J:909:ILE:CD1	2.42	0.50
3:J:64:PRO:HG3	3:J:90:VAL:CG1	2.41	0.50
1:A:38:THR:OG1	1:B:45:ARG:CG	2.58	0.49
2:C:1080:ASN:HB2	2:C:1085:MET:HE3	1.94	0.49
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.26	0.49
3:D:827:GLU:O	3:D:829:GLY:N	2.34	0.49
1:G:14:VAL:HG13	1:G:27:THR:HB	1.93	0.49
3:J:1273:ASP:HB3	3:J:1276:GLU:HG3	1.92	0.49
3:J:250:ARG:HB3	3:J:265:LEU:HD12	1.93	0.49
3:J:360:TYR:OH	3:J:442:ILE:HD11	2.12	0.49
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.93	0.49
1:A:53:GLY:O	1:A:177:TYR:HB3	2.12	0.49
2:C:471:VAL:CG2	2:C:498:ILE:HD11	2.41	0.49
2:I:700:VAL:HG13	2:I:1117:LEU:CD2	2.42	0.49
2:I:31:GLN:OE1	2:I:456:VAL:HG23	2.12	0.49
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.94	0.49
3:J:451:PRO:O	3:J:454:CYS:HB2	2.12	0.49
3:J:827:GLU:CG	3:J:832:LYS:HD2	2.41	0.49
5:L:597:LYS:O	5:L:603:ARG:HG3	2.12	0.49
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.94	0.49
2:C:921:PRO:O	2:C:924:VAL:HG22	2.12	0.49
3:D:450:HIS:CE1	3:D:452:LEU:HD12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:741:ALA:O	3:D:762:ASN:ND2	2.45	0.49
3:D:814:CYS:HB3	3:D:890:THR:OG1	2.12	0.49
1:H:59:VAL:N	1:H:171:LEU:O	2.35	0.49
1:H:43:LEU:HD21	1:H:221:ALA:HB2	1.92	0.49
2:I:796:LEU:O	2:I:1233:LEU:HD12	2.12	0.49
2:I:824:GLN:HE22	2:I:1082:ILE:HD11	1.77	0.49
3:J:1191:PRO:HB2	3:J:1194:ARG:HH11	1.77	0.49
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.27	0.49
3:J:290:ILE:CD1	3:J:290:ILE:H	2.23	0.49
3:J:609:TYR:HD1	3:J:610:ARG:HH11	1.60	0.49
5:L:224:LEU:HB2	5:L:259:PHE:CE1	2.48	0.49
5:L:281:ARG:CG	5:L:285:ARG:HH11	2.24	0.49
2:C:1146:GLN:NE2	2:C:1150:ASP:OD2	2.45	0.49
2:C:1272:GLU:N	3:D:343:LEU:HD11	2.27	0.49
2:C:593:LYS:CB	2:C:602:GLU:HG3	2.38	0.49
2:C:891:GLY:O	2:C:892:GLU:HG3	2.12	0.49
3:D:279:LEU:HD23	3:D:279:LEU:O	2.12	0.49
3:D:536:LEU:CD1	3:D:541:LEU:HB2	2.33	0.49
3:D:755:ILE:HG22	3:D:757:THR:H	1.76	0.49
3:D:885:VAL:HG12	3:D:894:VAL:CG1	2.43	0.49
5:F:494:ILE:O	5:F:498:LEU:CB	2.60	0.49
1:G:27:THR:HG21	1:G:200:LYS:HD3	1.94	0.49
1:G:230:ALA:HB3	1:G:231:PHE:CD2	2.46	0.49
2:I:1164:PHE:O	2:I:1169:VAL:HG23	2.12	0.49
2:I:1250:SER:OG	5:L:524:GLU:OE1	2.30	0.49
2:I:757:THR:C	2:I:833:ILE:HD12	2.32	0.49
3:J:545:HIS:NE2	3:J:719:PHE:HE1	2.10	0.49
2:C:1292:THR:HG22	2:C:1293:VAL:N	2.28	0.49
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.48	0.49
2:C:227:LYS:HZ2	2:C:298:ALA:HB1	1.74	0.49
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.94	0.49
3:D:16:GLU:CG	3:D:1369:ARG:NH2	2.74	0.49
3:D:536:LEU:HD12	3:D:542:ALA:CB	2.42	0.49
3:D:583:VAL:HG13	3:D:587:LEU:HD22	1.95	0.49
2:I:208:ILE:HD11	2:I:365:GLU:CB	2.42	0.49
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.48	0.49
2:I:39:ILE:CD1	2:I:75:LEU:HG	2.42	0.49
2:I:761:GLN:O	2:I:762:ASN:HB2	2.12	0.49
1:G:134:THR:O	2:I:773:LEU:HD11	2.13	0.49
3:J:418:GLU:HG3	4:K:45:LYS:H	1.77	0.49
4:K:26:ARG:NE	4:K:53:GLU:OE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:CG2	1:A:158:ARG:CZ	2.90	0.49
2:C:1066:MET:HE1	2:C:1076:ILE:HB	1.88	0.49
2:C:1180:MET:O	2:C:1182:ILE:HG13	2.11	0.49
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.27	0.49
3:D:510:LEU:O	3:D:514:THR:HG23	2.13	0.49
1:G:89:ALA:H	1:G:125:LYS:HD3	1.77	0.49
1:H:183:ILE:HD11	1:H:205:MET:HG3	1.94	0.49
2:I:981:ALA:HB1	2:I:1007:LYS:HZ2	1.77	0.49
2:I:979:LEU:HD13	2:I:1011:LEU:CD2	2.42	0.49
3:J:917:VAL:O	3:J:921:GLN:HG3	2.12	0.49
5:L:144:LEU:HG	5:L:221:PHE:HE1	1.77	0.49
5:L:287:ILE:CD1	5:L:344:LEU:HD22	2.42	0.49
2:C:98:VAL:HB	2:C:124:MET:HE2	1.95	0.49
2:C:520:PRO:HB3	2:C:714:VAL:HG21	1.95	0.49
2:C:733:VAL:HG11	2:C:966:ILE:HG21	1.93	0.49
2:C:691:PRO:HB3	2:C:788:SER:OG	2.13	0.49
2:C:854:ILE:HD11	2:C:885:GLY:HA3	1.94	0.49
3:D:1371:ARG:HB3	3:D:1371:ARG:CZ	2.43	0.49
3:D:518:VAL:HG13	3:D:519:ASN:N	2.26	0.49
3:D:824:PRO:HB2	3:D:826:ILE:HG23	1.94	0.49
5:F:583:THR:HG22	5:F:584:ARG:H	1.76	0.49
3:J:113:HIS:HD1	3:J:115:TRP:H	1.60	0.49
3:J:1344:LEU:HD12	3:J:1344:LEU:N	2.27	0.49
3:J:420:PRO:O	3:J:471:PRO:HD2	2.12	0.49
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.33	0.49
5:L:348:GLU:HG2	5:L:354:THR:HA	1.95	0.49
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.95	0.49
1:A:61:ILE:HD12	1:A:64:VAL:HG21	1.95	0.49
1:B:51:MET:HG3	1:B:52:PRO:CD	2.41	0.49
2:C:215:TYR:CE1	2:C:223:LEU:HD11	2.48	0.49
2:C:886:LYS:HE3	2:C:916:SER:HB3	1.95	0.49
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	1.93	0.49
5:F:420:GLU:OE1	5:F:423:ARG:NH2	2.45	0.49
2:I:1043:ALA:HB3	2:I:1046:VAL:HG11	1.94	0.49
2:I:1293:VAL:HG11	2:I:1304:MET:CE	2.43	0.49
2:I:192:ASP:CG	2:I:436:ARG:HH21	2.12	0.49
2:I:516:ASP:CG	2:I:522:SER:HG	2.16	0.49
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.47	0.49
3:J:1298:VAL:O	3:J:1298:VAL:HG13	2.13	0.49
1:B:19:VAL:HB	1:B:23:HIS:CD2	2.48	0.49
1:A:185:TYR:CE1	2:C:1087:TYR:OH	2.64	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:836:LEU:HD12	2:C:836:LEU:N	2.27	0.49
2:C:985:GLU:HG2	2:C:988:LYS:HD2	1.95	0.49
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.94	0.49
3:D:842:ARG:HD3	3:D:882:VAL:HG11	1.95	0.49
5:F:96:ASP:O	5:F:96:ASP:CG	2.52	0.49
1:G:172:LEU:HD12	1:G:172:LEU:H	1.77	0.49
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.95	0.49
2:I:1246:ARG:HG2	2:I:1247:SER:N	2.26	0.49
2:I:490:GLN:HG2	2:I:491:ASP:N	2.27	0.49
3:J:1371:ARG:HB3	3:J:1371:ARG:CZ	2.43	0.49
3:J:755:ILE:HD12	3:J:774:ILE:HG21	1.93	0.49
1:B:51:MET:O	1:B:150:ARG:HA	2.13	0.49
2:C:1158:LYS:O	2:C:1159:VAL:CG1	2.55	0.49
2:C:91:THR:HG21	2:C:503:LYS:HZ1	1.77	0.49
3:D:11:GLN:HG3	3:D:12:THR:N	2.28	0.49
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.93	0.49
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.52	0.49
3:D:795:TYR:CE2	3:D:799:ARG:NE	2.81	0.49
3:D:91:GLU:HG3	3:D:91:GLU:O	2.13	0.49
5:F:147:GLN:HB3	5:F:161:LEU:CD2	2.43	0.49
5:F:512:GLY:C	5:F:514:ASP:H	2.16	0.49
1:G:16:ILE:CG2	1:G:26:VAL:HG12	2.42	0.49
1:H:35:PHE:HA	1:H:38:THR:CG2	2.36	0.49
1:G:38:THR:HA	1:H:45:ARG:CD	2.43	0.49
2:I:105:TYR:HA	2:I:113:THR:HA	1.94	0.49
2:I:1294:LYS:HB3	3:J:347:VAL:HG13	1.94	0.49
2:I:488:MET:O	2:I:490:GLN:N	2.43	0.49
2:I:91:THR:CA	2:I:138:ILE:O	2.61	0.49
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.94	0.49
1:A:165:GLU:C	1:A:167:PRO:HD2	2.33	0.48
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.94	0.48
2:C:1264:GLN:HG2	2:C:1264:GLN:O	2.12	0.48
2:C:510:GLN:CA	6:C:2001:KNG:C49	2.83	0.48
3:D:1143:ASP:OD1	3:D:1148:ARG:NH1	2.45	0.48
5:F:568:ASN:O	5:F:569:THR:HG22	2.12	0.48
1:H:125:LYS:HE2	1:H:128:HIS:HB2	1.94	0.48
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.52	0.48
3:J:1263:LYS:NZ	3:J:1315:ALA:CB	2.76	0.48
3:J:885:VAL:HG12	3:J:894:VAL:CG1	2.43	0.48
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.95	0.48
5:L:341:LEU:O	5:L:344:LEU:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:560:ARG:O	5:L:567:MET:HE2	2.13	0.48
2:C:1131:MET:HE2	2:C:1141:LEU:CA	2.37	0.48
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.95	0.48
2:C:737:ASN:HB3	2:C:739:ASP:OD1	2.13	0.48
3:D:899:TYR:CE2	3:D:1251:LYS:HD2	2.48	0.48
3:D:622:ASP:HB3	3:D:626:TYR:CE2	2.41	0.48
5:F:494:ILE:O	5:F:498:LEU:HB3	2.13	0.48
2:I:975:ILE:HG23	2:I:1011:LEU:CD2	2.43	0.48
3:J:288:PRO:HD2	3:J:291:ILE:HD12	1.94	0.48
3:J:831:VAL:O	3:J:831:VAL:HG13	2.13	0.48
5:L:533:ASP:O	5:L:536:THR:N	2.46	0.48
1:A:14:VAL:HG22	1:A:15:ASP:N	2.21	0.48
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.41	0.48
2:C:548:ARG:HB3	2:C:569:ILE:O	2.12	0.48
2:C:650:VAL:HG23	2:C:650:VAL:O	2.13	0.48
2:C:4:SER:HB2	2:C:7:GLU:HG3	1.95	0.48
3:D:518:VAL:H	3:D:716:GLN:HE22	1.60	0.48
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.95	0.48
5:F:362:ASN:O	5:F:365:MET:HB3	2.13	0.48
3:D:291:ILE:CD1	5:F:409:ASN:HB3	2.43	0.48
2:I:886:LYS:NZ	2:I:916:SER:HB3	2.28	0.48
3:J:352:ARG:O	3:J:353:SER:HB3	2.14	0.48
3:J:839:VAL:HG12	3:J:839:VAL:O	2.12	0.48
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.94	0.48
5:L:147:GLN:HB3	5:L:161:LEU:HD13	1.95	0.48
1:A:172:LEU:HD12	1:A:172:LEU:H	1.78	0.48
1:B:144:ILE:HG23	1:B:144:ILE:O	2.12	0.48
2:C:1066:MET:CE	2:C:1076:ILE:CB	2.86	0.48
2:C:1148:ALA:HB1	2:C:1180:MET:CE	2.42	0.48
2:C:62:TYR:C	2:C:64:GLY:H	2.16	0.48
5:F:277:MET:CE	5:F:281:ARG:HH21	2.26	0.48
1:G:71:LYS:NZ	1:G:140:ILE:HG22	2.28	0.48
2:I:1172:LEU:O	2:I:1172:LEU:HD22	2.14	0.48
2:I:141:THR:O	2:I:143:ARG:HG3	2.13	0.48
2:I:119:GLU:HG2	2:I:489:PRO:HD2	1.96	0.48
2:I:737:ASN:HB3	2:I:739:ASP:OD1	2.13	0.48
3:J:1237:VAL:CG1	3:J:1253:ILE:HD13	2.43	0.48
3:J:507:VAL:HG21	3:J:598:LYS:HB2	1.94	0.48
5:L:468:ARG:O	5:L:471:LEU:HB2	2.13	0.48
5:L:544:THR:HG22	5:L:607:LEU:CD2	2.44	0.48
1:B:205:MET:CG	1:B:206:GLU:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1327:LEU:HD23	2:C:1331:ARG:HH21	1.78	0.48
2:C:180:ARG:NH1	2:C:465:ARG:HH12	2.12	0.48
2:C:805:MET:O	2:C:805:MET:HG3	2.13	0.48
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.96	0.48
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.96	0.48
5:F:162:ILE:HD13	5:F:221:PHE:HE2	1.78	0.48
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.95	0.48
5:F:312:SER:O	5:F:315:TRP:NE1	2.47	0.48
1:G:197:ASP:O	1:G:198:LEU:HD23	2.13	0.48
1:H:124:VAL:HG11	1:H:210:THR:HG23	1.96	0.48
2:I:1080:ASN:CB	2:I:1085:MET:HE3	2.44	0.48
2:I:1142:ARG:HD3	2:I:1161:LEU:HD11	1.90	0.48
2:I:106:GLU:HA	2:I:114:VAL:CG2	2.43	0.48
2:I:478:ARG:CZ	2:I:487:LEU:HD13	2.43	0.48
2:I:998:LEU:HD12	2:I:998:LEU:H	1.79	0.48
3:J:400:MET:HE2	3:J:405:GLU:OE1	2.14	0.48
3:J:355:ILE:HG22	3:J:447:ILE:HB	1.96	0.48
5:L:513:ASP:C	5:L:515:GLU:H	2.16	0.48
1:A:57:THR:CG2	1:A:158:ARG:NH2	2.76	0.48
2:C:241:LEU:CD2	2:C:246:LEU:HD11	2.36	0.48
2:C:911:SER:OG	2:C:913:VAL:HG12	2.13	0.48
3:D:1141:VAL:HG13	3:D:1237:VAL:HG23	1.96	0.48
2:C:1271:GLY:HA3	3:D:343:LEU:HD11	1.87	0.48
3:D:854:ALA:CB	3:J:1372:ARG:HE	2.26	0.48
5:F:163:THR:HG22	5:F:163:THR:O	2.13	0.48
5:F:400:GLN:HB2	5:F:403:ASP:OD2	2.13	0.48
2:I:101:ARG:NE	2:I:118:LYS:HD2	2.28	0.48
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.77	0.48
2:I:470:ARG:CZ	2:I:497:PRO:HA	2.44	0.48
2:I:720:ARG:NH2	2:I:736:VAL:HG21	2.28	0.48
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.47	0.48
3:J:510:LEU:O	3:J:514:THR:HG23	2.14	0.48
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.39	0.48
2:C:1149:TYR:HD1	2:C:1159:VAL:CG1	2.25	0.48
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.62	0.48
2:C:566:GLY:O	2:C:569:ILE:HG13	2.13	0.48
2:C:594:VAL:HG22	2:C:599:VAL:HA	1.95	0.48
2:C:614:TYR:CE1	2:C:652:TYR:CE1	3.01	0.48
2:C:74:ARG:C	2:C:75:LEU:HD22	2.33	0.48
3:D:1169:THR:CG2	3:D:1192:LYS:HD3	2.43	0.48
3:D:214:ARG:HA	3:D:217:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:412:LEU:O	3:D:415:VAL:HG22	2.13	0.48
3:D:514:THR:HG23	3:D:596:LEU:HB2	1.95	0.48
3:D:750:PRO:HA	3:D:777:HIS:NE2	2.28	0.48
2:C:672:GLU:HB3	3:D:767:LEU:O	2.13	0.48
3:D:77:ARG:NH1	3:D:78:LEU:HG	2.29	0.48
5:F:298:PRO:HD2	5:F:326:TRP:CB	2.43	0.48
1:G:71:LYS:HB3	1:G:74:VAL:CG1	2.44	0.48
1:G:75:GLN:HA	2:I:729:ALA:N	2.28	0.48
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.96	0.48
3:J:930:LEU:HD12	3:J:1138:LEU:HD13	1.94	0.48
3:J:1175:LEU:O	3:J:1187:GLU:HA	2.13	0.48
3:J:1184:ASP:OD2	3:J:1185:PRO:N	2.47	0.48
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.79	0.48
3:J:336:GLY:HA3	3:J:1324:SER:O	2.14	0.48
3:J:481:ARG:O	3:J:485:MET:HB2	2.13	0.48
1:A:207:THR:HG22	1:A:209:GLY:H	1.78	0.48
2:C:1165:SER:HA	2:C:1169:VAL:CG2	2.44	0.48
2:C:1262:LYS:HA	2:C:1262:LYS:HD3	1.62	0.48
2:C:757:THR:HG22	2:C:765:ILE:O	2.13	0.48
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.77	0.48
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.47	0.48
3:D:858:VAL:HG22	3:D:858:VAL:O	2.13	0.48
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.96	0.48
1:H:142:MET:HG3	1:H:144:ILE:CG1	2.41	0.48
1:H:76:GLU:HB3	1:H:81:ILE:HG13	1.95	0.48
2:I:1112:ILE:HD11	3:J:639:VAL:HG13	1.96	0.48
2:I:582:ASN:HB3	2:I:586:PHE:N	2.29	0.48
2:I:697:LYS:HD2	2:I:1181:PRO:HG3	1.96	0.48
2:I:896:THR:OG1	2:I:899:GLU:HG3	2.14	0.48
3:J:1167:LYS:HB2	3:J:1174:ARG:HD3	1.95	0.48
3:J:186:GLN:HG3	3:J:238:ILE:CB	2.30	0.48
1:A:82:LEU:HD11	1:A:171:LEU:HG	1.96	0.48
2:C:1149:TYR:CB	2:C:1159:VAL:HG11	2.44	0.48
3:D:905:ARG:NH2	3:D:907:HIS:HB2	2.17	0.48
1:G:13:LEU:HD23	1:H:230:ALA:HB1	1.96	0.48
1:G:163:GLU:O	1:G:164:ASP:HB3	2.14	0.48
1:G:38:THR:CB	1:H:45:ARG:HD3	2.43	0.48
2:I:981:ALA:O	2:I:1002:LEU:HD11	2.13	0.48
2:I:979:LEU:HD12	2:I:1011:LEU:HD11	1.95	0.48
2:I:1134:GLN:O	2:I:1135:GLN:HG2	2.14	0.48
2:I:1151:LEU:CD1	2:I:1198:LEU:HD23	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:292:ILE:HD12	2:I:322:LEU:HD11	1.96	0.48
2:I:43:PRO:O	2:I:44:GLU:HB3	2.13	0.48
2:I:38:PHE:HE1	2:I:461:GLU:HA	1.79	0.48
2:I:815:SER:OG	3:J:357:VAL:HG22	2.14	0.48
5:L:290:LEU:CD1	5:L:337:VAL:HG22	2.43	0.48
5:L:444:ALA:HB1	5:L:457:ILE:CD1	2.44	0.48
5:L:583:THR:HG22	5:L:584:ARG:H	1.78	0.48
1:A:13:LEU:H	1:A:13:LEU:CD2	2.06	0.48
1:A:27:THR:HA	1:A:201:LEU:O	2.13	0.48
1:B:14:VAL:O	1:B:16:ILE:HG13	2.14	0.48
2:C:1304:MET:HE2	3:D:472:LEU:CD1	2.44	0.48
2:C:243:PRO:CB	2:C:278:GLU:HG3	2.41	0.48
2:C:397:LEU:HD12	2:C:397:LEU:H	1.77	0.48
2:C:494:ASN:HB3	2:C:497:PRO:HD2	1.96	0.48
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.60	0.48
2:C:883:LEU:HA	2:C:883:LEU:HD23	1.57	0.48
3:D:113:HIS:HE1	3:D:115:TRP:HB2	1.69	0.48
5:F:513:ASP:OD2	5:F:515:GLU:OE1	2.32	0.48
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.96	0.48
3:J:518:VAL:N	3:J:716:GLN:HE22	2.12	0.48
3:J:615:LYS:NZ	4:K:7:GLN:CG	2.77	0.48
1:A:54:CYS:HB3	1:A:148:ARG:HG3	1.96	0.47
1:B:198:LEU:HD13	1:B:198:LEU:HA	1.56	0.47
2:C:91:THR:CB	2:C:138:ILE:O	2.62	0.47
2:C:159:SER:O	2:C:160:ASP:HB2	2.13	0.47
2:C:393:ASP:OD1	2:C:394:ARG:HD3	2.13	0.47
2:C:852:ALA:HB2	2:C:869:GLY:HA2	1.96	0.47
3:D:147:ILE:HG22	3:D:188:LEU:CG	2.43	0.47
3:D:197:GLU:O	3:D:201:LEU:HG	2.14	0.47
1:G:165:GLU:HG3	1:G:165:GLU:O	2.12	0.47
1:H:55:ALA:CB	1:H:176:CYS:H	2.27	0.47
2:I:179:TYR:OH	2:I:458:GLU:OE2	2.20	0.47
2:I:756:TYR:HD1	2:I:756:TYR:H	1.62	0.47
3:J:1165:PHE:CE1	3:J:1200:GLU:HB3	2.45	0.47
3:J:1314:LEU:HD11	3:J:1330:ARG:HH22	1.79	0.47
3:J:1343:GLU:C	3:J:1344:LEU:HD12	2.34	0.47
3:J:1356:LEU:HA	3:J:1356:LEU:HD23	1.72	0.47
5:L:315:TRP:O	5:L:319:ALA:HB3	2.14	0.47
5:L:297:MET:HA	5:L:326:TRP:HB3	1.95	0.47
5:L:101:TYR:CE2	5:L:405:ILE:HD12	2.49	0.47
5:L:397:ARG:HB3	5:L:443:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:513:ASP:OD2	5:L:515:GLU:HB2	2.13	0.47
5:L:96:ASP:O	5:L:98:VAL:HG13	2.14	0.47
1:B:89:ALA:CB	1:B:124:VAL:CG1	2.90	0.47
2:C:17:LYS:NZ	2:C:1154:ASP:HB2	2.29	0.47
2:C:374:GLU:HG3	2:C:374:GLU:O	2.13	0.47
2:C:818:VAL:HG23	2:C:1076:ILE:CD1	2.38	0.47
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.95	0.47
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.96	0.47
5:F:388:ILE:O	5:F:392:LYS:HG3	2.13	0.47
3:D:394:ILE:HG13	5:F:536:THR:HG22	1.96	0.47
2:I:1299:ASN:ND2	2:I:1303:LYS:HE2	2.29	0.47
2:I:14:ASP:OD2	2:I:1156:ARG:NE	2.46	0.47
2:I:60:GLN:HB3	2:I:67:GLU:HG3	1.96	0.47
3:J:1174:ARG:NH2	3:J:1187:GLU:OE2	2.47	0.47
3:J:148:GLU:H	3:J:156:ARG:HG3	1.78	0.47
4:K:38:LEU:HD23	4:K:58:LEU:HD13	1.96	0.47
1:A:43:LEU:CD1	1:A:203:ILE:HD11	2.44	0.47
1:B:195:ARG:HB2	1:B:198:LEU:CD2	2.45	0.47
1:B:29:GLU:HG2	1:B:30:PRO:HG3	1.96	0.47
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.33	0.47
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.95	0.47
2:C:6:THR:HG21	2:C:782:VAL:HG23	1.94	0.47
3:D:1372:ARG:HA	3:J:853:THR:HB	1.96	0.47
3:D:654:ILE:O	3:D:658:GLU:HB2	2.14	0.47
1:H:16:ILE:HG23	1:H:26:VAL:HG13	1.96	0.47
1:H:22:THR:O	1:H:207:THR:OG1	2.31	0.47
