Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:45 am BST

PDB ID	:	3QT1
Title	:	RNA polymerase II variant containing A Chimeric RPB9-C11 subunit
Authors	:	Ruan, W.; Lehmann, E.; Thomm, M.; Kostrewa, D.; Cramer, P.
Deposited on	:	2011-02-22
Resolution	:	4.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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

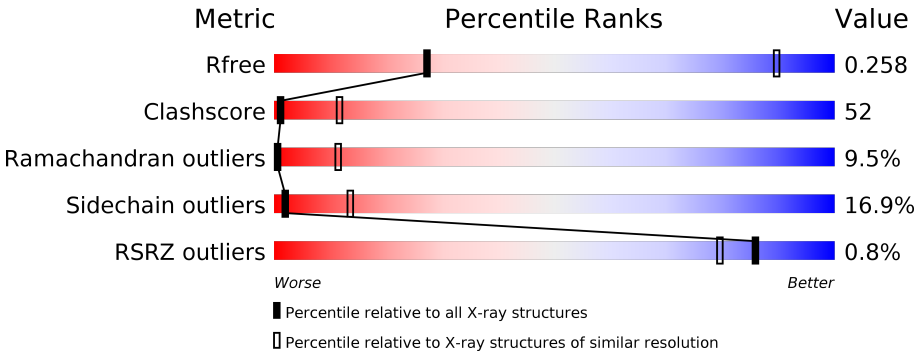
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	% 23% 44% 14% • 18%
2	B	1224	% 26% 49% 15% • 10%
3	C	318	26% 44% 13% 16%
4	D	219	21% 45% 14% • 19%
5	E	215	27% 60% 11% •
6	F	155	13% 34% 9% • 44%

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Mol	Chain	Length	Quality of chain
7	G	171	32% 54% 13%
8	H	146	3% 35% 42% 13% 8%
9	I	133	13% 17% 5% 65%
10	J	70	19% 61% 11% 7%
11	K	120	33% 39% 23% 5%
12	L	70	13% 26% 20% 7% 34%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 30535 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1416	11143	7021	1949	2111	62	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1103	8770	5554	1535	1626	55	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	178	1434	887	257	288	2	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	214	1752	1111	309	321	11	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	87	705	451	119	132	3	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	134	Total	C	N	O	S	0	0	0
			1076	677	182	213	4			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9, DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	47	Total	C	N	O	S	0	0	0
			398	246	72	75	5			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	J	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total Zn 1 1	0	0
13	I	1	Total Zn 1 1	0	0
13	C	1	Total Zn 1 1	0	0
13	A	2	Total Zn 2 2	0	0
13	L	1	Total Zn 1 1	0	0

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

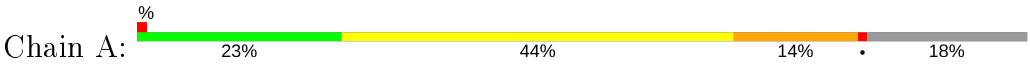
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total Mg 1 1	0	0

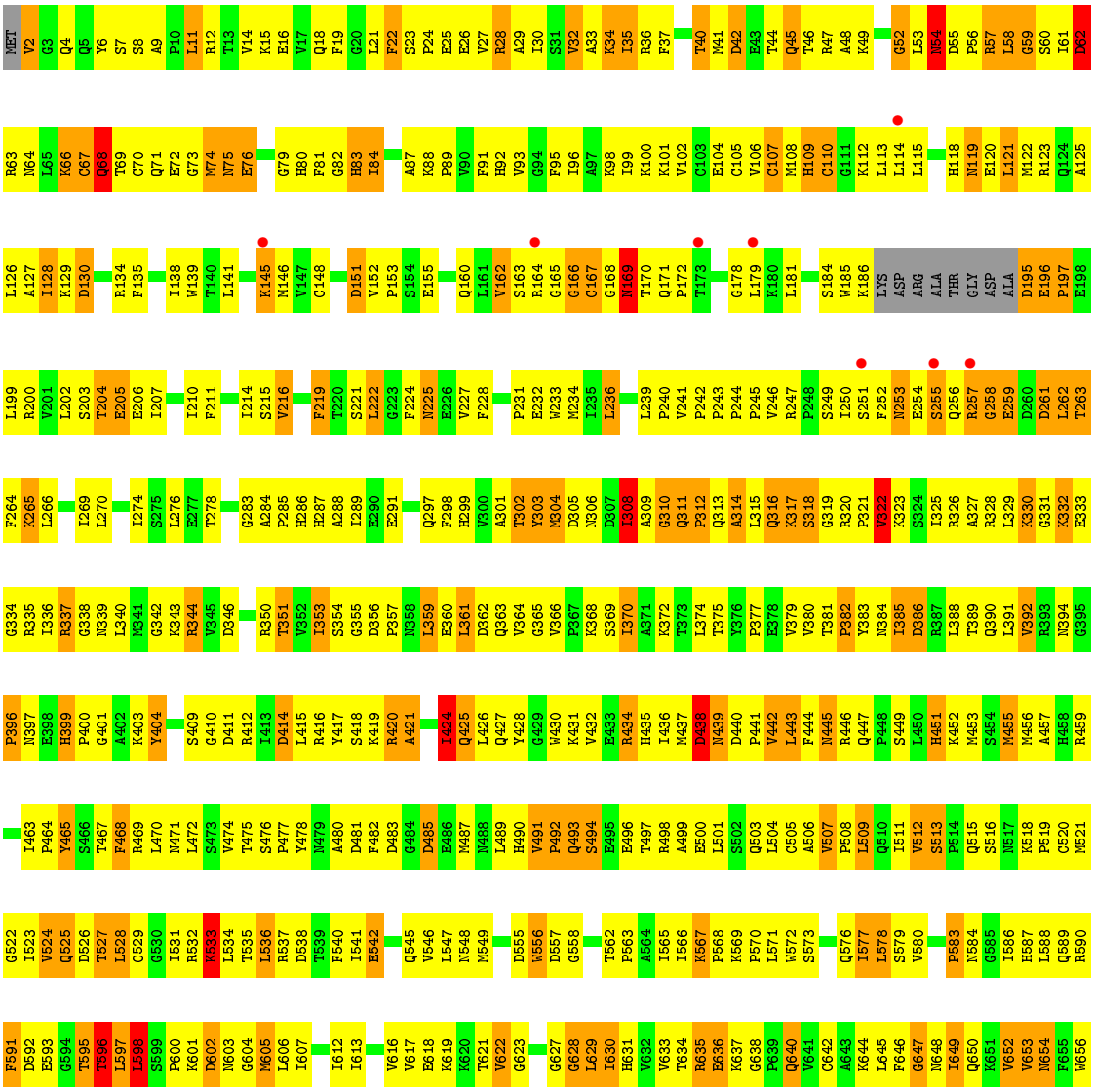
3 Residue-property plots (i)

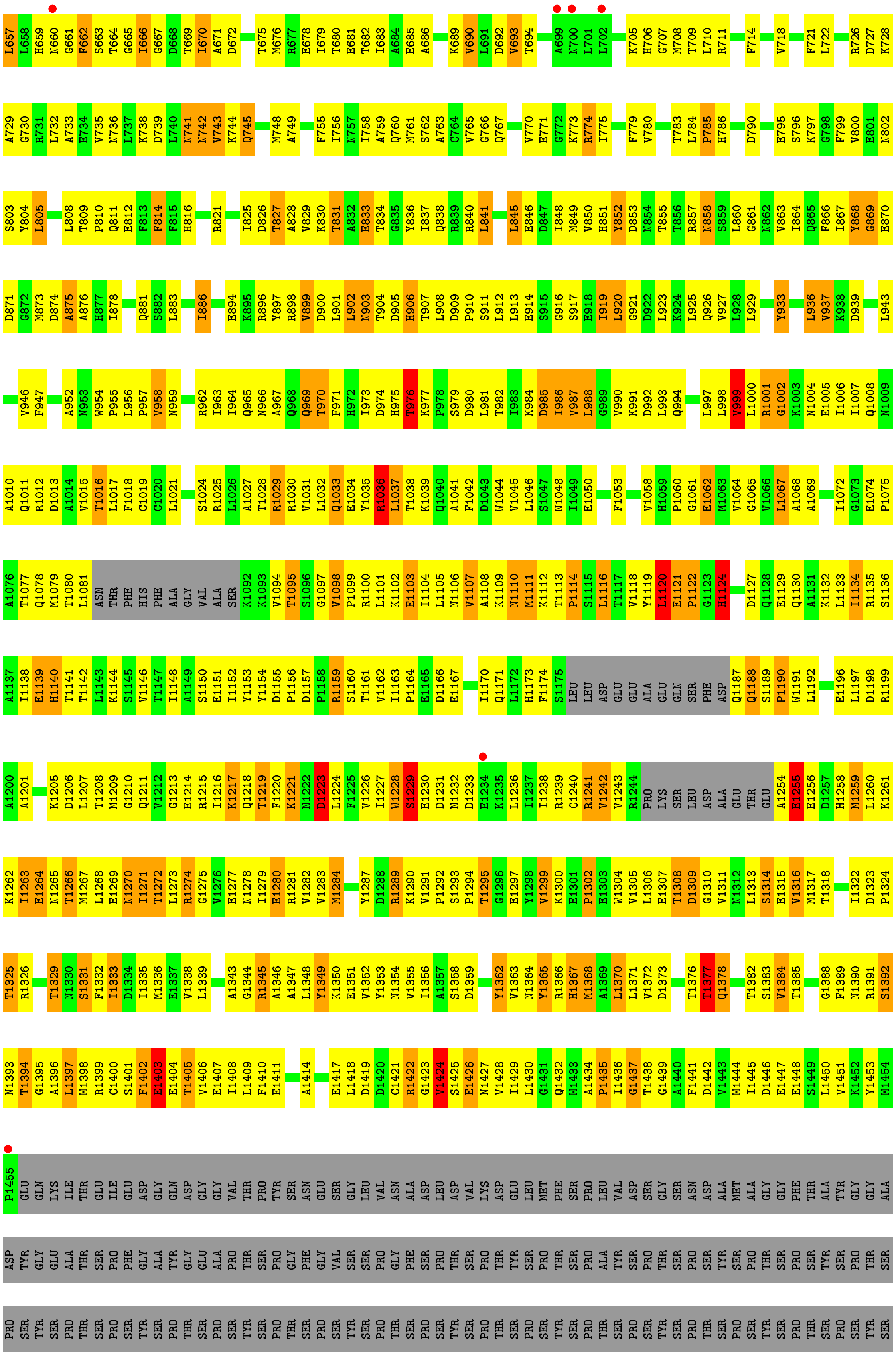
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

Chain A:



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A729 G730 R731 L732 A733 E734 V735 N736 L737 K738 D739 L740 N741 N742 V743 K744 Q745 M748 A749 F755 I756 N757 I758 A759 Q760 M761 S762 A763 C764 V765 G766 Q767 V770 E771 G772 K773 R774 I775 F779 V780 T783 L784 P785 H786 D790 E795 S796 K797 G798 F799 V800 E801 N802
S803 Y804 L805 L808 T809 P810 Q811 E812 F813 F814 F815 H816 R821 I825 D826 T827 A828 V829 K830 T831 A832 E833 T834 G835 Y836 I837 Q838 R839 R840 L841 L845 E846 D847 I848 M849 V850 H851 Y852 D853 N854 T855 T856 R857 N858 S859 L860 G861 N862 V863 I864 Q865 F866 I867 Y868 G869 E870
D871 G872 M873 D874 A875 A876 H877 I878 Q881 S882 L883 I886 E894 K895 R896 Y897 R898 V899 D900 L901 L902 N903 T904 D905 H906 T907 L908 D909 P910 S911 L912 L913 E914 S915 G916 S917 E918 I919 L920 G921 D922 L923 K924 L925 Q926 V927 L928 L929 Y933 L936 V937 K938 D939 L943
V946 F947 A952 N953 W954 P955 L956 P957 V958 N959 R962 I963 I964 Q965 N966 A967 Q968 Q969 T970 F971 H972 I973 D974 H975 T976 K977 P978 S979 D980 L981 T982 I983 K984 D985 I986 V987 L988 G989 V990 K991 D992 L993 Q994 L997 L998 V999 L1000 R1001 G1002 K1003 N1004 E1005 I1006 I1007 Q1008 N1009
A1010 Q1011 R1012 D1013 A1014 V1015 T1016 L1017 F1018 C1019 C1020 L1021 S1024 R1025 L1026 A1027 T1028 R1029 R1030 V1031 L1032 Q1033 E1034 Y1035 R1036 L1037 T1038 K1039 Q1040 A1041 F1042 D1043 W1044 V1045 L1046 S1047 N1048 I1049 E1050 F1053 V1058 H1059 P1060 G1061 E1062 M1063 V1064 G1065 V1066 L1067 A1068 A1069 I1072 G1073 E1074 P1075
A1076 T1077 Q1078 M1079 T1080 L1081 ASN THR PHE HIS PHE ALA GLY VAL ALA SER K1092 K1093 V1094 T1095 S1096 G1097 V1098 P1099 R1100 L1101 K1102 E1103 I1104 L1105 N1106 V1107 A1108 K1109 N1110 M1111 K1112 T1113 P1114 S1115 L1116 T1117 V1118 Y1119 L1120 E1121 P1122 G1123 H1124 D1127 Q1128 E1129 Q1130 A1131 K1132 L1133 I1134 R1135 S1136
A1137 I1138 E1139 H1140 T1141 T1142 L1143 K1144 S1145 V1146 T1147 I1148 A1149 S1150 E1151 I1152 Y1153 Y1154 D1155 P1156 D1157 P1158 R1159 S1160 T1161 V1162 I1163 P1164 E1165 D1166 E1167 I1170 Q1171 L1172 H1173 F1174 S1175 LEU LEU ASP GLU GLU ALA GLU GLN SER PHE ASP Q1187 Q1188 S1189 P1190 W1191 L1192 E1196 L1197 D1198 R1199
A1200 A1201 K1205 D1206 L1207 T1208 M1209 G1210 Q1211 V1212 G1213 E1214 R1215 I1216 K1217 Q1218 T1219 F1220 K1221 N1222 D1223 L1224 F1225 V1226 I1227 W1228 S1229 E1230 D1231 N1232 D1233 E1234 K1235 L1236 T1237 I1238 R1239 C1240 R1241 V1242 V1243 R1244 PRO LYS SER LEU ASP ALA GLU THR GLU A1254 E1255 E1256 D1257 H1258 M1259 L1260 K1261
K1262 I1263 E1264 N1265 T1266 M1267 L1268 E1269 N1270 I1271 T1272 L1273 R1274 G1275 V1276 E1277 N1278 I1279 E1280 R1281 V1282 V1283 M1284 Y1287 D1288 R1289 K1290 V1291 P1292 S1293 P1294 T1295 G1296 E1297 Y1298 V1299 K1300 E1301 P1302 E1303 W1304 V1305 L1306 E1307 T1308 D1309 G1310 V1311 N1312 L1313 S1314 E1315 V1316 M1317 T1318 I1322 D1323 P1324
T1325 R1326 T1329 N1330 S1331 F1332 I1333 D1334 I1335 M1336 E1337 V1338 L1339 A1343 G1344 R1345 A1346 A1347 L1348 Y1349 K1350 E1351 V1352 Y1353 N1354 V1355 I1356 A1357 S1358 D1359 Y1362 V1363 N1364 Y1365 R1366 H1367 M1368 A1369 L1370 L1371 V1372 D1373 T1376 T1377 Q1378 T1382 S1383 V1384 T1385 G1388 F1389 N1390 R1391 S1392
N1393 T1394 G1395 A1396 L1397 M1398 R1399 C1400 S1401 F1402 E1403 E1404 T1405 V1406 E1407 I1408 L1409 F1410 E1411 A1414 E1417 L1418 D1419 D1420 C1421 R1422 G1423 V1424 S1425 E1426 N1427 V1428 I1429 L1430 G1431 Q1432 M1433 A1434 P1435 I1436 G1437 T1438 G1439 A1440 F1441 D1442 V1443 M1444 I1445 D1446 E1447 E1448 S1449 L1450 V1451 K1452 Y1453 M1454
P1455 GLU GLN LYS ILE THR GLU ILE GLU ASP GLY GLN ASP GLY GLY VAL THR PRO TYR SER ASN GLU SER GLY LEU VAL ASN ALA ASP LEU ASP VAL LYS ASP GLU LEU MET PHE SER PRO LEU VAL ASP SER GLY SER ASN ASP ALA MET ALA GLY GLY PHE THR ALA TYR GLY GLY ALA
ASP TYR GLY GLU ALA THR SER PRO PHE GLY ALA TYR GLY GLU ALA PRO THR SER PRO GLY PHE GLY VAL SER SER PRO GLY PHE SER PRO THR SER PRO THR TYR SER PRO THR SER PRO ALA TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER
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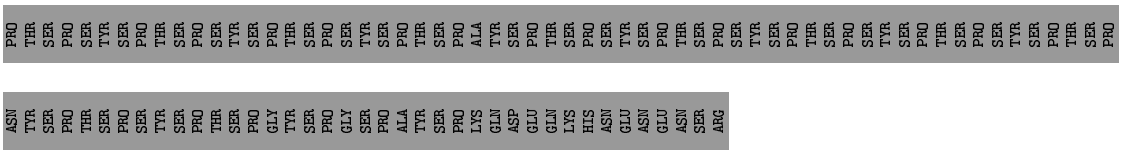
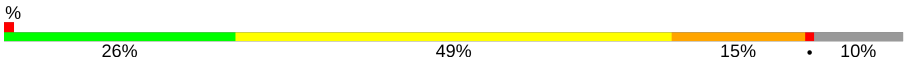
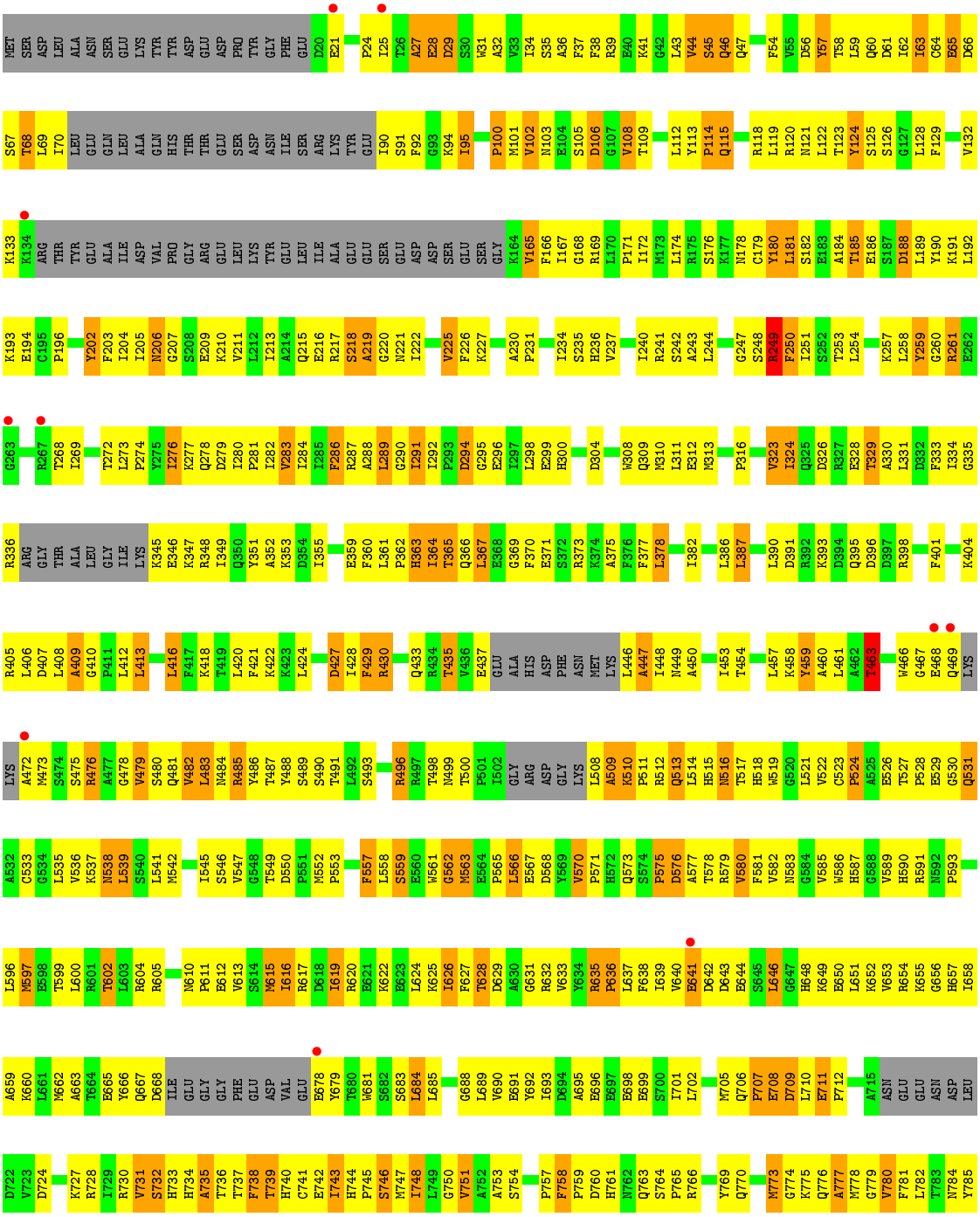
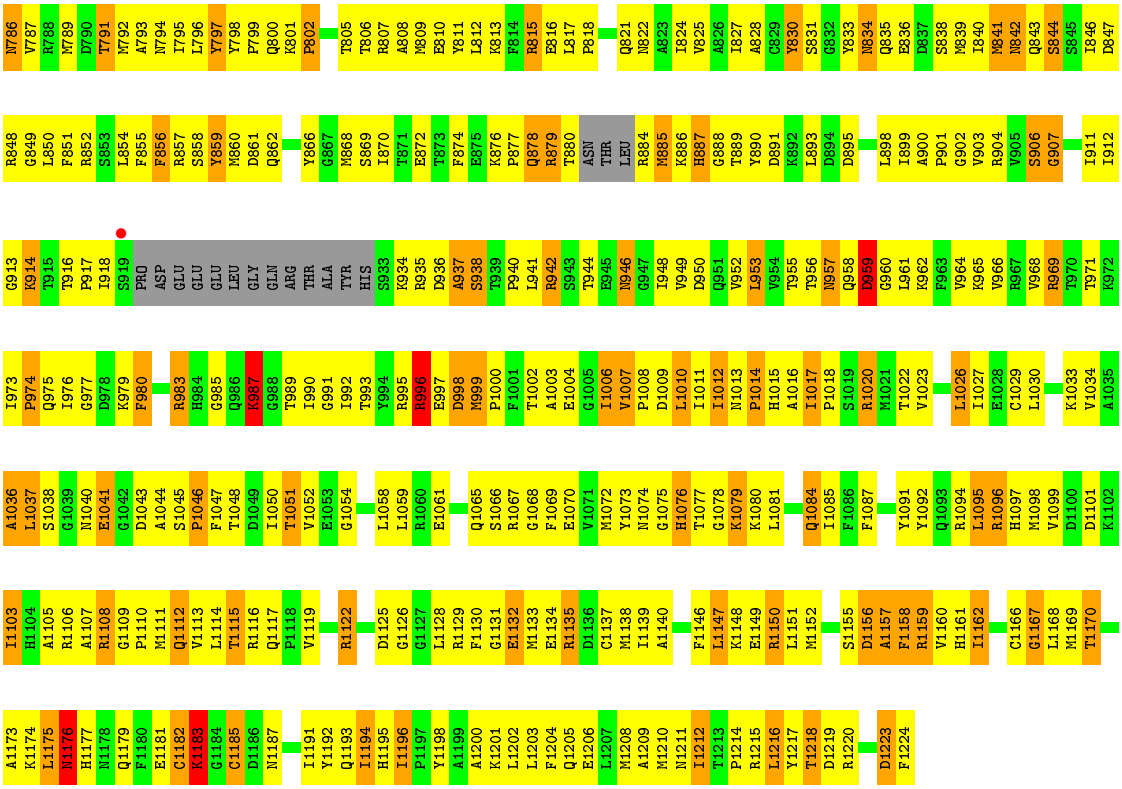


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

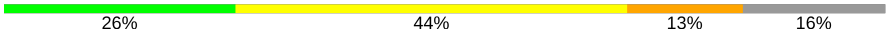


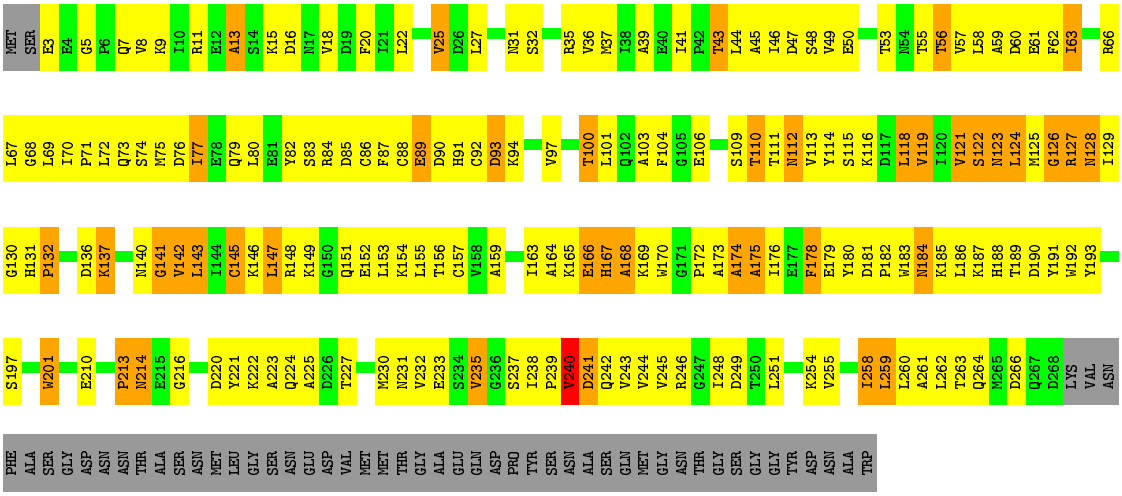




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

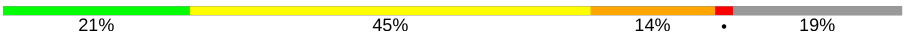
Chain C:

