Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:39 PM GMT

PDB ID	:	4YFK
Title	:	Escherichia coli RNA polymerase in complex with squaramide compound 8.
Authors	:	Molodtsov, V.; Fleming, P.R.; Eyermann, C.J.; Ferguson, A.D.; Foulk, M.A.; McKinney, D.C.; Masse, C.E.; Buurman, E.T.; Murakami, K.S.
Deposited on	:	2015-02-25
Resolution	:	3.57 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

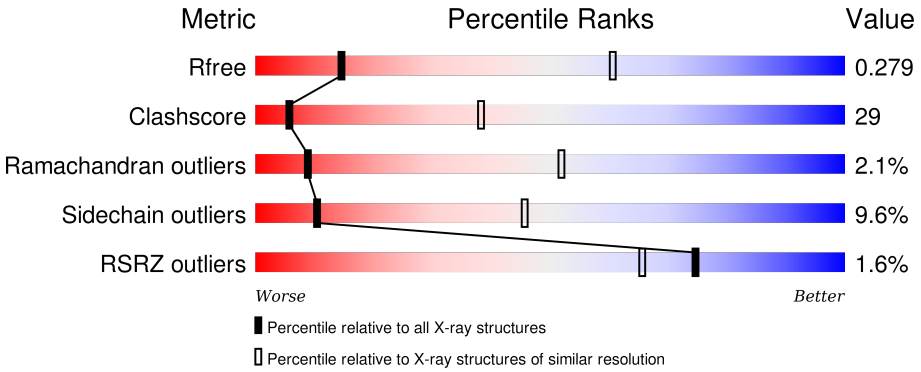
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.57 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}	91344	1261 (3.76-3.40)
Clashscore	102246	1026 (3.72-3.44)
Ramachandran outliers	100387	1028 (3.74-3.42)
Sidechain outliers	100360	1028 (3.74-3.42)
RSRZ outliers	91569	1268 (3.76-3.40)

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. 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	2% 37% 45% 14%
1	B	329	30% 33% 34%
1	G	329	33% 30% 6% 31%
1	H	329	2% 28% 34% 34%
2	C	1342	48% 46% 6%

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Mol	Chain	Length	Quality of chain
2	I	1342	3% 49% 45% 5%
3	D	1407	37% 40% 6% 17%
3	J	1407	% 39% 37% 5% 18%
4	E	91	60% 35%
4	K	91	9% 40% 43% 13%
5	F	613	2% 38% 33% 5% 24%
5	L	613	2% 33% 39% 5% 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	4C6	D	2004	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55782 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1163	Total	C	N	O	S	0	0	0
			9050	5690	1620	1694	46			
3	J	1152	Total	C	N	O	S	0	0	0
			8990	5654	1608	1682	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			

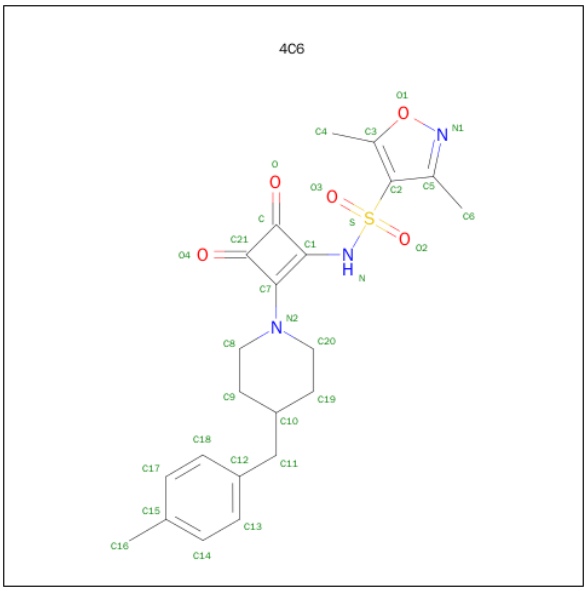
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 8 is 3,5-dimethyl-N-{2-[4-(4-methylbenzyl)piperidin-1-yl]-3,4-dioxocyclobut-1-en-1-yl}-1,2-oxazole-4-sulfonamide (three-letter code: 4C6) (formula: $C_{22}H_{25}N_3O_5S$).



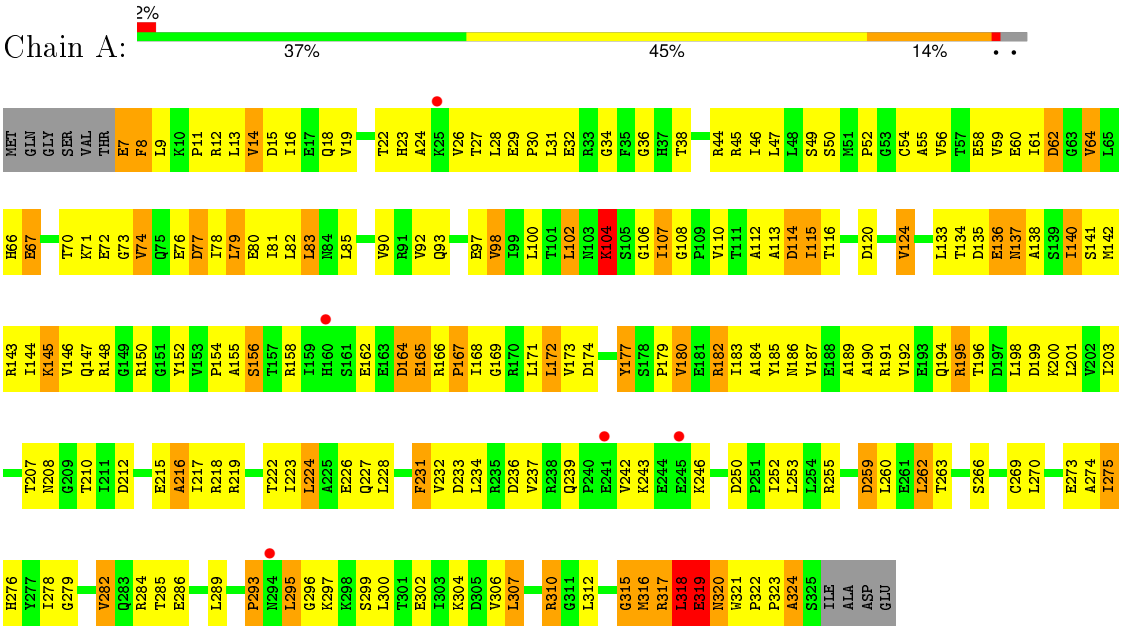
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			31	22	3	5	1		
8	J	1	Total	C	N	O	S	0	0
			31	22	3	5	1		

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 errors 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.

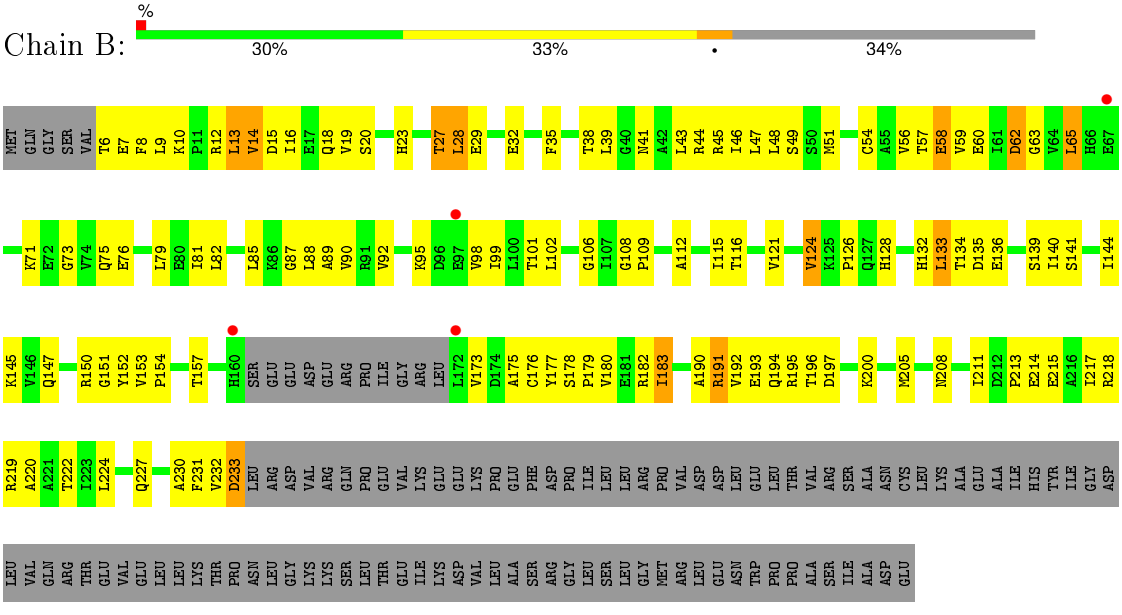
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



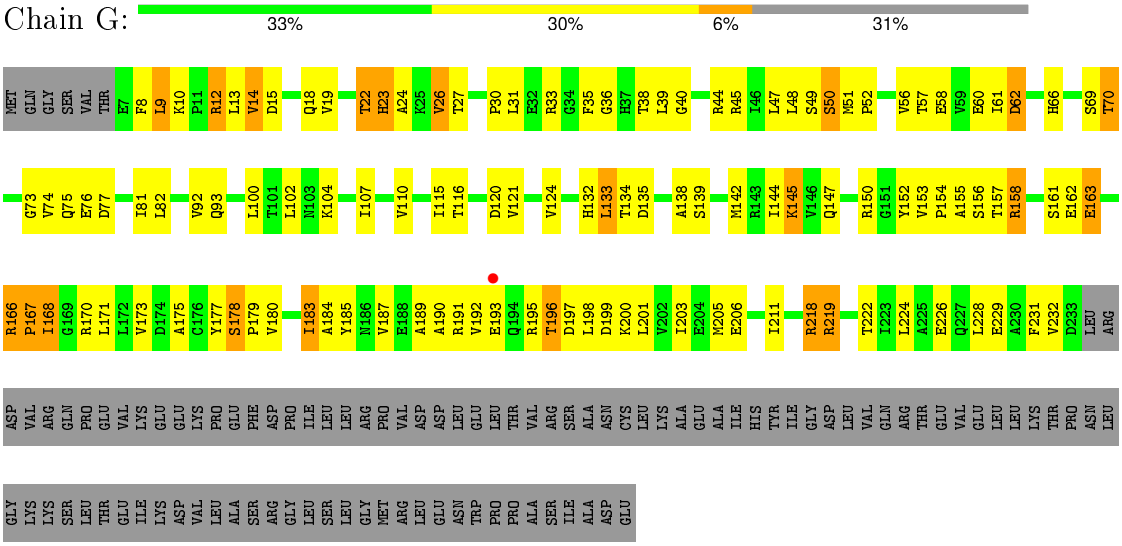
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



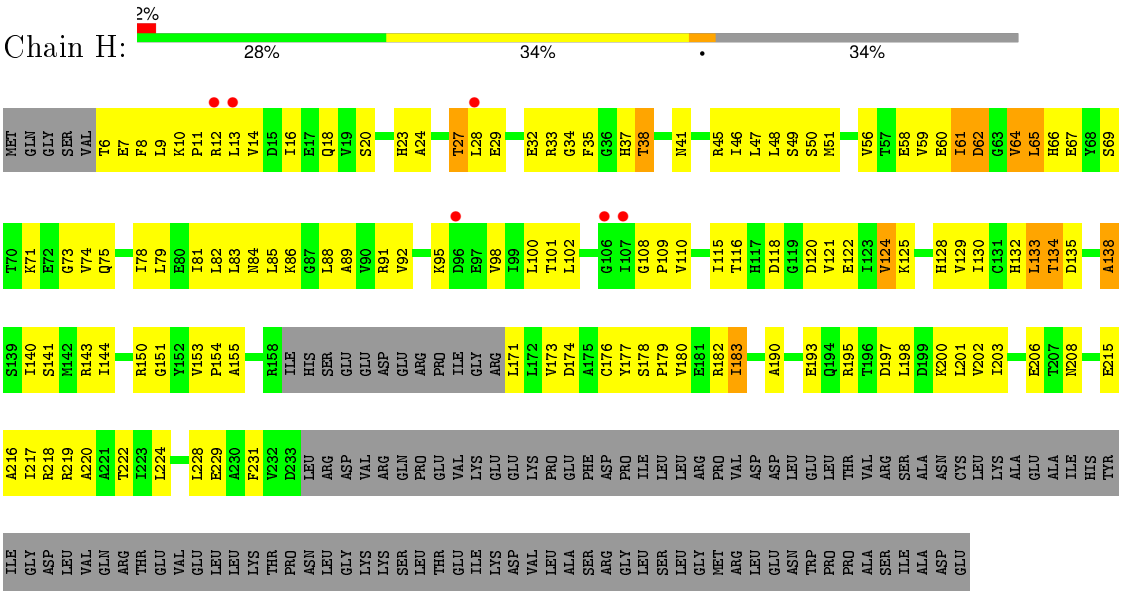
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G:



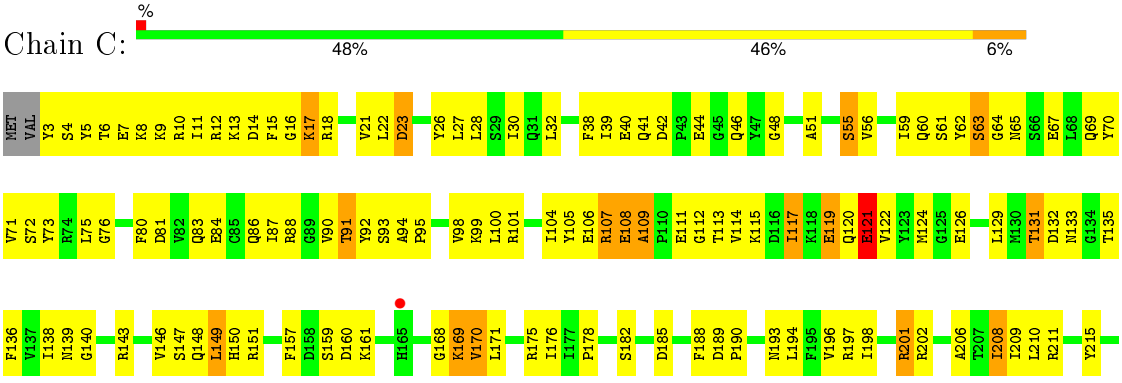
• Molecule 1: DNA-directed RNA polymerase subunit alpha

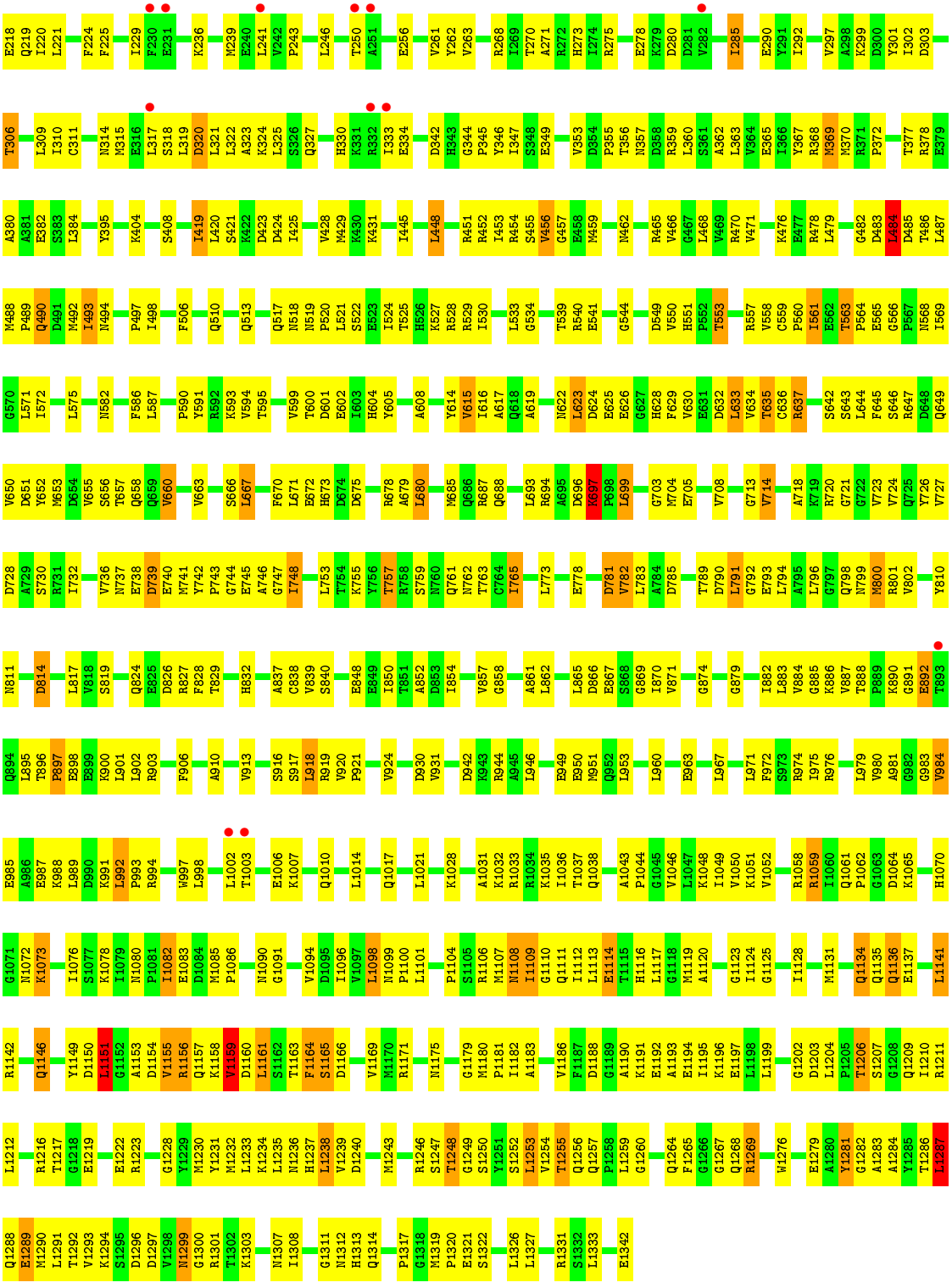
Chain H:



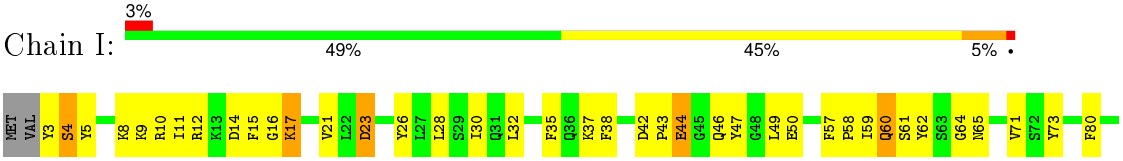
• Molecule 2: DNA-directed RNA polymerase subunit beta

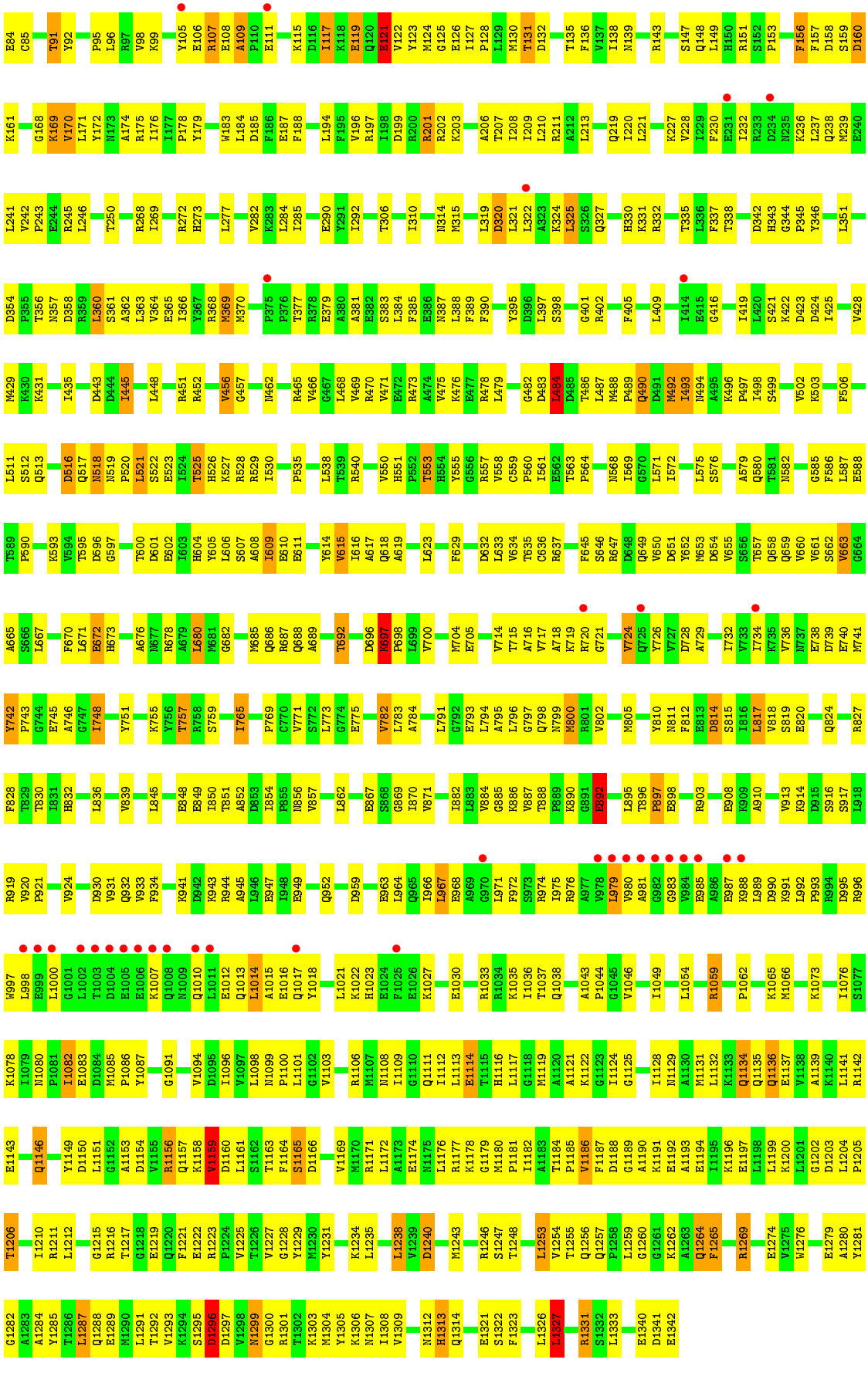
Chain C:





• Molecule 2: DNA-directed RNA polymerase subunit beta

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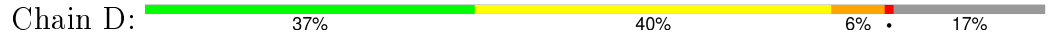
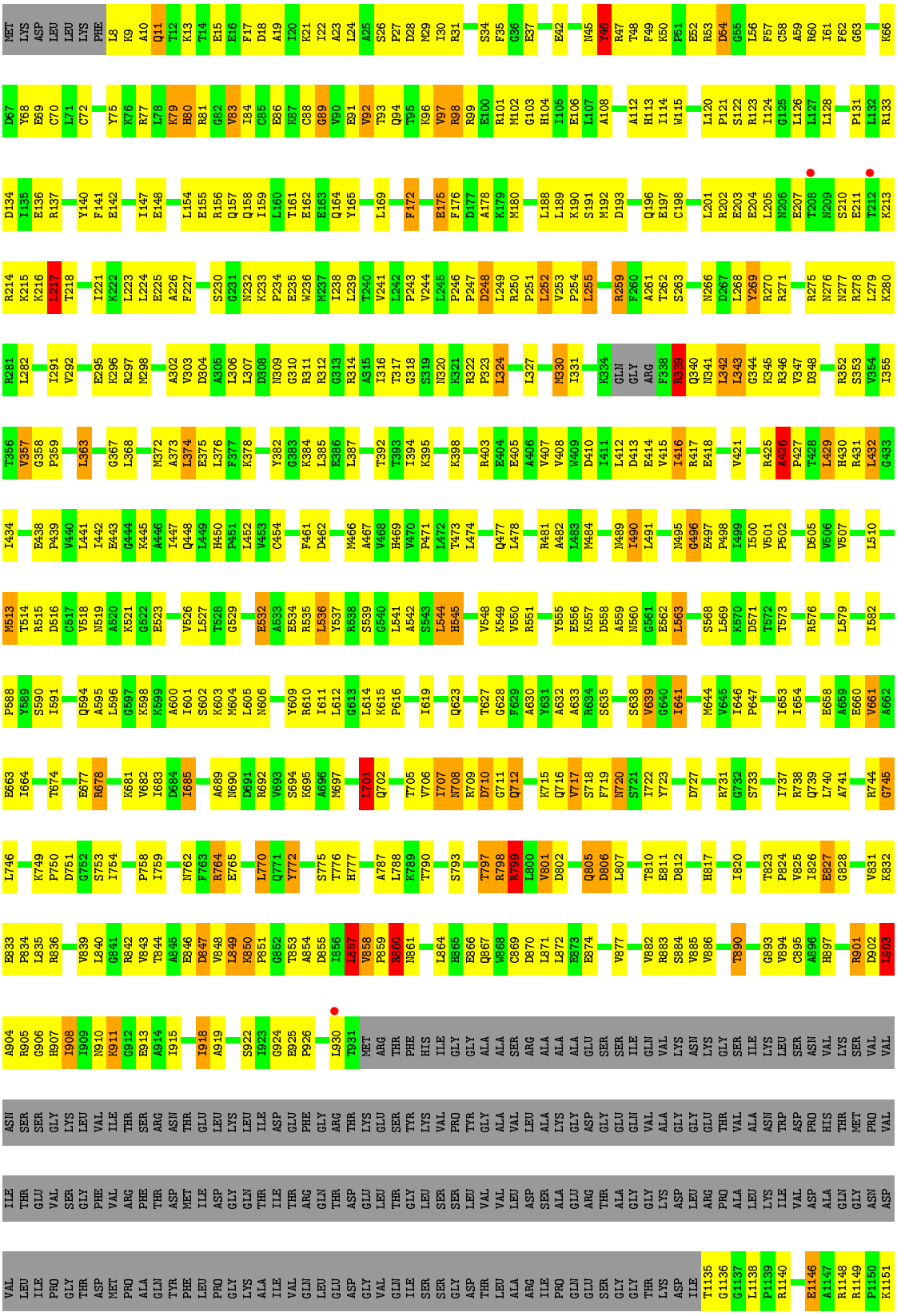
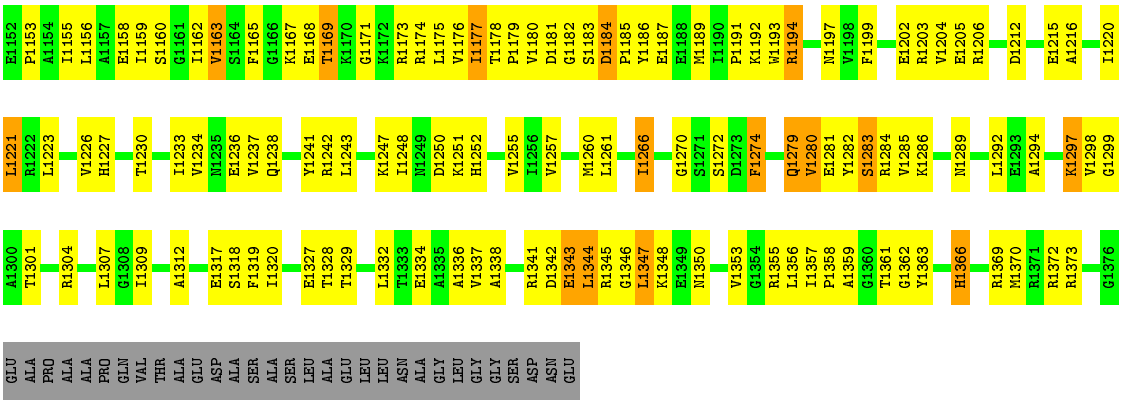
K161 G168 K169 V170 L171 Y172 N173 A174 R175 I176 I177 P178 Y179 W183 L184 D185 F186 E187 F188 L194 F195 V196 R197 I198 D199 R200 R201 R202 K203 A206 T207 I208 I209 L210 R211 A212 L213 Q219 I220 L221 K227 V228 I229 F230 E231 I232 R233 D234 N235 K236 L237 Q238 M239 E240
L241 V242 P243 E244 R245 L246 T250 R268 I269 R272 H273 L277 V282 K283 L284 I285 E290 Y291 I292 T306 I310 N314 M315 L319 D320 L321 L322 A323 K324 L325 S326 Q327 H330 K331 R332 T335 L336 F337 T338 D342 H343 G344 P345 Y346 L351
D354 P355 T356 N357 D358 R359 L360 S361 A362 L363 V364 E365 I366 Y367 R368 M369 M370 P375 P376 T377 R378 E379 A380 A381 E382 S383 L384 F385 E386 N387 L388 F389 F390 Y395 D396 L397 S398 G401 R402 F405 L409 T414 E415 G416 T419 L420 S421 K422 D423 D424 T425 V428
M429 K430 K431 I435 D443 D444 I445 L448 R451 R452 V456 G457 N462 R465 V466 G467 L468 V469 R470 V471 E472 R473 A474 V475 K476 E477 R478 L479 G482 D483 L484 D485 T486 L487 M488 P489 Q490 D491 M492 I493 N494 A495 K496 P497 I498 S499 V502 K503 F506
L511 S512 Q513 D516 Q517 N518 N519 P520 L521 S522 E523 I524 T525 H526 K527 R528 R529 I530 P535 L538 T539 R540 V550 H551 P552 T553 H554 Y555 G556 R557 V558 C559 P560 I561 E562 T563 P564 N568 I569 G570 L571 I572 L575 S576 A579 Q580 T581 N582 G585 F586 L587 E588
T589 P590 K593 V594 T595 D596 G597 T600 D601 E602 I603 H604 Y605 L606 S607 A608 I609 E610 E611 Y614 V615 I616 A617 Q618 A619 L623 F629 D632 L633 V634 T635 C636 R637 F645 S646 R647 D648 Q649 V650 D651 Y652 M653 D654 V655 S656 T657 Q658 Q659 V660 V661 S662 V663 G664
A665 S666 L667 F670 L671 E672 H673 A676 N677 R678 A679 L680 M681 G682 M685 Q686 R687 Q688 A689 T692 D696 K697 P698 L699 V700 M704 E705 V714 T715 A716 V717 A718 K719 R720 G721 V724 Q725 Y726 V727 D728 A729 I732 V733 I734 K735 V736 N737 E738 D739 E740 M741
Y742 P743 G744 E745 A746 G747 T748 Y751 K755 Y756 T757 R758 S759 I765 P769 G770 V771 S772 L773 G774 E775 V782 L783 A784 L791 G792 E793 L794 A795 L796 G797 Q798 N799 M800 R801 V802 M805 Y810 N811 F812 E813 D814 S815 I816 L817 V818 S819 E820 Q824 R827
F828 T829 T830 I831 H832 L836 V839 L845 E848 E849 I850 T851 A852 D853 I854 P855 N856 V857 L862 E867 S868 G869 I870 V871 I882 L883 V884 G885 K886 V887 T888 P889 K890 G891 E892 L895 T896 P897 E898 R903 E908 K909 A910 V913 K914 D915 S916 S917 L918
R919 V920 P921 V924 D930 V931 Q932 V933 F934 K941 D942 K943 R944 A945 L946 E947 I948 E949 Q952 D959 E963 L964 Q965 I966 L967 E968 A969 G970 L971 F972 S973 R974 I975 R976 A977 V978 L979 V980 A981 G982 G983 V984 E985 A986 E987 K988 L989 D990 K991 L992 P993 R994 D995 R996
W997 L998 E999 L1000 G1001 L1002 T1003 D1004 E1005 E1006 K1007 Q1008 N1009 Q1010 L1011 E1012 Q1013 L1014 A1015 E1016 Q1017 Y1018 L1021 K1022 H1023 E1024 F1025 E1026 K1027 E1030 R1033 R1034 K1035 I1036 I1037 Q1038 A1043 P1044 G1045 V1046 I1049 L1054 R1059 P1062 K1065 M1066 K1073 I1076 S1077
K1078 I1079 N1080 P1081 I1082 E1083 D1084 M1085 P1086 Y1087 G1091 V1094 D1095 I1096 V1097 L1098 N1099 P1100 L1101 G1102 V1103 R1106 M1107 N1108 I1109 G1110 Q1111 I1112 L1113 E1114 T1115 H1116 L1117 G1118 M1119 A1120 A1121 K1122 G1123 I1124 G1125 I1128 N1129 A1130 M1131 L1132 K1133 Q1134 Q1135 Q1136 E1137 V1138 A1139 K1140 L1141 R1142
E1143 Q1146 Y1149 D1150 L1151 G1152 A1153 D1154 V1155 R1156 Q1157 K1158 V1159 D1160 L1161 S1162 T1163 F1164 S1165 D1166 V1169 M1170 R1171 L1172 A1173 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 L1204 P1205
T1206 I1210 R1211 L1212 G1215 R1216 T1217 G1218 E1219 Q1220 F1221 E1222 R1223 P1224 V1225 T1226 V1227 G1228 Y1229 M1230 Y1231 K1234 L1235 L1238 V1239 D1240 M1243 R1246 S1247 T1248 L1253 V1254 T1255 R1269 E1274 V1275 W1276 E1279 A1280 Y1281
G1282 A1283 A1284 Y1285 T1286 L1287 Q1288 E1289 M1290 L1291 T1292 V1293 K1294 S1295 D1296 D1297 V1298 N1299 G1300 R1301 T1302 K1303 M1304 Y1305 K1306 N1307 I1308 V1309 N1312 H1313 Q1314 E1321 S1322 F1323 L1326 L1327 R1331 S1332 L1333 E1340 D1341 E1342

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

Chain D:

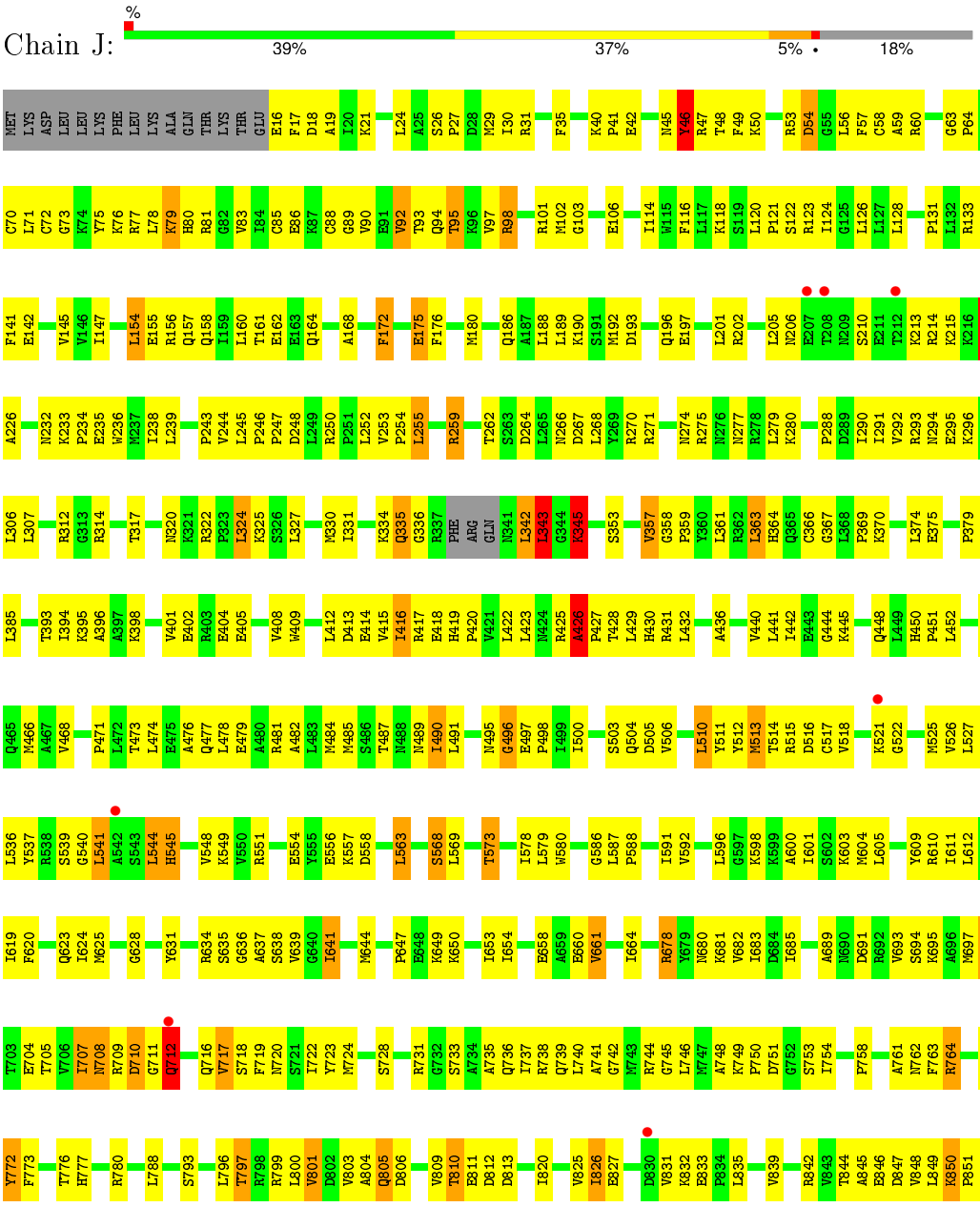


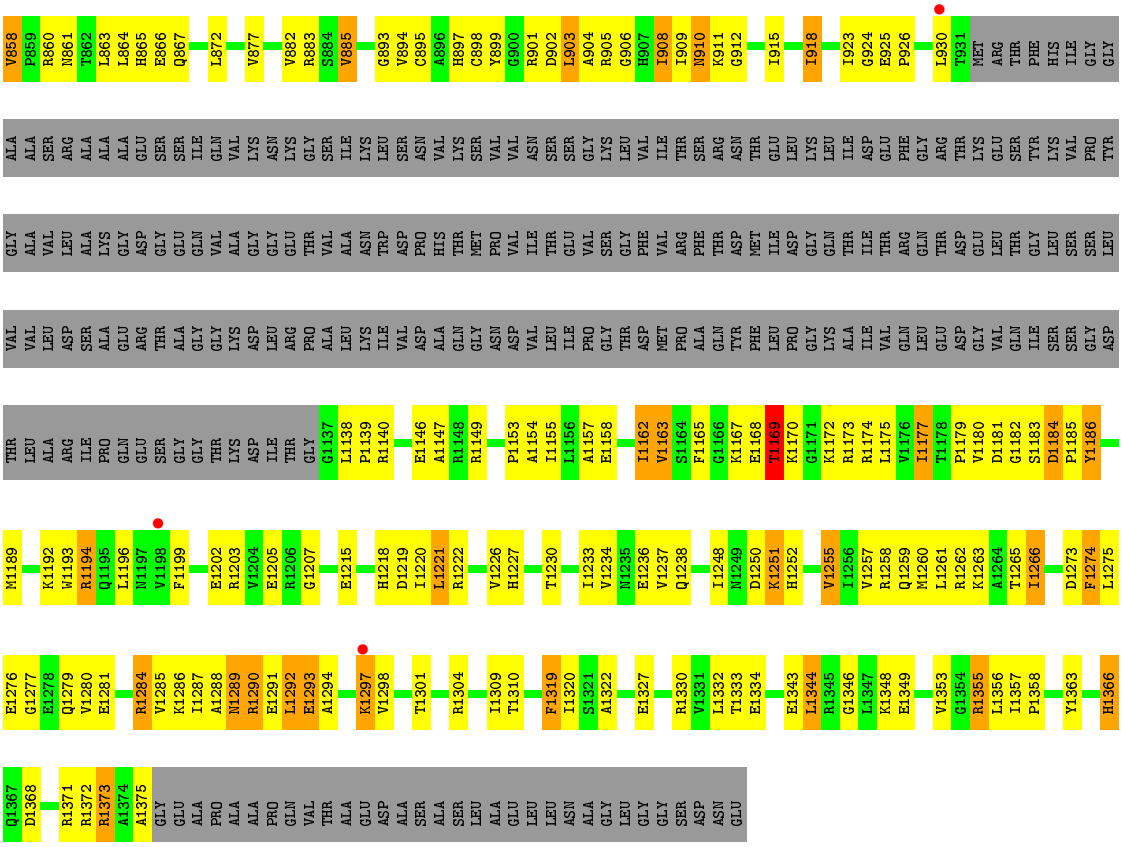




• Molecule 3: DNA-directed RNA polymerase subunit beta'