2:I:1066:MET:CE	2:I:1076:ILE:HB	2.44	0.47
2:I:765:ILE:HG13	2:I:787:PRO:HG3	1.96	0.47
3:J:290:ILE:N	3:J:290:ILE:HD12	2.22	0.47
3:J:572:THR:HG21	3:J:589:TYR:OH	2.14	0.47
3:J:693:VAL:HG21	3:J:743:MET:CE	2.45	0.47
1:A:40:GLY:HA3	1:A:185:TYR:CD2	2.49	0.47
1:B:31:LEU:O	1:B:198:LEU:HD12	2.14	0.47
2:C:23:ASP:N	2:C:23:ASP:OD1	2.44	0.47
2:C:530:ILE:HD12	2:C:530:ILE:HG23	1.59	0.47
2:C:564:PRO:HG2	2:C:568:ASN:O	2.14	0.47
2:C:738:GLU:HG2	2:C:741:MET:CE	2.44	0.47
2:C:882:ILE:HD12	2:C:882:ILE:N	2.29	0.47
3:D:22:ILE:HG23	3:D:1336:ALA:HA	1.95	0.47
3:D:490:ILE:O	3:D:490:ILE:HG13	2.14	0.47
5:F:280:VAL:HG13	5:F:355:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:291:ILE:HG12	5:F:409:ASN:HD22	1.79	0.47
5:F:540:LEU:HB2	5:F:610:PHE:CE1	2.49	0.47
2:I:828:PHE:HB3	2:I:1060:ILE:HD12	1.96	0.47
2:I:218:GLU:OE1	2:I:299:LYS:HE2	2.14	0.47
2:I:582:ASN:HB3	2:I:586:PHE:H	1.78	0.47
2:I:671:LEU:HD23	2:I:1186:VAL:HG12	1.97	0.47
2:I:705:GLU:HB2	2:I:794:LEU:H	1.80	0.47
3:J:1145:PHE:HB3	3:J:1309:ILE:HG23	1.95	0.47
3:J:502:PRO:HB3	3:J:506:VAL:CG1	2.44	0.47
3:J:608:CYS:HG	3:J:620:PHE:HD2	1.62	0.47
3:J:615:LYS:NZ	4:K:7:GLN:HG2	2.29	0.47
3:J:438:GLU:OE1	4:K:2:ALA:CB	2.62	0.47
1:A:59:VAL:HG21	1:A:85:LEU:HD12	1.97	0.47
1:B:210:THR:O	1:B:211:ILE:CD1	2.63	0.47
1:B:89:ALA:O	1:B:124:VAL:HG12	2.14	0.47
2:C:22:LEU:HD22	2:C:22:LEU:HA	1.61	0.47
2:C:894:GLN:O	2:C:894:GLN:HG3	2.14	0.47
1:B:152:TYR:HE2	3:D:536:LEU:HD21	1.75	0.47
3:D:684:ASP:O	3:D:687:ALA:HB3	2.15	0.47
3:D:705:THR:OG1	3:D:718:SER:HA	2.14	0.47
3:D:92:VAL:CG2	3:D:92:VAL:O	2.63	0.47
5:F:394:TYR:OH	5:F:436:ARG:HG3	2.13	0.47
5:F:562:ARG:HE	5:F:573:LEU:HB3	1.80	0.47
1:G:194:GLN:O	1:G:195:ARG:HB2	2.13	0.47
2:I:104:ILE:O	2:I:114:VAL:N	2.45	0.47
2:I:146:VAL:HG11	2:I:531:LEU:CD1	2.45	0.47
2:I:692:THR:OG1	2:I:693:LEU:N	2.47	0.47
3:J:267:ASP:HA	3:J:270:ARG:HH21	1.80	0.47
3:J:510:LEU:HA	3:J:513:MET:HE2	1.96	0.47
3:J:517:CYS:C	3:J:716:GLN:HE22	2.16	0.47
3:J:552:ILE:HG12	3:J:570:LYS:HG3	1.96	0.47
4:K:29:GLN:CD	4:K:35:LYS:HE2	2.34	0.47
5:L:124:GLU:O	5:L:127:ILE:HG13	2.13	0.47
1:A:76:GLU:HB3	1:A:81:ILE:HG12	1.97	0.47
2:C:104:ILE:O	2:C:113:THR:HA	2.14	0.47
2:C:1151:LEU:HD23	2:C:1197:GLU:OE2	2.14	0.47
3:D:1184:ASP:O	3:D:1186:TYR:N	2.48	0.47
3:D:35:PHE:HD1	3:D:101:ARG:CB	2.23	0.47
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.96	0.47
1:G:85:LEU:HD22	1:G:144:ILE:HD13	1.95	0.47
1:G:56:VAL:HG11	1:G:86:LYS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1291:GLU:HB3	3:J:1292:LEU:HD12	1.97	0.47
3:J:201:LEU:HD11	3:J:220:ARG:NH1	2.30	0.47
3:J:218:THR:HA	3:J:221:ILE:HG22	1.97	0.47
3:J:48:THR:HB	3:J:50:LYS:HG3	1.97	0.47
3:J:746:LEU:CD2	3:J:758:PRO:HG3	2.45	0.47
5:L:390:ILE:HD12	5:L:435:ILE:CG2	2.44	0.47
1:B:192:VAL:CG1	1:B:193:GLU:N	2.77	0.47
1:A:150:ARG:CD	1:B:8:PHE:CE2	2.98	0.47
2:C:1191:LYS:HD3	2:C:1193:ALA:N	2.24	0.47
2:C:739:ASP:N	2:C:739:ASP:OD1	2.47	0.47
2:C:741:MET:HG2	2:C:974:ARG:NH2	2.29	0.47
2:C:972:PHE:CD2	2:C:975:ILE:HD12	2.50	0.47
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.97	0.47
3:D:490:ILE:O	3:D:491:LEU:HD23	2.15	0.47
3:D:580:TRP:CZ3	3:D:589:TYR:HA	2.49	0.47
3:D:839:VAL:HG13	3:D:882:VAL:HG21	1.96	0.47
3:D:9:LYS:HE2	3:D:11:GLN:O	2.15	0.47
5:F:481:GLU:O	5:F:485:GLU:OE2	2.32	0.47
1:H:67:GLU:OE2	1:H:171:LEU:N	2.47	0.47
2:I:452:ARG:NH2	2:I:458:GLU:OE1	2.44	0.47
2:I:27:LEU:HD12	2:I:524:ILE:HD11	1.96	0.47
2:I:1272:GLU:CG	3:J:342:LEU:CB	2.92	0.47
3:J:858:VAL:O	3:J:858:VAL:HG22	2.14	0.47
5:L:573:LEU:HG	5:L:574:GLU:OE1	2.14	0.47
2:C:1024:GLU:HA	2:C:1027:LYS:HG2	1.95	0.47
2:C:185:ASP:O	2:C:196:VAL:HA	2.14	0.47
2:C:22:LEU:HD13	2:C:23:ASP:N	2.29	0.47
2:C:230:PHE:O	2:C:332:ARG:HA	2.15	0.47
2:C:697:LYS:CA	2:C:795:ALA:HB2	2.36	0.47
3:D:1250:ASP:O	3:D:1251:LYS:C	2.51	0.47
2:C:1279:GLU:HG2	3:D:1357:ILE:HD13	1.97	0.47
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.48	0.47
3:D:795:TYR:HE2	3:D:799:ARG:NE	2.12	0.47
3:D:861:ASN:OD1	3:D:861:ASN:O	2.33	0.47
1:G:61:ILE:HG22	1:G:62:ASP:H	1.79	0.47
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.15	0.47
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.97	0.47
3:J:1350:ASN:OD1	3:J:1355:ARG:HD2	2.14	0.47
3:J:479:GLU:HG3	4:K:20:VAL:CG1	2.37	0.47
5:L:511:ILE:HG23	5:L:511:ILE:O	2.14	0.47
1:A:165:GLU:HG3	1:A:165:GLU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:VAL:HG21	1:A:144:ILE:HG23	1.97	0.47
1:B:92:VAL:HA	1:B:120:ASP:O	2.15	0.47
2:C:842:ASP:HB2	2:C:1045:GLY:O	2.14	0.47
2:C:848:GLU:HG2	2:C:888:THR:HB	1.97	0.47
2:C:854:ILE:HD11	2:C:885:GLY:CA	2.45	0.47
2:C:896:THR:HG23	2:C:899:GLU:OE2	2.14	0.47
1:G:14:VAL:HG22	1:G:15:ASP:N	2.23	0.47
2:I:1196:LYS:O	2:I:1199:LEU:HB2	2.14	0.47
2:I:894:GLN:HG3	2:I:894:GLN:O	2.14	0.47
3:J:1146:GLU:HG2	3:J:1148:ARG:NH2	2.30	0.47
3:J:1263:LYS:CE	3:J:1279:GLN:NE2	2.78	0.47
3:J:418:GLU:OE1	4:K:2:ALA:HA	2.15	0.47
5:L:490:PRO:HG2	5:L:493:LYS:HE3	1.97	0.47
1:A:61:ILE:CD1	1:A:64:VAL:HG21	2.45	0.47
2:C:810:TYR:HD1	2:C:1078:LYS:HB2	1.78	0.47
2:C:1268:GLN:HE22	3:D:352:ARG:NH1	2.13	0.47
2:C:302:ILE:HG22	2:C:308:GLU:C	2.35	0.47
2:C:360:LEU:O	2:C:364:VAL:HG23	2.15	0.47
2:C:518:ASN:ND2	2:C:761:GLN:HG2	2.30	0.47
2:C:796:LEU:HB2	2:C:1233:LEU:CD1	2.45	0.47
3:D:139:LEU:HA	3:D:139:LEU:HD23	1.58	0.47
4:E:16:ARG:HG2	4:E:16:ARG:O	2.14	0.47
1:G:177:TYR:O	1:G:178:SER:HB2	2.15	0.47
1:H:66:HIS:HB3	1:H:68:TYR:CE2	2.49	0.47
2:I:1043:ALA:O	2:I:1046:VAL:CG1	2.63	0.47
1:G:67:GLU:OE1	2:I:1057:LYS:NZ	2.48	0.47
2:I:1337:ILE:O	2:I:1337:ILE:HG23	2.14	0.47
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.95	0.47
3:J:800:LEU:CD1	3:J:1309:ILE:CD1	2.93	0.47
3:J:303:VAL:O	3:J:307:LEU:HG	2.14	0.47
5:L:111:LEU:HD23	5:L:111:LEU:HA	1.48	0.47
2:C:103:VAL:HB	2:C:113:THR:HG21	1.97	0.47
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.79	0.47
3:D:440:VAL:O	3:D:442:ILE:HG12	2.15	0.47
3:D:45:ASN:O	3:D:46:TYR:CB	2.61	0.47
3:D:598:LYS:O	3:D:601:ILE:HG22	2.15	0.47
3:D:686:TRP:CE3	3:D:758:PRO:HG2	2.49	0.47
3:D:857:LEU:CD2	3:D:875:ASN:ND2	2.71	0.47
5:F:423:ARG:CD	5:F:425:TYR:CE2	2.98	0.47
1:G:110:VAL:O	1:G:130:ILE:HB	2.14	0.47
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:724:VAL:HG11	2:I:727:VAL:CG2	2.39	0.47
3:J:755:ILE:HG22	3:J:757:THR:H	1.80	0.47
1:A:59:VAL:CG2	1:A:85:LEU:HD13	2.44	0.46
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.80	0.46
2:C:1184:THR:HG23	2:C:1189:GLY:CA	2.45	0.46
2:C:1246:ARG:NH2	2:C:1249:GLY:H	2.13	0.46
3:D:1290:ARG:HA	3:D:1294:ALA:HB3	1.95	0.46
3:D:333:GLY:CA	3:D:338:PHE:CZ	2.98	0.46
5:F:244:THR:O	5:F:247:GLU:HG2	2.15	0.46
1:H:151:GLY:O	1:H:177:TYR:HB2	2.15	0.46
1:H:6:THR:O	1:H:6:THR:CG2	2.61	0.46
2:I:53:PHE:O	2:I:57:PHE:HB2	2.16	0.46
3:J:218:THR:HA	3:J:221:ILE:CG2	2.45	0.46
3:J:45:ASN:O	3:J:46:TYR:CD2	2.68	0.46
1:A:112:ALA:O	1:A:115:ILE:HG13	2.16	0.46
1:B:89:ALA:HB3	1:B:124:VAL:HG11	1.94	0.46
2:C:316:GLU:H	2:C:316:GLU:CD	2.19	0.46
3:D:1290:ARG:HA	3:D:1294:ALA:CB	2.45	0.46
5:F:470:MET:HE1	5:F:482:GLU:HG2	1.97	0.46
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.79	0.46
2:I:870:ILE:HG12	2:I:1050:VAL:HG11	1.95	0.46
2:I:1293:VAL:HG11	2:I:1304:MET:HE2	1.97	0.46
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.97	0.46
2:I:745:GLU:HG3	2:I:1017:GLN:CB	2.42	0.46
2:I:855:PRO:HG3	2:I:913:VAL:HG13	1.96	0.46
3:J:1203:ARG:NH1	3:J:1205:GLU:HG2	2.30	0.46
3:J:1280:VAL:CB	3:J:1304:ARG:HE	2.28	0.46
3:J:1307:LEU:HB3	3:J:1312:ALA:HB2	1.96	0.46
3:J:201:LEU:HD11	3:J:220:ARG:HH11	1.79	0.46
3:J:709:ARG:C	3:J:711:GLY:N	2.69	0.46
3:J:820:ILE:HD11	3:J:822:MET:CE	2.45	0.46
3:J:847:ASP:N	3:J:847:ASP:OD1	2.26	0.46
5:L:482:GLU:HA	5:L:485:GLU:OE2	2.15	0.46
5:L:601:PRO:HB2	5:L:605:GLU:HG2	1.97	0.46
1:A:233:ASP:CA	1:A:234:LEU:HD22	2.45	0.46
1:B:6:THR:N	1:B:7:GLU:OE2	2.48	0.46
1:A:50:SER:HB2	1:B:8:PHE:CZ	2.44	0.46
2:C:632:ASP:O	2:C:647:ARG:HB2	2.15	0.46
2:C:882:ILE:HG13	2:C:919:ARG:NH1	2.30	0.46
3:D:1319:PHE:HB3	3:D:1340:LYS:HD2	1.97	0.46
3:D:537:TYR:CZ	3:D:544:LEU:HD22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:CYS:SG	3:D:60:ARG:HB3	2.55	0.46
3:D:857:LEU:CD1	3:D:858:VAL:HG13	2.45	0.46
4:E:54:ILE:HD13	4:E:59:ILE:O	2.16	0.46
5:F:292:VAL:HA	5:F:297:MET:O	2.16	0.46
5:F:297:MET:HE3	5:F:330:LEU:HD11	1.96	0.46
1:H:100:LEU:HB3	1:H:115:ILE:CG2	2.45	0.46
1:G:38:THR:CA	1:H:45:ARG:HD3	2.44	0.46
2:I:106:GLU:HA	2:I:114:VAL:HG22	1.97	0.46
2:I:159:SER:O	2:I:160:ASP:HB2	2.15	0.46
3:J:1264:ALA:CB	3:J:1304:ARG:HA	2.44	0.46
3:J:681:LYS:O	3:J:685:ILE:HG23	2.16	0.46
3:J:518:VAL:HG12	3:J:707:ILE:HD13	1.97	0.46
5:L:137:TYR:CD2	5:L:273:MET:HG2	2.50	0.46
1:A:85:LEU:HD22	1:A:144:ILE:HD13	1.97	0.46
1:A:71:LYS:HB3	1:A:74:VAL:CG1	2.45	0.46
2:C:1151:LEU:HD23	2:C:1151:LEU:HA	1.71	0.46
2:C:1327:LEU:O	2:C:1331:ARG:HB2	2.15	0.46
2:C:883:LEU:CD1	2:C:920:VAL:HG22	2.41	0.46
3:D:902:ASP:OD1	3:D:903:LEU:N	2.48	0.46
5:F:584:ARG:HA	5:F:584:ARG:NH1	2.31	0.46
2:I:109:ALA:CB	2:I:111:GLU:HA	2.44	0.46
2:I:251:ALA:CA	2:I:269:ILE:HD11	2.45	0.46
2:I:238:GLN:OE1	2:I:284:LEU:HD21	2.16	0.46
3:J:1237:VAL:HG11	3:J:1253:ILE:HD13	1.96	0.46
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.97	0.46
3:J:816:THR:HB	3:J:889:ASP:HB2	1.98	0.46
3:J:843:VAL:HG23	3:J:862:THR:C	2.35	0.46
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.97	0.46
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.48	0.46
2:C:466:VAL:O	2:C:470:ARG:HG2	2.15	0.46
2:C:591:TYR:CD2	2:C:606:LEU:HD13	2.40	0.46
2:C:719:LYS:O	2:C:779:ARG:HG3	2.15	0.46
2:C:800:MET:HE1	2:C:822:VAL:HG21	1.96	0.46
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.98	0.46
3:D:142:GLU:HG3	5:F:100:MET:HE1	1.98	0.46
5:F:567:MET:HB2	5:F:567:MET:HE3	1.73	0.46
1:G:179:PRO:CG	1:G:211:ILE:HG13	2.45	0.46
2:I:253:PHE:CD1	2:I:288:PRO:HD3	2.50	0.46
2:I:56:VAL:HG11	2:I:468:LEU:CD1	2.41	0.46
3:J:34:SER:HB2	3:J:104:HIS:HB3	1.98	0.46
3:J:930:LEU:HB2	3:J:1138:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1145:PHE:CE1	3:J:1256:ILE:HG21	2.51	0.46
3:J:514:THR:HG21	3:J:596:LEU:CG	2.46	0.46
3:J:664:ILE:HG21	3:J:681:LYS:HB3	1.97	0.46
3:D:1372:ARG:HH21	3:J:854:ALA:CB	2.27	0.46
4:K:50:ALA:O	4:K:54:ILE:HG12	2.16	0.46
5:L:582:VAL:HG11	5:L:586:ARG:HG2	1.95	0.46
2:I:905:ILE:CD1	5:L:598:LEU:HD13	2.46	0.46
2:C:188:PHE:CZ	2:C:194:LEU:HD13	2.51	0.46
2:C:274:ILE:HG22	2:C:278:GLU:OE1	2.15	0.46
2:C:820:GLU:O	2:C:823:VAL:HG12	2.16	0.46
2:C:972:PHE:HD2	2:C:975:ILE:HD12	1.79	0.46
3:D:1167:LYS:CD	3:D:1174:ARG:HD2	2.42	0.46
2:C:1341:ASP:HB3	3:D:18:ASP:OD2	2.16	0.46
4:E:49:ILE:O	4:E:53:GLU:HG3	2.16	0.46
5:F:479:THR:HG23	5:F:481:GLU:H	1.79	0.46
1:G:166:ARG:O	1:G:167:PRO:C	2.54	0.46
1:G:27:THR:C	1:G:28:LEU:HD12	2.36	0.46
2:I:1149:TYR:CB	2:I:1159:VAL:HG11	2.46	0.46
2:I:237:LEU:HD11	2:I:292:ILE:CD1	2.45	0.46
2:I:30:ILE:CD1	2:I:30:ILE:H	2.13	0.46
2:I:455:SER:O	2:I:456:VAL:C	2.54	0.46
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.30	0.46
3:J:1341:ARG:NH1	3:J:1343:GLU:OE2	2.47	0.46
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.98	0.46
5:L:322:MET:SD	5:L:326:TRP:HH2	2.39	0.46
1:B:116:THR:O	1:B:116:THR:HG23	2.16	0.46
1:B:86:LYS:HD3	1:B:174:ASP:OD2	2.16	0.46
2:C:109:ALA:HB1	2:C:110:PRO:O	2.13	0.46
2:C:192:ASP:CG	2:C:436:ARG:HH21	2.19	0.46
3:D:16:GLU:HB3	3:D:1369:ARG:NH2	2.30	0.46
3:D:100:GLU:O	3:D:246:PRO:HG3	2.15	0.46
3:D:56:LEU:CD2	3:D:269:TYR:HB3	2.46	0.46
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.96	0.46
1:G:172:LEU:HD12	1:G:172:LEU:N	2.31	0.46
1:H:99:ILE:O	1:H:99:ILE:HG23	2.15	0.46
2:I:151:ARG:CZ	2:I:445:ILE:HD11	2.46	0.46
2:I:577:VAL:HG23	2:I:661:VAL:O	2.15	0.46
1:B:32:GLU:HA	1:B:198:LEU:HD12	1.97	0.46
2:C:494:ASN:HD22	2:C:497:PRO:CD	2.28	0.46
2:C:818:VAL:CB	2:C:1076:ILE:CD1	2.94	0.46
2:C:836:LEU:HD21	2:C:921:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:980:VAL:HG13	2:C:984:VAL:CB	2.46	0.46
3:D:478:LEU:HD12	4:E:24:ALA:HA	1.98	0.46
5:F:568:ASN:O	5:F:569:THR:CG2	2.64	0.46
1:G:156:SER:O	1:G:159:ILE:HG22	2.16	0.46
1:G:179:PRO:O	1:G:207:THR:HG23	2.15	0.46
1:G:223:ILE:HD13	1:H:8:PHE:CZ	2.50	0.46
2:I:1067:ALA:HB1	2:I:1072:ASN:O	2.16	0.46
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.79	0.46
2:I:62:TYR:C	2:I:64:GLY:N	2.70	0.46
2:I:850:ILE:O	2:I:850:ILE:HG22	2.16	0.46
3:J:1359:ALA:HA	3:J:1363:TYR:HB2	1.96	0.46
2:I:806:PRO:O	3:J:633:ALA:HA	2.15	0.46
1:A:145:LYS:HB2	1:A:170:ARG:HH12	1.80	0.46
2:C:1178:LYS:HA	2:C:1178:LYS:HD3	1.75	0.46
2:C:593:LYS:O	2:C:600:THR:HB	2.15	0.46
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.75	0.46
2:C:794:LEU:HD21	2:C:796:LEU:HD21	1.97	0.46
3:D:126:LEU:CD1	3:D:223:LEU:HD23	2.46	0.46
3:D:26:SER:HB2	3:D:236:TRP:CZ2	2.51	0.46
3:D:517:CYS:HA	3:D:716:GLN:NE2	2.31	0.46
3:D:64:PRO:HG3	3:D:90:VAL:CG1	2.46	0.46
5:F:551:LEU:HD11	5:F:598:LEU:HD21	1.98	0.46
2:I:1103:VAL:HG21	3:J:639:VAL:HG11	1.97	0.46
2:I:1119:MET:HG3	2:I:1204:LEU:HD13	1.97	0.46
3:J:1261:LEU:HD12	3:J:1261:LEU:C	2.36	0.46
3:J:741:ALA:O	3:J:762:ASN:ND2	2.49	0.46
1:B:192:VAL:HG12	1:B:193:GLU:N	2.30	0.46
1:B:26:VAL:HG21	1:B:217:ILE:HD12	1.98	0.46
2:C:407:ARG:HH21	2:C:414:ILE:HG22	1.81	0.46
2:C:448:LEU:HD23	2:C:451:ARG:HB2	1.97	0.46
3:D:515:ARG:HH21	3:D:717:VAL:HG23	1.79	0.46
2:C:1101:LEU:CD2	3:D:725:MET:SD	3.03	0.46
3:D:905:ARG:NH2	3:D:907:HIS:ND1	2.63	0.46
5:F:315:TRP:CH2	5:F:341:LEU:HD11	2.51	0.46
5:F:394:TYR:OH	5:F:436:ARG:CG	2.64	0.46
2:I:521:LEU:O	2:I:524:ILE:HG22	2.16	0.46
2:I:6:THR:HG21	2:I:782:VAL:CG2	2.44	0.46
2:I:81:ASP:O	2:I:85:CYS:HB2	2.15	0.46
2:I:88:ARG:HB2	2:I:88:ARG:NH1	2.30	0.46
3:J:1198:VAL:CG1	3:J:1210:ILE:HG23	2.46	0.46
3:J:72:CYS:SG	3:J:73:GLY:N	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:439:ILE:O	5:L:442:SER:HB3	2.16	0.46
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.65	0.45
1:A:232:VAL:O	1:A:233:ASP:HB3	2.16	0.45
2:C:197:ARG:NH2	2:C:203:LYS:HB2	2.31	0.45
3:D:357:VAL:HA	3:D:461:PHE:CE1	2.50	0.45
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.97	0.45
2:I:127:ILE:O	2:I:127:ILE:HG13	2.14	0.45
2:I:356:THR:HG21	2:I:362:ALA:HA	1.97	0.45
2:I:560:PRO:O	3:J:780:ARG:NH2	2.48	0.45
2:I:660:VAL:HG11	3:J:769:VAL:CG1	2.46	0.45
3:J:1234:VAL:HG23	3:J:1235:ASN:N	2.29	0.45
3:J:127:LEU:CD2	3:J:234:PRO:HB3	2.46	0.45
3:J:358:GLY:N	3:J:359:PRO:HD3	2.31	0.45
3:J:357:VAL:HA	3:J:461:PHE:CE1	2.51	0.45
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.97	0.45
1:A:19:VAL:HG11	1:A:23:HIS:CE1	2.50	0.45
1:B:51:MET:HG2	1:B:179:PRO:CD	2.47	0.45
2:C:11:ILE:HG22	2:C:1149:TYR:CZ	2.51	0.45
2:C:593:LYS:HG2	2:C:602:GLU:OE2	2.15	0.45
2:C:677:ASN:O	2:C:681:MET:HG3	2.16	0.45
2:C:818:VAL:CG2	2:C:1076:ILE:CD1	2.85	0.45
2:C:91:THR:HG21	2:C:503:LYS:HZ2	1.80	0.45
2:C:808:ASN:H	3:D:633:ALA:HB2	1.80	0.45
3:D:821:MET:CE	3:D:879:ALA:HB1	2.47	0.45
3:D:930:LEU:HA	3:D:1244:GLN:HG3	1.97	0.45
5:F:483:LEU:HB2	5:F:494:ILE:CD1	2.46	0.45
5:F:499:LYS:HE3	5:F:499:LYS:HB2	1.70	0.45
1:H:76:GLU:CB	1:H:81:ILE:HG12	2.45	0.45
2:I:974:ARG:HD3	2:I:1010:GLN:NE2	2.32	0.45
2:I:1043:ALA:HB3	2:I:1046:VAL:CG1	2.47	0.45
2:I:1120:ALA:HB2	2:I:1199:LEU:HG	1.97	0.45
3:J:95:THR:O	3:J:98:ARG:HB2	2.16	0.45
2:C:101:ARG:HH21	2:C:118:LYS:CE	2.25	0.45
2:C:1298:VAL:HG21	3:D:96:LYS:NZ	2.30	0.45
2:C:1333:LEU:HD21	3:D:327:LEU:CB	2.47	0.45
2:C:750:ILE:HD13	2:C:963:GLU:CD	2.37	0.45
3:D:688:ALA:O	3:D:692:ARG:HG3	2.16	0.45
5:F:322:MET:HE3	5:F:324:LYS:NZ	2.30	0.45
5:F:387:VAL:HG22	5:F:435:ILE:CD1	2.46	0.45
1:G:171:LEU:N	1:G:171:LEU:HD22	2.32	0.45
1:G:218:ARG:HH11	1:H:232:VAL:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:843:VAL:O	3:J:883:ARG:HG3	2.16	0.45
3:J:931:THR:O	3:J:931:THR:HG22	2.16	0.45
5:L:227:GLN:O	5:L:230:VAL:CG1	2.64	0.45
5:L:577:GLY:CA	5:L:583:THR:HG23	2.31	0.45