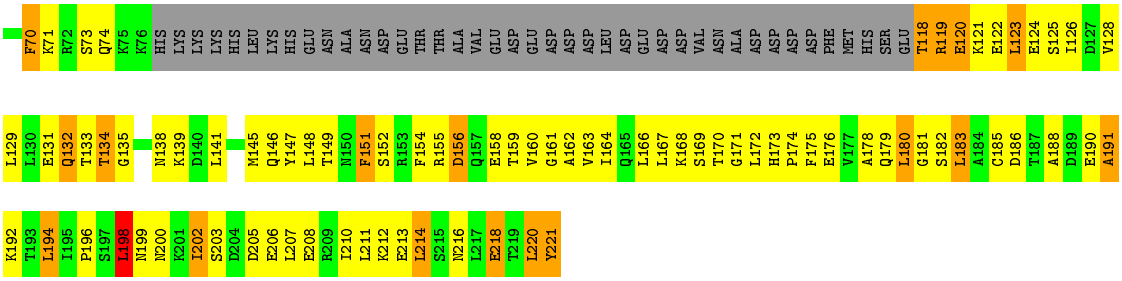




• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

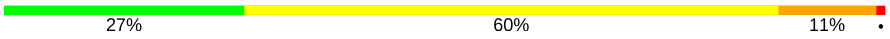
Chain D:

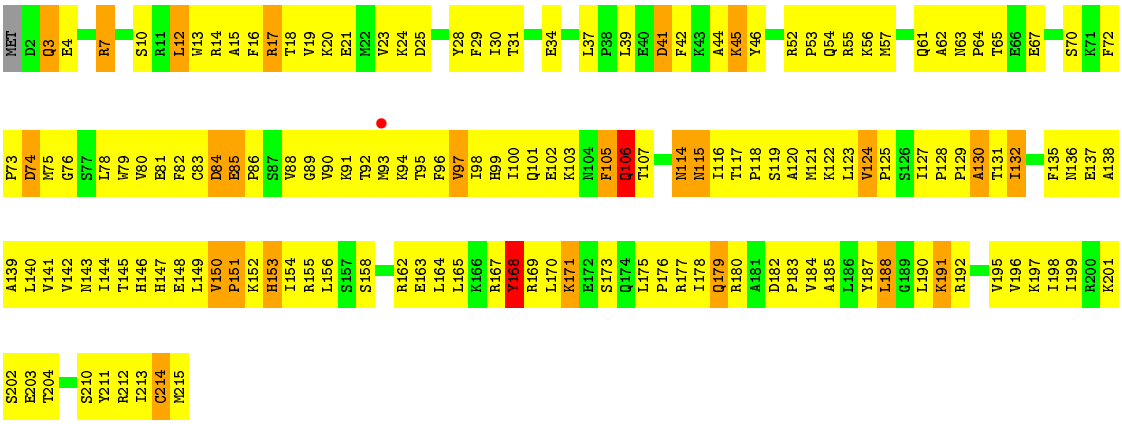




• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

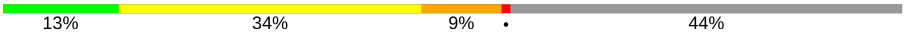
Chain E:

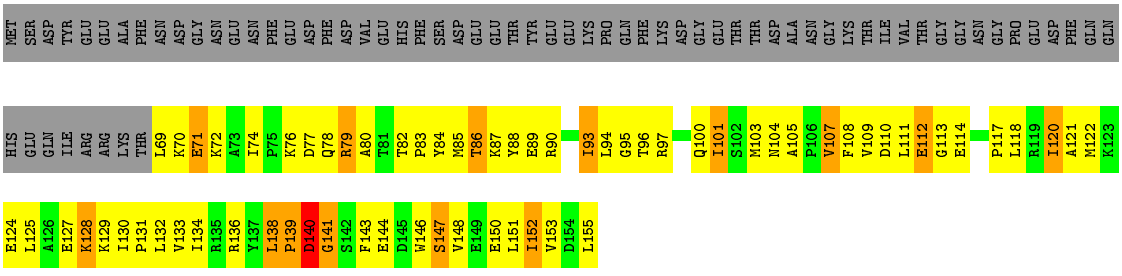




• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

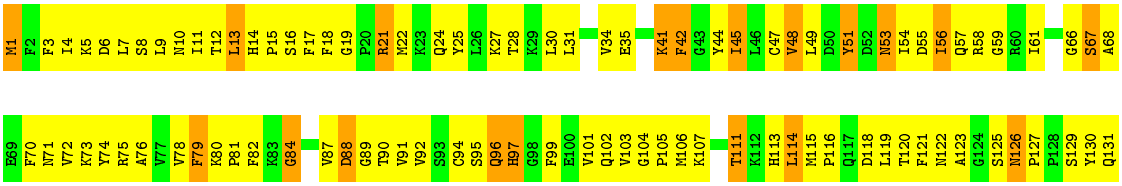
Chain F:

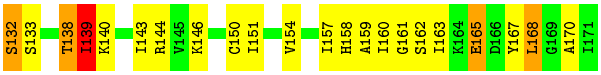




• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

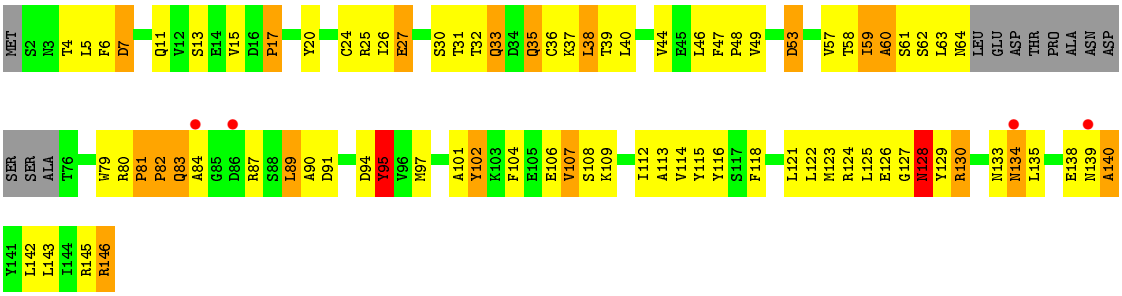
Chain G:





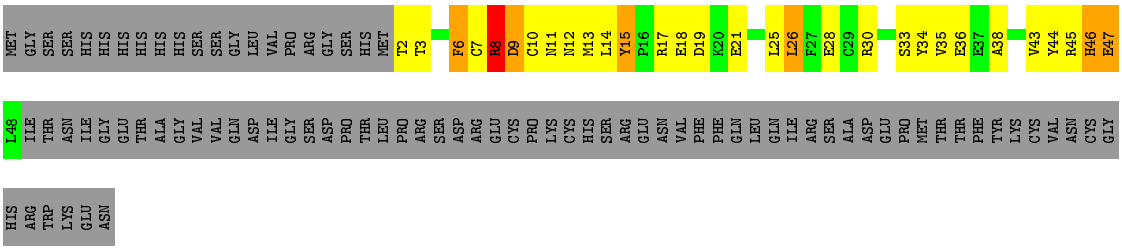
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



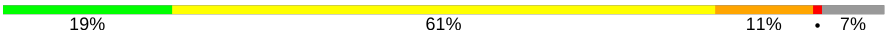
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9, DNA-directed RNA polymerase III subunit RPC10

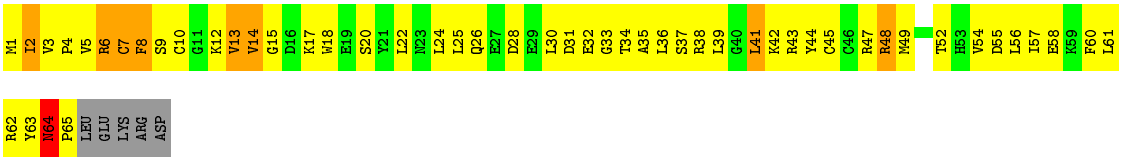
Chain I:



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

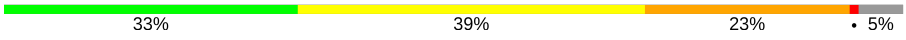
Chain J:

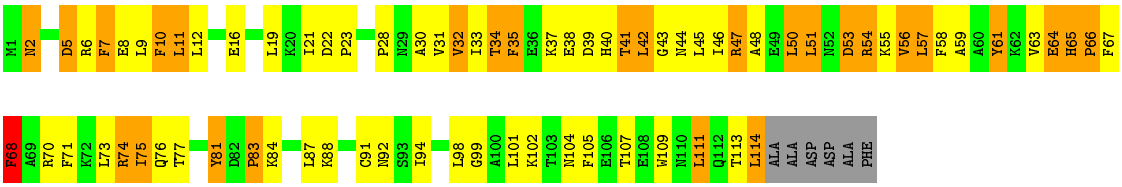




• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

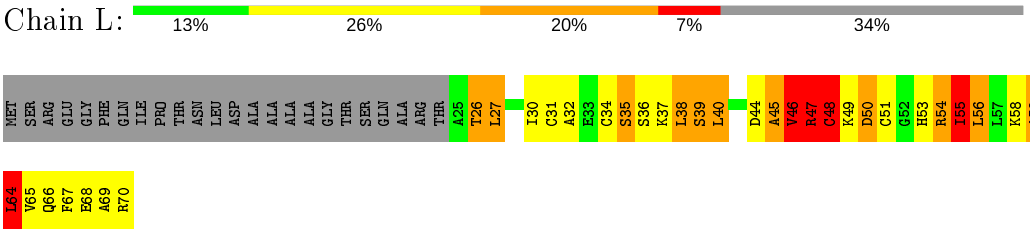
Chain K:





• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:


13%
26%
20%
7%
34%
MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA ALA GLY THR SER GLN ALA ARG THR A25 T26 L27 I30 C31 A32 E33 C34 S35 S36 K37 L38 S39 L40 D44 A45 V46 R47 C48 K49 D50 C51 G52 H53 R54 I55 L56 L57 K58 A59 R60 T61 K62 R63 L64 V65 Q66 F67 E68 A69 R70

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	222.38Å 393.38Å 281.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.60 – 4.30 48.66 – 4.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.60-4.30) 98.5 (48.66-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.235 , 0.281 0.209 , 0.258	Depositor DCC
R_{free} test set	2022 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å^2)	172.3	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 119.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.057 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.067 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	30535	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/11342	0.58	0/15337
2	B	0.34	0/8939	0.56	0/12051
3	C	0.33	0/2133	0.56	0/2891
4	D	0.32	0/1444	0.52	0/1935
5	E	0.32	0/1788	0.54	0/2406
6	F	0.40	0/717	0.63	0/967
7	G	0.33	0/1368	0.55	0/1844
8	H	0.29	0/1094	0.50	0/1481
9	I	0.36	0/406	0.57	0/546
10	J	0.33	0/541	0.57	0/727
11	K	0.38	0/937	0.56	0/1265
12	L	0.36	0/365	0.64	0/485
All	All	0.34	0/31074	0.56	0/41935

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11143	0	11217	1243	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8770	0	8795	984	0
3	C	2095	0	2051	223	0
4	D	1434	0	1460	163	0
5	E	1752	0	1776	172	0
6	F	705	0	731	101	0
7	G	1340	0	1357	153	0
8	H	1076	0	1046	97	0
9	I	398	0	370	37	0
10	J	532	0	542	92	0
11	K	919	0	929	113	0
12	L	363	0	386	65	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	1	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
14	A	1	0	0	0	0
All	All	30535	0	30660	3185	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 52.