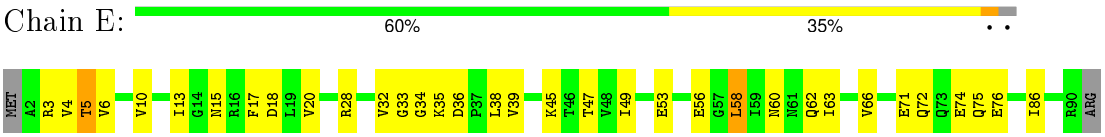
Chain J:





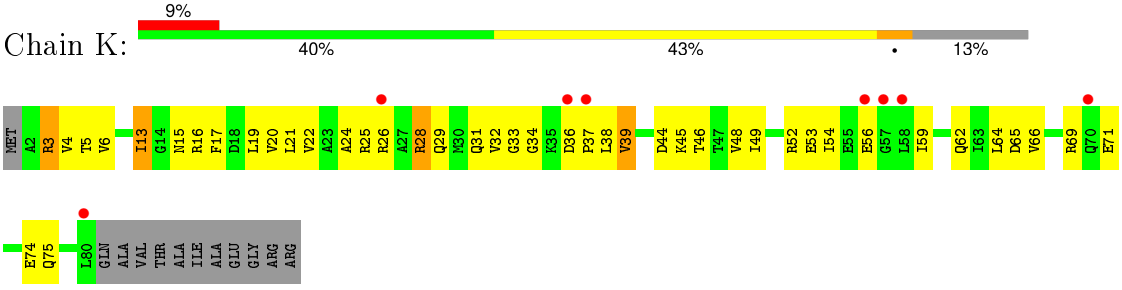
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



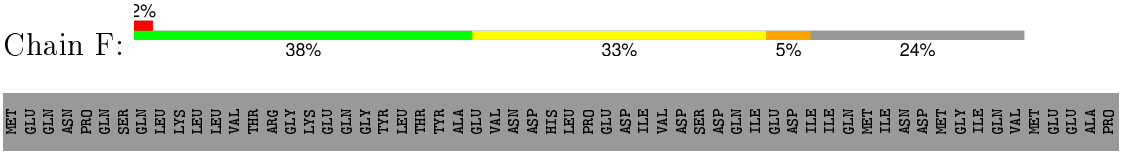
• Molecule 4: DNA-directed RNA polymerase subunit omega

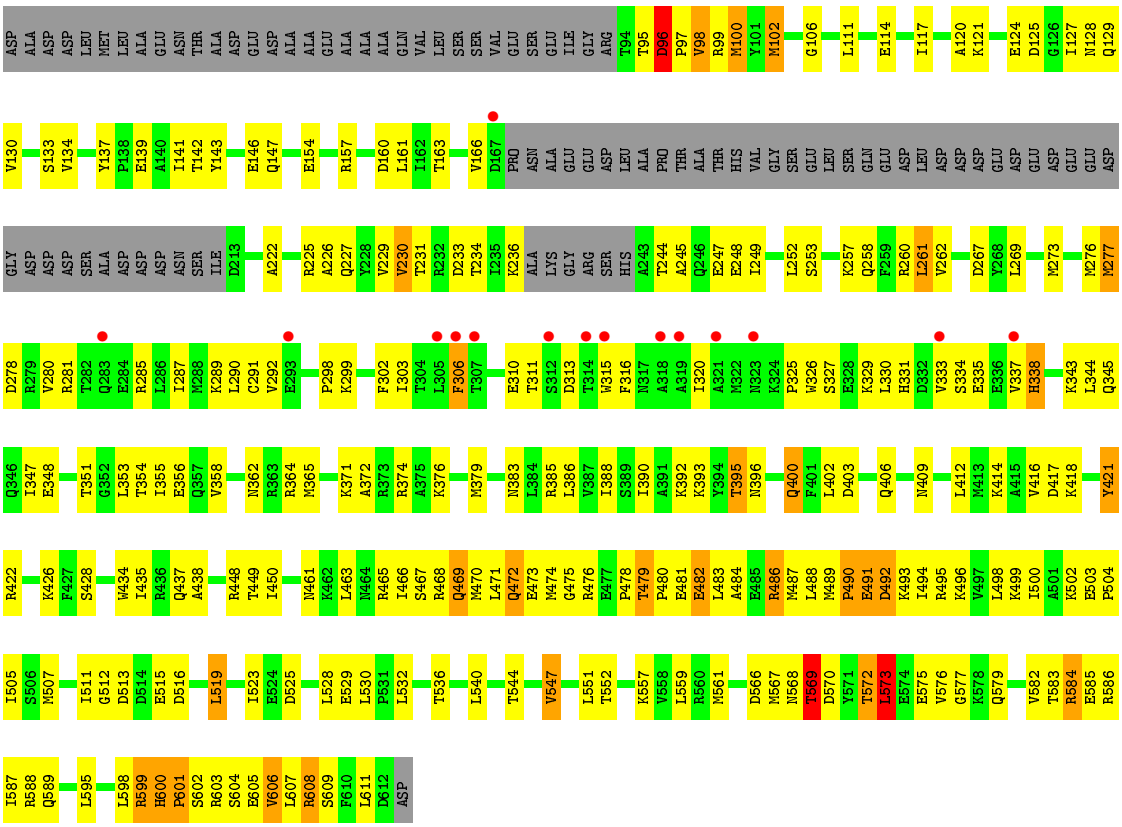
Chain K:



• Molecule 5: RNA polymerase sigma factor RpoD

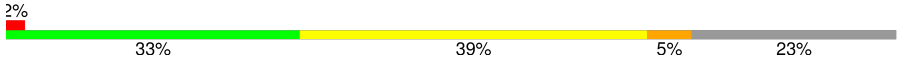
Chain F:

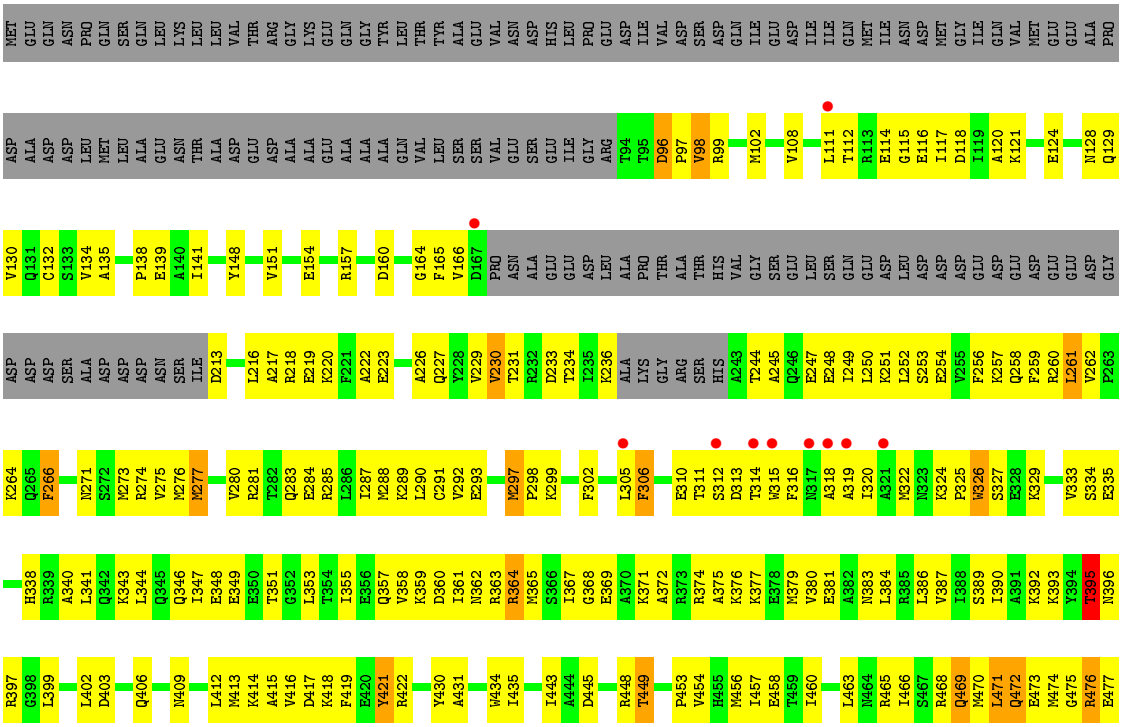


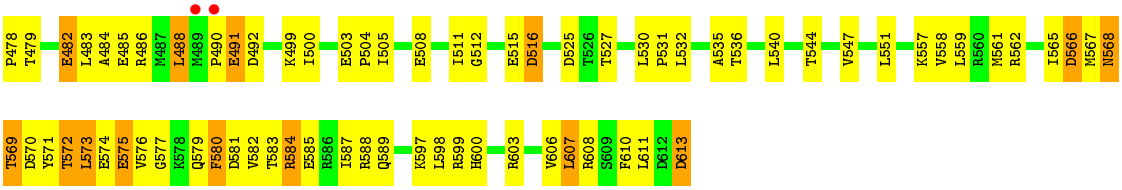


• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:



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T569 D570 Y571 T572 L573 E574 E575 V576 G577 R578 Q579 F580 D581 V582 T583 R584 E585 R586 I587 R588 Q589 K597 L598 R599 H600 R603 V606 I607 R608 S609 F610 L611 D612 D613

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	186.10Å 206.44Å 307.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.57 31.02 – 3.57	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.96-3.57) 92.3 (31.02-3.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.217 , 0.252 0.264 , 0.279	Depositor DCC
R_{free} test set	2000 reflections (1.56%)	DCC
Wilson B-factor (Å^2)	109.4	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 57.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 133164 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	55782	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 4C6, 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	0.80	0/2524	0.91	2/3421 (0.1%)
1	B	0.86	3/1697 (0.2%)	0.97	4/2300 (0.2%)
1	G	0.80	0/1777	0.92	1/2408 (0.0%)
1	H	0.83	1/1681 (0.1%)	0.94	1/2278 (0.0%)
2	C	0.84	1/10739 (0.0%)	0.89	9/14489 (0.1%)
2	I	0.79	2/10735 (0.0%)	0.87	10/14484 (0.1%)
3	D	0.90	6/9188 (0.1%)	0.95	18/12404 (0.1%)
3	J	0.78	2/9128 (0.0%)	0.89	10/12322 (0.1%)
4	E	0.73	0/693	0.75	0/935
4	K	1.03	0/629	0.89	0/847
5	F	0.83	1/3864 (0.0%)	0.87	3/5194 (0.1%)
5	L	0.83	1/3872 (0.0%)	0.83	2/5205 (0.0%)
All	All	0.83	17/56527 (0.0%)	0.90	60/76287 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
2	I	0	4
3	D	0	2
3	J	0	1
5	F	0	1
All	All	0	11

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	799	ARG	CB-CG	-10.16	1.25	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	339	ARG	CZ-NH2	8.46	1.44	1.33
3	D	799	ARG	CG-CD	8.42	1.73	1.51
2	I	1296	ASP	CG-OD2	8.26	1.44	1.25
3	D	339	ARG	CB-CG	-8.08	1.30	1.52
3	J	345	LYS	CE-NZ	-6.64	1.32	1.49
3	D	339	ARG	CG-CD	-6.43	1.35	1.51
1	B	233	ASP	CA-CB	6.32	1.67	1.53
1	B	232	VAL	CB-CG1	-6.17	1.39	1.52
1	B	233	ASP	CB-CG	-5.75	1.39	1.51
2	I	1269	ARG	NE-CZ	-5.72	1.25	1.33
1	H	14	VAL	CA-CB	5.28	1.65	1.54
5	L	326	TRP	CB-CG	5.27	1.59	1.50
3	D	827	GLU	CG-CD	5.21	1.59	1.51
5	F	315	TRP	CB-CG	5.16	1.59	1.50
3	J	831	VAL	CA-CB	5.09	1.65	1.54
2	C	1112	ILE	CA-CB	-5.01	1.43	1.54

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1269	ARG	NE-CZ-NH1	15.48	128.04	120.30
2	I	1269	ARG	NE-CZ-NH2	-11.03	114.79	120.30
2	I	484	LEU	CA-CB-CG	9.30	136.69	115.30
2	I	1269	ARG	CD-NE-CZ	9.27	136.57	123.60
2	C	1161	LEU	CA-CB-CG	-9.26	94.01	115.30
3	D	799	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	B	233	ASP	CB-CG-OD2	-9.13	110.08	118.30
3	D	798	ARG	NE-CZ-NH1	8.43	124.51	120.30
3	D	426	ALA	C-N-CD	7.94	145.07	128.40
3	J	1344	LEU	CA-CB-CG	-7.84	97.25	115.30
3	D	799	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	C	1151	LEU	CA-CB-CG	-7.57	97.88	115.30
5	L	530	LEU	CA-CB-CG	7.37	132.24	115.30
2	I	817	LEU	CA-CB-CG	6.71	130.74	115.30
3	D	339	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	B	28	LEU	CB-CG-CD2	-6.56	99.84	111.00
1	B	65	LEU	CA-CB-CG	6.54	130.34	115.30
3	J	217	LEU	CA-CB-CG	6.28	129.74	115.30
3	D	799	ARG	CB-CG-CD	6.21	127.74	111.60
3	D	860	ARG	NE-CZ-NH1	6.18	123.39	120.30
5	F	486	ARG	NE-CZ-NH1	6.05	123.33	120.30
3	D	701	LEU	CA-CB-CG	6.01	129.13	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	857	LEU	CA-CB-CG	6.00	129.11	115.30
3	D	432	LEU	CB-CG-CD2	-5.98	100.84	111.00
3	D	799	ARG	CA-CB-CG	5.97	126.54	113.40
2	I	1296	ASP	CB-CG-OD2	5.94	123.64	118.30
3	J	426	ALA	C-N-CD	5.82	140.62	128.40
3	D	217	LEU	CA-CB-CG	5.77	128.58	115.30
3	D	605	LEU	CA-CB-CG	-5.73	102.12	115.30
2	C	1326	LEU	CB-CG-CD2	-5.67	101.37	111.00
2	I	1327	LEU	CB-CG-CD1	-5.63	101.43	111.00
3	D	1347	LEU	CA-CB-CG	5.60	128.18	115.30
3	D	342	LEU	CA-CB-CG	5.55	128.06	115.30
3	D	339	ARG	CB-CA-C	-5.54	99.33	110.40
3	D	911	LYS	CD-CE-NZ	5.53	124.41	111.70
2	C	149	LEU	CB-CG-CD2	-5.52	101.61	111.00
3	J	343	LEU	CB-CG-CD2	5.47	120.30	111.00
3	J	701	LEU	CA-CB-CG	5.47	127.88	115.30
1	H	29	GLU	C-N-CD	-5.47	108.58	120.60
5	F	573	LEU	CA-CB-CG	-5.41	102.86	115.30
5	L	488	LEU	CA-CB-CG	5.38	127.69	115.30
1	A	318	LEU	CA-CB-CG	5.36	127.62	115.30
2	I	1014	LEU	CA-CB-CG	-5.24	103.26	115.30
2	C	484	LEU	CA-CB-CG	5.23	127.33	115.30
2	C	1287	LEU	CA-CB-CG	-5.23	103.27	115.30
1	A	224	LEU	CA-CB-CG	-5.19	103.36	115.30
2	C	667	LEU	CB-CG-CD1	-5.17	102.20	111.00
5	F	519	LEU	CB-CG-CD1	-5.17	102.20	111.00
3	J	857	LEU	CA-CB-CG	5.17	127.20	115.30
3	J	1275	LEU	CA-CB-CG	5.16	127.18	115.30
3	D	903	LEU	CA-CB-CG	5.14	127.13	115.30
3	J	541	LEU	CA-CB-CG	5.12	127.08	115.30
3	J	1373	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	C	544	GLY	N-CA-C	-5.09	100.38	113.10
2	I	1295	SER	N-CA-C	5.06	124.66	111.00
3	J	343	LEU	CB-CG-CD1	-5.06	102.40	111.00
1	G	177	TYR	CA-CB-CG	5.04	122.98	113.40
1	B	233	ASP	CB-CG-OD1	5.04	122.84	118.30
2	I	325	LEU	CA-CB-CG	5.01	126.83	115.30
2	C	448	LEU	CA-CB-CG	-5.01	103.78	115.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	1264	GLN	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
2	I	1264	GLN	Peptide
2	I	1296	ASP	Mainchain
2	I	236	LYS	Peptide
3	J	1184	ASP	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	2490	0	2542	204	0
1	B	1677	0	1703	105	0
1	G	1755	0	1773	122	0
1	H	1662	0	1687	131	0
2	C	10570	0	10582	606	0
2	I	10566	0	10576	626	0
3	D	9050	0	9218	641	0
3	J	8990	0	9173	595	0
4	E	691	0	695	24	0
4	K	627	0	634	47	0
5	F	3813	0	3880	203	0
5	L	3821	0	3884	244	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
8	D	31	0	25	1	0
8	J	31	0	25	2	0
All	All	55782	0	56397	3255	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 29.