1:B:205:MET:CE	1:B:213:PRO:CB	2.94	0.45
2:C:1075:VAL:O	2:C:1076:ILE:C	2.54	0.45
2:C:1271:GLY:HA2	3:D:343:LEU:CG	2.46	0.45
2:C:1285:TYR:CD1	3:D:475:GLU:HB3	2.52	0.45
2:C:614:TYR:CE1	2:C:652:TYR:HE1	2.34	0.45
2:C:981:ALA:HB1	2:C:1007:LYS:HZ1	1.81	0.45
3:D:1140:ARG:NH2	3:D:1236:GLU:HG2	2.30	0.45
3:D:112:ALA:HB3	3:D:300:GLN:HE22	1.82	0.45
3:D:664:ILE:HG21	3:D:681:LYS:HB3	1.99	0.45
5:F:399:LEU:CB	5:F:404:LEU:HD21	2.39	0.45
1:H:118:ASP:HB2	1:H:121:VAL:CG2	2.46	0.45
2:I:1103:VAL:HB	2:I:1104:PRO:HD3	1.97	0.45
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.31	0.45
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.81	0.45
2:I:634:VAL:HG13	2:I:636:CYS:SG	2.57	0.45
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.97	0.45
3:J:1252:HIS:CA	3:J:1255:VAL:HG13	2.46	0.45
2:I:815:SER:OG	3:J:461:PHE:CD1	2.70	0.45
2:I:1313:HIS:HD2	3:J:477:GLN:NE2	2.14	0.45
3:J:644:MET:HE3	3:J:764:ARG:HG2	1.98	0.45
3:J:788:LEU:HG	3:J:792:ASN:ND2	2.31	0.45
3:J:804:ALA:HB1	3:J:916:GLY:HA3	1.98	0.45
3:J:850:LYS:HD3	3:J:875:ASN:ND2	2.29	0.45
3:J:908:ILE:HD13	3:J:909:ILE:N	2.32	0.45
4:K:49:ILE:HA	4:K:52:ARG:HD3	1.98	0.45
2:C:852:ALA:HB2	2:C:869:GLY:CA	2.47	0.45
3:D:1203:ARG:HH22	3:D:1205:GLU:CG	2.19	0.45
3:D:1280:VAL:HG21	3:D:1304:ARG:CD	2.45	0.45
3:D:646:ILE:HG12	3:D:646:ILE:H	1.60	0.45
5:F:290:LEU:HD12	5:F:337:VAL:HG22	1.97	0.45
5:F:322:MET:HE3	5:F:324:LYS:HZ1	1.82	0.45
5:F:587:ILE:HG22	5:F:588:ARG:N	2.31	0.45
1:G:14:VAL:CG1	1:G:27:THR:HB	2.46	0.45
1:H:139:SER:O	1:H:140:ILE:HG23	2.16	0.45
1:H:86:LYS:CD	1:H:174:ASP:HB2	2.45	0.45
2:I:617:ALA:HB3	2:I:653:MET:CG	2.43	0.45
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:902:ASP:HB3	3:J:1251:LYS:HE3	1.96	0.45
3:J:114:ILE:HB	3:J:304:ASP:OD1	2.16	0.45
3:J:447:ILE:HG21	3:J:447:ILE:HD13	1.64	0.45
3:J:79:LYS:HB2	5:L:569:THR:H	1.82	0.45
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.97	0.45
2:C:202:ARG:NH2	2:C:368:ARG:HH12	2.14	0.45
2:C:964:LEU:HD12	2:C:964:LEU:HA	1.73	0.45
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	1.98	0.45
3:D:1368:ASP:HA	3:D:1371:ARG:HH22	1.81	0.45
5:F:607:LEU:HD12	5:F:607:LEU:N	2.31	0.45
1:G:67:GLU:H	1:G:67:GLU:HG2	1.41	0.45
1:G:74:VAL:HG22	1:G:76:GLU:H	1.81	0.45
2:I:1236:ASN:HB2	2:I:1238:LEU:HD11	1.99	0.45
2:I:1326:LEU:HA	2:I:1326:LEU:HD12	1.82	0.45
2:I:593:LYS:HE3	2:I:595:THR:HG23	1.94	0.45
2:I:669:PRO:O	2:I:1070:HIS:HE1	1.99	0.45
2:I:996:ARG:HD2	2:I:999:GLU:CD	2.37	0.45
3:J:800:LEU:CD1	3:J:1309:ILE:HD13	2.47	0.45
3:J:45:ASN:O	3:J:46:TYR:CB	2.64	0.45
3:J:364:HIS:CB	4:K:4:VAL:HG23	2.45	0.45
1:A:154:PRO:O	1:A:158:ARG:HG3	2.17	0.45
1:B:37:HIS:HA	1:B:185:TYR:HE1	1.82	0.45
1:B:29:GLU:CG	1:B:30:PRO:HG3	2.46	0.45
2:C:100:LEU:HD12	2:C:122:VAL:CG1	2.47	0.45
2:C:210:LEU:CD1	2:C:224:PHE:HE2	2.30	0.45
2:C:494:ASN:O	2:C:498:ILE:CD1	2.64	0.45
2:C:678:ARG:HG3	2:C:1106:ARG:HB3	1.98	0.45
3:D:1257:VAL:HG22	3:D:1260:MET:HE1	1.97	0.45
3:D:1350:ASN:OD1	3:D:1355:ARG:CD	2.65	0.45
2:C:1269:ARG:CD	3:D:343:LEU:HB3	2.30	0.45
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.67	0.45
3:D:848:VAL:CG2	3:D:858:VAL:CG1	2.88	0.45
5:F:308:GLY:HA2	5:F:356:GLU:OE1	2.17	0.45
5:F:547:VAL:CG2	5:F:603:ARG:HH11	2.30	0.45
5:F:583:THR:HG22	5:F:584:ARG:N	2.31	0.45
5:F:602:SER:OG	5:F:603:ARG:N	2.49	0.45
1:G:195:ARG:HG2	1:G:198:LEU:CG	2.45	0.45
2:I:445:ILE:HG22	2:I:446:ASP:OD1	2.16	0.45
2:I:854:ILE:O	2:I:857:VAL:HG22	2.17	0.45
3:J:242:LEU:HD23	3:J:243:PRO:O	2.16	0.45
3:J:827:GLU:HB3	3:J:832:LYS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.98	0.45
2:C:1149:TYR:CG	2:C:1159:VAL:HG11	2.50	0.45
2:C:796:LEU:HB2	2:C:1233:LEU:HD12	1.99	0.45
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.99	0.45
3:D:641:ILE:HD13	3:D:641:ILE:O	2.17	0.45
5:F:467:SER:O	5:F:471:LEU:HB2	2.17	0.45
2:I:158:ASP:HB3	2:I:173:ASN:OD1	2.17	0.45
2:I:361:SER:O	2:I:364:VAL:HB	2.17	0.45
2:I:10:ARG:NH2	2:I:697:LYS:HD3	2.31	0.45
3:J:109:SER:HB2	3:J:296:LYS:HE2	1.99	0.45
3:J:750:PRO:HA	3:J:777:HIS:NE2	2.32	0.45
2:C:489:PRO:HA	2:C:492:MET:HE3	1.99	0.45
2:C:848:GLU:CD	2:C:888:THR:HG22	2.37	0.45
2:C:5:TYR:CD1	2:C:8:LYS:HD3	2.30	0.45
1:H:22:THR:O	1:H:213:PRO:HG3	2.17	0.45
2:I:565:GLU:HB2	2:I:680:LEU:HD21	1.98	0.45
2:I:57:PHE:CE2	2:I:70:TYR:HB2	2.51	0.45
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.32	0.45
3:J:205:LEU:O	3:J:205:LEU:HD13	2.16	0.45
3:J:351:GLY:O	3:J:352:ARG:HB3	2.15	0.45
3:J:908:ILE:HD13	3:J:908:ILE:HG23	1.77	0.45
5:L:316:PHE:CE2	5:L:334:SER:HA	2.48	0.45
1:A:227:GLN:HB3	1:B:39:LEU:HD11	1.99	0.45
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.99	0.45
1:A:64:VAL:HG11	1:A:78:ILE:HG21	1.99	0.45
1:B:151:GLY:H	1:B:177:TYR:HB2	1.81	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.57	0.45
2:C:233:ARG:NH1	2:C:332:ARG:HH12	2.15	0.45
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.52	0.45
2:C:705:GLU:CD	2:C:705:GLU:H	2.20	0.45
3:D:115:TRP:NE1	3:D:1329:THR:CG2	2.79	0.45
3:D:174:ASP:O	3:D:175:GLU:HG2	2.16	0.45
3:D:514:THR:CG2	3:D:596:LEU:CB	2.94	0.45
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.81	0.45
3:D:825:VAL:HG21	3:D:832:LYS:CB	2.47	0.45
2:I:801:ARG:HG2	2:I:1094:VAL:HG23	1.98	0.45
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.81	0.45
3:J:450:HIS:HE1	3:J:452:LEU:HD12	1.80	0.45
5:L:298:PRO:HD2	5:L:326:TRP:CD1	2.52	0.45
1:A:57:THR:HG22	1:A:158:ARG:HH21	1.80	0.44
2:C:1259:LEU:HA	2:C:1259:LEU:HD12	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	1.98	0.44
2:C:262:TYR:CZ	2:C:282:VAL:HG21	2.51	0.44
2:C:80:PHE:CE2	2:C:88:ARG:HD2	2.53	0.44
3:D:209:ASN:HA	3:D:214:ARG:HE	1.82	0.44
3:D:591:ILE:HG13	3:D:604:MET:HE2	1.98	0.44
3:D:863:LEU:HA	3:D:863:LEU:HD12	1.58	0.44
5:F:227:GLN:O	5:F:230:VAL:HG12	2.17	0.44
1:H:205:MET:SD	1:H:217:ILE:HG12	2.57	0.44
2:I:207:THR:HA	2:I:210:LEU:HD12	1.99	0.44
3:J:1280:VAL:O	3:J:1280:VAL:HG12	2.17	0.44
3:J:141:PHE:CD1	3:J:293:ARG:HD3	2.52	0.44
2:I:1271:GLY:CA	3:J:343:LEU:HD12	2.47	0.44
3:J:518:VAL:O	3:J:547:ARG:NH1	2.50	0.44
3:J:658:GLU:C	3:J:661:VAL:HG13	2.37	0.44
3:J:647:PRO:HG3	3:J:697:MET:N	2.32	0.44
3:J:748:ALA:O	3:J:777:HIS:CD2	2.64	0.44
5:L:562:ARG:HH21	5:L:573:LEU:HB3	1.82	0.44
1:B:205:MET:CE	1:B:213:PRO:CA	2.95	0.44
2:C:1142:ARG:CG	2:C:1161:LEU:HD11	2.47	0.44
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	1.98	0.44
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.60	0.44
2:C:481:LEU:N	2:C:481:LEU:HD22	2.32	0.44
2:C:562:GLU:OE2	2:C:662:SER:OG	2.28	0.44
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.73	0.44
2:C:62:TYR:O	2:C:64:GLY:N	2.50	0.44
3:D:114:ILE:HB	3:D:304:ASP:OD1	2.17	0.44
3:D:140:TYR:CE2	5:F:95:THR:CG2	2.92	0.44
3:D:140:TYR:O	3:D:141:PHE:HB2	2.17	0.44
3:D:74:LYS:HD3	3:D:75:TYR:HE1	1.82	0.44
5:F:277:MET:HE3	5:F:281:ARG:HH21	1.81	0.44
5:F:421:TYR:CE2	5:F:422:ARG:HG3	2.53	0.44
2:I:1077:SER:HA	3:J:356:THR:HG1	1.78	0.44
2:I:10:ARG:HH12	2:I:697:LYS:NZ	2.15	0.44
2:I:1101:LEU:HD12	3:J:505:ASP:OD2	2.17	0.44
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.80	0.44
2:I:1301:ARG:HH11	2:I:1301:ARG:HD2	1.66	0.44
2:I:1334:GLY:O	3:J:25:ALA:CB	2.65	0.44
2:I:208:ILE:CD1	2:I:365:GLU:HB3	2.47	0.44
2:I:520:PRO:HB3	2:I:714:VAL:HG21	1.99	0.44
3:J:317:THR:HB	3:J:324:LEU:HB3	1.99	0.44
3:J:520:ALA:HB1	3:J:543:SER:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:83:VAL:HG13	3:J:92:VAL:HG13	1.99	0.44
5:L:519:LEU:C	5:L:519:LEU:HD23	2.37	0.44
5:L:592:ALA:O	5:L:596:ARG:HB2	2.17	0.44
3:D:1193:TRP:HB2	3:D:1194:ARG:HH12	1.73	0.44
3:D:825:VAL:HG21	3:D:832:LYS:HB3	1.99	0.44
5:F:279:ARG:NH2	5:F:350:GLU:OE2	2.42	0.44
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.53	0.44
3:J:1346:GLY:O	3:J:1358:PRO:HG3	2.17	0.44
3:J:930:LEU:HD23	3:J:930:LEU:HA	1.72	0.44
1:B:152:TYR:HA	1:B:175:ALA:O	2.18	0.44
2:C:1149:TYR:CD1	2:C:1159:VAL:CG1	2.92	0.44
2:C:13:LYS:NZ	2:C:1151:LEU:HB2	2.32	0.44
2:C:1199:LEU:HD23	2:C:1204:LEU:HD12	1.99	0.44
2:C:120:GLN:HB2	2:C:120:GLN:HE21	1.59	0.44
2:C:289:VAL:HG13	2:C:319:LEU:CD1	2.47	0.44
2:C:393:ASP:OD1	2:C:394:ARG:HG2	2.17	0.44
3:D:706:VAL:HG12	3:D:715:LYS:CB	2.47	0.44
1:G:79:LEU:HD13	1:G:83:LEU:HD13	2.00	0.44
1:G:218:ARG:HH12	1:H:232:VAL:H	1.65	0.44
2:I:119:GLU:CG	2:I:489:PRO:CD	2.88	0.44
2:I:17:LYS:NZ	2:I:1154:ASP:CB	2.80	0.44
3:J:1156:LEU:CD2	3:J:1219:ASP:HB3	2.44	0.44
3:J:137:ARG:HD3	3:J:143:SER:OG	2.16	0.44
3:J:244:VAL:O	3:J:244:VAL:CG2	2.64	0.44
3:J:615:LYS:HZ3	4:K:7:GLN:CG	2.30	0.44
3:J:638:SER:OG	3:J:639:VAL:N	2.50	0.44
3:J:654:ILE:HG12	3:J:743:MET:HE1	1.99	0.44
3:J:670:SER:HB2	3:J:672:LEU:HD13	1.99	0.44
1:A:78:ILE:HD12	1:A:78:ILE:HG23	1.64	0.44
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.99	0.44
2:C:1240:ASP:HB3	3:D:445:LYS:CD	2.40	0.44
3:D:121:PRO:HG2	3:D:123:ARG:HH22	1.83	0.44
3:D:450:HIS:HE1	3:D:452:LEU:CD1	2.30	0.44
3:D:857:LEU:HD13	3:D:858:VAL:CG1	2.47	0.44
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.78	0.44
1:H:28:LEU:HD21	1:H:31:LEU:HD21	2.00	0.44
2:I:18:ARG:NH1	2:I:621:SER:O	2.48	0.44
2:I:250:THR:HG23	2:I:268:ARG:N	2.33	0.44
3:J:213:LYS:O	3:J:217:LEU:HB2	2.18	0.44
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.88	0.44
3:J:478:LEU:HD12	4:K:24:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ARG:O	1:B:223:ILE:HG13	2.17	0.44
1:A:38:THR:CG2	1:B:45:ARG:HG2	2.48	0.44
2:C:818:VAL:CB	2:C:1076:ILE:HD13	2.46	0.44
2:C:448:LEU:HA	2:C:448:LEU:HD23	1.81	0.44
2:C:848:GLU:CG	2:C:888:THR:HG22	2.47	0.44
2:C:886:LYS:HZ1	2:C:916:SER:HB3	1.82	0.44
3:D:66:LYS:HE2	3:D:69:GLU:OE1	2.17	0.44
3:D:839:VAL:CG1	3:D:864:LEU:HD12	2.44	0.44
5:F:295:CYS:O	5:F:329:LYS:HB3	2.17	0.44
1:H:172:LEU:HD12	1:H:172:LEU:H	1.83	0.44
1:H:67:GLU:HG2	1:H:82:LEU:HD11	1.99	0.44
1:H:83:LEU:HD11	3:J:526:VAL:HG21	1.92	0.44
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.98	0.44
2:I:1279:GLU:CG	3:J:1357:ILE:HD13	2.47	0.44
2:I:494:ASN:ND2	2:I:497:PRO:HD3	2.26	0.44
3:J:1286:LYS:HD3	3:J:1286:LYS:HA	1.85	0.44
3:J:1314:LEU:HD12	3:J:1326:GLN:OE1	2.18	0.44
2:I:1272:GLU:CB	3:J:342:LEU:CB	2.95	0.44
3:J:474:LEU:HB2	4:K:28:ARG:NH1	2.33	0.44
5:L:118:ASP:O	5:L:122:ARG:HG3	2.18	0.44
5:L:388:ILE:O	5:L:392:LYS:HG3	2.18	0.44
5:L:556:ALA:O	5:L:560:ARG:HG3	2.18	0.44
1:A:149:GLY:HA3	1:A:177:TYR:CE2	2.52	0.44
2:C:68:LEU:HD11	2:C:489:PRO:HB3	2.00	0.44
2:C:847:PRO:HB3	2:C:1047:LEU:HD11	1.99	0.44
3:D:352:ARG:O	3:D:353:SER:HB3	2.17	0.44
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.83	0.44
5:F:147:GLN:HB3	5:F:161:LEU:CD1	2.48	0.44
1:H:67:GLU:HA	1:H:78:ILE:HG21	1.99	0.44
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.99	0.44
2:I:496:LYS:HE3	2:I:496:LYS:HB3	1.63	0.44
2:I:453:ILE:HD12	2:I:587:LEU:HD21	2.00	0.44
3:J:127:LEU:HD21	3:J:234:PRO:CG	2.47	0.44
5:L:227:GLN:O	5:L:230:VAL:HG12	2.18	0.44
1:B:92:VAL:HG21	1:B:95:LYS:O	2.17	0.44
1:B:99:ILE:HG23	1:B:99:ILE:O	2.18	0.44
2:C:13:LYS:HA	2:C:1157:GLN:OE1	2.18	0.44
2:C:452:ARG:HH21	2:C:458:GLU:CD	2.20	0.44
2:C:854:ILE:O	2:C:857:VAL:HG22	2.18	0.44
3:D:294:ASN:HD22	5:F:406:GLN:HE21	1.66	0.44
3:D:74:LYS:HD3	3:D:75:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:495:ALA:HB3	5:F:471:LEU:HD22	1.99	0.44
5:F:96:ASP:O	5:F:98:VAL:N	2.50	0.44
1:G:168:ILE:H	1:G:168:ILE:HG12	1.60	0.44
2:I:149:LEU:HD11	2:I:451:ARG:HB3	1.98	0.44
2:I:191:LYS:HB3	2:I:191:LYS:HE2	1.79	0.44
2:I:253:PHE:CZ	2:I:287:VAL:HG12	2.52	0.44
2:I:838:CYS:HB2	2:I:918:LEU:HB2	2.00	0.44
3:J:1241:TYR:CE2	3:J:1248:ILE:HD11	2.52	0.44
3:J:1344:LEU:HA	3:J:1349:GLU:HG3	2.00	0.44
3:J:334:LYS:HA	3:J:335:GLN:HA	1.76	0.44
3:J:56:LEU:HD11	3:J:273:ILE:CD1	2.47	0.44
3:J:825:VAL:CG1	3:J:833:GLU:HB3	2.47	0.44
5:L:443:ILE:O	5:L:447:ALA:HB3	2.18	0.44
1:A:9:LEU:CD1	1:A:198:LEU:HD11	2.48	0.44
1:A:27:THR:O	1:A:28:LEU:HD12	2.17	0.44
1:B:6:THR:CG2	1:B:6:THR:O	2.52	0.44
2:C:1217:THR:CB	2:C:1219:GLU:HG2	2.48	0.44
2:C:496:LYS:HE3	2:C:497:PRO:HD3	2.00	0.44
2:C:591:TYR:O	2:C:603:ILE:HA	2.18	0.44
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.17	0.44
3:D:1290:ARG:HA	3:D:1290:ARG:HD3	1.77	0.44
3:D:1264:ALA:HB2	3:D:1304:ARG:HA	2.00	0.44
3:D:16:GLU:HB3	3:D:1369:ARG:HH21	1.82	0.44
3:D:875:ASN:N	3:D:875:ASN:OD1	2.51	0.44
1:G:169:GLY:O	1:G:171:LEU:CD2	2.66	0.44
1:G:218:ARG:HG3	1:H:231:PHE:HB3	1.99	0.44
2:I:1165:SER:HA	2:I:1169:VAL:HG21	2.00	0.44
3:J:596:LEU:HD11	3:J:604:MET:CE	2.48	0.44
3:J:71:LEU:C	3:J:71:LEU:HD22	2.36	0.44
3:J:755:ILE:HD12	3:J:774:ILE:CG2	2.48	0.44
1:B:48:LEU:HA	1:B:48:LEU:HD23	1.77	0.43
2:C:338:THR:HG22	2:C:345:PRO:HB3	2.00	0.43
3:D:9:LYS:HZ3	3:D:11:GLN:HA	1.83	0.43
3:D:334:LYS:HA	3:D:335:GLN:HA	1.75	0.43
3:D:43:THR:OG1	3:D:44:ILE:N	2.51	0.43
5:F:400:GLN:O	5:F:404:LEU:HG	2.18	0.43
3:D:259:ARG:CG	5:F:502:LYS:HE3	2.44	0.43
5:F:561:MET:HG3	5:F:571:TYR:HD2	1.82	0.43
1:G:88:LEU:CD1	1:G:112:ALA:HB1	2.47	0.43
1:G:231:PHE:CB	1:H:218:ARG:HG2	2.45	0.43
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:156:PHE:CZ	2:I:445:ILE:HG13	2.52	0.43
2:I:198:ILE:HD13	2:I:388:LEU:HD13	2.00	0.43
2:I:241:LEU:HD21	2:I:246:LEU:HD11	2.00	0.43
2:I:895:LEU:H	2:I:895:LEU:HG	1.56	0.43
3:J:349:TYR:CG	3:J:472:LEU:HD21	2.52	0.43
5:L:291:CYS:SG	5:L:330:LEU:HD22	2.58	0.43
1:A:36:GLY:C	1:A:187:VAL:HG11	2.38	0.43
1:A:218:ARG:NH1	1:B:231:PHE:CA	2.78	0.43
1:B:225:ALA:O	1:B:228:LEU:HB2	2.18	0.43
2:C:74:ARG:HG2	2:C:75:LEU:N	2.33	0.43
2:C:961:SER:O	2:C:965:GLN:HG3	2.18	0.43
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.18	0.43
2:C:1269:ARG:NE	3:D:343:LEU:O	2.48	0.43
3:D:394:ILE:CG1	5:F:536:THR:HG22	2.48	0.43
3:D:419:HIS:CE1	3:D:477:GLN:OE1	2.71	0.43
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.55	0.43
5:F:225:ARG:O	5:F:229:VAL:HG13	2.18	0.43
5:F:595:LEU:O	5:F:599:ARG:HB2	2.17	0.43
1:G:89:ALA:HB3	1:G:124:VAL:CG1	2.48	0.43
2:I:1327:LEU:HD21	2:I:1339:LEU:HD11	2.00	0.43
2:I:235:ASN:OD1	2:I:236:LYS:HG2	2.18	0.43
2:I:545:PHE:HA	2:I:548:ARG:CD	2.47	0.43
3:J:1221:LEU:HD13	3:J:1221:LEU:C	2.38	0.43
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.17	0.43
5:L:276:MET:O	5:L:280:VAL:HG23	2.18	0.43
5:L:380:VAL:HG13	5:L:412:LEU:HD23	2.01	0.43
1:A:150:ARG:HD2	1:B:8:PHE:CE2	2.53	0.43
1:B:210:THR:C	1:B:211:ILE:HG12	2.39	0.43
2:C:101:ARG:HE	2:C:118:LYS:HD2	1.83	0.43
3:D:1248:ILE:HD13	3:D:1248:ILE:HG21	1.69	0.43
3:D:218:THR:HA	3:D:221:ILE:CG2	2.47	0.43
3:D:250:ARG:HB3	3:D:265:LEU:HD12	2.00	0.43
3:D:140:TYR:OH	3:D:312:ARG:CZ	2.65	0.43
2:C:844:LYS:HD3	3:D:49:PHE:CD2	2.53	0.43
1:G:100:LEU:HD23	1:G:115:ILE:HG21	2.00	0.43
1:G:158:ARG:NH2	1:G:172:LEU:HD23	2.33	0.43
1:G:53:GLY:O	1:G:148:ARG:HG3	2.18	0.43
1:H:68:TYR:O	1:H:69:SER:HB3	2.18	0.43
2:I:1271:GLY:HA2	3:J:344:GLY:HA3	1.99	0.43
2:I:737:ASN:O	2:I:741:MET:HB2	2.18	0.43
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:596:LEU:HD11	3:J:604:MET:HE3	2.00	0.43
5:L:244:THR:O	5:L:244:THR:HG22	2.18	0.43
5:L:575:GLU:O	5:L:579:GLN:HG2	2.18	0.43
1:A:134:THR:HG23	2:C:726:TYR:HE1	1.83	0.43
2:C:866:ASP:HB3	2:C:872:TYR:CE1	2.53	0.43
2:C:898:GLU:OE1	2:C:898:GLU:N	2.47	0.43
3:D:884:SER:OG	3:D:886:VAL:HG12	2.18	0.43
5:F:254:GLU:HA	5:F:257:LYS:HD3	2.00	0.43
5:F:137:TYR:HD2	5:F:273:MET:HE2	1.82	0.43
1:G:57:THR:CG2	1:G:158:ARG:CZ	2.96	0.43
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	2.01	0.43
2:I:208:ILE:O	2:I:362:ALA:HB1	2.19	0.43
2:I:119:GLU:HB2	2:I:489:PRO:HB2	2.00	0.43
2:I:981:ALA:HB1	2:I:1007:LYS:NZ	2.33	0.43
3:J:165:TYR:CE2	3:J:169:LEU:HD12	2.53	0.43
3:J:421:VAL:CG2	3:J:439:PRO:HG3	2.45	0.43
3:J:528:THR:HG22	3:J:532:GLU:CD	2.39	0.43
5:L:132:CYS:SG	5:L:257:LYS:HE3	2.58	0.43
5:L:489:MET:CB	5:L:490:PRO:HD2	2.48	0.43
1:A:232:VAL:O	1:A:233:ASP:CB	2.66	0.43
2:C:1112:ILE:CD1	3:D:639:VAL:HG22	2.48	0.43