All (3185) 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:A:775:ILE:HB	1:A:797:LYS:O	1.37	1.23
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.21	1.17
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.26	1.15
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.17	1.14
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.30	1.13
4:D:134:THR:HG22	4:D:135:GLY:H	1.06	1.10
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.30	1.10
1:A:482:PHE:HB2	2:B:836:GLU:O	1.52	1.09
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.35	1.07
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.14	1.03
2:B:1116:ARG:HG3	2:B:1198:TYR:CD2	1.93	1.03
2:B:295:GLY:H	2:B:298:LEU:HD23	1.19	1.03
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.37	1.02
1:A:855:THR:HG21	1:A:857:ARG:HE	1.23	1.01
11:K:65:HIS:CD2	11:K:67:PHE:H	1.80	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.44	0.99
4:D:66:ARG:HH22	7:G:48:VAL:HG23	1.26	0.98
2:B:210:LYS:HD3	2:B:482:VAL:HG13	1.41	0.98
4:D:188:ALA:HA	4:D:191:ALA:HB3	1.44	0.98
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.44	0.98
2:B:1130:PHE:HE2	2:B:1151:LEU:HD21	1.27	0.97
2:B:706:GLN:HB2	2:B:709:ASP:HB2	1.47	0.97
2:B:273:LEU:HD21	2:B:360:PHE:HD1	1.28	0.96
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.47	0.96
1:A:741:ASN:HD21	1:A:743:VAL:HG23	1.26	0.96
3:C:103:ALA:HB3	3:C:153:LEU:HB3	1.47	0.96
1:A:814:PHE:HD1	2:B:519:TRP:HE3	1.03	0.95
1:A:95:PHE:HD1	1:A:234:MET:HG2	1.30	0.95
7:G:13:LEU:HD21	7:G:17:PHE:HD2	1.32	0.95
2:B:430:ARG:HG2	2:B:430:ARG:HH11	1.29	0.95
1:A:903:ASN:HD22	1:A:905:ASP:H	1.01	0.94
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.45	0.94
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.49	0.94
1:A:361:LEU:HA	1:A:471:ASN:HD22	1.32	0.94
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.47	0.93
2:B:846:ILE:HD13	2:B:974:PRO:HB2	1.51	0.93
2:B:996:ARG:HH22	3:C:175:ALA:H	1.07	0.93
1:A:121:LEU:HD22	1:A:141:LEU:HD21	1.48	0.93
2:B:848:ARG:HH22	2:B:996:ARG:HD2	1.33	0.93
1:A:1156:PRO:HA	1:A:1190:PRO:HB3	1.51	0.93
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.32	0.92
1:A:600:PRO:HG2	1:A:601:LYS:HG3	1.51	0.92
2:B:515:HIS:HD2	2:B:517:THR:H	1.08	0.92
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.51	0.91
2:B:1162:ILE:HD11	2:B:1194:ILE:HG21	1.51	0.91
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.05	0.90
2:B:1034:VAL:HG22	2:B:1059:LEU:HD13	1.51	0.90
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.53	0.90
1:A:95:PHE:CD1	1:A:234:MET:HG2	2.06	0.90
1:A:53:LEU:HD23	1:A:54:ASN:H	1.35	0.90
1:A:591:PHE:HD2	1:A:595:THR:HB	1.34	0.90
7:G:139:ILE:HG23	7:G:140:LYS:HG3	1.53	0.90
1:A:216:VAL:O	1:A:219:PHE:HB2	1.71	0.90
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.54	0.90
8:H:130:ARG:H	8:H:130:ARG:HH11	1.16	0.90
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.53	0.90
2:B:1181:GLU:HA	2:B:1187:ASN:O	1.72	0.89
1:A:265:LYS:HD2	1:A:322:VAL:HG21	1.55	0.89
1:A:254:GLU:HB2	2:B:935:ARG:HH22	1.36	0.89
11:K:65:HIS:HD2	11:K:67:PHE:N	1.70	0.89
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.01	0.89
6:F:90:ARG:HD2	6:F:155:LEU:HD13	1.55	0.89
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.51	0.89
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.55	0.89
2:B:515:HIS:CD2	2:B:517:THR:H	1.90	0.88
4:D:134:THR:HG22	4:D:135:GLY:N	1.87	0.88
2:B:975:GLN:HG3	2:B:976:ILE:H	1.38	0.88
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.56	0.88
2:B:824:ILE:HG12	10:J:48:ARG:NH1	1.88	0.88
11:K:65:HIS:HD2	11:K:67:PHE:H	0.90	0.88
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.54	0.87
4:D:71:LYS:HG3	4:D:74:GLN:HG3	1.54	0.87
1:A:524:VAL:HG12	1:A:525:GLN:H	1.40	0.87
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.57	0.87
1:A:425:GLN:NE2	1:A:425:GLN:H	1.72	0.87
1:A:506:ALA:HB1	1:A:508:PRO:HD2	1.57	0.87
6:F:101:ILE:HD13	6:F:120:ILE:HG21	1.55	0.87
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.22	0.87
2:B:408:LEU:HD11	2:B:545:ILE:HG13	1.55	0.87
4:D:56:ARG:HA	4:D:59:ILE:HD12	1.55	0.87
1:A:814:PHE:CD1	2:B:519:TRP:HE3	1.92	0.86
1:A:506:ALA:HB3	1:A:509:LEU:HG	1.56	0.86
4:D:179:GLN:HE22	7:G:1:MET:HB2	1.38	0.86
11:K:56:VAL:HA	11:K:77:THR:HG22	1.56	0.86
1:A:933:TYR:O	1:A:933:TYR:HD2	1.59	0.85
3:C:115:SER:HB3	3:C:141:GLY:O	1.76	0.85
1:A:1318:THR:HB	5:E:141:VAL:HG11	1.57	0.85
1:A:814:PHE:HD1	2:B:519:TRP:CE3	1.93	0.85
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.58	0.85
3:C:88:CYS:SG	3:C:91:HIS:HA	2.16	0.85
12:L:39:SER:O	12:L:40:LEU:HG	1.77	0.85
2:B:1130:PHE:CE2	2:B:1151:LEU:HD21	2.12	0.84
1:A:492:PRO:HG3	1:A:501:LEU:HD12	1.59	0.84
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.06	0.84
2:B:810:GLU:HA	2:B:815:ARG:HH22	1.42	0.84
10:J:36:LEU:HB2	10:J:47:ARG:NH1	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:PHE:HZ	1:A:1397:LEU:HD21	1.41	0.84
1:A:256:GLN:O	1:A:257:ARG:HB2	1.76	0.84
1:A:35:ILE:HD12	1:A:35:ILE:H	1.42	0.84
1:A:1035:TYR:O	1:A:1036:ARG:HB2	1.77	0.84
2:B:65:GLU:OE1	2:B:418:LYS:HE3	1.76	0.84
1:A:1094:VAL:HG13	1:A:1113:THR:HB	1.57	0.84
1:A:110:CYS:HB2	1:A:167:CYS:SG	2.17	0.84
2:B:613:VAL:HG13	2:B:627:PHE:O	1.77	0.84
4:D:134:THR:CG2	4:D:135:GLY:H	1.89	0.84
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.08	0.84
1:A:40:THR:HB	1:A:41:MET:HG2	1.60	0.84
8:H:4:THR:HA	8:H:60:ALA:HB2	1.58	0.83
9:I:35:VAL:HG12	9:I:36:GLU:H	1.43	0.83
1:A:19:PHE:CZ	1:A:1397:LEU:HD21	2.13	0.83
1:A:770:VAL:HG12	1:A:771:GLU:HG3	1.61	0.83
7:G:13:LEU:HD21	7:G:17:PHE:CD2	2.14	0.83
2:B:405:ARG:HB3	2:B:631:GLY:HA3	1.61	0.83
1:A:868:TYR:HE1	1:A:1064:VAL:HG13	1.43	0.83
2:B:408:LEU:O	2:B:412:LEU:HG	1.79	0.83
2:B:241:ARG:HA	2:B:253:THR:HG22	1.58	0.83
1:A:664:THR:HA	1:A:742:ASN:HD22	1.43	0.82
6:F:100:GLN:O	6:F:105:ALA:HB2	1.80	0.82
11:K:21:ILE:HG12	11:K:33:ILE:HG23	1.58	0.82
1:A:591:PHE:CD2	1:A:595:THR:HB	2.14	0.82
1:A:335:ARG:HD3	1:A:339:ASN:HD22	1.43	0.82
1:A:903:ASN:ND2	1:A:905:ASP:H	1.77	0.82
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.44	0.82
9:I:6:PHE:HA	9:I:14:LEU:HG	1.59	0.82
1:A:954:TRP:CZ3	5:E:203:GLU:HB2	2.15	0.82
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.62	0.82
7:G:158:HIS:HD2	7:G:159:ALA:H	1.25	0.82
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.45	0.82
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.45	0.82
1:A:414:ASP:HB3	1:A:417:TYR:HB2	1.60	0.82
10:J:8:PHE:HD2	10:J:8:PHE:H	1.27	0.82
1:A:107:CYS:HA	1:A:171:GLN:HE22	1.45	0.82
2:B:430:ARG:CG	2:B:430:ARG:HH11	1.93	0.82
2:B:570:VAL:HB	2:B:573:GLN:HB3	1.61	0.82
3:C:166:GLU:O	11:K:6:ARG:HG3	1.80	0.82
12:L:26:THR:HG22	12:L:27:LEU:H	1.44	0.82
2:B:202:TYR:H	2:B:202:TYR:HD2	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:ILE:CB	1:A:797:LYS:O	2.26	0.81
1:A:254:GLU:HB2	2:B:935:ARG:NH2	1.95	0.81
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.62	0.81
2:B:211:VAL:O	2:B:480:SER:HA	1.78	0.81
2:B:406:LEU:HD12	2:B:545:ILE:HD11	1.62	0.81
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.62	0.81
1:A:342:GLY:HA3	2:B:1131:GLY:HA2	1.59	0.81
2:B:345:LYS:HG2	2:B:346:GLU:H	1.44	0.81
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.63	0.81
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.10	0.80
1:A:845:LEU:CD1	1:A:1069:ALA:HB2	2.11	0.80
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.64	0.80
1:A:590:ARG:O	1:A:591:PHE:HB2	1.81	0.80
2:B:1076:HIS:HD2	11:K:40:HIS:CE1	1.99	0.80
3:C:148:ARG:H	3:C:151:GLN:HG3	1.46	0.80
10:J:6:ARG:HA	10:J:12:LYS:O	1.81	0.80
1:A:1354:ASN:O	1:A:1358:SER:HB3	1.81	0.80
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.62	0.80
1:A:332:LYS:HG2	1:A:333:GLU:HG2	1.64	0.80
2:B:801:LYS:O	10:J:52:THR:HG23	1.82	0.80
3:C:118:LEU:HD12	3:C:132:PRO:HG3	1.63	0.80
1:A:362:ASP:HB3	1:A:507:VAL:HG12	1.61	0.80
1:A:868:TYR:CE1	1:A:1064:VAL:HG13	2.17	0.80
2:B:1157:ALA:O	2:B:1158:PHE:HB2	1.82	0.80
2:B:277:LYS:HE2	2:B:336:ARG:C	2.02	0.80
7:G:158:HIS:CD2	7:G:159:ALA:H	1.99	0.80
10:J:1:MET:O	10:J:2:ILE:HG22	1.81	0.80
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.64	0.79
2:B:1158:PHE:HE2	2:B:1160:VAL:HG22	1.47	0.79
4:D:54:GLU:O	4:D:58:VAL:HG23	1.81	0.79
11:K:5:ASP:HB2	11:K:7:PHE:CZ	2.17	0.79
2:B:295:GLY:N	2:B:298:LEU:HD23	1.98	0.79
2:B:843:GLN:HB2	2:B:993:THR:HB	1.64	0.79
2:B:996:ARG:NH2	3:C:175:ALA:H	1.78	0.79
1:A:1094:VAL:HG22	1:A:1113:THR:HG21	1.65	0.79
8:H:102:TYR:H	8:H:102:TYR:HD2	1.28	0.79
3:C:259:LEU:HD21	11:K:92:ASN:OD1	1.83	0.79
4:D:53:SER:HB3	4:D:152:SER:HB3	1.65	0.79
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.63	0.79
8:H:13:SER:HB3	8:H:27:GLU:O	1.83	0.79
7:G:111:THR:HG22	7:G:114:LEU:HD22	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:THR:CG2	1:A:857:ARG:HE	1.95	0.78
4:D:25:ALA:CB	4:D:196:PRO:HG2	2.13	0.78
2:B:94:LYS:HG2	2:B:95:ILE:H	1.48	0.78
1:A:391:LEU:HD23	1:A:400:PRO:O	1.84	0.78
3:C:242:GLN:HE21	3:C:246:ARG:HE	1.27	0.78
4:D:138:ASN:HB3	4:D:141:LEU:HB3	1.65	0.78
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.46	0.78
3:C:184:ASN:HD21	3:C:189:THR:H	1.31	0.78
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.18	0.78
11:K:113:THR:HG22	11:K:114:LEU:H	1.49	0.78
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.19	0.78
2:B:280:ILE:HG23	2:B:284:ILE:HD12	1.66	0.78
7:G:31:LEU:HD22	7:G:48:VAL:HG21	1.64	0.78
1:A:1124:HIS:H	1:A:1124:HIS:CD2	2.02	0.78
2:B:955:THR:HG22	2:B:956:THR:N	1.98	0.78
1:A:1102:LYS:HG2	1:A:1106:ASN:HD21	1.48	0.78
6:F:87:LYS:HG3	6:F:88:TYR:CD1	2.19	0.78
2:B:702:LEU:HD23	2:B:738:PHE:H	1.49	0.77
1:A:1205:LYS:O	1:A:1207:LEU:HG	1.84	0.77
10:J:35:ALA:O	10:J:39:LEU:HD12	1.84	0.77
1:A:134:ARG:HG2	1:A:138:ILE:HD11	1.67	0.77
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.65	0.77
2:B:174:LEU:HD21	2:B:204:ILE:HD11	1.67	0.77
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.67	0.77
3:C:70:ILE:O	3:C:72:LEU:HD12	1.83	0.77
1:A:70:CYS:O	1:A:72:GLU:HG2	1.84	0.77
1:A:899:VAL:HG13	1:A:908:LEU:HD21	1.67	0.77
2:B:326:ASP:O	2:B:330:ALA:HB2	1.85	0.77
1:A:351:THR:HG23	1:A:468:PHE:CE1	2.20	0.77
1:A:66:LYS:HD3	1:A:67:CYS:N	2.00	0.77
1:A:108:MET:HB3	1:A:210:ILE:HD13	1.67	0.77
1:A:34:LYS:HE3	1:A:57:ARG:HH12	1.47	0.77
1:A:881:GLN:NE2	1:A:959:ASN:HA	1.99	0.77
2:B:36:ALA:HA	2:B:39:ARG:HD2	1.65	0.77
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.66	0.77
1:A:336:ILE:HD11	2:B:1203:LEU:CD1	2.15	0.77
2:B:619:ILE:HG22	2:B:620:ARG:HG3	1.66	0.77
3:C:41:ILE:O	3:C:163:ILE:HG22	1.84	0.76
5:E:202:SER:OG	5:E:204:THR:HG22	1.85	0.76
3:C:111:THR:HB	3:C:147:LEU:HG	1.67	0.76
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:VAL:HG22	3:C:157:CYS:SG	2.25	0.76
4:D:56:ARG:HD3	4:D:149:THR:HA	1.65	0.76
7:G:115:MET:HB3	7:G:119:LEU:HD23	1.67	0.76
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.16	0.76
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.66	0.76
1:A:672:ASP:HB3	1:A:736:ASN:HD21	1.51	0.76
2:B:613:VAL:HG22	2:B:628:THR:HA	1.67	0.76
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.68	0.76
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.68	0.76
4:D:206:GLU:O	4:D:210:ILE:HG13	1.85	0.76
10:J:8:PHE:HD2	10:J:8:PHE:N	1.82	0.76
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.68	0.76
2:B:559:SER:HA	2:B:563:MET:HB3	1.66	0.76
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.50	0.76
1:A:855:THR:HG21	1:A:857:ARG:NE	1.99	0.76
1:A:755:PHE:HA	1:A:758:ILE:HD12	1.66	0.76
4:D:15:LEU:O	4:D:17:LYS:HG3	1.85	0.76
1:A:600:PRO:HA	8:H:25:ARG:NH1	2.01	0.75
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.67	0.75
1:A:706:HIS:CD2	1:A:1283:VAL:HG22	2.21	0.75
6:F:100:GLN:HB3	7:G:15:PRO:HB3	1.65	0.75
7:G:55:ASP:HB3	7:G:73:LYS:HB2	1.68	0.75
1:A:79:GLY:HA3	1:A:243:PRO:HB2	1.66	0.75
2:B:824:ILE:CG1	10:J:48:ARG:HH12	1.98	0.75
2:B:616:ILE:HD12	2:B:625:LYS:HB2	1.69	0.75
10:J:48:ARG:HG2	10:J:48:ARG:HH11	1.52	0.75
2:B:351:TYR:O	2:B:355:ILE:HG13	1.85	0.75
2:B:387:LEU:HD23	2:B:393:LYS:HG3	1.69	0.75
1:A:53:LEU:HD23	1:A:54:ASN:HD22	1.49	0.75
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.69	0.75
4:D:25:ALA:HB1	4:D:196:PRO:HG2	1.69	0.75
1:A:606:LEU:HG	1:A:613:ILE:HG13	1.69	0.75
2:B:975:GLN:HG3	2:B:976:ILE:N	2.00	0.75
2:B:1202:LEU:O	2:B:1206:GLU:HG3	1.87	0.74
3:C:56:THR:HG21	3:C:145:CYS:SG	2.27	0.74
1:A:356:ASP:HB3	1:A:359:LEU:HD21	1.68	0.74
1:A:56:PRO:O	1:A:57:ARG:HG3	1.87	0.74
4:D:56:ARG:NH2	4:D:155:ARG:HG2	2.02	0.74
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.68	0.74
1:A:427:GLN:HB2	1:A:430:TRP:CD2	2.21	0.74
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:GLY:HA2	1:A:1228:TRP:HE1	1.50	0.74
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.23	0.74
2:B:1158:PHE:CE2	2:B:1160:VAL:HG22	2.23	0.74
4:D:35:LEU:H	4:D:35:LEU:HD12	1.52	0.74
5:E:44:ALA:O	5:E:45:LYS:HB2	1.87	0.74
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.53	0.74
10:J:64:ASN:CB	10:J:65:PRO:HD3	2.15	0.74
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.70	0.73
4:D:47:LEU:HB3	4:D:174:PRO:HG2	1.70	0.73
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.70	0.73
2:B:1099:VAL:O	2:B:1103:ILE:HG22	1.88	0.73
1:A:283:GLY:O	1:A:285:PRO:HD3	1.88	0.73
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	2.02	0.73
1:A:1148:ILE:O	9:I:47:GLU:HA	1.89	0.73
2:B:406:LEU:O	2:B:408:LEU:HD12	1.88	0.73
4:D:208:GLU:HG3	4:D:212:LYS:HE3	1.69	0.73
2:B:842:ASN:HD21	2:B:844:SER:HB2	1.54	0.73
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.24	0.73
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.16	0.73
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.28	0.73
12:L:49:LYS:O	12:L:50:ASP:HB2	1.87	0.73
2:B:770:GLN:HB2	2:B:985:GLY:H	1.52	0.73
1:A:549:MET:HE1	1:A:656:TRP:CD1	2.23	0.73
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.52	0.73
1:A:115:LEU:HD13	1:A:122:MET:HB2	1.71	0.73
7:G:121:PHE:CZ	7:G:123:ALA:HB2	2.24	0.73
6:F:96:THR:O	6:F:100:GLN:HG3	1.89	0.72
7:G:111:THR:HG22	7:G:114:LEU:HD13	1.70	0.72
1:A:635:ARG:NH1	1:A:635:ARG:HA	2.04	0.72
2:B:794:ASN:C	2:B:795:ILE:HD12	2.09	0.72
4:D:59:ILE:HG22	4:D:63:LEU:HD12	1.71	0.72
5:E:96:PHE:CE1	5:E:100:ILE:HD11	2.24	0.72
1:A:962:ARG:HA	1:A:965:GLN:HG3	1.71	0.72
7:G:129:SER:HB2	7:G:138:THR:HG23	1.71	0.72
2:B:850:LEU:HB2	10:J:8:PHE:HD1	1.55	0.72
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.54	0.72
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.70	0.72
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.55	0.72
2:B:261:ARG:NH1	2:B:261:ARG:HB3	2.05	0.72
1:A:1269:GLU:O	1:A:1270:ASN:HB2	1.90	0.72
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:LYS:O	2:B:347:LYS:HG2	1.89	0.72
1:A:1148:ILE:HB	1:A:1196:GLU:HG2	1.72	0.72
5:E:16:PHE:CE1	5:E:20:LYS:HE3	2.25	0.72
7:G:81:PRO:HG3	7:G:106:MET:SD	2.29	0.72
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.25	0.72
1:A:726:ARG:HD2	1:A:765:VAL:O	1.89	0.72
1:A:853:ASP:OD1	1:A:855:THR:HG22	1.90	0.72
2:B:777:ALA:HA	2:B:1095:LEU:CB	2.19	0.72
2:B:25:ILE:HD11	2:B:651:LEU:HD12	1.71	0.72
3:C:183:TRP:O	3:C:185:LYS:HG3	1.89	0.72
1:A:706:HIS:HD2	1:A:1283:VAL:HG22	1.53	0.72
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.04	0.72
1:A:1304:TRP:O	1:A:1305:VAL:HG23	1.89	0.71
4:D:66:ARG:NH2	7:G:48:VAL:HG23	2.03	0.71
11:K:5:ASP:OD2	11:K:5:ASP:N	2.21	0.71
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.04	0.71
2:B:165:VAL:HG12	2:B:167:ILE:HD11	1.72	0.71
6:F:109:VAL:HG12	6:F:110:ASP:N	2.05	0.71
1:A:1155:ASP:OD2	1:A:1161:THR:HA	1.90	0.71
2:B:457:LEU:O	2:B:461:LEU:HB2	1.90	0.71
7:G:97:HIS:H	7:G:97:HIS:CD2	2.09	0.71
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.55	0.71
7:G:119:LEU:HD12	7:G:131:GLN:O	1.91	0.71
1:A:814:PHE:CE1	2:B:519:TRP:HB2	2.26	0.71
2:B:711:GLU:HB2	2:B:712:PRO:HD3	1.72	0.71
6:F:87:LYS:HG3	6:F:88:TYR:HD1	1.56	0.71
1:A:34:LYS:HE3	1:A:57:ARG:NH1	2.05	0.71
1:A:427:GLN:HB2	1:A:430:TRP:CG	2.26	0.71
1:A:53:LEU:HD23	1:A:54:ASN:N	2.04	0.71
3:C:18:VAL:HG21	11:K:109:TRP:HZ3	1.53	0.71
4:D:51:ASN:HD22	4:D:178:ALA:HA	1.55	0.71
8:H:101:ALA:HB2	8:H:116:TYR:HE2	1.56	0.71
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.52	0.71
1:A:362:ASP:OD1	1:A:459:ARG:HD3	1.91	0.71
2:B:1138:MET:HB2	2:B:1147:LEU:HD21	1.72	0.71
2:B:291:ILE:HG12	2:B:300:HIS:NE2	2.06	0.71
2:B:996:ARG:HH22	3:C:175:ALA:N	1.87	0.71
12:L:27:LEU:HD22	12:L:37:LYS:HD2	1.72	0.71
1:A:1028:THR:O	1:A:1032:LEU:HD12	1.91	0.71
1:A:511:ILE:O	1:A:519:PRO:HA	1.91	0.71
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HD23	2:B:1212:ILE:HG13	1.73	0.70
1:A:535:THR:HG21	1:A:617:VAL:H	1.55	0.70
1:A:901:LEU:H	1:A:926:GLN:NE2	1.89	0.70
2:B:522:VAL:HG12	2:B:523:CYS:N	2.06	0.70
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.21	0.70
7:G:143:ILE:HG12	7:G:170:ALA:HA	1.71	0.70
1:A:947:PHE:CE1	1:A:954:TRP:CE2	2.79	0.70
2:B:745:PRO:O	2:B:748:ILE:HG12	1.91	0.70
3:C:67:LEU:HD23	3:C:70:ILE:HD11	1.72	0.70
4:D:205:ASP:O	4:D:208:GLU:HB3	1.91	0.70
2:B:313:MET:O	2:B:316:PRO:HD2	1.90	0.70
2:B:705:MET:H	2:B:710:LEU:HD12	1.57	0.70
7:G:56:ILE:HG23	7:G:57:GLN:H	1.57	0.70
11:K:47:ARG:HD3	11:K:59:ALA:O	1.91	0.70
1:A:984:LYS:O	1:A:988:LEU:HB2	1.90	0.70
1:A:913:LEU:HD12	1:A:914:GLU:N	2.06	0.70
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.72	0.70
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.56	0.70