All (3255) 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)
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.29	1.14
1:A:45:ARG:HG2	1:B:38:THR:HB	1.31	1.12
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.30	1.08
2:I:1269:ARG:HD3	3:J:343:LEU:HD21	1.35	1.08
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.17	1.07
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.33	1.06
3:D:1280:VAL:HG21	3:D:1304:ARG:HH21	1.19	1.05
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.39	1.04
1:G:12:ARG:H	1:G:30:PRO:HD2	1.24	1.02
2:I:17:LYS:HZ1	2:I:1154:ASP:HB3	1.24	1.02
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.40	1.00
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.23	0.99
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.45	0.99
1:A:156:SER:HB3	2:C:1059:ARG:HH22	1.30	0.96
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.47	0.96
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.48	0.95
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.46	0.94
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.49	0.94
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.13	0.94
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.48	0.94
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.50	0.93
2:C:324:LYS:O	2:C:327:GLN:NE2	1.99	0.93
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.49	0.93
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.05	0.92
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.52	0.92
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.47	0.92
1:G:45:ARG:HG2	1:H:38:THR:HB	1.51	0.92
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.49	0.92
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.53	0.91
1:G:187:VAL:HG12	1:G:201:LEU:HD13	1.52	0.90
3:D:310:GLY:HA2	3:D:314:ARG:HD2	1.53	0.90
5:F:600:HIS:CD2	5:F:601:PRO:HD3	2.07	0.90
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.37	0.90
2:I:148:GLN:NE2	2:I:535:PRO:O	2.04	0.89
3:D:156:ARG:NH2	3:D:191:SER:OG	2.05	0.89
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.55	0.88
1:A:45:ARG:NH2	2:C:1216:ARG:HA	1.87	0.88
2:C:4:SER:HB3	2:C:7:GLU:HG3	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLY:HA3	1:B:71:LYS:HE3	1.54	0.87
5:F:121:LYS:NZ	5:F:421:TYR:OH	2.08	0.87
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.56	0.87
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.38	0.87
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.55	0.87
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.55	0.86
2:I:1269:ARG:CD	3:J:343:LEU:HD21	2.05	0.86
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.56	0.86
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.58	0.86
2:C:810:TYR:HE1	2:C:1078:LYS:HZ3	1.23	0.86
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.41	0.86
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.38	0.86
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.41	0.86
2:I:742:TYR:HD2	2:I:743:PRO:HD2	1.41	0.86
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.11	0.86
5:F:493:LYS:HG2	5:F:496:LYS:HE2	1.57	0.86
1:H:9:LEU:HD12	1:H:195:ARG:HH21	1.41	0.86
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.58	0.85
2:I:1296:ASP:OD2	2:I:1322:SER:N	2.08	0.85
1:A:77:ASP:OD1	1:A:77:ASP:N	2.09	0.85
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.10	0.85
3:D:430:HIS:HD2	3:D:432:LEU:HB2	1.38	0.85
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.40	0.85
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.38	0.85
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.59	0.85
3:D:418:GLU:HG3	4:E:45:LYS:H	1.40	0.84
3:D:339:ARG:HD3	3:D:798:ARG:HH11	1.42	0.84
2:C:974:ARG:HD2	2:C:1014:LEU:HD21	1.60	0.84
5:L:132:CYS:SG	5:L:257:LYS:NZ	2.49	0.84
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.58	0.84
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.58	0.84
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.59	0.84
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.56	0.84
1:A:296:GLY:H	1:A:299:SER:HB2	1.43	0.84
1:B:102:LEU:O	1:B:141:SER:HA	1.78	0.83
2:I:490:GLN:HG3	5:L:472:GLN:HG3	1.60	0.83
1:A:133:LEU:HD21	1:A:140:ILE:HD11	1.59	0.83
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.59	0.83
5:L:470:MET:HB2	5:L:478:PRO:HG3	1.59	0.83
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.42	0.83
3:D:1159:ILE:HG22	3:D:1177:ILE:HD12	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.12	0.83
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.60	0.82
2:C:1281:TYR:HD1	3:D:484:MET:HG2	1.44	0.82
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.60	0.82
1:H:74:VAL:HG11	1:H:81:ILE:HD11	1.60	0.82
3:D:425:ARG:HG2	3:D:426:ALA:H	1.42	0.82
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.61	0.82
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.25	0.82
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.61	0.82
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.59	0.82
3:D:1280:VAL:HG21	3:D:1304:ARG:NH2	1.93	0.82
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.14	0.82
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.13	0.82
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.13	0.82
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.60	0.81
5:L:316:PHE:HZ	5:L:334:SER:HA	1.44	0.81
2:C:703:GLY:N	2:C:705:GLU:OE2	2.11	0.81
3:D:317:THR:HG22	3:D:322:ARG:O	1.81	0.81
2:I:30:ILE:HD12	2:I:30:ILE:H	1.44	0.81
1:G:166:ARG:HH11	1:G:168:ILE:HG12	1.46	0.81
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.63	0.81
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.14	0.80
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.16	0.80
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.61	0.80
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.62	0.80
2:I:17:LYS:NZ	2:I:1154:ASP:HB3	1.96	0.80
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.62	0.80
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.61	0.80
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.64	0.80
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.28	0.80
1:G:229:GLU:HA	1:G:231:PHE:CE2	2.17	0.80
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.64	0.80
2:I:1176:LEU:HD13	2:I:1180:MET:HG3	1.64	0.80
3:D:339:ARG:HD2	3:D:798:ARG:HD3	1.64	0.79
2:C:975:ILE:HG13	2:C:1014:LEU:HD22	1.64	0.79
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.28	0.79
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.63	0.79
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.62	0.79
1:A:227:GLN:HG3	1:B:39:LEU:HD11	1.64	0.79
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.64	0.79
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.64	0.79
3:J:1265:THR:HG22	3:J:1277:GLY:HA2	1.63	0.78
2:I:600:THR:HG21	2:I:602:GLU:HG2	1.63	0.78
2:I:550:VAL:HG11	3:J:776:THR:HG22	1.64	0.78
1:B:191:ARG:NH2	3:D:410:ASP:OD2	2.16	0.78
2:C:483:ASP:HB2	2:C:486:THR:CG2	2.12	0.78
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.17	0.78
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.19	0.78
3:J:384:LYS:NZ	3:J:414:GLU:OE1	2.16	0.78
1:A:166:ARG:O	1:A:168:ILE:N	2.17	0.78
5:L:572:THR:HG23	5:L:575:GLU:HB2	1.66	0.78
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.66	0.78
2:I:119:GLU:HG3	2:I:489:PRO:HD2	1.64	0.78
3:J:1289:ASN:OD1	3:J:1290:ARG:NH1	2.17	0.78
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	1.98	0.77
3:D:854:ALA:HB2	3:J:1372:ARG:HG3	1.66	0.77
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.00	0.77
1:H:98:VAL:HG21	1:H:121:VAL:HG23	1.67	0.77
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.49	0.77
5:L:561:MET:HA	5:L:567:MET:HE1	1.65	0.77
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.65	0.77
5:F:281:ARG:O	5:F:285:ARG:HG3	1.85	0.77
2:C:117:ILE:HD12	2:C:488:MET:HG2	1.66	0.77
2:I:227:LYS:O	2:I:245:ARG:NH2	2.18	0.77
3:J:395:LYS:HG2	5:L:536:THR:HG21	1.67	0.76
1:G:218:ARG:NH1	1:H:231:PHE:O	2.18	0.76
2:C:1134:GLN:HB3	2:C:1136:GLN:HG2	1.67	0.76
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.20	0.76
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.66	0.76
2:I:170:VAL:HG21	2:I:172:TYR:CZ	2.20	0.76
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.67	0.76
1:H:61:ILE:HB	1:H:64:VAL:O	1.85	0.76
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.14	0.76
1:A:16:ILE:HG12	1:A:26:VAL:HB	1.67	0.76
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.67	0.76
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.67	0.76
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.66	0.76
3:J:425:ARG:HG2	3:J:426:ALA:H	1.51	0.76
3:D:414:GLU:O	4:E:45:LYS:NZ	2.18	0.75
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.68	0.75
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:TYR:HD1	2:C:112:GLY:H	1.31	0.75
3:D:844:THR:OG1	3:D:860:ARG:O	2.02	0.75
2:I:1156:ARG:HH11	2:I:1156:ARG:HB2	1.51	0.75
2:C:810:TYR:CE2	3:D:359:PRO:HD2	2.21	0.75
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.67	0.75
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.52	0.75
5:F:470:MET:HB2	5:F:478:PRO:HG3	1.68	0.75
2:I:724:VAL:HG23	2:I:775:GLU:H	1.52	0.75
1:A:92:VAL:O	1:A:148:ARG:NH1	2.18	0.75
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.69	0.75
3:D:1191:PRO:HB3	3:D:1194:ARG:HH11	1.52	0.75
3:D:1320:ILE:HG23	8:D:2004:4C6:H9	1.68	0.75
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.06	0.75
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.16	0.75
4:E:56:GLU:HB2	4:E:58:LEU:HD11	1.68	0.75
5:F:547:VAL:HG13	5:F:598:LEU:HD22	1.69	0.75
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.67	0.75
3:J:128:LEU:HA	3:J:192:MET:HE1	1.69	0.74
1:H:108:GLY:O	1:H:133:LEU:HB2	1.86	0.74
1:A:115:ILE:HG22	1:A:116:THR:H	1.52	0.74
3:J:201:LEU:O	3:J:217:LEU:HD11	1.87	0.74
1:A:49:SER:OG	1:A:50:SER:N	2.17	0.74
3:J:1179:PRO:HD2	3:J:1184:ASP:HA	1.69	0.74
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.18	0.74
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.50	0.74
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.23	0.74
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.68	0.74
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.68	0.74
2:I:892:GLU:OE2	3:J:66:LYS:NZ	2.19	0.74
5:L:281:ARG:O	5:L:285:ARG:HG3	1.88	0.74
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.69	0.74
1:A:76:GLU:OE2	1:A:76:GLU:N	2.21	0.74
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.53	0.74
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.70	0.73
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.52	0.73
5:L:571:TYR:CD1	5:L:575:GLU:HG2	2.23	0.73
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.52	0.73
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.16	0.73
3:J:846:GLU:HA	3:J:860:ARG:HD2	1.70	0.73
3:J:264:ASP:HB3	3:J:324:LEU:HB2	1.70	0.73
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1281:TYR:CE2	3:D:431:ARG:HB2	2.23	0.73
3:D:392:THR:HG21	5:F:606:VAL:HA	1.69	0.73
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.70	0.73
2:I:742:TYR:CD2	2:I:743:PRO:HD2	2.23	0.73
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.24	0.73
1:G:190:ALA:HB2	1:G:200:LYS:CB	2.15	0.73
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.18	0.73
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.70	0.73
3:J:19:ALA:HB2	3:J:1373:ARG:HH22	1.53	0.73
2:C:197:ARG:NH1	2:C:201:ARG:O	2.21	0.73
5:F:595:LEU:HB3	5:F:599:ARG:HH21	1.53	0.73
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.69	0.73
2:I:600:THR:HG22	2:I:602:GLU:H	1.53	0.73
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.70	0.73
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.54	0.72
1:B:73:GLY:HA2	1:B:134:THR:CG2	2.19	0.72
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.71	0.72
3:J:708:ASN:HB3	3:J:712:GLN:O	1.87	0.72
3:J:709:ARG:O	3:J:711:GLY:N	2.21	0.72
3:D:860:ARG:HB3	3:D:860:ARG:HH11	1.55	0.72
5:F:600:HIS:HD2	5:F:601:PRO:HD3	1.52	0.72
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.54	0.72
1:G:75:GLN:HA	2:I:729:ALA:N	2.05	0.72
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.22	0.72
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.71	0.72
3:J:682:VAL:HG13	3:J:685:ILE:HD11	1.70	0.72
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.70	0.72
1:B:152:TYR:CE1	1:B:176:CYS:HB3	2.24	0.72
1:H:101:THR:H	1:H:116:THR:HG22	1.54	0.72
3:J:430:HIS:HD2	3:J:432:LEU:HB2	1.53	0.72
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.23	0.72
1:H:51:MET:HB3	1:H:178:SER:HB2	1.71	0.72
2:C:972:PHE:HB2	2:C:994:ARG:HH21	1.54	0.72
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.72	0.72
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.54	0.72
2:C:201:ARG:NH2	2:C:370:MET:O	2.21	0.72
1:G:12:ARG:N	1:G:30:PRO:HD2	2.02	0.71
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.72	0.71
1:H:18:GLN:HA	1:H:24:ALA:HA	1.72	0.71
1:A:190:ALA:HB2	1:A:200:LYS:HE3	1.71	0.71
1:A:73:GLY:O	1:A:134:THR:HG22	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:515:ARG:NH2	3:D:717:VAL:O	2.23	0.71
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.71	0.71
1:G:61:ILE:HG22	1:G:62:ASP:H	1.55	0.71
5:F:311:THR:HG21	5:F:348:GLU:OE2	1.91	0.71
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.72	0.71
2:C:550:VAL:HG11	3:D:776:THR:HG22	1.73	0.71
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.72	0.71
5:F:354:THR:O	5:F:358:VAL:HG23	1.91	0.71
5:F:532:LEU:O	5:F:536:THR:HG23	1.91	0.71
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.24	0.71
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.71	0.71
2:I:963:GLU:O	2:I:967:LEU:HB2	1.91	0.71
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.71	0.71
2:C:593:LYS:HG3	2:C:595:THR:HG23	1.72	0.71
3:D:707:ILE:H	3:D:707:ILE:HD12	1.56	0.71
2:I:798:GLN:HB2	2:I:828:PHE:HE1	1.53	0.71
2:I:839:VAL:HG12	2:I:1049:ILE:HG12	1.72	0.71
2:I:123:TYR:OH	2:I:126:GLU:HG3	1.91	0.70
5:L:262:VAL:HG11	5:L:264:LYS:NZ	2.06	0.70
3:J:70:CYS:SG	3:J:71:LEU:N	2.63	0.70
1:A:158:ARG:NH2	1:A:172:LEU:HB3	2.05	0.70
1:A:58:GLU:HG2	1:A:158:ARG:HH22	1.55	0.70
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.73	0.70
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.07	0.70
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.55	0.70
2:I:748:ILE:HD11	2:I:966:ILE:HG22	1.72	0.70
2:C:1269:ARG:HD3	3:D:343:LEU:HD11	1.72	0.70
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.25	0.70
5:F:320:ILE:HG21	5:F:331:HIS:CE1	2.25	0.70
2:I:499:SER:HA	2:I:502:VAL:HG12	1.74	0.70
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.74	0.70
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.24	0.70
2:I:59:ILE:HG23	2:I:476:LYS:HE3	1.72	0.70
3:J:48:THR:O	3:J:50:LYS:N	2.25	0.70
3:J:210:SER:O	3:J:214:ARG:HG2	1.91	0.70
3:D:495:ASN:O	3:D:497:GLU:N	2.23	0.70
2:I:206:ALA:O	2:I:209:ILE:HG22	1.90	0.70
3:D:805:GLN:O	3:D:807:LEU:N	2.25	0.70
3:D:48:THR:O	3:D:50:LYS:N	2.23	0.70
1:A:7:GLU:OE1	1:B:150:ARG:NH1	2.25	0.70
2:I:885:GLY:HA2	2:I:917:SER:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.73	0.70
1:B:112:ALA:HB3	1:B:126:PRO:HA	1.74	0.70
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.72	0.70
5:L:274:ARG:NH2	5:L:369:GLU:OE2	2.25	0.70
5:F:575:GLU:O	5:F:579:GLN:HG2	1.91	0.70
2:C:798:GLN:OE1	2:C:827:ARG:HB2	1.92	0.69
2:C:564:PRO:HG3	2:C:572:ILE:HG13	1.74	0.69
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.72	0.69
2:I:143:ARG:HH21	2:I:513:GLN:HA	1.56	0.69
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.22	0.69
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.74	0.69
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.25	0.69
1:A:50:SER:HB3	1:B:8:PHE:CZ	2.27	0.69
2:C:1269:ARG:CD	3:D:343:LEU:HD11	2.22	0.69
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.74	0.69
3:D:918:ILE:O	3:D:922:SER:OG	2.09	0.69
5:L:386:LEU:O	5:L:389:SER:OG	2.10	0.69
3:D:853:THR:HG22	3:D:854:ALA:H	1.56	0.69
3:D:591:ILE:HG13	3:D:604:MET:HE2	1.74	0.69
2:C:972:PHE:CB	2:C:994:ARG:HH21	2.05	0.69
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.75	0.69
2:I:848:GLU:HG2	2:I:888:THR:HG22	1.73	0.69
2:C:5:TYR:O	2:C:8:LYS:HG2	1.93	0.69
1:G:92:VAL:HA	1:G:120:ASP:O	1.92	0.69
5:L:395:THR:OG1	5:L:396:ASN:N	2.26	0.69
5:F:493:LYS:HA	5:F:496:LYS:HG3	1.75	0.69
3:D:210:SER:O	3:D:214:ARG:HG2	1.92	0.69
3:D:425:ARG:HG2	3:D:426:ALA:N	2.03	0.69
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.75	0.69
2:C:1289:GLU:OE2	3:D:473:THR:HG22	1.91	0.69
2:C:930:ASP:OD2	2:C:931:VAL:N	2.26	0.69
2:C:615:VAL:HG13	2:C:651:ASP:H	1.58	0.69
3:J:1262:ARG:HD2	3:J:1279:GLN:HE22	1.57	0.69
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.58	0.69
1:H:61:ILE:HG12	1:H:171:LEU:HD12	1.75	0.69
1:A:32:GLU:HG2	1:A:198:LEU:HD22	1.75	0.69
3:J:259:ARG:HD2	5:L:505:ILE:HD13	1.73	0.69
1:A:113:ALA:O	1:A:115:ILE:N	2.25	0.68
3:J:915:ILE:HA	3:J:918:ILE:HG23	1.73	0.68
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.75	0.68
3:D:709:ARG:HD2	3:D:710:ASP:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:566:GLY:O	2:C:569:ILE:HG13	1.94	0.68
3:J:320:ASN:OD1	3:J:322:ARG:HB3	1.93	0.68
5:F:469:GLN:O	5:F:473:GLU:HB2	1.93	0.68
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.75	0.68
2:C:17:LYS:NZ	2:C:1194:GLU:OE1	2.26	0.68
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.74	0.68
3:J:902:ASP:OD1	3:J:903:LEU:N	2.26	0.68
3:D:1149:ARG:NH2	3:D:1153:PRO:HG2	2.07	0.68
1:A:66:HIS:HD2	2:C:874:GLY:HA2	1.59	0.68
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.76	0.68
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.74	0.68
1:H:109:PRO:HA	1:H:132:HIS:HA	1.73	0.68
5:L:233:ASP:O	5:L:236:LYS:HE2	1.93	0.68
2:I:670:PHE:CD2	2:I:1113:LEU:HB3	2.29	0.68
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.76	0.68
2:C:670:PHE:CD2	2:C:1113:LEU:HB3	2.28	0.68
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.75	0.68
3:D:1227:HIS:HB2	3:J:1293:GLU:CD	2.14	0.68
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.58	0.68
2:C:1281:TYR:HE2	3:D:431:ARG:HB2	1.59	0.68
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.75	0.68
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.76	0.68
2:I:125:GLY:HA3	2:I:499:SER:HB2	1.76	0.68
3:J:1157:ALA:HB3	3:J:1207:GLY:H	1.59	0.68
1:H:35:PHE:HA	1:H:38:THR:HG22	1.76	0.67
1:H:195:ARG:HB3	1:H:198:LEU:HD21	1.76	0.67
1:A:60:GLU:CD	1:A:143:ARG:HH21	1.96	0.67
3:J:1203:ARG:NH2	3:J:1205:GLU:HG2	2.10	0.67
3:D:75:TYR:HD2	3:D:80:HIS:HD2	1.41	0.67
3:D:83:VAL:HG13	3:D:92:VAL:HG13	1.75	0.67
3:J:1193:TRP:HB2	3:J:1194:ARG:HH12	1.60	0.67
2:I:1124:ILE:O	2:I:1128:ILE:HG13	1.94	0.67
2:I:871:VAL:O	2:I:944:ARG:NH1	2.27	0.67
3:D:482:ALA:HB3	4:E:20:VAL:HG22	1.75	0.67
5:F:163:THR:O	5:F:260:ARG:NH2	2.28	0.67
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.75	0.67
1:A:250:ASP:HA	5:F:605:GLU:HG3	1.77	0.67
2:C:854:ILE:O	2:C:857:VAL:HG22	1.95	0.67
1:H:47:LEU:HD22	1:H:180:VAL:HG11	1.76	0.67
3:D:339:ARG:HD3	3:D:798:ARG:NH1	2.08	0.67
3:D:161:THR:HG22	3:D:164:GLN:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.29	0.67
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.77	0.67
3:J:450:HIS:HE1	3:J:452:LEU:HD12	1.60	0.67
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.75	0.67
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.28	0.67
4:K:52:ARG:O	4:K:56:GLU:HG2	1.95	0.67
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.09	0.67
3:J:425:ARG:HG2	3:J:426:ALA:N	2.09	0.67
2:I:1197:GLU:HA	2:I:1200:LYS:HD2	1.75	0.67
3:D:515:ARG:O	3:D:545:HIS:HB3	1.94	0.67
3:J:1203:ARG:HH22	3:J:1205:GLU:HG2	1.60	0.67
3:J:797:THR:O	3:J:801:VAL:HG12	1.94	0.67
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.77	0.67
1:G:161:SER:O	1:G:163:GLU:N	2.28	0.67
2:I:998:LEU:HD12	2:I:998:LEU:H	1.59	0.66
2:I:1013:GLN:O	2:I:1017:GLN:HG2	1.95	0.66
2:I:499:SER:O	2:I:503:LYS:HB2	1.95	0.66
1:B:215:GLU:HA	1:B:218:ARG:HG3	1.77	0.66
3:D:510:LEU:O	3:D:514:THR:HG22	1.95	0.66
3:J:45:ASN:HB3	3:J:48:THR:O	1.95	0.66
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.08	0.66
2:C:303:ASP:HB3	2:C:306:THR:HG23	1.78	0.66
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.77	0.66
1:A:31:LEU:HB2	1:A:199:ASP:O	1.95	0.66
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.10	0.66
3:J:903:LEU:HB3	3:J:905:ARG:HG3	1.77	0.66
1:A:135:ASP:O	1:A:138:ALA:N	2.27	0.66
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.27	0.66
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.59	0.66
4:E:4:VAL:HG13	4:E:5:THR:HG23	1.77	0.66
5:L:453:PRO:O	5:L:456:MET:HB2	1.95	0.66
3:D:114:ILE:HD11	3:D:311:ARG:HB2	1.77	0.66
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.77	0.66
3:J:370:LYS:HG2	3:J:441:LEU:HD12	1.78	0.66
2:I:629:PHE:CD2	2:I:634:VAL:HG11	2.31	0.66
2:C:1289:GLU:OE1	2:C:1294:LYS:HE2	1.95	0.66
3:J:853:THR:HG22	3:J:854:ALA:H	1.60	0.66
5:F:276:MET:O	5:F:280:VAL:HG23	1.95	0.66
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.76	0.66
5:F:261:LEU:HD12	5:F:261:LEU:H	1.60	0.66
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4:SER:OG	2:I:5:TYR:N	2.27	0.66
3:J:16:GLU:HG3	3:J:17:PHE:H	1.61	0.66
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.77	0.66
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.77	0.66
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.77	0.66
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.77	0.66
1:B:196:THR:CG2	3:D:443:GLU:HG3	2.26	0.66
2:C:721:GLY:N	2:C:740:GLU:OE1	2.25	0.66
2:I:799:ASN:HB3	2:I:1231:TYR:HD1	1.61	0.66
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.61	0.66
2:C:27:LEU:O	2:C:528:ARG:NH1	2.29	0.65
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.25	0.65
3:J:700:ASN:O	3:J:704:GLU:HB2	1.97	0.65
3:D:709:ARG:HD2	3:D:710:ASP:N	2.11	0.65
3:D:594:GLN:HG3	3:D:596:LEU:HD22	1.78	0.65
5:F:343:LYS:O	5:F:347:ILE:HG13	1.97	0.65
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.77	0.65
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.76	0.65
2:C:1161:LEU:HG	2:C:1161:LEU:O	1.91	0.65
3:D:1183:SER:HA	3:J:206:ASN:ND2	2.11	0.65
2:I:870:ILE:HG13	2:I:884:VAL:HG22	1.78	0.65
1:H:69:SER:HB2	1:H:78:ILE:HD11	1.76	0.65
5:F:418:LYS:HD2	5:F:434:TRP:CZ2	2.32	0.65
1:A:13:LEU:HD12	1:A:16:ILE:HD11	1.79	0.65
2:C:1243:MET:HA	3:D:353:SER:HB3	1.78	0.65
3:J:827:GLU:CB	3:J:832:LYS:HD2	2.27	0.65
2:C:600:THR:HG22	2:C:602:GLU:H	1.61	0.65
2:C:624:ASP:OD1	2:C:625:GLU:N	2.26	0.65
3:D:709:ARG:O	3:D:711:GLY:N	2.30	0.65
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.32	0.65
1:H:101:THR:HG22	1:H:116:THR:HB	1.79	0.65
2:C:4:SER:OG	2:C:5:TYR:N	2.30	0.65
2:I:12:ARG:NH1	2:I:1182:ILE:O	2.28	0.65
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.77	0.65
3:J:479:GLU:HG2	4:K:20:VAL:HG11	1.77	0.65
3:J:850:LYS:HB3	3:J:851:PRO:HD2	1.77	0.65
3:J:495:ASN:O	3:J:497:GLU:N	2.30	0.65
1:H:27:THR:HB	1:H:202:VAL:HG22	1.79	0.65
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.77	0.65
1:H:81:ILE:HG23	1:H:130:ILE:O	1.97	0.65
5:L:306:PHE:CZ	5:L:310:GLU:HG3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:SER:HB3	1:B:8:PHE:HZ	1.62	0.65
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.78	0.65
2:C:1017:GLN:O	2:C:1021:LEU:HG	1.97	0.65
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.79	0.65
5:L:343:LYS:O	5:L:347:ILE:HG13	1.96	0.65
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.79	0.65
5:L:476:ARG:HH11	5:L:476:ARG:HB3	1.61	0.65
2:C:483:ASP:HB2	2:C:486:THR:HG22	1.77	0.65
5:F:483:LEU:HD12	5:F:483:LEU:H	1.62	0.65
1:H:59:VAL:HG22	1:H:144:ILE:HG13	1.78	0.65
3:D:833:GLU:OE2	3:D:1247:LYS:NZ	2.30	0.65
1:G:23:HIS:HB2	1:G:205:MET:O	1.97	0.65
3:J:1147:ALA:O	3:J:1218:HIS:NE2	2.29	0.65
3:J:58:CYS:SG	3:J:60:ARG:HB3	2.37	0.64
1:H:13:LEU:HA	1:H:28:LEU:HD13	1.79	0.64
1:G:49:SER:HB3	2:I:1083:GLU:CD	2.16	0.64
1:H:62:ASP:N	1:H:62:ASP:OD1	2.30	0.64
5:F:466:ILE:CG2	5:F:486:ARG:HG3	2.27	0.64
5:F:125:ASP:O	5:F:129:GLN:HG3	1.97	0.64
3:J:17:PHE:O	3:J:1355:ARG:NH2	2.30	0.64
2:I:746:ALA:HA	2:I:974:ARG:HH21	1.62	0.64
3:D:1191:PRO:HB3	3:D:1194:ARG:NH1	2.11	0.64
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.80	0.64
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.32	0.64
2:C:1321:GLU:OE2	3:D:99:ARG:HD3	1.96	0.64
2:I:798:GLN:OE1	2:I:827:ARG:HB2	1.98	0.64
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.80	0.64
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.79	0.64
2:C:367:TYR:HA	2:C:384:LEU:HD22	1.78	0.64
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.77	0.64
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.78	0.64
1:A:104:LYS:HD3	1:A:114:ASP:OD2	1.98	0.64
1:H:35:PHE:HA	1:H:38:THR:CG2	2.28	0.64
2:I:478:ARG:NH1	2:I:482:GLY:HA2	2.10	0.64
2:C:40:GLU:HG2	2:C:41:GLN:N	2.12	0.64
1:H:79:LEU:HA	1:H:82:LEU:HD12	1.79	0.64
5:L:573:LEU:HD23	5:L:573:LEU:H	1.61	0.64
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.33	0.64
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.13	0.64
2:I:888:THR:OG1	2:I:914:LYS:HB3	1.97	0.64
5:F:306:PHE:CZ	5:F:310:GLU:HG3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.80	0.64
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.29	0.64
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.78	0.64
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.79	0.64
3:J:770:LEU:H	3:J:770:LEU:HD22	1.63	0.64
5:F:298:PRO:HD2	5:F:326:TRP:CG	2.33	0.64
2:C:619:ALA:HB1	2:C:657:THR:HA	1.80	0.64
3:J:1167:LYS:HE3	3:J:1174:ARG:HD2	1.80	0.64
3:D:140:TYR:HB3	5:F:100:MET:SD	2.37	0.64
3:D:259:ARG:HG3	5:F:502:LYS:HD2	1.79	0.64
1:G:45:ARG:NH2	1:H:37:HIS:HB3	2.13	0.64
1:H:9:LEU:HD12	1:H:195:ARG:NH2	2.10	0.64
3:D:66:LYS:HE2	3:D:69:GLU:OE1	1.97	0.64
5:F:463:LEU:HD21	5:F:487:MET:HG3	1.81	0.64
3:J:24:LEU:HD23	3:J:232:ASN:ND2	2.13	0.63
2:C:1259:LEU:HD12	2:C:1260:GLY:N	2.13	0.63
1:H:102:LEU:O	1:H:141:SER:HA	1.98	0.63
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.78	0.63
1:G:35:PHE:CE1	1:H:46:ILE:HG12	2.33	0.63
2:I:617:ALA:HA	2:I:636:CYS:SG	2.37	0.63
3:D:327:LEU:HA	3:D:330:MET:HG3	1.81	0.63
3:D:60:ARG:HA	3:D:89:GLY:O	1.99	0.63
3:J:430:HIS:CE1	3:J:925:GLU:HG3	2.34	0.63
1:B:112:ALA:HA	1:B:115:ILE:HG13	1.80	0.63
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.79	0.63
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.80	0.63
2:I:705:GLU:HB2	2:I:794:LEU:H	1.62	0.63
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.63	0.63
2:I:1065:LYS:HE2	3:J:462:ASP:O	1.98	0.63
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.63	0.63
3:D:1280:VAL:CG2	3:D:1304:ARG:HH21	2.04	0.63
3:D:750:PRO:HA	3:D:777:HIS:CE1	2.34	0.63
1:A:14:VAL:HG22	1:A:15:ASP:H	1.63	0.63
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.14	0.63
1:A:158:ARG:HH21	1:A:172:LEU:HB3	1.60	0.63
3:J:510:LEU:O	3:J:514:THR:HG22	1.99	0.63
2:C:510:GLN:NE2	2:C:534:GLY:HA2	2.14	0.63
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.81	0.63
3:D:902:ASP:OD1	3:D:903:LEU:N	2.32	0.63
3:J:432:LEU:HD21	3:J:489:ASN:HB3	1.79	0.63
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:244:THR:O	5:L:247:GLU:HG2	1.99	0.63
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.81	0.63
2:C:209:ILE:HD11	2:C:425:ILE:HD13	1.81	0.63
2:C:1255:THR:O	2:C:1257:GLN:N	2.32	0.63
3:D:1179:PRO:HG2	3:D:1183:SER:O	1.99	0.63
2:I:857:VAL:HG21	2:I:862:LEU:HD21	1.80	0.63
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.80	0.63
1:A:55:ALA:HB3	1:A:177:TYR:HD1	1.61	0.63
3:J:102:MET:HE2	3:J:246:PRO:HD3	1.80	0.63
2:C:356:THR:HG21	2:C:362:ALA:HA	1.81	0.63
2:C:325:LEU:O	2:C:330:HIS:HB2	1.98	0.62
5:L:245:ALA:O	5:L:249:ILE:HG13	1.99	0.62
5:F:470:MET:HA	5:F:473:GLU:HB3	1.81	0.62
4:E:38:LEU:HB2	4:E:53:GLU:OE1	1.99	0.62
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.81	0.62
3:D:491:LEU:HD22	3:D:496:GLY:O	1.99	0.62
2:I:975:ILE:HD13	2:I:998:LEU:HG	1.80	0.62
3:J:1183:SER:C	3:J:1185:PRO:HD3	2.20	0.62
3:J:19:ALA:CB	3:J:1373:ARG:HH22	2.11	0.62
3:D:507:VAL:HG11	3:D:598:LYS:HG3	1.81	0.62
3:D:701:LEU:HD12	3:D:723:TYR:HD2	1.64	0.62
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	1.80	0.62
2:I:771:VAL:HG21	2:I:783:LEU:HD13	1.82	0.62
4:K:49:ILE:HA	4:K:52:ARG:HD3	1.81	0.62
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.80	0.62
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.64	0.62
3:J:515:ARG:NH2	3:J:717:VAL:O	2.32	0.62
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.81	0.62
5:L:470:MET:O	5:L:478:PRO:HD3	1.99	0.62
3:J:75:TYR:CE2	3:J:83:VAL:HG21	2.35	0.62
3:D:79:LYS:HG3	3:D:80:HIS:ND1	2.14	0.62
3:D:271:ARG:HG2	3:D:302:ALA:HB1	1.80	0.62
3:D:1233:ILE:O	3:D:1237:VAL:HG12	1.98	0.62
1:A:156:SER:HB3	2:C:1059:ARG:NH2	2.08	0.62
2:I:1192:GLU:O	2:I:1196:LYS:HG2	1.98	0.62
2:I:1297:ASP:OD1	2:I:1300:GLY:N	2.30	0.62
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.81	0.62
1:H:41:ASN:O	1:H:45:ARG:HG3	1.99	0.62
3:D:432:LEU:HD21	3:D:489:ASN:HB3	1.80	0.62
2:I:498:ILE:H	2:I:498:ILE:HD12	1.65	0.62
2:I:358:ASP:OD2	2:I:361:SER:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.32	0.62
2:C:886:LYS:H	2:C:917:SER:HB3	1.65	0.62
3:J:600:ALA:O	3:J:603:LYS:HG2	1.99	0.62
2:C:744:GLY:C	2:C:746:ALA:H	2.03	0.62
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.35	0.62
3:D:197:GLU:O	3:D:201:LEU:HG	1.99	0.62
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.81	0.62
1:H:9:LEU:HB3	1:H:32:GLU:HG2	1.81	0.62
2:I:490:GLN:HA	2:I:493:ILE:HG23	1.82	0.62
1:A:54:CYS:HA	1:A:148:ARG:HA	1.82	0.62
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.34	0.62
2:C:138:ILE:O	2:C:139:ASN:ND2	2.33	0.62
2:C:421:SER:H	2:C:424:ASP:HB2	1.64	0.62
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.82	0.62
5:L:544:THR:HG22	5:L:607:LEU:HD11	1.81	0.62
3:D:339:ARG:CD	3:D:798:ARG:HD3	2.30	0.62
2:C:796:LEU:HD12	2:C:796:LEU:H	1.64	0.62
2:I:720:ARG:NH2	2:I:736:VAL:HG21	2.15	0.62
2:C:561:ILE:O	2:C:680:LEU:HD12	2.00	0.62
2:C:377:THR:HB	2:C:380:ALA:H	1.65	0.62
2:C:1292:THR:HG22	2:C:1293:VAL:N	2.15	0.62
1:A:145:LYS:HZ2	1:A:147:GLN:HG3	1.64	0.62
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.82	0.62
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.82	0.62
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.30	0.61
2:I:560:PRO:O	3:J:780:ARG:NH2	2.32	0.61
1:G:93:GLN:H	1:G:120:ASP:HB3	1.63	0.61
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.81	0.61
3:D:248:ASP:O	3:D:251:PRO:HG3	2.00	0.61
2:I:356:THR:HG21	2:I:362:ALA:HA	1.82	0.61
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.33	0.61
1:G:135:ASP:HB3	1:G:138:ALA:HB2	1.80	0.61
3:J:322:ARG:NH1	3:J:322:ARG:HB2	2.15	0.61
3:D:203:GLU:O	3:D:207:GLU:HG2	1.99	0.61
2:I:968:GLU:HG3	2:I:1018:TYR:CE1	2.32	0.61
2:I:519:ASN:O	2:I:523:GLU:HG3	1.99	0.61
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.65	0.61
3:D:661:VAL:CG1	3:D:685:ILE:HD11	2.30	0.61
3:D:310:GLY:HA2	3:D:314:ARG:CD	2.29	0.61
3:D:1344:LEU:O	3:D:1346:GLY:N	2.27	0.61
3:J:1179:PRO:CD	3:J:1184:ASP:HA	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:582:ASN:HB3	2:I:586:PHE:H	1.65	0.61
1:G:14:VAL:HG22	1:G:15:ASP:H	1.66	0.61
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.83	0.61
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.00	0.61
5:F:311:THR:HB	5:F:345:GLN:HG2	1.81	0.61
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.34	0.61
5:L:515:GLU:HG2	5:L:516:ASP:H	1.66	0.61
3:D:827:GLU:HB3	3:D:832:LYS:HD2	1.83	0.61
2:I:232:ILE:HD12	2:I:330:HIS:O	2.00	0.61
1:H:101:THR:H	1:H:116:THR:CG2	2.14	0.61
2:I:518:ASN:OD1	2:I:518:ASN:N	2.33	0.61
1:G:156:SER:HB2	2:I:1059:ARG:HH22	1.65	0.61
2:C:448:LEU:HB2	2:C:553:THR:HB	1.81	0.61
2:I:724:VAL:HA	2:I:734:ILE:HD13	1.82	0.61
2:I:360:LEU:O	2:I:364:VAL:HG23	1.99	0.61
3:D:244:VAL:HA	3:D:269:TYR:OH	2.01	0.61
5:L:465:ARG:HD2	5:L:468:ARG:HH22	1.65	0.61
3:J:812:ASP:HB2	3:J:911:LYS:HE3	1.83	0.61
1:H:151:GLY:O	1:H:177:TYR:HB2	1.99	0.61
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.82	0.61
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.83	0.61
5:L:299:LYS:HA	5:L:302:PHE:CB	2.28	0.61
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.65	0.61
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.66	0.61
3:J:514:THR:HG21	3:J:596:LEU:HG	1.82	0.61
2:C:149:LEU:HD12	2:C:452:ARG:O	2.01	0.61
5:L:414:LYS:HD3	5:L:434:TRP:HZ3	1.66	0.61
2:I:596:ASP:CG	2:I:597:GLY:H	2.05	0.61
2:C:55:SER:OG	2:C:465:ARG:NH1	2.34	0.61
3:D:632:ALA:O	3:D:635:SER:OG	2.18	0.61
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.82	0.61
5:L:340:ALA:HA	5:L:343:LYS:NZ	2.15	0.61
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.82	0.61
3:D:1301:THR:HG23	3:J:1301:THR:HG23	1.83	0.61
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.33	0.61
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.82	0.60
5:F:244:THR:O	5:F:247:GLU:HG2	2.00	0.60
3:J:751:ASP:HB3	3:J:753:SER:H	1.66	0.60
5:L:134:VAL:HG22	5:L:273:MET:HE3	1.82	0.60
5:F:573:LEU:H	5:F:573:LEU:HD23	1.66	0.60
3:J:1280:VAL:HG11	3:J:1304:ARG:NH2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:798:GLN:HB2	2:I:828:PHE:CE1	2.35	0.60
3:D:1183:SER:C	3:D:1185:PRO:HD3	2.22	0.60
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.84	0.60
3:D:75:TYR:OH	3:D:86:GLU:OE1	2.18	0.60
2:I:797:GLY:O	2:I:1231:TYR:OH	2.19	0.60
2:C:582:ASN:HB3	2:C:586:PHE:H	1.66	0.60
3:J:215:LYS:O	3:J:218:THR:HG22	2.01	0.60
1:G:8:PHE:O	1:G:9:LEU:HB2	2.00	0.60
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.35	0.60
1:H:49:SER:O	1:H:151:GLY:HA2	2.00	0.60
1:A:61:ILE:HB	1:A:64:VAL:CG2	2.31	0.60
3:J:267:ASP:HA	3:J:270:ARG:HH21	1.66	0.60
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.83	0.60
3:D:1270:GLY:HA3	3:D:1297:LYS:O	2.01	0.60
3:J:551:ARG:HA	3:J:568:SER:O	2.01	0.60
2:I:1327:LEU:O	2:I:1331:ARG:HB2	2.00	0.60
2:C:1191:LYS:O	2:C:1195:ILE:HG13	1.99	0.60
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.66	0.60
2:C:483:ASP:HB2	2:C:486:THR:HG21	1.83	0.60
5:L:557:LYS:HG3	5:L:561:MET:HE1	1.83	0.60
5:F:466:ILE:HG23	5:F:486:ARG:HG3	1.83	0.60
2:I:941:LYS:HD3	2:I:949:GLU:OE1	2.01	0.60
1:B:73:GLY:CA	1:B:134:THR:HG22	2.27	0.60
3:D:427:PRO:HB2	3:D:429:LEU:HD22	1.84	0.60
3:D:75:TYR:HD2	3:D:80:HIS:CD2	2.18	0.60
3:J:827:GLU:HB3	3:J:832:LYS:HD2	1.83	0.60
3:J:649:LYS:O	3:J:653:ILE:HG13	2.01	0.60
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.83	0.60
5:L:379:MET:O	5:L:383:ASN:ND2	2.33	0.60
3:D:224:LEU:O	3:D:227:PHE:N	2.34	0.60
2:C:148:GLN:NE2	2:C:533:LEU:O	2.26	0.60
5:L:371:LYS:HA	5:L:374:ARG:NH1	2.17	0.60
2:I:520:PRO:HG3	2:I:714:VAL:HG11	1.82	0.60
5:L:326:TRP:HA	5:L:329:LYS:HD2	1.84	0.60
5:F:130:VAL:HB	5:F:365:MET:HG3	1.83	0.60
2:I:117:ILE:HD12	2:I:488:MET:HG2	1.83	0.60
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.42	0.60
2:C:5:TYR:HB2	2:C:781:ASP:OD1	2.02	0.60
2:I:971:LEU:HD21	2:I:1014:LEU:O	2.02	0.60
5:F:348:GLU:HG2	5:F:354:THR:HA	1.84	0.60
3:J:473:THR:HG23	3:J:476:ALA:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.84	0.60
2:C:1032:LYS:O	2:C:1036:ILE:HG13	2.01	0.60
2:C:949:GLU:HG2	2:C:1036:ILE:HG22	1.83	0.60
3:D:1226:VAL:HB	3:J:1293:GLU:H	1.67	0.60
3:D:1167:LYS:NZ	3:D:1168:GLU:O	2.35	0.60
3:D:27:PRO:O	3:D:31:ARG:HG3	2.02	0.60
5:F:573:LEU:HD13	5:F:588:ARG:NE	2.17	0.60
1:H:48:LEU:HD22	3:J:539:SER:HB3	1.83	0.60
2:I:1142:ARG:HH11	2:I:1161:LEU:HD11	1.67	0.59
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.32	0.59
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.83	0.59
3:D:825:VAL:HG22	3:D:833:GLU:H	1.67	0.59
2:I:57:PHE:HD1	2:I:58:PRO:HA	1.67	0.59
2:I:475:VAL:HG22	2:I:492:MET:HB2	1.83	0.59
3:J:405:GLU:O	3:J:408:VAL:HG22	2.02	0.59
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.14	0.59
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.17	0.59
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.84	0.59
2:I:169:LYS:O	2:I:170:VAL:HG22	2.02	0.59
5:L:465:ARG:HB3	5:L:468:ARG:HH12	1.67	0.59
2:I:57:PHE:CD1	2:I:58:PRO:HA	2.37	0.59
2:I:528:ARG:NH2	2:I:576:SER:O	2.35	0.59
1:G:195:ARG:HG3	1:G:198:LEU:HG	1.84	0.59
3:J:619:ILE:O	3:J:623:GLN:HG2	2.03	0.59
2:C:310:ILE:HD13	2:C:325:LEU:HA	1.83	0.59
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.84	0.59
3:D:482:ALA:HA	4:E:6:VAL:HG11	1.83	0.59
3:D:421:VAL:CG1	3:D:439:PRO:HG3	2.32	0.59
2:I:462:ASN:O	2:I:466:VAL:HG23	2.02	0.59
3:J:1163:VAL:HG21	3:J:1175:LEU:HD21	1.83	0.59
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.03	0.59
1:A:49:SER:HG	1:A:50:SER:HG	1.51	0.59
5:F:299:LYS:O	5:F:303:ILE:HG12	2.02	0.59
2:I:1100:PRO:HB3	3:J:639:VAL:HG12	1.84	0.59
5:L:290:LEU:HD22	5:L:333:VAL:HG21	1.83	0.59
2:C:41:GLN:NE2	2:C:73:TYR:O	2.34	0.59
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.85	0.59
1:A:71:LYS:HD3	1:A:72:GLU:N	2.17	0.59
5:L:390:ILE:O	5:L:393:LYS:HB2	2.03	0.59
3:D:1158:GLU:HA	3:D:1223:LEU:HD11	1.83	0.59
1:B:47:LEU:O	1:B:180:VAL:HG21	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:491:LEU:HD23	3:D:498:PRO:HA	1.85	0.59
2:I:12:ARG:NH2	2:I:698:PRO:O	2.27	0.59
3:J:418:GLU:H	4:K:45:LYS:NZ	2.01	0.59
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.84	0.59
2:I:629:PHE:HE2	2:I:650:VAL:HG21	1.64	0.59
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.36	0.59
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.83	0.59
2:I:685:MET:HA	2:I:688:GLN:HE21	1.66	0.59
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	1.85	0.59
2:I:384:LEU:O	2:I:388:LEU:HG	2.03	0.59
2:C:62:TYR:O	2:C:64:GLY:N	2.36	0.59
1:A:253:LEU:HA	1:A:278:ILE:HG13	1.85	0.59
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.36	0.59
3:D:1191:PRO:CB	3:D:1194:ARG:HH11	2.16	0.59
2:I:151:ARG:HH22	2:I:175:ARG:HD2	1.67	0.59
5:L:139:GLU:HG2	5:L:351:THR:HA	1.84	0.59
5:F:245:ALA:O	5:F:249:ILE:HG13	2.03	0.59
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.85	0.59
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.03	0.59
1:A:296:GLY:N	1:A:299:SER:HB2	2.16	0.59
5:L:320:ILE:HG23	5:L:327:SER:O	2.02	0.59
2:C:705:GLU:HB2	2:C:794:LEU:H	1.68	0.59
3:D:854:ALA:HB2	3:J:1372:ARG:CG	2.33	0.59
2:I:168:GLY:O	2:I:170:VAL:N	2.24	0.59
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.85	0.59
5:L:348:GLU:HA	5:L:353:LEU:O	2.03	0.59
3:J:735:ALA:O	3:J:739:GLN:HG3	2.03	0.59
5:L:547:VAL:HG13	5:L:598:LEU:HD22	1.85	0.59
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.84	0.59
2:I:1313:HIS:O	4:K:28:ARG:NH1	2.36	0.58
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.83	0.58
3:J:1158:GLU:HB3	3:J:1186:TYR:CE1	2.38	0.58
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.67	0.58
2:C:486:THR:HG23	2:C:487:LEU:N	2.18	0.58
3:J:733:SER:O	3:J:737:ILE:HG12	2.04	0.58
1:B:35:PHE:HA	1:B:38:THR:HG22	1.84	0.58
3:J:128:LEU:HD23	3:J:192:MET:HE1	1.86	0.58
3:D:26:SER:HA	3:D:236:TRP:NE1	2.19	0.58
5:L:284:GLU:OE2	5:L:359:LYS:HD2	2.03	0.58
3:D:872:LEU:HB3	3:D:877:VAL:HG11	1.84	0.58
1:A:236:ASP:HA	1:B:14:VAL:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:678:ARG:O	3:D:682:VAL:HG23	2.03	0.58
3:D:1181:ASP:OD1	3:D:1182:GLY:N	2.36	0.58
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.85	0.58
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.69	0.58
5:F:388:ILE:HG22	5:F:392:LYS:HE3	1.85	0.58
3:J:689:ALA:O	3:J:693:VAL:HG23	2.03	0.58
1:A:250:ASP:HB2	5:F:601:PRO:HB3	1.85	0.58
5:L:230:VAL:O	5:L:234:THR:HG23	2.03	0.58
1:B:101:THR:H	1:B:116:THR:CG2	2.15	0.58
3:D:1270:GLY:HA3	3:D:1297:LYS:C	2.24	0.58
2:C:517:GLN:O	2:C:517:GLN:HG2	2.02	0.58
2:C:998:LEU:HD12	2:C:998:LEU:H	1.68	0.58
4:K:32:VAL:O	4:K:34:GLY:N	2.34	0.58
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.85	0.58
5:F:379:MET:O	5:F:383:ASN:ND2	2.37	0.58
3:D:490:ILE:HA	3:D:500:ILE:CG1	2.33	0.58
5:L:111:LEU:HD13	5:L:116:GLU:HA	1.85	0.58
2:I:1269:ARG:NE	3:J:343:LEU:HD21	2.17	0.58
3:J:155:GLU:CB	3:J:158:GLN:HB2	2.25	0.58
2:C:323:ALA:O	2:C:327:GLN:HG3	2.04	0.58
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.85	0.58
2:C:39:ILE:HD11	2:C:75:LEU:HG	1.84	0.58
5:L:561:MET:HA	5:L:567:MET:CE	2.33	0.58
3:J:1167:LYS:CE	3:J:1174:ARG:HD2	2.34	0.58
3:D:140:TYR:HE2	5:F:95:THR:HG22	1.67	0.58
5:F:226:ALA:O	5:F:229:VAL:HG22	2.03	0.58
3:J:291:ILE:HG23	5:L:406:GLN:HE22	1.69	0.58
1:B:49:SER:O	1:B:151:GLY:HA2	2.04	0.58
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.34	0.58
2:I:1046:VAL:HG21	2:I:1049:ILE:HD11	1.85	0.58
3:D:48:THR:C	3:D:50:LYS:H	2.06	0.58
1:A:187:VAL:HG12	1:A:201:LEU:HD13	1.85	0.58
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.19	0.58
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.85	0.58
3:D:1372:ARG:NE	3:J:854:ALA:HB2	2.19	0.58
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.85	0.58
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.36	0.58
5:L:515:GLU:HG2	5:L:516:ASP:N	2.18	0.58
1:A:279:GLY:HA3	1:A:321:TRP:CZ2	2.38	0.58
2:C:643:SER:HG	2:C:645:PHE:HE1	1.52	0.58
2:I:852:ALA:HB2	2:I:869:GLY:CA	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1333:LEU:HD23	3:D:307:LEU:HD22	1.84	0.58
2:C:696:ASP:O	2:C:697:LYS:HB3	2.03	0.58
1:B:101:THR:H	1:B:116:THR:HG21	1.69	0.58
2:C:70:TYR:HA	2:C:100:LEU:HD23	1.85	0.58
3:J:57:PHE:CE1	3:J:252:LEU:HB2	2.38	0.58
3:J:810:THR:HG23	3:J:811:GLU:H	1.69	0.58
3:D:374:LEU:HD23	3:D:412:LEU:HD12	1.85	0.58
2:C:906:PHE:CE2	5:F:608:ARG:HD3	2.38	0.58
2:C:119:GLU:HB2	2:C:489:PRO:HD2	1.85	0.58
3:J:66:LYS:HE2	3:J:69:GLU:OE1	2.04	0.58
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.85	0.58
3:J:510:LEU:HD22	3:J:601:ILE:HD11	1.86	0.58
3:D:161:THR:H	3:D:164:GLN:HB2	1.69	0.58
1:H:50:SER:HA	1:H:150:ARG:O	2.04	0.58
2:I:483:ASP:HB2	2:I:486:THR:CG2	2.34	0.58
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.69	0.58
2:I:80:PHE:HZ	2:I:1038:GLN:HE22	1.52	0.58
1:G:12:ARG:H	1:G:30:PRO:CD	2.09	0.57
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.85	0.57
5:L:357:GLN:O	5:L:361:ILE:HG13	2.04	0.57
3:D:215:LYS:HE3	3:D:216:LYS:HG3	1.86	0.57
2:C:685:MET:HA	2:C:688:GLN:HE21	1.69	0.57
3:J:47:ARG:NH1	5:L:500:ILE:HD11	2.19	0.57
1:A:134:THR:HG23	2:C:726:TYR:HE1	1.70	0.57
2:C:138:ILE:HD11	2:C:506:PHE:HB3	1.84	0.57
2:C:561:ILE:HD12	2:C:679:ALA:HB1	1.85	0.57
3:D:474:LEU:HA	3:D:477:GLN:HG3	1.85	0.57
3:D:72:CYS:HB3	3:D:88:CYS:SG	2.43	0.57
1:G:70:THR:CG2	2:I:755:LYS:HE2	2.34	0.57
2:I:519:ASN:ND2	2:I:689:ALA:O	2.37	0.57
3:D:438:GLU:OE2	3:D:481:ARG:NH2	2.28	0.57
3:D:268:LEU:HG	3:D:324:LEU:HD22	1.86	0.57
2:I:1281:TYR:CE1	3:J:484:MET:HE3	2.40	0.57
2:I:138:ILE:HD11	2:I:506:PHE:HB3	1.86	0.57
3:D:787:ALA:O	3:D:790:THR:HB	2.04	0.57
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.85	0.57
3:D:161:THR:HG23	3:D:164:GLN:H	1.69	0.57
2:C:748:ILE:HD11	2:C:967:LEU:HD12	1.86	0.57
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.33	0.57
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.69	0.57
5:F:479:THR:HG23	5:F:481:GLU:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1333:LEU:HD23	3:J:307:LEU:HD22	1.85	0.57
3:D:653:ILE:HG23	3:D:692:ARG:CZ	2.35	0.57
2:I:800:MET:O	2:I:1229:TYR:HA	2.04	0.57
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.86	0.57
5:L:338:HIS:CE1	5:L:341:LEU:HD13	2.40	0.57
1:B:89:ALA:HB3	1:B:124:VAL:CG1	2.34	0.57
3:D:514:THR:CG2	3:D:596:LEU:HB2	2.35	0.57
3:D:279:LEU:HD12	3:D:295:GLU:HG3	1.85	0.57
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.69	0.57
1:G:189:ALA:HB1	1:G:191:ARG:CZ	2.35	0.57
1:H:100:LEU:HD23	1:H:116:THR:O	2.05	0.57
3:J:664:ILE:HG21	3:J:681:LYS:HB3	1.86	0.57
2:C:1160:ASP:HB2	2:C:1161:LEU:HD12	1.86	0.57
1:A:234:LEU:N	1:B:218:ARG:HH12	2.02	0.57
3:D:690:ASN:HD21	3:D:745:GLY:HA2	1.68	0.57
2:I:1313:HIS:N	4:K:31:GLN:OE1	2.28	0.57
5:L:288:MET:HG2	5:L:299:LYS:HE2	1.86	0.57
2:C:802:VAL:HG12	2:C:1228:GLY:O	2.04	0.57
1:H:64:VAL:HG12	1:H:66:HIS:H	1.68	0.57
1:G:47:LEU:O	1:G:180:VAL:HG11	2.04	0.57
2:I:897:PRO:HB2	2:I:898:GLU:OE1	2.05	0.57
1:A:71:LYS:HB3	1:A:74:VAL:HG13	1.86	0.57
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.87	0.57
2:C:211:ARG:NH1	2:C:357:ASN:O	2.38	0.57
5:F:494:ILE:O	5:F:498:LEU:HB2	2.05	0.57
2:I:32:LEU:HD23	2:I:130:MET:SD	2.45	0.57
3:J:26:SER:HA	3:J:236:TRP:NE1	2.20	0.57
2:I:5:TYR:O	2:I:8:LYS:HG2	2.04	0.57
5:L:474:MET:O	5:L:476:ARG:N	2.28	0.57
5:F:484:ALA:O	5:F:491:GLU:HB2	2.05	0.57
3:J:79:LYS:HB2	5:L:569:THR:H	1.70	0.57
3:J:147:ILE:HG13	3:J:147:ILE:O	2.05	0.57
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.69	0.57
5:L:465:ARG:CD	5:L:468:ARG:HH22	2.18	0.57
3:D:363:LEU:HA	3:D:450:HIS:CD2	2.39	0.57
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.86	0.57
5:L:148:TYR:OH	5:L:218:ARG:HA	2.04	0.57
2:I:1106:ARG:NE	3:J:731:ARG:HH21	2.02	0.57
3:D:45:ASN:HB3	3:D:48:THR:O	2.04	0.57
5:L:503:GLU:OE1	5:L:504:PRO:HD2	2.04	0.57
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:870:ILE:HG22	2:I:944:ARG:NH1	2.20	0.56
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.85	0.56
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.69	0.56
1:A:106:GLY:O	1:A:108:GLY:N	2.38	0.56
2:I:726:TYR:OH	2:I:728:ASP:OD2	2.19	0.56
2:C:27:LEU:HB2	2:C:524:ILE:HD11	1.86	0.56
2:I:5:TYR:HD1	2:I:8:LYS:HD3	1.70	0.56
2:I:12:ARG:NE	2:I:793:GLU:OE1	2.27	0.56
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.45	0.56
2:C:86:GLN:HA	2:C:140:GLY:HA2	1.86	0.56
2:I:157:PHE:O	2:I:443:ASP:N	2.36	0.56
1:B:35:PHE:HA	1:B:38:THR:CG2	2.35	0.56
1:H:11:PRO:HB2	1:H:28:LEU:HD11	1.87	0.56
1:A:112:ALA:O	1:A:115:ILE:HG13	2.05	0.56
5:L:281:ARG:HG3	5:L:285:ARG:HH11	1.68	0.56
3:D:514:THR:HG21	3:D:596:LEU:HB2	1.87	0.56
5:L:456:MET:O	5:L:460:ILE:HG13	2.05	0.56
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.86	0.56
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.71	0.56
3:J:749:LYS:HG2	3:J:753:SER:O	2.05	0.56
1:G:195:ARG:HD2	1:G:196:THR:H	1.69	0.56
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.87	0.56
2:C:541:GLU:OE1	2:C:541:GLU:N	2.36	0.56
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.88	0.56
2:C:898:GLU:OE1	2:C:898:GLU:N	2.30	0.56
8:J:2004:4C6:O	8:J:2004:4C6:H20	2.04	0.56
4:K:54:ILE:HD13	4:K:59:ILE:HG22	1.87	0.56
1:H:216:ALA:O	1:H:220:ALA:N	2.37	0.56
3:J:522:GLY:O	3:J:525:MET:HG2	2.06	0.56
2:I:1269:ARG:HD3	3:J:343:LEU:CD2	2.24	0.56
2:C:802:VAL:HG21	2:C:1098:LEU:HD22	1.87	0.56
2:C:673:HIS:HB3	2:C:1109:ILE:CG2	2.35	0.56
1:G:224:LEU:CD2	1:G:228:LEU:HD22	2.35	0.56
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.21	0.56
3:J:393:THR:HG23	3:J:396:ALA:H	1.71	0.56
2:C:1035:LYS:O	2:C:1038:GLN:HG2	2.06	0.56
2:C:782:VAL:HG11	2:C:792:GLY:HA2	1.87	0.56
2:I:908:GLU:OE2	5:L:611:LEU:HD13	2.05	0.56
2:C:778:GLU:O	2:C:781:ASP:HB2	2.05	0.56
2:C:976:ARG:HB2	2:C:997:TRP:CZ3	2.41	0.56
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:277:MET:SD	5:L:359:LYS:HG2	2.46	0.56
2:C:359:ARG:CZ	2:C:363:LEU:HD11	2.36	0.56
2:C:498:ILE:H	2:C:498:ILE:HD12	1.70	0.56
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.86	0.56
2:I:1247:SER:HB3	3:J:375:GLU:O	2.05	0.56
1:H:60:GLU:HG3	1:H:143:ARG:O	2.06	0.56
2:I:1280:ALA:HB3	3:J:431:ARG:HB3	1.87	0.56
3:J:1199:PHE:HB2	3:J:1202:GLU:CB	2.34	0.56
2:C:73:TYR:HB2	2:C:98:VAL:HG22	1.86	0.56
1:H:78:ILE:O	1:H:82:LEU:HG	2.06	0.56
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.86	0.56
3:J:418:GLU:H	4:K:45:LYS:HZ2	1.51	0.56
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	1.88	0.56
2:I:149:LEU:HD12	2:I:452:ARG:O	2.06	0.56
2:I:135:THR:HG22	2:I:527:LYS:HE2	1.87	0.56
2:C:8:LYS:HE3	2:C:1171:ARG:NH2	2.21	0.56
1:G:166:ARG:NH1	1:G:168:ILE:HG12	2.19	0.56
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.87	0.56
2:C:486:THR:HG23	2:C:487:LEU:H	1.70	0.56
3:D:1284:ARG:HH22	3:J:1292:LEU:HD11	1.69	0.56
3:J:805:GLN:NE2	3:J:1348:LYS:HD3	2.21	0.56
5:L:314:THR:O	5:L:318:ALA:HB3	2.06	0.56
1:A:219:ARG:O	1:A:222:THR:HB	2.06	0.56
2:C:737:ASN:HB3	2:C:739:ASP:OD1	2.06	0.56
3:D:797:THR:O	3:D:801:VAL:HG12	2.05	0.56
2:I:810:TYR:HD2	3:J:359:PRO:HG2	1.70	0.56
5:F:421:TYR:CE2	5:F:422:ARG:HG3	2.41	0.56
3:D:1226:VAL:HG21	3:J:1292:LEU:HA	1.86	0.56
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.87	0.56
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	1.87	0.56
1:B:88:LEU:HD12	1:B:89:ALA:H	1.71	0.56
1:A:318:LEU:O	1:A:320:ASN:N	2.38	0.56
2:C:105:TYR:CD1	2:C:111:GLU:HB3	2.40	0.56
1:A:11:PRO:HA	1:A:30:PRO:HB2	1.88	0.56
2:I:16:GLY:O	2:I:1156:ARG:HG2	2.06	0.56
1:A:61:ILE:HB	1:A:64:VAL:HG21	1.88	0.56
2:I:1225:VAL:HG12	3:J:636:GLY:O	2.06	0.56
2:C:1002:LEU:HD22	2:C:1007:LYS:HB2	1.87	0.56
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.30	0.56
2:I:1131:MET:HB3	2:I:1141:LEU:HD11	1.88	0.56
3:J:844:THR:HG21	3:J:858:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.06	0.56
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.87	0.56
3:J:905:ARG:NH1	4:K:16:ARG:HB2	2.21	0.56
2:I:618:GLN:CG	3:J:770:LEU:HD21	2.35	0.56
3:J:1167:LYS:HD3	3:J:1174:ARG:HH11	1.71	0.56
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.88	0.56
2:C:76:GLY:O	2:C:94:ALA:HB1	2.05	0.56
5:F:561:MET:HA	5:F:567:MET:HE1	1.86	0.56
3:D:619:ILE:O	3:D:623:GLN:HG2	2.05	0.56
3:D:707:ILE:HD12	3:D:707:ILE:N	2.20	0.55
5:F:320:ILE:HG23	5:F:327:SER:O	2.05	0.55
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.20	0.55
2:I:73:TYR:HB2	2:I:98:VAL:HG22	1.88	0.55
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.87	0.55
1:B:219:ARG:HA	1:B:222:THR:HB	1.87	0.55
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.87	0.55
1:A:212:ASP:O	1:A:215:GLU:HB3	2.06	0.55
3:D:210:SER:HB2	3:D:213:LYS:CB	2.32	0.55
2:I:746:ALA:HB2	2:I:974:ARG:HE	1.70	0.55
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.89	0.55
5:F:306:PHE:CE1	5:F:310:GLU:HG3	2.42	0.55
5:F:513:ASP:C	5:F:515:GLU:H	2.09	0.55
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.88	0.55
3:J:418:GLU:HG3	4:K:45:LYS:H	1.72	0.55
2:I:1281:TYR:HE1	3:J:484:MET:HE3	1.72	0.55
3:J:1320:ILE:HG23	8:J:2004:4C6:H9	1.87	0.55
2:C:1207:SER:C	2:C:1209:GLN:H	2.08	0.55
2:I:425:ILE:O	2:I:429:MET:HG3	2.05	0.55
3:D:905:ARG:NH1	4:E:10:VAL:HG11	2.22	0.55
1:H:102:LEU:HD11	1:H:130:ILE:HG21	1.88	0.55
2:C:708:VAL:HG11	2:C:794:LEU:HD22	1.89	0.55
1:A:194:GLN:OE1	1:A:195:ARG:N	2.40	0.55
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.21	0.55
3:D:810:THR:HG23	3:D:811:GLU:H	1.71	0.55
3:J:1167:LYS:NZ	3:J:1170:LYS:HB2	2.22	0.55
5:L:280:VAL:O	5:L:284:GLU:HG3	2.06	0.55
1:B:81:ILE:O	1:B:85:LEU:HG	2.05	0.55
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.88	0.55
2:C:320:ASP:OD1	2:C:324:LYS:HE3	2.05	0.55
2:C:1281:TYR:HE2	3:D:431:ARG:CB	2.20	0.55
5:L:231:THR:CG2	5:L:249:ILE:HG12	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:109:ALA:HB1	2:C:111:GLU:HA	1.86	0.55
5:L:346:GLN:HA	5:L:349:GLU:OE2	2.07	0.55
3:D:54:ASP:OD1	3:D:54:ASP:N	2.39	0.55
1:A:145:LYS:NZ	1:A:147:GLN:HG3	2.21	0.55
2:C:1164:PHE:O	2:C:1166:ASP:N	2.38	0.55
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.41	0.55
1:A:47:LEU:O	1:A:180:VAL:HG11	2.07	0.55
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.22	0.55
3:J:598:LYS:O	3:J:601:ILE:HG22	2.06	0.55
5:L:340:ALA:HA	5:L:343:LYS:HZ3	1.72	0.55
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.88	0.55
3:D:327:LEU:O	3:D:330:MET:HB2	2.06	0.55
3:D:638:SER:OG	3:D:639:VAL:N	2.39	0.55
1:A:253:LEU:HA	1:A:278:ILE:CG1	2.37	0.55
2:I:800:MET:SD	2:I:1096:ILE:HD11	2.47	0.55
2:I:431:LYS:O	2:I:435:ILE:HG13	2.07	0.55