2:C:62:TYR:C	2:C:64:GLY:N	2.70	0.43
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.38	0.43
3:D:156:ARG:NH1	3:D:157:GLN:NE2	2.67	0.43
3:D:244:VAL:HG23	3:D:244:VAL:O	2.18	0.43
3:D:360:TYR:OH	3:D:442:ILE:HD11	2.18	0.43
3:D:75:TYR:CD2	3:D:83:VAL:HG21	2.52	0.43
4:E:39:VAL:HG22	4:E:40:PRO:HD2	2.00	0.43
5:F:141:ILE:HG23	5:F:224:LEU:HD11	2.00	0.43
5:F:280:VAL:HG22	5:F:347:ILE:HG21	1.99	0.43
1:G:231:PHE:CA	1:H:218:ARG:HH11	2.31	0.43
2:I:131:THR:HG22	2:I:132:ASP:N	2.34	0.43
2:I:145:ILE:HB	2:I:456:VAL:CG2	2.39	0.43
2:I:27:LEU:CD1	2:I:524:ILE:HD11	2.48	0.43
2:I:650:VAL:HG23	2:I:650:VAL:O	2.19	0.43
3:J:1237:VAL:HG13	3:J:1238:GLN:N	2.33	0.43
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.84	0.43
3:J:490:ILE:HG21	3:J:490:ILE:HD13	1.80	0.43
2:C:1152:GLY:O	2:C:1153:ALA:CB	2.65	0.43
2:C:98:VAL:HB	2:C:124:MET:CE	2.47	0.43
2:C:231:GLU:HG2	2:C:332:ARG:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:556:GLY:HA2	2:C:659:GLN:O	2.18	0.43
2:C:754:THR:O	2:C:755:LYS:HD2	2.19	0.43
3:D:291:ILE:CD1	5:F:409:ASN:HD22	2.31	0.43
3:D:647:PRO:CD	3:D:697:MET:HB3	2.49	0.43
3:D:909:ILE:O	3:D:909:ILE:HG23	2.17	0.43
5:F:290:LEU:HD13	5:F:333:VAL:HG22	2.01	0.43
5:F:558:VAL:HG21	5:F:587:ILE:HG12	2.00	0.43
2:I:974:ARG:HD2	2:I:1014:LEU:HD11	2.01	0.43
2:I:1013:GLN:O	2:I:1017:GLN:HG2	2.18	0.43
2:I:49:LEU:HD12	2:I:73:TYR:HE2	1.84	0.43
2:I:720:ARG:HB2	2:I:749:ASP:OD1	2.19	0.43
2:I:759:SER:OG	2:I:763:THR:N	2.48	0.43
2:I:74:ARG:NH2	2:I:97:ARG:HG3	2.33	0.43
3:J:24:LEU:HD11	3:J:116:PHE:CE2	2.54	0.43
3:J:179:LYS:CB	3:J:184:ALA:HB2	2.47	0.43
5:L:491:GLU:O	5:L:491:GLU:HG3	2.17	0.43
2:C:1124:ILE:HG22	2:C:1180:MET:HG3	2.01	0.43
2:C:1131:MET:CB	2:C:1141:LEU:HD11	2.47	0.43
2:C:1160:ASP:HB2	2:C:1163:THR:OG1	2.19	0.43
2:C:325:LEU:HD13	2:C:333:ILE:CG1	2.48	0.43
2:C:407:ARG:HH21	2:C:414:ILE:CG2	2.31	0.43
2:C:157:PHE:HE2	2:C:431:LYS:HZ3	1.66	0.43
2:C:589:THR:HG1	2:C:659:GLN:NE2	2.14	0.43
2:C:800:MET:HE1	2:C:822:VAL:CG2	2.49	0.43
2:C:848:GLU:OE1	2:C:886:LYS:NZ	2.51	0.43
2:C:934:PHE:CD2	2:C:934:PHE:N	2.85	0.43
3:D:578:ILE:HG21	3:D:631:TYR:OH	2.18	0.43
3:D:609:TYR:HD1	3:D:610:ARG:HH11	1.65	0.43
3:D:653:ILE:HD13	3:D:692:ARG:HB3	2.01	0.43
3:D:722:ILE:HD13	3:D:722:ILE:HG21	1.62	0.43
3:D:903:LEU:HD22	3:D:909:ILE:HD12	2.01	0.43
5:F:606:VAL:HG13	5:F:607:LEU:CD1	2.49	0.43
1:G:13:LEU:HD22	1:H:231:PHE:CE1	2.54	0.43
1:G:8:PHE:N	1:H:150:ARG:HH12	2.16	0.43
2:I:168:GLY:C	2:I:170:VAL:H	2.22	0.43
2:I:20:GLN:NE2	2:I:23:ASP:HB3	2.34	0.43
2:I:548:ARG:HH21	2:I:568:ASN:HA	1.83	0.43
2:I:548:ARG:O	2:I:570:GLY:HA3	2.19	0.43
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.83	0.43
3:J:123:ARG:O	3:J:126:LEU:HD12	2.18	0.43
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:474:LEU:HA	3:J:474:LEU:HD12	1.81	0.43
3:J:647:PRO:CD	3:J:697:MET:HB3	2.49	0.43
3:J:820:ILE:HD11	3:J:822:MET:HE3	2.01	0.43
5:L:244:THR:O	5:L:247:GLU:HG2	2.19	0.43
1:B:14:VAL:HG13	1:B:14:VAL:O	2.19	0.43
1:B:188:GLU:O	1:B:200:LYS:N	2.49	0.43
1:B:51:MET:HB3	1:B:179:PRO:HD3	2.00	0.43
2:C:590:PRO:CB	2:C:655:VAL:HG21	2.48	0.43
2:C:74:ARG:HH22	2:C:97:ARG:HG3	1.81	0.43
3:D:1273:ASP:CB	3:D:1276:GLU:CD	2.87	0.43
2:C:1336:ASN:ND2	3:D:29:MET:HE2	2.34	0.43
3:D:342:LEU:CB	3:D:343:LEU:HD13	2.47	0.43
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.78	0.43
5:F:305:LEU:HD13	5:F:315:TRP:HA	2.00	0.43
1:G:175:ALA:HB1	1:G:177:TYR:CZ	2.54	0.43
1:G:26:VAL:HG22	1:G:203:ILE:HB	2.01	0.43
1:G:35:PHE:HE1	1:H:46:ILE:HG23	1.83	0.43
2:I:802:VAL:HA	2:I:1096:ILE:O	2.19	0.43
2:I:1222:GLU:O	2:I:1223:ARG:CB	2.64	0.43
2:I:149:LEU:HB2	2:I:530:ILE:HG21	1.99	0.43
2:I:708:VAL:CG1	2:I:794:LEU:HD22	2.48	0.43
3:J:138:VAL:CG2	3:J:145:VAL:HB	2.43	0.43
3:J:478:LEU:HD21	4:K:47:THR:O	2.18	0.43
3:J:505:ASP:HB2	3:J:629:PHE:CE1	2.47	0.43
3:J:514:THR:HG21	3:J:596:LEU:HG	2.00	0.43
2:C:607:SER:H	2:C:610:GLU:HB2	1.84	0.43
3:D:9:LYS:CE	3:D:11:GLN:HA	2.49	0.43
3:D:126:LEU:C	3:D:126:LEU:HD12	2.38	0.43
2:C:1271:GLY:C	3:D:343:LEU:HD11	2.38	0.43
3:D:510:LEU:O	3:D:514:THR:CG2	2.67	0.43
5:F:391:ALA:CB	5:F:405:ILE:HG22	2.46	0.43
5:F:588:ARG:HG3	5:F:588:ARG:H	1.48	0.43
1:H:33:ARG:HD2	2:I:1081:PRO:HG3	2.00	0.43
1:G:38:THR:OG1	1:H:45:ARG:HB3	2.18	0.43
2:I:815:SER:HB3	2:I:1077:SER:HB3	2.00	0.43
2:I:98:VAL:CG2	2:I:124:MET:CE	2.96	0.43
2:I:483:ASP:HB2	2:I:486:THR:HG21	1.99	0.43
2:I:496:LYS:O	2:I:500:ALA:CB	2.67	0.43
2:I:755:LYS:O	2:I:757:THR:HG22	2.19	0.43
2:I:807:TRP:HE1	2:I:1086:PRO:HD3	1.84	0.43
1:B:84:ASN:ND2	1:B:129:VAL:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:ILE:HG21	2:C:456:VAL:HG22	1.96	0.43
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.34	0.43
3:D:1252:HIS:HA	3:D:1255:VAL:HG13	2.01	0.43
3:D:678:ARG:C	3:D:678:ARG:CD	2.86	0.43
3:D:755:ILE:HD12	3:D:774:ILE:HG21	1.99	0.43
3:D:479:GLU:CG	4:E:20:VAL:HG11	2.46	0.43
5:F:470:MET:HA	5:F:473:GLU:HB3	2.01	0.43
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.33	0.43
2:I:228:VAL:HB	2:I:335:THR:OG1	2.19	0.43
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.90	0.43
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.33	0.43
3:J:1229:VAL:HG22	3:J:1233:ILE:HD13	2.01	0.43
2:I:1245:ALA:HB2	3:J:372:MET:HE3	2.00	0.43
3:J:821:MET:HE3	3:J:879:ALA:HB1	2.01	0.43
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.59	0.43
3:J:810:THR:CG2	3:J:893:GLY:HA3	2.44	0.43
5:L:111:LEU:CD1	5:L:119:ILE:HD12	2.49	0.43
5:L:234:THR:HG21	5:L:248:GLU:OE2	2.19	0.43
5:L:490:PRO:O	5:L:491:GLU:HG2	2.18	0.43
5:L:499:LYS:HA	5:L:502:LYS:HE2	2.00	0.43
2:C:103:VAL:HA	2:C:116:ASP:HB3	2.00	0.42
2:C:91:THR:HB	2:C:138:ILE:O	2.19	0.42
2:C:230:PHE:HE1	2:C:287:VAL:HG21	1.83	0.42
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.62	0.42
2:C:412:GLU:HB3	2:C:413:GLU:OE1	2.18	0.42
2:C:593:LYS:O	2:C:600:THR:CB	2.67	0.42
3:D:639:VAL:O	3:D:639:VAL:HG13	2.19	0.42
4:E:4:VAL:HG13	4:E:5:THR:HG23	2.01	0.42
5:F:322:MET:CE	5:F:324:LYS:NZ	2.82	0.42
1:G:191:ARG:HH12	1:G:197:ASP:CA	2.28	0.42
2:I:13:LYS:HD3	2:I:1149:TYR:HA	2.01	0.42
2:I:44:GLU:HA	2:I:54:ARG:NH1	2.34	0.42
2:I:676:ALA:HB3	3:J:779:ALA:HB2	2.01	0.42
3:J:1191:PRO:CB	3:J:1194:ARG:HH11	2.31	0.42
3:J:805:GLN:CD	3:J:1348:LYS:HD3	2.37	0.42
5:L:226:ALA:O	5:L:229:VAL:HG22	2.19	0.42
5:L:341:LEU:CG	5:L:344:LEU:HD23	2.49	0.42
1:B:102:LEU:HD22	1:B:103:ASN:N	2.35	0.42
1:B:12:ARG:O	1:B:13:LEU:HG	2.19	0.42
1:B:64:VAL:HG11	1:B:69:SER:HB3	1.98	0.42
1:A:154:PRO:CB	2:C:1059:ARG:NH2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:528:ARG:NH2	2:C:576:SER:O	2.51	0.42
3:D:1314:LEU:HD12	3:D:1326:GLN:OE1	2.19	0.42
3:D:536:LEU:CD1	3:D:541:LEU:CB	2.96	0.42
3:D:842:ARG:CD	3:D:882:VAL:HG11	2.49	0.42
3:D:8:LEU:HD22	3:D:9:LYS:O	2.19	0.42
3:D:382:TYR:HE2	5:F:532:LEU:HD23	1.84	0.42
1:G:13:LEU:H	1:G:13:LEU:CD2	2.24	0.42
1:G:29:GLU:HB3	1:G:30:PRO:HD3	2.01	0.42
2:I:29:SER:HB3	2:I:33:ASP:OD2	2.19	0.42
2:I:979:LEU:HA	2:I:1002:LEU:HD12	2.01	0.42
3:J:357:VAL:HG22	3:J:461:PHE:CE1	2.54	0.42
3:J:494:ALA:HB2	3:J:922:SER:CB	2.49	0.42
3:J:62:PHE:CG	3:J:247:PRO:CG	3.02	0.42
3:J:660:GLU:O	3:J:663:GLU:HB2	2.19	0.42
4:K:32:VAL:O	4:K:34:GLY:N	2.52	0.42
5:L:127:ILE:HG13	5:L:127:ILE:H	1.64	0.42
1:A:47:LEU:HA	1:A:47:LEU:HD23	1.78	0.42
1:B:140:ILE:O	1:B:140:ILE:CG2	2.67	0.42
1:B:183:ILE:HD12	1:B:183:ILE:N	2.34	0.42
1:B:19:VAL:HG21	1:B:23:HIS:CE1	2.55	0.42
2:C:1080:ASN:HD22	2:C:1085:MET:CE	2.32	0.42
2:C:218:GLU:O	2:C:222:ASP:HB2	2.19	0.42
2:C:817:LEU:HD23	2:C:1078:LYS:HB3	2.01	0.42
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.77	0.42
2:C:1332:SER:HB3	3:D:245:LEU:HD13	2.01	0.42
3:D:364:HIS:CD2	4:E:4:VAL:HG23	2.54	0.42
3:D:369:PRO:HB3	3:D:444:GLY:O	2.19	0.42
3:D:441:LEU:HD13	3:D:441:LEU:HA	1.70	0.42
3:D:664:ILE:HD12	3:D:681:LYS:HG2	2.01	0.42
2:I:250:THR:HG23	2:I:268:ARG:CA	2.49	0.42
2:I:560:PRO:HG3	3:J:773:PHE:HE2	1.85	0.42
2:I:568:ASN:HB3	2:I:571:LEU:HD12	2.01	0.42
2:I:590:PRO:HG3	2:I:605:TYR:CE2	2.53	0.42
2:I:696:ASP:O	2:I:697:LYS:CB	2.67	0.42
2:I:818:VAL:HG12	2:I:819:SER:O	2.18	0.42
2:I:812:PHE:CE2	3:J:451:PRO:HB3	2.55	0.42
3:J:47:ARG:HD2	3:J:47:ARG:HA	1.81	0.42
3:J:650:LYS:HE2	3:J:654:ILE:HD11	2.02	0.42
3:J:808:VAL:HG12	3:J:809:VAL:N	2.35	0.42
3:J:903:LEU:HD23	3:J:905:ARG:HD3	2.00	0.42
1:B:14:VAL:HA	1:B:27:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	2.01	0.42
2:C:175:ARG:HG2	2:C:177:ILE:CG1	2.50	0.42
2:C:271:ALA:O	2:C:275:ARG:HG3	2.19	0.42
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.77	0.42
2:C:680:LEU:O	2:C:684:ASN:HB2	2.18	0.42
2:C:800:MET:HE2	2:C:1095:ASP:HB3	2.01	0.42
3:D:1217:PRO:HG3	3:D:1232:TYR:HE2	1.84	0.42
3:D:614:LEU:HD23	4:E:7:GLN:HB2	2.01	0.42
3:D:64:PRO:HG3	3:D:90:VAL:HG12	2.01	0.42
4:E:59:ILE:HD12	4:E:59:ILE:HG23	1.55	0.42
1:H:158:ARG:HB3	1:H:172:LEU:HD23	2.01	0.42
2:I:830:THR:HG22	2:I:1234:LYS:NZ	2.35	0.42
2:I:233:ARG:HH12	2:I:332:ARG:HH12	1.66	0.42
2:I:62:TYR:OH	2:I:476:LYS:HB3	2.19	0.42
5:L:101:TYR:O	5:L:102:MET:C	2.56	0.42
5:L:96:ASP:O	5:L:96:ASP:CG	2.57	0.42
1:A:172:LEU:N	1:A:172:LEU:HD12	2.34	0.42
2:C:1124:ILE:HG21	2:C:1180:MET:HG3	2.02	0.42
2:C:2:VAL:O	2:C:2:VAL:CG1	2.66	0.42
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.34	0.42
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.71	0.42
3:D:520:ALA:HB1	3:D:543:SER:HB3	2.00	0.42
3:D:438:GLU:OE1	4:E:2:ALA:CB	2.68	0.42
5:F:444:ALA:HB1	5:F:457:ILE:HD13	1.96	0.42
1:G:73:GLY:C	1:G:134:THR:HG22	2.39	0.42
1:G:195:ARG:HG2	1:G:198:LEU:CD1	2.50	0.42
2:I:1080:ASN:CB	2:I:1085:MET:CE	2.97	0.42
2:I:1337:ILE:O	2:I:1337:ILE:CG2	2.67	0.42
2:I:22:LEU:HA	2:I:22:LEU:HD22	1.69	0.42
2:I:556:GLY:O	2:I:589:THR:HB	2.18	0.42
2:I:681:MET:HE1	2:I:1073:LYS:NZ	2.35	0.42
2:I:804:PHE:O	2:I:805:MET:HB3	2.19	0.42
3:J:1146:GLU:O	3:J:1147:ALA:HB3	2.19	0.42
3:J:800:LEU:HB3	3:J:920:ALA:CB	2.49	0.42
3:J:846:GLU:HA	3:J:860:ARG:HD2	2.00	0.42
4:K:26:ARG:HB2	4:K:64:LEU:HD21	2.01	0.42
5:L:147:GLN:CB	5:L:161:LEU:CD1	2.97	0.42
5:L:277:MET:CE	5:L:281:ARG:NH2	2.81	0.42
5:L:470:MET:HB2	5:L:478:PRO:HG3	2.00	0.42
1:B:61:ILE:HG23	1:B:142:MET:HE2	2.02	0.42
2:C:1111:GLN:HB2	2:C:1230:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1241:TYR:HD2	3:D:1246:VAL:CG1	2.28	0.42
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.49	0.42
3:D:141:PHE:CG	3:D:293:ARG:HD3	2.54	0.42
3:D:342:LEU:HA	3:D:343:LEU:HA	1.67	0.42
3:D:848:VAL:HG22	3:D:858:VAL:HG22	2.00	0.42
5:F:423:ARG:HD2	5:F:425:TYR:CD2	2.54	0.42
1:G:13:LEU:CD2	1:H:230:ALA:HB1	2.50	0.42
1:G:86:LYS:HB2	1:G:86:LYS:HE3	1.83	0.42
1:H:9:LEU:HB3	1:H:32:GLU:CG	2.49	0.42
2:I:1043:ALA:O	2:I:1046:VAL:HG12	2.19	0.42
1:G:156:SER:HB2	2:I:1059:ARG:NH2	2.35	0.42
2:I:1327:LEU:HG	2:I:1337:ILE:HG23	2.00	0.42
2:I:397:LEU:O	2:I:398:SER:OG	2.34	0.42
2:I:606:LEU:N	2:I:606:LEU:HD12	2.35	0.42
2:I:807:TRP:NE1	2:I:1086:PRO:HD3	2.34	0.42
2:I:85:CYS:SG	2:I:92:TYR:HA	2.60	0.42
3:J:97:VAL:CG1	3:J:101:ARG:CZ	2.91	0.42
3:J:1158:GLU:HB3	3:J:1186:TYR:CE1	2.54	0.42
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.83	0.42
3:J:1361:THR:CG2	4:K:21:LEU:HD13	2.46	0.42
3:J:141:PHE:O	3:J:180:MET:HE1	2.20	0.42
3:J:282:LEU:HD23	3:J:282:LEU:HA	1.84	0.42
3:J:702:GLN:HG2	3:J:703:THR:N	2.31	0.42
5:L:324:LYS:HG3	5:L:326:TRP:CZ2	2.54	0.42
2:C:245:ARG:O	2:C:249:GLU:OE1	2.37	0.42
2:C:250:THR:HA	2:C:268:ARG:HA	2.02	0.42
2:C:363:LEU:HD13	2:C:382:GLU:HG2	2.01	0.42
2:C:719:LYS:HD2	2:C:751:TYR:HE1	1.84	0.42
3:D:527:LEU:HD21	3:D:536:LEU:HG	2.02	0.42
3:D:527:LEU:HB3	3:D:532:GLU:CG	2.49	0.42
3:D:749:LYS:HG2	3:D:753:SER:HB2	2.01	0.42
5:F:405:ILE:HD13	5:F:405:ILE:HG21	1.60	0.42
5:F:568:ASN:C	5:F:569:THR:HG22	2.40	0.42
1:H:47:LEU:HD22	1:H:180:VAL:CG1	2.47	0.42
2:I:1119:MET:CE	2:I:1210:ILE:HD11	2.50	0.42
2:I:1246:ARG:NH2	2:I:1258:PRO:HB3	2.34	0.42
2:I:1250:SER:HB3	2:I:1259:LEU:O	2.20	0.42
2:I:170:VAL:CG2	2:I:171:LEU:N	2.76	0.42
2:I:494:ASN:HB3	2:I:497:PRO:HG2	2.01	0.42
2:I:794:LEU:HG	2:I:796:LEU:CD1	2.49	0.42
3:J:1221:LEU:HD13	3:J:1222:ARG:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:418:GLU:HG3	4:K:44:ASP:CA	2.36	0.42
5:L:405:ILE:HG21	5:L:405:ILE:HD13	1.61	0.42
1:A:44:ARG:CZ	1:A:48:LEU:HD11	2.50	0.42
1:B:152:TYR:HD2	3:D:541:LEU:CD1	2.33	0.42
2:C:1217:THR:C	2:C:1219:GLU:H	2.22	0.42
2:C:1222:GLU:H	2:C:1222:GLU:HG3	1.47	0.42
2:C:1225:VAL:HG23	2:C:1227:VAL:HG13	2.01	0.42
2:C:840:SER:CB	2:C:850:ILE:HD11	2.50	0.42
2:C:850:ILE:O	2:C:850:ILE:HG22	2.19	0.42
3:D:137:ARG:CD	3:D:143:SER:HB2	2.45	0.42
3:D:733:SER:O	3:D:736:GLN:N	2.53	0.42
3:D:826:ILE:HD12	3:D:826:ILE:O	2.20	0.42
5:F:112:THR:OG1	5:F:114:GLU:HG3	2.19	0.42
5:F:94:THR:O	5:F:95:THR:OG1	2.33	0.42
2:I:587:LEU:HA	2:I:587:LEU:HD23	1.75	0.42
2:I:617:ALA:HA	2:I:636:CYS:SG	2.60	0.42
2:I:996:ARG:NH1	2:I:999:GLU:OE2	2.49	0.42
3:J:1144:LEU:HA	3:J:1144:LEU:HD23	1.83	0.42
3:J:242:LEU:C	3:J:242:LEU:HD23	2.41	0.42
3:J:528:THR:O	3:J:551:ARG:HB3	2.20	0.42
3:J:610:ARG:HG2	3:J:866:GLU:OE1	2.19	0.42
5:L:289:LYS:HG2	5:L:293:GLU:OE1	2.19	0.42
5:L:583:THR:HG22	5:L:584:ARG:N	2.34	0.42
1:A:38:THR:CB	1:B:45:ARG:HG2	2.49	0.42
2:C:1042:LEU:HD23	2:C:1042:LEU:HA	1.81	0.42
2:C:690:VAL:HG23	2:C:763:THR:HG21	2.01	0.42
3:D:1287:ILE:HG22	3:D:1300:ALA:H	1.84	0.42
3:D:1289:ASN:O	3:D:1292:LEU:O	2.38	0.42
3:D:116:PHE:CD1	3:D:1333:THR:HG22	2.55	0.42
3:D:285:LEU:HD23	5:F:413:MET:HE2	2.02	0.42
3:D:423:LEU:N	3:D:423:LEU:HD12	2.34	0.42
3:D:544:LEU:O	3:D:574:VAL:HB	2.20	0.42
3:D:609:TYR:HA	3:D:617:THR:OG1	2.19	0.42
3:D:765:GLU:H	3:D:765:GLU:HG3	1.66	0.42
4:E:86:ILE:O	4:E:86:ILE:HG22	2.20	0.42
1:G:201:LEU:HD12	1:G:201:LEU:HA	1.75	0.42
2:I:678:ARG:NH2	2:I:1106:ARG:HG2	2.33	0.42
2:I:830:THR:HG22	2:I:1234:LYS:HZ2	1.85	0.42
2:I:1285:TYR:CD1	3:J:475:GLU:HB3	2.54	0.42
3:J:1183:SER:OG	3:J:1185:PRO:HD3	2.19	0.42
3:J:1177:ILE:CD1	3:J:1186:TYR:HB3	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:252:LEU:HD23	3:J:262:THR:HB	2.00	0.42
3:J:357:VAL:HA	3:J:461:PHE:CZ	2.54	0.42
3:J:93:THR:HG22	3:J:94:GLN:H	1.84	0.42
5:L:111:LEU:HD11	5:L:119:ILE:CD1	2.49	0.42
5:L:141:ILE:HG23	5:L:224:LEU:HD11	2.00	0.42
1:B:101:THR:CG2	1:B:103:ASN:HD21	2.32	0.42
2:C:1176:LEU:HD23	2:C:1176:LEU:HA	1.69	0.42
2:C:122:VAL:HG13	2:C:122:VAL:O	2.20	0.42
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.55	0.42
2:C:653:MET:HG2	2:C:654:ASP:N	2.35	0.42
2:C:1285:TYR:CZ	3:D:1356:LEU:HD11	2.53	0.42
2:C:1333:LEU:HD23	3:D:327:LEU:HD13	2.01	0.42
3:D:395:LYS:O	3:D:398:LYS:HB3	2.20	0.42
3:D:614:LEU:O	3:D:615:LYS:C	2.56	0.42
3:D:702:GLN:O	3:D:718:SER:N	2.35	0.42
3:D:646:ILE:CD1	3:D:741:ALA:HA	2.50	0.42
3:D:843:VAL:CG2	3:D:861:ASN:HB2	2.50	0.42
2:I:800:MET:HE2	2:I:1095:ASP:HB3	2.00	0.42
2:I:229:ILE:CD1	2:I:334:GLU:HG2	2.50	0.42
2:I:402:ARG:NH2	2:I:419:ILE:O	2.52	0.42
2:I:478:ARG:NH2	2:I:487:LEU:HB3	2.35	0.42
2:I:967:LEU:HD23	2:I:1021:LEU:HD22	2.01	0.42
3:J:1286:LYS:HD2	3:J:1290:ARG:HH22	1.85	0.42
3:J:1343:GLU:O	3:J:1344:LEU:HB2	2.20	0.42
2:I:1287:LEU:HD21	3:J:1351:VAL:HG22	2.02	0.42
3:J:645:VAL:HB	3:J:701:LEU:HD23	2.02	0.42
5:L:161:LEU:O	5:L:262:VAL:HG23	2.20	0.42
5:L:363:ARG:NH2	5:L:367:ILE:HD11	2.34	0.42
5:L:375:ALA:O	5:L:378:GLU:HB3	2.20	0.42
1:A:153:VAL:HB	1:A:175:ALA:HB3	2.02	0.41
2:C:100:LEU:HA	2:C:100:LEU:HD23	1.84	0.41
2:C:1337:ILE:HD13	2:C:1337:ILE:HG21	1.88	0.41
2:C:24:VAL:CG1	2:C:27:LEU:HD21	2.49	0.41
2:C:724:VAL:HA	2:C:734:ILE:HD13	2.02	0.41
2:C:80:PHE:CZ	2:C:88:ARG:HD2	2.54	0.41
2:C:867:GLU:HG3	2:C:867:GLU:H	1.46	0.41
3:D:1337:VAL:HG23	3:D:1338:ALA:N	2.35	0.41
3:D:35:PHE:CD1	3:D:101:ARG:CD	2.94	0.41
3:D:49:PHE:HE1	5:F:500:ILE:HD12	1.85	0.41
5:F:548:LEU:CD2	5:F:551:LEU:HD12	2.47	0.41
1:G:44:ARG:CG	1:G:183:ILE:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:964:LEU:CD1	2:I:1021:LEU:HB3	2.49	0.41