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.21	0.70
1:A:265:LYS:O	1:A:269:ILE:HG13	1.91	0.70
2:B:1002:THR:OG1	2:B:1006:ILE:HD12	1.92	0.70
3:C:121:VAL:HG12	3:C:122:SER:N	2.05	0.70
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.72	0.70
2:B:123:THR:OG1	2:B:458:LYS:HE2	1.92	0.70
2:B:573:GLN:O	2:B:575:PRO:HD3	1.91	0.70
2:B:616:ILE:CD1	2:B:625:LYS:HB2	2.21	0.70
1:A:483:ASP:CB	2:B:987:LYS:HG3	2.22	0.70
3:C:242:GLN:NE2	3:C:246:ARG:HE	1.89	0.70
2:B:190:TYR:CE1	10:J:62:ARG:HD3	2.26	0.70
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.73	0.70
4:D:39:ASN:CG	4:D:40:HIS:H	1.94	0.69
11:K:63:VAL:HG23	11:K:63:VAL:O	1.91	0.69
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.20	0.69
6:F:101:ILE:HG22	6:F:117:PRO:HB3	1.74	0.69
1:A:107:CYS:HA	1:A:171:GLN:NE2	2.07	0.69
4:D:188:ALA:HA	4:D:191:ALA:CB	2.22	0.69
4:D:220:LEU:HD23	4:D:221:TYR:H	1.56	0.69
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.75	0.69
1:A:1216:ILE:O	1:A:1219:THR:HG22	1.93	0.69
1:A:463:ILE:HB	1:A:464:PRO:CD	2.22	0.69
1:A:565:ILE:CG2	1:A:567:LYS:HG2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:112:ILE:CG2	8:H:130:ARG:HH22	2.06	0.69
2:B:54:PHE:CZ	2:B:59:LEU:HD13	2.27	0.69
1:A:664:THR:HG23	1:A:664:THR:O	1.93	0.69
2:B:398:ARG:HB2	2:B:398:ARG:CZ	2.22	0.69
4:D:12:ARG:HD3	4:D:14:ARG:HG2	1.74	0.69
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.75	0.69
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.28	0.69
2:B:113:TYR:CD2	2:B:114:PRO:HD2	2.28	0.69
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.74	0.69
7:G:138:THR:HG22	7:G:139:ILE:H	1.58	0.69
8:H:102:TYR:CE2	8:H:115:TYR:HB3	2.28	0.69
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.51	0.69
2:B:780:VAL:O	2:B:817:LEU:HD22	1.93	0.69
3:C:46:ILE:HD12	3:C:67:LEU:HB3	1.75	0.69
1:A:240:PRO:O	1:A:242:PRO:HD3	1.93	0.69
7:G:31:LEU:CD2	7:G:48:VAL:HG21	2.21	0.69
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.28	0.68
6:F:111:LEU:C	6:F:113:GLY:H	1.96	0.68
7:G:21:ARG:HD2	7:G:24:GLN:HB3	1.74	0.68
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.33	0.68
1:A:1217:LYS:O	1:A:1221:LYS:HA	1.92	0.68
1:A:997:LEU:HB3	1:A:1053:PHE:CE2	2.28	0.68
2:B:1007:VAL:HG23	2:B:1008:PRO:HD2	1.74	0.68
3:C:58:LEU:HD21	10:J:57:ILE:HD13	1.75	0.68
1:A:1036:ARG:NH1	1:A:1036:ARG:HG2	2.06	0.68
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.94	0.68
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.28	0.68
4:D:190:GLU:HA	7:G:167:TYR:CD1	2.27	0.68
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.29	0.68
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.76	0.68
5:E:153:HIS:C	5:E:154:ILE:HD12	2.14	0.68
4:D:179:GLN:NE2	7:G:1:MET:HB2	2.07	0.68
11:K:51:LEU:HD11	11:K:59:ALA:HB3	1.76	0.68
3:C:174:ALA:HA	10:J:10:CYS:O	1.94	0.68
3:C:67:LEU:O	3:C:70:ILE:HG13	1.94	0.68
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.29	0.68
3:C:75:MET:HG3	3:C:76:ASP:OD1	1.92	0.68
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.75	0.68
1:A:1101:LEU:HA	1:A:1104:ILE:HD12	1.75	0.68
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.09	0.68
1:A:251:SER:HA	1:A:257:ARG:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:CD2	1:A:54:ASN:HD22	2.06	0.68
1:A:584:ASN:O	1:A:637:LYS:HE2	1.93	0.68
1:A:671:ALA:H	1:A:676:MET:HE3	1.57	0.68
2:B:731:VAL:O	2:B:732:SER:HB2	1.93	0.68
2:B:797:TYR:HB3	2:B:798:TYR:HD2	1.59	0.68
1:A:1404:GLU:O	1:A:1408:ILE:HG13	1.94	0.68
1:A:434:ARG:NH2	1:A:437:MET:HG3	2.09	0.67
3:C:63:ILE:CA	3:C:66:ARG:HG3	2.23	0.67
8:H:26:ILE:HG22	8:H:40:LEU:O	1.94	0.67
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.28	0.67
1:A:492:PRO:O	1:A:493:GLN:NE2	2.26	0.67
1:A:869:GLY:O	5:E:204:THR:HG21	1.94	0.67
2:B:785:TYR:HE2	10:J:60:PHE:CE1	2.12	0.67
11:K:46:ILE:O	11:K:50:LEU:HB2	1.94	0.67
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.76	0.67
4:D:30:GLY:C	4:D:32:GLU:H	1.97	0.67
6:F:111:LEU:HD21	6:F:120:ILE:HD11	1.76	0.67
1:A:34:LYS:CE	1:A:57:ARG:HH12	2.08	0.67
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.76	0.67
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.76	0.67
11:K:113:THR:HG22	11:K:114:LEU:N	2.09	0.67
1:A:666:ILE:HD12	1:A:667:GLY:H	1.60	0.67
1:A:933:TYR:O	1:A:933:TYR:CD2	2.44	0.67
2:B:955:THR:HG22	2:B:956:THR:H	1.60	0.67
2:B:1076:HIS:HD2	11:K:40:HIS:NE2	1.91	0.67
1:A:91:PHE:H	1:A:297:GLN:HE22	1.41	0.67
1:A:330:LYS:O	1:A:334:GLY:HA3	1.95	0.67
1:A:845:LEU:HA	1:A:848:ILE:HD12	1.76	0.67
2:B:973:ILE:HG22	2:B:974:PRO:HD2	1.77	0.67
5:E:15:ALA:HA	5:E:140:LEU:O	1.93	0.67
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.10	0.67
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.10	0.67
5:E:180:ARG:HB2	5:E:215:MET:OXT	1.95	0.67
1:A:1112:LYS:O	1:A:1114:PRO:HD3	1.95	0.67
1:A:219:PHE:CZ	1:A:231:PRO:HD2	2.30	0.67
2:B:102:VAL:HB	2:B:112:LEU:HB2	1.77	0.67
2:B:215:GLN:HB2	2:B:407:ASP:HB2	1.76	0.67
2:B:496:ARG:HH12	2:B:541:LEU:HA	1.60	0.67
3:C:45:ALA:HA	3:C:72:LEU:HD22	1.77	0.67
2:B:1138:MET:CB	2:B:1147:LEU:HD21	2.25	0.67
2:B:817:LEU:N	2:B:818:PRO:HD3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:213:ILE:HG12	5:E:214:CYS:N	2.10	0.67
8:H:139:ASN:O	8:H:140:ALA:HB2	1.95	0.67
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.76	0.67
1:A:649:ILE:O	1:A:653:VAL:HG23	1.95	0.67
1:A:760:GLN:HE21	1:A:765:VAL:HG13	1.59	0.67
1:A:32:VAL:HG23	1:A:33:ALA:H	1.59	0.66
1:A:589:GLN:HA	1:A:605:MET:O	1.94	0.66
1:A:69:THR:HG21	2:B:1174:LYS:NZ	2.08	0.66
2:B:36:ALA:O	2:B:39:ARG:HB2	1.95	0.66
10:J:57:ILE:HG23	10:J:58:GLU:N	2.11	0.66
1:A:1445:ILE:O	1:A:1445:ILE:HD12	1.94	0.66
1:A:262:LEU:HD12	1:A:328:ARG:NH2	2.10	0.66
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.77	0.66
2:B:363:HIS:O	2:B:364:ILE:HB	1.95	0.66
7:G:144:ARG:O	7:G:168:LEU:HD22	1.95	0.66
10:J:12:LYS:O	10:J:14:VAL:HG23	1.95	0.66
2:B:824:ILE:HB	2:B:1009:ASP:OD2	1.94	0.66
2:B:559:SER:HA	2:B:563:MET:CB	2.25	0.66
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.30	0.66
1:A:351:THR:HG23	1:A:468:PHE:CD1	2.31	0.66
6:F:120:ILE:HG22	6:F:121:ALA:N	2.10	0.66
11:K:32:VAL:HG23	11:K:74:ARG:HG3	1.77	0.66
1:A:1138:ILE:O	1:A:1140:HIS:N	2.29	0.66
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.77	0.66
1:A:205:GLU:CD	1:A:205:GLU:H	1.98	0.66
1:A:361:LEU:CA	1:A:471:ASN:HD22	2.07	0.66
1:A:795:GLU:CD	1:A:795:GLU:H	1.99	0.66
2:B:1114:LEU:CD1	2:B:1202:LEU:HD11	2.26	0.66
4:D:40:HIS:ND1	7:G:6:ASP:HB3	2.10	0.66
1:A:494:SER:O	1:A:497:THR:HB	1.96	0.66
2:B:1107:ALA:O	2:B:1108:ARG:CB	2.44	0.66
2:B:643:ASP:OD2	2:B:652:LYS:HE3	1.95	0.66
2:B:806:THR:HG22	2:B:808:ALA:H	1.61	0.66
2:B:886:LYS:HE2	2:B:940:PRO:HG3	1.76	0.66
12:L:47:ARG:O	12:L:48:CYS:HB2	1.95	0.66
1:A:1100:ARG:O	1:A:1104:ILE:HG13	1.96	0.66
1:A:1119:TYR:CD2	1:A:1305:VAL:HG21	2.31	0.66
1:A:359:LEU:HD23	1:A:359:LEU:H	1.59	0.66
2:B:1160:VAL:HG12	2:B:1161:HIS:H	1.59	0.66
2:B:810:GLU:CA	2:B:815:ARG:HH22	2.08	0.66
2:B:878:GLN:H	2:B:934:LYS:HZ3	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:89:GLU:O	6:F:93:ILE:HG13	1.96	0.66
1:A:474:VAL:HG23	1:A:521:MET:HE1	1.78	0.66
2:B:418:LYS:HG2	2:B:422:LYS:HE3	1.78	0.66
7:G:21:ARG:NH1	7:G:24:GLN:HB2	2.10	0.66
1:A:672:ASP:HB3	1:A:736:ASN:ND2	2.10	0.66
2:B:204:ILE:HG23	2:B:207:GLY:O	1.95	0.66
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.77	0.66
3:C:112:ASN:ND2	3:C:146:LYS:HG2	2.10	0.66
4:D:48:ILE:O	4:D:48:ILE:HG22	1.94	0.66
12:L:55:ILE:H	12:L:55:ILE:HD13	1.60	0.66
1:A:1120:LEU:HD22	1:A:1124:HIS:O	1.95	0.65
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.78	0.65
2:B:879:ARG:H	2:B:879:ARG:HE	1.44	0.65
4:D:52:LEU:HD12	4:D:182:SER:HB2	1.76	0.65
1:A:1004:ASN:ND2	1:A:1007:ILE:HG13	2.11	0.65
1:A:350:ARG:N	2:B:1128:LEU:HD11	2.11	0.65
1:A:622:VAL:O	1:A:630:ILE:HD11	1.96	0.65
4:D:66:ARG:O	4:D:70:PHE:HB2	1.96	0.65
6:F:84:TYR:HA	6:F:152:ILE:HD12	1.78	0.65
1:A:58:LEU:CD1	1:A:244:PRO:HD3	2.26	0.65
2:B:1194:ILE:HG12	2:B:1196:ILE:HG22	1.77	0.65
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.77	0.65
2:B:542:MET:SD	2:B:747:MET:HE2	2.37	0.65
2:B:94:LYS:HG2	2:B:95:ILE:N	2.11	0.65
10:J:5:VAL:HA	10:J:15:GLY:H	1.61	0.65
1:A:1453:TYR:CE2	6:F:129:LYS:HA	2.32	0.65
2:B:299:GLU:HB3	2:B:571:PRO:HG2	1.77	0.65
1:A:1434:ALA:O	1:A:1436:ILE:N	2.29	0.65
1:A:63:ARG:CG	1:A:74:MET:HE1	2.26	0.65
2:B:227:LYS:H	2:B:395:GLN:NE2	1.94	0.65
4:D:46:GLU:HG2	4:D:47:LEU:H	1.62	0.65
9:I:45:ARG:HG3	9:I:46:HIS:N	2.12	0.65
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	1.95	0.65
1:A:709:THR:HG22	1:A:710:LEU:N	2.12	0.65
1:A:112:LYS:HG2	1:A:113:LEU:H	1.62	0.65
1:A:1308:THR:HG21	1:A:1310:GLY:O	1.97	0.65
1:A:30:ILE:HD11	2:B:1168:LEU:HD13	1.78	0.65
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.79	0.65
1:A:714:PHE:O	1:A:718:VAL:HG23	1.96	0.65
1:A:966:ASN:O	1:A:970:THR:HB	1.97	0.65
2:B:1065:GLN:HG3	2:B:1068:GLY:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:8:PHE:CZ	4:D:37:GLN:HB2	2.31	0.65
5:E:198:ILE:HD13	5:E:212:ARG:HH11	1.62	0.65
1:A:1223:ASP:HA	1:A:1243:VAL:CG2	2.27	0.65
1:A:864:ILE:HD12	1:A:864:ILE:N	2.11	0.65
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.31	0.65
2:B:488:TYR:HE2	2:B:813:LYS:HB2	1.61	0.65
5:E:78:LEU:HG	5:E:107:THR:HG21	1.77	0.65
6:F:94:LEU:HD21	6:F:122:MET:HG2	1.76	0.65
1:A:59:GLY:C	1:A:244:PRO:HG2	2.16	0.65
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.80	0.65
3:C:55:THR:OG1	3:C:152:GLU:N	2.30	0.65
3:C:197:SER:O	3:C:201:TRP:HB2	1.97	0.65
2:B:780:VAL:HG11	10:J:56:LEU:CD1	2.27	0.65
1:A:1027:ALA:O	1:A:1031:VAL:HG23	1.96	0.65
1:A:532:ARG:HD2	1:A:749:ALA:HB2	1.77	0.65
3:C:112:ASN:ND2	3:C:143:LEU:HD21	2.12	0.65
1:A:1280:GLU:O	1:A:1282:VAL:HG23	1.97	0.64
1:A:456:MET:HE3	1:A:507:VAL:HG23	1.79	0.64
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.31	0.64
1:A:2:VAL:O	2:B:1158:PHE:HA	1.97	0.64
2:B:549:THR:HG22	2:B:550:ASP:H	1.61	0.64
2:B:638:PHE:CE1	2:B:743:ILE:HA	2.32	0.64
1:A:537:ARG:HD2	8:H:20:TYR:CZ	2.32	0.64
1:A:982:THR:HG22	1:A:984:LYS:H	1.61	0.64
1:A:467:THR:HG21	2:B:976:ILE:HG22	1.79	0.64
1:A:58:LEU:HD12	1:A:244:PRO:HD3	1.78	0.64
2:B:169:ARG:O	2:B:457:LEU:HD12	1.98	0.64
2:B:430:ARG:HG2	2:B:430:ARG:NH1	2.04	0.64
2:B:807:ARG:HG2	2:B:1045:SER:OG	1.97	0.64
5:E:10:SER:O	5:E:13:TRP:HB3	1.97	0.64
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.79	0.64
1:A:642:CYS:O	1:A:645:LEU:HB3	1.97	0.64
5:E:100:ILE:HG23	5:E:105:PHE:CD1	2.32	0.64
5:E:61:GLN:HG2	5:E:62:ALA:H	1.63	0.64
1:A:1118:VAL:O	1:A:1305:VAL:HG13	1.97	0.64
5:E:19:VAL:O	5:E:23:VAL:HG23	1.97	0.64
1:A:135:PHE:HD1	1:A:222:LEU:CD2	2.10	0.64
1:A:441:PRO:HG2	1:A:498:ARG:HB2	1.79	0.64
2:B:1162:ILE:CD1	2:B:1194:ILE:HG21	2.27	0.64
5:E:187:TYR:HD2	5:E:188:LEU:CD2	2.11	0.64
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1226:VAL:HG22	1:A:1240:CYS:HB3	1.80	0.64
2:B:1096:ARG:HG2	2:B:1097:HIS:H	1.61	0.64
2:B:213:ILE:CG2	2:B:499:ASN:HB2	2.27	0.64
2:B:798:TYR:CE1	10:J:4:PRO:HB3	2.33	0.64
2:B:955:THR:CG2	2:B:956:THR:N	2.61	0.64
7:G:158:HIS:HD2	7:G:159:ALA:N	1.96	0.64
11:K:23:PRO:HA	11:K:31:VAL:HG13	1.80	0.64
1:A:332:LYS:HA	1:A:337:ARG:HB3	1.80	0.64
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.80	0.64
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.79	0.64
1:A:91:PHE:HZ	1:A:207:ILE:HD12	1.62	0.64
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.28	0.64
2:B:619:ILE:HG22	2:B:620:ARG:N	2.13	0.64
1:A:115:LEU:HB3	1:A:122:MET:HG2	1.79	0.64
11:K:46:ILE:HG22	11:K:50:LEU:HD12	1.78	0.64
11:K:65:HIS:CD2	11:K:67:PHE:N	2.55	0.64
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.80	0.63
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.98	0.63
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.79	0.63
2:B:69:LEU:HB3	2:B:429:PHE:HE1	1.63	0.63
2:B:1116:ARG:HG3	2:B:1198:TYR:CE2	2.32	0.63
2:B:948:ILE:HG22	2:B:949:VAL:O	1.98	0.63
4:D:194:LEU:HD23	4:D:194:LEU:N	2.13	0.63
1:A:1223:ASP:HA	1:A:1243:VAL:HG21	1.80	0.63
3:C:182:PRO:HD2	3:C:210:GLU:OE1	1.98	0.63
3:C:191:TYR:CD2	3:C:201:TRP:CD1	2.87	0.63
1:A:93:VAL:HG21	1:A:304:MET:HB2	1.80	0.63
8:H:82:PRO:C	8:H:84:ALA:H	2.00	0.63
12:L:66:GLN:C	12:L:67:PHE:CD1	2.72	0.63
1:A:336:ILE:HD11	2:B:1203:LEU:HD13	1.79	0.63
1:A:685:GLU:HG3	1:A:686:ALA:N	2.12	0.63
3:C:260:LEU:O	3:C:264:GLN:HG3	1.98	0.63
5:E:41:ASP:HA	5:E:44:ALA:HB3	1.79	0.63
1:A:256:GLN:O	1:A:257:ARG:CB	2.47	0.63
1:A:997:LEU:HD22	1:A:1053:PHE:CG	2.33	0.63
2:B:702:LEU:HD23	2:B:738:PHE:N	2.14	0.63
4:D:159:THR:O	4:D:163:VAL:HG23	1.98	0.63
4:D:163:VAL:HG13	4:D:214:LEU:HD21	1.79	0.63
4:D:60:LYS:O	4:D:64:VAL:HG23	1.98	0.63
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.80	0.63
7:G:42:PHE:O	7:G:80:LYS:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.33	0.63
2:B:859:TYR:HD1	2:B:859:TYR:H	1.47	0.63
1:A:265:LYS:HE3	1:A:265:LYS:CA	2.27	0.63
2:B:277:LYS:HG3	2:B:336:ARG:HG2	1.79	0.63
2:B:696:GLU:O	2:B:699:GLU:HB2	1.97	0.63
1:A:999:VAL:HG12	1:A:1000:LEU:HG	1.79	0.63
1:A:1227:ILE:HA	1:A:1228:TRP:CE3	2.34	0.63
1:A:59:GLY:CA	1:A:244:PRO:HG2	2.29	0.63
1:A:634:THR:O	1:A:638:GLY:HA2	1.99	0.63
10:J:25:LEU:HD21	10:J:32:GLU:HG3	1.81	0.63
11:K:40:HIS:NE2	11:K:63:VAL:HG11	2.13	0.63
12:L:53:HIS:HB3	12:L:55:ILE:HD13	1.80	0.63
1:A:767:GLN:NE2	1:A:774:ARG:HB2	2.14	0.62
2:B:650:GLU:HG3	2:B:651:LEU:N	2.14	0.62
5:E:117:THR:HB	5:E:120:ALA:HB2	1.81	0.62
11:K:45:LEU:O	11:K:48:ALA:HB3	1.99	0.62
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.81	0.62
1:A:350:ARG:C	1:A:351:THR:HG22	2.18	0.62
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.28	0.62
1:A:535:THR:HG21	1:A:616:VAL:HA	1.80	0.62
2:B:126:SER:OG	2:B:172:ILE:HD11	1.98	0.62
2:B:948:ILE:O	2:B:968:VAL:HG13	1.99	0.62
8:H:127:GLY:O	8:H:128:ASN:HB2	1.98	0.62
1:A:1107:VAL:CG2	1:A:1383:SER:HB3	2.29	0.62
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.79	0.62
2:B:613:VAL:CG2	2:B:628:THR:HA	2.30	0.62
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.35	0.62
6:F:129:LYS:C	6:F:130:ILE:HG13	2.20	0.62
10:J:48:ARG:HD2	10:J:48:ARG:O	1.99	0.62
1:A:1402:PHE:C	1:A:1403:GLU:HG2	2.19	0.62
1:A:82:GLY:O	1:A:241:VAL:HB	1.99	0.62
1:A:262:LEU:HD12	1:A:328:ARG:CZ	2.30	0.62
1:A:403:LYS:O	1:A:415:LEU:HB2	2.00	0.62
3:C:169:LYS:HZ2	12:L:69:ALA:HB3	1.64	0.62
6:F:128:LYS:HD3	6:F:148:VAL:O	1.98	0.62
7:G:30:LEU:HD13	7:G:72:VAL:HG11	1.81	0.62
9:I:46:HIS:O	9:I:47:GLU:HG2	1.99	0.62
1:A:377:PRO:HB2	1:A:431:LYS:NZ	2.15	0.62
2:B:770:GLN:HG2	2:B:983:ARG:O	2.00	0.62
4:D:147:TYR:O	4:D:151:PHE:CD1	2.51	0.62
6:F:100:GLN:O	6:F:105:ALA:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:PHE:HE1	2:B:519:TRP:HB2	1.64	0.62
5:E:156:LEU:HG	5:E:195:VAL:O	2.00	0.62
7:G:17:PHE:CE2	7:G:25:TYR:HE2	2.16	0.62
4:D:147:TYR:O	4:D:151:PHE:HD1	1.82	0.62
8:H:145:ARG:O	8:H:146:ARG:HB2	1.99	0.62
1:A:1119:TYR:HA	1:A:1305:VAL:HG22	1.80	0.62
1:A:1207:LEU:HD13	1:A:1273:LEU:HD23	1.82	0.62
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.65	0.62
1:A:49:LYS:NZ	1:A:61:ILE:H	1.98	0.62
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.34	0.62
2:B:638:PHE:HA	2:B:690:VAL:HG12	1.81	0.62
2:B:898:LEU:HD21	2:B:964:VAL:HG21	1.82	0.62
4:D:167:LEU:C	4:D:169:SER:H	2.03	0.62
5:E:16:PHE:CZ	5:E:20:LYS:HE3	2.34	0.62
7:G:90:THR:HG23	7:G:140:LYS:O	2.00	0.62
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.82	0.62
1:A:1210:GLY:HA2	1:A:1228:TRP:NE1	2.14	0.62
1:A:58:LEU:HB3	1:A:80:HIS:O	1.99	0.62
3:C:220:ASP:OD2	3:C:223:ALA:HB2	2.00	0.62
5:E:61:GLN:HG2	5:E:62:ALA:N	2.14	0.62
2:B:174:LEU:HD21	2:B:204:ILE:CD1	2.29	0.62
2:B:879:ARG:N	2:B:879:ARG:HE	1.97	0.62
11:K:53:ASP:HB3	11:K:56:VAL:HB	1.82	0.62
1:A:1107:VAL:HG23	1:A:1383:SER:HB3	1.80	0.61
1:A:604:GLY:O	1:A:605:MET:HB2	2.00	0.61
2:B:515:HIS:HD2	2:B:517:THR:N	1.90	0.61
5:E:119:SER:O	5:E:122:LYS:HB2	2.00	0.61
1:A:1154:TYR:CZ	1:A:1156:PRO:HG3	2.34	0.61
1:A:506:ALA:CB	1:A:508:PRO:HD2	2.28	0.61
1:A:40:THR:HG23	1:A:54:ASN:HD21	1.63	0.61
1:A:601:LYS:HD3	1:A:603:ASN:HD21	1.65	0.61
9:I:35:VAL:HG12	9:I:36:GLU:N	2.12	0.61
1:A:1153:TYR:HB2	1:A:1192:LEU:HD23	1.81	0.61
1:A:224:PHE:HD2	1:A:231:PRO:HD3	1.63	0.61
1:A:317:LYS:O	1:A:318:SER:HB3	1.99	0.61
1:A:419:LYS:HG3	1:A:420:ARG:N	2.14	0.61
1:A:621:THR:O	1:A:629:LEU:HB2	2.00	0.61
3:C:237:SER:O	3:C:238:ILE:HG13	1.99	0.61
11:K:63:VAL:O	11:K:65:HIS:N	2.33	0.61
2:B:486:TYR:CD1	2:B:1096:ARG:NH2	2.68	0.61
2:B:234:ILE:HG12	2:B:257:LYS:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:45:ILE:O	7:G:45:ILE:HG22	1.99	0.61
2:B:105:SER:O	2:B:106:ASP:HB2	1.99	0.61
2:B:68:THR:HG22	2:B:91:SER:HA	1.82	0.61
3:C:3:GLU:HB3	11:K:104:ASN:HD21	1.65	0.61
4:D:29:LEU:HD23	4:D:33:PHE:HB3	1.81	0.61
8:H:130:ARG:HH11	8:H:130:ARG:N	1.92	0.61
12:L:62:LYS:O	12:L:64:LEU:N	2.32	0.61
1:A:1146:VAL:O	1:A:1197:LEU:HA	2.00	0.61
1:A:253:ASN:HB2	2:B:884:ARG:NH1	2.14	0.61
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.36	0.61
2:B:999:MET:HG2	2:B:1007:VAL:CG2	2.30	0.61
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.36	0.61
2:B:309:GLN:O	2:B:312:GLU:HB3	2.00	0.61
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.30	0.61
2:B:955:THR:CG2	2:B:956:THR:H	2.12	0.61
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.83	0.61
12:L:47:ARG:HH21	12:L:54:ARG:HG2	1.65	0.61
1:A:1079:MET:HG2	1:A:1359:ASP:OD1	2.01	0.61
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.16	0.61
5:E:178:ILE:HB	5:E:212:ARG:HD3	1.82	0.61