1:A:282:VAL:O	1:A:315:GLY:N	2.40	0.55
1:A:323:PRO:HB2	1:A:324:ALA:HB2	1.88	0.55
3:D:557:LYS:HA	3:D:563:LEU:HA	1.89	0.55
5:F:465:ARG:CD	5:F:468:ARG:HH22	2.20	0.55
3:J:638:SER:OG	3:J:639:VAL:N	2.39	0.55
5:F:230:VAL:O	5:F:234:THR:HG23	2.05	0.55
5:F:313:ASP:OD1	5:F:338:HIS:NE2	2.40	0.55
3:J:580:TRP:HH2	3:J:587:LEU:O	1.89	0.55
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.07	0.55
5:F:372:ALA:O	5:F:376:LYS:HG3	2.07	0.55
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.87	0.55
2:C:9:LYS:HD2	2:C:791:LEU:HD11	1.89	0.55
3:J:511:TYR:HE1	3:J:724:MET:HG2	1.72	0.55
3:J:1140:ARG:HH21	3:J:1236:GLU:HG3	1.71	0.55
3:D:1146:GLU:HA	3:D:1146:GLU:OE2	2.05	0.55
1:G:190:ALA:CB	1:G:200:LYS:HB2	2.20	0.55
1:H:134:THR:HG23	1:H:135:ASP:H	1.70	0.55
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.15	0.55
3:D:1193:TRP:HB2	3:D:1194:ARG:CZ	2.37	0.55
3:J:197:GLU:O	3:J:201:LEU:HG	2.06	0.55
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.36	0.55
2:I:888:THR:HG23	2:I:916:SER:OG	2.07	0.55
3:D:161:THR:CG2	3:D:164:GLN:H	2.20	0.55
3:D:799:ARG:HG2	3:D:1309:ILE:HD12	1.89	0.55
3:D:102:MET:HE2	3:D:246:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.87	0.55
4:K:62:GLN:O	4:K:66:VAL:HG23	2.07	0.55
5:F:106:GLY:HA2	5:F:385:ARG:HH22	1.72	0.55
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.22	0.55
3:D:128:LEU:HD21	3:D:189:LEU:HD23	1.89	0.55
3:D:514:THR:O	3:D:595:ALA:HA	2.07	0.55
5:L:562:ARG:NH2	5:L:573:LEU:HD22	2.22	0.55
3:D:535:ARG:O	3:D:539:SER:OG	2.24	0.55
2:I:615:VAL:HG21	2:I:645:PHE:CD2	2.42	0.55
5:F:137:TYR:O	5:F:141:ILE:HG12	2.06	0.55
1:B:12:ARG:O	1:B:13:LEU:HB3	2.06	0.55
3:D:739:GLN:OE1	3:D:744:ARG:NE	2.40	0.55
2:I:715:THR:HG23	2:I:717:VAL:HG23	1.89	0.55
2:I:715:THR:OG1	2:I:782:VAL:HG12	2.06	0.55
3:D:606:ASN:OD1	3:D:610:ARG:NE	2.40	0.55
2:I:245:ARG:HG2	2:I:337:PHE:CE2	2.42	0.55
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.88	0.55
1:A:233:ASP:HA	1:B:218:ARG:NH1	2.22	0.55
1:H:67:GLU:HA	1:H:78:ILE:HG21	1.89	0.55
1:B:59:VAL:HG22	1:B:144:ILE:HG13	1.89	0.55
3:D:27:PRO:HB3	3:D:241:VAL:HG23	1.88	0.54
3:J:172:PHE:HB3	3:J:175:GLU:OE2	2.07	0.54
2:C:494:ASN:HB3	2:C:497:PRO:HG2	1.89	0.54
5:F:143:TYR:CE2	5:F:147:GLN:HG3	2.43	0.54
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.07	0.54
2:C:1142:ARG:NH1	2:C:1165:SER:HA	2.15	0.54
5:L:470:MET:HA	5:L:473:GLU:HB3	1.88	0.54
3:J:1262:ARG:HD2	3:J:1279:GLN:NE2	2.21	0.54
2:I:971:LEU:HD22	2:I:1018:TYR:CD1	2.43	0.54
3:J:517:CYS:HA	3:J:716:GLN:NE2	2.21	0.54
1:G:76:GLU:OE1	1:G:132:HIS:N	2.36	0.54
1:H:109:PRO:HB3	1:H:132:HIS:HD2	1.72	0.54
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.42	0.54
5:F:400:GLN:HB2	5:F:403:ASP:OD2	2.07	0.54
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.88	0.54
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.88	0.54
3:J:161:THR:HG22	3:J:164:GLN:HB2	1.89	0.54
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.88	0.54
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.89	0.54
3:D:79:LYS:HE3	3:D:80:HIS:HA	1.90	0.54
3:J:1167:LYS:HD3	3:J:1174:ARG:NH1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:35:PHE:CD2	2:I:130:MET:HB3	2.42	0.54
1:A:133:LEU:HD11	1:A:140:ILE:HG12	1.89	0.54
3:D:848:VAL:O	3:D:857:LEU:HD12	2.08	0.54
2:I:896:THR:HB	2:I:897:PRO:HD2	1.89	0.54
5:F:343:LYS:H	5:F:343:LYS:HD2	1.72	0.54
1:H:46:ILE:HD11	1:H:224:LEU:HD13	1.90	0.54
5:L:511:ILE:HG13	5:L:512:GLY:H	1.73	0.54
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.43	0.54
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.90	0.54
3:J:694:SER:O	3:J:698:MET:HB2	2.07	0.54
3:J:516:ASP:HB3	3:J:573:THR:HG21	1.90	0.54
2:I:802:VAL:HG23	2:I:1098:LEU:HD13	1.89	0.54
5:L:577:GLY:O	5:L:581:ASP:N	2.40	0.54
1:H:65:LEU:HD22	1:H:171:LEU:HD21	1.89	0.54
3:J:850:LYS:HB2	3:J:852:GLY:O	2.07	0.54
2:I:21:VAL:HG13	2:I:655:VAL:HG13	1.89	0.54
5:L:248:GLU:HG2	5:L:251:LYS:NZ	2.23	0.54
3:D:1297:LYS:N	3:D:1298:VAL:HA	2.22	0.54
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.22	0.54
3:D:694:SER:OG	3:D:738:ARG:NE	2.40	0.54
1:G:10:LYS:NZ	1:H:229:GLU:OE1	2.36	0.54
1:B:92:VAL:CG1	1:B:95:LYS:HB3	2.37	0.54
3:J:1179:PRO:HG2	3:J:1183:SER:O	2.08	0.54
4:K:71:GLU:O	4:K:75:GLN:HG3	2.08	0.54
3:J:793:SER:O	3:J:797:THR:HG23	2.08	0.54
2:C:209:ILE:HD13	2:C:425:ILE:HG21	1.89	0.54
3:D:560:ASN:ND2	3:D:560:ASN:O	2.40	0.54
3:J:279:LEU:HD12	3:J:295:GLU:HG3	1.89	0.54
2:C:1082:ILE:HD12	2:C:1082:ILE:H	1.72	0.54
1:A:124:VAL:HG11	1:A:210:THR:HG23	1.89	0.54
3:D:22:ILE:HG23	3:D:1336:ALA:HA	1.90	0.54
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.90	0.54
3:D:48:THR:HB	3:D:50:LYS:HG3	1.90	0.54
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.89	0.54
2:I:930:ASP:OD2	2:I:931:VAL:N	2.40	0.54
2:I:131:THR:HG22	2:I:132:ASP:H	1.71	0.54
1:A:226:GLU:HB3	1:B:10:LYS:HE2	1.90	0.54
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.89	0.54
3:D:903:LEU:HB3	3:D:905:ARG:H	1.71	0.54
1:A:135:ASP:O	1:A:137:ASN:N	2.41	0.54
2:I:1305:TYR:CD2	5:L:531:PRO:HB2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.90	0.54
3:J:122:SER:O	3:J:126:LEU:HG	2.07	0.54
1:A:137:ASN:N	1:A:137:ASN:OD1	2.41	0.54
2:I:389:PHE:HD1	2:I:395:TYR:HE1	1.54	0.54
3:J:1167:LYS:HZ3	3:J:1170:LYS:HB2	1.71	0.54
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.43	0.54
2:I:810:TYR:CE1	2:I:1078:LYS:HD2	2.43	0.54
2:I:1131:MET:HB3	2:I:1141:LEU:CD1	2.37	0.54
2:C:92:TYR:CD2	2:C:129:LEU:HB2	2.43	0.54
1:A:310:ARG:HA	1:A:310:ARG:NE	2.23	0.54
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.89	0.54
3:D:871:LEU:HA	3:D:874:GLU:HG3	1.89	0.54
1:H:37:HIS:CD2	2:I:1216:ARG:HD2	2.43	0.53
3:D:930:LEU:HB2	3:D:1138:LEU:HB2	1.89	0.53
2:I:1184:THR:HG23	2:I:1189:GLY:HA2	1.90	0.53
2:I:810:TYR:CD2	3:J:359:PRO:HG2	2.43	0.53
2:C:759:SER:OG	2:C:763:THR:N	2.41	0.53
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.42	0.53
3:D:140:TYR:CE2	5:F:95:THR:HG22	2.43	0.53
5:F:225:ARG:O	5:F:229:VAL:HG13	2.08	0.53
2:I:812:PHE:CZ	3:J:503:SER:HB2	2.42	0.53
1:H:195:ARG:CB	1:H:198:LEU:HD21	2.38	0.53
2:C:976:ARG:HB2	2:C:997:TRP:HZ3	1.73	0.53
2:C:994:ARG:HD2	2:C:997:TRP:CZ2	2.43	0.53
4:K:26:ARG:NH1	4:K:29:GLN:OE1	2.42	0.53
1:G:39:LEU:HD21	1:H:224:LEU:HD11	1.89	0.53
2:C:1236:ASN:HB2	2:C:1238:LEU:HD11	1.90	0.53
2:I:615:VAL:HG13	2:I:651:ASP:H	1.72	0.53
3:J:647:PRO:HG3	3:J:697:MET:N	2.23	0.53
3:J:697:MET:HG3	3:J:698:MET:N	2.23	0.53
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.91	0.53
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.91	0.53
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.89	0.53
3:J:363:LEU:HD21	3:J:487:THR:HG22	1.90	0.53
5:F:280:VAL:HG13	5:F:355:ILE:HD12	1.91	0.53
1:H:125:LYS:HB3	1:H:128:HIS:HB2	1.88	0.53
2:I:952:GLN:OE1	2:I:1036:ILE:HG23	2.09	0.53
3:D:223:LEU:O	3:D:226:ALA:HB3	2.09	0.53
2:C:1192:GLU:OE2	3:D:764:ARG:HD3	2.09	0.53
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.91	0.53
1:H:62:ASP:HB3	1:H:141:SER:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.44	0.53
5:L:387:VAL:HG22	5:L:435:ILE:HD13	1.91	0.53
5:L:377:LYS:O	5:L:381:GLU:HG3	2.09	0.53
1:H:182:ARG:HD3	1:H:206:GLU:OE2	2.09	0.53
5:L:306:PHE:CE1	5:L:310:GLU:HG3	2.44	0.53
3:J:773:PHE:O	3:J:776:THR:HB	2.09	0.53
3:D:54:ASP:HB2	3:D:61:ILE:HD11	1.90	0.53
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.90	0.53
1:A:263:THR:HG22	1:A:302:GLU:HG2	1.89	0.53
2:I:1243:MET:HA	3:J:353:SER:HB3	1.90	0.53
5:F:395:THR:OG1	5:F:396:ASN:N	2.42	0.53
5:L:298:PRO:HD2	5:L:326:TRP:CD1	2.43	0.53
3:J:845:ALA:O	3:J:860:ARG:NE	2.40	0.53
3:J:322:ARG:HH11	3:J:322:ARG:HB2	1.72	0.53
1:G:156:SER:HB2	2:I:1059:ARG:NH2	2.24	0.53
1:A:319:GLU:O	1:A:320:ASN:HB2	2.08	0.53
5:F:511:ILE:HG13	5:F:512:GLY:H	1.74	0.53
1:H:215:GLU:OE1	1:H:219:ARG:NH1	2.41	0.53
3:D:751:ASP:HB3	3:D:753:SER:H	1.73	0.53
2:C:1296:ASP:OD2	2:C:1322:SER:HB3	2.09	0.53
3:J:720:ASN:OD1	3:J:722:ILE:HG22	2.09	0.53
5:F:233:ASP:O	5:F:236:LYS:HE2	2.07	0.53
3:J:660:GLU:O	3:J:664:ILE:HG12	2.08	0.53
3:D:817:HIS:CE1	3:D:860:ARG:HH21	2.26	0.53
3:J:709:ARG:HD2	3:J:710:ASP:N	2.24	0.53
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.89	0.53
1:H:82:LEU:O	1:H:86:LYS:HG3	2.09	0.53
2:C:425:ILE:O	2:C:429:MET:HG3	2.09	0.53
2:I:338:THR:CG2	2:I:345:PRO:HB3	2.39	0.53
3:D:500:ILE:O	3:D:500:ILE:HG22	2.08	0.53
5:F:234:THR:HG21	5:F:248:GLU:OE2	2.09	0.53
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.91	0.53
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.91	0.53
1:H:98:VAL:HG11	1:H:121:VAL:CG2	2.39	0.53
1:G:45:ARG:HH22	1:H:37:HIS:CB	2.22	0.53
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.74	0.53
3:J:903:LEU:HD22	3:J:909:ILE:HD12	1.91	0.53
5:F:127:ILE:O	5:F:130:VAL:HG22	2.08	0.53
3:D:211:GLU:O	3:D:215:LYS:HB3	2.08	0.53
3:J:588:PRO:O	3:J:591:ILE:HG22	2.09	0.53
2:C:568:ASN:HB2	2:C:571:LEU:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:166:VAL:HG23	5:F:258:GLN:O	2.09	0.53
1:G:154:PRO:HG2	1:G:157:THR:OG1	2.08	0.53
3:J:761:ALA:H	3:J:771:GLN:HE22	1.56	0.53
2:I:692:THR:OG1	2:I:827:ARG:O	2.27	0.53
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.90	0.53
3:J:1154:ALA:HB3	3:J:1215:GLU:HB3	1.90	0.53
5:F:316:PHE:HZ	5:F:334:SER:HA	1.74	0.53
3:J:903:LEU:HB3	3:J:905:ARG:H	1.74	0.53
1:G:195:ARG:CG	1:G:198:LEU:HG	2.38	0.53
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.90	0.53
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.91	0.53
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.91	0.53
2:C:150:HIS:CE1	2:C:454:ARG:HE	2.27	0.53
2:C:720:ARG:CZ	2:C:736:VAL:HG21	2.38	0.53
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.08	0.53
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.90	0.52
3:J:872:LEU:O	3:J:877:VAL:HG12	2.09	0.52
5:F:465:ARG:HD2	5:F:468:ARG:HH22	1.74	0.52
3:J:1140:ARG:HH21	3:J:1236:GLU:CG	2.23	0.52
2:I:1238:LEU:H	2:I:1238:LEU:HD12	1.74	0.52
3:D:733:SER:O	3:D:737:ILE:HG12	2.09	0.52
5:L:419:PHE:HD1	5:L:430:TYR:CD2	2.27	0.52
3:J:537:TYR:CZ	3:J:544:LEU:HD22	2.44	0.52
3:D:600:ALA:O	3:D:603:LYS:HG2	2.09	0.52
3:J:156:ARG:HH12	3:J:157:GLN:NE2	2.07	0.52
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.91	0.52
3:J:1252:HIS:O	3:J:1255:VAL:HG13	2.08	0.52
3:J:682:VAL:O	3:J:685:ILE:HG12	2.09	0.52
2:C:1281:TYR:CE1	3:D:484:MET:HA	2.44	0.52
2:C:98:VAL:O	2:C:121:GLU:HA	2.08	0.52
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.09	0.52
3:J:903:LEU:CB	3:J:905:ARG:HG3	2.39	0.52
3:D:705:THR:OG1	3:D:718:SER:HA	2.09	0.52
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.91	0.52
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.74	0.52
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.29	0.52
1:G:60:GLU:HB2	1:G:170:ARG:CG	2.39	0.52
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.92	0.52
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.35	0.52
1:A:190:ALA:CB	1:A:200:LYS:HB2	2.39	0.52
1:G:76:GLU:OE2	1:G:76:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.24	0.52
1:A:36:GLY:CA	1:A:187:VAL:HG11	2.38	0.52
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.92	0.52
3:J:767:LEU:HD23	3:J:771:GLN:HB3	1.91	0.52
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.73	0.52
3:D:706:VAL:HG12	3:D:715:LYS:HB2	1.91	0.52
2:C:565:GLU:HG2	2:C:565:GLU:O	2.09	0.52
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.10	0.52
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.44	0.52
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.92	0.52
5:L:569:THR:OG1	5:L:570:ASP:N	2.42	0.52
1:A:44:ARG:NH2	2:C:1091:GLY:O	2.42	0.52
5:L:460:ILE:O	5:L:463:LEU:HB2	2.10	0.52
3:D:825:VAL:HG13	3:D:833:GLU:HB3	1.90	0.52
5:F:326:TRP:HA	5:F:329:LYS:HD2	1.90	0.52
5:L:608:ARG:O	5:L:611:LEU:N	2.30	0.52
5:F:557:LYS:O	5:F:561:MET:HB2	2.09	0.52
2:I:521:LEU:O	2:I:525:THR:HB	2.09	0.52
3:D:529:GLY:HA2	3:D:551:ARG:O	2.09	0.52
3:D:347:VAL:HG12	3:D:348:ASP:O	2.09	0.52
2:I:517:GLN:O	2:I:517:GLN:HG2	2.09	0.52
1:H:92:VAL:HG13	1:H:120:ASP:O	2.10	0.52
3:J:436:ALA:HB3	3:J:485:MET:HA	1.91	0.52
3:D:615:LYS:HE2	3:D:616:PRO:HD3	1.91	0.52
1:G:36:GLY:C	1:G:187:VAL:HG11	2.30	0.52
1:A:102:LEU:HD23	1:A:115:ILE:HA	1.91	0.52
2:C:726:TYR:CZ	2:C:728:ASP:HB2	2.45	0.52
1:A:73:GLY:HA2	2:C:726:TYR:OH	2.10	0.52
2:I:143:ARG:NH2	2:I:512:SER:O	2.42	0.52
3:J:363:LEU:HG	3:J:363:LEU:O	2.10	0.52
1:G:23:HIS:HB2	1:G:206:GLU:HA	1.91	0.52
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.90	0.52
2:C:466:VAL:O	2:C:470:ARG:HG2	2.09	0.52
3:D:310:GLY:CA	3:D:314:ARG:HD2	2.34	0.52
2:I:990:ASP:HA	2:I:997:TRP:HZ2	1.74	0.52
3:D:84:ILE:HG22	3:D:91:GLU:HB3	1.90	0.52
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.91	0.52
3:J:1168:GLU:O	3:J:1170:LYS:N	2.43	0.52
3:J:266:ASN:O	3:J:270:ARG:HB2	2.10	0.52
3:D:490:ILE:HA	3:D:500:ILE:HG12	1.91	0.52
3:D:1160:SER:HA	3:D:1204:VAL:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:262:TYR:HE1	2:C:280:ASP:OD2	1.93	0.52
2:I:331:LYS:HB2	2:I:332:ARG:NH2	2.23	0.52
2:I:159:SER:O	2:I:160:ASP:HB2	2.09	0.52
2:C:169:LYS:HE2	2:C:190:PRO:O	2.09	0.52
5:L:288:MET:HA	5:L:302:PHE:CZ	2.45	0.52
3:D:19:ALA:HB2	3:D:1343:GLU:HG3	1.90	0.52
3:J:1265:THR:HG22	3:J:1277:GLY:CA	2.34	0.52
1:A:233:ASP:O	1:A:234:LEU:HG	2.09	0.52
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	1.92	0.52
2:I:908:GLU:OE1	5:L:611:LEU:HD22	2.09	0.52
2:I:796:LEU:H	2:I:796:LEU:HD12	1.74	0.52
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.91	0.52
2:I:320:ASP:OD1	2:I:324:LYS:HE3	2.08	0.52
3:D:772:TYR:O	3:D:775:SER:HB3	2.10	0.52
4:E:60:ASN:OD1	4:E:63:ILE:HD13	2.09	0.52
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.37	0.52
2:I:1259:LEU:HD12	2:I:1260:GLY:N	2.23	0.52
5:F:354:THR:OG1	5:F:356:GLU:HB3	2.10	0.52
1:A:195:ARG:HG2	1:A:198:LEU:HD11	1.91	0.52
2:C:637:ARG:HA	2:C:642:SER:HA	1.92	0.52
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.74	0.52
1:B:56:VAL:HG11	1:B:144:ILE:HD11	1.92	0.52
2:I:158:ASP:OD1	2:I:159:SER:N	2.42	0.52
2:C:667:LEU:CD2	2:C:704:MET:HB2	2.40	0.52
2:I:757:THR:O	2:I:765:ILE:HG23	2.10	0.52
2:I:993:PRO:HB2	2:I:995:ASP:OD2	2.10	0.52
2:I:721:GLY:N	2:I:740:GLU:OE1	2.38	0.52
1:A:66:HIS:CD2	2:C:874:GLY:HA2	2.44	0.52
3:J:1344:LEU:O	3:J:1346:GLY:N	2.40	0.52
2:C:550:VAL:HG11	3:D:776:THR:CG2	2.39	0.52
5:L:262:VAL:HG11	5:L:264:LYS:HZ1	1.72	0.52
5:L:457:ILE:HA	5:L:460:ILE:HD12	1.92	0.52
3:J:611:ILE:HB	3:J:612:LEU:HD12	1.92	0.52
3:J:705:THR:OG1	3:J:718:SER:HA	2.10	0.52
5:L:261:LEU:HD12	5:L:261:LEU:H	1.75	0.52
5:L:421:TYR:CE2	5:L:422:ARG:HG3	2.44	0.52
2:C:182:SER:O	2:C:395:TYR:HE1	1.93	0.52
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.90	0.52
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.08	0.52
4:E:32:VAL:O	4:E:34:GLY:N	2.43	0.52
5:F:569:THR:OG1	5:F:570:ASP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:313:ASP:CG	5:L:338:HIS:HE2	2.13	0.52
1:B:152:TYR:HE1	1:B:176:CYS:HB3	1.73	0.52
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.91	0.52
3:J:48:THR:C	3:J:50:LYS:H	2.13	0.52
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.92	0.52
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.91	0.52
4:K:49:ILE:O	4:K:53:GLU:HG3	2.10	0.52
1:B:214:GLU:HG2	1:B:218:ARG:NH2	2.25	0.52
2:C:1238:LEU:H	2:C:1238:LEU:CD1	2.20	0.52
2:C:635:THR:HG23	2:C:644:LEU:HD22	1.92	0.52
2:C:800:MET:HG3	2:C:1096:ILE:HD11	1.92	0.52
2:I:1082:ILE:HD12	2:I:1082:ILE:H	1.75	0.52
2:I:1119:MET:HB2	2:I:1228:GLY:CA	2.40	0.52
2:I:981:ALA:HB1	2:I:1007:LYS:NZ	2.25	0.52
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.42	0.52
2:C:135:THR:HG22	2:C:527:LYS:HE2	1.92	0.52
3:J:154:LEU:HD22	3:J:160:LEU:HD11	1.91	0.52
1:H:95:LYS:NZ	1:H:98:VAL:HG23	2.25	0.51
3:D:384:LYS:NZ	3:D:414:GLU:OE1	2.35	0.51
5:L:135:ALA:HB1	5:L:253:SER:HB3	1.91	0.51
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.45	0.51
5:F:348:GLU:HA	5:F:353:LEU:O	2.10	0.51
3:D:598:LYS:O	3:D:601:ILE:HG22	2.09	0.51
3:D:825:VAL:C	3:D:826:ILE:HG13	2.30	0.51
2:I:362:ALA:O	2:I:366:ILE:HG13	2.10	0.51
3:D:227:PHE:O	3:D:230:SER:HB3	2.10	0.51
3:J:1177:ILE:HD12	3:J:1186:TYR:HB3	1.91	0.51
5:F:465:ARG:HA	5:F:468:ARG:NH2	2.24	0.51
1:B:75:GLN:HG2	1:B:76:GLU:OE1	2.10	0.51
3:D:537:TYR:CE2	3:D:544:LEU:HD22	2.45	0.51
2:C:837:ALA:HB2	2:C:1051:LYS:HG2	1.90	0.51
2:I:886:LYS:NZ	2:I:916:SER:HB3	2.25	0.51
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.10	0.51
1:A:55:ALA:HB3	1:A:177:TYR:CD1	2.44	0.51
3:J:419:HIS:HB2	4:K:45:LYS:HE2	1.92	0.51
1:B:151:GLY:O	1:B:177:TYR:HB2	2.10	0.51
3:J:503:SER:H	3:J:506:VAL:HG11	1.75	0.51
3:J:156:ARG:NH1	3:J:157:GLN:HE21	2.08	0.51
2:I:564:PRO:HG3	2:I:572:ILE:HG13	1.92	0.51
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.92	0.51
1:B:99:ILE:HD12	1:B:145:LYS:HB2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1149:ARG:NH2	3:J:1153:PRO:HG2	2.26	0.51
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.43	0.51
1:H:73:GLY:CA	1:H:134:THR:HG22	2.33	0.51
1:A:150:ARG:HD2	1:B:8:PHE:CZ	2.45	0.51
2:I:448:LEU:HB2	2:I:553:THR:HB	1.93	0.51
1:G:13:LEU:H	1:G:13:LEU:HD23	1.74	0.51
2:I:277:LEU:HD23	2:I:282:VAL:HG21	1.92	0.51
2:C:1124:ILE:O	2:C:1128:ILE:HG13	2.11	0.51
2:I:228:VAL:HB	2:I:335:THR:OG1	2.11	0.51
5:F:471:LEU:HD23	5:F:476:ARG:O	2.09	0.51
2:C:1247:SER:HB3	3:D:375:GLU:O	2.10	0.51
1:A:134:THR:HG23	2:C:726:TYR:CE1	2.45	0.51
1:A:187:VAL:O	1:A:187:VAL:HG23	2.10	0.51
5:F:325:PRO:HG2	5:F:326:TRP:CD1	2.45	0.51
1:G:197:ASP:O	1:G:198:LEU:HD23	2.09	0.51
2:I:136:PHE:CZ	2:I:456:VAL:HG11	2.46	0.51
3:J:697:MET:O	3:J:701:LEU:N	2.32	0.51
3:J:1349:GLU:O	3:J:1353:VAL:HG12	2.11	0.51
2:I:468:LEU:O	2:I:471:VAL:HG12	2.09	0.51
3:J:825:VAL:CG1	3:J:833:GLU:HB3	2.40	0.51
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.45	0.51
1:A:218:ARG:HG3	1:B:231:PHE:O	2.09	0.51
3:J:412:LEU:O	3:J:415:VAL:HG22	2.09	0.51
3:D:1257:VAL:HA	3:D:1260:MET:HG3	1.92	0.51
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.74	0.51
5:L:121:LYS:O	5:L:124:GLU:HB2	2.11	0.51
2:I:696:ASP:O	2:I:697:LYS:HB3	2.09	0.51
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.41	0.51
2:I:1142:ARG:NH2	2:I:1165:SER:HB2	2.26	0.51
2:C:1269:ARG:HG2	3:D:343:LEU:HD11	1.93	0.51
3:J:1170:LYS:C	3:J:1172:LYS:H	2.13	0.51
1:G:224:LEU:HD22	1:H:228:LEU:HD11	1.92	0.51
3:J:102:MET:CE	3:J:246:PRO:HD3	2.41	0.51
5:F:426:LYS:HD3	5:F:428:SER:HB2	1.93	0.51
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.93	0.51
5:L:372:ALA:O	5:L:376:LYS:HG3	2.11	0.51
3:J:121:PRO:HG2	3:J:123:ARG:NH2	2.25	0.51
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.17	0.51
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.10	0.51
2:C:1006:GLU:O	2:C:1010:GLN:N	2.44	0.51
1:G:219:ARG:HA	1:G:222:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1134:GLN:O	2:C:1135:GLN:HG2	2.09	0.51
2:C:106:GLU:O	2:C:109:ALA:HB2	2.10	0.51
3:J:205:LEU:CD2	3:J:214:ARG:HB2	2.41	0.51
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.93	0.51
3:D:102:MET:CE	3:D:246:PRO:HD3	2.40	0.51
2:C:147:SER:OG	2:C:455:SER:HB3	2.10	0.51
3:D:1282:TYR:O	3:D:1285:VAL:HG22	2.11	0.51
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.41	0.51
3:D:432:LEU:HD21	3:D:489:ASN:CB	2.40	0.51
2:C:21:VAL:HG13	2:C:655:VAL:HG13	1.92	0.51
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.11	0.51
2:I:582:ASN:HB3	2:I:586:PHE:N	2.25	0.51
2:C:268:ARG:HD2	2:C:270:THR:CG2	2.40	0.51
2:I:1174:GLU:O	2:I:1177:ARG:HG2	2.11	0.51
3:J:680:ASN:O	3:J:683:ILE:HG22	2.09	0.51
2:I:494:ASN:HB3	2:I:497:PRO:HG2	1.91	0.51
2:C:670:PHE:CE2	2:C:1113:LEU:HB3	2.46	0.51
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.92	0.51
5:L:247:GLU:O	5:L:251:LYS:HG3	2.10	0.51
3:D:702:GLN:HG3	3:D:723:TYR:OH	2.09	0.51
3:D:266:ASN:O	3:D:270:ARG:HB2	2.10	0.51
2:C:629:PHE:CE2	2:C:634:VAL:HG11	2.44	0.51
2:I:1012:GLU:O	2:I:1016:GLU:HG3	2.10	0.51
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.93	0.51
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.46	0.51
3:J:857:LEU:HD13	3:J:858:VAL:HG13	1.92	0.51
2:I:1197:GLU:O	2:I:1200:LYS:HB2	2.11	0.51
3:J:615:LYS:HE2	3:J:616:PRO:HD3	1.92	0.51
3:J:420:PRO:O	3:J:471:PRO:HD2	2.11	0.51
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.93	0.51
3:D:850:LYS:HB3	3:D:851:PRO:HD2	1.93	0.51
3:J:750:PRO:HA	3:J:777:HIS:NE2	2.26	0.51
1:G:56:VAL:HG21	1:G:144:ILE:HG23	1.91	0.51
2:I:1158:LYS:HG3	2:I:1159:VAL:N	2.25	0.51
2:C:887:VAL:HB	2:C:913:VAL:HG22	1.93	0.51
3:J:557:LYS:HA	3:J:563:LEU:HA	1.93	0.51
2:C:882:ILE:HD12	2:C:882:ILE:H	1.76	0.51
2:C:42:ASP:O	2:C:44:GLU:N	2.36	0.51
1:A:228:LEU:O	1:A:231:PHE:N	2.42	0.50
2:C:4:SER:HB3	2:C:7:GLU:CG	2.34	0.50
2:C:1142:ARG:NH1	2:C:1169:VAL:HG21	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:168:GLY:C	2:I:170:VAL:H	2.13	0.50
3:D:811:GLU:OE1	3:D:890:THR:OG1	2.29	0.50
2:C:600:THR:HG22	2:C:601:ASP:N	2.26	0.50
2:C:987:GLU:O	2:C:991:LYS:HE3	2.10	0.50
2:I:465:ARG:O	2:I:469:VAL:HG13	2.11	0.50
1:A:318:LEU:HD23	1:A:321:TRP:HB2	1.93	0.50
4:K:59:ILE:HG23	4:K:64:LEU:HD21	1.93	0.50
3:D:147:ILE:HG13	3:D:147:ILE:O	2.11	0.50
3:D:1160:SER:OG	3:D:1203:ARG:NH1	2.43	0.50
5:L:124:GLU:O	5:L:128:ASN:HB2	2.11	0.50
2:C:263:VAL:HG21	2:C:273:HIS:CG	2.46	0.50
2:I:561:ILE:HD11	2:I:665:ALA:HB1	1.93	0.50
1:A:255:ARG:HD3	1:A:259:ASP:OD2	2.10	0.50
3:J:1280:VAL:O	3:J:1284:ARG:N	2.37	0.50
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.76	0.50
2:C:802:VAL:CG2	2:C:1098:LEU:HD22	2.41	0.50
3:D:847:ASP:HB3	3:D:859:PRO:HA	1.94	0.50
3:D:1227:HIS:HA	3:D:1230:THR:CG2	2.39	0.50
2:I:959:ASP:O	2:I:963:GLU:HG2	2.11	0.50
5:F:572:THR:HG23	5:F:575:GLU:HG3	1.94	0.50
2:I:557:ARG:NH2	2:I:608:ALA:HA	2.26	0.50
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.74	0.50
5:L:117:ILE:HA	5:L:120:ALA:HB3	1.92	0.50
1:A:152:TYR:CE2	1:A:154:PRO:HB3	2.46	0.50
3:D:501:VAL:HG21	3:D:602:SER:HB2	1.93	0.50
2:I:998:LEU:HD23	2:I:1015:ALA:HA	1.92	0.50
1:A:12:ARG:H	1:A:30:PRO:HD2	1.76	0.50
3:D:812:ASP:HB2	3:D:911:LYS:NZ	2.26	0.50
2:C:551:HIS:ND1	2:C:553:THR:OG1	2.44	0.50
3:J:40:LYS:HB3	3:J:42:GLU:OE1	2.11	0.50
2:I:887:VAL:HB	2:I:913:VAL:HG21	1.93	0.50
3:J:923:ILE:O	3:J:926:PRO:HD2	2.11	0.50
3:D:45:ASN:O	3:D:46:TYR:HD2	1.94	0.50
3:D:11:GLN:HE21	3:D:15:GLU:CD	2.15	0.50
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.92	0.50
3:J:277:ASN:HA	3:J:280:LYS:HG3	1.92	0.50
5:F:142:THR:O	5:F:146:GLU:HG3	2.12	0.50
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.46	0.50
2:I:998:LEU:HD12	2:I:998:LEU:N	2.26	0.50
5:L:234:THR:O	5:L:245:ALA:HB2	2.11	0.50
3:J:514:THR:HG21	3:J:596:LEU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:347:ILE:HB	5:L:355:ILE:HD11	1.93	0.50
2:I:486:THR:HG23	2:I:487:LEU:H	1.77	0.50
3:D:793:SER:O	3:D:797:THR:HG23	2.10	0.50
5:F:585:GLU:O	5:F:589:GLN:HG3	2.11	0.50
3:D:849:LEU:CB	3:D:853:THR:HG23	2.41	0.50
1:H:51:MET:HB3	1:H:178:SER:CB	2.41	0.50
3:J:1263:LYS:HE2	3:J:1279:GLN:NE2	2.26	0.50
3:D:702:GLN:O	3:D:718:SER:N	2.37	0.50
2:C:93:SER:OG	2:C:126:GLU:OE1	2.26	0.50
3:D:706:VAL:HG12	3:D:715:LYS:CB	2.41	0.50
2:I:156:PHE:CZ	2:I:158:ASP:HB2	2.47	0.50
3:D:261:ALA:HA	5:F:505:ILE:H	1.76	0.50
5:L:551:LEU:CD2	5:L:597:LYS:HD2	2.41	0.50
1:A:113:ALA:C	1:A:115:ILE:H	2.14	0.50
3:D:849:LEU:HA	3:D:855:ASP:O	2.10	0.50
3:D:80:HIS:CB	3:D:83:VAL:HG11	2.41	0.50
3:D:833:GLU:OE1	3:D:1242:ARG:HD3	2.12	0.50
2:C:886:LYS:HB3	2:C:917:SER:HA	1.93	0.50
2:C:60:GLN:O	2:C:476:LYS:HE2	2.11	0.50
4:K:19:LEU:HD13	4:K:54:ILE:HG21	1.93	0.50
5:L:108:VAL:HG11	5:L:381:GLU:O	2.11	0.50
3:J:761:ALA:H	3:J:771:GLN:NE2	2.09	0.50
3:D:21:LYS:NZ	3:D:23:ALA:HB2	2.26	0.50
2:C:799:ASN:HB3	2:C:1231:TYR:HD1	1.76	0.50
2:I:607:SER:OG	2:I:609:ILE:HG13	2.12	0.50
1:H:88:LEU:HD21	1:H:115:ILE:HD11	1.92	0.50
5:F:484:ALA:HB1	5:F:491:GLU:CG	2.41	0.50
5:L:305:LEU:HB3	5:L:315:TRP:HB3	1.93	0.50
3:D:697:MET:SD	3:D:741:ALA:HB3	2.51	0.50
3:D:536:LEU:HD13	3:D:541:LEU:HB2	1.92	0.50
5:F:414:LYS:O	5:F:417:ASP:N	2.43	0.50
1:A:71:LYS:HD3	1:A:72:GLU:H	1.76	0.50
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.24	0.50
5:L:483:LEU:H	5:L:483:LEU:HD12	1.76	0.50
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.93	0.50
3:D:770:LEU:HD22	3:D:770:LEU:H	1.77	0.50
3:D:1165:PHE:HD2	3:D:1173:ARG:HD2	1.77	0.50
2:C:345:PRO:O	2:C:349:GLU:HG2	2.12	0.50
2:I:250:THR:HA	2:I:268:ARG:HA	1.94	0.50
1:A:45:ARG:HE	2:C:1083:GLU:HB3	1.77	0.50
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1353:VAL:HG13	3:D:1355:ARG:HG2	1.94	0.50
5:L:341:LEU:HD23	5:L:344:LEU:HD23	1.93	0.50
1:G:47:LEU:HB3	1:G:183:ILE:HD13	1.94	0.50
1:B:57:THR:HG22	1:B:58:GLU:HG2	1.93	0.50
5:F:606:VAL:O	5:F:609:SER:OG	2.30	0.50
1:A:201:LEU:HG	1:A:203:ILE:HG13	1.94	0.50
2:C:897:PRO:HB2	2:C:898:GLU:OE1	2.12	0.50
2:I:494:ASN:OD1	5:L:471:LEU:HD13	2.11	0.50
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.94	0.50
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.27	0.50
2:C:884:VAL:HG21	2:C:1050:VAL:HB	1.93	0.50
2:C:188:PHE:CE1	2:C:194:LEU:HD13	2.47	0.50
1:A:274:ALA:O	1:A:275:ILE:HG13	2.12	0.50
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.93	0.50
1:A:250:ASP:CB	5:F:601:PRO:HB3	2.42	0.49
2:I:974:ARG:HD3	2:I:1010:GLN:NE2	2.27	0.49
2:I:1156:ARG:NH1	2:I:1156:ARG:HB2	2.23	0.49
3:J:905:ARG:CZ	3:J:910:ASN:HD21	2.25	0.49
5:F:298:PRO:HD2	5:F:326:TRP:CD1	2.48	0.49
1:A:252:ILE:HG22	1:A:278:ILE:HD11	1.94	0.49
2:I:1305:TYR:OH	5:L:532:LEU:HG	2.12	0.49
2:I:1129:ASN:CB	2:I:1177:ARG:HB2	2.41	0.49
2:I:187:GLU:OE2	2:I:197:ARG:NH2	2.38	0.49
5:F:134:VAL:HG13	5:F:273:MET:HE3	1.93	0.49
3:J:518:VAL:CG1	3:J:707:ILE:HD13	2.42	0.49
1:G:45:ARG:CD	2:I:1083:GLU:HB3	2.42	0.49
5:L:341:LEU:CD2	5:L:344:LEU:HD23	2.42	0.49
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.47	0.49
2:C:303:ASP:HB3	2:C:306:THR:CG2	2.42	0.49
3:J:515:ARG:O	3:J:545:HIS:HB3	2.12	0.49
3:J:515:ARG:HH21	3:J:717:VAL:HG23	1.77	0.49
3:D:106:GLU:OE2	3:D:241:VAL:HG22	2.12	0.49
2:I:138:ILE:O	2:I:139:ASN:ND2	2.44	0.49
4:K:3:ARG:NE	4:K:3:ARG:HA	2.27	0.49
4:E:72:GLN:O	4:E:76:GLU:HG3	2.12	0.49
3:D:660:GLU:O	3:D:663:GLU:HB2	2.11	0.49
2:I:972:PHE:CD2	2:I:975:ILE:HD12	2.48	0.49
1:A:295:LEU:HD23	1:A:299:SER:HB2	1.94	0.49
3:D:647:PRO:HG3	3:D:697:MET:CB	2.42	0.49
3:D:1299:GLY:HA2	3:J:1301:THR:CG2	2.42	0.49
2:I:810:TYR:HE1	2:I:1078:LYS:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:156:ARG:HH12	3:J:157:GLN:HE21	1.59	0.49
3:J:825:VAL:HG22	3:J:833:GLU:H	1.78	0.49
5:L:574:GLU:N	5:L:574:GLU:OE1	2.45	0.49
3:D:1359:ALA:O	3:D:1363:TYR:N	2.44	0.49
2:C:104:ILE:O	2:C:113:THR:HA	2.11	0.49
5:L:289:LYS:HG2	5:L:293:GLU:OE1	2.13	0.49
3:D:901:ARG:HA	3:D:908:ILE:HA	1.94	0.49
3:J:514:THR:CG2	3:J:596:LEU:HB2	2.41	0.49
3:J:363:LEU:HB2	3:J:450:HIS:CE1	2.48	0.49
5:L:379:MET:HG2	5:L:416:VAL:HG22	1.94	0.49
3:D:292:VAL:O	3:D:296:LYS:HG3	2.12	0.49
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.94	0.49
3:D:1307:LEU:HD23	3:D:1312:ALA:HA	1.94	0.49
2:C:696:ASP:CB	2:C:798:GLN:HG2	2.32	0.49
2:I:96:LEU:HD23	2:I:124:MET:HG3	1.93	0.49
2:I:933:VAL:HG11	2:I:945:ALA:HB2	1.94	0.49
2:I:26:TYR:OH	2:I:28:LEU:HD12	2.13	0.49
2:C:1268:GLN:HE22	3:D:352:ARG:NE	2.10	0.49
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.45	0.49
2:C:1182:ILE:HG22	2:C:1183:ALA:N	2.28	0.49
3:J:416:ILE:HG12	3:J:441:LEU:CD2	2.34	0.49
3:D:849:LEU:HD22	3:D:849:LEU:H	1.77	0.49
1:A:11:PRO:HD3	1:B:227:GLN:OE1	2.11	0.49
3:D:1230:THR:O	3:D:1234:VAL:HG13	2.12	0.49
2:C:617:ALA:HA	2:C:636:CYS:SG	2.52	0.49
3:D:1167:LYS:CD	3:D:1174:ARG:HD2	2.41	0.49
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.95	0.49
3:D:161:THR:HG22	3:D:164:GLN:CB	2.41	0.49
3:J:518:VAL:HG11	3:J:707:ILE:HD13	1.94	0.49
2:I:84:GLU:OE1	2:I:1035:LYS:HD2	2.11	0.49
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.76	0.49
3:J:1257:VAL:HA	3:J:1260:MET:HG3	1.95	0.49
5:L:325:PRO:HG2	5:L:326:TRP:CD1	2.47	0.49
2:C:122:VAL:CG1	2:C:493:ILE:HD13	2.42	0.49
3:D:1174:ARG:NE	3:D:1187:GLU:OE2	2.46	0.49
2:C:448:LEU:HA	2:C:448:LEU:HD23	1.57	0.49
2:C:292:ILE:HG22	2:C:317:LEU:HB2	1.94	0.49
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	1.93	0.49
1:B:95:LYS:NZ	1:B:98:VAL:HG23	2.28	0.49
3:J:290:ILE:HD12	3:J:290:ILE:H	1.77	0.49
2:C:290:GLU:HG2	2:C:319:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:25:ARG:NH1	4:K:65:ASP:OD1	2.39	0.49
1:A:273:GLU:OE2	1:A:293:PRO:HD2	2.12	0.49
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.48	0.49
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.95	0.49
1:B:115:ILE:HG22	1:B:116:THR:N	2.28	0.49
3:J:1309:ILE:HG13	3:J:1310:THR:H	1.77	0.49
1:A:187:VAL:CG1	1:A:201:LEU:HD13	2.42	0.49
3:J:16:GLU:HG3	3:J:17:PHE:CD2	2.45	0.49
2:I:698:PRO:HA	2:I:1231:TYR:CD1	2.48	0.49
2:I:619:ALA:HB1	2:I:657:THR:HA	1.94	0.49
1:H:56:VAL:HG21	1:H:144:ILE:HD11	1.94	0.49
5:F:326:TRP:O	5:F:330:LEU:HG	2.12	0.49
5:F:390:ILE:HD12	5:F:435:ILE:HG21	1.95	0.49
3:J:56:LEU:H	3:J:56:LEU:HD12	1.78	0.49
2:C:1131:MET:HE2	2:C:1141:LEU:HA	1.94	0.49
2:C:891:GLY:O	2:C:892:GLU:HG3	2.13	0.49
5:L:469:GLN:O	5:L:473:GLU:HB2	2.13	0.49
5:L:262:VAL:HG11	5:L:264:LYS:HZ2	1.75	0.49
2:I:60:GLN:O	2:I:476:LYS:HE2	2.12	0.49
5:L:585:GLU:HA	5:L:588:ARG:HD2	1.95	0.49
2:I:37:LYS:HD3	2:I:37:LYS:HA	1.63	0.49
1:B:108:GLY:O	1:B:133:LEU:HB2	2.12	0.49
3:J:901:ARG:HA	3:J:908:ILE:HA	1.94	0.49
2:C:1246:ARG:NH1	2:C:1249:GLY:HA3	2.27	0.49
1:A:59:VAL:HG21	1:A:85:LEU:HD12	1.95	0.49
2:I:560:PRO:HG3	3:J:773:PHE:CE2	2.48	0.49
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.12	0.49
3:J:517:CYS:HB2	3:J:716:GLN:OE1	2.13	0.49
2:I:848:GLU:CG	2:I:888:THR:HG22	2.43	0.49
2:C:421:SER:N	2:C:424:ASP:OD2	2.45	0.49
5:F:231:THR:CG2	5:F:249:ILE:HG12	2.43	0.49
3:J:358:GLY:N	3:J:359:PRO:HD3	2.28	0.49
5:F:465:ARG:HA	5:F:468:ARG:CZ	2.42	0.49
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.39	0.49
2:I:1134:GLN:O	2:I:1135:GLN:HG2	2.13	0.49
2:C:229:ILE:HD13	2:C:334:GLU:HG2	1.95	0.49
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.27	0.48
1:A:233:ASP:HA	1:B:218:ARG:HH11	1.78	0.48
3:D:842:ARG:HB3	3:D:882:VAL:CG1	2.43	0.48
5:F:503:GLU:OE1	5:F:504:PRO:HD2	2.13	0.48
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PHE:HE2	1:B:39:LEU:HB3	1.78	0.48
1:A:77:ASP:O	1:A:80:GLU:N	2.46	0.48
3:J:81:ARG:C	3:J:83:VAL:H	2.16	0.48
1:G:166:ARG:N	1:G:167:PRO:HD2	2.28	0.48
3:J:848:VAL:HG11	3:J:877:VAL:HG21	1.94	0.48
1:A:234:LEU:HD12	1:B:218:ARG:NH1	2.28	0.48
2:C:510:GLN:CD	2:C:534:GLY:HA2	2.34	0.48
3:D:201:LEU:O	3:D:217:LEU:HD11	2.13	0.48
3:D:204:GLU:HB3	3:D:217:LEU:HD21	1.94	0.48
2:C:70:TYR:HA	2:C:100:LEU:CD2	2.42	0.48
2:C:1234:LYS:HE2	2:C:1238:LEU:HD23	1.94	0.48
2:I:1132:LEU:HD22	2:I:1177:ARG:NH1	2.28	0.48
2:C:981:ALA:HB1	2:C:1007:LYS:NZ	2.28	0.48
3:J:554:GLU:HA	3:J:580:TRP:HZ2	1.78	0.48
2:I:470:ARG:HA	2:I:473:ARG:HD2	1.95	0.48
2:I:243:PRO:O	2:I:246:LEU:HD12	2.13	0.48
3:D:1286:LYS:HA	3:D:1289:ASN:HB2	1.95	0.48
3:J:288:PRO:O	3:J:292:VAL:HG13	2.13	0.48
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.13	0.48
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.95	0.48
5:L:577:GLY:HA3	5:L:583:THR:CG2	2.32	0.48
1:B:63:GLY:CA	1:B:71:LYS:HE3	2.36	0.48
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.94	0.48
3:J:317:THR:HB	3:J:324:LEU:HB3	1.95	0.48
2:C:487:LEU:H	2:C:487:LEU:HD23	1.79	0.48
2:I:971:LEU:HD22	2:I:1018:TYR:HD1	1.79	0.48
3:D:1227:HIS:CA	3:D:1230:THR:HG22	2.42	0.48
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.14	0.48
3:J:363:LEU:HA	3:J:450:HIS:CD2	2.48	0.48
2:C:1065:LYS:CD	2:C:1235:LEU:HD12	2.43	0.48
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.96	0.48
3:J:615:LYS:O	3:J:619:ILE:HG22	2.13	0.48
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.95	0.48
5:L:283:GLN:O	5:L:287:ILE:HG13	2.14	0.48
1:A:82:LEU:HB3	1:A:173:VAL:HG12	1.95	0.48
2:I:30:ILE:CD1	2:I:30:ILE:H	2.17	0.48
2:I:974:ARG:HD2	2:I:1014:LEU:HD11	1.94	0.48
2:C:488:MET:O	2:C:490:GLN:N	2.44	0.48
3:J:48:THR:HB	3:J:50:LYS:HG3	1.96	0.48
2:I:1285:TYR:CZ	3:J:1356:LEU:HD11	2.48	0.48
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:528:ARG:HD3	2:I:663:VAL:HG21	1.96	0.48
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.95	0.48
3:D:739:GLN:OE1	3:D:744:ARG:HB2	2.14	0.48
2:C:1101:LEU:O	3:D:731:ARG:HD3	2.14	0.48
2:I:818:VAL:HB	2:I:1076:ILE:HD11	1.93	0.48
2:I:632:ASP:O	2:I:647:ARG:HB2	2.13	0.48
2:C:590:PRO:HG3	2:C:605:TYR:OH	2.14	0.48
1:G:226:GLU:O	1:G:229:GLU:HG3	2.13	0.48
2:C:615:VAL:HG11	2:C:649:GLN:O	2.13	0.48
2:I:655:VAL:N	2:I:659:GLN:OE1	2.46	0.48
2:I:151:ARG:NH2	2:I:175:ARG:HD2	2.28	0.48
2:C:553:THR:O	2:C:557:ARG:HD2	2.12	0.48
2:I:1282:GLY:O	2:I:1284:ALA:N	2.47	0.48
3:J:123:ARG:HH22	3:J:1334:GLU:HG3	1.78	0.48
3:D:1165:PHE:CD1	3:D:1165:PHE:N	2.81	0.48
2:I:646:SER:HB3	2:I:649:GLN:CG	2.44	0.48
2:I:850:ILE:O	2:I:850:ILE:HG22	2.13	0.48
2:I:1217:THR:OG1	2:I:1219:GLU:HG2	2.14	0.48
1:A:27:THR:C	1:A:28:LEU:HD12	2.33	0.48
2:C:832:HIS:CE1	2:C:1058:ARG:HD2	2.48	0.48
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	1.93	0.48
1:A:227:GLN:CG	1:B:39:LEU:HD11	2.41	0.48
1:G:231:PHE:CD1	1:G:231:PHE:O	2.66	0.48
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.48	0.48
3:D:1149:ARG:HG3	3:D:1216:ALA:HB2	1.95	0.48
3:D:810:THR:HG23	3:D:811:GLU:N	2.28	0.48
2:C:906:PHE:HE2	5:F:608:ARG:HH11	1.61	0.48
3:J:647:PRO:HD3	3:J:697:MET:HB3	1.96	0.48
2:C:143:ARG:HH21	2:C:513:GLN:HA	1.79	0.48
2:C:243:PRO:HB2	2:C:278:GLU:HG3	1.96	0.48
3:J:1284:ARG:NH1	3:J:1288:ALA:HB2	2.29	0.48
4:E:39:VAL:HG21	4:E:56:GLU:HG3	1.95	0.48
2:I:1192:GLU:OE2	3:J:764:ARG:NH1	2.47	0.48
1:G:77:ASP:O	1:G:81:ILE:HG13	2.13	0.48
3:D:141:PHE:CD1	3:D:180:MET:HG3	2.42	0.48
1:G:142:MET:HG3	1:G:144:ILE:HG13	1.95	0.48
3:D:83:VAL:O	3:D:91:GLU:HA	2.13	0.48
5:L:343:LYS:HD2	5:L:343:LYS:H	1.79	0.48
3:D:683:ILE:CD1	3:D:754:ILE:HG23	2.43	0.48
3:D:537:TYR:CZ	3:D:544:LEU:HD22	2.49	0.48
5:F:507:MET:O	5:F:519:LEU:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:478:LEU:HD13	4:K:24:ALA:HA	1.96	0.48
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.14	0.48
2:C:13:LYS:O	2:C:1183:ALA:N	2.45	0.48
5:L:316:PHE:O	5:L:320:ILE:HG13	2.14	0.48
3:D:518:VAL:HG11	3:D:707:ILE:HB	1.94	0.48
3:D:83:VAL:HG13	3:D:92:VAL:CG1	2.44	0.48
3:D:839:VAL:CG1	3:D:864:LEU:HD12	2.42	0.48
3:D:363:LEU:HB2	3:D:450:HIS:CE1	2.49	0.48
2:I:810:TYR:CE2	3:J:359:PRO:HD2	2.49	0.48
2:I:607:SER:N	2:I:610:GLU:HB2	2.28	0.48
2:I:646:SER:HB3	2:I:649:GLN:CD	2.34	0.48
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.47	0.48
1:B:46:ILE:HD12	1:B:224:LEU:HB2	1.95	0.48
1:H:13:LEU:O	1:H:13:LEU:HD12	2.14	0.48
3:D:905:ARG:HH12	4:E:10:VAL:HG11	1.79	0.48
3:D:233:LYS:HB3	3:D:235:GLU:OE2	2.14	0.48
5:F:292:VAL:HG21	5:F:299:LYS:CG	2.44	0.48
2:C:617:ALA:HB3	2:C:653:MET:CB	2.44	0.48
3:D:77:ARG:HB3	3:D:80:HIS:CE1	2.48	0.48
2:I:897:PRO:HD3	3:J:77:ARG:HH22	1.78	0.48
3:D:331:ILE:HG22	3:D:1328:THR:HG21	1.96	0.48
5:L:130:VAL:HG23	5:L:266:PHE:HZ	1.79	0.48
1:A:323:PRO:CB	1:A:324:ALA:HB2	2.43	0.48
5:F:511:ILE:CG1	5:F:512:GLY:H	2.27	0.48
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.94	0.48
2:C:1156:ARG:HB2	2:C:1156:ARG:HH11	1.78	0.48
2:I:369:MET:SD	2:I:370:MET:SD	3.12	0.48
3:J:744:ARG:HH11	3:J:763:PHE:HZ	1.61	0.48
1:A:231:PHE:CE2	1:B:39:LEU:HD13	2.49	0.48
5:F:577:GLY:CA	5:F:583:THR:HG23	2.34	0.48
2:I:1322:SER:HB3	3:J:345:LYS:HZ1	1.79	0.48
2:C:73:TYR:CB	2:C:98:VAL:HG22	2.44	0.48
3:D:215:LYS:CE	3:D:216:LYS:HG3	2.43	0.48
1:B:92:VAL:HG12	1:B:95:LYS:HB3	1.96	0.48
2:C:169:LYS:HD3	2:C:190:PRO:HA	1.96	0.48
2:C:178:PRO:HG3	2:C:395:TYR:CE1	2.48	0.48
3:D:1292:LEU:HA	3:J:1226:VAL:HG21	1.96	0.48
2:I:1099:ASN:ND2	3:J:505:ASP:OD2	2.45	0.48
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.46	0.47
2:C:1142:ARG:HD3	2:C:1161:LEU:HD13	1.96	0.47
2:I:976:ARG:HB2	2:I:997:TRP:CZ3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1162:ILE:O	3:D:1178:THR:N	2.47	0.47
5:F:348:GLU:CG	5:F:354:THR:HA	2.44	0.47
2:I:885:GLY:HA2	2:I:917:SER:CB	2.41	0.47
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.49	0.47
2:C:62:TYR:C	2:C:64:GLY:H	2.18	0.47
1:A:252:ILE:HG22	1:A:278:ILE:CD1	2.44	0.47
3:J:647:PRO:HG3	3:J:697:MET:CA	2.44	0.47
3:D:252:LEU:HD23	3:D:262:THR:HB	1.96	0.47
3:D:165:TYR:CE2	3:D:178:ALA:HB3	2.49	0.47
2:C:189:ASP:OD1	2:C:193:ASN:N	2.38	0.47
2:C:408:SER:O	2:C:431:LYS:NZ	2.46	0.47
3:J:490:ILE:HA	3:J:500:ILE:CG1	2.43	0.47
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.96	0.47
1:A:224:LEU:O	1:A:228:LEU:HD12	2.14	0.47
1:H:11:PRO:O	1:H:12:ARG:HG3	2.14	0.47
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.47	0.47
2:I:972:PHE:CZ	2:I:998:LEU:HD11	2.47	0.47
3:J:517:CYS:CA	3:J:716:GLN:HE22	2.25	0.47
3:J:259:ARG:HD2	5:L:505:ILE:CD1	2.40	0.47
3:D:75:TYR:CD2	3:D:80:HIS:HD2	2.27	0.47
3:D:99:ARG:HG3	3:D:249:LEU:HD21	1.95	0.47
3:D:58:CYS:SG	3:D:60:ARG:HB3	2.55	0.47
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.78	0.47
3:D:861:ASN:HD22	3:D:883:ARG:NH1	2.12	0.47
2:I:38:PHE:HB2	2:I:457:GLY:O	2.13	0.47
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.30	0.47
2:I:383:SER:O	2:I:387:ASN:HB2	2.14	0.47
2:I:667:LEU:HD23	2:I:704:MET:HB2	1.95	0.47
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.97	0.47
2:I:409:LEU:HD11	2:I:428:VAL:HG23	1.97	0.47
3:J:1319:PHE:O	3:J:1322:ALA:HB3	2.14	0.47
2:C:1099:ASN:ND2	3:D:505:ASP:OD2	2.40	0.47
2:I:10:ARG:NH2	2:I:791:LEU:HB2	2.28	0.47
2:I:1142:ARG:NH1	2:I:1169:VAL:HG21	2.29	0.47
2:C:39:ILE:O	2:C:39:ILE:HG23	2.14	0.47
2:I:971:LEU:CD2	2:I:1018:TYR:HB2	2.45	0.47
1:A:12:ARG:HG2	1:A:13:LEU:H	1.80	0.47
1:H:110:VAL:HG23	1:H:133:LEU:HD13	1.97	0.47
2:C:519:ASN:HB3	2:C:522:SER:CB	2.44	0.47
2:C:522:SER:O	2:C:525:THR:HG22	2.13	0.47
3:J:510:LEU:HA	3:J:513:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:GLU:O	1:H:78:ILE:HB	2.14	0.47
2:I:153:PRO:HB2	2:I:401:GLY:HA2	1.96	0.47
2:C:1267:GLY:HA3	3:D:347:VAL:O	2.14	0.47
2:I:202:ARG:NH1	2:I:369:MET:HA	2.29	0.47
3:D:630:ALA:O	3:D:633:ALA:HB3	2.15	0.47
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.96	0.47
3:J:474:LEU:HD12	3:J:477:GLN:NE2	2.21	0.47
5:L:558:VAL:HG23	5:L:580:PHE:HE2	1.79	0.47
2:I:1116:HIS:HE1	3:J:641:ILE:N	2.03	0.47
1:H:89:ALA:HB3	1:H:124:VAL:CG1	2.39	0.47
3:J:133:ARG:O	3:J:137:ARG:HB2	2.15	0.47
2:C:493:ILE:HG12	2:C:493:ILE:O	2.13	0.47
2:I:1191:LYS:HD3	2:I:1192:GLU:N	2.29	0.47
3:J:709:ARG:HD2	3:J:710:ASP:H	1.78	0.47
5:L:392:LYS:O	5:L:395:THR:HG22	2.14	0.47
2:I:1184:THR:HG23	2:I:1189:GLY:CA	2.45	0.47
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.96	0.47
3:J:482:ALA:HB3	4:K:20:VAL:HG22	1.96	0.47
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.96	0.47
1:G:156:SER:CB	2:I:1059:ARG:HH22	2.26	0.47
5:L:362:ASN:HA	5:L:365:MET:HB2	1.96	0.47
2:I:568:ASN:HB2	2:I:571:LEU:HB2	1.95	0.47
2:C:395:TYR:HB3	2:C:419:ILE:CG2	2.45	0.47
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.97	0.47
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.95	0.47
2:C:171:LEU:HA	2:C:171:LEU:HD23	1.61	0.47
2:I:932:GLN:HB3	2:I:934:PHE:CE2	2.50	0.47
2:I:849:GLU:HB2	2:I:851:THR:HG22	1.96	0.47
2:I:122:VAL:HG11	2:I:493:ILE:HD13	1.97	0.47
5:L:311:THR:O	5:L:341:LEU:HD21	2.14	0.47
2:C:1269:ARG:CG	3:D:343:LEU:HD11	2.43	0.47
2:I:670:PHE:CD1	2:I:1113:LEU:HD23	2.49	0.47
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.97	0.47
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.96	0.47
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.79	0.47
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.96	0.47
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.46	0.47
2:I:1299:ASN:O	2:I:1303:LYS:HG2	2.15	0.47
2:I:1222:GLU:OE1	3:J:512:TYR:OH	2.21	0.47
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.97	0.47
2:C:1281:TYR:OH	3:D:431:ARG:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:HD2	1:B:227:GLN:O	2.15	0.47
1:A:58:GLU:HG2	1:A:158:ARG:NH2	2.25	0.47
2:C:594:VAL:HG11	2:C:650:VAL:HG23	1.96	0.47
5:L:454:VAL:O	5:L:458:GLU:HG3	2.15	0.47
3:D:810:THR:O	3:D:911:LYS:HE2	2.14	0.47
1:H:79:LEU:O	1:H:82:LEU:HB2	2.14	0.47
5:L:585:GLU:O	5:L:589:GLN:HG3	2.14	0.47
2:C:785:ASP:OD2	2:C:791:LEU:N	2.46	0.47
2:C:861:ALA:HB1	2:C:882:ILE:CD1	2.45	0.47
4:E:15:ASN:HB3	4:E:18:ASP:H	1.80	0.47
3:D:122:SER:O	3:D:126:LEU:HG	2.15	0.47
3:J:1280:VAL:CG1	3:J:1304:ARG:HH21	2.27	0.47
5:F:583:THR:O	5:F:584:ARG:HB2	2.14	0.47
1:A:44:ARG:HG3	1:A:183:ILE:CG2	2.44	0.47
2:C:1106:ARG:O	2:C:1108:ASN:N	2.45	0.47
2:C:670:PHE:CD1	2:C:1113:LEU:HD23	2.50	0.47
3:D:514:THR:HG21	3:D:596:LEU:HG	1.97	0.47
1:A:36:GLY:HA3	1:A:187:VAL:HG11	1.96	0.47
3:D:1327:GLU:OE2	3:D:1329:THR:HB	2.14	0.47
3:J:418:GLU:HB3	4:K:48:VAL:HG23	1.97	0.47
2:C:785:ASP:HB3	2:C:789:THR:O	2.13	0.47
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.97	0.47
2:I:802:VAL:CG2	2:I:1098:LEU:HD13	2.45	0.47
3:D:239:LEU:HA	3:D:239:LEU:HD23	1.62	0.47
2:I:700:VAL:HG11	2:I:1114:GLU:HG2	1.97	0.47
2:I:1086:PRO:O	2:I:1094:VAL:HG12	2.14	0.47
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.48	0.47
2:C:256:GLU:OE2	2:C:261:VAL:HG22	2.14	0.47
3:D:322:ARG:HH11	3:D:322:ARG:HB2	1.79	0.47
3:D:384:LYS:HD2	3:D:387:LEU:HD23	1.97	0.47
3:D:536:LEU:HD12	3:D:542:ALA:CB	2.44	0.47
2:C:857:VAL:HG21	2:C:862:LEU:HD21	1.97	0.47
3:J:658:GLU:O	3:J:661:VAL:HG22	2.14	0.47
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.97	0.47
3:J:1162:ILE:HD12	3:J:1163:VAL:H	1.80	0.47
1:A:321:TRP:HA	1:A:322:PRO:HA	1.83	0.47
5:L:415:ALA:O	5:L:419:PHE:N	2.48	0.47
2:C:667:LEU:HD23	2:C:704:MET:HB2	1.96	0.47
3:D:238:ILE:HA	3:D:238:ILE:HD13	1.70	0.47
2:I:964:LEU:HD13	2:I:1021:LEU:O	2.14	0.47
2:C:520:PRO:HB3	2:C:714:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:337:PHE:CE2	2:I:343:HIS:CD2	3.03	0.47
1:A:180:VAL:HG12	1:A:183:ILE:HD11	1.97	0.47
2:C:1028:LYS:O	2:C:1032:LYS:HB2	2.15	0.47
3:D:124:ILE:HG23	3:D:189:LEU:HD21	1.96	0.47
3:D:518:VAL:HB	3:D:707:ILE:HD13	1.97	0.47
2:C:1259:LEU:HD12	2:C:1260:GLY:H	1.78	0.47
1:G:73:GLY:HA2	1:G:134:THR:HG22	1.96	0.47
2:C:62:TYR:C	2:C:64:GLY:N	2.68	0.47
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.96	0.47
3:D:412:LEU:HD23	3:D:416:ILE:HG12	1.96	0.47
1:A:263:THR:HG23	1:A:266:SER:H	1.78	0.47
3:J:481:ARG:O	4:K:6:VAL:HG11	2.15	0.47
2:C:980:VAL:HA	2:C:984:VAL:HA	1.97	0.47
1:G:190:ALA:C	1:G:191:ARG:HD3	2.36	0.47
2:I:1014:LEU:O	2:I:1018:TYR:HB2	2.15	0.47
2:I:551:HIS:CE1	2:I:553:THR:OG1	2.68	0.47
3:J:850:LYS:HB3	3:J:851:PRO:CD	2.42	0.47
2:I:1223:ARG:HG3	3:J:635:SER:O	2.15	0.47
2:I:519:ASN:HB3	2:I:522:SER:HB2	1.97	0.47
2:C:210:LEU:O	2:C:215:TYR:HB2	2.15	0.47
3:D:870:ASP:O	3:D:874:GLU:N	2.44	0.47
2:I:561:ILE:O	2:I:680:LEU:HD12	2.15	0.47
3:D:746:LEU:HG	3:D:758:PRO:HG3	1.96	0.47
5:L:288:MET:CG	5:L:299:LYS:HE2	2.45	0.46
2:I:975:ILE:O	2:I:979:LEU:HB2	2.15	0.46
3:J:189:LEU:HB3	3:J:234:PRO:CB	2.43	0.46
2:C:490:GLN:HG3	5:F:472:GLN:CG	2.43	0.46
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.97	0.46
3:D:647:PRO:HG3	3:D:697:MET:CA	2.45	0.46
2:I:389:PHE:HD1	2:I:395:TYR:CE1	2.33	0.46
2:C:60:GLN:HA	2:C:67:GLU:HA	1.97	0.46
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.50	0.46
1:A:310:ARG:HA	1:A:310:ARG:HE	1.79	0.46
2:I:324:LYS:O	2:I:327:GLN:NE2	2.48	0.46
3:J:707:ILE:HD12	3:J:707:ILE:H	1.80	0.46
3:J:691:ASP:O	3:J:695:LYS:HG2	2.15	0.46
3:D:905:ARG:HH12	4:E:10:VAL:CG1	2.28	0.46
2:C:746:ALA:CB	2:C:974:ARG:HE	2.28	0.46
3:D:19:ALA:H	3:D:1344:LEU:HD12	1.80	0.46
1:G:166:ARG:O	1:G:168:ILE:N	2.48	0.46
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:281:ARG:CG	5:L:285:ARG:HH11	2.28	0.46
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.97	0.46
2:I:985:GLU:CG	2:I:988:LYS:HD2	2.46	0.46
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.97	0.46
2:I:98:VAL:C	2:I:121:GLU:HA	2.34	0.46
2:C:1222:GLU:OE2	3:D:537:TYR:OH	2.28	0.46
2:C:632:ASP:O	2:C:647:ARG:HB2	2.15	0.46
2:C:879:GLY:HA2	2:C:920:VAL:HG12	1.97	0.46
1:H:201:LEU:HG	1:H:203:ILE:CD1	2.46	0.46
3:D:1156:LEU:N	3:D:1156:LEU:HD22	2.29	0.46
3:J:556:GLU:HG2	3:J:558:ASP:HB2	1.97	0.46
2:C:1253:LEU:HA	5:F:525:ASP:HB2	1.97	0.46
3:J:68:TYR:C	3:J:92:VAL:HG23	2.34	0.46
2:I:1101:LEU:O	3:J:731:ARG:HD3	2.15	0.46
5:L:324:LYS:HB3	5:L:325:PRO:HD2	1.98	0.46
3:J:233:LYS:H	3:J:236:TRP:HE3	1.63	0.46
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.50	0.46
5:F:311:THR:HG21	5:F:348:GLU:CD	2.35	0.46
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.96	0.46
1:G:22:THR:OG1	1:G:23:HIS:N	2.48	0.46
5:F:97:PRO:HA	5:F:100:MET:HG3	1.98	0.46
3:D:24:LEU:HD23	3:D:232:ASN:ND2	2.30	0.46
5:F:479:THR:OG1	5:F:480:PRO:HD2	2.15	0.46
3:D:744:ARG:HG3	3:D:744:ARG:O	2.15	0.46
3:J:697:MET:SD	3:J:741:ALA:HB3	2.55	0.46
2:C:169:LYS:O	2:C:170:VAL:HG22	2.15	0.46
3:J:683:ILE:HD11	3:J:754:ILE:HG21	1.98	0.46
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.73	0.46
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.44	0.46
1:B:106:GLY:O	1:B:133:LEU:HB3	2.15	0.46
3:D:385:LEU:HA	3:D:385:LEU:HD23	1.76	0.46
3:J:1281:GLU:O	3:J:1285:VAL:HB	2.16	0.46
5:L:129:GLN:HB2	5:L:368:GLY:HA3	1.98	0.46
2:I:1146:GLN:NE2	2:I:1150:ASP:OD2	2.47	0.46
5:L:253:SER:O	5:L:257:LYS:HG3	2.15	0.46
3:J:801:VAL:O	3:J:805:GLN:HB2	2.15	0.46
5:L:346:GLN:O	5:L:346:GLN:HG2	2.14	0.46
2:C:1252:SER:HB3	2:C:1255:THR:O	2.16	0.46
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.45	0.46
3:D:872:LEU:HD23	3:D:872:LEU:HA	1.67	0.46
4:E:71:GLU:O	4:E:75:GLN:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:VAL:O	1:B:175:ALA:N	2.22	0.46
5:L:114:GLU:HG3	5:L:115:GLY:H	1.81	0.46
5:L:572:THR:O	5:L:576:VAL:HG23	2.15	0.46
3:D:367:GLY:HA3	3:D:448:GLN:CB	2.38	0.46
3:D:848:VAL:HG13	3:D:857:LEU:CD1	2.46	0.46
3:D:1284:ARG:NH2	3:J:1292:LEU:HD11	2.30	0.46
3:D:128:LEU:HB3	3:D:157:GLN:HE22	1.80	0.46
5:F:287:ILE:O	5:F:291:CYS:SG	2.70	0.46
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.13	0.46
3:D:702:GLN:HA	3:D:723:TYR:CE2	2.50	0.46
2:I:593:LYS:HE3	2:I:595:THR:CG2	2.44	0.46
2:I:582:ASN:O	2:I:585:GLY:N	2.47	0.46
3:J:293:ARG:O	3:J:296:LYS:N	2.49	0.46
2:I:1305:TYR:CE1	3:J:379:PRO:HG3	2.51	0.46
2:C:229:ILE:CD1	2:C:334:GLU:HG2	2.46	0.46
3:D:112:ALA:HA	3:D:238:ILE:CD1	2.45	0.46
2:I:671:LEU:HD23	2:I:1186:VAL:CG1	2.46	0.46
2:I:921:PRO:HB2	2:I:924:VAL:HG22	1.97	0.46
3:J:103:GLY:C	3:J:244:VAL:HG22	2.36	0.46
2:I:124:MET:HE2	2:I:493:ILE:HD11	1.98	0.46
3:D:1163:VAL:HG21	3:D:1175:LEU:HD21	1.98	0.46
3:J:848:VAL:H	3:J:858:VAL:HG22	1.81	0.46
1:B:191:ARG:O	1:B:191:ARG:HG2	2.15	0.46
3:D:847:ASP:N	3:D:847:ASP:OD1	2.42	0.46
3:D:647:PRO:CG	3:D:697:MET:HB3	2.42	0.46
2:I:553:THR:O	2:I:557:ARG:HD2	2.16	0.46
2:C:600:THR:HG22	2:C:601:ASP:H	1.81	0.46
5:F:461:ASN:O	5:F:465:ARG:HG2	2.15	0.46
5:L:108:VAL:HG11	5:L:381:GLU:C	2.35	0.46
2:C:1247:SER:OG	2:C:1248:THR:N	2.49	0.46
2:I:1023:HIS:O	2:I:1027:LYS:HG2	2.15	0.46
3:J:245:LEU:O	3:J:250:ARG:NE	2.46	0.46
1:A:224:LEU:HA	1:A:224:LEU:HD12	1.53	0.46
2:I:1180:MET:HA	2:I:1181:PRO:HD3	1.78	0.46
2:C:1142:ARG:HH11	2:C:1161:LEU:CD1	2.28	0.46
1:A:296:GLY:H	1:A:299:SER:CB	2.20	0.46
1:A:115:ILE:HG22	1:A:116:THR:N	2.26	0.46
2:C:953:LEU:HD13	2:C:1036:ILE:HD12	1.97	0.46
3:J:1266:ILE:HD12	3:J:1273:ASP:O	2.15	0.46
3:D:710:ASP:OD1	3:D:711:GLY:N	2.49	0.46
3:J:1157:ALA:HB3	3:J:1207:GLY:N	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:825:VAL:CG1	3:D:833:GLU:HB3	2.46	0.46
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.15	0.46
2:I:852:ALA:HB2	2:I:869:GLY:HA2	1.97	0.46
2:C:95:PRO:CA	2:C:126:GLU:HG2	2.46	0.46
5:L:372:ALA:O	5:L:375:ALA:HB3	2.16	0.46
3:J:1319:PHE:CD1	3:J:1319:PHE:C	2.89	0.46
2:I:738:GLU:HA	2:I:741:MET:CE	2.46	0.46
2:C:867:GLU:HG3	2:C:867:GLU:H	1.17	0.46
2:I:811:ASN:N	2:I:811:ASN:OD1	2.48	0.46
2:I:42:ASP:O	2:I:44:GLU:N	2.43	0.46
2:I:1255:THR:O	2:I:1257:GLN:N	2.48	0.46
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.46	0.46
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.80	0.46
3:D:318:GLY:C	3:D:320:ASN:H	2.19	0.46
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.97	0.46
2:C:119:GLU:HG3	2:C:488:MET:HB3	1.97	0.46
1:B:57:THR:OG1	1:B:147:GLN:HB3	2.16	0.46
3:J:596:LEU:HD11	3:J:604:MET:CE	2.45	0.46
2:C:91:THR:HB	2:C:138:ILE:O	2.16	0.46
3:D:232:ASN:HA	3:D:236:TRP:HZ3	1.81	0.46
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.73	0.46
5:F:383:ASN:O	5:F:386:LEU:HB3	2.15	0.46
2:I:106:GLU:O	2:I:109:ALA:HB2	2.16	0.46
3:D:901:ARG:HD2	3:D:906:GLY:O	2.15	0.46
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.97	0.46
3:D:1197:ASN:HB2	3:D:1212:ASP:OD2	2.16	0.46
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.97	0.46
2:I:1139:ALA:O	2:I:1143:GLU:HB2	2.16	0.46
5:F:489:MET:O	5:F:491:GLU:N	2.49	0.46
5:L:288:MET:O	5:L:292:VAL:HG23	2.16	0.46
2:C:1269:ARG:HD3	3:D:343:LEU:HD21	1.96	0.46
5:F:316:PHE:O	5:F:320:ILE:HG13	2.15	0.46
2:I:886:LYS:CE	2:I:916:SER:HB3	2.46	0.46
3:D:123:ARG:NH1	3:D:1334:GLU:HG3	2.31	0.46
2:C:55:SER:OG	2:C:56:VAL:N	2.49	0.46
3:J:267:ASP:OD1	3:J:271:ARG:NH2	2.49	0.46
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.98	0.46
5:L:138:PRO:HD2	5:L:353:LEU:HD11	1.98	0.46
5:F:226:ALA:O	5:F:230:VAL:HG12	2.15	0.46
1:A:106:GLY:HA2	1:A:136:GLU:O	2.16	0.46
1:H:217:ILE:HA	1:H:220:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1101:LEU:O	2:C:1104:PRO:HD2	2.16	0.46
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.51	0.46
3:D:708:ASN:HB3	3:D:712:GLN:O	2.16	0.46
1:B:217:ILE:HA	1:B:220:ALA:HB3	1.96	0.46
2:C:1086:PRO:HB3	2:C:1212:LEU:HD23	1.96	0.46
3:J:813:ASP:OD1	3:J:883:ARG:NH2	2.41	0.46
3:J:861:ASN:HD22	3:J:883:ARG:NH1	2.13	0.46
3:J:491:LEU:HD22	3:J:496:GLY:O	2.16	0.46
2:C:976:ARG:HD2	2:C:989:LEU:CD2	2.46	0.46
5:L:482:GLU:HA	5:L:485:GLU:OE2	2.16	0.46
3:D:1167:LYS:HE3	3:D:1167:LYS:HB3	1.85	0.46
3:J:514:THR:HG21	3:J:596:LEU:CG	2.46	0.46
3:J:452:LEU:HD11	3:J:625:MET:HB2	1.98	0.46
3:D:137:ARG:CG	3:D:142:GLU:HB2	2.45	0.46
3:D:58:CYS:SG	3:D:59:ALA:N	2.89	0.46
2:I:1131:MET:CE	2:I:1141:LEU:HD12	2.46	0.46
3:D:744:ARG:O	3:D:759:ILE:HB	2.15	0.46
1:H:215:GLU:HA	1:H:218:ARG:HG3	1.97	0.46
3:J:825:VAL:C	3:J:826:ILE:HG13	2.36	0.46
2:C:730:SER:O	2:C:753:LEU:HB2	2.15	0.46
3:J:1298:VAL:O	3:J:1298:VAL:HG13	2.16	0.46
2:I:290:GLU:HG2	2:I:319:LEU:HD12	1.97	0.46
2:C:131:THR:HG22	2:C:132:ASP:H	1.81	0.46
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.51	0.46
1:B:38:THR:HG23	1:B:39:LEU:N	2.32	0.45
3:J:474:LEU:HB2	4:K:28:ARG:NH1	2.31	0.45
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.80	0.45
2:I:1296:ASP:OD2	2:I:1321:GLU:N	2.49	0.45
2:C:744:GLY:O	2:C:746:ALA:N	2.48	0.45
3:J:844:THR:HG23	3:J:864:LEU:HD21	1.98	0.45
2:C:811:ASN:N	2:C:811:ASN:OD1	2.48	0.45
3:D:860:ARG:CB	3:D:860:ARG:HH11	2.26	0.45
3:D:45:ASN:O	3:D:46:TYR:HB3	2.15	0.45
3:J:805:GLN:HE22	3:J:1348:LYS:HD3	1.80	0.45
5:L:476:ARG:HB3	5:L:476:ARG:NH1	2.31	0.45
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.41	0.45
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.49	0.45
5:F:222:ALA:O	5:F:226:ALA:N	2.45	0.45
1:G:110:VAL:CG2	1:G:133:LEU:HD23	2.45	0.45
2:I:91:THR:HB	2:I:138:ILE:O	2.16	0.45
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:555:TYR:OH	2:I:654:ASP:OD1	2.16	0.45
3:D:627:THR:HG23	3:D:628:GLY:N	2.31	0.45
5:L:99:ARG:HD3	5:L:99:ARG:HA	1.68	0.45
3:J:385:LEU:HD23	3:J:385:LEU:HA	1.73	0.45
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.50	0.45
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.80	0.45
3:J:93:THR:HG22	3:J:94:GLN:H	1.80	0.45
1:B:62:ASP:HB3	1:B:141:SER:O	2.15	0.45
2:C:1161:LEU:HD12	2:C:1161:LEU:HA	1.65	0.45