2:I:403:MET:HE3	2:I:403:MET:HB3	1.98	0.41
2:I:448:LEU:HG	2:I:553:THR:OG1	2.20	0.41
3:J:1198:VAL:HG11	3:J:1210:ILE:CG2	2.48	0.41
3:J:68:TYR:HA	3:J:92:VAL:HG23	2.02	0.41
5:L:287:ILE:HG21	5:L:315:TRP:HH2	1.82	0.41
1:B:104:LYS:O	1:B:140:ILE:HG22	2.19	0.41
1:B:205:MET:CG	1:B:206:GLU:H	2.32	0.41
1:B:82:LEU:HA	1:B:82:LEU:HD23	1.74	0.41
3:D:430:HIS:ND1	3:D:430:HIS:N	2.65	0.41
5:F:298:PRO:HD3	5:F:326:TRP:HB3	2.02	0.41
1:G:221:ALA:HB1	1:H:228:LEU:CD2	2.50	0.41
1:G:97:GLU:OE2	1:G:145:LYS:HD3	2.18	0.41
2:I:978:VAL:HG21	2:I:1010:GLN:OE1	2.21	0.41
2:I:1219:GLU:OE2	3:J:634:ARG:NE	2.52	0.41
2:I:511:LEU:CD2	2:I:531:LEU:HD13	2.49	0.41
2:I:91:THR:HG21	2:I:503:LYS:HZ1	1.85	0.41
3:J:112:ALA:HA	3:J:238:ILE:HD13	2.01	0.41
3:J:693:VAL:HG21	3:J:743:MET:HE2	2.02	0.41
3:J:930:LEU:HD22	3:J:1240:VAL:HG12	2.02	0.41
2:C:1301:ARG:HG3	2:C:1302:THR:N	2.35	0.41
2:C:135:THR:HG21	2:C:515:MET:SD	2.60	0.41
3:D:1237:VAL:CG1	3:D:1253:ILE:HD13	2.48	0.41
3:D:156:ARG:NH1	3:D:157:GLN:HE21	2.18	0.41
3:D:416:ILE:O	3:D:417:ARG:C	2.58	0.41
3:D:9:LYS:HE2	3:D:11:GLN:CA	2.51	0.41
2:I:1290:MET:SD	2:I:1294:LYS:HE3	2.59	0.41
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.20	0.41
3:J:147:ILE:HD11	3:J:177:ASP:OD2	2.20	0.41
3:J:244:VAL:O	3:J:244:VAL:HG23	2.19	0.41
4:K:26:ARG:HH22	4:K:38:LEU:HD13	1.85	0.41
5:L:362:ASN:O	5:L:365:MET:HB3	2.20	0.41
1:A:161:SER:O	1:A:163:GLU:N	2.52	0.41
1:A:31:LEU:HA	1:A:31:LEU:HD23	1.81	0.41
1:B:153:VAL:HB	1:B:175:ALA:CB	2.46	0.41
1:B:212:ASP:OD2	1:B:215:GLU:HB2	2.20	0.41
2:C:131:THR:OG1	2:C:135:THR:O	2.37	0.41
2:C:596:ASP:O	2:C:648:ASP:OD1	2.38	0.41
2:C:1332:SER:HB3	3:D:245:LEU:CD1	2.50	0.41
3:D:478:LEU:CD1	4:E:24:ALA:N	2.83	0.41
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:489:MET:H	5:F:489:MET:HG2	1.41	0.41
5:F:533:ASP:O	5:F:536:THR:N	2.54	0.41
1:G:89:ALA:O	1:G:124:VAL:HG12	2.20	0.41
1:G:27:THR:HA	1:G:201:LEU:O	2.21	0.41
1:H:14:VAL:HG13	1:H:15:ASP:N	2.35	0.41
2:I:1209:GLN:HB3	2:I:1224:PRO:HB2	2.02	0.41
2:I:353:VAL:O	2:I:353:VAL:HG12	2.20	0.41
2:I:588:GLU:HA	2:I:606:LEU:O	2.21	0.41
3:J:138:VAL:HG13	3:J:180:MET:HA	2.03	0.41
3:J:210:SER:HB2	3:J:213:LYS:CB	2.50	0.41
3:J:591:ILE:HG23	3:J:592:VAL:HG13	2.03	0.41
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	2.32	0.41
5:L:101:TYR:O	5:L:104:GLU:N	2.49	0.41
5:L:322:MET:SD	5:L:326:TRP:CH2	3.13	0.41
1:A:90:VAL:HG22	1:A:91:ARG:H	1.84	0.41
1:B:57:THR:HA	1:B:173:VAL:HG22	2.02	0.41
2:C:1066:MET:HE3	2:C:1076:ILE:HB	1.92	0.41
2:C:1087:TYR:O	2:C:1213:TYR:N	2.41	0.41
2:C:498:ILE:H	2:C:498:ILE:HD12	1.85	0.41
2:C:569:ILE:HD13	2:C:569:ILE:HG21	1.79	0.41
2:C:755:LYS:HA	2:C:766:ASN:OD1	2.21	0.41
3:D:1150:PRO:O	3:D:1153:PRO:HG3	2.20	0.41
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	2.02	0.41
3:D:317:THR:CG2	3:D:320:ASN:HB3	2.42	0.41
3:D:667:GLN:HB3	3:D:673:VAL:HG22	2.02	0.41
3:D:748:ALA:HB1	3:D:753:SER:O	2.20	0.41
3:D:844:THR:HB	3:D:860:ARG:O	2.19	0.41
3:D:68:TYR:HA	3:D:92:VAL:HG23	2.03	0.41
5:F:515:GLU:C	5:F:517:SER:N	2.74	0.41
5:F:515:GLU:HG2	5:F:516:ASP:N	2.35	0.41
2:I:1067:ALA:CB	2:I:1072:ASN:O	2.69	0.41
2:I:802:VAL:HG21	2:I:1098:LEU:HD13	2.01	0.41
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	1.97	0.41
2:I:1184:THR:O	2:I:1184:THR:HG22	2.20	0.41
2:I:210:LEU:CD1	2:I:220:ILE:HD13	2.50	0.41
2:I:239:MET:HG2	2:I:240:GLU:O	2.20	0.41
2:I:498:ILE:H	2:I:498:ILE:HD12	1.86	0.41
2:I:803:ALA:HB2	2:I:1094:VAL:HG21	2.02	0.41
3:J:1328:THR:O	3:J:1332:LEU:HD23	2.20	0.41
3:J:18:ASP:HB2	3:J:1373:ARG:NH1	2.35	0.41
3:J:337:ARG:HB3	3:J:340:GLN:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:707:ILE:HD12	3:J:707:ILE:H	1.86	0.41
3:J:800:LEU:HD12	3:J:1309:ILE:HD12	2.01	0.41
2:C:1082:ILE:HD12	2:C:1082:ILE:H	1.85	0.41
2:C:28:LEU:HA	2:C:28:LEU:HD23	1.56	0.41
2:C:484:LEU:HG	2:C:484:LEU:H	1.56	0.41
2:C:75:LEU:HA	2:C:75:LEU:HD13	1.79	0.41
2:C:796:LEU:HD12	2:C:796:LEU:N	2.35	0.41
2:C:888:THR:HG23	2:C:916:SER:OG	2.21	0.41
3:D:1221:LEU:HD13	3:D:1222:ARG:N	2.36	0.41
3:D:60:ARG:HA	3:D:89:GLY:O	2.20	0.41
3:D:418:GLU:N	4:E:45:LYS:HZ3	2.11	0.41
1:G:153:VAL:HB	1:G:175:ALA:HB3	2.01	0.41
2:I:1211:ARG:HB2	2:I:1220:GLN:HE21	1.85	0.41
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.00	0.41
3:J:1280:VAL:HG21	3:J:1304:ARG:HD3	2.02	0.41
5:L:163:THR:HG22	5:L:163:THR:O	2.21	0.41
1:B:78:ILE:HA	1:B:81:ILE:HD12	2.02	0.41
2:C:1101:LEU:HA	2:C:1101:LEU:HD23	1.62	0.41
2:C:1144:PHE:HE1	2:C:1201:LEU:HD11	1.85	0.41
2:C:201:ARG:HE	2:C:370:MET:HA	1.86	0.41
3:D:147:ILE:HG22	3:D:188:LEU:CD2	2.51	0.41
3:D:518:VAL:CG1	3:D:519:ASN:N	2.84	0.41
5:F:99:ARG:HA	5:F:99:ARG:HD3	1.89	0.41
2:I:105:TYR:HA	2:I:112:GLY:O	2.21	0.41
2:I:1289:GLU:OE2	3:J:473:THR:CG2	2.48	0.41
2:I:720:ARG:HB3	2:I:736:VAL:HG13	2.01	0.41
2:I:791:LEU:HD23	2:I:791:LEU:HA	1.88	0.41
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.55	0.41
3:J:1311:LYS:O	3:J:1314:LEU:HB3	2.21	0.41
3:J:695:LYS:HD3	3:J:695:LYS:HA	1.72	0.41
3:J:821:MET:HE2	3:J:879:ALA:HB1	2.02	0.41
3:J:60:ARG:HA	3:J:89:GLY:O	2.20	0.41
5:L:164:GLY:O	5:L:260:ARG:HB2	2.21	0.41
1:B:195:ARG:HB2	1:B:198:LEU:HD21	2.02	0.41
2:C:1142:ARG:CZ	2:C:1142:ARG:HB2	2.50	0.41
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	2.01	0.41
2:C:958:LYS:O	2:C:962:GLU:CG	2.69	0.41
3:D:931:THR:HG22	3:D:1244:GLN:HE21	1.84	0.41
3:D:1291:GLU:CG	3:D:1297:LYS:NZ	2.84	0.41
3:D:161:THR:HG22	3:D:164:GLN:HG3	2.02	0.41
3:D:255:LEU:HA	3:D:255:LEU:HD13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:442:ILE:HA	3:D:442:ILE:HD13	1.85	0.41
1:G:86:LYS:HE2	1:G:174:ASP:O	2.21	0.41
1:G:79:LEU:O	1:G:79:LEU:HD13	2.21	0.41
1:H:133:LEU:CD1	1:H:140:ILE:HD13	2.50	0.41
1:H:43:LEU:CD1	1:H:43:LEU:N	2.83	0.41
2:I:1069:ARG:NH2	2:I:1231:TYR:HB3	2.35	0.41
2:I:1278:LEU:HD21	3:J:484:MET:HE1	2.03	0.41
2:I:660:VAL:HG11	3:J:769:VAL:HG13	2.03	0.41
2:I:699:LEU:HA	2:I:699:LEU:HD23	1.44	0.41
2:I:882:ILE:HG13	2:I:919:ARG:NH1	2.36	0.41
3:J:1372:ARG:O	3:J:1375:ALA:HB3	2.20	0.41
3:J:57:PHE:CD2	3:J:57:PHE:N	2.87	0.41
3:J:582:ILE:HG22	3:J:620:PHE:CE1	2.55	0.41
3:J:814:CYS:SG	3:J:889:ASP:N	2.93	0.41
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.77	0.41
5:L:557:LYS:O	5:L:561:MET:HB2	2.20	0.41
1:B:95:LYS:HG3	1:B:120:ASP:OD2	2.21	0.41
2:C:1259:LEU:HG	2:C:1260:GLY:N	2.31	0.41
2:C:531:LEU:HD11	6:C:2001:KNG:C14	2.50	0.41
2:C:568:ASN:HA	2:C:571:LEU:HD12	2.03	0.41
2:C:857:VAL:HB	2:C:861:ALA:HB3	2.01	0.41
2:C:953:LEU:HD12	2:C:953:LEU:HA	1.76	0.41
3:D:1343:GLU:C	3:D:1344:LEU:HD12	2.41	0.41
3:D:147:ILE:O	3:D:147:ILE:HG13	2.21	0.41
3:D:337:ARG:O	3:D:341:ASN:CB	2.68	0.41
3:D:363:LEU:HD23	3:D:487:THR:HG22	2.02	0.41
3:D:474:LEU:HD23	4:E:28:ARG:HG2	2.03	0.41
3:D:528:THR:HG23	3:D:529:GLY:N	2.36	0.41
3:D:93:THR:CG2	3:D:94:GLN:N	2.84	0.41
3:D:298:MET:SD	5:F:406:GLN:HG3	2.61	0.41
5:F:490:PRO:O	5:F:491:GLU:HG2	2.21	0.41
2:I:978:VAL:HG21	2:I:1010:GLN:CD	2.41	0.41
2:I:1287:LEU:HD22	3:J:1357:ILE:HG13	2.02	0.41
2:I:623:LEU:HD23	2:I:623:LEU:N	2.36	0.41
3:J:1263:LYS:HZ2	3:J:1315:ALA:CB	2.32	0.41
3:J:139:LEU:HD23	3:J:139:LEU:HA	1.84	0.41
3:J:22:ILE:O	3:J:1339:GLY:HA2	2.20	0.41
3:J:38:VAL:HG13	3:J:55:GLY:C	2.41	0.41
3:J:722:ILE:HD11	3:J:740:LEU:CD2	2.40	0.41
3:J:701:LEU:HD13	3:J:723:TYR:HB2	2.01	0.41
3:J:93:THR:HG22	3:J:94:GLN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:276:MET:HG2	5:L:351:THR:HG21	2.03	0.41
5:L:296:LYS:HB2	5:L:329:LYS:HD3	2.03	0.41
2:C:1037:THR:O	2:C:1037:THR:HG22	2.20	0.41
2:C:1112:ILE:HD11	3:D:639:VAL:CG1	2.50	0.41
2:C:1308:ILE:HG23	3:D:380:PHE:CD2	2.56	0.41
2:C:247:ARG:HB2	2:C:274:ILE:CD1	2.51	0.41
2:C:637:ARG:HB3	2:C:642:SER:HB3	2.02	0.41
3:D:124:ILE:HG12	3:D:237:MET:SD	2.61	0.41
3:D:239:LEU:HA	3:D:239:LEU:HD23	1.77	0.41
3:D:310:GLY:HA2	3:D:314:ARG:HD2	2.02	0.41
2:C:1240:ASP:HB3	3:D:445:LYS:NZ	2.35	0.41
3:D:517:CYS:CA	3:D:716:GLN:HE22	2.34	0.41
3:D:825:VAL:O	3:D:826:ILE:HG13	2.21	0.41
2:C:898:GLU:OE2	5:F:541:ARG:NH1	2.54	0.41
1:H:107:ILE:HG13	1:H:136:GLU:O	2.21	0.41
1:H:28:LEU:HD23	1:H:31:LEU:HD11	2.03	0.41
2:I:1294:LYS:CB	3:J:347:VAL:HG13	2.51	0.41
2:I:239:MET:O	2:I:284:LEU:HD12	2.21	0.41
2:I:26:TYR:HE2	2:I:32:LEU:CD1	2.28	0.41
2:I:27:LEU:HD12	2:I:524:ILE:CD1	2.50	0.41
2:I:41:GLN:NE2	2:I:73:TYR:O	2.53	0.41
2:I:496:LYS:O	2:I:500:ALA:HB2	2.21	0.41
2:I:516:ASP:CG	2:I:522:SER:OG	2.58	0.41
2:I:590:PRO:CB	2:I:655:VAL:HG21	2.50	0.41
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.54	0.41
3:J:923:ILE:HD13	3:J:923:ILE:HG21	1.81	0.41
5:L:489:MET:CB	5:L:490:PRO:CD	2.99	0.41
1:A:65:LEU:HA	1:A:65:LEU:HD13	1.63	0.41
1:B:125:LYS:HG3	1:B:128:HIS:HB2	2.03	0.41
1:A:218:ARG:NH1	1:B:231:PHE:C	2.75	0.41
2:C:290:GLU:HG2	2:C:319:LEU:HD12	1.99	0.41
2:C:385:PHE:CE2	2:C:390:PHE:HE2	2.39	0.41
2:C:615:VAL:HG21	2:C:645:PHE:CD2	2.55	0.41
3:D:806:ASP:HA	3:D:1347:LEU:HD13	2.02	0.41
3:D:657:ALA:O	3:D:661:VAL:HG12	2.21	0.41
3:D:664:ILE:CD1	3:D:681:LYS:HG2	2.51	0.41
3:D:801:VAL:O	3:D:805:GLN:HB2	2.21	0.41
5:F:324:LYS:HB3	5:F:325:PRO:HD2	2.03	0.41
1:H:124:VAL:HB	1:H:210:THR:HG22	2.03	0.41
2:I:972:PHE:CZ	2:I:1018:TYR:CE1	3.09	0.41
2:I:976:ARG:HD2	2:I:989:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:883:ARG:HH12	3:J:897:HIS:HD2	1.66	0.41
1:B:51:MET:HG2	1:B:179:PRO:HD2	2.03	0.40
1:B:210:THR:O	1:B:211:ILE:HG12	2.20	0.40
2:C:1293:VAL:HG11	2:C:1304:MET:HE2	2.02	0.40
2:C:606:LEU:N	2:C:606:LEU:HD12	2.36	0.40
2:C:716:ALA:HB2	2:C:767:GLN:HE22	1.86	0.40
2:C:803:ALA:HB2	2:C:1094:VAL:HG21	2.03	0.40
3:D:174:ASP:O	3:D:175:GLU:CG	2.69	0.40
3:D:349:TYR:CG	3:D:472:LEU:HD21	2.56	0.40
3:D:647:PRO:HD3	3:D:697:MET:HB3	2.03	0.40
3:D:478:LEU:HD12	4:E:24:ALA:CA	2.51	0.40
1:G:104:LYS:HG2	1:G:110:VAL:CG2	2.38	0.40
1:G:31:LEU:HA	1:G:31:LEU:HD23	1.79	0.40
1:G:46:ILE:HD11	1:H:38:THR:HG21	2.03	0.40
1:G:231:PHE:CB	1:H:218:ARG:HD3	2.51	0.40
2:I:971:LEU:CD2	2:I:1018:TYR:HB2	2.50	0.40
2:I:1113:LEU:HD12	2:I:1113:LEU:N	2.36	0.40
2:I:11:ILE:HG22	2:I:1149:TYR:CZ	2.56	0.40
3:J:1264:ALA:HB3	3:J:1280:VAL:HG22	2.02	0.40
3:J:688:ALA:O	3:J:691:ASP:HB2	2.20	0.40
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.31	0.40
5:L:470:MET:HE2	5:L:478:PRO:CB	2.32	0.40
1:B:11:PRO:HB2	1:B:28:LEU:CD1	2.44	0.40
2:C:1015:ALA:O	2:C:1018:TYR:HB3	2.21	0.40
2:C:1158:LYS:O	2:C:1159:VAL:CB	2.69	0.40
2:C:1271:GLY:HA3	3:D:343:LEU:CD2	2.45	0.40
2:C:13:LYS:O	2:C:1183:ALA:N	2.47	0.40
2:C:513:GLN:HG3	2:C:526:HIS:CE1	2.56	0.40
2:C:548:ARG:NH2	2:C:571:LEU:CD1	2.84	0.40
2:C:738:GLU:HG2	2:C:741:MET:HE1	2.02	0.40
3:D:245:LEU:HA	3:D:245:LEU:HD12	1.84	0.40
2:C:1271:GLY:CA	3:D:343:LEU:HD21	2.45	0.40
3:D:34:SER:HB2	3:D:104:HIS:HB3	2.02	0.40
3:D:564:VAL:HG12	3:D:565:ALA:N	2.36	0.40
3:D:844:THR:HG21	3:D:858:VAL:HG21	2.02	0.40
3:D:902:ASP:O	3:D:903:LEU:HB2	2.20	0.40
4:E:39:VAL:HG21	4:E:56:GLU:HG3	2.03	0.40
1:G:13:LEU:HB3	1:H:231:PHE:HZ	1.85	0.40
1:G:228:LEU:HA	1:G:228:LEU:HD23	1.79	0.40
1:G:231:PHE:CE1	1:H:221:ALA:HB3	2.56	0.40
1:H:228:LEU:HD23	1:H:228:LEU:HA	1.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1290:MET:O	3:J:347:VAL:HG21	2.21	0.40
2:I:306:THR:OG1	2:I:308:GLU:HB2	2.21	0.40
2:I:525:THR:HG21	2:I:687:ARG:HD2	2.02	0.40
2:I:905:ILE:HD11	5:L:598:LEU:HD13	2.03	0.40
2:I:9:LYS:HG2	2:I:1171:ARG:HD3	2.03	0.40
3:J:162:GLU:O	3:J:163:GLU:C	2.58	0.40
5:L:224:LEU:HB2	5:L:259:PHE:CZ	2.57	0.40
5:L:437:GLN:HG3	5:L:438:ALA:N	2.35	0.40
5:L:481:GLU:O	5:L:484:ALA:HB3	2.22	0.40
5:L:484:ALA:CB	5:L:491:GLU:OE2	2.69	0.40
1:B:112:ALA:O	1:B:115:ILE:CD1	2.68	0.40
1:B:197:ASP:O	1:B:197:ASP:CG	2.59	0.40
1:B:74:VAL:HG12	1:B:76:GLU:H	1.86	0.40
2:C:971:LEU:HG	2:C:1014:LEU:HD23	2.03	0.40
2:C:1151:LEU:HD12	2:C:1198:LEU:HD23	2.01	0.40
2:C:11:ILE:HG22	2:C:11:ILE:O	2.21	0.40
2:C:79:VAL:HG23	2:C:80:PHE:H	1.86	0.40
3:D:1231:ARG:HA	3:D:1234:VAL:HG22	2.02	0.40
3:D:238:ILE:HA	3:D:238:ILE:HD13	1.82	0.40
3:D:242:LEU:HD23	3:D:243:PRO:N	2.36	0.40
3:D:638:SER:O	3:D:721:SER:CB	2.70	0.40
3:D:755:ILE:HD12	3:D:774:ILE:CG2	2.50	0.40
3:D:478:LEU:CD1	4:E:24:ALA:HA	2.52	0.40
4:E:26:ARG:NE	4:E:53:GLU:OE1	2.55	0.40
5:F:105:MET:HE2	5:F:385:ARG:HG2	2.00	0.40
1:H:19:VAL:HB	1:H:23:HIS:NE2	2.37	0.40
1:H:79:LEU:C	1:H:79:LEU:HD13	2.41	0.40
1:H:92:VAL:HA	1:H:120:ASP:O	2.21	0.40
2:I:15:PHE:CE1	2:I:1151:LEU:HD13	2.57	0.40
2:I:299:LYS:HG2	2:I:334:GLU:OE1	2.21	0.40
2:I:208:ILE:HD11	2:I:356:THR:HG21	2.04	0.40
2:I:617:ALA:HB3	2:I:653:MET:CB	2.52	0.40
2:I:646:SER:CB	2:I:649:GLN:HG3	2.36	0.40
3:J:288:PRO:CG	3:J:291:ILE:HD12	2.52	0.40
3:J:427:PRO:O	3:J:429:LEU:HD22	2.21	0.40
5:L:295:CYS:SG	5:L:333:VAL:HB	2.61	0.40
5:L:518:HIS:O	5:L:519:LEU:C	2.59	0.40
1:A:211:ILE:HG22	1:A:216:ALA:HB2	1.98	0.40
1:B:89:ALA:CB	1:B:124:VAL:HG12	2.49	0.40
1:B:71:LYS:HE2	1:B:139:SER:O	2.21	0.40
1:B:14:VAL:O	1:B:15:ASP:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:TYR:CE2	3:D:536:LEU:CD2	2.99	0.40
2:C:263:VAL:CG2	2:C:273:HIS:HB3	2.52	0.40
2:C:557:ARG:HH21	2:C:608:ALA:HA	1.86	0.40
2:C:623:LEU:HA	2:C:630:VAL:HG23	2.02	0.40
2:C:592:ARG:O	2:C:652:TYR:HA	2.22	0.40
3:D:161:THR:HG22	3:D:164:GLN:H	1.86	0.40
3:D:221:ILE:HG23	3:D:222:LYS:N	2.37	0.40
3:D:522:GLY:O	3:D:525:MET:HG2	2.21	0.40
2:C:1112:ILE:CD1	3:D:639:VAL:HG13	2.50	0.40
5:F:530:LEU:O	5:F:533:ASP:HB2	2.22	0.40
1:G:110:VAL:HG13	1:G:114:ASP:OD2	2.21	0.40
1:G:96:ASP:OD2	1:G:148:ARG:NH2	2.39	0.40
2:I:978:VAL:HG13	2:I:1007:LYS:HB3	2.03	0.40
2:I:870:ILE:CG1	2:I:1050:VAL:HG11	2.51	0.40
2:I:1065:LYS:HD3	2:I:1235:LEU:CD1	2.47	0.40
2:I:1301:ARG:HG3	2:I:1302:THR:N	2.36	0.40
2:I:632:ASP:O	2:I:647:ARG:HB2	2.21	0.40
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.73	0.40
3:J:127:LEU:HD23	3:J:189:LEU:HD22	2.04	0.40
3:J:395:LYS:HG2	5:L:536:THR:HG21	2.04	0.40
3:J:611:ILE:CG2	3:J:612:LEU:HD12	2.48	0.40
3:J:914:ALA:O	3:J:918:ILE:HG23	2.21	0.40
4:K:10:VAL:CG1	4:K:16:ARG:HB2	2.49	0.40
5:L:253:SER:O	5:L:257:LYS:HG3	2.22	0.40
1:B:124:VAL:HG21	1:B:209:GLY:O	2.21	0.40
2:C:1106:ARG:HD2	2:C:1106:ARG:N	2.34	0.40
2:C:209:ILE:HD13	2:C:209:ILE:HG21	1.81	0.40
2:C:325:LEU:O	2:C:330:HIS:HB2	2.21	0.40
2:C:517:GLN:O	2:C:517:GLN:HG2	2.21	0.40
2:C:698:PRO:HD3	2:C:795:ALA:CA	2.51	0.40
2:C:818:VAL:O	2:C:1079:ILE:HD12	2.20	0.40
3:D:1291:GLU:CG	3:D:1297:LYS:HZ3	2.35	0.40
3:D:434:ILE:HG21	3:D:434:ILE:HD13	1.73	0.40
3:D:822:MET:SD	3:D:838:ARG:HB3	2.61	0.40
3:D:8:LEU:CD2	3:D:9:LYS:N	2.85	0.40
5:F:311:THR:HG21	5:F:348:GLU:OE2	2.21	0.40
1:G:107:ILE:HG13	1:G:136:GLU:HA	2.02	0.40
2:I:1246:ARG:NH2	2:I:1249:GLY:H	2.19	0.40
2:I:690:VAL:HG22	2:I:691:PRO:HD2	2.04	0.40
2:I:708:VAL:HG11	2:I:794:LEU:HD22	2.03	0.40
2:I:1334:GLY:O	3:J:25:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:557:LYS:CD	3:J:611:ILE:HG23	2.52	0.40
3:J:814:CYS:SG	3:J:889:ASP:HB3	2.61	0.40
3:J:850:LYS:CD	3:J:875:ASN:ND2	2.85	0.40
5:L:251:LYS:HA	5:L:254:GLU:HG2	2.03	0.40
5:L:296:LYS:HD3	5:L:296:LYS:HA	1.97	0.40
5:L:544:THR:HA	5:L:547:VAL:HG12	2.03	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	225/329 (68%)	198 (88%)	20 (9%)	7 (3%)	4 31
1	B	210/329 (64%)	186 (89%)	19 (9%)	5 (2%)	6 35
1	G	222/329 (68%)	194 (87%)	23 (10%)	5 (2%)	6 36
1	H	211/329 (64%)	187 (89%)	17 (8%)	7 (3%)	4 29
2	C	1335/1342 (100%)	1226 (92%)	100 (8%)	9 (1%)	22 60
2	I	1324/1342 (99%)	1220 (92%)	96 (7%)	8 (1%)	25 63
3	D	1162/1407 (83%)	1068 (92%)	86 (7%)	8 (1%)	22 60
3	J	1151/1407 (82%)	1060 (92%)	78 (7%)	13 (1%)	14 50
4	E	87/91 (96%)	82 (94%)	4 (5%)	1 (1%)	14 50
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100 100
5	F	462/613 (75%)	426 (92%)	35 (8%)	1 (0%)	47 80
5	L	463/613 (76%)	426 (92%)	36 (8%)	1 (0%)	47 80
All	All	6929/8222 (84%)	6347 (92%)	517 (8%)	65 (1%)	17 54