6:F:111:LEU:O	6:F:113:GLY:N	2.33	0.61
9:I:17:ARG:HG3	9:I:18:GLU:H	1.65	0.61
3:C:262:LEU:HD13	11:K:88:LYS:HG2	1.82	0.61
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.82	0.61
1:A:969:GLN:O	1:A:969:GLN:HG2	2.01	0.61
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.14	0.61
2:B:644:GLU:HG3	2:B:646:LEU:H	1.66	0.61
2:B:656:GLY:O	2:B:660:LYS:HB2	1.99	0.61
7:G:13:LEU:HD23	7:G:14:HIS:N	2.15	0.61
9:I:25:LEU:CB	9:I:38:ALA:HB2	2.11	0.61
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.82	0.61
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.81	0.61
1:A:1255:GLU:CD	1:A:1258:HIS:HB2	2.20	0.61
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.35	0.61
1:A:321:PRO:O	1:A:322:VAL:HG12	2.00	0.61
1:A:370:ILE:HG22	1:A:374:LEU:CD1	2.30	0.61
1:A:873:MET:O	1:A:1058:VAL:HG23	2.01	0.61
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.81	0.61
2:B:999:MET:HE3	2:B:999:MET:HA	1.81	0.61
3:C:124:LEU:HD23	3:C:127:ARG:H	1.65	0.61
3:C:80:LEU:HD12	3:C:94:LYS:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.82	0.61
1:A:1259:MET:O	1:A:1263:ILE:HG13	2.01	0.61
1:A:27:VAL:C	1:A:29:ALA:H	2.04	0.61
1:A:648:ASN:O	1:A:652:VAL:HG23	2.00	0.61
2:B:791:THR:HA	2:B:858:SER:HB2	1.82	0.61
3:C:186:LEU:HD21	3:C:225:ALA:HB2	1.82	0.61
4:D:120:GLU:O	4:D:123:LEU:HB2	2.01	0.61
8:H:59:ILE:O	8:H:60:ALA:HB3	2.01	0.61
1:A:709:THR:HG22	1:A:710:LEU:H	1.66	0.60
2:B:1079:LYS:HZ2	3:C:188:HIS:CE1	2.18	0.60
7:G:30:LEU:CD1	7:G:72:VAL:HG11	2.31	0.60
10:J:8:PHE:CD2	10:J:8:PHE:N	2.56	0.60
1:A:1263:ILE:HA	1:A:1266:THR:HB	1.83	0.60
1:A:219:PHE:CE2	1:A:231:PRO:HD2	2.36	0.60
1:A:42:ASP:HB3	1:A:45:GLN:HA	1.83	0.60
1:A:463:ILE:CB	1:A:464:PRO:HD2	2.27	0.60
1:A:741:ASN:ND2	1:A:743:VAL:N	2.49	0.60
2:B:1096:ARG:HB2	2:B:1096:ARG:CZ	2.30	0.60
2:B:168:GLY:H	2:B:450:ALA:HB1	1.65	0.60
8:H:104:PHE:CE2	8:H:114:VAL:HG12	2.36	0.60
2:B:1013:ASN:HD21	2:B:1015:HIS:HD2	1.48	0.60
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.37	0.60
6:F:100:GLN:NE2	7:G:18:PHE:HE2	1.99	0.60
1:A:1010:ALA:O	1:A:1013:ASP:HB2	2.00	0.60
1:A:106:VAL:HG13	1:A:112:LYS:O	2.01	0.60
1:A:1227:ILE:C	1:A:1228:TRP:HE3	2.04	0.60
1:A:75:ASN:O	1:A:76:GLU:CB	2.48	0.60
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.82	0.60
2:B:777:ALA:HA	2:B:1095:LEU:HB3	1.82	0.60
2:B:493:SER:HA	2:B:751:VAL:HG21	1.82	0.60
7:G:120:THR:OG1	7:G:131:GLN:HB2	2.00	0.60
1:A:102:VAL:HG11	1:A:211:PHE:HE1	1.66	0.60
1:A:359:LEU:HD23	1:A:359:LEU:N	2.15	0.60
2:B:549:THR:HG22	2:B:550:ASP:N	2.17	0.60
9:I:17:ARG:HH21	9:I:30:ARG:NH2	2.00	0.60
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.83	0.60
1:A:49:LYS:HZ2	1:A:61:ILE:H	1.48	0.60
1:A:679:ILE:HD11	1:A:733:ALA:HB2	1.82	0.60
1:A:84:ILE:HG22	1:A:84:ILE:O	2.01	0.60
2:B:959:ASP:OD2	2:B:961:LEU:HD12	2.02	0.60
7:G:51:TYR:O	7:G:51:TYR:CD2	2.55	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1349:TYR:O	1:A:1350:LYS:C	2.40	0.60
1:A:744:LYS:O	1:A:748:MET:HB2	2.01	0.60
2:B:210:LYS:HD2	2:B:480:SER:OG	2.01	0.60
2:B:508:LEU:O	2:B:509:ALA:HB3	2.01	0.60
2:B:841:MET:HG2	2:B:846:ILE:HD11	1.84	0.60
4:D:190:GLU:O	4:D:194:LEU:HG	2.01	0.60
8:H:102:TYR:N	8:H:102:TYR:HD2	1.98	0.60
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.83	0.60
1:A:1152:ILE:HG23	1:A:1260:LEU:HD23	1.81	0.60
6:F:86:THR:HG23	6:F:89:GLU:CD	2.23	0.60
12:L:38:LEU:O	12:L:39:SER:CB	2.49	0.60
1:A:118:HIS:O	1:A:119:ASN:HB2	2.01	0.60
1:A:528:LEU:HG	1:A:529:CYS:N	2.16	0.60
5:E:14:ARG:HB3	5:E:141:VAL:O	2.02	0.60
5:E:56:LYS:HE2	5:E:84:ASP:HB2	1.84	0.60
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.83	0.60
1:A:346:ASP:OD1	2:B:1108:ARG:HA	2.02	0.60
3:C:121:VAL:HG12	3:C:122:SER:H	1.66	0.60
4:D:8:PHE:HZ	4:D:37:GLN:HB2	1.67	0.60
1:A:1208:THR:HG23	1:A:1231:ASP:OD2	2.02	0.59
1:A:135:PHE:HA	1:A:138:ILE:HD12	1.83	0.59
1:A:49:LYS:HD3	1:A:54:ASN:O	2.02	0.59
2:B:1023:VAL:HG12	2:B:1027:ILE:HD11	1.82	0.59
2:B:879:ARG:N	2:B:879:ARG:NE	2.49	0.59
4:D:192:LYS:HG2	4:D:198:LEU:HD12	1.83	0.59
5:E:122:LYS:O	5:E:123:LEU:HG	2.02	0.59
6:F:109:VAL:HG12	6:F:110:ASP:H	1.65	0.59
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.67	0.59
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.83	0.59
2:B:126:SER:CB	2:B:172:ILE:HD11	2.32	0.59
2:B:652:LYS:HD3	2:B:688:GLY:O	2.01	0.59
3:C:13:ALA:HB1	3:C:18:VAL:HG22	1.83	0.59
4:D:59:ILE:O	4:D:63:LEU:HB2	2.02	0.59
5:E:124:VAL:O	5:E:132:ILE:HD13	2.02	0.59
5:E:55:ARG:C	5:E:57:MET:H	2.05	0.59
6:F:111:LEU:HD23	6:F:114:GLU:O	2.02	0.59
6:F:140:ASP:CG	6:F:141:GLY:N	2.56	0.59
7:G:158:HIS:CD2	7:G:159:ALA:N	2.69	0.59
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.83	0.59
3:C:147:LEU:N	3:C:147:LEU:HD23	2.16	0.59
3:C:163:ILE:HD12	3:C:165:LYS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:25:LEU:HB3	9:I:38:ALA:CB	2.11	0.59
9:I:6:PHE:N	9:I:6:PHE:CD1	2.69	0.59
11:K:65:HIS:CD2	11:K:65:HIS:C	2.76	0.59
1:A:66:LYS:HD3	1:A:67:CYS:H	1.67	0.59
1:A:979:SER:OG	1:A:980:ASP:N	2.35	0.59
3:C:241:ASP:O	3:C:244:VAL:HB	2.02	0.59
5:E:79:TRP:HD1	5:E:96:PHE:HE1	1.49	0.59
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.16	0.59
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.83	0.59
1:A:883:LEU:HD23	1:A:1021:LEU:HD13	1.84	0.59
2:B:188:ASP:O	2:B:192:LEU:HD12	2.03	0.59
2:B:446:LEU:O	2:B:447:ALA:HB3	2.03	0.59
2:B:880:THR:HB	2:B:934:LYS:HB2	1.85	0.59
11:K:16:GLU:OE1	11:K:37:LYS:HE3	2.02	0.59
1:A:1094:VAL:HG22	1:A:1113:THR:CG2	2.32	0.59
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.85	0.59
1:A:916:GLY:O	1:A:919:ILE:HG22	2.03	0.59
1:A:923:LEU:O	1:A:927:VAL:HG23	2.03	0.59
2:B:596:LEU:HD11	2:B:600:LEU:HD11	1.85	0.59
2:B:734:HIS:O	2:B:735:ALA:CB	2.51	0.59
2:B:872:GLU:OE1	2:B:914:LYS:HE3	2.02	0.59
8:H:63:LEU:HB3	8:H:90:ALA:H	1.68	0.59
11:K:53:ASP:CB	11:K:56:VAL:HB	2.33	0.59
1:A:597:LEU:O	1:A:598:LEU:HB2	2.02	0.59
2:B:1110:PRO:HG2	2:B:1125:ASP:O	2.03	0.59
3:C:167:HIS:ND1	3:C:169:LYS:HG2	2.18	0.59
5:E:152:LYS:HG3	5:E:154:ILE:HD11	1.85	0.59
1:A:12:ARG:CB	2:B:1218:THR:HG22	2.33	0.59
1:A:92:HIS:HB3	1:A:95:PHE:HB2	1.85	0.59
2:B:115:GLN:O	2:B:119:LEU:HD12	2.02	0.59
2:B:100:PRO:HA	2:B:126:SER:HB3	1.83	0.59
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.38	0.59
4:D:73:SER:HB3	7:G:21:ARG:HH21	1.68	0.59
1:A:35:ILE:HG12	1:A:241:VAL:HG11	1.85	0.59
1:A:306:ASN:HD22	1:A:322:VAL:HG12	1.67	0.59
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.83	0.59
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.03	0.59
2:B:1195:HIS:C	2:B:1196:ILE:HG22	2.24	0.59
4:D:53:SER:HB3	4:D:152:SER:CB	2.33	0.59
1:A:356:ASP:OD2	2:B:833:TYR:HE2	1.86	0.58
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ILE:N	2:B:205:ILE:HD12	2.18	0.58
2:B:597:MET:CE	2:B:597:MET:HA	2.32	0.58
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.85	0.58
2:B:728:ARG:HH11	2:B:730:ARG:NH2	2.01	0.58
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.85	0.58
2:B:957:ASN:H	2:B:957:ASN:HD22	1.50	0.58
1:A:1343:ALA:HA	5:E:149:LEU:O	2.03	0.58
7:G:49:LEU:HG	7:G:76:ALA:HA	1.85	0.58
10:J:36:LEU:O	10:J:41:LEU:HG	2.02	0.58
2:B:1034:VAL:HA	2:B:1037:LEU:CD1	2.32	0.58
2:B:1159:ARG:NH1	2:B:1159:ARG:HB3	2.15	0.58
2:B:815:ARG:HH11	2:B:815:ARG:HB2	1.68	0.58
3:C:112:ASN:HD21	3:C:146:LYS:HE2	1.67	0.58
6:F:100:GLN:NE2	7:G:61:ILE:HD11	2.17	0.58
7:G:9:LEU:HD12	7:G:10:ASN:N	2.19	0.58
1:A:1226:VAL:HG13	1:A:1239:ARG:O	2.03	0.58
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.68	0.58
2:B:1174:LYS:HB2	2:B:1179:GLN:O	2.02	0.58
2:B:119:LEU:HD23	2:B:953:LEU:HD11	1.85	0.58
2:B:681:TRP:CE3	2:B:684:LEU:HD12	2.38	0.58
2:B:901:PRO:HG3	2:B:952:VAL:HG23	1.84	0.58
4:D:147:TYR:CZ	7:G:103:VAL:HG13	2.38	0.58
2:B:308:TRP:CH2	9:I:45:ARG:HG2	2.37	0.58
1:A:1012:ARG:O	1:A:1013:ASP:C	2.42	0.58
1:A:1316:VAL:O	1:A:1316:VAL:HG12	2.03	0.58
1:A:392:VAL:HG13	1:A:415:LEU:HD21	1.85	0.58
2:B:663:ALA:O	2:B:667:GLN:HG3	2.04	0.58
2:B:69:LEU:HD13	2:B:429:PHE:CD1	2.37	0.58
3:C:242:GLN:HE21	3:C:246:ARG:NE	1.99	0.58
11:K:70:ARG:O	11:K:70:ARG:HG3	2.02	0.58
1:A:148:CYS:O	1:A:168:GLY:HA2	2.03	0.58
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.84	0.58
2:B:912:ILE:HD11	2:B:966:VAL:CG2	2.34	0.58
6:F:77:ASP:O	6:F:78:GLN:HB3	2.02	0.58
7:G:51:TYR:HD2	7:G:51:TYR:O	1.86	0.58
8:H:59:ILE:HG22	8:H:60:ALA:N	2.18	0.58
1:A:973:ILE:HD13	1:A:1038:THR:HG23	1.84	0.58
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.85	0.58
1:A:449:SER:HB2	2:B:1133:MET:HB3	1.85	0.58
1:A:515:GLN:HA	1:A:1367:HIS:NE2	2.19	0.58
1:A:595:THR:O	1:A:596:THR:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:GLY:N	2:B:450:ALA:HB1	2.18	0.58
2:B:469:GLN:C	2:B:472:ALA:HB3	2.23	0.58
5:E:169:ARG:HD3	6:F:140:ASP:OD1	2.04	0.58
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.67	0.58
1:A:391:LEU:O	1:A:394:ASN:HB2	2.03	0.58
1:A:71:GLN:O	1:A:73:GLY:N	2.35	0.58
2:B:842:ASN:HD22	2:B:842:ASN:C	2.06	0.58
3:C:18:VAL:HG21	11:K:109:TRP:CZ3	2.37	0.58
10:J:37:SER:OG	10:J:47:ARG:NH2	2.36	0.58
3:C:8:VAL:HG12	3:C:9:LYS:N	2.18	0.58
4:D:39:ASN:ND2	4:D:40:HIS:H	2.01	0.58
5:E:213:ILE:HG12	5:E:214:CYS:H	1.68	0.58
10:J:2:ILE:HG23	10:J:3:VAL:O	2.04	0.58
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.33	0.58
1:A:172:PRO:HG3	1:A:185:TRP:CE2	2.39	0.58
1:A:664:THR:CG2	2:B:1014:PRO:HB3	2.34	0.58
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	1.86	0.58
2:B:108:VAL:HG23	2:B:109:THR:H	1.68	0.58
3:C:44:LEU:HD23	3:C:44:LEU:C	2.24	0.58
4:D:52:LEU:HB2	4:D:182:SER:HB2	1.84	0.58
5:E:187:TYR:HD2	5:E:188:LEU:HD23	1.69	0.58
7:G:79:PHE:CD1	7:G:79:PHE:C	2.72	0.58
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.69	0.58
1:A:1350:LYS:O	1:A:1353:TYR:HB3	2.03	0.58
1:A:741:ASN:HD22	1:A:741:ASN:C	2.06	0.58
1:A:827:THR:HG22	1:A:828:ALA:N	2.19	0.58
1:A:858:ASN:HD22	1:A:858:ASN:H	1.52	0.58
2:B:326:ASP:O	2:B:330:ALA:CB	2.50	0.58
2:B:453:ILE:O	2:B:457:LEU:HG	2.03	0.58
2:B:833:TYR:C	2:B:835:GLN:H	2.05	0.58
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.86	0.58
6:F:87:LYS:CE	6:F:88:TYR:HE1	2.16	0.58
1:A:1150:SER:H	9:I:46:HIS:HB3	1.68	0.58
1:A:1349:TYR:CE2	1:A:1353:TYR:HB2	2.39	0.57
1:A:617:VAL:HG12	1:A:622:VAL:HG12	1.85	0.57
2:B:975:GLN:CG	2:B:976:ILE:N	2.67	0.57
2:B:770:GLN:CD	2:B:983:ARG:HA	2.24	0.57
3:C:45:ALA:CB	3:C:72:LEU:HD13	2.33	0.57
6:F:130:ILE:O	6:F:132:LEU:N	2.36	0.57
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.43	0.57
1:A:1406:VAL:HG12	1:A:1410:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.38	0.57
1:A:524:VAL:HG12	1:A:525:GLN:N	2.15	0.57
1:A:808:LEU:HB3	1:A:812:GLU:HB2	1.86	0.57
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.39	0.57
2:B:1166:CYS:O	2:B:1168:LEU:N	2.36	0.57
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.86	0.57
2:B:879:ARG:H	2:B:879:ARG:NE	2.02	0.57
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.22	0.57
10:J:57:ILE:HG23	10:J:58:GLU:H	1.69	0.57
1:A:98:LYS:O	1:A:102:VAL:HG23	2.04	0.57
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.05	0.57
1:A:206:GLU:O	1:A:210:ILE:HG13	2.04	0.57
1:A:6:TYR:CG	1:A:7:SER:N	2.72	0.57
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.58	0.57
2:B:898:LEU:HD12	12:L:58:LYS:HD2	1.86	0.57
3:C:213:PRO:O	3:C:214:ASN:HB3	2.04	0.57
6:F:90:ARG:CD	6:F:155:LEU:HD13	2.32	0.57
1:A:247:ARG:HD2	1:A:263:THR:HG23	1.85	0.57
1:A:546:VAL:O	1:A:549:MET:HB2	2.05	0.57
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.86	0.57
1:A:975:HIS:O	1:A:976:THR:HG23	2.05	0.57
2:B:777:ALA:HA	2:B:1095:LEU:HB2	1.87	0.57
1:A:447:GLN:HG2	2:B:1134:GLU:OE2	2.04	0.57
2:B:365:THR:HG23	2:B:367:LEU:H	1.69	0.57
2:B:655:LYS:HD2	2:B:658:ILE:HG22	1.84	0.57
3:C:50:GLU:HB3	3:C:156:THR:HB	1.86	0.57
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.86	0.57
1:A:1444:MET:HG3	7:G:59:GLY:O	2.04	0.57
12:L:58:LYS:O	12:L:59:ALA:O	2.22	0.57
1:A:443:LEU:HD23	1:A:501:LEU:HD22	1.87	0.57
6:F:76:LYS:HA	6:F:79:ARG:HD2	1.85	0.57
7:G:115:MET:CB	7:G:119:LEU:HD23	2.35	0.57
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.39	0.57
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.04	0.57
1:A:1279:ILE:HG23	1:A:1308:THR:OG1	2.04	0.57
1:A:409:SER:O	1:A:411:ASP:HB2	2.05	0.57
2:B:345:LYS:HG2	2:B:346:GLU:N	2.17	0.57
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.87	0.57
2:B:405:ARG:NH1	2:B:632:ARG:HG2	2.19	0.57
3:C:16:ASP:O	3:C:233:GLU:HA	2.04	0.57
6:F:101:ILE:HD13	6:F:120:ILE:CG2	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:9:SER:CB	10:J:45:CYS:HB2	2.35	0.57
11:K:63:VAL:O	11:K:64:GLU:C	2.42	0.57
1:A:1354:ASN:O	1:A:1358:SER:CB	2.51	0.57
1:A:270:LEU:O	1:A:274:ILE:HG13	2.05	0.57
1:A:355:GLY:N	1:A:482:PHE:CZ	2.72	0.57
2:B:977:GLY:HA3	2:B:1099:VAL:HG11	1.86	0.57
2:B:467:GLY:H	2:B:475:SER:HB2	1.69	0.57
2:B:593:PRO:HB2	2:B:617:ARG:CZ	2.35	0.57
9:I:15:TYR:N	9:I:15:TYR:CD1	2.73	0.57
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.34	0.57
1:A:1315:GLU:O	1:A:1317:MET:N	2.37	0.57
1:A:850:VAL:HG23	1:A:1064:VAL:HG21	1.87	0.57
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.40	0.57
2:B:990:ILE:HG22	2:B:992:ILE:H	1.69	0.57
5:E:185:ALA:O	5:E:190:LEU:HG	2.05	0.57
5:E:15:ALA:O	5:E:19:VAL:HG23	2.04	0.57
7:G:111:THR:CG2	7:G:114:LEU:HD13	2.34	0.57
12:L:26:THR:HG22	12:L:27:LEU:N	2.15	0.57
1:A:1356:ILE:HD13	1:A:1363:VAL:HG21	1.86	0.57
1:A:202:LEU:HB3	1:A:207:ILE:HD11	1.87	0.57
2:B:361:LEU:HD21	2:B:377:PHE:HD2	1.69	0.57
2:B:398:ARG:NH1	2:B:398:ARG:HB2	2.20	0.57
6:F:129:LYS:O	6:F:130:ILE:HG13	2.05	0.57
7:G:126:ASN:HD22	7:G:127:PRO:N	2.03	0.57
11:K:39:ASP:OD1	11:K:41:THR:HG22	2.05	0.57
1:A:1029:ARG:O	1:A:1033:GLN:HB3	2.04	0.57
1:A:403:LYS:HE2	1:A:404:TYR:HE1	1.70	0.57
1:A:933:TYR:O	1:A:937:VAL:HG23	2.04	0.57
2:B:1098:MET:O	2:B:1101:ASP:HB2	2.05	0.57
2:B:1166:CYS:C	2:B:1168:LEU:H	2.08	0.57
2:B:192:LEU:O	2:B:193:LYS:HB2	2.05	0.57
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.86	0.57
2:B:797:TYR:HB2	2:B:852:ARG:O	2.04	0.57
4:D:170:THR:O	4:D:172:LEU:N	2.38	0.57
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.86	0.57
1:A:567:LYS:HZ2	8:H:46:LEU:HB2	1.70	0.57
2:B:363:HIS:O	2:B:364:ILE:CB	2.52	0.56
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.86	0.56
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.05	0.56
11:K:57:LEU:HD13	11:K:76:GLN:NE2	2.18	0.56
1:A:1351:GLU:O	1:A:1355:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:HE1	1:A:1410:PHE:CE2	2.22	0.56
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.86	0.56
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.05	0.56
3:C:76:ASP:C	3:C:129:ILE:HD11	2.26	0.56
5:E:153:HIS:HB3	5:E:196:VAL:HG21	1.86	0.56
1:A:1116:LEU:N	1:A:1308:THR:HG22	2.20	0.56
1:A:134:ARG:HD2	1:A:221:SER:O	2.05	0.56
1:A:490:HIS:ND1	2:B:1150:ARG:NH1	2.53	0.56
1:A:903:ASN:HB3	1:A:906:HIS:HB2	1.87	0.56
2:B:230:ALA:CB	2:B:231:PRO:HD3	2.33	0.56
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.40	0.56
2:B:792:MET:HA	2:B:856:PHE:O	2.05	0.56
5:E:155:ARG:O	5:E:156:LEU:HD23	2.05	0.56
1:A:12:ARG:HB2	2:B:1218:THR:HG22	1.86	0.56
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.87	0.56
1:A:640:GLN:CD	1:A:640:GLN:N	2.57	0.56
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.05	0.56
2:B:1157:ALA:O	2:B:1158:PHE:CB	2.52	0.56
2:B:510:LYS:CG	2:B:511:PRO:HD3	2.24	0.56
8:H:30:SER:CB	8:H:36:CYS:HB3	2.35	0.56
1:A:92:HIS:HE1	1:A:1410:PHE:HE2	1.51	0.56
1:A:185:TRP:CZ3	1:A:200:ARG:HB3	2.41	0.56
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.70	0.56
1:A:549:MET:CE	1:A:656:TRP:HD1	2.18	0.56
2:B:486:TYR:HD1	2:B:1096:ARG:NH2	2.03	0.56
1:A:810:PRO:HD3	2:B:730:ARG:HH21	1.70	0.56
4:D:24:ALA:HB3	4:D:26:THR:HG23	1.88	0.56
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.41	0.56
6:F:97:ARG:NH2	6:F:108:PHE:HE1	2.03	0.56
7:G:111:THR:HG22	7:G:114:LEU:CD2	2.34	0.56
3:C:35:ARG:NH1	11:K:41:THR:HB	2.20	0.56
1:A:108:MET:O	1:A:109:HIS:HB3	2.04	0.56
1:A:1260:LEU:HA	1:A:1263:ILE:HD12	1.86	0.56
1:A:81:PHE:CD2	1:A:243:PRO:HD3	2.41	0.56
1:A:363:GLN:HA	1:A:459:ARG:O	2.05	0.56
1:A:850:VAL:HG12	1:A:1060:PRO:HA	1.87	0.56
2:B:65:GLU:HG3	2:B:66:ASP:H	1.71	0.56
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.70	0.56
6:F:130:ILE:HG22	6:F:132:LEU:HG	1.88	0.56
2:B:900:ALA:HB1	12:L:61:THR:OG1	2.05	0.56
1:A:11:LEU:HG	1:A:12:ARG:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1362:TYR:HD1	1:A:1363:VAL:N	2.04	0.56
1:A:361:LEU:HA	1:A:471:ASN:ND2	2.11	0.56
1:A:399:HIS:C	1:A:399:HIS:ND1	2.58	0.56
2:B:1065:GLN:HB2	2:B:1069:PHE:O	2.06	0.56
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.74	0.56
2:B:798:TYR:CD1	10:J:4:PRO:HB3	2.41	0.56
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.69	0.56
1:A:1210:GLY:O	1:A:1214:GLU:HG2	2.05	0.56
1:A:528:LEU:O	1:A:531:ILE:HG22	2.06	0.56
1:A:617:VAL:HG12	1:A:622:VAL:CG1	2.35	0.56
1:A:868:TYR:HE2	1:A:1366:ARG:HE	1.53	0.56
2:B:1131:GLY:O	2:B:1132:GLU:C	2.44	0.56
2:B:515:HIS:CD2	2:B:516:ASN:H	2.24	0.56
3:C:31:ASN:O	3:C:35:ARG:HG3	2.05	0.56
3:C:32:SER:O	3:C:36:VAL:HG23	2.05	0.56
4:D:123:LEU:HB3	4:D:124:GLU:OE2	2.06	0.56
4:D:151:PHE:N	4:D:151:PHE:CD1	2.74	0.56
8:H:11:GLN:HA	8:H:53:ASP:O	2.06	0.56
1:A:1152:ILE:CD1	9:I:44:TYR:HD2	2.18	0.56
1:A:547:LEU:HD13	11:K:58:PHE:CD1	2.41	0.56
1:A:1110:ASN:H	1:A:1110:ASN:ND2	2.04	0.56
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.86	0.56
3:C:148:ARG:N	3:C:151:GLN:HG3	2.19	0.56