2:C:1119:MET:HB2	2:C:1228:GLY:CA	2.46	0.45
2:C:960:LEU:HD11	2:C:1028:LYS:HE2	1.97	0.45
3:D:521:LYS:HB3	3:D:541:LEU:O	2.16	0.45
5:L:474:MET:C	5:L:476:ARG:H	2.15	0.45
2:I:175:ARG:HD3	2:I:183:TRP:CE3	2.52	0.45
3:J:267:ASP:HA	3:J:270:ARG:NH2	2.28	0.45
2:I:1212:LEU:HD11	2:I:1227:VAL:HG11	1.98	0.45
1:A:321:TRP:CD2	1:A:322:PRO:HB3	2.50	0.45
2:C:946:LEU:HA	2:C:946:LEU:HD23	1.75	0.45
2:I:1292:THR:HG22	2:I:1293:VAL:N	2.31	0.45
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.97	0.45
3:J:1327:GLU:OE1	3:J:1330:ARG:HB2	2.17	0.45
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.52	0.45
3:D:210:SER:OG	3:D:213:LYS:HD2	2.16	0.45
5:L:557:LYS:HG3	5:L:561:MET:CE	2.46	0.45
2:I:1196:LYS:O	2:I:1200:LYS:HG3	2.17	0.45
5:F:99:ARG:HA	5:F:99:ARG:HD3	1.72	0.45
3:D:58:CYS:SG	3:D:60:ARG:N	2.87	0.45
5:F:386:LEU:O	5:F:390:ILE:HG13	2.17	0.45
2:I:486:THR:HG23	2:I:487:LEU:N	2.31	0.45
2:C:210:LEU:HB2	2:C:220:ILE:HD11	1.97	0.45
2:C:800:MET:HG3	2:C:1096:ILE:CD1	2.46	0.45
5:F:290:LEU:O	5:F:333:VAL:HG11	2.16	0.45
2:C:30:ILE:HD12	2:C:30:ILE:H	1.82	0.45
2:C:83:GLN:O	2:C:87:ILE:HG13	2.17	0.45
2:C:883:LEU:HB3	2:C:1052:VAL:HG21	1.99	0.45
1:A:189:ALA:HB1	1:A:191:ARG:NH2	2.31	0.45
2:I:95:PRO:HB3	2:I:123:TYR:CE1	2.51	0.45
2:I:814:ASP:N	2:I:814:ASP:OD1	2.49	0.45
5:L:310:GLU:O	5:L:344:LEU:HD21	2.16	0.45
2:C:1307:ASN:O	2:C:1311:GLY:N	2.50	0.45
2:I:119:GLU:CG	2:I:489:PRO:HD2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:O	1:A:180:VAL:HG21	2.17	0.45
2:I:985:GLU:HB3	2:I:988:LYS:HD2	1.99	0.45
3:D:247:PRO:HA	3:D:250:ARG:CZ	2.47	0.45
3:D:298:MET:SD	5:F:402:LEU:HB3	2.57	0.45
3:D:255:LEU:HA	3:D:255:LEU:HD13	1.82	0.45
1:G:150:ARG:HH11	1:H:6:THR:HG23	1.81	0.45
2:C:15:PHE:CD2	2:C:1190:ALA:HB2	2.51	0.45
5:L:558:VAL:HG23	5:L:580:PHE:CE2	2.51	0.45
2:C:1117:LEU:HD21	2:C:1182:ILE:HD12	1.99	0.45
1:G:166:ARG:O	1:G:167:PRO:C	2.55	0.45
3:J:861:ASN:HD22	3:J:883:ARG:HH11	1.63	0.45
2:I:974:ARG:HD3	2:I:1010:GLN:HE21	1.82	0.45
2:C:117:ILE:H	2:C:117:ILE:HG12	1.59	0.45
2:C:106:GLU:HG3	2:C:107:ARG:N	2.32	0.45
2:C:1230:MET:HG2	2:C:1232:MET:HG3	1.99	0.45
3:D:311:ARG:NH2	3:D:1329:THR:HG21	2.32	0.45
3:D:810:THR:HG21	3:D:893:GLY:HA3	1.95	0.45
3:J:532:GLU:HB2	3:J:535:ARG:NH2	2.30	0.45
3:D:490:ILE:HA	3:D:500:ILE:HG13	1.98	0.45
3:J:811:GLU:O	3:J:895:CYS:HA	2.16	0.45
2:C:87:ILE:H	2:C:87:ILE:HG13	1.51	0.45
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.81	0.45
2:C:826:ASP:O	2:C:829:THR:HB	2.16	0.45
3:J:193:ASP:HB3	3:J:196:GLN:HG2	1.98	0.45
3:J:398:LYS:O	3:J:402:GLU:HB2	2.16	0.45
2:I:716:ALA:HB3	2:I:784:ALA:HB3	1.98	0.45
2:I:676:ALA:HB2	3:J:772:TYR:HE1	1.82	0.45
2:C:1319:MET:HG3	2:C:1320:PRO:HD2	1.98	0.45
3:D:1350:ASN:OD1	3:D:1355:ARG:HD2	2.17	0.45
1:A:54:CYS:HB3	1:A:148:ARG:HB2	1.97	0.45
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.16	0.45
2:C:478:ARG:CZ	2:C:487:LEU:HD13	2.47	0.45
3:J:73:GLY:O	3:J:76:LYS:HG3	2.17	0.45
2:I:361:SER:O	2:I:364:VAL:HB	2.16	0.45
2:I:516:ASP:HB3	2:I:522:SER:HG	1.81	0.45
1:A:237:VAL:O	1:B:13:LEU:HA	2.17	0.45
5:L:565:ILE:HG22	5:L:566:ASP:OD1	2.16	0.45
3:D:405:GLU:O	3:D:408:VAL:HG22	2.17	0.45
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.99	0.45
2:I:526:HIS:O	2:I:529:ARG:HB2	2.17	0.45
3:D:491:LEU:HA	3:D:491:LEU:HD23	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:583:THR:HG22	5:L:584:ARG:N	2.32	0.45
2:C:810:TYR:HE2	3:D:359:PRO:HD2	1.80	0.45
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.98	0.45
2:C:615:VAL:HG13	2:C:651:ASP:N	2.29	0.45
2:I:898:GLU:CB	5:L:540:LEU:HD22	2.46	0.45
3:J:451:PRO:HD2	3:J:625:MET:SD	2.57	0.45
4:K:38:LEU:HB2	4:K:53:GLU:OE1	2.17	0.45
2:I:1297:ASP:O	2:I:1301:ARG:HG2	2.17	0.45
5:F:96:ASP:O	5:F:99:ARG:N	2.42	0.45
3:D:98:ARG:O	3:D:247:PRO:HD2	2.17	0.45
2:C:62:TYR:CZ	2:C:476:LYS:HB3	2.52	0.45
2:C:378:ARG:NH1	2:C:382:GLU:OE2	2.50	0.45
3:D:1279:GLN:H	3:D:1279:GLN:HG2	1.42	0.45
3:D:276:ASN:O	3:D:280:LYS:HG2	2.17	0.45
2:I:1306:LYS:HE2	5:L:535:ALA:HA	1.97	0.45
3:J:474:LEU:CD2	4:K:28:ARG:HG2	2.47	0.45
3:J:35:PHE:HE1	3:J:101:ARG:HH11	1.64	0.45
2:I:976:ARG:O	2:I:980:VAL:HG23	2.17	0.45
1:G:166:ARG:HD2	1:G:166:ARG:C	2.37	0.45
2:C:870:ILE:HG22	2:C:944:ARG:NH1	2.32	0.45
3:J:596:LEU:HD11	3:J:604:MET:HE1	1.98	0.45
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.31	0.45
1:G:35:PHE:HE1	1:H:46:ILE:HG12	1.82	0.45
3:D:327:LEU:HD23	3:D:327:LEU:HA	1.74	0.45
1:G:150:ARG:NH1	1:H:7:GLU:O	2.42	0.45
3:D:47:ARG:NH1	5:F:500:ILE:HD11	2.31	0.45
2:C:239:MET:N	2:C:285:ILE:O	2.48	0.45
2:I:1066:MET:HG2	2:I:1234:LYS:HA	1.98	0.45
2:I:1340:GLU:HG2	3:J:21:LYS:HB2	1.98	0.45
1:G:51:MET:HA	1:G:52:PRO:HD3	1.80	0.45
2:I:1262:LYS:C	2:I:1264:GLN:H	2.20	0.45
1:A:228:LEU:HD21	1:B:43:LEU:HD11	1.99	0.45
2:C:1146:GLN:HG2	2:C:1160:ASP:OD1	2.16	0.45
1:H:65:LEU:HD22	1:H:171:LEU:HD11	1.99	0.45
3:D:342:LEU:O	3:D:343:LEU:C	2.54	0.45
2:C:871:VAL:O	2:C:944:ARG:NH1	2.50	0.45
2:C:796:LEU:HD12	2:C:796:LEU:N	2.30	0.45
3:J:510:LEU:HD12	3:J:628:GLY:HA2	1.99	0.45
1:A:60:GLU:HG3	1:A:169:GLY:O	2.17	0.45
1:A:31:LEU:HD12	1:A:201:LEU:HB2	1.99	0.45
3:D:1356:LEU:HA	3:D:1356:LEU:HD23	1.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.97	0.45
3:D:513:MET:CE	3:D:579:LEU:HD13	2.47	0.45
1:A:90:VAL:O	1:A:210:THR:HG21	2.17	0.45
3:J:193:ASP:HB3	3:J:196:GLN:CG	2.46	0.45
2:I:272:ARG:HD3	2:I:273:HIS:CD2	2.52	0.45
1:A:312:LEU:H	1:A:312:LEU:HD12	1.81	0.45
2:I:682:GLY:O	2:I:686:GLN:HB2	2.17	0.45
2:C:159:SER:O	2:C:160:ASP:HB2	2.17	0.45
3:D:654:ILE:O	3:D:658:GLU:HB2	2.16	0.45
1:G:50:SER:HG	1:H:35:PHE:HE1	1.64	0.45
2:I:490:GLN:CG	5:L:472:GLN:HG3	2.40	0.45
3:J:317:THR:CG2	3:J:320:ASN:HB3	2.41	0.45
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.99	0.45
3:D:121:PRO:HD2	3:D:123:ARG:NH2	2.31	0.45
1:A:185:TYR:HB2	1:A:201:LEU:HD11	1.98	0.45
2:I:618:GLN:OE1	3:J:769:VAL:HB	2.16	0.45
2:C:688:GLN:OE1	2:C:1237:HIS:CE1	2.69	0.45
1:A:282:VAL:HG22	1:A:316:MET:SD	2.56	0.45
2:C:1276:TRP:HA	2:C:1279:GLU:OE1	2.17	0.45
5:F:289:LYS:HE2	5:F:289:LYS:HB3	1.86	0.45
2:I:658:GLN:O	2:I:661:VAL:HG22	2.17	0.45
2:I:1287:LEU:HD23	2:I:1288:GLN:N	2.32	0.45
3:D:478:LEU:HG	4:E:47:THR:HG23	1.98	0.45
3:J:578:ILE:HG21	3:J:631:TYR:OH	2.17	0.45
2:C:353:VAL:O	2:C:355:PRO:HD3	2.17	0.45
3:D:1250:ASP:O	3:D:1251:LYS:C	2.55	0.45
2:C:202:ARG:NH1	2:C:368:ARG:HH22	2.14	0.44
5:L:292:VAL:HG21	5:L:299:LYS:CG	2.47	0.44
3:D:427:PRO:HB2	3:D:429:LEU:CD2	2.47	0.44
3:D:853:THR:HG22	3:D:854:ALA:N	2.29	0.44
2:C:865:LEU:HD23	2:C:871:VAL:HA	1.99	0.44
3:J:24:LEU:HA	3:J:24:LEU:HD13	1.71	0.44
1:G:14:VAL:HG13	1:G:27:THR:HB	1.98	0.44
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.32	0.44
2:I:106:GLU:HG3	2:I:107:ARG:N	2.31	0.44
3:J:1149:ARG:HH21	3:J:1153:PRO:HG2	1.80	0.44
2:I:588:GLU:HB3	2:I:607:SER:HA	1.99	0.44
3:J:118:LYS:HE2	3:J:118:LYS:HB3	1.72	0.44
1:A:285:THR:OG1	1:A:286:GLU:N	2.50	0.44
2:C:175:ARG:HG3	2:C:185:ASP:OD1	2.17	0.44
3:D:903:LEU:HD23	3:D:905:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:357:VAL:HB	3:D:358:GLY:H	1.67	0.44
3:J:845:ALA:HB3	3:J:846:GLU:HG2	1.99	0.44
2:C:950:GLU:O	2:C:953:LEU:HB3	2.16	0.44
1:G:77:ASP:CG	2:I:755:LYS:HZ1	2.18	0.44
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.81	0.44
2:C:814:ASP:N	2:C:814:ASP:OD1	2.50	0.44
3:D:518:VAL:N	3:D:716:GLN:HE22	2.15	0.44
3:D:343:LEU:HD13	3:D:344:GLY:N	2.33	0.44
5:F:572:THR:O	5:F:576:VAL:HG23	2.18	0.44
2:I:670:PHE:CE1	2:I:1184:THR:HG21	2.52	0.44
3:D:123:ARG:HH12	3:D:1334:GLU:HG3	1.83	0.44
2:C:1239:VAL:HG13	2:C:1240:ASP:N	2.32	0.44
2:C:557:ARG:HB3	2:C:587:LEU:HD13	2.00	0.44
2:I:945:ALA:O	2:I:949:GLU:HB2	2.17	0.44
5:L:362:ASN:HA	5:L:365:MET:CB	2.46	0.44
3:D:412:LEU:O	3:D:415:VAL:HG22	2.17	0.44
3:D:1146:GLU:HG2	3:D:1148:ARG:NH2	2.33	0.44
3:J:1291:GLU:HG2	3:J:1297:LYS:NZ	2.32	0.44
2:I:981:ALA:HB1	2:I:1007:LYS:HZ3	1.81	0.44
2:C:18:ARG:HG2	2:C:1188:ASP:OD1	2.17	0.44
1:G:200:LYS:HB2	1:G:200:LYS:HE2	1.60	0.44
1:H:34:GLY:O	1:H:38:THR:HG22	2.18	0.44
1:B:6:THR:OG1	1:B:7:GLU:N	2.50	0.44
3:D:45:ASN:O	3:D:46:TYR:CD2	2.69	0.44
2:C:858:GLY:O	2:C:862:LEU:HG	2.18	0.44
2:I:153:PRO:HB2	2:I:401:GLY:CA	2.48	0.44
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.86	0.44
5:F:130:VAL:HA	5:F:133:SER:HB2	1.98	0.44
2:I:1212:LEU:HB3	2:I:1221:PHE:HD2	1.82	0.44
3:D:416:ILE:HA	3:D:416:ILE:HD12	1.72	0.44
3:D:108:ALA:HB3	3:D:279:LEU:HD22	1.98	0.44
2:C:1031:ALA:O	2:C:1035:LYS:HG3	2.17	0.44
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.98	0.44
1:A:285:THR:O	1:A:289:LEU:HG	2.18	0.44
2:C:699:LEU:HA	2:C:699:LEU:HD23	1.80	0.44
2:I:269:ILE:HD12	2:I:269:ILE:H	1.81	0.44
2:C:992:LEU:HB2	2:C:993:PRO:HD2	2.00	0.44
5:L:584:ARG:HA	5:L:584:ARG:HD2	1.68	0.44
2:C:202:ARG:HH11	2:C:369:MET:HB2	1.83	0.44
3:D:205:LEU:CD2	3:D:214:ARG:HB2	2.47	0.44
3:J:844:THR:OG1	3:J:860:ARG:O	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:48:THR:C	3:D:50:LYS:N	2.67	0.44
3:J:800:LEU:HD12	3:J:1309:ILE:HD13	1.98	0.44
2:I:812:PHE:N	2:I:815:SER:OG	2.50	0.44
5:F:143:TYR:CD2	5:F:269:LEU:HD21	2.52	0.44
5:L:511:ILE:CG1	5:L:512:GLY:H	2.30	0.44
2:C:1082:ILE:CD1	2:C:1082:ILE:H	2.29	0.44
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.32	0.44
2:C:629:PHE:CD2	2:C:634:VAL:HG11	2.52	0.44
3:D:1283:SER:O	3:D:1286:LYS:N	2.50	0.44
3:J:490:ILE:HA	3:J:500:ILE:HG13	2.00	0.44
3:J:695:LYS:HD3	3:J:695:LYS:HA	1.69	0.44
2:I:1210:ILE:HG22	2:I:1211:ARG:N	2.32	0.44
3:D:56:LEU:HD12	3:D:56:LEU:H	1.82	0.44
3:J:327:LEU:HA	3:J:327:LEU:HD23	1.65	0.44
3:D:291:ILE:CD1	5:F:409:ASN:HB3	2.47	0.44
3:J:1219:ASP:O	3:J:1222:ARG:N	2.50	0.44
2:C:5:TYR:CD2	2:C:778:GLU:HB2	2.53	0.44
2:C:810:TYR:CD2	3:D:359:PRO:HD2	2.53	0.44
3:D:1183:SER:HA	3:J:206:ASN:HD21	1.80	0.44
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.21	0.44
2:C:616:ILE:HG22	2:C:617:ALA:O	2.18	0.44
3:J:510:LEU:HD22	3:J:601:ILE:CD1	2.48	0.44
3:J:513:MET:HE3	3:J:579:LEU:HD22	1.99	0.44
5:L:476:ARG:HD2	5:L:477:GLU:H	1.83	0.44
2:I:178:PRO:HB3	2:I:395:TYR:CE2	2.53	0.44
3:D:53:ARG:HA	3:D:54:ASP:HA	1.72	0.44
3:D:26:SER:OG	3:D:28:ASP:N	2.50	0.44
5:L:139:GLU:CG	5:L:351:THR:HA	2.46	0.44
3:J:736:GLN:O	3:J:739:GLN:N	2.44	0.44
3:D:268:LEU:HD23	3:D:268:LEU:HA	1.66	0.44
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.83	0.44
1:A:219:ARG:O	1:A:223:ILE:HG13	2.17	0.44
5:L:363:ARG:O	5:L:367:ILE:HG13	2.17	0.44
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.98	0.44
3:D:469:HIS:O	3:D:471:PRO:HD3	2.18	0.44
2:C:895:LEU:HD11	2:C:900:LYS:HG3	1.99	0.44
1:G:185:TYR:HB2	1:G:201:LEU:HD11	1.99	0.44
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.99	0.44
2:C:708:VAL:CG1	2:C:794:LEU:HD22	2.47	0.44
1:G:75:GLN:HA	2:I:729:ALA:H	1.81	0.44
3:D:128:LEU:HA	3:D:192:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:710:ASP:CG	3:D:711:GLY:H	2.20	0.44
3:J:1167:LYS:NZ	3:J:1168:GLU:O	2.50	0.44
1:H:224:LEU:O	1:H:228:LEU:HG	2.17	0.44
2:I:617:ALA:HB3	2:I:653:MET:CB	2.48	0.44
1:G:14:VAL:HG22	1:G:15:ASP:N	2.33	0.44
3:D:827:GLU:CB	3:D:832:LYS:HD2	2.48	0.44
2:C:898:GLU:HB3	5:F:544:THR:HG21	1.99	0.44
3:J:761:ALA:N	3:J:771:GLN:HE22	2.15	0.44
2:C:742:TYR:HD2	2:C:743:PRO:HD2	1.82	0.44
5:F:227:GLN:CG	5:F:252:LEU:HA	2.48	0.44
4:E:62:GLN:O	4:E:66:VAL:HG23	2.16	0.44
3:D:94:GLN:HB2	3:D:96:LYS:HB2	1.99	0.44
1:B:192:VAL:O	1:B:195:ARG:N	2.50	0.44
2:C:1193:ALA:O	2:C:1197:GLU:HB2	2.18	0.44
5:F:484:ALA:C	5:F:491:GLU:HB2	2.38	0.44
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.18	0.44
3:D:81:ARG:C	3:D:83:VAL:H	2.20	0.44
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.99	0.44
2:I:1223:ARG:HD3	3:J:637:ALA:HA	1.98	0.44
2:I:157:PHE:CD1	2:I:174:ALA:HB2	2.53	0.44
3:J:161:THR:H	3:J:164:GLN:HB2	1.83	0.44
3:J:748:ALA:HA	3:J:754:ILE:HA	2.00	0.44
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.81	0.44
2:C:903:ARG:NE	2:C:910:ALA:HB2	2.32	0.44
3:D:442:ILE:HD13	3:D:442:ILE:HA	1.81	0.44
2:C:866:ASP:OD2	2:C:869:GLY:N	2.51	0.44
2:I:1122:LYS:NZ	2:I:1178:LYS:O	2.41	0.44
3:D:660:GLU:O	3:D:664:ILE:HG12	2.18	0.44
5:L:297:MET:HA	5:L:326:TRP:HB3	2.00	0.44
3:J:872:LEU:CD2	3:J:877:VAL:HG11	2.43	0.44
2:C:122:VAL:HG11	2:C:493:ILE:HG21	1.99	0.44
3:D:849:LEU:HB2	3:D:853:THR:HG23	1.99	0.44
2:C:960:LEU:O	2:C:963:GLU:HB2	2.18	0.44
3:J:47:ARG:HH12	5:L:500:ILE:HD11	1.82	0.44
1:H:179:PRO:HA	1:H:208:ASN:HD21	1.81	0.44
3:D:532:GLU:O	3:D:536:LEU:HB2	2.17	0.44
2:I:870:ILE:CG2	2:I:944:ARG:HD3	2.47	0.44
5:F:466:ILE:HG21	5:F:486:ARG:HG3	1.99	0.44
5:F:390:ILE:O	5:F:393:LYS:HB2	2.18	0.44
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.99	0.44
3:D:279:LEU:HD11	3:D:296:LYS:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1132:LEU:HD13	2:I:1177:ARG:HD2	2.00	0.44
2:C:494:ASN:HB3	2:C:497:PRO:CG	2.48	0.44
2:C:1043:ALA:O	2:C:1046:VAL:HG12	2.18	0.44
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.33	0.44
3:J:121:PRO:HG2	3:J:123:ARG:HH21	1.82	0.44
1:B:109:PRO:HA	1:B:132:HIS:HA	2.00	0.44
5:L:114:GLU:HG3	5:L:115:GLY:N	2.32	0.44
3:J:442:ILE:HA	3:J:442:ILE:HD13	1.80	0.44
2:C:1291:LEU:O	3:D:345:LYS:NZ	2.50	0.44
2:I:614:TYR:CD1	2:I:652:TYR:CE1	3.06	0.44
5:L:575:GLU:O	5:L:579:GLN:HG2	2.17	0.44
5:L:322:MET:HB3	5:L:324:LYS:HZ3	1.83	0.44
3:J:416:ILE:HD12	3:J:416:ILE:HA	1.70	0.44
5:L:226:ALA:O	5:L:230:VAL:HG12	2.18	0.44
3:D:847:ASP:CA	3:D:860:ARG:H	2.31	0.44
3:J:53:ARG:HA	3:J:54:ASP:HA	1.59	0.44
1:A:71:LYS:HB3	1:A:74:VAL:CG1	2.48	0.44
1:A:317:ARG:O	1:A:318:LEU:HD13	2.18	0.44
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.00	0.44
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.48	0.44
1:B:54:CYS:O	1:B:90:VAL:HB	2.18	0.44
2:I:867:GLU:H	2:I:867:GLU:HG3	1.61	0.44
3:J:238:ILE:HD13	3:J:238:ILE:HA	1.74	0.44
3:D:169:LEU:HA	3:D:169:LEU:HD23	1.82	0.44
2:C:484:LEU:HB2	2:C:485:ASP:H	1.62	0.44
2:C:61:SER:HB3	2:C:479:LEU:HB3	2.00	0.44
5:F:157:ARG:HB3	5:F:160:ASP:OD2	2.18	0.44
3:D:172:PHE:HB3	3:D:175:GLU:OE2	2.17	0.44
3:J:59:ALA:HA	3:J:63:GLY:O	2.18	0.44
3:D:678:ARG:HD3	3:D:682:VAL:CG2	2.48	0.43
1:H:115:ILE:HG22	1:H:116:THR:N	2.33	0.43
1:A:295:LEU:CD2	1:A:300:LEU:HB2	2.48	0.43
3:D:1159:ILE:HA	3:D:1206:ARG:HB3	2.00	0.43
3:J:858:VAL:HG11	3:J:872:LEU:HD21	2.00	0.43
2:I:600:THR:CG2	2:I:602:GLU:HG2	2.41	0.43
2:I:971:LEU:O	2:I:1014:LEU:HD23	2.18	0.43
2:C:198:ILE:O	2:C:201:ARG:HB2	2.18	0.43
2:C:593:LYS:HE3	2:C:595:THR:HG22	2.00	0.43
3:D:707:ILE:HD11	3:D:716:GLN:CG	2.46	0.43
4:K:39:VAL:HG21	4:K:56:GLU:HG3	2.00	0.43
1:H:86:LYS:HG2	1:H:173:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:476:ARG:HD2	5:L:477:GLU:HG2	2.00	0.43
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.99	0.43
3:J:298:MET:SD	5:L:406:GLN:HG3	2.58	0.43
1:A:319:GLU:OE2	1:A:319:GLU:HA	2.18	0.43
3:J:525:MET:O	3:J:548:VAL:HG13	2.18	0.43
3:D:772:TYR:O	3:D:775:SER:N	2.51	0.43
3:J:123:ARG:HD3	3:J:123:ARG:HA	1.91	0.43
3:J:68:TYR:CA	3:J:92:VAL:HG23	2.48	0.43
1:H:84:ASN:ND2	1:H:129:VAL:O	2.50	0.43
2:C:80:PHE:HB3	2:C:84:GLU:CB	2.48	0.43
1:B:9:LEU:HB3	1:B:32:GLU:HG2	1.99	0.43
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.33	0.43
3:D:660:GLU:HB3	3:D:685:ILE:CD1	2.23	0.43
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.99	0.43
5:L:316:PHE:HZ	5:L:334:SER:CA	2.22	0.43
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.48	0.43
3:D:1169:THR:CG2	3:D:1192:LYS:HD3	2.42	0.43
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.17	0.43
3:D:846:GLU:HA	3:D:860:ARG:HD3	2.00	0.43
1:B:57:THR:O	1:B:173:VAL:N	2.47	0.43
5:L:412:LEU:CD1	5:L:435:ILE:HD11	2.42	0.43
5:F:316:PHE:CZ	5:F:334:SER:HA	2.52	0.43
3:D:61:ILE:HB	3:D:62:PHE:CD2	2.53	0.43
2:I:466:VAL:O	2:I:469:VAL:HG22	2.17	0.43
5:L:276:MET:O	5:L:280:VAL:HG23	2.18	0.43
3:J:57:PHE:CZ	3:J:252:LEU:HB2	2.53	0.43
5:L:148:TYR:O	5:L:151:VAL:N	2.41	0.43
3:D:799:ARG:HD2	3:D:1146:GLU:OE1	2.17	0.43
2:I:158:ASP:CG	2:I:159:SER:H	2.21	0.43
2:I:1134:GLN:HB3	2:I:1136:GLN:HG2	2.01	0.43
5:L:115:GLY:HA2	5:L:118:ASP:HB2	2.00	0.43
3:D:919:ALA:CB	3:D:1255:VAL:HG21	2.47	0.43
2:I:188:PHE:CE1	2:I:194:LEU:HD13	2.53	0.43
2:C:1308:ILE:HD12	2:C:1308:ILE:HG23	1.72	0.43
5:L:166:VAL:HG23	5:L:258:GLN:HA	2.00	0.43
3:J:930:LEU:HD12	3:J:1138:LEU:HD13	1.99	0.43
3:D:316:ILE:HA	3:D:323:PRO:HA	2.00	0.43
2:I:987:GLU:HG2	2:I:991:LYS:HE3	2.00	0.43
5:L:292:VAL:HG21	5:L:299:LYS:HG3	2.00	0.43
2:C:490:GLN:HG3	5:F:472:GLN:HG3	1.99	0.43
3:J:69:GLU:HG3	3:J:76:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:80:HIS:ND1	3:D:80:HIS:N	2.66	0.43
2:I:151:ARG:NE	2:I:445:ILE:HD11	2.34	0.43
2:I:1308:ILE:HD12	3:J:380:PHE:CZ	2.52	0.43
1:H:125:LYS:HB3	1:H:125:LYS:HE2	1.77	0.43
2:C:15:PHE:HA	2:C:1155:VAL:HG11	2.01	0.43
3:D:93:THR:HG22	3:D:94:GLN:H	1.83	0.43
3:D:806:ASP:HA	3:D:1347:LEU:HD13	2.00	0.43
2:I:882:ILE:HG13	2:I:919:ARG:NH1	2.33	0.43
3:J:1165:PHE:HD2	3:J:1173:ARG:NE	2.15	0.43
2:C:218:GLU:HG3	2:C:299:LYS:HA	2.00	0.43
2:C:761:GLN:O	2:C:762:ASN:HB2	2.16	0.43
2:I:1083:GLU:HG3	2:I:1083:GLU:H	1.58	0.43
5:L:576:VAL:O	5:L:580:PHE:HB2	2.19	0.43
2:I:972:PHE:HD2	2:I:975:ILE:HD12	1.84	0.43
2:C:811:ASN:HD22	2:C:1098:LEU:C	2.21	0.43
2:I:600:THR:HG22	2:I:601:ASP:N	2.33	0.43
2:C:985:GLU:O	2:C:989:LEU:N	2.42	0.43
3:D:1171:GLY:O	3:D:1193:TRP:HZ3	2.02	0.43
3:D:395:LYS:HG2	5:F:536:THR:HG21	2.01	0.43
2:C:599:VAL:HG21	2:C:623:LEU:HD13	2.00	0.43
3:J:905:ARG:HH11	4:K:16:ARG:HB2	1.83	0.43
2:I:184:LEU:HD12	2:I:184:LEU:HA	1.64	0.43
2:C:987:GLU:HG2	2:C:991:LYS:CE	2.46	0.43
3:D:452:LEU:HA	3:D:452:LEU:HD23	1.84	0.43
4:K:19:LEU:CD1	4:K:54:ILE:HG21	2.48	0.43
3:J:511:TYR:CD2	3:J:728:SER:HB3	2.54	0.43
3:J:746:LEU:HD22	3:J:754:ILE:HD11	2.00	0.43
3:J:500:ILE:O	3:J:500:ILE:HG22	2.18	0.43
2:I:1340:GLU:CG	3:J:21:LYS:HB2	2.48	0.43
3:J:1138:LEU:HB3	3:J:1139:PRO:HD3	2.01	0.43
2:C:902:LEU:HD12	5:F:607:LEU:HD23	2.01	0.43
2:I:377:THR:HG22	2:I:379:GLU:OE2	2.19	0.43
2:C:848:GLU:CD	2:C:888:THR:HG22	2.37	0.43
2:I:1164:PHE:O	2:I:1166:ASP:N	2.51	0.43
2:I:1274:GLU:HA	3:J:428:THR:HG21	2.00	0.43
1:A:227:GLN:HA	1:A:227:GLN:OE1	2.17	0.43
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.19	0.43
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.49	0.43
3:J:79:LYS:HG3	3:J:80:HIS:ND1	2.34	0.43
3:J:128:LEU:HD23	3:J:192:MET:CE	2.47	0.43
1:B:152:TYR:CD1	1:B:176:CYS:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:707:ILE:HD11	3:D:716:GLN:CD	2.39	0.43
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	2.00	0.43
5:F:573:LEU:HD13	5:F:588:ARG:CZ	2.48	0.43
2:C:318:SER:O	2:C:322:LEU:HG	2.19	0.43
3:D:363:LEU:HG	3:D:363:LEU:O	2.17	0.43
2:C:462:ASN:O	2:C:466:VAL:HG23	2.18	0.43
3:D:1292:LEU:HA	3:J:1226:VAL:CG2	2.48	0.43
3:J:1319:PHE:HD1	3:J:1319:PHE:C	2.22	0.43
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.31	0.43
3:D:193:ASP:HB3	3:D:196:GLN:CG	2.48	0.43
2:C:1110:GLY:O	2:C:1114:GLU:HB2	2.19	0.43
5:L:213:ASP:HB2	5:L:216:LEU:HB3	1.99	0.43
3:J:899:TYR:CE1	3:J:1251:LYS:HD2	2.52	0.43
2:C:202:ARG:HH12	2:C:368:ARG:HH22	1.66	0.43
2:C:1010:GLN:O	2:C:1014:LEU:HD12	2.19	0.43
3:D:1355:ARG:NH2	3:D:1369:ARG:HH12	2.17	0.43
3:D:848:VAL:HG13	3:D:857:LEU:HD13	2.00	0.43
3:D:1171:GLY:C	3:D:1193:TRP:HZ3	2.21	0.43
3:J:46:TYR:CD1	5:L:500:ILE:HG21	2.41	0.43
3:J:1371:ARG:O	3:J:1371:ARG:HG2	2.16	0.43
3:J:768:ASN:HD21	3:J:770:LEU:HD23	1.84	0.43
5:L:449:THR:OG1	5:L:503:GLU:OE1	2.36	0.43
2:C:1282:GLY:HA3	4:E:17:PHE:HE1	1.82	0.43
3:J:698:MET:O	3:J:702:GLN:HB3	2.19	0.43
2:I:107:ARG:HA	2:I:108:GLU:HA	1.71	0.43
3:D:262:THR:OG1	3:D:263:SER:N	2.52	0.43
2:C:1268:GLN:HE22	3:D:352:ARG:CD	2.31	0.43
3:J:41:PRO:HG3	3:J:274:ASN:OD1	2.19	0.43
2:C:30:ILE:N	2:C:30:ILE:HD12	2.34	0.43
5:F:227:GLN:HG3	5:F:252:LEU:HA	2.00	0.43
2:I:14:ASP:N	2:I:1157:GLN:OE1	2.29	0.43
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.71	0.43
3:D:516:ASP:HA	3:D:545:HIS:HB2	2.00	0.43
2:I:617:ALA:HB3	2:I:653:MET:HB2	2.00	0.43
5:L:414:LYS:HD3	5:L:434:TRP:CZ3	2.51	0.43
2:C:211:ARG:HA	2:C:215:TYR:O	2.18	0.43
4:K:13:ILE:HD11	4:K:54:ILE:HG23	2.01	0.43
3:J:120:LEU:HB3	3:J:121:PRO:HD3	2.01	0.43
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	2.01	0.43
2:I:1204:LEU:HB3	2:I:1205:PRO:HD2	2.00	0.43
3:D:588:PRO:HB2	3:D:590:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:324:LYS:C	2:C:327:GLN:HE21	2.16	0.43
1:H:37:HIS:NE2	2:I:1216:ARG:HD2	2.34	0.43
3:D:1175:LEU:HD12	3:D:1175:LEU:HA	1.86	0.43
3:D:1184:ASP:N	3:D:1185:PRO:HD3	2.33	0.43
3:J:75:TYR:OH	3:J:86:GLU:OE2	2.35	0.43
2:I:974:ARG:HB3	2:I:1014:LEU:CD2	2.47	0.43
5:L:561:MET:HB2	5:L:561:MET:HE3	1.52	0.43
2:I:170:VAL:CG2	2:I:172:TYR:CZ	2.99	0.43
3:J:19:ALA:H	3:J:1344:LEU:HD12	1.84	0.43
3:J:592:VAL:HA	3:J:596:LEU:HD21	2.01	0.43
2:C:600:THR:HG21	2:C:602:GLU:HG2	2.00	0.43
3:D:825:VAL:HG22	3:D:833:GLU:N	2.32	0.43
5:L:414:LYS:O	5:L:417:ASP:N	2.51	0.43
3:J:528:THR:HG22	3:J:532:GLU:HB3	1.99	0.43
2:C:739:ASP:N	2:C:739:ASP:OD1	2.45	0.43
1:H:219:ARG:HA	1:H:222:THR:HB	2.01	0.43
2:I:470:ARG:HE	2:I:497:PRO:HB3	1.83	0.43
1:A:270:LEU:HD22	1:A:275:ILE:HG21	2.00	0.43
3:D:582:ILE:CD1	3:D:627:THR:HG21	2.49	0.43
3:D:1279:GLN:NE2	3:D:1317:GLU:OE2	2.52	0.43
2:I:805:MET:HE3	2:I:805:MET:HB2	1.74	0.43
2:C:738:GLU:HA	2:C:741:MET:CE	2.48	0.43
1:A:78:ILE:HA	1:A:81:ILE:HG13	2.00	0.43
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.99	0.43
1:H:8:PHE:HB2	1:H:10:LYS:NZ	2.33	0.43
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.51	0.43
5:L:96:ASP:OD2	5:L:98:VAL:HG13	2.19	0.43
1:A:66:HIS:O	1:A:66:HIS:ND1	2.49	0.43
1:A:166:ARG:O	1:A:167:PRO:C	2.52	0.43
1:G:61:ILE:HG23	1:G:142:MET:HB3	1.99	0.43
2:C:865:LEU:HD23	2:C:865:LEU:HA	1.86	0.43
5:L:343:LYS:HA	5:L:346:GLN:HB3	2.01	0.43
3:J:654:ILE:O	3:J:658:GLU:HB2	2.18	0.43
1:G:107:ILE:HG12	1:G:135:ASP:O	2.19	0.43
3:D:303:VAL:O	3:D:306:LEU:HB3	2.19	0.43
3:D:278:ARG:O	3:D:282:LEU:HG	2.19	0.43
2:I:1305:TYR:CG	5:L:531:PRO:HB2	2.53	0.43
3:D:797:THR:HG22	3:D:924:GLY:HA3	2.00	0.43
2:C:95:PRO:HA	2:C:126:GLU:HA	2.01	0.43
3:J:223:LEU:O	3:J:226:ALA:HB3	2.18	0.43
5:F:467:SER:O	5:F:471:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:616:ILE:HG13	2:I:652:TYR:HB2	2.00	0.43
2:I:171:LEU:HD23	2:I:171:LEU:HA	1.86	0.43
5:L:250:LEU:O	5:L:254:GLU:HG2	2.19	0.43
5:L:227:GLN:HG3	5:L:252:LEU:HA	2.00	0.43
5:L:141:ILE:HD13	5:L:256:PHE:CD1	2.54	0.43
5:L:397:ARG:HB3	5:L:443:ILE:HD13	2.00	0.43
5:F:139:GLU:HG2	5:F:351:THR:HA	2.01	0.43
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.54	0.43
2:I:1246:ARG:HD2	2:I:1265:PHE:O	2.19	0.43
3:D:681:LYS:O	3:D:685:ILE:HG23	2.19	0.43
2:C:1180:MET:HA	2:C:1181:PRO:HD3	1.76	0.43
3:D:309:ASN:OD1	3:D:314:ARG:HA	2.18	0.43
2:C:971:LEU:HG	2:C:1014:LEU:HD23	2.01	0.43
2:C:744:GLY:C	2:C:746:ALA:N	2.71	0.43
1:A:300:LEU:HD13	1:A:304:LYS:HE2	2.00	0.43
5:L:312:SER:OG	5:L:313:ASP:N	2.52	0.43
1:H:65:LEU:CD2	1:H:171:LEU:HD21	2.47	0.43
2:I:125:GLY:CA	2:I:499:SER:HB2	2.45	0.43
2:I:854:ILE:HD11	2:I:885:GLY:HA3	2.00	0.43
2:I:985:GLU:HG2	2:I:988:LYS:HD2	2.01	0.43
2:I:799:ASN:HA	2:I:1231:TYR:HA	2.01	0.43
3:D:749:LYS:HB2	3:D:750:PRO:HD2	2.01	0.43
3:J:545:HIS:CD2	3:J:719:PHE:HE1	2.37	0.43
2:C:250:THR:HA	2:C:268:ARG:HA	2.01	0.43
2:I:365:GLU:CD	2:I:368:ARG:HH21	2.22	0.43
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.43	0.43
3:D:762:ASN:OD1	3:D:765:GLU:HG3	2.19	0.43
3:J:404:GLU:HG2	3:J:409:TRP:CZ2	2.54	0.43
2:I:15:PHE:CD2	2:I:1190:ALA:HB2	2.54	0.43
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	2.00	0.42
3:D:1163:VAL:HG23	3:D:1177:ILE:HG23	2.01	0.42
3:D:847:ASP:CB	3:D:860:ARG:H	2.32	0.42
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.34	0.42
3:D:1199:PHE:HB2	3:D:1202:GLU:CB	2.46	0.42
3:D:84:ILE:H	3:D:84:ILE:HG13	1.67	0.42
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.54	0.42
3:J:1167:LYS:O	3:J:1168:GLU:HG2	2.18	0.42
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.60	0.42
3:D:872:LEU:HD22	3:D:877:VAL:HG11	2.01	0.42
3:J:825:VAL:HG11	3:J:833:GLU:HB3	2.00	0.42
3:D:1281:GLU:O	3:D:1285:VAL:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:PHE:HB2	2:C:457:GLY:O	2.19	0.42
2:C:69:GLN:HG2	2:C:101:ARG:O	2.19	0.42
2:C:1299:ASN:O	2:C:1303:LYS:HG2	2.20	0.42
2:C:819:SER:HB3	2:C:1085:MET:SD	2.59	0.42
2:I:17:LYS:HZ3	2:I:17:LYS:HG3	1.30	0.42
1:B:134:THR:HG23	1:B:135:ASP:N	2.34	0.42
1:G:31:LEU:HA	1:G:31:LEU:HD23	1.67	0.42
3:J:75:TYR:CD2	3:J:83:VAL:HG21	2.54	0.42
3:D:427:PRO:O	3:D:429:LEU:HD22	2.19	0.42
3:J:641:ILE:HD13	3:J:644:MET:CE	2.48	0.42
2:C:63:SER:C	2:C:65:ASN:H	2.21	0.42
2:I:734:ILE:O	2:I:748:ILE:HB	2.18	0.42
2:I:870:ILE:HG22	2:I:944:ARG:HH11	1.81	0.42
2:I:47:TYR:OH	2:I:398:SER:HB2	2.19	0.42
1:B:48:LEU:CD2	3:D:535:ARG:HG3	2.48	0.42
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.18	0.42
5:L:357:GLN:HA	5:L:360:ASP:HB2	2.01	0.42
3:J:901:ARG:HD2	3:J:906:GLY:O	2.19	0.42
3:D:1252:HIS:O	3:D:1255:VAL:HG22	2.20	0.42
3:J:620:PHE:CZ	3:J:624:ILE:HD11	2.54	0.42
2:I:315:MET:HB2	2:I:315:MET:HE3	1.92	0.42
1:G:18:GLN:HG3	1:G:24:ALA:HB2	2.02	0.42
3:J:742:GLY:O	3:J:762:ASN:HB3	2.19	0.42
3:D:198:CYS:HA	3:D:221:ILE:CD1	2.49	0.42
3:J:521:LYS:NZ	3:J:540:GLY:O	2.51	0.42
1:H:33:ARG:HD3	1:H:197:ASP:OD2	2.18	0.42
3:J:912:GLY:HA2	3:J:1363:TYR:CD1	2.53	0.42
5:L:338:HIS:HA	5:L:341:LEU:HB2	2.00	0.42
2:C:994:ARG:HD2	2:C:997:TRP:CH2	2.54	0.42
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.01	0.42
3:D:817:HIS:CE1	3:D:860:ARG:NH2	2.87	0.42
1:H:178:SER:HA	1:H:179:PRO:HD3	1.76	0.42
2:C:1290:MET:SD	2:C:1294:LYS:HE3	2.59	0.42
5:F:486:ARG:HG2	5:F:486:ARG:NH1	2.34	0.42
3:D:140:TYR:O	3:D:297:ARG:NH1	2.52	0.42
4:E:49:ILE:O	4:E:53:GLU:HG3	2.19	0.42
3:D:1301:THR:HG23	3:J:1301:THR:CG2	2.49	0.42
3:J:271:ARG:HB2	3:J:271:ARG:HE	1.40	0.42
2:C:301:TYR:CE2	2:C:333:ILE:HA	2.53	0.42
3:J:1175:LEU:HD12	3:J:1175:LEU:HA	1.84	0.42
5:L:280:VAL:HG21	5:L:358:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:810:THR:HG22	3:J:894:VAL:H	1.84	0.42
2:C:1002:LEU:HD23	2:C:1003:THR:O	2.19	0.42
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.34	0.42
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.55	0.42
3:J:382:TYR:CE1	3:J:398:LYS:HA	2.53	0.42
3:J:186:GLN:HG3	3:J:238:ILE:HB	2.02	0.42
3:D:193:ASP:CG	3:D:196:GLN:HG2	2.39	0.42
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.84	0.42
1:G:82:LEU:HD13	1:G:173:VAL:HG12	2.01	0.42
5:F:98:VAL:O	5:F:102:MET:HB2	2.18	0.42
3:D:519:ASN:HA	3:D:523:GLU:OE1	2.19	0.42
3:D:317:THR:CG2	3:D:320:ASN:HB3	2.40	0.42
2:I:976:ARG:CD	2:I:989:LEU:HD23	2.41	0.42
3:D:1183:SER:CB	3:D:1185:PRO:HD3	2.50	0.42
3:J:26:SER:O	3:J:30:ILE:HG13	2.19	0.42
2:C:972:PHE:HB3	2:C:994:ARG:HH21	1.81	0.42
2:C:1230:MET:HE3	2:C:1230:MET:HB2	1.91	0.42
3:D:128:LEU:HA	3:D:192:MET:CE	2.50	0.42
2:I:503:LYS:HD2	2:I:503:LYS:HA	1.60	0.42
3:D:98:ARG:O	3:D:248:ASP:HB2	2.19	0.42
3:J:809:VAL:HG12	3:J:911:LYS:HA	2.00	0.42
3:D:1301:THR:CG2	3:J:1301:THR:HG23	2.50	0.42
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.76	0.42
2:I:800:MET:HE3	2:I:800:MET:HB3	1.87	0.42
2:I:1304:MET:HE3	2:I:1308:ILE:HD11	2.01	0.42
3:J:168:ALA:O	3:J:172:PHE:HD2	2.03	0.42
2:I:1119:MET:HB2	2:I:1228:GLY:HA3	2.00	0.42
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.54	0.42
2:I:671:LEU:HD23	2:I:1186:VAL:HG11	2.02	0.42
5:L:220:LYS:O	5:L:223:GLU:HB3	2.20	0.42
2:C:404:LYS:HA	2:C:404:LYS:HD2	1.80	0.42
2:I:719:LYS:N	2:I:751:TYR:OH	2.52	0.42
1:B:87:GLY:O	1:B:128:HIS:NE2	2.52	0.42
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.33	0.42
2:I:1106:ARG:HB3	2:I:1108:ASN:ND2	2.34	0.42
1:G:222:THR:O	1:G:226:GLU:HB2	2.19	0.42
5:L:226:ALA:O	5:L:229:VAL:HG22	2.20	0.42
2:C:614:TYR:CE1	2:C:652:TYR:HE1	2.37	0.42
3:J:1273:ASP:HB3	3:J:1276:GLU:CD	2.40	0.42
4:K:26:ARG:NH2	4:K:38:LEU:HD13	2.34	0.42
3:D:811:GLU:O	3:D:895:CYS:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:175:ARG:HG3	2:I:185:ASP:OD1	2.19	0.42
3:J:735:ALA:O	3:J:738:ARG:HB3	2.19	0.42
3:D:872:LEU:O	3:D:877:VAL:HG12	2.19	0.42
3:J:894:VAL:HG22	3:J:1258:ARG:HH11	1.85	0.42
3:J:810:THR:HG23	3:J:811:GLU:N	2.35	0.42
1:H:60:GLU:OE2	1:H:143:ARG:HB2	2.19	0.42
3:J:537:TYR:OH	3:J:634:ARG:NH2	2.53	0.42
1:A:82:LEU:HB3	1:A:173:VAL:CG1	2.50	0.42
1:A:307:LEU:HA	1:A:307:LEU:HD12	1.78	0.42
2:I:845:LEU:H	2:I:845:LEU:HG	1.49	0.42
3:J:255:LEU:HA	3:J:255:LEU:HD13	1.85	0.42
3:D:253:VAL:HG21	5:F:523:ILE:HG21	2.01	0.42
3:D:42:GLU:HG2	3:D:52:GLU:HG2	2.00	0.42
1:B:154:PRO:HD2	1:B:157:THR:OG1	2.20	0.42
3:D:609:TYR:CE2	3:D:614:LEU:HD12	2.54	0.42
3:J:1181:ASP:OD1	3:J:1182:GLY:N	2.52	0.42
1:A:236:ASP:HA	1:B:14:VAL:HG13	2.01	0.42
2:C:202:ARG:HH11	2:C:369:MET:CB	2.31	0.42
2:I:1106:ARG:O	2:I:1108:ASN:N	2.44	0.42
2:C:1142:ARG:HH12	2:C:1169:VAL:HG21	1.83	0.42
1:B:196:THR:HG22	1:B:197:ASP:N	2.35	0.42
2:C:98:VAL:HB	2:C:124:MET:HE3	2.00	0.42
1:A:150:ARG:HH11	1:B:6:THR:N	2.18	0.42
3:J:364:HIS:CG	4:K:4:VAL:HG23	2.55	0.42
1:G:224:LEU:HD22	1:H:228:LEU:CD1	2.49	0.42
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.20	0.42
2:C:885:GLY:HA2	2:C:917:SER:HB3	2.02	0.42
2:C:138:ILE:HG22	2:C:139:ASN:N	2.35	0.42
2:C:557:ARG:NH2	2:C:608:ALA:HA	2.34	0.42
1:A:61:ILE:HB	1:A:64:VAL:HG23	1.99	0.42
3:J:885:VAL:HG22	3:J:885:VAL:H	1.49	0.42
1:G:58:GLU:CD	1:G:145:LYS:HE3	2.39	0.42
2:I:812:PHE:HZ	3:J:503:SER:CB	2.32	0.42
1:A:315:GLY:C	1:A:316:MET:HG3	2.39	0.42
3:J:126:LEU:HD13	3:J:223:LEU:CD2	2.50	0.42
2:C:168:GLY:O	2:C:170:VAL:N	2.34	0.42
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.54	0.42
3:J:863:LEU:HD11	3:J:901:ARG:HD3	2.01	0.42
2:I:147:SER:HB2	2:I:529:ARG:O	2.20	0.42
2:I:127:ILE:HA	2:I:128:PRO:HD3	1.71	0.42
3:D:641:ILE:HD13	3:D:644:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:O	1:A:183:ILE:HD12	2.20	0.42
2:C:960:LEU:HD13	2:C:960:LEU:HA	1.75	0.42
3:J:64:PRO:HB3	3:J:69:GLU:O	2.20	0.42
1:A:61:ILE:HG22	1:A:62:ASP:N	2.34	0.42
2:C:317:LEU:HD11	2:C:333:ILE:HG21	2.02	0.42
1:H:48:LEU:HG	1:H:183:ILE:HD11	2.01	0.42
5:L:112:THR:O	5:L:116:GLU:HG3	2.19	0.42
5:F:479:THR:HG22	5:F:482:GLU:HB2	2.01	0.42
3:D:689:ALA:O	3:D:692:ARG:HB2	2.19	0.42
2:I:672:GLU:HG3	2:I:672:GLU:H	1.27	0.42
2:I:673:HIS:HB3	2:I:1109:ILE:CG2	2.49	0.42
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.87	0.42
5:L:399:LEU:HG	5:L:403:ASP:HB3	2.02	0.42
2:I:23:ASP:N	2:I:23:ASP:OD1	2.38	0.42
2:C:1217:THR:OG1	2:C:1219:GLU:HG2	2.19	0.42
1:H:153:VAL:HA	1:H:154:PRO:HD3	1.91	0.42
2:I:697:LYS:HA	2:I:795:ALA:HB2	2.02	0.42
3:D:148:GLU:H	3:D:156:ARG:HG3	1.84	0.42
2:C:1191:LYS:HD3	2:C:1193:ALA:N	2.30	0.42
2:C:1149:TYR:CB	2:C:1159:VAL:HG21	2.49	0.42
5:L:292:VAL:HA	5:L:297:MET:O	2.19	0.42
2:C:39:ILE:O	2:C:40:GLU:HB2	2.20	0.42
3:J:30:ILE:CG2	3:J:243:PRO:HG3	2.50	0.42
2:I:718:ALA:HB2	2:I:783:LEU:CD2	2.50	0.42
3:D:710:ASP:CG	3:D:711:GLY:N	2.73	0.42
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	2.01	0.42
2:I:395:TYR:HE2	2:I:397:LEU:CD1	2.32	0.42
2:I:856:ASN:CB	5:L:613:ASP:HA	2.50	0.42
2:C:150:HIS:CD2	2:C:150:HIS:N	2.87	0.42
3:J:521:LYS:HD2	3:J:541:LEU:O	2.18	0.42
5:L:448:ARG:HE	5:L:448:ARG:HB3	1.51	0.42
5:F:111:LEU:HD23	5:F:111:LEU:HA	1.77	0.42
3:D:372:MET:O	3:D:376:LEU:HD12	2.20	0.42
5:F:253:SER:O	5:F:257:LYS:HG3	2.20	0.42
2:I:943:LYS:O	2:I:947:GLU:HG3	2.20	0.42
2:I:210:LEU:HB2	2:I:220:ILE:HD11	2.02	0.42
2:C:88:ARG:HB3	2:C:90:VAL:HG23	2.01	0.42
5:F:117:ILE:HA	5:F:120:ALA:HB3	2.00	0.42
2:I:830:THR:HG23	2:I:832:HIS:NE2	2.35	0.42
1:G:40:GLY:HA2	1:G:201:LEU:HD21	2.02	0.42
3:D:903:LEU:HB3	3:D:905:ARG:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:835:LEU:HG	3:J:839:VAL:CG2	2.49	0.42
3:J:857:LEU:HD12	3:J:858:VAL:H	1.84	0.42
2:I:971:LEU:HG	2:I:1014:LEU:HD23	2.01	0.42
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.48	0.42
2:C:615:VAL:HG22	2:C:650:VAL:HA	2.01	0.42
3:D:510:LEU:HD22	3:D:601:ILE:HD11	2.02	0.42
5:F:414:LYS:HD3	5:F:434:TRP:CZ3	2.55	0.42
5:F:499:LYS:HA	5:F:502:LYS:HE2	2.00	0.42
5:F:463:LEU:HA	5:F:463:LEU:HD23	1.70	0.42
3:D:63:GLY:HA3	3:D:98:ARG:HG3	2.01	0.42
3:D:718:SER:OG	3:D:720:ASN:HB3	2.20	0.42
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.54	0.42
3:J:885:VAL:HG12	3:J:894:VAL:CG1	2.50	0.42
3:D:278:ARG:HH11	3:D:295:GLU:CD	2.23	0.42
3:J:701:LEU:HD12	3:J:723:TYR:HD2	1.85	0.42
3:J:1173:ARG:HH21	3:J:1196:LEU:HD21	1.85	0.42
2:C:819:SER:HB2	2:C:1085:MET:HG3	2.02	0.42
5:F:448:ARG:HE	5:F:448:ARG:HB3	1.70	0.42
3:J:423:LEU:HB3	3:J:466:MET:CE	2.50	0.42
1:G:153:VAL:HB	1:G:175:ALA:HB3	2.02	0.42
2:I:421:SER:H	2:I:424:ASP:HB2	1.85	0.42
2:C:48:GLY:H	2:C:51:ALA:HB3	1.84	0.42
3:J:422:LEU:O	3:J:468:VAL:HA	2.19	0.42
3:D:1162:ILE:HD12	3:D:1163:VAL:H	1.85	0.42
3:D:823:THR:HA	3:D:835:LEU:HD13	2.02	0.42
1:G:115:ILE:HG22	1:G:116:THR:N	2.35	0.42
3:D:915:ILE:HA	3:D:918:ILE:HG23	2.01	0.42
1:H:47:LEU:O	1:H:180:VAL:HG21	2.20	0.42
3:J:800:LEU:O	3:J:803:VAL:HG12	2.19	0.42
3:J:54:ASP:HB3	3:J:60:ARG:HH11	1.85	0.42
5:L:418:LYS:HD2	5:L:434:TRP:CH2	2.55	0.42
2:I:1225:VAL:HA	3:J:638:SER:CB	2.50	0.42
2:I:98:VAL:O	2:I:121:GLU:HA	2.20	0.42
3:D:690:ASN:ND2	3:D:745:GLY:HA2	2.34	0.42
4:K:54:ILE:HA	4:K:59:ILE:O	2.20	0.42
1:A:46:ILE:CG2	1:A:223:ILE:HD12	2.50	0.42
2:C:1164:PHE:C	2:C:1166:ASP:H	2.23	0.42
3:J:537:TYR:CE2	3:J:544:LEU:HD22	2.54	0.42
3:J:116:PHE:O	3:J:123:ARG:HB2	2.20	0.42
2:I:1134:GLN:NE2	2:I:1136:GLN:OE1	2.53	0.42
2:I:836:LEU:HD21	2:I:921:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:42:ASP:HA	2:I:43:PRO:HD3	1.90	0.42
2:C:622:ASN:O	2:C:630:VAL:HB	2.20	0.42
1:A:231:PHE:HE1	1:B:28:LEU:HD23	1.85	0.41
1:H:10:LYS:HA	1:H:11:PRO:HD3	1.82	0.41
2:C:202:ARG:NH1	2:C:369:MET:HB2	2.35	0.41
3:D:358:GLY:N	3:D:359:PRO:HD3	2.35	0.41
3:J:641:ILE:HD13	3:J:644:MET:HE3	2.01	0.41
2:I:170:VAL:HG21	2:I:172:TYR:OH	2.19	0.41
2:C:1256:GLN:HB3	2:C:1301:ARG:NH2	2.28	0.41
2:C:1111:GLN:HB2	2:C:1230:MET:CE	2.50	0.41
1:A:73:GLY:C	1:A:134:THR:HG22	2.41	0.41
2:I:898:GLU:HB3	5:L:540:LEU:CD2	2.45	0.41
2:I:1121:ALA:HB2	2:I:1182:ILE:CD1	2.49	0.41
2:I:397:LEU:O	2:I:398:SER:OG	2.22	0.41
3:J:419:HIS:HA	3:J:420:PRO:HD3	1.73	0.41
3:D:1140:ARG:NH2	3:D:1236:GLU:HG2	2.33	0.41
3:J:810:THR:CG2	3:J:893:GLY:HA3	2.50	0.41
2:C:6:THR:HG21	2:C:782:VAL:HG23	2.01	0.41
5:F:313:ASP:CG	5:F:338:HIS:HE2	2.23	0.41
2:I:525:THR:HG21	2:I:687:ARG:CD	2.50	0.41
5:L:117:ILE:HG23	5:L:421:TYR:CE1	2.55	0.41
5:F:504:PRO:C	5:F:505:ILE:HD12	2.40	0.41
3:J:1250:ASP:O	3:J:1251:LYS:C	2.58	0.41
2:I:1276:TRP:HA	2:I:1279:GLU:OE1	2.19	0.41
4:K:21:LEU:HD12	4:K:21:LEU:HA	1.66	0.41
2:I:62:TYR:O	2:I:64:GLY:N	2.53	0.41
3:J:88:CYS:O	3:J:90:VAL:N	2.53	0.41
3:D:658:GLU:O	3:D:661:VAL:HG22	2.19	0.41
1:H:73:GLY:HA2	1:H:134:THR:CG2	2.36	0.41
2:C:1192:GLU:O	2:C:1195:ILE:HB	2.20	0.41
3:J:85:CYS:SG	3:J:86:GLU:N	2.93	0.41
2:C:1281:TYR:CD2	3:D:431:ARG:HB2	2.55	0.41
1:A:98:VAL:HG22	1:A:100:LEU:HD12	2.02	0.41
3:J:491:LEU:HD23	3:J:498:PRO:HA	2.00	0.41
5:F:470:MET:O	5:F:478:PRO:HD3	2.20	0.41
3:J:64:PRO:O	3:J:95:THR:OG1	2.33	0.41
2:I:718:ALA:HB2	2:I:783:LEU:HD23	2.01	0.41
5:L:380:VAL:HG13	5:L:412:LEU:HD23	2.02	0.41
2:I:670:PHE:CD1	2:I:1184:THR:HG21	2.55	0.41
2:C:1107:MET:HG2	3:D:740:LEU:HD11	2.02	0.41
3:D:885:VAL:HG12	3:D:894:VAL:CG1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:698:PRO:HA	2:I:1231:TYR:CE1	2.54	0.41
3:J:810:THR:HG21	3:J:893:GLY:HA3	2.02	0.41
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.85	0.41
2:C:494:ASN:HB3	2:C:497:PRO:CD	2.50	0.41
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.85	0.41
5:L:165:PHE:HE1	5:L:259:PHE:CD2	2.37	0.41
2:C:455:SER:HA	2:C:459:MET:HE2	2.02	0.41
1:A:27:THR:O	1:A:28:LEU:HD12	2.20	0.41
2:I:202:ARG:HG3	2:I:202:ARG:H	1.73	0.41
2:C:632:ASP:HB2	2:C:633:LEU:HD23	2.02	0.41
2:I:920:VAL:HG13	2:I:921:PRO:HD2	2.01	0.41
3:D:712:GLN:HG2	3:D:712:GLN:H	1.51	0.41
2:C:360:LEU:HD22	2:C:378:ARG:HH21	1.86	0.41
3:J:72:CYS:HB3	3:J:88:CYS:SG	2.60	0.41
1:B:211:ILE:HD12	1:B:211:ILE:HA	1.87	0.41
5:F:161:LEU:C	5:F:262:VAL:HG23	2.41	0.41
2:I:820:GLU:N	2:I:1080:ASN:O	2.53	0.41
1:G:189:ALA:HB1	1:G:191:ARG:NH2	2.35	0.41
1:A:92:VAL:HA	1:A:120:ASP:O	2.21	0.41
2:I:971:LEU:HD11	2:I:1014:LEU:O	2.19	0.41
2:I:971:LEU:HD22	2:I:1018:TYR:HB2	2.02	0.41
1:G:44:ARG:HG3	1:G:183:ILE:CG2	2.45	0.41
3:D:382:TYR:CE1	3:D:398:LYS:HA	2.55	0.41
2:C:593:LYS:HA	2:C:652:TYR:CD2	2.55	0.41
5:F:320:ILE:O	5:F:327:SER:HB3	2.21	0.41
3:D:591:ILE:HD12	3:D:591:ILE:HA	1.83	0.41
1:A:8:PHE:HE1	1:A:32:GLU:OE1	2.04	0.41
1:A:36:GLY:C	1:A:187:VAL:HG11	2.40	0.41
2:I:395:TYR:HE2	2:I:397:LEU:HD12	1.84	0.41
3:J:515:ARG:NH2	3:J:717:VAL:HG23	2.34	0.41
3:J:1162:ILE:HD12	3:J:1163:VAL:N	2.35	0.41
3:J:293:ARG:O	3:J:294:ASN:C	2.57	0.41
3:D:278:ARG:O	3:D:278:ARG:HG2	2.20	0.41
3:J:587:LEU:HD23	3:J:591:ILE:HG21	2.02	0.41
3:D:1366:HIS:O	3:D:1370:MET:HB2	2.20	0.41
2:C:848:GLU:HG2	2:C:888:THR:HG22	2.02	0.41
2:I:15:PHE:CE1	2:I:1194:GLU:HB3	2.56	0.41
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.70	0.41
2:I:237:LEU:HA	2:I:237:LEU:HD13	1.72	0.41
2:C:671:LEU:HD23	2:C:1186:VAL:CG1	2.50	0.41
5:L:271:ASN:O	5:L:275:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:HA	1:A:24:ALA:CB	2.49	0.41
1:G:190:ALA:HA	1:G:200:LYS:HE2	2.02	0.41
2:I:696:ASP:HB3	2:I:697:LYS:H	1.65	0.41
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.83	0.41
2:I:550:VAL:CG1	3:J:777:HIS:HA	2.50	0.41
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.54	0.41
3:J:1356:LEU:O	3:J:1366:HIS:CE1	2.73	0.41
5:F:344:LEU:O	5:F:355:ILE:HD11	2.19	0.41
2:I:1256:GLN:HB3	2:I:1301:ARG:NH2	2.33	0.41
3:D:701:LEU:HD12	3:D:723:TYR:CD2	2.51	0.41
3:D:723:TYR:CE1	3:D:727:ASP:HB2	2.55	0.41
2:C:896:THR:HB	2:C:897:PRO:HD2	2.02	0.41
5:L:381:GLU:O	5:L:384:LEU:HG	2.20	0.41
2:I:571:LEU:HD23	2:I:571:LEU:HA	1.62	0.41
3:D:646:ILE:HG12	3:D:646:ILE:H	1.58	0.41
3:J:796:LEU:HA	3:J:796:LEU:HD12	1.64	0.41
5:L:157:ARG:HB3	5:L:160:ASP:OD2	2.19	0.41
2:C:658:GLN:O	2:C:660:VAL:N	2.54	0.41
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.02	0.41
1:A:97:GLU:HA	1:A:146:VAL:O	2.19	0.41
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.84	0.41
2:C:12:ARG:NE	2:C:793:GLU:OE1	2.39	0.41
3:D:654:ILE:O	3:D:658:GLU:N	2.49	0.41
1:H:134:THR:HG23	1:H:135:ASP:N	2.34	0.41
1:A:92:VAL:HG11	1:A:98:VAL:HG11	2.03	0.41
2:I:629:PHE:CE2	2:I:634:VAL:HG11	2.55	0.41
1:G:102:LEU:HD23	1:G:115:ILE:CG1	2.45	0.41
2:I:1043:ALA:O	2:I:1046:VAL:HG12	2.21	0.41
4:K:44:ASP:HB2	4:K:49:ILE:HG13	2.01	0.41
2:C:549:ASP:OD1	3:D:750:PRO:HB3	2.20	0.41
3:D:832:LYS:NZ	3:D:1243:LEU:HD12	2.35	0.41
3:J:616:PRO:HA	3:J:619:ILE:HG22	2.03	0.41
5:F:388:ILE:O	5:F:392:LYS:HG3	2.21	0.41
2:I:49:LEU:HB2	2:I:73:TYR:CZ	2.56	0.41
2:C:850:ILE:O	2:C:850:ILE:HG22	2.21	0.41
3:J:825:VAL:HG13	3:J:833:GLU:HB3	2.02	0.41
3:J:116:PHE:O	3:J:124:ILE:HG13	2.20	0.41
5:L:551:LEU:HD23	5:L:597:LYS:HD2	2.03	0.41
2:I:1299:ASN:ND2	2:I:1303:LYS:HE2	2.36	0.41
2:C:980:VAL:HG13	2:C:984:VAL:HB	2.02	0.41
2:I:836:LEU:HD11	2:I:1054:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:848:GLU:CG	2:C:888:THR:HG22	2.50	0.41
2:C:208:ILE:HD11	2:C:365:GLU:HG2	2.02	0.41
1:B:51:MET:HB3	1:B:178:SER:HB2	2.01	0.41
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	2.02	0.41
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	2.02	0.41
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.55	0.41
1:A:22:THR:O	1:A:207:THR:N	2.37	0.41
3:J:138:VAL:HG21	3:J:145:VAL:HB	2.02	0.41
5:F:124:GLU:O	5:F:128:ASN:HB2	2.21	0.41
3:D:526:VAL:HG12	3:D:549:LYS:HB2	2.02	0.41
5:F:583:THR:HG22	5:F:584:ARG:N	2.35	0.41
3:J:678:ARG:O	3:J:682:VAL:HG23	2.20	0.41
1:A:295:LEU:HD22	1:A:300:LEU:HB2	2.02	0.41
3:J:860:ARG:HD2	3:J:860:ARG:HA	1.89	0.41
1:A:54:CYS:HB3	1:A:148:ARG:HD3	2.02	0.41
3:J:133:ARG:HA	3:J:133:ARG:HD2	1.86	0.41
5:F:281:ARG:HH11	5:F:281:ARG:HD2	1.71	0.41
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.03	0.41
2:I:209:ILE:HD13	2:I:209:ILE:HG21	1.84	0.41
3:D:368:LEU:CD2	3:D:373:ALA:HB2	2.48	0.41
1:G:57:THR:OG1	1:G:147:GLN:HG2	2.20	0.41
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	2.01	0.41
1:B:98:VAL:HG11	1:B:121:VAL:HG22	2.03	0.41
1:B:108:GLY:HA2	1:B:109:PRO:HD3	1.83	0.41
2:I:1062:PRO:HA	2:I:1076:ILE:O	2.19	0.41
5:F:519:LEU:C	5:F:519:LEU:HD23	2.41	0.41
2:C:520:PRO:HG3	2:C:714:VAL:HG11	2.02	0.41
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.94	0.41
2:I:62:TYR:C	2:I:64:GLY:N	2.74	0.41
2:C:921:PRO:HB2	2:C:924:VAL:HG22	2.03	0.41
5:F:611:LEU:HD23	5:F:611:LEU:HA	1.78	0.41
1:A:56:VAL:CG2	1:A:144:ILE:HG23	2.51	0.41
2:C:626:GLU:HB2	2:C:628:HIS:CE1	2.56	0.41
1:G:49:SER:HB3	2:I:1083:GLU:OE2	2.21	0.41
3:D:1178:THR:HA	3:D:1179:PRO:HD3	1.75	0.41
3:D:19:ALA:HB2	3:D:1373:ARG:NH2	2.36	0.41
3:J:395:LYS:CG	5:L:536:THR:HG21	2.45	0.41
2:I:1192:GLU:OE2	3:J:764:ARG:HD3	2.19	0.41
3:J:903:LEU:CD2	3:J:909:ILE:HD12	2.51	0.41
5:F:310:GLU:O	5:F:344:LEU:HD21	2.21	0.41
2:I:1065:LYS:CD	2:I:1235:LEU:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:421:SER:H	2:C:424:ASP:CB	2.33	0.41
5:L:607:LEU:O	5:L:610:PHE:HB2	2.21	0.41
2:I:1323:PHE:CE1	2:I:1327:LEU:HD11	2.56	0.41
2:C:906:PHE:HE2	5:F:608:ARG:NH1	2.19	0.41
3:D:1345:ARG:HG2	3:D:1370:MET:CE	2.51	0.41
1:H:203:ILE:HD12	1:H:203:ILE:N	2.36	0.41
2:C:136:PHE:HE2	2:C:456:VAL:HG11	1.85	0.41
1:A:18:GLN:HA	1:A:24:ALA:HB2	2.03	0.41
2:I:511:LEU:HA	2:I:511:LEU:HD23	1.77	0.41
3:D:1266:ILE:HD12	3:D:1274:PHE:N	2.36	0.41
2:C:297:VAL:HG12	2:C:315:MET:O	2.20	0.41
2:I:385:PHE:CE2	2:I:390:PHE:HE2	2.38	0.41
1:A:260:LEU:HB2	1:A:262:LEU:HG	2.02	0.41
1:B:15:ASP:O	1:B:27:THR:HG23	2.21	0.41
3:D:884:SER:OG	3:D:886:VAL:HG12	2.21	0.41
2:I:95:PRO:HB3	2:I:123:TYR:HE1	1.85	0.41
1:G:50:SER:HB3	1:H:8:PHE:CZ	2.56	0.41
1:G:31:LEU:HB2	1:G:199:ASP:O	2.21	0.41
2:C:1281:TYR:CD2	2:C:1281:TYR:N	2.88	0.41
1:A:102:LEU:O	1:A:141:SER:HA	2.20	0.41
5:L:315:TRP:O	5:L:319:ALA:HB3	2.21	0.41
2:C:594:VAL:HG22	2:C:599:VAL:HG22	2.03	0.41
2:I:745:GLU:N	2:I:1017:GLN:HG3	2.35	0.41
2:C:224:PHE:CD2	2:C:347:ILE:HG21	2.56	0.41
2:C:1288:GLN:O	2:C:1292:THR:HB	2.20	0.41
1:A:321:TRP:CE2	1:A:322:PRO:HB3	2.56	0.41
2:I:487:LEU:HD23	2:I:487:LEU:H	1.85	0.41
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.55	0.41
3:D:555:TYR:HB3	3:D:563:LEU:HD23	2.02	0.41
5:F:474:MET:O	5:F:476:ARG:N	2.48	0.41
1:A:216:ALA:O	1:A:218:ARG:N	2.54	0.41
1:A:173:VAL:HG23	1:A:174:ASP:O	2.21	0.41
1:G:51:MET:HB3	1:G:51:MET:HE3	1.93	0.41
2:I:1274:GLU:HG3	3:J:428:THR:OG1	2.19	0.41
3:D:441:LEU:HA	3:D:441:LEU:HD13	1.83	0.41
2:C:59:ILE:HG21	2:C:59:ILE:HD13	1.75	0.41
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.75	0.41
2:I:230:PHE:CE1	2:I:239:MET:HB2	2.56	0.41
3:J:335:GLN:CB	3:J:336:GLY:HA3	2.51	0.41
2:I:211:ARG:NE	2:I:354:ASP:OD2	2.35	0.41
3:D:1337:VAL:HG23	3:D:1338:ALA:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:LEU:HD11	1:H:121:VAL:CG2	2.50	0.41
1:H:95:LYS:HZ3	1:H:98:VAL:HG23	1.84	0.41
5:L:291:CYS:HB3	5:L:297:MET:SD	2.61	0.41
5:L:96:ASP:O	5:L:98:VAL:N	2.54	0.41
3:J:1372:ARG:HE	3:J:1372:ARG:HB2	1.64	0.41
2:I:161:LYS:HA	2:I:170:VAL:HA	2.03	0.41
4:K:15:ASN:O	4:K:16:ARG:HB3	2.21	0.41
3:J:805:GLN:HB3	3:J:806:ASP:H	1.73	0.41
3:D:601:ILE:HG21	3:D:601:ILE:HD13	1.78	0.41
3:D:840:LEU:HD12	3:D:864:LEU:O	2.20	0.41
5:F:483:LEU:N	5:F:483:LEU:HD12	2.34	0.41
5:L:573:LEU:CD1	5:L:588:ARG:HE	2.33	0.41
2:I:590:PRO:HG3	2:I:605:TYR:CE1	2.55	0.41
3:J:1174:ARG:HG2	3:J:1189:MET:CG	2.51	0.41
2:C:1250:SER:HB3	2:C:1259:LEU:O	2.21	0.41
1:G:39:LEU:CD2	1:H:224:LEU:HD11	2.51	0.41
2:I:519:ASN:HB3	2:I:522:SER:CB	2.51	0.41
3:J:527:LEU:HB3	3:J:532:GLU:CG	2.51	0.41
2:C:62:TYR:HE1	2:C:476:LYS:O	2.03	0.41
5:L:138:PRO:HB2	5:L:351:THR:O	2.20	0.41
3:J:294:ASN:O	3:J:298:MET:HG3	2.21	0.41
1:A:318:LEU:HD22	1:A:318:LEU:N	2.36	0.41
3:J:357:VAL:HB	3:J:358:GLY:H	1.75	0.41
3:J:722:ILE:HD11	3:J:740:LEU:HD23	2.01	0.41
3:J:156:ARG:NH1	3:J:157:GLN:NE2	2.69	0.41
2:C:420:LEU:HD23	2:C:420:LEU:HA	1.76	0.41
2:C:395:TYR:CE2	2:C:420:LEU:HG	2.56	0.41
1:A:155:ALA:H	1:A:174:ASP:HA	1.86	0.41
3:J:504:GLN:HG3	3:J:505:ASP:H	1.86	0.41
1:B:192:VAL:O	1:B:194:GLN:N	2.53	0.41
2:C:852:ALA:HB2	2:C:869:GLY:CA	2.51	0.41
5:L:166:VAL:HG23	5:L:258:GLN:O	2.21	0.41
3:D:1347:LEU:O	3:D:1348:LYS:C	2.59	0.41
5:L:227:GLN:CG	5:L:252:LEU:HA	2.50	0.41
2:I:207:THR:HG21	2:I:351:LEU:HG	2.02	0.41
3:J:331:ILE:HD13	3:J:331:ILE:HG21	1.76	0.41
1:A:208:ASN:OD1	1:A:208:ASN:N	2.53	0.41
3:J:842:ARG:HB3	3:J:882:VAL:HG11	2.02	0.41
2:C:757:THR:O	2:C:765:ILE:HG23	2.21	0.41
1:G:178:SER:HA	1:G:179:PRO:HD3	1.91	0.41
1:B:38:THR:HG23	1:B:39:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:369:MET:O	2:C:372:PRO:HD3	2.21	0.41
3:D:339:ARG:O	3:D:340:GLN:HG2	2.20	0.41
2:I:974:ARG:HD2	2:I:1014:LEU:CD2	2.51	0.41
3:J:234:PRO:HD2	3:J:235:GLU:OE2	2.21	0.41
1:A:134:THR:HG21	2:C:727:VAL:O	2.21	0.41
1:A:165:GLU:OE1	1:A:172:LEU:HD21	2.21	0.41
5:L:463:LEU:HA	5:L:463:LEU:HD23	1.73	0.41
5:F:95:THR:O	5:F:96:ASP:C	2.59	0.41
1:B:48:LEU:CD1	1:B:183:ILE:HD11	2.50	0.41
3:D:53:ARG:NH2	3:D:60:ARG:HD2	2.36	0.41
1:G:134:THR:HG23	1:G:135:ASP:N	2.36	0.41
3:D:307:LEU:HA	3:D:307:LEU:HD23	1.81	0.41
5:F:465:ARG:HB3	5:F:468:ARG:HH12	1.86	0.41
2:I:569:ILE:C	2:I:571:LEU:H	2.23	0.41
2:C:666:SER:OG	2:C:704:MET:HG3	2.21	0.41
3:D:501:VAL:HG22	3:D:502:PRO:O	2.21	0.41
2:I:405:PHE:CE2	2:I:409:LEU:HD12	2.56	0.41
3:J:440:VAL:O	3:J:442:ILE:HG12	2.21	0.41
2:I:211:ARG:NH2	2:I:351:LEU:HD22	2.36	0.41
3:J:369:PRO:HB3	3:J:444:GLY:O	2.20	0.41
2:I:996:ARG:HA	2:I:996:ARG:HD3	1.95	0.41
1:A:107:ILE:H	1:A:107:ILE:HG13	1.71	0.41
2:C:22:LEU:HD22	2:C:23:ASP:N	2.36	0.41
3:D:664:ILE:HG22	3:D:678:ARG:HG2	2.02	0.40
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.21	0.40
3:D:97:VAL:HG11	3:D:101:ARG:CZ	2.52	0.40
3:J:233:LYS:HA	3:J:234:PRO:HD3	1.96	0.40
1:A:182:ARG:HG2	1:A:183:ILE:N	2.36	0.40
2:C:886:LYS:NZ	2:C:916:SER:HB3	2.36	0.40
2:I:559:CYS:CB	2:I:662:SER:HB3	2.50	0.40
2:I:663:VAL:H	2:I:663:VAL:HG22	1.51	0.40
5:L:409:ASN:O	5:L:413:MET:HG3	2.22	0.40
3:J:481:ARG:O	3:J:485:MET:HB2	2.20	0.40
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.36	0.40
2:I:197:ARG:HH12	2:I:203:LYS:HB2	1.86	0.40
1:B:133:LEU:HD11	1:B:140:ILE:HG21	2.03	0.40
1:H:6:THR:O	1:H:6:THR:HG22	2.21	0.40
3:D:277:ASN:HA	3:D:280:LYS:HG3	2.03	0.40
2:C:80:PHE:HB3	2:C:84:GLU:HB2	2.03	0.40
2:C:1303:LYS:HD3	2:C:1303:LYS:HA	1.78	0.40
3:D:113:HIS:ND1	3:D:113:HIS:C	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:VAL:HG22	1:G:203:ILE:HB	2.04	0.40
2:I:1309:VAL:HA	3:J:383:GLY:HA3	2.03	0.40
2:I:402:ARG:HG2	2:I:416:GLY:H	1.86	0.40
3:D:611:ILE:HG22	3:D:612:LEU:HD12	2.03	0.40
3:D:489:ASN:HA	3:D:904:ALA:HB1	2.03	0.40
1:G:45:ARG:CG	1:H:38:THR:HB	2.36	0.40
2:C:1146:GLN:O	2:C:1150:ASP:OD2	2.39	0.40
2:C:121:GLU:HG3	2:C:121:GLU:H	1.57	0.40
5:F:599:ARG:O	5:F:604:SER:HB2	2.21	0.40
1:G:75:GLN:HG3	1:G:76:GLU:OE2	2.21	0.40
3:D:189:LEU:HB3	3:D:234:PRO:HB2	2.03	0.40
2:C:530:ILE:O	2:C:572:ILE:O	2.40	0.40
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.51	0.40
3:D:1327:GLU:HG2	3:D:1328:THR:N	2.35	0.40
1:H:86:LYS:HD2	1:H:174:ASP:HB2	2.03	0.40
2:C:62:TYR:CE1	2:C:476:LYS:HB3	2.56	0.40
2:I:136:PHE:CE1	2:I:506:PHE:HE2	2.40	0.40
2:I:564:PRO:HG2	2:I:568:ASN:O	2.20	0.40
3:J:1233:ILE:HG22	3:J:1234:VAL:N	2.36	0.40
3:D:403:ARG:HB3	3:D:405:GLU:HG3	2.02	0.40
3:D:1357:ILE:O	3:D:1362:GLY:HA3	2.21	0.40
2:C:271:ALA:O	2:C:275:ARG:HG3	2.21	0.40
3:D:466:MET:HB3	3:D:466:MET:HE2	1.98	0.40
5:F:528:LEU:HD23	5:F:528:LEU:HA	1.90	0.40
3:J:239:LEU:HA	3:J:239:LEU:HD23	1.77	0.40
1:A:83:LEU:HB3	2:C:694:ARG:NH2	2.36	0.40
5:L:164:GLY:O	5:L:260:ARG:HB2	2.20	0.40
2:I:85:CYS:SG	2:I:92:TYR:HA	2.61	0.40
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.86	0.40
1:H:100:LEU:HB3	1:H:115:ILE:HG22	2.02	0.40
5:F:584:ARG:HA	5:F:584:ARG:HD2	1.74	0.40
3:D:1353:VAL:O	3:D:1353:VAL:HG22	2.22	0.40
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.86	0.40
2:C:1281:TYR:OH	3:D:434:ILE:O	2.39	0.40
3:J:860:ARG:HB3	3:J:861:ASN:H	1.73	0.40
2:C:72:SER:O	2:C:98:VAL:HG13	2.21	0.40
2:C:616:ILE:HG13	2:C:652:TYR:HB2	2.03	0.40
2:C:1064:ASP:OD1	2:C:1239:VAL:HG12	2.22	0.40
3:J:401:VAL:HA	3:J:408:VAL:HG11	2.02	0.40
2:I:726:TYR:CZ	2:I:728:ASP:HB2	2.56	0.40
2:C:92:TYR:CE2	2:C:129:LEU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:LYS:O	2:C:1175:ASN:ND2	2.53	0.40
3:J:511:TYR:HE1	3:J:724:MET:CG	2.33	0.40
3:J:511:TYR:CE1	3:J:724:MET:HG2	2.53	0.40
2:I:517:GLN:NE2	2:I:759:SER:HA	2.37	0.40
2:C:800:MET:HB3	2:C:800:MET:HE3	1.81	0.40
2:I:496:LYS:HB3	2:I:497:PRO:HD3	2.03	0.40
2:C:1268:GLN:HG2	3:D:467:ALA:HB1	2.03	0.40
2:I:920:VAL:HA	2:I:921:PRO:HD3	1.92	0.40
2:C:656:SER:OG	2:C:658:GLN:HB2	2.21	0.40
3:D:57:PHE:CD2	3:D:57:PHE:N	2.88	0.40
5:L:568:ASN:ND2	5:L:568:ASN:H	2.19	0.40
5:F:406:GLN:NE2	5:F:406:GLN:HA	2.36	0.40
2:I:579:ALA:O	2:I:580:GLN:HG3	2.21	0.40
2:I:606:LEU:HD23	2:I:611:GLU:HA	2.04	0.40
1:H:88:LEU:HD21	1:H:115:ILE:CD1	2.51	0.40
2:C:10:ARG:HD3	2:C:1181:PRO:CG	2.46	0.40
2:I:337:PHE:CE2	2:I:343:HIS:HD2	2.40	0.40
5:F:551:LEU:HD11	5:F:598:LEU:HD21	2.02	0.40
1:G:74:VAL:HG21	1:G:81:ILE:HD11	2.04	0.40
5:F:316:PHE:CE1	5:F:337:VAL:HB	2.57	0.40
3:D:45:ASN:O	3:D:46:TYR:CB	2.70	0.40
3:J:452:LEU:HD23	3:J:452:LEU:HA	1.81	0.40
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	2.04	0.40
3:D:1372:ARG:HE	3:D:1372:ARG:HB2	1.73	0.40
3:J:268:LEU:HD22	3:J:306:LEU:HA	2.03	0.40
2:C:838:CYS:HB2	2:C:918:LEU:HB3	2.03	0.40
2:I:151:ARG:HE	2:I:445:ILE:HD11	1.85	0.40
5:L:431:ALA:O	5:L:434:TRP:N	2.55	0.40
4:K:22:VAL:HG13	4:K:64:LEU:CD1	2.51	0.40
3:J:722:ILE:HG21	3:J:722:ILE:HD13	1.79	0.40
5:F:426:LYS:HE2	5:F:428:SER:OG	2.22	0.40
2:I:197:ARG:HH22	2:I:203:LYS:HE2	1.86	0.40
3:J:41:PRO:HA	3:J:56:LEU:HD11	2.02	0.40
2:I:964:LEU:HD21	2:I:1022:LYS:HD2	2.03	0.40
1:H:71:LYS:HA	1:H:71:LYS:HD2	1.84	0.40
1:B:19:VAL:O	1:B:23:HIS:HB3	2.21	0.40
2:I:979:LEU:HD23	2:I:989:LEU:CD2	2.52	0.40
2:I:989:LEU:HD13	2:I:1000:LEU:HD13	2.04	0.40
1:G:219:ARG:HB2	1:G:219:ARG:HE	1.68	0.40
3:J:1286:LYS:HD2	3:J:1290:ARG:HH22	1.87	0.40
2:C:107:ARG:HA	2:C:108:GLU:HA	1.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:547:VAL:HG13	5:F:598:LEU:CD2	2.46	0.40
3:D:647:PRO:HD3	3:D:697:MET:HB3	2.04	0.40
3:J:1262:ARG:HH11	3:J:1262:ARG:HD3	1.73	0.40
3:D:121:PRO:HD2	3:D:123:ARG:HH21	1.86	0.40
3:J:804:ALA:O	3:J:806:ASP:N	2.54	0.40
1:A:34:GLY:C	1:A:36:GLY:N	2.75	0.40
1:H:155:ALA:HB2	1:H:174:ASP:N	2.36	0.40
3:D:833:GLU:HA	3:D:834:PRO:HD3	1.66	0.40
1:G:224:LEU:HD23	1:G:224:LEU:O	2.22	0.40
2:I:810:TYR:HB3	2:I:817:LEU:HD23	2.03	0.40
2:C:161:LYS:HA	2:C:170:VAL:HA	2.04	0.40
2:C:723:VAL:HG12	2:C:724:VAL:N	2.37	0.40
2:C:901:LEU:HD12	2:C:901:LEU:O	2.21	0.40
1:A:67:GLU:HG2	1:A:67:GLU:H	1.46	0.40
5:F:437:GLN:HG3	5:F:438:ALA:N	2.35	0.40
1:G:155:ALA:HA	1:G:158:ARG:HG3	2.03	0.40
3:D:34:SER:OG	3:D:103:GLY:HA2	2.21	0.40
2:C:133:ASN:ND2	2:C:713:GLY:HA3	2.37	0.40
5:L:219:GLU:O	5:L:222:ALA:HB3	2.21	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	317/329 (96%)	243 (77%)	48 (15%)	26 (8%)	1 15
1	B	213/329 (65%)	193 (91%)	15 (7%)	5 (2%)	8 50
1	G	225/329 (68%)	195 (87%)	21 (9%)	9 (4%)	4 35
1	H	212/329 (64%)	193 (91%)	15 (7%)	4 (2%)	10 53
2	C	1338/1342 (100%)	1210 (90%)	111 (8%)	17 (1%)	15 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	I	1338/1342 (100%)	1207 (90%)	112 (8%)	19 (1%)	14 59
3	D	1157/1407 (82%)	1031 (89%)	101 (9%)	25 (2%)	8 51
3	J	1146/1407 (81%)	1032 (90%)	92 (8%)	22 (2%)	10 53
4	E	87/91 (96%)	81 (93%)	4 (5%)	2 (2%)	8 50
4	K	77/91 (85%)	73 (95%)	3 (4%)	1 (1%)	15 61
5	F	462/613 (75%)	424 (92%)	30 (6%)	8 (2%)	11 55
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	11 55
All	All	7035/8222 (86%)	6307 (90%)	582 (8%)	146 (2%)	9 52