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PRO
1	B	13	LEU
1	B	29	GLU
2	C	2	VAL
2	C	3	TYR
2	C	535	PRO
2	C	697	LYS
2	C	1159	VAL
3	D	332	LYS
1	G	162	GLU
1	G	167	PRO
1	H	135	ASP
2	I	1159	VAL
3	J	332	LYS
1	A	162	GLU
1	A	233	ASP
1	B	135	ASP
1	B	136	GLU
2	C	170	VAL
1	G	14	VAL
1	H	136	GLU
1	H	177	TYR
2	I	170	VAL
3	J	334	LYS
2	C	1158	LYS
2	I	697	LYS
3	J	337	ARG
2	C	484	LEU
3	D	710	ASP
3	D	806	ASP
1	G	62	ASP
1	H	20	SER
1	H	62	ASP
1	H	138	ALA
1	H	157	THR
2	I	484	LEU
3	J	338	PHE
3	J	342	LEU
3	J	344	GLY
3	J	710	ASP
1	A	14	VAL
1	A	196	THR
1	A	232	VAL

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Mol	Chain	Res	Type
3	D	12	THR
2	I	1136	GLN
2	I	1158	LYS
3	J	333	GLY
3	J	345	LYS
3	J	806	ASP
1	B	14	VAL
3	D	345	LYS
3	D	831	VAL
2	I	63	SER
2	C	1186	VAL
4	E	86	ILE
3	J	831	VAL
5	F	477	GLU
1	G	159	ILE
3	J	826	ILE
3	D	826	ILE
5	L	477	GLU
3	D	1180	VAL
2	I	1186	VAL
3	J	336	GLY
1	A	159	ILE