6:F:100:GLN:NE2	7:G:18:PHE:CE2	2.73	0.56
7:G:51:TYR:O	7:G:54:ILE:HG13	2.05	0.56
1:A:664:THR:HG22	2:B:1014:PRO:HB3	1.87	0.56
2:B:120:ARG:HH12	12:L:54:ARG:HH11	1.54	0.56
2:B:220:GLY:HA2	2:B:241:ARG:NH1	2.21	0.56
2:B:334:ILE:O	2:B:334:ILE:HG22	2.05	0.56
3:C:101:LEU:HB3	3:C:155:LEU:HB2	1.86	0.56
4:D:35:LEU:H	4:D:35:LEU:CD1	2.18	0.56
5:E:90:VAL:HG22	5:E:90:VAL:O	2.06	0.56
6:F:139:PRO:O	6:F:140:ASP:C	2.44	0.56
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.46	0.56
1:A:1396:ALA:HA	1:A:1399:ARG:NH2	2.21	0.56
2:B:222:ILE:HD11	2:B:627:PHE:CZ	2.40	0.56
6:F:111:LEU:C	6:F:113:GLY:N	2.59	0.56
7:G:13:LEU:CD2	7:G:17:PHE:HD2	2.12	0.56
1:A:541:ILE:HG22	1:A:542:GLU:N	2.21	0.55
2:B:362:PRO:HB3	2:B:366:GLN:OE1	2.06	0.55
2:B:542:MET:HG2	2:B:747:MET:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:485:ARG:HH12	2:B:782:LEU:HD21	1.71	0.55
2:B:828:ALA:HB2	2:B:1085:ILE:HG12	1.88	0.55
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.41	0.55
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.88	0.55
5:E:148:GLU:HG2	5:E:149:LEU:HD23	1.87	0.55
2:B:679:TYR:CE1	2:B:683:SER:HB2	2.41	0.55
3:C:43:THR:HG22	3:C:74:SER:OG	2.06	0.55
4:D:208:GLU:O	4:D:212:LYS:HG3	2.06	0.55
8:H:82:PRO:O	8:H:84:ALA:N	2.40	0.55
1:A:873:MET:C	1:A:1058:VAL:HG23	2.26	0.55
1:A:145:LYS:HE3	1:A:146:MET:H	1.71	0.55
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.40	0.55
1:A:718:VAL:O	1:A:721:PHE:HB2	2.06	0.55
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.40	0.55
3:C:123:ASN:OD1	3:C:125:MET:HG2	2.07	0.55
5:E:63:ASN:HB3	5:E:64:PRO:HD2	1.88	0.55
8:H:130:ARG:HB3	8:H:134:ASN:H	1.72	0.55
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.72	0.55
1:A:1011:GLN:HG3	1:A:1012:ARG:N	2.20	0.55
2:B:522:VAL:HG13	2:B:537:LYS:HB3	1.88	0.55
2:B:805:THR:HG22	2:B:806:THR:O	2.06	0.55
3:C:113:VAL:O	3:C:143:LEU:HD13	2.07	0.55
4:D:134:THR:HG21	4:D:138:ASN:HB2	1.88	0.55
5:E:114:ASN:O	5:E:115:ASN:HB3	2.06	0.55
5:E:122:LYS:C	5:E:123:LEU:HG	2.25	0.55
7:G:160:ILE:HG22	7:G:161:GLY:N	2.21	0.55
11:K:32:VAL:HA	11:K:73:LEU:O	2.06	0.55
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.36	0.55
1:A:16:GLU:HA	1:A:1419:ASP:O	2.06	0.55
1:A:335:ARG:HD3	1:A:339:ASN:ND2	2.19	0.55
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.53	0.55
2:B:120:ARG:NH1	12:L:54:ARG:HH11	2.02	0.55
2:B:530:GLY:C	2:B:531:GLN:HG2	2.25	0.55
1:A:308:ILE:HG22	1:A:309:ALA:H	1.71	0.55
1:A:481:ASP:HB2	1:A:483:ASP:OD2	2.07	0.55
1:A:353:ILE:HG23	1:A:485:ASP:O	2.07	0.55
1:A:670:ILE:CG2	1:A:805:LEU:HD21	2.37	0.55
1:A:679:ILE:O	1:A:683:ILE:HG13	2.06	0.55
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.06	0.55
2:B:416:LEU:O	2:B:420:LEU:HB2	2.07	0.55
2:B:459:TYR:C	2:B:459:TYR:CD2	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:GLY:H	2:B:475:SER:CB	2.19	0.55
2:B:785:TYR:CE2	10:J:60:PHE:CE1	2.95	0.55
2:B:876:LYS:NZ	2:B:891:ASP:HA	2.22	0.55
4:D:39:ASN:HD22	4:D:41:GLN:H	1.53	0.55
11:K:37:LYS:O	11:K:38:GLU:HG2	2.05	0.55
11:K:68:PHE:CD2	11:K:68:PHE:N	2.71	0.55
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.72	0.55
1:A:711:ARG:O	1:A:714:PHE:HB3	2.06	0.55
2:B:806:THR:HB	2:B:809:MET:HG3	1.87	0.55
2:B:842:ASN:HD21	2:B:844:SER:CB	2.19	0.55
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.70	0.55
5:E:143:ASN:ND2	5:E:146:HIS:ND1	2.55	0.55
1:A:95:PHE:CE2	1:A:1410:PHE:HD2	2.25	0.55
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.53	0.55
2:B:1174:LYS:HB2	2:B:1179:GLN:H	1.72	0.55
1:A:1004:ASN:O	1:A:1008:GLN:HG2	2.06	0.55
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.89	0.55
1:A:1105:LEU:O	1:A:1384:VAL:HG23	2.07	0.55
1:A:1287:TYR:O	1:A:1302:PRO:HA	2.07	0.55
1:A:556:TRP:O	1:A:558:GLY:N	2.40	0.55
1:A:666:ILE:HG23	2:B:1026:LEU:CB	2.34	0.55
2:B:1012:ILE:O	2:B:1014:PRO:HD3	2.07	0.55
2:B:185:THR:O	2:B:189:LEU:HG	2.07	0.55
2:B:230:ALA:HB3	2:B:231:PRO:CD	2.32	0.55
2:B:251:ILE:HG22	2:B:251:ILE:O	2.07	0.55
2:B:999:MET:HA	2:B:999:MET:CE	2.35	0.55
3:C:82:TYR:HB2	3:C:85:ASP:OD2	2.06	0.55
7:G:126:ASN:HD22	7:G:126:ASN:C	2.10	0.55
1:A:224:PHE:HD2	1:A:231:PRO:CD	2.19	0.55
1:A:909:ASP:O	1:A:911:SER:N	2.40	0.55
4:D:25:ALA:HB3	4:D:196:PRO:HG2	1.88	0.55
1:A:474:VAL:C	1:A:477:PRO:HD2	2.27	0.54
1:A:866:PHE:C	1:A:867:ILE:HD12	2.27	0.54
2:B:1137:CYS:O	2:B:1140:ALA:HB3	2.07	0.54
2:B:179:CYS:SG	2:B:181:LEU:HD12	2.47	0.54
2:B:57:TYR:CD1	2:B:57:TYR:N	2.72	0.54
2:B:754:SER:HB2	2:B:812:LEU:HD11	1.89	0.54
8:H:130:ARG:H	8:H:130:ARG:NH1	1.96	0.54
10:J:17:LYS:HB3	10:J:39:LEU:CD2	2.38	0.54
1:A:1050:GLU:O	1:A:1053:PHE:HB3	2.07	0.54
1:A:1400:CYS:SG	1:A:1409:LEU:HD21	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLY:C	1:A:312:PRO:HD2	2.26	0.54
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.37	0.54
1:A:541:ILE:HD12	1:A:577:ILE:HD11	1.87	0.54
2:B:859:TYR:CD1	2:B:859:TYR:N	2.71	0.54
3:C:88:CYS:SG	3:C:91:HIS:CA	2.93	0.54
4:D:118:THR:HG21	4:D:121:LYS:HD2	1.88	0.54
4:D:39:ASN:CG	4:D:40:HIS:N	2.60	0.54
11:K:113:THR:CG2	11:K:114:LEU:H	2.20	0.54
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.37	0.54
1:A:1224:LEU:N	1:A:1243:VAL:HG13	2.22	0.54
1:A:1344:GLY:O	1:A:1345:ARG:C	2.46	0.54
1:A:364:VAL:O	1:A:366:VAL:HG23	2.07	0.54
1:A:636:GLU:CD	1:A:966:ASN:HD21	2.10	0.54
1:A:986:ILE:HG22	1:A:987:VAL:N	2.22	0.54
2:B:856:PHE:CD1	2:B:856:PHE:N	2.74	0.54
2:B:955:THR:HG22	2:B:956:THR:O	2.07	0.54
5:E:177:ARG:HH11	5:E:215:MET:CE	2.20	0.54
5:E:178:ILE:HG22	5:E:213:ILE:O	2.07	0.54
8:H:102:TYR:N	8:H:102:TYR:CD2	2.69	0.54
10:J:30:LEU:HD22	10:J:34:THR:HG21	1.89	0.54
10:J:48:ARG:CG	10:J:48:ARG:HH11	2.20	0.54
11:K:7:PHE:C	11:K:9:LEU:H	2.11	0.54
1:A:1313:LEU:O	1:A:1315:GLU:N	2.41	0.54
1:A:1390:ASN:HD21	1:A:1402:PHE:HB3	1.72	0.54
1:A:374:LEU:O	1:A:436:ILE:HG12	2.07	0.54
1:A:665:GLY:O	1:A:667:GLY:N	2.40	0.54
1:A:830:LYS:HG3	1:A:1098:VAL:HG11	1.89	0.54
1:A:982:THR:O	1:A:985:ASP:HB2	2.07	0.54
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.07	0.54
2:B:1152:MET:O	2:B:1157:ALA:HB2	2.07	0.54
2:B:1168:LEU:HB2	2:B:1170:THR:OG1	2.07	0.54
2:B:955:THR:HG23	12:L:54:ARG:O	2.08	0.54
4:D:56:ARG:HD2	4:D:122:GLU:OE1	2.08	0.54
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.42	0.54
12:L:66:GLN:C	12:L:67:PHE:HD1	2.10	0.54
1:A:164:ARG:HG2	1:A:165:GLY:N	2.23	0.54
1:A:707:GLY:HA2	1:A:1281:ARG:HD3	1.90	0.54
2:B:516:ASN:HD22	2:B:516:ASN:H	1.55	0.54
2:B:515:HIS:H	2:B:518:HIS:CD2	2.25	0.54
2:B:936:ASP:CG	2:B:937:ALA:N	2.61	0.54
1:A:102:VAL:CG1	1:A:211:PHE:HE1	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1315:GLU:C	1:A:1317:MET:H	2.09	0.54
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.71	0.54
1:A:741:ASN:O	1:A:745:GLN:HG3	2.08	0.54
2:B:210:LYS:CD	2:B:482:VAL:HG13	2.28	0.54
2:B:521:LEU:HD22	2:B:633:VAL:CG1	2.35	0.54
2:B:541:LEU:HB2	2:B:747:MET:CE	2.38	0.54
2:B:911:ILE:HG21	2:B:966:VAL:HG11	1.89	0.54
8:H:89:LEU:O	8:H:89:LEU:HD12	2.07	0.54
9:I:13:MET:HG2	9:I:14:LEU:N	2.23	0.54
12:L:55:ILE:O	12:L:56:LEU:HB2	2.08	0.54
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.27	0.54
1:A:826:ASP:HB2	1:A:830:LYS:HD3	1.90	0.54
2:B:581:PHE:O	2:B:582:VAL:HG23	2.08	0.54
3:C:167:HIS:O	3:C:168:ALA:C	2.45	0.54
4:D:192:LYS:HD2	4:D:199:ASN:H	1.72	0.54
7:G:79:PHE:CD2	7:G:105:PRO:HD2	2.42	0.54
1:A:1100:ARG:HH12	1:A:1111:MET:HE2	1.73	0.54
1:A:1427:ASN:O	1:A:1430:LEU:N	2.40	0.54
1:A:16:GLU:OE1	4:D:13:ARG:NH2	2.41	0.54
8:H:128:ASN:C	8:H:128:ASN:HD22	2.11	0.54
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.43	0.54
1:A:224:PHE:CD2	1:A:231:PRO:HD3	2.42	0.54
2:B:126:SER:HB3	2:B:172:ILE:HD11	1.89	0.54
2:B:213:ILE:HG21	2:B:499:ASN:HB2	1.88	0.54
4:D:190:GLU:HG2	4:D:194:LEU:HD11	1.88	0.54
6:F:121:ALA:HA	6:F:124:GLU:HB2	1.90	0.54
1:A:500:GLU:O	1:A:504:LEU:HB2	2.08	0.54
1:A:741:ASN:ND2	1:A:743:VAL:H	2.07	0.54
1:A:669:THR:O	1:A:762:SER:HB3	2.07	0.54
1:A:998:LEU:HD23	1:A:1001:ARG:HG3	1.88	0.54
1:A:69:THR:HG21	2:B:1174:LYS:HZ2	1.72	0.54
2:B:291:ILE:HD12	2:B:291:ILE:H	1.72	0.54
2:B:611:PRO:O	2:B:692:TYR:HB2	2.08	0.54
2:B:662:MET:HA	2:B:665:GLU:HB2	1.88	0.54
2:B:899:ILE:HG23	2:B:903:VAL:HG21	1.89	0.54
3:C:111:THR:O	3:C:147:LEU:HD23	2.08	0.54
1:A:1098:VAL:HB	1:A:1099:PRO:CD	2.38	0.53
1:A:1119:TYR:HA	1:A:1305:VAL:CG2	2.38	0.53
1:A:196:GLU:HG2	1:A:197:PRO:HD2	1.90	0.53
1:A:404:TYR:CD2	1:A:412:ARG:HD3	2.43	0.53
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:PHE:HZ	8:H:121:LEU:HD11	1.73	0.53
1:A:567:LYS:HE3	8:H:46:LEU:CD1	2.38	0.53
1:A:908:LEU:HD23	1:A:1029:ARG:NH2	2.23	0.53
2:B:828:ALA:CB	2:B:1085:ILE:HG12	2.37	0.53
2:B:37:PHE:HE1	2:B:41:LYS:HG3	1.73	0.53
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.82	0.53
1:A:964:ILE:HG22	1:A:964:ILE:O	2.08	0.53
2:B:1198:TYR:O	2:B:1201:LYS:HB3	2.09	0.53
2:B:508:LEU:O	2:B:509:ALA:CB	2.57	0.53
2:B:917:PRO:O	2:B:918:ILE:HG13	2.07	0.53
4:D:167:LEU:O	4:D:169:SER:N	2.41	0.53
4:D:39:ASN:ND2	4:D:41:GLN:H	2.05	0.53
5:E:155:ARG:C	5:E:156:LEU:HD23	2.29	0.53
6:F:118:LEU:O	6:F:122:MET:HG3	2.07	0.53
11:K:30:ALA:HA	11:K:75:ILE:O	2.08	0.53
1:A:605:MET:SD	1:A:621:THR:HG21	2.49	0.53
1:A:640:GLN:H	1:A:640:GLN:CD	2.11	0.53
2:B:172:ILE:HG21	2:B:178:ASN:HB3	1.90	0.53
2:B:654:ARG:O	2:B:657:HIS:HB2	2.08	0.53
2:B:744:HIS:CD2	2:B:746:SER:OG	2.60	0.53
3:C:62:PHE:O	3:C:66:ARG:CG	2.57	0.53
4:D:170:THR:O	4:D:172:LEU:HG	2.08	0.53
8:H:114:VAL:HG22	8:H:125:LEU:HB3	1.91	0.53
9:I:6:PHE:HB3	9:I:12:ASN:O	2.08	0.53
1:A:236:LEU:N	1:A:236:LEU:HD23	2.23	0.53
1:A:317:LYS:O	1:A:318:SER:CB	2.55	0.53
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.38	0.53
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.72	0.53
2:B:323:VAL:O	2:B:324:ILE:HG13	2.08	0.53
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.44	0.53
2:B:533:CYS:C	2:B:535:LEU:H	2.12	0.53
2:B:763:GLN:O	2:B:766:ARG:HB2	2.07	0.53
7:G:30:LEU:HD23	7:G:31:LEU:HD23	1.91	0.53
8:H:142:LEU:C	8:H:143:LEU:HD12	2.29	0.53
9:I:7:CYS:SG	9:I:8:ARG:O	2.66	0.53
10:J:24:LEU:HD11	10:J:38:ARG:HG2	1.89	0.53
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.91	0.53
2:B:522:VAL:CG1	2:B:523:CYS:N	2.70	0.53
2:B:583:ASN:OD1	2:B:628:THR:HG22	2.08	0.53
1:A:954:TRP:HZ3	5:E:203:GLU:HB2	1.68	0.53
6:F:83:PRO:HA	6:F:146:TRP:CZ3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:113:ALA:HA	8:H:125:LEU:O	2.08	0.53
1:A:178:GLY:C	1:A:179:LEU:HD23	2.29	0.53
1:A:453:MET:HE3	1:A:513:SER:HB2	1.90	0.53
2:B:324:ILE:HD11	2:B:329:THR:HG22	1.91	0.53
5:E:158:SER:O	5:E:162:ARG:HG3	2.07	0.53
3:C:244:VAL:HG11	11:K:105:PHE:CE2	2.43	0.53
1:A:1016:THR:O	1:A:1019:CYS:HB2	2.09	0.53
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	1.91	0.53
1:A:535:THR:O	1:A:536:LEU:O	2.27	0.53
1:A:664:THR:HA	1:A:742:ASN:ND2	2.19	0.53
2:B:825:VAL:HG11	2:B:1012:ILE:HD11	1.90	0.53
2:B:64:CYS:HA	2:B:67:SER:OG	2.08	0.53
2:B:990:ILE:HG22	2:B:991:GLY:N	2.24	0.53
5:E:28:TYR:C	5:E:65:THR:HG23	2.29	0.53
1:A:23:SER:HB2	1:A:233:TRP:CE2	2.44	0.53
1:A:381:THR:O	1:A:384:ASN:OD1	2.27	0.53
2:B:124:TYR:CD2	2:B:124:TYR:O	2.61	0.53
2:B:652:LYS:O	2:B:689:LEU:HD22	2.09	0.53
2:B:941:LEU:HG	2:B:942:ARG:N	2.23	0.53
6:F:69:LEU:HB3	6:F:71:GLU:OE1	2.09	0.53
7:G:56:ILE:O	7:G:57:GLN:HB2	2.09	0.53
1:A:1037:LEU:HD13	1:A:1041:ALA:HB1	1.90	0.53
1:A:852:TYR:HD2	1:A:1060:PRO:CB	2.22	0.53
1:A:386:ASP:N	1:A:386:ASP:OD1	2.38	0.53
1:A:396:PRO:O	1:A:397:ASN:OD1	2.27	0.53
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	2.17	0.53
2:B:1096:ARG:CG	2:B:1097:HIS:H	2.22	0.53
2:B:1130:PHE:CE1	2:B:1134:GLU:HB3	2.44	0.53
2:B:581:PHE:HA	2:B:585:VAL:O	2.08	0.53
4:D:56:ARG:HH21	4:D:155:ARG:HG2	1.73	0.53
6:F:87:LYS:HE2	6:F:88:TYR:HE1	1.73	0.53
7:G:121:PHE:CE2	7:G:123:ALA:HB2	2.44	0.53
6:F:133:VAL:HG21	7:G:58:ARG:HE	1.74	0.53
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.44	0.53
1:A:1098:VAL:HB	1:A:1099:PRO:HD3	1.90	0.53
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.37	0.53
1:A:1376:THR:O	1:A:1377:THR:C	2.48	0.53
1:A:315:LEU:HD22	1:A:319:GLY:O	2.08	0.53
2:B:1084:GLN:HE21	2:B:1084:GLN:N	2.07	0.53
1:A:15:LYS:HB3	2:B:1220:ARG:NH2	2.23	0.53
2:B:553:PRO:O	2:B:557:PHE:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:SER:N	2:B:751:VAL:HG11	2.24	0.53
5:E:78:LEU:HG	5:E:107:THR:CG2	2.39	0.53
7:G:5:LYS:HG3	7:G:6:ASP:N	2.23	0.53
2:B:120:ARG:HH12	12:L:54:ARG:NH1	2.07	0.53
1:A:970:THR:HG22	1:A:971:PHE:CD1	2.44	0.52
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.91	0.52
2:B:655:LYS:HD2	2:B:658:ILE:CG2	2.39	0.52
2:B:801:LYS:O	2:B:801:LYS:HG3	2.09	0.52
4:D:185:CYS:SG	4:D:190:GLU:HB3	2.49	0.52
7:G:55:ASP:HB3	7:G:73:LYS:CB	2.39	0.52
8:H:145:ARG:O	8:H:146:ARG:CB	2.56	0.52
11:K:40:HIS:CE1	11:K:63:VAL:HG11	2.43	0.52
12:L:30:ILE:CD1	12:L:59:ALA:HB2	2.40	0.52
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.24	0.52
2:B:259:TYR:H	2:B:259:TYR:HD1	1.56	0.52
2:B:744:HIS:HD2	2:B:746:SER:OG	1.92	0.52
3:C:62:PHE:O	3:C:66:ARG:HG3	2.09	0.52
1:A:1258:HIS:O	1:A:1262:LYS:HE3	2.10	0.52
1:A:122:MET:HA	1:A:141:LEU:HD13	1.91	0.52
1:A:285:PRO:O	1:A:287:HIS:N	2.42	0.52
1:A:34:LYS:HB2	1:A:36:ARG:NH1	2.24	0.52
1:A:894:GLU:O	1:A:898:ARG:HB3	2.10	0.52
2:B:1194:ILE:HD11	2:B:1196:ILE:HG21	1.90	0.52
2:B:102:VAL:HG21	2:B:122:LEU:HD13	1.91	0.52
2:B:126:SER:O	2:B:169:ARG:HA	2.09	0.52
2:B:732:SER:HB3	2:B:734:HIS:CE1	2.45	0.52
2:B:899:ILE:HG22	2:B:900:ALA:O	2.09	0.52
2:B:878:GLN:H	2:B:934:LYS:NZ	2.07	0.52
3:C:115:SER:CB	3:C:142:VAL:HB	2.39	0.52
3:C:46:ILE:HA	3:C:159:ALA:HA	1.91	0.52
5:E:85:GLU:OE1	5:E:88:VAL:HA	2.10	0.52
1:A:129:LYS:O	1:A:130:ASP:CB	2.56	0.52
1:A:257:ARG:HG2	1:A:259:GLU:HG2	1.92	0.52
1:A:370:ILE:C	1:A:372:LYS:H	2.13	0.52
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.75	0.52
2:B:421:PHE:CE1	2:B:424:LEU:HD23	2.43	0.52
2:B:508:LEU:N	2:B:512:ARG:HH21	2.07	0.52
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.92	0.52
2:B:848:ARG:NH2	2:B:996:ARG:HD2	2.15	0.52
4:D:216:ASN:C	4:D:218:GLU:H	2.13	0.52
6:F:109:VAL:CG1	6:F:110:ASP:N	2.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:84:ALA:HA	8:H:87:ARG:HD2	1.92	0.52
10:J:52:THR:HG22	10:J:52:THR:O	2.08	0.52
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.92	0.52
1:A:1036:ARG:NH1	1:A:1036:ARG:CG	2.72	0.52
1:A:1037:LEU:HD12	1:A:1042:PHE:HA	1.91	0.52
1:A:967:ALA:CA	1:A:1044:TRP:HZ3	2.22	0.52
1:A:164:ARG:HG2	1:A:165:GLY:H	1.74	0.52
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.91	0.52
1:A:962:ARG:O	1:A:965:GLN:N	2.38	0.52
4:D:59:ILE:HG23	7:G:47:CYS:SG	2.49	0.52
5:E:55:ARG:HD2	5:E:84:ASP:HA	1.92	0.52
6:F:78:GLN:O	6:F:78:GLN:HG2	2.10	0.52
7:G:27:LYS:O	7:G:31:LEU:HG	2.10	0.52
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.43	0.52
1:A:1219:THR:CG2	1:A:1220:PHE:N	2.72	0.52
1:A:388:LEU:O	1:A:392:VAL:HG23	2.09	0.52
1:A:438:ASP:O	1:A:439:ASN:C	2.47	0.52
1:A:596:THR:O	1:A:598:LEU:N	2.42	0.52
1:A:692:ASP:C	1:A:694:THR:H	2.13	0.52
1:A:864:ILE:HG21	1:A:1370:LEU:CD2	2.39	0.52
1:A:929:LEU:H	1:A:929:LEU:CD2	2.22	0.52
2:B:274:PRO:HB2	2:B:359:GLU:HB3	1.91	0.52
2:B:203:PHE:CD2	2:B:461:LEU:HD21	2.45	0.52
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.40	0.52
2:B:655:LYS:HE3	2:B:659:ALA:HB2	1.92	0.52
5:E:136:ASN:O	5:E:140:LEU:HG	2.09	0.52
6:F:117:PRO:HA	6:F:120:ILE:HB	1.90	0.52
7:G:139:ILE:HD13	7:G:140:LYS:HG3	1.92	0.52
8:H:89:LEU:C	8:H:91:ASP:H	2.13	0.52
1:A:1289:ARG:HD3	1:A:1290:LYS:O	2.10	0.52
1:A:1329:THR:HG23	1:A:1331:SER:H	1.74	0.52
2:B:427:ASP:O	2:B:430:ARG:HB2	2.10	0.52
2:B:702:LEU:O	2:B:739:THR:N	2.42	0.52
2:B:791:THR:O	2:B:792:MET:HB3	2.09	0.52
2:B:860:MET:HG2	2:B:861:ASP:N	2.24	0.52
7:G:111:THR:CG2	7:G:114:LEU:HD22	2.38	0.52
8:H:30:SER:HB3	8:H:36:CYS:HB3	1.91	0.52
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.09	0.52
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.39	0.52
1:A:1259:MET:HE2	1:A:1259:MET:O	2.09	0.52
1:A:1378:GLN:O	5:E:177:ARG:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	1:A:568:PRO:CD	2.74	0.52
1:A:28:ARG:HG3	1:A:83:HIS:ND1	2.24	0.52
2:B:345:LYS:HA	2:B:348:ARG:HG2	1.91	0.52
2:B:766:ARG:NH2	2:B:1020:ARG:HB3	2.25	0.52
5:E:153:HIS:ND1	5:E:153:HIS:N	2.58	0.52
1:A:1365:TYR:HB2	5:E:203:GLU:OE1	2.10	0.52
5:E:55:ARG:C	5:E:57:MET:N	2.61	0.52
1:A:645:LEU:O	1:A:649:ILE:HG13	2.09	0.52
1:A:814:PHE:HE1	2:B:519:TRP:CA	2.23	0.52
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.92	0.52
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.90	0.52
1:A:130:ASP:H	1:A:134:ARG:HH21	1.58	0.52
1:A:1377:THR:HG22	5:E:176:PRO:HB3	1.92	0.52
2:B:483:LEU:HD12	2:B:484:ASN:N	2.25	0.52
2:B:582:VAL:HG22	2:B:626:ILE:CG2	2.39	0.52
11:K:33:ILE:HB	11:K:35:PHE:HE1	1.76	0.52
11:K:53:ASP:C	11:K:55:LYS:H	2.11	0.52
3:C:166:GLU:HA	11:K:6:ARG:HB3	1.92	0.52
1:A:172:PRO:HG3	1:A:185:TRP:CZ2	2.46	0.51
1:A:401:GLY:H	1:A:435:HIS:HD2	1.58	0.51
1:A:446:ARG:HB2	1:A:487:MET:HE3	1.92	0.51
1:A:693:VAL:HG12	1:A:693:VAL:O	2.10	0.51
2:B:479:VAL:O	2:B:480:SER:HB3	2.09	0.51
2:B:781:PHE:HD1	2:B:782:LEU:HG	1.75	0.51
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.50	0.51
6:F:140:ASP:CG	6:F:141:GLY:H	2.13	0.51
6:F:146:TRP:HB3	6:F:151:LEU:HD11	1.92	0.51
1:A:1218:GLN:O	1:A:1221:LYS:HE3	2.10	0.51
1:A:1345:ARG:O	1:A:1348:LEU:HB3	2.10	0.51
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.09	0.51
2:B:770:GLN:HB2	2:B:985:GLY:N	2.24	0.51
5:E:96:PHE:CD1	5:E:100:ILE:HD11	2.45	0.51
6:F:134:ILE:HG22	6:F:136:ARG:HG3	1.92	0.51