All (146) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	107	ILE
1	A	114	ASP
1	A	136	GLU
1	A	195	ARG
1	A	217	ILE
1	A	232	VAL
1	A	320	ASN
1	B	193	GLU
2	C	169	LYS
2	C	170	VAL
2	C	484	LEU
2	C	697	LYS
2	C	1137	GLU
2	C	1159	VAL
3	D	339	ARG
3	D	341	ASN
3	D	426	ALA
3	D	496	GLY
3	D	710	ASP
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO
5	F	566	ASP
5	F	584	ARG
1	G	162	GLU
1	G	167	PRO

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Mol	Chain	Res	Type
1	G	193	GLU
2	I	121	GLU
2	I	169	LYS
2	I	170	VAL
2	I	484	LEU
2	I	697	LYS
2	I	897	PRO
2	I	1137	GLU
2	I	1153	ALA
2	I	1159	VAL
2	I	1203	ASP
3	J	426	ALA
3	J	710	ASP
3	J	850	LYS
3	J	1169	THR
3	J	1294	ALA
5	L	490	PRO
5	L	569	THR
5	L	584	ARG
1	A	14	VAL
1	A	104	LYS
1	A	162	GLU
1	A	167	PRO
1	A	177	TYR
1	A	179	PRO
1	A	242	VAL
1	A	319	GLU
2	C	121	GLU
2	C	747	GLY
2	C	897	PRO
2	C	1059	ARG
2	C	1153	ALA
2	C	1165	SER
3	D	10	ALA
3	D	13	LYS
3	D	49	PHE
3	D	417	ARG
3	D	745	GLY
3	D	805	GLN
3	D	850	LYS
5	F	569	THR
1	G	9	LEU