5.3.2 Protein sidechains (i)

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	194/286 (68%)	180 (93%)	14 (7%)	14 42
1	B	182/286 (64%)	172 (94%)	10 (6%)	21 50
1	G	191/286 (67%)	177 (93%)	14 (7%)	14 41
1	H	184/286 (64%)	176 (96%)	8 (4%)	29 56
2	C	1151/1157 (100%)	1045 (91%)	106 (9%)	9 32
2	I	1147/1157 (99%)	1042 (91%)	105 (9%)	9 32
3	D	970/1168 (83%)	868 (90%)	102 (10%)	7 27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	J	960/1168 (82%)	863 (90%)	97 (10%)	7 28
4	E	72/75 (96%)	64 (89%)	8 (11%)	6 25
4	K	67/75 (89%)	63 (94%)	4 (6%)	19 47
5	F	417/540 (77%)	375 (90%)	42 (10%)	7 28
5	L	418/540 (77%)	377 (90%)	41 (10%)	8 29
All	All	5953/7024 (85%)	5402 (91%)	551 (9%)	9 32

All (551) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	19	VAL
1	A	26	VAL
1	A	50	SER
1	A	61	ILE
1	A	74	VAL
1	A	115	ILE
1	A	133	LEU
1	A	145	LYS
1	A	168	ILE
1	A	215	GLU
1	A	219	ARG
1	A	231	PHE
1	B	8	PHE
1	B	9	LEU
1	B	13	LEU
1	B	50	SER
1	B	61	ILE
1	B	115	ILE
1	B	186	ASN
1	B	194	GLN
1	B	215	GLU
1	B	231	PHE
2	C	11	ILE
2	C	22	LEU
2	C	39	ILE
2	C	46	GLN
2	C	60	GLN
2	C	70	TYR

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Mol	Chain	Res	Type
2	C	82	VAL
2	C	85	CYS
2	C	90	VAL
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	132	ASP
2	C	167	SER
2	C	189	ASP
2	C	285	ILE
2	C	299	LYS
2	C	306	THR
2	C	320	ASP
2	C	360	LEU
2	C	369	MET
2	C	377	THR
2	C	394	ARG
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	496	LYS
2	C	518	ASN
2	C	531	LEU
2	C	554	HIS
2	C	589	THR
2	C	604	HIS
2	C	607	SER
2	C	609	ILE
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU

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Mol	Chain	Res	Type
2	C	633	LEU
2	C	639	LYS
2	C	657	THR
2	C	672	GLU
2	C	680	LEU
2	C	684	ASN
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER
2	C	799	ASN
2	C	800	MET
2	C	814	ASP
2	C	817	LEU
2	C	819	SER
2	C	826	ASP
2	C	840	SER
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	919	ARG
2	C	944	ARG
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	992	LEU
2	C	1002	LEU
2	C	1006	GLU
2	C	1040	ASP
2	C	1073	LYS
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN

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Mol	Chain	Res	Type
2	C	1136	GLN
2	C	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1159	VAL
2	C	1198	LEU
2	C	1210	ILE
2	C	1237	HIS
2	C	1238	LEU
2	C	1264	GLN
2	C	1265	PHE
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1341	ASP
2	C	1342	GLU
3	D	8	LEU
3	D	18	ASP
3	D	26	SER
3	D	29	MET
3	D	46	TYR
3	D	54	ASP
3	D	79	LYS
3	D	84	ILE
3	D	92	VAL
3	D	94	GLN
3	D	95	THR
3	D	98	ARG
3	D	159	ILE
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	217	LEU
3	D	230	SER
3	D	252	LEU
3	D	312	ARG
3	D	324	LEU
3	D	352	ARG
3	D	363	LEU
3	D	374	LEU
3	D	425	ARG

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Mol	Chain	Res	Type
3	D	430	HIS
3	D	454	CYS
3	D	490	ILE
3	D	506	VAL
3	D	507	VAL
3	D	513	MET
3	D	514	THR
3	D	523	GLU
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	567	THR
3	D	568	SER
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	704	GLU
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	740	LEU
3	D	746	LEU
3	D	754	ILE
3	D	764	ARG
3	D	770	LEU
3	D	788	LEU
3	D	798	ARG
3	D	805	GLN
3	D	810	THR
3	D	844	THR

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Mol	Chain	Res	Type
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	881	LYS
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	931	THR
3	D	1135	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1202	GLU
3	D	1221	LEU
3	D	1255	VAL
3	D	1273	ASP
3	D	1274	PHE
3	D	1275	LEU
3	D	1278	GLU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1298	VAL
3	D	1333	THR
3	D	1343	GLU
4	E	5	THR
4	E	13	ILE
4	E	16	ARG
4	E	28	ARG
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
4	E	84	THR

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Mol	Chain	Res	Type
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	154	GLU
5	F	267	ASP
5	F	297	MET
5	F	301	ASN
5	F	306	PHE
5	F	310	GLU
5	F	335	GLU
5	F	341	LEU
5	F	395	THR
5	F	417	ASP
5	F	422	ARG
5	F	429	THR
5	F	437	GLN
5	F	445	ASP
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	482	GLU
5	F	485	GLU
5	F	486	ARG
5	F	488	LEU
5	F	489	MET
5	F	491	GLU
5	F	492	ASP
5	F	508	GLU
5	F	530	LEU
5	F	547	VAL
5	F	558	VAL
5	F	561	MET
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	580	PHE
5	F	587	ILE
5	F	606	VAL
5	F	612	ASP

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Mol	Chain	Res	Type
1	G	9	LEU
1	G	13	LEU
1	G	19	VAL
1	G	26	VAL
1	G	50	SER
1	G	61	ILE
1	G	74	VAL
1	G	115	ILE
1	G	133	LEU
1	G	145	LYS
1	G	168	ILE
1	G	215	GLU
1	G	219	ARG
1	G	231	PHE
1	H	13	LEU
1	H	19	VAL
1	H	26	VAL
1	H	45	ARG
1	H	50	SER
1	H	61	ILE
1	H	115	ILE
1	H	215	GLU
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	60	GLN
2	I	70	TYR
2	I	82	VAL
2	I	85	CYS
2	I	90	VAL
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	119	GLU
2	I	121	GLU
2	I	132	ASP
2	I	167	SER
2	I	189	ASP
2	I	285	ILE
2	I	299	LYS

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Mol	Chain	Res	Type
2	I	306	THR
2	I	320	ASP
2	I	360	LEU
2	I	369	MET
2	I	377	THR
2	I	394	ARG
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	445	ILE
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	487	LEU
2	I	490	GLN
2	I	493	ILE
2	I	496	LYS
2	I	518	ASN
2	I	554	HIS
2	I	589	THR
2	I	604	HIS
2	I	607	SER
2	I	609	ILE
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU
2	I	633	LEU
2	I	639	LYS
2	I	657	THR
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	799	ASN
2	I	800	MET
2	I	814	ASP

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Mol	Chain	Res	Type
2	I	817	LEU
2	I	819	SER
2	I	826	ASP
2	I	840	SER
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	919	ARG
2	I	944	ARG
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	984	VAL
2	I	992	LEU
2	I	1002	LEU
2	I	1006	GLU
2	I	1040	ASP
2	I	1073	LYS
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1159	VAL
2	I	1198	LEU
2	I	1210	ILE
2	I	1237	HIS
2	I	1238	LEU
2	I	1246	ARG
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1327	LEU
2	I	1331	ARG
2	I	1341	ASP

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Mol	Chain	Res	Type
2	I	1342	GLU
3	J	18	ASP
3	J	26	SER
3	J	29	MET
3	J	46	TYR
3	J	54	ASP
3	J	79	LYS
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR
3	J	159	ILE
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	217	LEU
3	J	251	PRO
3	J	252	LEU
3	J	312	ARG
3	J	324	LEU
3	J	352	ARG
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	425	ARG
3	J	454	CYS
3	J	490	ILE
3	J	507	VAL
3	J	513	MET
3	J	514	THR
3	J	523	GLU
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	567	THR
3	J	568	SER
3	J	573	THR
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL
3	J	678	ARG

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Mol	Chain	Res	Type
3	J	680	ASN
3	J	683	ILE
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	702	GLN
3	J	704	GLU
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN
3	J	740	LEU
3	J	746	LEU
3	J	754	ILE
3	J	770	LEU
3	J	788	LEU
3	J	798	ARG
3	J	803	VAL
3	J	805	GLN
3	J	810	THR
3	J	844	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
3	J	881	LYS
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	931	THR
3	J	1155	ILE
3	J	1163	VAL
3	J	1170	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG

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Mol	Chain	Res	Type
3	J	1221	LEU
3	J	1255	VAL
3	J	1273	ASP
3	J	1274	PHE
3	J	1275	LEU
3	J	1278	GLU
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1298	VAL
3	J	1333	THR
3	J	1343	GLU
4	K	13	ILE
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	154	GLU
5	L	266	PHE
5	L	267	ASP
5	L	297	MET
5	L	301	ASN
5	L	306	PHE
5	L	310	GLU
5	L	335	GLU
5	L	341	LEU
5	L	395	THR
5	L	417	ASP
5	L	422	ARG
5	L	429	THR
5	L	437	GLN
5	L	445	ASP
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	485	GLU