1:A:1170:ILE:HG22	1:A:1174:PHE:CE1	2.46	0.51
1:A:364:VAL:O	1:A:364:VAL:HG13	2.09	0.51
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.92	0.51
1:A:577:ILE:HA	1:A:580:VAL:CG2	2.39	0.51
1:A:913:LEU:HD12	1:A:914:GLU:H	1.73	0.51
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.92	0.51
2:B:459:TYR:CE1	2:B:469:GLN:HB2	2.46	0.51
2:B:54:PHE:CE2	2:B:59:LEU:HD13	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:100:GLN:O	6:F:103:MET:HB2	2.10	0.51
7:G:165:GLU:HG3	7:G:168:LEU:HD12	1.90	0.51
12:L:61:THR:HG21	12:L:63:ARG:NE	2.25	0.51
1:A:1037:LEU:HD12	1:A:1042:PHE:CA	2.40	0.51
1:A:492:PRO:HG3	1:A:501:LEU:CD1	2.36	0.51
2:B:378:LEU:O	2:B:382:ILE:HG13	2.10	0.51
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.40	0.51
2:B:408:LEU:CD1	2:B:545:ILE:HG21	2.41	0.51
2:B:640:VAL:O	2:B:640:VAL:HG12	2.09	0.51
2:B:886:LYS:HE2	2:B:940:PRO:CG	2.40	0.51
1:A:151:ASP:HA	1:A:162:VAL:O	2.11	0.51
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.91	0.51
1:A:496:GLU:O	1:A:499:ALA:HB3	2.11	0.51
2:B:203:PHE:HD2	2:B:461:LEU:HD21	1.75	0.51
2:B:408:LEU:HD13	2:B:545:ILE:HG21	1.93	0.51
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.45	0.51
1:A:1324:PRO:CB	5:E:142:VAL:HG11	2.40	0.51
7:G:122:ASN:HB2	7:G:131:GLN:HG2	1.92	0.51
1:A:1008:GLN:O	1:A:1011:GLN:HB3	2.11	0.51
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.92	0.51
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.92	0.51
1:A:340:LEU:HD21	2:B:1200:ALA:N	2.26	0.51
1:A:981:LEU:HD23	1:A:1039:LYS:HA	1.93	0.51
2:B:294:ASP:C	2:B:296:GLU:H	2.14	0.51
2:B:638:PHE:HE1	2:B:743:ILE:HA	1.74	0.51
1:A:853:ASP:HB3	6:F:138:LEU:HD21	1.93	0.51
11:K:12:LEU:HA	11:K:37:LYS:HG3	1.91	0.51
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.25	0.51
1:A:441:PRO:O	1:A:492:PRO:HG2	2.11	0.51
1:A:44:THR:O	1:A:45:GLN:HB2	2.10	0.51
1:A:68:GLN:NE2	1:A:68:GLN:O	2.43	0.51
2:B:114:PRO:O	2:B:118:ARG:HG3	2.09	0.51
2:B:514:LEU:HD12	2:B:518:HIS:HD2	1.76	0.51
2:B:822:ASN:HD22	2:B:822:ASN:N	2.08	0.51
3:C:115:SER:HB2	3:C:142:VAL:HB	1.93	0.51
3:C:77:ILE:N	3:C:129:ILE:HD11	2.25	0.51
4:D:18:VAL:O	4:D:19:GLU:CB	2.57	0.51
8:H:31:THR:HG22	8:H:31:THR:O	2.10	0.51
2:B:800:GLN:CB	10:J:52:THR:HG22	2.38	0.51
12:L:44:ASP:O	12:L:45:ALA:HB3	2.10	0.51
1:A:332:LYS:C	1:A:334:GLY:H	2.15	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.75	0.51
1:A:370:ILE:C	1:A:372:LYS:N	2.64	0.51
1:A:855:THR:HA	1:A:866:PHE:O	2.11	0.51
2:B:1022:THR:HG23	2:B:1022:THR:O	2.10	0.51
2:B:575:PRO:HG2	2:B:576:ASP:H	1.76	0.51
2:B:759:PRO:C	2:B:761:HIS:H	2.13	0.51
2:B:795:ILE:HD12	2:B:795:ILE:N	2.26	0.51
3:C:53:THR:HG21	3:C:152:GLU:HB3	1.92	0.51
3:C:57:VAL:HG23	3:C:58:LEU:N	2.26	0.51
7:G:111:THR:HG22	7:G:114:LEU:CD1	2.39	0.51
8:H:63:LEU:CB	8:H:90:ALA:HB3	2.41	0.51
8:H:95:TYR:HE2	8:H:97:MET:SD	2.34	0.51
12:L:34:CYS:O	12:L:35:SER:C	2.48	0.51
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.11	0.51
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.92	0.51
1:A:1437:GLY:O	1:A:1441:PHE:CE2	2.64	0.51
1:A:518:LYS:CB	1:A:519:PRO:HD2	2.40	0.51
1:A:586:ILE:HD11	1:A:633:VAL:HG22	1.93	0.51
1:A:666:ILE:HD12	1:A:667:GLY:N	2.24	0.51
1:A:866:PHE:O	1:A:867:ILE:HD12	2.09	0.51
2:B:1116:ARG:HG3	2:B:1198:TYR:CG	2.45	0.51
2:B:1212:ILE:HG22	2:B:1212:ILE:O	2.11	0.51
2:B:32:ALA:HB3	2:B:658:ILE:HD11	1.92	0.51
2:B:698:GLU:HA	2:B:701:ILE:HG12	1.93	0.51
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.45	0.51
3:C:184:ASN:ND2	3:C:189:THR:H	2.04	0.51
4:D:4:SER:O	4:D:5:THR:HB	2.11	0.51
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.45	0.51
8:H:59:ILE:O	8:H:60:ALA:CB	2.59	0.51
3:C:49:VAL:O	12:L:66:GLN:HA	2.10	0.51
1:A:868:TYR:CE1	1:A:1064:VAL:HG22	2.45	0.51
1:A:1384:VAL:HA	1:A:1389:PHE:CE2	2.46	0.51
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.46	0.51
2:B:957:ASN:ND2	2:B:961:LEU:HB2	2.21	0.51
4:D:160:VAL:HG12	4:D:161:GLY:N	2.26	0.51
4:D:50:LEU:H	4:D:50:LEU:HD23	1.75	0.51
6:F:84:TYR:CA	6:F:152:ILE:HD12	2.41	0.51
8:H:59:ILE:HG22	8:H:60:ALA:H	1.75	0.51
10:J:8:PHE:CE2	10:J:49:MET:SD	3.04	0.51
11:K:68:PHE:HD2	11:K:68:PHE:N	2.08	0.51
1:A:993:LEU:HB2	1:A:1046:LEU:HD22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.11	0.50
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.11	0.50
1:A:331:GLY:O	1:A:332:LYS:O	2.29	0.50
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.92	0.50
1:A:490:HIS:CD2	1:A:490:HIS:N	2.79	0.50
2:B:345:LYS:HE3	2:B:349:ILE:HD11	1.93	0.50
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.45	0.50
3:C:18:VAL:O	3:C:18:VAL:HG12	2.10	0.50
6:F:147:SER:OG	6:F:150:GLU:HG3	2.12	0.50
11:K:56:VAL:HG12	11:K:56:VAL:O	2.11	0.50
11:K:75:ILE:N	11:K:75:ILE:HD13	2.26	0.50
12:L:38:LEU:HD12	12:L:39:SER:N	2.26	0.50
1:A:332:LYS:H	1:A:337:ARG:CB	2.23	0.50
1:A:532:ARG:CD	1:A:749:ALA:HB2	2.41	0.50
2:B:1058:LEU:HD23	2:B:1061:GLU:OE2	2.10	0.50
2:B:240:ILE:HD12	2:B:241:ARG:N	2.25	0.50
2:B:390:LEU:O	2:B:391:ASP:C	2.49	0.50
2:B:785:TYR:HE2	10:J:60:PHE:CZ	2.29	0.50
6:F:101:ILE:HD11	6:F:107:VAL:HG13	1.92	0.50
3:C:66:ARG:NH2	10:J:3:VAL:O	2.45	0.50
11:K:68:PHE:O	11:K:70:ARG:HG2	2.11	0.50
11:K:83:PRO:O	11:K:84:LYS:C	2.49	0.50
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.92	0.50
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.45	0.50
1:A:881:GLN:HE22	1:A:959:ASN:HA	1.75	0.50
2:B:1037:LEU:HD12	2:B:1037:LEU:H	1.77	0.50
2:B:221:ASN:OD1	2:B:242:SER:HA	2.10	0.50
2:B:91:SER:OG	2:B:133:LYS:HB2	2.12	0.50
8:H:63:LEU:CG	8:H:90:ALA:HB3	2.41	0.50
1:A:1349:TYR:HD2	1:A:1349:TYR:C	2.14	0.50
1:A:63:ARG:HG3	1:A:74:MET:HE1	1.93	0.50
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.42	0.50
2:B:60:GLN:NE2	2:B:95:ILE:HB	2.25	0.50
2:B:831:SER:HG	2:B:833:TYR:HD1	1.59	0.50
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.12	0.50
3:C:37:MET:HE3	3:C:176:ILE:HD13	1.94	0.50
3:C:76:ASP:O	3:C:79:GLN:HG2	2.11	0.50
4:D:47:LEU:HD13	4:D:48:ILE:N	2.26	0.50
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.45	0.50
5:E:89:GLY:C	5:E:91:LYS:H	2.13	0.50
1:A:1329:THR:HG22	1:A:1329:THR:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:O	1:A:457:ALA:HA	2.10	0.50
1:A:593:GLU:C	1:A:595:THR:H	2.15	0.50
1:A:966:ASN:O	1:A:970:THR:CB	2.60	0.50
2:B:323:VAL:HG12	2:B:323:VAL:O	2.10	0.50
2:B:796:LEU:HD21	2:B:821:GLN:HG3	1.92	0.50
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.92	0.50
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.12	0.50
4:D:156:ASP:C	4:D:158:GLU:H	2.14	0.50
4:D:35:LEU:HD11	4:D:173:HIS:CD2	2.46	0.50
7:G:81:PRO:O	7:G:82:PHE:CD2	2.65	0.50
8:H:118:PHE:HD1	8:H:121:LEU:O	1.95	0.50
8:H:58:THR:HG22	8:H:59:ILE:N	2.26	0.50
11:K:22:ASP:C	11:K:31:VAL:HG13	2.31	0.50
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.12	0.50
1:A:302:THR:HA	1:A:305:ASP:O	2.12	0.50
1:A:353:ILE:HG21	1:A:487:MET:CG	2.40	0.50
1:A:354:SER:HA	1:A:482:PHE:CE2	2.47	0.50
1:A:464:PRO:O	1:A:465:TYR:O	2.30	0.50
1:A:573:SER:OG	1:A:576:GLN:HB2	2.11	0.50
1:A:633:VAL:O	1:A:634:THR:C	2.48	0.50
1:A:858:ASN:ND2	1:A:861:GLY:H	2.09	0.50
2:B:1077:THR:OG1	2:B:1079:LYS:HB3	2.11	0.50
2:B:1183:LYS:HD2	2:B:1183:LYS:O	2.11	0.50
2:B:628:THR:O	2:B:628:THR:HG23	2.10	0.50
2:B:637:LEU:HB3	2:B:740:HIS:HB3	1.93	0.50
2:B:780:VAL:HG21	10:J:56:LEU:HD11	1.94	0.50
4:D:128:VAL:O	4:D:131:GLU:HB3	2.12	0.50
5:E:80:VAL:HG12	5:E:82:PHE:HE1	1.77	0.50
7:G:106:MET:HG2	7:G:107:LYS:N	2.25	0.50
1:A:973:ILE:HG21	1:A:1036:ARG:O	2.12	0.50
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.77	0.50
1:A:185:TRP:HE3	1:A:185:TRP:H	1.58	0.50
1:A:82:GLY:C	1:A:241:VAL:HB	2.32	0.50
2:B:1107:ALA:O	2:B:1108:ARG:HB2	2.11	0.50
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.77	0.50
2:B:429:PHE:CD2	2:B:433:GLN:NE2	2.79	0.50
2:B:429:PHE:HD2	2:B:433:GLN:NE2	2.10	0.50
2:B:213:ILE:HD11	2:B:481:GLN:CD	2.32	0.50
4:D:13:ARG:C	4:D:15:LEU:H	2.15	0.50
5:E:117:THR:HG22	5:E:119:SER:H	1.76	0.50
12:L:27:LEU:HD13	12:L:37:LYS:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.75	0.50
1:A:129:LYS:O	1:A:130:ASP:HB2	2.12	0.50
1:A:1323:ASP:OD2	1:A:1325:THR:HG22	2.12	0.50
1:A:379:VAL:HG12	1:A:380:VAL:H	1.76	0.50
2:B:60:GLN:HE22	2:B:95:ILE:HB	1.76	0.50
2:B:844:SER:O	2:B:847:ASP:HB2	2.12	0.50
4:D:220:LEU:HD23	4:D:221:TYR:N	2.23	0.50
5:E:23:VAL:O	5:E:28:TYR:HB2	2.11	0.50
7:G:1:MET:HE3	7:G:80:LYS:O	2.11	0.50
7:G:53:ASN:HD22	7:G:53:ASN:N	2.10	0.50
8:H:106:GLU:HG2	8:H:112:ILE:HD11	1.92	0.50
8:H:139:ASN:O	8:H:140:ALA:CB	2.59	0.50
1:A:1198:ASP:HB3	1:A:1201:ALA:CB	2.41	0.50
1:A:1445:ILE:HD11	7:G:70:PHE:CE2	2.47	0.50
1:A:476:SER:N	1:A:477:PRO:CD	2.75	0.50
1:A:79:GLY:HA3	1:A:243:PRO:CB	2.37	0.50
1:A:947:PHE:CD2	1:A:947:PHE:N	2.80	0.50
2:B:1160:VAL:CG1	2:B:1161:HIS:H	2.25	0.50
3:C:127:ARG:O	3:C:129:ILE:N	2.45	0.50
4:D:125:SER:O	4:D:128:VAL:HB	2.12	0.50
11:K:35:PHE:CD1	11:K:35:PHE:N	2.78	0.50
1:A:100:LYS:HE2	1:A:104:GLU:OE2	2.12	0.49
1:A:1103:GLU:C	1:A:1108:ALA:HB2	2.32	0.49
1:A:1331:SER:OG	1:A:1333:ILE:HG22	2.12	0.49
1:A:24:PRO:O	1:A:28:ARG:HB2	2.12	0.49
1:A:40:THR:CG2	1:A:54:ASN:HD21	2.24	0.49
1:A:903:ASN:HD22	1:A:905:ASP:N	1.87	0.49
2:B:1096:ARG:HB2	2:B:1096:ARG:NH1	2.27	0.49
3:C:70:ILE:O	3:C:72:LEU:CD1	2.56	0.49
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.93	0.49
3:C:93:ASP:OD2	3:C:122:SER:HB2	2.11	0.49
7:G:9:LEU:HG	7:G:11:ILE:CG1	2.41	0.49
7:G:159:ALA:C	7:G:160:ILE:HD12	2.32	0.49
1:A:1198:ASP:HB3	1:A:1201:ALA:HB3	1.94	0.49
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.58	0.49
1:A:490:HIS:HE1	2:B:1130:PHE:HB2	1.77	0.49
2:B:58:THR:O	2:B:62:ILE:HG13	2.12	0.49
4:D:40:HIS:CD2	7:G:73:LYS:HE3	2.47	0.49
5:E:100:ILE:HG23	5:E:105:PHE:HD1	1.74	0.49
5:E:106:GLN:HA	5:E:130:ALA:HB2	1.95	0.49
5:E:182:ASP:OD1	5:E:183:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1322:ILE:HG13	1:A:1323:ASP:N	2.26	0.49
1:A:58:LEU:HD13	1:A:243:PRO:HA	1.94	0.49
1:A:91:PHE:N	1:A:297:GLN:HE22	2.09	0.49
1:A:525:GLN:O	1:A:526:ASP:C	2.50	0.49
1:A:9:ALA:HB3	2:B:1193:GLN:HB2	1.93	0.49
1:A:374:LEU:HD11	2:B:1105:ALA:HB1	1.94	0.49
2:B:545:ILE:HG22	2:B:546:SER:O	2.12	0.49
4:D:155:ARG:NH2	4:D:221:TYR:CD1	2.81	0.49
5:E:3:GLN:HE21	5:E:52:ARG:HH12	1.58	0.49
4:D:6:SER:HB3	7:G:8:SER:OG	2.11	0.49
10:J:57:ILE:CG2	10:J:58:GLU:N	2.75	0.49
1:A:1030:ARG:HD3	1:A:1035:TYR:OH	2.13	0.49
1:A:1197:LEU:HD12	1:A:1209:MET:SD	2.52	0.49
1:A:370:ILE:HG22	1:A:374:LEU:HD13	1.92	0.49
2:B:1016:ALA:HB1	2:B:1020:ARG:HE	1.76	0.49
2:B:269:ILE:HG21	2:B:282:ILE:HD13	1.95	0.49
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.12	0.49
2:B:780:VAL:HB	2:B:817:LEU:HD22	1.93	0.49
1:A:253:ASN:HB3	2:B:935:ARG:NH1	2.28	0.49
6:F:139:PRO:O	6:F:141:GLY:N	2.45	0.49
7:G:8:SER:HA	7:G:72:VAL:O	2.12	0.49
11:K:57:LEU:H	11:K:77:THR:HA	1.77	0.49
3:C:165:LYS:O	11:K:6:ARG:HD2	2.13	0.49
12:L:38:LEU:O	12:L:39:SER:HB2	2.12	0.49
1:A:670:ILE:H	1:A:670:ILE:HD13	1.78	0.49
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.92	0.49
2:B:222:ILE:HD11	2:B:627:PHE:HZ	1.77	0.49
2:B:458:LYS:O	2:B:459:TYR:C	2.51	0.49
3:C:185:LYS:C	3:C:186:LEU:HD12	2.33	0.49
3:C:86:CYS:SG	3:C:87:PHE:N	2.86	0.49
4:D:156:ASP:C	4:D:158:GLU:N	2.64	0.49
4:D:25:ALA:C	4:D:27:LEU:H	2.15	0.49
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.76	0.49
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.27	0.49
12:L:61:THR:HG21	12:L:63:ARG:HE	1.77	0.49
2:B:900:ALA:CB	12:L:61:THR:OG1	2.61	0.49
1:A:528:LEU:C	1:A:528:LEU:HD12	2.33	0.49
1:A:741:ASN:HD21	1:A:743:VAL:CG2	2.12	0.49
1:A:761:MET:HA	1:A:804:TYR:HB2	1.95	0.49
2:B:176:SER:O	2:B:182:SER:HB3	2.13	0.49
2:B:604:ARG:HG3	2:B:611:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.42	0.49
9:I:17:ARG:NH2	9:I:30:ARG:NH2	2.61	0.49
1:A:1146:VAL:HG12	1:A:1201:ALA:O	2.12	0.49
1:A:335:ARG:O	1:A:339:ASN:HB2	2.13	0.49
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.47	0.49
2:B:1170:THR:HB	2:B:1182:CYS:HB2	1.95	0.49
3:C:45:ALA:HB1	3:C:72:LEU:HD13	1.94	0.49
1:A:1325:THR:O	5:E:147:HIS:CD2	2.66	0.49
5:E:93:MET:O	5:E:97:VAL:HG23	2.13	0.49
12:L:45:ALA:C	12:L:46:VAL:HG22	2.33	0.49
1:A:14:VAL:N	1:A:1432:GLN:HE22	2.01	0.49
1:A:316:GLN:HG2	1:A:317:LYS:HG2	1.93	0.49
1:A:34:LYS:CE	1:A:57:ARG:NH1	2.71	0.49
2:B:226:PHE:CE2	2:B:398:ARG:NH2	2.80	0.49
2:B:298:LEU:HD22	2:B:298:LEU:N	2.27	0.49
2:B:361:LEU:N	2:B:362:PRO:HD3	2.26	0.49
2:B:167:ILE:HG22	2:B:453:ILE:HG13	1.94	0.49
2:B:635:ARG:HH22	2:B:742:GLU:CD	2.16	0.49
3:C:112:ASN:HB3	3:C:114:TYR:HE1	1.78	0.49
3:C:15:LYS:O	3:C:240:VAL:HG22	2.13	0.49
4:D:71:LYS:HA	4:D:74:GLN:HG3	1.93	0.49
6:F:88:TYR:O	6:F:89:GLU:C	2.50	0.49
7:G:13:LEU:HD23	7:G:14:HIS:H	1.75	0.49
8:H:115:TYR:CZ	8:H:124:ARG:HG3	2.48	0.49
8:H:62:SER:C	8:H:63:LEU:HD12	2.33	0.49
11:K:42:LEU:O	11:K:46:ILE:HG13	2.13	0.49
1:A:1116:LEU:HB2	1:A:1311:VAL:HG22	1.93	0.49
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.80	0.49
1:A:224:PHE:CD2	1:A:231:PRO:CD	2.95	0.49
1:A:362:ASP:HB3	1:A:507:VAL:CG1	2.39	0.49
1:A:41:MET:CB	1:A:49:LYS:HA	2.43	0.49
1:A:572:TRP:HH2	8:H:79:TRP:CZ3	2.31	0.49
1:A:63:ARG:HG2	1:A:74:MET:HE1	1.93	0.49
1:A:883:LEU:HD21	1:A:956:LEU:HD11	1.95	0.49
2:B:1203:LEU:HA	2:B:1206:GLU:OE1	2.13	0.49
2:B:705:MET:N	2:B:710:LEU:HD12	2.25	0.49
2:B:980:PHE:HE1	2:B:990:ILE:HG13	1.78	0.49
3:C:8:VAL:HG12	3:C:9:LYS:H	1.78	0.49
4:D:138:ASN:O	4:D:139:LYS:C	2.51	0.49
4:D:52:LEU:O	4:D:54:GLU:N	2.44	0.49
6:F:109:VAL:CG1	6:F:110:ASP:H	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:55:ILE:O	12:L:56:LEU:CB	2.60	0.49
1:A:1437:GLY:O	1:A:1441:PHE:HE2	1.96	0.49
1:A:567:LYS:CB	8:H:95:TYR:HA	2.43	0.49
1:A:563:PRO:HB3	1:A:572:TRP:CZ2	2.47	0.49
1:A:741:ASN:HD22	1:A:743:VAL:N	2.11	0.49
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.94	0.49
1:A:997:LEU:HD22	1:A:1053:PHE:CD2	2.48	0.49
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.78	0.49
2:B:188:ASP:C	2:B:192:LEU:HD12	2.33	0.49
2:B:227:LYS:H	2:B:395:GLN:CD	2.16	0.49
2:B:290:GLY:O	2:B:292:ILE:HG13	2.13	0.49
2:B:288:ALA:HB1	2:B:331:LEU:HG	1.94	0.49
2:B:581:PHE:O	2:B:626:ILE:HB	2.12	0.49
2:B:757:PRO:O	2:B:758:PHE:HB2	2.13	0.49
4:D:179:GLN:O	4:D:183:LEU:HD12	2.13	0.49
5:E:185:ALA:HA	5:E:190:LEU:HG	1.95	0.49
5:E:198:ILE:HB	5:E:210:SER:HB3	1.94	0.49
7:G:17:PHE:C	7:G:19:GLY:H	2.16	0.49
1:A:14:VAL:HB	1:A:1430:LEU:CD1	2.43	0.48
1:A:252:PHE:O	1:A:253:ASN:HB3	2.13	0.48
1:A:28:ARG:HG3	1:A:83:HIS:CE1	2.48	0.48
1:A:426:LEU:O	1:A:427:GLN:HG2	2.13	0.48
1:A:453:MET:HG2	1:A:520:CYS:SG	2.53	0.48
1:A:491:VAL:HG13	1:A:492:PRO:O	2.13	0.48
1:A:58:LEU:CB	1:A:80:HIS:O	2.61	0.48
1:A:863:VAL:HG12	1:A:864:ILE:N	2.28	0.48
1:A:998:LEU:O	1:A:999:VAL:HG23	2.13	0.48
2:B:188:ASP:N	2:B:188:ASP:OD2	2.44	0.48
2:B:446:LEU:HD23	2:B:448:ILE:HD11	1.94	0.48
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.66	0.48
2:B:876:LYS:HG3	2:B:893:LEU:HD12	1.95	0.48
3:C:167:HIS:CD2	12:L:70:ARG:HG2	2.49	0.48
12:L:47:ARG:NH1	12:L:47:ARG:HB2	2.27	0.48
1:A:1152:ILE:HD11	9:I:44:TYR:HD2	1.77	0.48
1:A:125:ALA:O	1:A:128:ILE:HB	2.13	0.48
1:A:1329:THR:CG2	1:A:1331:SER:H	2.26	0.48
1:A:1362:TYR:C	1:A:1362:TYR:CD1	2.85	0.48
1:A:360:GLU:O	1:A:361:LEU:C	2.51	0.48
1:A:81:PHE:CE2	1:A:243:PRO:HD3	2.48	0.48
1:A:874:ASP:O	1:A:876:ALA:N	2.46	0.48
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:PHE:O	2:B:361:LEU:C	2.52	0.48
3:C:61:GLU:O	3:C:62:PHE:C	2.50	0.48
4:D:51:ASN:HB3	4:D:178:ALA:O	2.13	0.48
6:F:76:LYS:O	6:F:79:ARG:HD3	2.13	0.48
6:F:80:ALA:HB3	6:F:144:GLU:OE2	2.13	0.48
7:G:30:LEU:CD2	7:G:31:LEU:HD23	2.43	0.48
10:J:17:LYS:O	10:J:20:SER:N	2.45	0.48
2:B:190:TYR:HD2	10:J:63:TYR:CE2	2.31	0.48
1:A:380:VAL:HB	1:A:430:TRP:H	1.78	0.48
2:B:1007:VAL:HG23	2:B:1008:PRO:CD	2.43	0.48
2:B:1079:LYS:N	3:C:27:LEU:HD21	2.29	0.48
2:B:202:TYR:CD2	2:B:202:TYR:N	2.65	0.48
2:B:659:ALA:HA	2:B:662:MET:HE2	1.94	0.48
3:C:68:GLY:O	3:C:169:LYS:HB2	2.13	0.48
3:C:235:VAL:HG12	10:J:13:VAL:CG1	2.43	0.48
5:E:152:LYS:HG3	5:E:154:ILE:CD1	2.43	0.48
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.95	0.48
11:K:109:TRP:C	11:K:109:TRP:CD1	2.87	0.48
11:K:31:VAL:HG12	11:K:32:VAL:N	2.28	0.48
1:A:1393:ASN:O	1:A:1394:THR:O	2.30	0.48
1:A:298:PHE:C	1:A:298:PHE:CD2	2.87	0.48
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.95	0.48
1:A:588:LEU:HB3	1:A:607:ILE:HB	1.95	0.48
1:A:763:ALA:C	1:A:803:SER:HB3	2.33	0.48
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.42	0.48
2:B:108:VAL:HG23	2:B:109:THR:N	2.29	0.48
2:B:1206:GLU:O	2:B:1209:ALA:HB3	2.13	0.48
2:B:516:ASN:ND2	2:B:516:ASN:N	2.62	0.48
2:B:541:LEU:CD1	2:B:747:MET:HE1	2.44	0.48
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.78	0.48
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.95	0.48
3:C:167:HIS:O	3:C:169:LYS:N	2.47	0.48
4:D:56:ARG:HD3	4:D:149:THR:CA	2.41	0.48
11:K:34:THR:HG22	11:K:34:THR:O	2.13	0.48
1:A:1005:GLU:O	1:A:1006:ILE:C	2.51	0.48
1:A:255:SER:OG	2:B:918:ILE:HD13	2.14	0.48
1:A:463:ILE:CB	1:A:464:PRO:CD	2.87	0.48
1:A:728:LYS:O	1:A:732:LEU:HB2	2.14	0.48
1:A:81:PHE:HA	1:A:243:PRO:HG3	1.96	0.48
2:B:582:VAL:HB	2:B:587:HIS:CD2	2.48	0.48
2:B:736:THR:O	2:B:736:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ARG:CD	2:B:955:THR:HG21	2.44	0.48
3:C:57:VAL:HG23	3:C:58:LEU:HD23	1.96	0.48
5:E:79:TRP:HB2	5:E:105:PHE:CE1	2.48	0.48
7:G:150:CYS:C	7:G:151:ILE:HD12	2.33	0.48
4:D:73:SER:CB	7:G:21:ARG:HH21	2.26	0.48
10:J:6:ARG:N	10:J:14:VAL:HB	2.28	0.48