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Mol	Chain	Res	Type
1	G	14	VAL
1	G	196	THR
1	H	138	ALA
2	I	44	GLU
3	J	334	LYS
3	J	335	GLN
3	J	342	LEU
3	J	496	GLY
3	J	745	GLY
3	J	805	GLN
4	K	33	GLY
5	L	395	THR
5	L	475	GLY
5	L	566	ASP
1	A	52	PRO
1	A	196	THR
1	A	216	ALA
2	C	983	GLY
2	C	1154	ASP
3	D	46	TYR
3	D	806	ASP
3	D	1274	PHE
5	F	602	SER
1	G	62	ASP
1	H	193	GLU
2	I	983	GLY
2	I	1059	ARG
2	I	1165	SER
3	J	49	PHE
3	J	417	ARG
1	A	164	ASP
1	A	324	ALA
1	B	13	LEU
1	B	14	VAL
1	B	20	SER
2	C	63	SER
3	D	1297	LYS
3	D	1344	LEU
1	H	134	THR
2	I	201	ARG
3	J	46	TYR
5	L	96	ASP

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Mol	Chain	Res	Type
1	A	124	VAL
1	A	275	ILE
2	C	1151	LEU
3	D	454	CYS
5	F	96	ASP
5	F	395	THR
1	G	22	THR
1	H	20	SER
2	I	160	ASP
3	J	1180	VAL
3	J	1297	LYS
1	A	115	ILE
1	A	315	GLY
1	B	136	GLU
3	D	1180	VAL
1	G	232	VAL
2	I	892	GLU
3	J	314	ARG
3	J	712	GLN
3	D	89	GLY
3	D	831	VAL
5	F	475	GLY
2	C	1317	PRO
3	D	357	VAL
3	J	826	ILE
1	A	293	PRO
2	I	1186	VAL
3	J	89	GLY
5	L	97	PRO
3	D	828	GLY
4	E	86	ILE
2	I	1202	GLY
3	J	357	VAL
3	J	586	GLY