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Mol	Chain	Res	Type
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	491	GLU
5	L	508	GLU
5	L	530	LEU
5	L	547	VAL
5	L	558	VAL
5	L	561	MET
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	580	PHE
5	L	587	ILE
5	L	606	VAL
5	L	612	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	132	HIS
1	B	66	HIS
1	B	227	GLN
2	C	69	GLN
2	C	120	GLN
2	C	133	ASN
2	C	139	ASN
2	C	150	HIS
2	C	327	GLN
2	C	494	ASN
2	C	513	GLN
2	C	620	ASN
2	C	628	HIS
2	C	659	GLN
2	C	684	ASN
2	C	725	GLN
2	C	1080	ASN
2	C	1116	HIS
2	C	1134	GLN
2	C	1136	GLN

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Mol	Chain	Res	Type
2	C	1146	GLN
2	C	1237	HIS
2	C	1299	ASN
2	C	1313	HIS
3	D	94	GLN
3	D	200	GLN
3	D	419	HIS
3	D	424	ASN
3	D	435	GLN
3	D	560	ASN
3	D	669	GLN
3	D	702	GLN
3	D	716	GLN
3	D	777	HIS
3	D	929	GLN
3	D	1244	GLN
3	D	1295	ASN
5	F	131	GLN
5	F	362	ASN
5	F	383	ASN
5	F	406	GLN
5	F	409	ASN
5	F	446	GLN
5	F	455	HIS
5	F	472	GLN
5	F	518	HIS
1	H	66	HIS
1	H	132	HIS
2	I	20	GLN
2	I	69	GLN
2	I	139	ASN
2	I	343	HIS
2	I	494	ASN
2	I	513	GLN
2	I	824	GLN
2	I	1038	GLN
2	I	1116	HIS
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1220	GLN
2	I	1288	GLN

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Mol	Chain	Res	Type
2	I	1299	ASN
2	I	1313	HIS
2	I	1314	GLN
3	J	94	GLN
3	J	200	GLN
3	J	419	HIS
3	J	450	HIS
3	J	469	HIS
3	J	488	ASN
3	J	594	GLN
3	J	669	GLN
3	J	702	GLN
3	J	716	GLN
3	J	777	HIS
3	J	792	ASN
3	J	861	ASN
3	J	897	HIS
3	J	1259	GLN
3	J	1279	GLN
3	J	1366	HIS
4	K	61	ASN
5	L	131	GLN
5	L	147	GLN
5	L	227	GLN
5	L	362	ASN
5	L	446	GLN
5	L	455	HIS
5	L	472	GLN

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 (i)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	KNG	C	2001	-	72,75,75	3.87	30 (41%)	101,114,114	3.01	40 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	KNG	C	2001	-	-	36/74/113/113	0/5/6/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2001	KNG	O18-C46	-14.63	1.20	1.44
6	C	2001	KNG	O17-C47	-9.86	1.21	1.43
6	C	2001	KNG	O03-C06	9.82	1.56	1.37
6	C	2001	KNG	C04-C10	8.96	1.59	1.43
6	C	2001	KNG	O16-C37	8.26	1.62	1.42
6	C	2001	KNG	O11-C04	-6.12	1.19	1.36
6	C	2001	KNG	C12-C11	-5.77	1.31	1.54
6	C	2001	KNG	C02-C01	5.38	1.55	1.40
6	C	2001	KNG	O17-C50	5.38	1.50	1.41
6	C	2001	KNG	O06-C37	-5.36	1.27	1.41
6	C	2001	KNG	O12-C39	5.36	1.44	1.34
6	C	2001	KNG	C03-C02	5.32	1.47	1.39
6	C	2001	KNG	C03-C04	5.31	1.49	1.37
6	C	2001	KNG	O18-C50	5.18	1.50	1.41
6	C	2001	KNG	C19-C18	-5.18	1.35	1.53
6	C	2001	KNG	C01-C09	5.14	1.59	1.43
6	C	2001	KNG	O07-C25	-4.83	1.37	1.44
6	C	2001	KNG	O01-C01	-4.65	1.20	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2001	KNG	C47-C48	4.24	1.60	1.52
6	C	2001	KNG	C43-C40	-4.04	1.51	1.56
6	C	2001	KNG	C47-C46	3.44	1.62	1.52
6	C	2001	KNG	C02-N01	3.28	1.48	1.41
6	C	2001	KNG	C15-N01	3.25	1.42	1.35
6	C	2001	KNG	O10-C15	-2.78	1.18	1.23
6	C	2001	KNG	C32-C22	-2.75	1.47	1.53
6	C	2001	KNG	C27-C28	2.61	1.59	1.50
6	C	2001	KNG	O05-C29	2.34	1.45	1.39
6	C	2001	KNG	C49-C48	-2.28	1.46	1.51
6	C	2001	KNG	O04-C11	-2.25	1.18	1.21
6	C	2001	KNG	O16-C48	2.25	1.49	1.44

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	2001	KNG	C34-C26-C27	-8.72	93.15	110.93
6	C	2001	KNG	C49-C48-C47	8.51	126.36	113.41
6	C	2001	KNG	C25-C26-C27	7.48	132.41	112.02
6	C	2001	KNG	C24-C23-C22	7.46	127.92	115.43
6	C	2001	KNG	O03-C06-C07	6.85	132.93	121.14
6	C	2001	KNG	O07-C35-C36	6.85	123.69	111.09
6	C	2001	KNG	C23-C22-C21	-6.79	98.90	112.54
6	C	2001	KNG	C45-C46-C47	-6.21	107.46	114.78
6	C	2001	KNG	C12-C11-C05	6.19	119.42	107.30
6	C	2001	KNG	C25-O07-C35	-6.14	108.21	117.72
6	C	2001	KNG	O07-C25-C26	-5.70	94.25	107.50
6	C	2001	KNG	O10-C15-N01	-5.16	112.92	123.92
6	C	2001	KNG	O04-C11-C05	-4.75	122.75	131.81
6	C	2001	KNG	C33-C24-C23	-4.26	102.78	111.39
6	C	2001	KNG	C34-C26-C25	-4.15	103.96	111.40
6	C	2001	KNG	O13-C39-C40	-4.03	112.56	123.82
6	C	2001	KNG	C18-C19-C20	3.95	122.11	114.59
6	C	2001	KNG	C23-C24-C25	3.70	117.84	110.61
6	C	2001	KNG	C02-N01-C15	-3.62	116.70	126.80
6	C	2001	KNG	C18-C17-C16	-3.46	121.72	129.08
6	C	2001	KNG	O07-C35-O08	-3.42	116.17	122.96
6	C	2001	KNG	C19-C20-C21	3.29	118.28	112.43
6	C	2001	KNG	C37-C45-C46	-3.04	105.25	111.11
6	C	2001	KNG	C13-C12-C11	-2.92	106.67	113.90
6	C	2001	KNG	C26-C25-C24	2.82	120.44	114.68
6	C	2001	KNG	C01-C02-N01	2.80	125.80	117.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	2001	KNG	C16-C15-N01	2.75	125.85	116.11
6	C	2001	KNG	C03-C02-N01	-2.72	114.71	121.90
6	C	2001	KNG	O19-C23-C24	-2.70	103.47	109.49
6	C	2001	KNG	O09-C21-C22	-2.61	103.67	109.49
6	C	2001	KNG	C38-C31-C20	2.56	117.98	113.39
6	C	2001	KNG	C43-C40-C39	-2.52	101.34	109.26
6	C	2001	KNG	O03-C06-C05	-2.44	106.80	113.57
6	C	2001	KNG	O11-C04-C03	-2.39	114.16	121.17
6	C	2001	KNG	O18-C50-O17	-2.30	103.41	107.44
6	C	2001	KNG	O16-C48-C49	-2.20	101.95	106.70
6	C	2001	KNG	O16-C48-C47	-2.18	105.07	109.13
6	C	2001	KNG	C32-C22-C23	2.13	115.69	111.39
6	C	2001	KNG	C05-C06-C07	-2.07	120.23	125.29
6	C	2001	KNG	C41-C40-C43	2.01	112.70	109.78

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	2001	KNG	C21-C22-C23-O19
6	C	2001	KNG	O19-C23-C24-C25
6	C	2001	KNG	O19-C23-C24-C33
6	C	2001	KNG	C23-C24-C25-C26
6	C	2001	KNG	C23-C24-C25-O07
6	C	2001	KNG	C33-C24-C25-C26
6	C	2001	KNG	C33-C24-C25-O07
6	C	2001	KNG	C26-C27-C28-C29
6	C	2001	KNG	O06-C27-C28-C29
6	C	2001	KNG	C38-C31-O12-C39
6	C	2001	KNG	C41-C40-C43-C44
6	C	2001	KNG	C32-C22-C23-C24
6	C	2001	KNG	C36-C35-O07-C25
6	C	2001	KNG	C32-C22-C23-O19
6	C	2001	KNG	C22-C23-C24-C33
6	C	2001	KNG	C21-C22-C23-C24
6	C	2001	KNG	C22-C23-C24-C25
6	C	2001	KNG	O08-C35-O07-C25
6	C	2001	KNG	C40-C39-O12-C31
6	C	2001	KNG	C31-C20-C21-O09
6	C	2001	KNG	C20-C21-C22-C23
6	C	2001	KNG	O10-C15-C16-C30
6	C	2001	KNG	O13-C39-O12-C31

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Mol	Chain	Res	Type	Atoms
6	C	2001	KNG	N01-C15-C16-C17
6	C	2001	KNG	C20-C21-C22-C32
6	C	2001	KNG	C39-C40-C43-C44
6	C	2001	KNG	N01-C15-C16-C30
6	C	2001	KNG	C28-C29-O05-C12
6	C	2001	KNG	C11-C12-O05-C29
6	C	2001	KNG	O03-C12-O05-C29
6	C	2001	KNG	O09-C21-C22-C32
6	C	2001	KNG	C01-C02-N01-C15
6	C	2001	KNG	O10-C15-C16-C17
6	C	2001	KNG	C42-C40-C43-C44
6	C	2001	KNG	O12-C39-C40-C43
6	C	2001	KNG	C03-C02-N01-C15

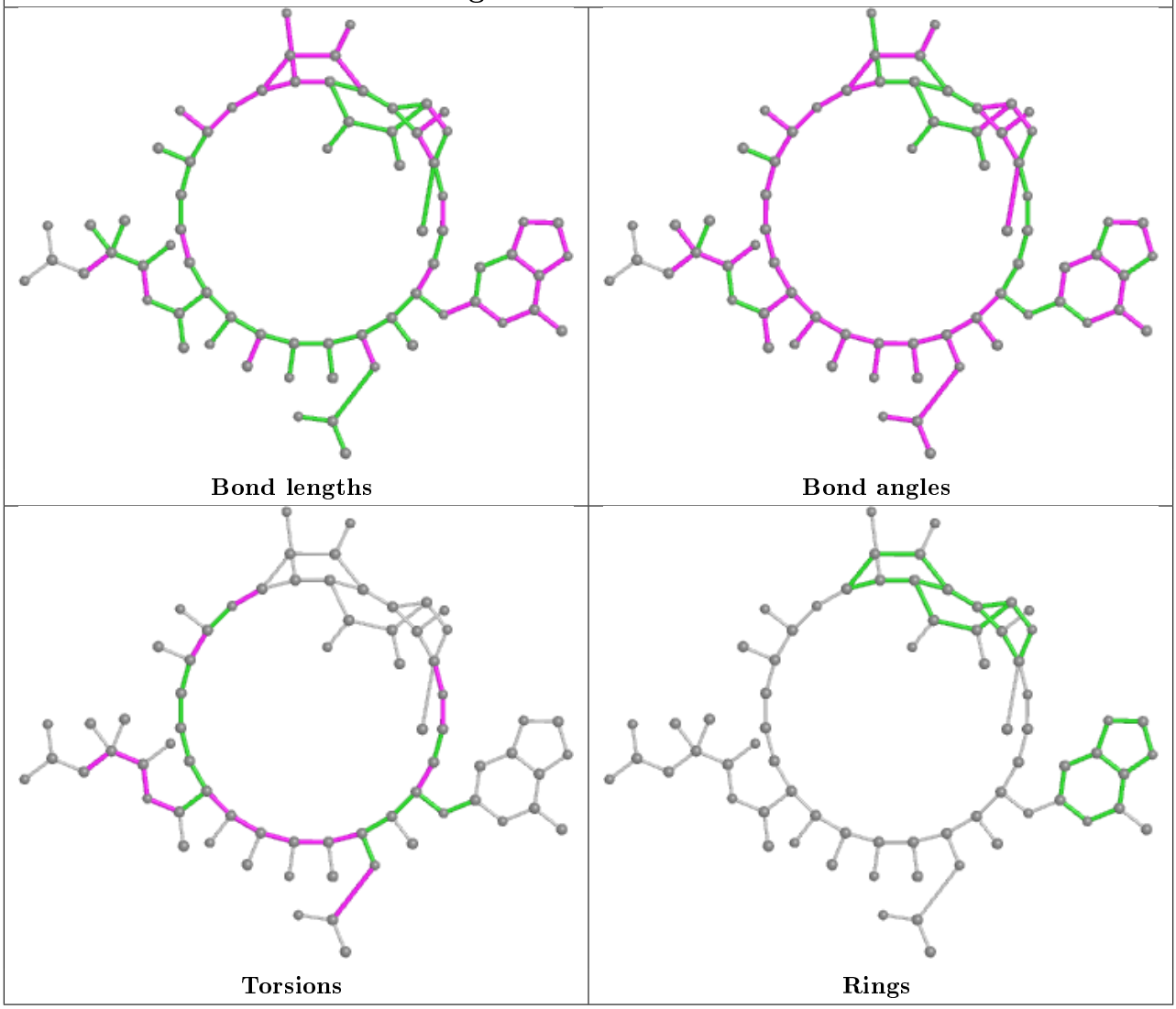
There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2001	KNG	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand KNG C 2001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	227/329 (68%)	-0.31	0 100 100	160, 212, 279, 349	0
1	B	214/329 (65%)	-0.19	4 (1%) 66 58	155, 250, 349, 390	0
1	G	224/329 (68%)	-0.28	2 (0%) 84 77	194, 274, 328, 348	0
1	H	215/329 (65%)	0.09	8 (3%) 41 33	247, 309, 348, 370	0
2	C	1339/1342 (99%)	-0.21	17 (1%) 77 68	124, 208, 314, 382	0
2	I	1328/1342 (98%)	-0.13	31 (2%) 60 51	186, 241, 336, 473	0
3	D	1166/1407 (82%)	-0.29	4 (0%) 94 90	129, 188, 298, 360	0
3	J	1155/1407 (82%)	-0.20	15 (1%) 77 68	164, 229, 312, 374	0
4	E	89/91 (97%)	-0.10	0 100 100	198, 267, 290, 306	0
4	K	79/91 (86%)	0.73	10 (12%) 3 5	329, 403, 484, 493	0
5	F	468/613 (76%)	-0.18	14 (2%) 50 39	156, 283, 413, 445	0
5	L	469/613 (76%)	-0.23	7 (1%) 73 63	193, 275, 393, 414	0
All	All	6973/8222 (84%)	-0.19	112 (1%) 72 62	124, 232, 349, 493	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	9.5
2	I	983	GLY	6.9
2	I	987	GLU	6.3
2	I	980	VAL	5.6
2	I	976	ARG	5.3
5	F	167	ASP	5.2
5	F	165	PHE	5.0
2	I	986	ALA	4.7
3	J	1175	LEU	4.5
2	I	981	ALA	4.5
2	I	979	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
5	F	301	ASN	3.8
2	C	1	MET	3.7
5	F	162	ILE	3.6
1	H	96	ASP	3.5
1	H	112	ALA	3.5
2	C	317	LEU	3.4
2	I	1003	THR	3.3
5	F	300	LYS	3.3
1	H	205	MET	3.2
4	K	5	THR	3.2
2	C	248	GLY	3.2
1	H	28	LEU	3.2
3	J	1296	GLY	3.1
5	F	305	LEU	3.1
2	C	1000	LEU	3.1
2	C	116	ASP	3.0
2	I	991	LYS	3.0
2	I	985	GLU	3.0
2	I	1006	GLU	3.0
2	I	984	VAL	2.8
2	I	1018	TYR	2.8
2	I	998	LEU	2.8
5	F	164	GLY	2.8
4	K	37	PRO	2.8
1	H	12	ARG	2.8
2	I	990	ASP	2.7
2	I	988	LYS	2.7
2	I	1020	GLU	2.7
1	H	98	VAL	2.7
2	I	973	SER	2.6
2	I	1021	LEU	2.6
3	J	849	LEU	2.6
4	K	36	ASP	2.6
5	F	259	PHE	2.6
2	C	282	VAL	2.5
4	K	61	ASN	2.5
1	H	24	ALA	2.5
2	C	272	ARG	2.5
5	F	288	MET	2.5
3	J	1151	LYS	2.4
5	L	165	PHE	2.4
2	C	292	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	100	LEU	2.4
4	K	22	VAL	2.4
2	C	206	ALA	2.4
2	I	977	ALA	2.4
2	I	975	ILE	2.3
3	J	1196	LEU	2.3
4	K	75	GLN	2.3
1	G	95	LYS	2.3
1	B	59	VAL	2.3
5	L	167	ASP	2.3
2	I	970	GLY	2.3
4	K	35	LYS	2.3
3	D	1165	PHE	2.3
2	C	266	GLY	2.3
2	C	265	LYS	2.3
3	D	213	LYS	2.3
5	F	314	THR	2.3
2	I	190	PRO	2.2
3	J	312	ARG	2.2
3	J	880	VAL	2.2
3	J	732	GLY	2.2
3	J	1297	LYS	2.2
2	C	322	LEU	2.2
2	I	989	LEU	2.2
5	L	287	ILE	2.2
5	L	427	PHE	2.2
3	D	149	GLY	2.2
4	K	47	THR	2.2
2	C	376	PRO	2.2
2	C	115	LYS	2.1
5	F	299	LYS	2.1
5	F	323	ASN	2.1
1	B	98	VAL	2.1
3	J	857	LEU	2.1
5	L	305	LEU	2.1
3	J	1165	PHE	2.1
3	J	1152	GLU	2.1
2	I	1022	LYS	2.1
2	C	253	PHE	2.1
4	K	13	ILE	2.1
2	I	1005	GLU	2.1
2	I	1017	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	J	747	MET	2.1
5	F	304	THR	2.1
3	J	1198	VAL	2.1
5	L	261	LEU	2.1
1	G	211	ILE	2.1
3	J	1201	GLY	2.0
5	L	309	ASN	2.0
1	B	97	GLU	2.0
2	I	1000	LEU	2.0
4	K	58	LEU	2.0
1	B	144	ILE	2.0
2	C	276	GLN	2.0
3	D	1186	TYR	2.0
1	H	26	VAL	2.0
2	I	1015	ALA	2.0
2	C	261	VAL	2.0
5	F	306	PHE	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	KNG	C	2001	70/70	0.93	0.28	155,226,287,292	0
8	ZN	D	1502	1/1	0.95	0.11	192,192,192,192	0
7	MG	J	1501	1/1	0.96	0.34	154,154,154,154	0
8	ZN	J	1502	1/1	0.96	0.06	215,215,215,215	0
7	MG	D	1501	1/1	0.98	0.46	196,196,196,196	0
8	ZN	D	1503	1/1	0.99	0.29	258,258,258,258	0

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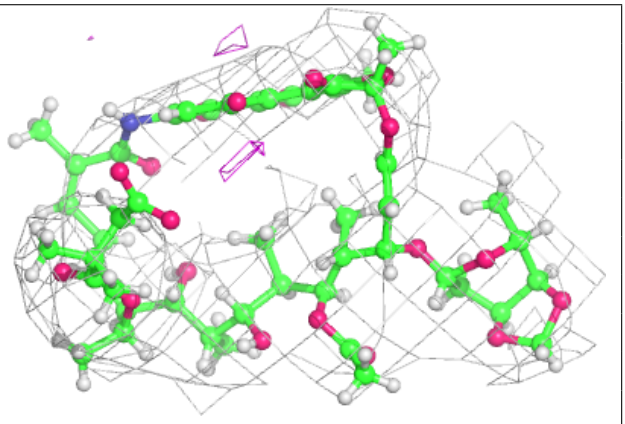
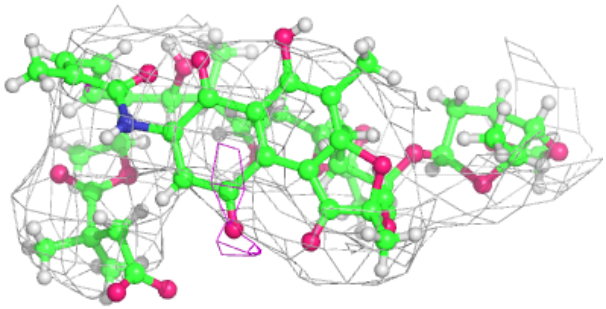
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	ZN	J	1503	1/1	0.99	0.28	197,197,197,197	0

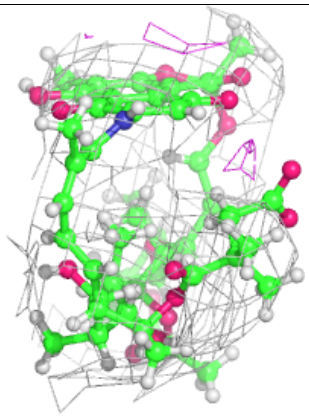
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around KNG C 2001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.