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	278/286 (97%)	231 (83%)	47 (17%)	2 18
1	B	186/286 (65%)	172 (92%)	14 (8%)	17 57
1	G	193/286 (68%)	170 (88%)	23 (12%)	6 34
1	H	183/286 (64%)	170 (93%)	13 (7%)	18 59
2	C	1155/1157 (100%)	1048 (91%)	107 (9%)	11 48
2	I	1154/1157 (100%)	1055 (91%)	99 (9%)	13 51
3	D	964/1168 (82%)	867 (90%)	97 (10%)	9 43
3	J	962/1168 (82%)	869 (90%)	93 (10%)	10 45
4	E	72/75 (96%)	67 (93%)	5 (7%)	19 60
4	K	67/75 (89%)	63 (94%)	4 (6%)	24 65
5	F	417/540 (77%)	376 (90%)	41 (10%)	10 44
5	L	418/540 (77%)	378 (90%)	40 (10%)	10 46
All	All	6049/7024 (86%)	5466 (90%)	583 (10%)	10 46

All (583) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	PHE
1	A	9	LEU
1	A	19	VAL
1	A	23	HIS
1	A	29	GLU
1	A	64	VAL
1	A	67	GLU
1	A	70	THR
1	A	74	VAL
1	A	77	ASP
1	A	79	LEU
1	A	83	LEU
1	A	98	VAL
1	A	102	LEU
1	A	104	LYS
1	A	110	VAL
1	A	137	ASN
1	A	140	ILE
1	A	145	LYS
1	A	156	SER
1	A	164	ASP

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Mol	Chain	Res	Type
1	A	165	GLU
1	A	172	LEU
1	A	180	VAL
1	A	182	ARG
1	A	186	ASN
1	A	192	VAL
1	A	231	PHE
1	A	239	GLN
1	A	243	LYS
1	A	246	LYS
1	A	259	ASP
1	A	262	LEU
1	A	269	CYS
1	A	276	HIS
1	A	282	VAL
1	A	284	ARG
1	A	295	LEU
1	A	297	LYS
1	A	306	VAL
1	A	307	LEU
1	A	310	ARG
1	A	316	MET
1	A	317	ARG
1	A	318	LEU
1	A	319	GLU
1	B	16	ILE
1	B	18	GLN
1	B	27	THR
1	B	58	GLU
1	B	60	GLU
1	B	62	ASP
1	B	65	LEU
1	B	79	LEU
1	B	124	VAL
1	B	133	LEU
1	B	139	SER
1	B	183	ILE
1	B	191	ARG
1	B	233	ASP
2	C	3	TYR
2	C	11	ILE
2	C	17	LYS

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Mol	Chain	Res	Type
2	C	23	ASP
2	C	46	GLN
2	C	55	SER
2	C	81	ASP
2	C	91	THR
2	C	107	ARG
2	C	108	GLU
2	C	115	LYS
2	C	117	ILE
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	131	THR
2	C	201	ARG
2	C	208	ILE
2	C	219	GLN
2	C	285	ILE
2	C	306	THR
2	C	320	ASP
2	C	321	LEU
2	C	342	ASP
2	C	369	MET
2	C	419	ILE
2	C	423	ASP
2	C	451	ARG
2	C	456	VAL
2	C	484	LEU
2	C	490	GLN
2	C	492	MET
2	C	493	ILE
2	C	518	ASN
2	C	521	LEU
2	C	539	THR
2	C	540	ARG
2	C	553	THR
2	C	558	VAL
2	C	561	ILE
2	C	563	THR
2	C	604	HIS
2	C	615	VAL
2	C	623	LEU
2	C	633	LEU

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Mol	Chain	Res	Type
2	C	635	THR
2	C	637	ARG
2	C	660	VAL
2	C	663	VAL
2	C	672	GLU
2	C	680	LEU
2	C	697	LYS
2	C	699	LEU
2	C	714	VAL
2	C	739	ASP
2	C	748	ILE
2	C	757	THR
2	C	765	ILE
2	C	773	LEU
2	C	781	ASP
2	C	782	VAL
2	C	791	LEU
2	C	800	MET
2	C	814	ASP
2	C	890	LYS
2	C	892	GLU
2	C	918	LEU
2	C	919	ARG
2	C	951	MET
2	C	979	LEU
2	C	984	VAL
2	C	992	LEU
2	C	1037	THR
2	C	1073	LYS
2	C	1076	ILE
2	C	1082	ILE
2	C	1090	ASN
2	C	1098	LEU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1136	GLN
2	C	1141	LEU
2	C	1146	GLN
2	C	1151	LEU
2	C	1155	VAL

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Mol	Chain	Res	Type
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1164	PHE
2	C	1206	THR
2	C	1233	LEU
2	C	1238	LEU
2	C	1248	THR
2	C	1253	LEU
2	C	1255	THR
2	C	1265	PHE
2	C	1269	ARG
2	C	1281	TYR
2	C	1287	LEU
2	C	1289	GLU
2	C	1299	ASN
2	C	1313	HIS
2	C	1327	LEU
2	C	1331	ARG
2	C	1342	GLU
3	D	8	LEU
3	D	11	GLN
3	D	18	ASP
3	D	29	MET
3	D	46	TYR
3	D	54	ASP
3	D	70	CYS
3	D	79	LYS
3	D	80	HIS
3	D	83	VAL
3	D	92	VAL
3	D	97	VAL
3	D	98	ARG
3	D	154	LEU
3	D	159	ILE
3	D	162	GLU
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	217	LEU
3	D	218	THR
3	D	248	ASP

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Mol	Chain	Res	Type
3	D	252	LEU
3	D	255	LEU
3	D	259	ARG
3	D	269	TYR
3	D	324	LEU
3	D	330	MET
3	D	343	LEU
3	D	346	ARG
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	407	VAL
3	D	413	ASP
3	D	416	ILE
3	D	429	LEU
3	D	490	ILE
3	D	513	MET
3	D	532	GLU
3	D	536	LEU
3	D	544	LEU
3	D	545	HIS
3	D	563	LEU
3	D	568	SER
3	D	569	LEU
3	D	571	ASP
3	D	573	THR
3	D	576	ARG
3	D	639	VAL
3	D	641	ILE
3	D	661	VAL
3	D	678	ARG
3	D	685	ILE
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	764	ARG
3	D	770	LEU
3	D	772	TYR
3	D	788	LEU

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Mol	Chain	Res	Type
3	D	797	THR
3	D	799	ARG
3	D	801	VAL
3	D	847	ASP
3	D	849	LEU
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	867	GLN
3	D	890	THR
3	D	897	HIS
3	D	903	LEU
3	D	908	ILE
3	D	910	ASN
3	D	913	GLU
3	D	918	ILE
3	D	1146	GLU
3	D	1155	ILE
3	D	1163	VAL
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1221	LEU
3	D	1261	LEU
3	D	1266	ILE
3	D	1272	SER
3	D	1279	GLN
3	D	1280	VAL
3	D	1283	SER
3	D	1332	LEU
3	D	1343	GLU
3	D	1361	THR
3	D	1366	HIS
4	E	3	ARG
4	E	5	THR
4	E	13	ILE
4	E	36	ASP
4	E	58	LEU
5	F	96	ASP
5	F	98	VAL
5	F	100	MET
5	F	102	MET

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Mol	Chain	Res	Type
5	F	114	GLU
5	F	154	GLU
5	F	230	VAL
5	F	261	LEU
5	F	267	ASP
5	F	277	MET
5	F	306	PHE
5	F	335	GLU
5	F	338	HIS
5	F	364	ARG
5	F	400	GLN
5	F	421	TYR
5	F	449	THR
5	F	450	ILE
5	F	469	GLN
5	F	472	GLN
5	F	479	THR
5	F	482	GLU
5	F	488	LEU
5	F	491	GLU
5	F	492	ASP
5	F	516	ASP
5	F	529	GLU
5	F	530	LEU
5	F	547	VAL
5	F	552	THR
5	F	559	LEU
5	F	568	ASN
5	F	569	THR
5	F	572	THR
5	F	573	LEU
5	F	587	ILE
5	F	599	ARG
5	F	600	HIS
5	F	603	ARG
5	F	606	VAL
5	F	608	ARG
1	G	12	ARG
1	G	19	VAL
1	G	23	HIS
1	G	26	VAL
1	G	33	ARG

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Mol	Chain	Res	Type
1	G	50	SER
1	G	70	THR
1	G	121	VAL
1	G	124	VAL
1	G	133	LEU
1	G	139	SER
1	G	145	LYS
1	G	158	ARG
1	G	163	GLU
1	G	166	ARG
1	G	168	ILE
1	G	171	LEU
1	G	178	SER
1	G	183	ILE
1	G	192	VAL
1	G	211	ILE
1	G	218	ARG
1	G	219	ARG
1	H	16	ILE
1	H	27	THR
1	H	38	THR
1	H	58	GLU
1	H	61	ILE
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	124	VAL
1	H	133	LEU
1	H	176	CYS
1	H	183	ILE
2	I	3	TYR
2	I	4	SER
2	I	11	ILE
2	I	17	LYS
2	I	23	ASP
2	I	46	GLN
2	I	60	GLN
2	I	91	THR
2	I	107	ARG
2	I	115	LYS
2	I	117	ILE

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Mol	Chain	Res	Type
2	I	119	GLU
2	I	121	GLU
2	I	131	THR
2	I	156	PHE
2	I	179	TYR
2	I	201	ARG
2	I	208	ILE
2	I	219	GLN
2	I	285	ILE
2	I	306	THR
2	I	320	ASP
2	I	321	LEU
2	I	342	ASP
2	I	360	LEU
2	I	369	MET
2	I	419	ILE
2	I	423	ASP
2	I	445	ILE
2	I	451	ARG
2	I	456	VAL
2	I	484	LEU
2	I	490	GLN
2	I	492	MET
2	I	493	ILE
2	I	516	ASP
2	I	518	ASN
2	I	521	LEU
2	I	525	THR
2	I	530	ILE
2	I	538	LEU
2	I	540	ARG
2	I	553	THR
2	I	558	VAL
2	I	604	HIS
2	I	609	ILE
2	I	615	VAL
2	I	623	LEU
2	I	633	LEU
2	I	635	THR
2	I	637	ARG
2	I	660	VAL
2	I	663	VAL

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Mol	Chain	Res	Type
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	724	VAL
2	I	739	ASP
2	I	742	TYR
2	I	748	ILE
2	I	757	THR
2	I	765	ILE
2	I	773	LEU
2	I	782	VAL
2	I	800	MET
2	I	814	ASP
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	967	LEU
2	I	979	LEU
2	I	992	LEU
2	I	1037	THR
2	I	1082	ILE
2	I	1114	GLU
2	I	1117	LEU
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	1163	THR
2	I	1206	THR
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1253	LEU
2	I	1265	PHE
2	I	1287	LEU
2	I	1291	LEU
2	I	1299	ASN
2	I	1313	HIS
2	I	1326	LEU

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Mol	Chain	Res	Type
2	I	1327	LEU
2	I	1331	ARG
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	29	MET
3	J	46	TYR
3	J	54	ASP
3	J	78	LEU
3	J	79	LYS
3	J	92	VAL
3	J	95	THR
3	J	97	VAL
3	J	98	ARG
3	J	154	LEU
3	J	162	GLU
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	217	LEU
3	J	218	THR
3	J	248	ASP
3	J	255	LEU
3	J	259	ARG
3	J	324	LEU
3	J	330	MET
3	J	342	LEU
3	J	343	LEU
3	J	345	LYS
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	413	ASP
3	J	416	ILE
3	J	429	LEU
3	J	490	ILE
3	J	510	LEU
3	J	513	MET
3	J	532	GLU
3	J	536	LEU
3	J	544	LEU
3	J	545	HIS

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Mol	Chain	Res	Type
3	J	563	LEU
3	J	568	SER
3	J	569	LEU
3	J	573	THR
3	J	605	LEU
3	J	641	ILE
3	J	661	VAL
3	J	678	ARG
3	J	698	MET
3	J	707	ILE
3	J	708	ASN
3	J	712	GLN
3	J	717	VAL
3	J	764	ARG
3	J	772	TYR
3	J	788	LEU
3	J	797	THR
3	J	801	VAL
3	J	810	THR
3	J	847	ASP
3	J	849	LEU
3	J	857	LEU
3	J	858	VAL
3	J	885	VAL
3	J	897	HIS
3	J	898	CYS
3	J	903	LEU
3	J	908	ILE
3	J	910	ASN
3	J	918	ILE
3	J	1146	GLU
3	J	1155	ILE
3	J	1162	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG
3	J	1221	LEU
3	J	1251	LYS
3	J	1255	VAL
3	J	1261	LEU

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Mol	Chain	Res	Type
3	J	1266	ILE
3	J	1274	PHE
3	J	1284	ARG
3	J	1289	ASN
3	J	1290	ARG
3	J	1292	LEU
3	J	1293	GLU
3	J	1319	PHE
3	J	1332	LEU
3	J	1333	THR
3	J	1343	GLU
3	J	1355	ARG
3	J	1366	HIS
4	K	3	ARG
4	K	13	ILE
4	K	28	ARG
4	K	39	VAL
5	L	98	VAL
5	L	102	MET
5	L	154	GLU
5	L	230	VAL
5	L	261	LEU
5	L	266	PHE
5	L	277	MET
5	L	297	MET
5	L	306	PHE
5	L	335	GLU
5	L	364	ARG
5	L	395	THR
5	L	421	TYR
5	L	445	ASP
5	L	449	THR
5	L	469	GLN
5	L	471	LEU
5	L	472	GLN
5	L	476	ARG
5	L	482	GLU
5	L	486	ARG
5	L	488	LEU
5	L	491	GLU
5	L	492	ASP
5	L	516	ASP

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Mol	Chain	Res	Type
5	L	527	THR
5	L	559	LEU
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	575	GLU
5	L	580	PHE
5	L	582	VAL
5	L	587	ILE
5	L	599	ARG
5	L	600	HIS
5	L	603	ARG
5	L	606	VAL
5	L	607	LEU
5	L	613	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	268	ASN
1	B	84	ASN
1	B	117	HIS
2	C	120	GLN
2	C	139	ASN
2	C	150	HIS
2	C	343	HIS
2	C	604	HIS
2	C	1116	HIS
2	C	1136	GLN
2	C	1236	ASN
2	C	1237	HIS
2	C	1314	GLN
3	D	200	GLN
3	D	424	ASN
3	D	450	HIS
3	D	690	ASN
3	D	702	GLN
3	D	716	GLN
3	D	861	ASN
5	F	129	GLN
5	F	301	ASN

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Mol	Chain	Res	Type
5	F	362	ASN
5	F	446	GLN
5	F	518	HIS
5	F	579	GLN
5	F	600	HIS
1	G	84	ASN
1	H	132	HIS
2	I	139	ASN
2	I	343	HIS
2	I	510	GLN
2	I	658	GLN
2	I	688	GLN
2	I	1010	GLN
2	I	1038	GLN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1146	GLN
2	I	1220	GLN
2	I	1237	HIS
2	I	1299	ASN
2	I	1314	GLN
3	J	157	GLN
3	J	200	GLN
3	J	206	ASN
3	J	320	ASN
3	J	450	HIS
3	J	465	GLN
3	J	477	GLN
3	J	702	GLN
3	J	716	GLN
3	J	771	GLN
3	J	817	HIS
3	J	861	ASN
3	J	910	ASN
3	J	1259	GLN
3	J	1366	HIS
4	K	7	GLN
5	L	131	GLN
5	L	406	GLN
5	L	446	GLN
5	L	469	GLN

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Mol	Chain	Res	Type
5	L	568	ASN

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

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
8	4C6	D	2004	-	31,34,34	1.12	3 (9%)	39,51,51	0.80	1 (2%)
8	4C6	J	2004	-	31,34,34	0.72	0	39,51,51	1.22	4 (10%)

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
8	4C6	D	2004	-	-	0/7/45/45	0/3/4/4
8	4C6	J	2004	-	-	0/7/45/45	0/3/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2004	4C6	C2-S	-4.32	1.71	1.79
8	D	2004	4C6	S-N	-2.11	1.60	1.64
8	D	2004	4C6	C4-C3	-2.07	1.46	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	2004	4C6	C3-C2-C5	-3.93	104.58	107.52
8	D	2004	4C6	C3-C2-C5	-2.99	105.28	107.52
8	J	2004	4C6	C7-C21-C	-2.69	85.26	88.13
8	J	2004	4C6	C7-C1-N	2.55	135.43	130.19
8	J	2004	4C6	O3-S-C2	2.69	112.70	108.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	2004	4C6	1	0
8	J	2004	4C6	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	319/329 (96%)	-0.30	5 (1%) 74 65	105, 138, 176, 185	0
1	B	217/329 (65%)	-0.13	4 (1%) 71 62	114, 172, 192, 198	0
1	G	227/329 (68%)	-0.35	1 (0%) 93 90	138, 159, 175, 192	0
1	H	216/329 (65%)	-0.04	6 (2%) 56 46	130, 174, 192, 201	0
2	C	1340/1342 (99%)	-0.34	13 (0%) 84 77	88, 126, 202, 228	0
2	I	1340/1342 (99%)	-0.16	35 (2%) 59 49	108, 154, 212, 314	0
3	D	1163/1407 (82%)	-0.33	3 (0%) 94 92	90, 119, 164, 197	0
3	J	1152/1407 (81%)	-0.23	10 (0%) 85 79	103, 137, 181, 211	0
4	E	89/91 (97%)	-0.20	0 100 100	129, 159, 178, 184	0
4	K	79/91 (86%)	0.66	8 (10%) 9 8	186, 221, 249, 254	0
5	F	468/613 (76%)	-0.21	15 (3%) 51 41	113, 159, 233, 249	0
5	L	469/613 (76%)	-0.18	12 (2%) 59 49	127, 168, 244, 260	0
All	All	7079/8222 (86%)	-0.24	112 (1%) 74 65	88, 143, 205, 314	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	9.1
2	I	1003	THR	7.1
5	F	167	ASP	5.6
2	I	1002	LEU	5.1
2	I	1004	ASP	5.0
2	I	979	LEU	4.9
5	L	167	ASP	4.8
2	I	1006	GLU	4.7
2	I	983	GLY	4.5
2	C	231	GLU	4.2
3	J	208	THR	4.1

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Mol	Chain	Res	Type	RSRZ
2	I	999	GLU	4.0
2	I	1005	GLU	4.0
4	K	36	ASP	4.0
5	L	315	TRP	3.9
5	F	318	ALA	3.9
5	L	111	LEU	3.8
2	C	332	ARG	3.7
5	L	318	ALA	3.7
3	J	830	ASP	3.6
5	F	319	ALA	3.5
2	I	985	GLU	3.5
2	C	251	ALA	3.5
5	F	305	LEU	3.4
3	J	212	THR	3.4
2	C	333	ILE	3.4
5	L	490	PRO	3.3
2	I	1011	LEU	3.3
5	F	307	THR	3.3
2	I	981	ALA	3.2
1	H	107	ILE	3.2
2	C	241	LEU	3.1
2	C	1003	THR	3.1
5	F	337	VAL	3.0
2	I	970	GLY	3.0
2	I	984	VAL	3.0
2	I	105	TYR	3.0
1	H	13	LEU	3.0
5	F	315	TRP	2.9
4	K	58	LEU	2.9
5	L	321	ALA	2.9
2	C	230	PHE	2.9
4	K	37	PRO	2.9
1	A	294	ASN	2.9
5	L	314	THR	2.8
5	L	319	ALA	2.8
2	I	1008	GLN	2.8
3	J	1198	VAL	2.8
3	J	542	ALA	2.7
2	I	725	GLN	2.7
2	I	111	GLU	2.7
2	I	1010	GLN	2.7
2	C	250	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	234	ASP	2.6
1	H	28	LEU	2.6
1	H	96	ASP	2.6
1	A	241	GLU	2.6
2	C	1002	LEU	2.6
4	K	56	GLU	2.6
5	F	323	ASN	2.6
2	I	1017	GLN	2.6
2	C	282	VAL	2.5
5	L	489	MET	2.5
1	A	160	HIS	2.5
2	I	1007	LYS	2.5
1	A	245	GLU	2.5
2	I	980	VAL	2.5
2	C	317	LEU	2.5
4	K	57	GLY	2.5
3	J	207	GLU	2.5
1	B	160	HIS	2.4
2	I	987	GLU	2.4
2	I	978	VAL	2.4
5	F	314	THR	2.4
3	J	930	LEU	2.4
1	B	97	GLU	2.4
1	B	172	LEU	2.4
2	I	998	LEU	2.4
5	F	321	ALA	2.4
2	I	322	LEU	2.3
3	D	212	THR	2.3
5	F	312	SER	2.3
2	I	720	ARG	2.3
5	L	305	LEU	2.3
3	J	1297	LYS	2.3
2	I	414	ILE	2.3
3	J	712	GLN	2.3
1	H	106	GLY	2.3
2	C	165	HIS	2.3
4	K	70	GLN	2.2
5	F	293	GLU	2.2
5	F	333	VAL	2.2
2	I	988	LYS	2.2
3	D	208	THR	2.2
1	B	67	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	893	THR	2.2
1	H	12	ARG	2.2
5	F	283	GLN	2.1
5	F	306	PHE	2.1
2	I	231	GLU	2.1
2	I	1025	PHE	2.1
4	K	26	ARG	2.1
2	I	734	ILE	2.1
3	D	930	LEU	2.1
1	A	25	LYS	2.0
2	I	375	PRO	2.0
5	L	312	SER	2.0
1	G	193	GLU	2.0
5	L	317	ASN	2.0
4	K	80	LEU	2.0
3	J	521	LYS	2.0
2	I	1000	LEU	2.0

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

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

6.3 Carbohydrates (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
8	4C6	D	2004	31/31	0.97	0.34	2.36	127,127,127,127	0
8	4C6	J	2004	31/31	0.95	0.32	1.45	127,127,128,141	0
7	ZN	D	2003	1/1	0.99	0.22	0.54	127,127,127,127	0
7	ZN	J	2003	1/1	0.96	0.20	-0.02	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	ZN	D	2002	1/1	0.98	0.18	-0.34	164,164,164,164	0
7	ZN	J	2002	1/1	0.97	0.12	-1.08	190,190,190,190	0
6	MG	D	2001	1/1	0.93	0.27	-	127,127,127,127	0
6	MG	C	1401	1/1	0.86	0.35	-	127,127,127,127	0
6	MG	J	2001	1/1	0.95	0.23	-	127,127,127,127	0
6	MG	I	1401	1/1	0.85	0.37	-	127,127,127,127	0

6.5 Other polymers

There are no such residues in this entry.