12:L:38:LEU:HD21	12:L:48:CYS:HA	1.95	0.48
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.13	0.48
1:A:1151:GLU:HG2	9:I:45:ARG:HB2	1.96	0.48
1:A:257:ARG:HG2	1:A:258:GLY:H	1.78	0.48
1:A:58:LEU:HD12	1:A:244:PRO:CD	2.44	0.48
1:A:67:CYS:O	1:A:68:GLN:C	2.52	0.48
1:A:773:LYS:HD2	1:A:773:LYS:H	1.78	0.48
1:A:722:LEU:HD23	1:A:799:PHE:CD1	2.49	0.48
2:B:642:ASP:HA	2:B:649:LYS:HG3	1.95	0.48
3:C:124:LEU:HB3	3:C:126:GLY:H	1.77	0.48
3:C:179:GLU:HG2	3:C:180:TYR:N	2.28	0.48
3:C:183:TRP:O	3:C:185:LYS:N	2.47	0.48
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.43	0.48
5:E:151:PRO:HD2	5:E:153:HIS:HE1	1.77	0.48
6:F:138:LEU:O	6:F:139:PRO:C	2.52	0.48
6:F:72:LYS:O	6:F:143:PHE:CD2	2.67	0.48
9:I:33:SER:O	9:I:35:VAL:HG23	2.13	0.48
12:L:59:ALA:O	12:L:60:ARG:O	2.31	0.48
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.96	0.48
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.14	0.48
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.94	0.48
1:A:722:LEU:HD12	1:A:722:LEU:N	2.29	0.48
2:B:637:LEU:HB2	2:B:693:ILE:HD12	1.94	0.48
3:C:173:ALA:O	3:C:174:ALA:HB3	2.14	0.48
8:H:58:THR:HG22	8:H:59:ILE:H	1.79	0.48
3:C:57:VAL:CG1	10:J:60:PHE:HB3	2.37	0.48
12:L:51:CYS:HB3	12:L:53:HIS:HB2	1.94	0.48
1:A:967:ALA:HA	1:A:1044:TRP:HZ3	1.77	0.48
1:A:1430:LEU:O	1:A:1432:GLN:HG3	2.12	0.48
1:A:145:LYS:HA	1:A:145:LYS:HE3	1.96	0.48
1:A:492:PRO:HA	1:A:497:THR:HG21	1.96	0.48
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.28	0.48
1:A:245:PRO:O	2:B:1114:LEU:CD1	2.61	0.48
2:B:247:GLY:HA2	2:B:418:LYS:NZ	2.28	0.48
6:F:100:GLN:HA	6:F:103:MET:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:48:PRO:O	8:H:49:VAL:HG23	2.14	0.48
1:A:1227:ILE:CA	1:A:1228:TRP:CE3	2.96	0.48
1:A:1227:ILE:C	1:A:1228:TRP:CE3	2.86	0.48
1:A:350:ARG:O	1:A:351:THR:HG22	2.13	0.48
1:A:388:LEU:HB3	1:A:432:VAL:HG21	1.95	0.48
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.96	0.48
1:A:756:ILE:O	1:A:759:ALA:HB3	2.14	0.48
1:A:831:THR:O	1:A:834:THR:HB	2.14	0.48
2:B:1114:LEU:HD11	2:B:1202:LEU:HD11	1.94	0.48
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.54	0.48
2:B:496:ARG:O	2:B:539:LEU:HD12	2.14	0.48
2:B:796:LEU:O	2:B:799:PRO:HD3	2.14	0.48
3:C:97:VAL:HG21	3:C:129:ILE:HG22	1.96	0.48
3:C:70:ILE:HG22	3:C:71:PRO:HD2	1.95	0.48
4:D:32:GLU:HB3	4:D:33:PHE:CD1	2.49	0.48
5:E:153:HIS:CD2	5:E:184:VAL:HG11	2.49	0.48
5:E:61:GLN:HB2	5:E:79:TRP:CE3	2.49	0.48
7:G:61:ILE:HG13	7:G:68:ALA:HB2	1.94	0.48
8:H:125:LEU:HG	8:H:126:GLU:N	2.28	0.48
1:A:105:CYS:O	1:A:114:LEU:HG	2.12	0.48
1:A:1227:ILE:CA	1:A:1228:TRP:HE3	2.27	0.48
1:A:523:ILE:HG23	1:A:527:THR:HB	1.95	0.48
1:A:89:PRO:O	1:A:204:THR:HG21	2.14	0.48
1:A:974:ASP:OD2	1:A:977:LYS:HB2	2.14	0.48
2:B:1003:ALA:CB	3:C:179:GLU:HB2	2.43	0.48
2:B:1084:GLN:C	2:B:1085:ILE:HD12	2.34	0.48
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.47	0.48
2:B:409:ALA:O	2:B:413:LEU:HD12	2.14	0.48
3:C:3:GLU:HB3	11:K:104:ASN:ND2	2.29	0.48
4:D:4:SER:O	4:D:5:THR:CB	2.62	0.48
5:E:119:SER:HA	5:E:122:LYS:CG	2.43	0.48
5:E:151:PRO:HD2	5:E:153:HIS:CE1	2.49	0.48
1:A:1001:ARG:O	1:A:1002:GLY:O	2.32	0.47
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.43	0.47
1:A:1260:LEU:HA	1:A:1263:ILE:CD1	2.44	0.47
1:A:535:THR:CG2	1:A:616:VAL:HA	2.44	0.47
1:A:850:VAL:HG23	1:A:1064:VAL:CG2	2.44	0.47
2:B:1192:TYR:CD1	2:B:1218:THR:HG21	2.48	0.47
2:B:500:THR:O	2:B:535:LEU:HD22	2.14	0.47
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.49	0.47
2:B:862:GLN:HA	2:B:962:LYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:49:ALA:HB3	4:D:174:PRO:O	2.13	0.47
8:H:130:ARG:HB3	8:H:133:ASN:HB2	1.96	0.47
9:I:17:ARG:HB3	9:I:26:LEU:HB3	1.96	0.47
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.92	0.47
1:A:515:GLN:HE22	1:A:1074:GLU:HB3	1.80	0.47
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.14	0.47
1:A:1346:ALA:O	1:A:1347:ALA:C	2.52	0.47
1:A:425:GLN:CD	1:A:425:GLN:H	2.16	0.47
1:A:947:PHE:N	1:A:947:PHE:HD2	2.11	0.47
2:B:1046:PRO:O	2:B:1048:THR:HG23	2.14	0.47
2:B:113:TYR:HD2	2:B:114:PRO:HD2	1.77	0.47
2:B:1193:GLN:C	2:B:1194:ILE:HG22	2.34	0.47
2:B:27:ALA:O	2:B:29:ASP:N	2.47	0.47
2:B:485:ARG:NH1	2:B:782:LEU:HD21	2.29	0.47
2:B:785:TYR:C	2:B:787:VAL:N	2.67	0.47
2:B:797:TYR:HB3	2:B:798:TYR:CD2	2.43	0.47
3:C:141:GLY:O	3:C:142:VAL:HB	2.14	0.47
3:C:82:TYR:CD2	3:C:84:ARG:NH2	2.82	0.47
5:E:84:ASP:O	5:E:86:PRO:HD3	2.14	0.47
7:G:56:ILE:HG23	7:G:57:GLN:N	2.26	0.47
8:H:37:LYS:HD2	8:H:126:GLU:OE2	2.13	0.47
11:K:22:ASP:O	11:K:31:VAL:HG13	2.13	0.47
1:A:1226:VAL:HG22	1:A:1240:CYS:CB	2.43	0.47
2:B:1101:ASP:O	2:B:1122:ARG:CZ	2.63	0.47
2:B:276:ILE:HD11	2:B:334:ILE:HG23	1.96	0.47
2:B:277:LYS:HG2	2:B:336:ARG:O	2.14	0.47
2:B:409:ALA:C	2:B:413:LEU:HD12	2.34	0.47
2:B:706:GLN:HA	2:B:707:PRO:HD2	1.72	0.47
2:B:743:ILE:H	2:B:743:ILE:HG12	1.41	0.47
4:D:71:LYS:HA	4:D:74:GLN:CG	2.44	0.47
5:E:143:ASN:HB3	5:E:146:HIS:HB2	1.95	0.47
5:E:131:THR:HG21	5:E:191:LYS:NZ	2.29	0.47
1:A:1289:ARG:HH22	1:A:1326:ARG:NH1	2.12	0.47
1:A:1364:ASN:O	1:A:1365:TYR:C	2.53	0.47
1:A:1364:ASN:O	1:A:1366:ARG:N	2.47	0.47
1:A:1391:ARG:O	1:A:1392:SER:O	2.33	0.47
2:B:1205:GLN:O	2:B:1208:MET:HB2	2.15	0.47
2:B:365:THR:HG23	2:B:367:LEU:N	2.29	0.47
2:B:612:GLU:HG2	2:B:613:VAL:N	2.28	0.47
2:B:582:VAL:HG22	2:B:626:ILE:HG21	1.96	0.47
2:B:918:ILE:HD12	2:B:935:ARG:CZ	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:ILE:HD12	3:C:243:VAL:HG13	1.96	0.47
4:D:154:PHE:HZ	4:D:214:LEU:CD1	2.28	0.47
5:E:124:VAL:CG1	5:E:132:ILE:HB	2.32	0.47
1:A:1037:LEU:HD12	1:A:1042:PHE:N	2.30	0.47
1:A:1173:HIS:HB3	1:A:1227:ILE:HD13	1.97	0.47
1:A:127:ALA:O	1:A:129:LYS:HG3	2.15	0.47
1:A:1444:MET:HB2	1:A:1444:MET:HE2	1.63	0.47
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.79	0.47
2:B:310:MET:O	2:B:311:LEU:C	2.52	0.47
2:B:32:ALA:O	2:B:35:SER:HB2	2.15	0.47
2:B:43:LEU:HD11	2:B:811:TYR:O	2.14	0.47
3:C:125:MET:HB2	3:C:127:ARG:HE	1.78	0.47
7:G:151:ILE:N	7:G:151:ILE:HD12	2.30	0.47
9:I:7:CYS:C	9:I:8:ARG:O	2.51	0.47
12:L:38:LEU:CD1	12:L:49:LYS:HE2	2.44	0.47
1:A:1400:CYS:HA	1:A:1408:ILE:HD12	1.97	0.47
1:A:390:GLN:HE21	1:A:394:ASN:HD21	1.63	0.47
1:A:451:HIS:N	1:A:451:HIS:ND1	2.62	0.47
1:A:501:LEU:HD21	2:B:1146:PHE:CD1	2.49	0.47
1:A:675:THR:O	1:A:675:THR:HG22	2.15	0.47
1:A:852:TYR:HE2	1:A:1060:PRO:HB2	1.72	0.47
1:A:864:ILE:CD1	1:A:864:ILE:N	2.78	0.47
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.15	0.47
1:A:336:ILE:HD11	2:B:1203:LEU:HD12	1.92	0.47
2:B:190:TYR:CD1	10:J:62:ARG:HD3	2.49	0.47
2:B:498:THR:HB	2:B:537:LYS:O	2.14	0.47
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.50	0.47
3:C:178:PHE:C	3:C:178:PHE:HD2	2.18	0.47
7:G:8:SER:HB2	7:G:71:ASN:OD1	2.13	0.47
9:I:17:ARG:HG3	9:I:18:GLU:N	2.30	0.47
10:J:41:LEU:HD23	10:J:41:LEU:N	2.29	0.47
3:C:241:ASP:HB3	11:K:109:TRP:CZ3	2.49	0.47
11:K:61:TYR:C	11:K:61:TYR:CD1	2.88	0.47
12:L:30:ILE:HG22	12:L:31:CYS:O	2.15	0.47
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.34	0.47
1:A:1313:LEU:C	1:A:1315:GLU:N	2.68	0.47
1:A:434:ARG:CZ	1:A:437:MET:HG3	2.44	0.47
1:A:444:PHE:HE2	1:A:470:LEU:HD13	1.80	0.47
1:A:578:LEU:C	1:A:580:VAL:H	2.18	0.47
1:A:826:ASP:O	1:A:830:LYS:HB2	2.14	0.47
2:B:774:GLY:C	2:B:776:GLN:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:958:GLN:C	2:B:960:GLY:H	2.18	0.47
7:G:27:LYS:HE2	7:G:54:ILE:HD12	1.97	0.47
1:A:600:PRO:CA	8:H:25:ARG:NH1	2.75	0.47
1:A:1111:MET:SD	1:A:1114:PRO:HB3	2.54	0.47
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.14	0.47
1:A:1446:ASP:O	1:A:1447:GLU:C	2.52	0.47
1:A:19:PHE:CZ	1:A:1397:LEU:CD2	2.92	0.47
1:A:377:PRO:HB2	1:A:431:LYS:HZ2	1.80	0.47
1:A:591:PHE:HD2	1:A:595:THR:CB	2.17	0.47
1:A:649:ILE:O	1:A:650:GLN:C	2.53	0.47
1:A:705:LYS:HB2	1:A:708:MET:HE3	1.96	0.47
1:A:933:TYR:C	1:A:933:TYR:HD2	2.17	0.47
2:B:1023:VAL:HG13	2:B:1026:LEU:HD12	1.95	0.47
2:B:25:ILE:HD11	2:B:651:LEU:CD1	2.41	0.47
2:B:335:GLY:O	2:B:336:ARG:HB2	2.14	0.47
2:B:523:CYS:SG	2:B:524:PRO:HD2	2.55	0.47
2:B:579:ARG:HA	2:B:589:VAL:HG22	1.97	0.47
3:C:178:PHE:C	3:C:178:PHE:CD2	2.88	0.47
3:C:213:PRO:O	3:C:214:ASN:CB	2.63	0.47
4:D:198:LEU:HB2	4:D:199:ASN:H	1.53	0.47
5:E:177:ARG:HH11	5:E:215:MET:HE1	1.79	0.47
7:G:111:THR:H	7:G:114:LEU:HD22	1.79	0.47
4:D:40:HIS:HD2	7:G:73:LYS:HE3	1.80	0.47
1:A:1308:THR:HG23	1:A:1310:GLY:N	2.26	0.47
1:A:164:ARG:CG	1:A:165:GLY:N	2.78	0.47
1:A:26:GLU:O	1:A:30:ILE:HG13	2.14	0.47
1:A:496:GLU:O	1:A:500:GLU:HG3	2.14	0.47
1:A:532:ARG:HH12	1:A:745:GLN:NE2	2.13	0.47
1:A:653:VAL:O	1:A:654:ASN:C	2.53	0.47
1:A:857:ARG:HA	1:A:864:ILE:HD13	1.97	0.47
2:B:1076:HIS:ND1	2:B:1076:HIS:N	2.63	0.47
2:B:204:ILE:HG22	2:B:204:ILE:O	2.13	0.47
2:B:421:PHE:CD1	2:B:424:LEU:HD23	2.50	0.47
2:B:782:LEU:HB3	2:B:784:ASN:OD1	2.15	0.47
2:B:822:ASN:HD22	2:B:822:ASN:H	1.62	0.47
3:C:112:ASN:HD21	3:C:146:LYS:HG2	1.79	0.47
3:C:148:ARG:NH1	10:J:64:ASN:HA	2.30	0.47
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.40	0.47
3:C:44:LEU:HD13	3:C:129:ILE:HG23	1.96	0.47
3:C:46:ILE:HG22	3:C:47:ASP:N	2.29	0.47
3:C:70:ILE:HG23	3:C:142:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:163:GLU:OE2	5:E:167:ARG:HG3	2.13	0.47
9:I:8:ARG:O	9:I:9:ASP:HB2	2.15	0.47
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.29	0.47
1:A:1139:GLU:O	1:A:1139:GLU:HG2	2.14	0.47
1:A:339:ASN:O	1:A:343:LYS:HE2	2.15	0.47
1:A:501:LEU:HD21	2:B:1146:PHE:CE1	2.49	0.47
1:A:656:TRP:CH2	1:A:660:ASN:CG	2.88	0.47
1:A:678:GLU:O	1:A:681:GLU:HG2	2.15	0.47
1:A:808:LEU:HD21	1:A:816:HIS:HD2	1.80	0.47
1:A:929:LEU:N	1:A:929:LEU:HD22	2.29	0.47
1:A:933:TYR:C	1:A:933:TYR:CD2	2.88	0.47
2:B:850:LEU:HD12	2:B:851:PHE:N	2.30	0.47
3:C:128:ASN:OD1	3:C:131:HIS:HD2	1.98	0.47
10:J:57:ILE:CG2	10:J:58:GLU:H	2.28	0.47
1:A:1219:THR:HG21	1:A:1271:ILE:HD11	1.96	0.47
1:A:416:ARG:C	1:A:417:TYR:HD2	2.18	0.47
1:A:690:VAL:O	1:A:690:VAL:HG13	2.14	0.47
2:B:802:PRO:HG3	2:B:1091:TYR:CZ	2.50	0.47
2:B:821:GLN:HE22	2:B:851:PHE:H	1.63	0.47
1:A:356:ASP:OD2	2:B:833:TYR:CE2	2.67	0.47
4:D:15:LEU:O	4:D:17:LYS:N	2.48	0.47
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.97	0.47
12:L:47:ARG:NH2	12:L:54:ARG:HG2	2.30	0.47
1:A:166:GLY:O	1:A:167:CYS:O	2.33	0.46
1:A:227:VAL:HG12	1:A:228:PHE:CD1	2.51	0.46
1:A:809:THR:HB	1:A:810:PRO:HD2	1.97	0.46
1:A:990:VAL:HG12	1:A:991:LYS:N	2.31	0.46
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.27	0.46
2:B:1065:GLN:NE2	2:B:1066:SER:H	2.12	0.46
1:A:659:HIS:ND1	2:B:1074:ASN:ND2	2.63	0.46
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.73	0.46
2:B:311:LEU:O	2:B:312:GLU:C	2.54	0.46
2:B:615:MET:HB3	2:B:626:ILE:HA	1.96	0.46
2:B:711:GLU:CB	2:B:712:PRO:HD3	2.43	0.46
2:B:899:ILE:HD12	2:B:911:ILE:HG23	1.96	0.46
2:B:916:THR:HB	2:B:935:ARG:HG3	1.97	0.46
2:B:999:MET:HG2	2:B:1007:VAL:HG23	1.97	0.46
4:D:30:GLY:C	4:D:32:GLU:N	2.64	0.46
5:E:136:ASN:OD1	5:E:137:GLU:N	2.48	0.46
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.15	0.46
7:G:94:CYS:SG	7:G:130:TYR:CE1	3.08	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:130:ARG:CZ	8:H:130:ARG:HB2	2.44	0.46
8:H:63:LEU:HG	8:H:90:ALA:HB3	1.97	0.46
1:A:1436:ILE:O	1:A:1438:THR:N	2.47	0.46
1:A:1450:LEU:HD13	6:F:131:PRO:HG2	1.97	0.46
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.80	0.46
1:A:357:PRO:HD2	2:B:833:TYR:CE2	2.51	0.46
1:A:913:LEU:HB2	1:A:1032:LEU:HD22	1.97	0.46
2:B:739:THR:HB	2:B:740:HIS:ND1	2.29	0.46
3:C:175:ALA:HB2	10:J:10:CYS:CB	2.46	0.46
4:D:159:THR:O	4:D:162:ALA:HB3	2.15	0.46
5:E:153:HIS:HB3	5:E:196:VAL:CG2	2.45	0.46
5:E:156:LEU:HD12	5:E:195:VAL:HB	1.96	0.46
5:E:83:CYS:HB3	5:E:85:GLU:HG3	1.98	0.46
7:G:115:MET:SD	7:G:119:LEU:HD23	2.56	0.46
1:A:1313:LEU:HB3	1:A:1338:VAL:HG21	1.96	0.46
1:A:1421:CYS:C	1:A:1423:GLY:H	2.19	0.46
1:A:986:ILE:HD13	1:A:1031:VAL:HG21	1.97	0.46
2:B:132:VAL:HG23	2:B:165:VAL:HB	1.96	0.46
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.96	0.46
3:C:238:ILE:HG23	3:C:239:PRO:HD2	1.97	0.46
4:D:26:THR:C	4:D:28:GLN:H	2.18	0.46
11:K:32:VAL:HG23	11:K:74:ARG:CG	2.43	0.46
1:A:868:TYR:HE2	1:A:1366:ARG:NE	2.14	0.46
1:A:583:PRO:HB2	1:A:637:LYS:HE3	1.98	0.46
1:A:682:THR:HG22	1:A:682:THR:O	2.15	0.46
1:A:814:PHE:HE1	2:B:519:TRP:CB	2.26	0.46
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.32	0.46
2:B:226:PHE:HA	2:B:395:GLN:CG	2.45	0.46
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.30	0.46
2:B:596:LEU:O	2:B:600:LEU:HG	2.15	0.46
2:B:405:ARG:NH1	2:B:632:ARG:CG	2.79	0.46
2:B:63:ILE:HG23	2:B:63:ILE:O	2.14	0.46
2:B:856:PHE:HD1	2:B:856:PHE:N	2.14	0.46
3:C:191:TYR:HB3	3:C:201:TRP:CD1	2.51	0.46
5:E:31:THR:OG1	5:E:34:GLU:HB2	2.16	0.46
5:E:80:VAL:HG12	5:E:82:PHE:CE1	2.50	0.46
6:F:101:ILE:HA	6:F:105:ALA:HB3	1.96	0.46
8:H:143:LEU:N	8:H:143:LEU:HD12	2.30	0.46
10:J:1:MET:N	10:J:56:LEU:N	2.63	0.46
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.61	0.46
1:A:245:PRO:O	2:B:1114:LEU:HD11	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LYS:HE2	1:A:533:LYS:HB3	1.69	0.46
1:A:566:ILE:O	1:A:566:ILE:HG22	2.15	0.46
1:A:66:LYS:O	1:A:67:CYS:CB	2.63	0.46
1:A:1422:ARG:HH12	2:B:1224:PHE:HD2	1.62	0.46
2:B:244:LEU:HD21	2:B:366:GLN:NE2	2.31	0.46
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.51	0.46
2:B:858:SER:HA	2:B:966:VAL:O	2.15	0.46
2:B:906:SER:O	2:B:907:GLY:C	2.54	0.46
3:C:123:ASN:HD21	3:C:125:MET:HG2	1.81	0.46
3:C:39:ALA:HA	3:C:164:ALA:CB	2.41	0.46
6:F:95:GLY:O	6:F:96:THR:C	2.54	0.46
7:G:139:ILE:HG23	7:G:140:LYS:N	2.31	0.46
8:H:107:VAL:O	8:H:108:SER:HB2	2.16	0.46
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.15	0.46
1:A:204:THR:O	1:A:205:GLU:C	2.54	0.46
1:A:288:ALA:HA	1:A:291:GLU:CD	2.36	0.46
1:A:382:PRO:HD3	1:A:428:TYR:CZ	2.50	0.46
1:A:503:GLN:O	1:A:504:LEU:HD12	2.15	0.46
1:A:541:ILE:HG22	1:A:542:GLU:H	1.81	0.46
1:A:898:ARG:HA	1:A:933:TYR:CE1	2.50	0.46
1:A:964:ILE:O	1:A:964:ILE:CG2	2.64	0.46
2:B:1004:GLU:HB3	2:B:1006:ILE:HD11	1.97	0.46
2:B:191:LYS:HB3	2:B:191:LYS:HE2	1.78	0.46
2:B:241:ARG:HG2	2:B:253:THR:CG2	2.46	0.46
2:B:611:PRO:CB	2:B:685:LEU:HD11	2.44	0.46
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.51	0.46
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.98	0.46
2:B:834:ASN:O	2:B:1013:ASN:CB	2.63	0.46
5:E:191:LYS:HB3	5:E:191:LYS:HE2	1.69	0.46
5:E:3:GLN:NE2	5:E:52:ARG:HH12	2.13	0.46
8:H:130:ARG:HA	8:H:133:ASN:HB2	1.97	0.46
8:H:63:LEU:HD23	8:H:90:ALA:C	2.36	0.46
1:A:1159:ARG:O	1:A:1160:SER:HB3	2.16	0.46
1:A:1282:VAL:HA	1:A:1307:GLU:O	2.16	0.46
1:A:92:HIS:HD2	1:A:236:LEU:HD21	1.81	0.46
1:A:535:THR:CG2	1:A:617:VAL:HG23	2.46	0.46
1:A:58:LEU:HD12	1:A:244:PRO:HG3	1.98	0.46
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.97	0.46
1:A:692:ASP:O	1:A:694:THR:N	2.49	0.46
1:A:863:VAL:C	1:A:864:ILE:HD12	2.36	0.46
1:A:881:GLN:NE2	1:A:958:VAL:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:861:ASP:OD1	2:B:862:GLN:N	2.48	0.46
2:B:770:GLN:HG2	2:B:983:ARG:C	2.36	0.46
5:E:198:ILE:CD1	5:E:212:ARG:HH11	2.27	0.46
6:F:120:ILE:CG2	6:F:121:ALA:N	2.78	0.46
11:K:74:ARG:C	11:K:75:ILE:HD13	2.36	0.46
1:A:521:MET:O	1:A:646:PHE:CE2	2.68	0.46
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.49	0.46
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.80	0.46
1:A:95:PHE:CE2	1:A:1410:PHE:CD2	3.03	0.46
2:B:103:ASN:HB2	2:B:169:ARG:NH2	2.31	0.46
2:B:887:HIS:CD2	2:B:888:GLY:N	2.84	0.46
3:C:167:HIS:HA	11:K:6:ARG:NH1	2.30	0.46
5:E:121:MET:HA	5:E:124:VAL:HG23	1.97	0.46
5:E:178:ILE:O	5:E:178:ILE:HG23	2.16	0.46
6:F:89:GLU:HB3	6:F:134:ILE:CD1	2.45	0.46
6:F:70:LYS:HD3	6:F:70:LYS:HA	1.42	0.46
8:H:38:LEU:HD12	8:H:39:THR:N	2.31	0.46
11:K:65:HIS:CD2	11:K:66:PRO:N	2.84	0.46
1:A:1167:GLU:HA	1:A:1170:ILE:CD1	2.45	0.46
1:A:1215:ARG:O	1:A:1218:GLN:N	2.49	0.46
1:A:222:LEU:HD13	1:A:222:LEU:O	2.16	0.46
1:A:381:THR:HG23	6:F:104:ASN:OD1	2.16	0.46
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.51	0.46
1:A:56:PRO:O	1:A:57:ARG:CG	2.60	0.46
1:A:923:LEU:HD23	1:A:923:LEU:HA	1.54	0.46
2:B:1013:ASN:HD21	2:B:1015:HIS:CD2	2.31	0.46
2:B:698:GLU:HG2	2:B:701:ILE:HD11	1.98	0.46
2:B:906:SER:HA	2:B:946:ASN:HB3	1.97	0.46
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.50	0.46
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.98	0.46
4:D:14:ARG:O	4:D:16:LYS:N	2.43	0.46
5:E:168:TYR:HD2	5:E:168:TYR:HA	1.69	0.46
7:G:95:SER:O	7:G:121:PHE:CE1	2.68	0.46
8:H:38:LEU:HD13	8:H:125:LEU:HD12	1.97	0.46
10:J:12:LYS:O	10:J:13:VAL:C	2.54	0.46
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.81	0.46
1:A:1228:TRP:N	1:A:1228:TRP:CE3	2.84	0.46
1:A:41:MET:CE	1:A:257:ARG:HG3	2.46	0.46
1:A:850:VAL:O	1:A:850:VAL:HG12	2.16	0.46
1:A:805:LEU:HD13	2:B:1052:VAL:HG21	1.98	0.46
2:B:1095:LEU:O	2:B:1096:ARG:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:HD22	2:B:1200:ALA:HB2	1.97	0.46
2:B:241:ARG:HG2	2:B:253:THR:HG21	1.97	0.46
2:B:446:LEU:O	2:B:447:ALA:CB	2.64	0.46
3:C:131:HIS:HA	3:C:132:PRO:HD2	1.76	0.46
3:C:22:LEU:HD22	3:C:230:MET:HE1	1.98	0.46
3:C:251:LEU:O	3:C:255:VAL:HG23	2.15	0.46
4:D:208:GLU:CG	4:D:212:LYS:HE3	2.43	0.46
5:E:132:ILE:N	5:E:132:ILE:HD12	2.31	0.46
5:E:61:GLN:HB2	5:E:79:TRP:HE3	1.81	0.46
2:B:308:TRP:HH2	9:I:45:ARG:HG2	1.81	0.46
11:K:58:PHE:HE2	11:K:74:ARG:HB3	1.80	0.46
1:A:1267:MET:O	1:A:1271:ILE:HB	2.15	0.45
1:A:445:ASN:HA	1:A:478:TYR:HE2	1.81	0.45
1:A:814:PHE:C	1:A:814:PHE:HD2	2.19	0.45
1:A:917:SER:C	1:A:919:ILE:H	2.19	0.45
2:B:1072:MET:HG3	2:B:1085:ILE:HD13	1.99	0.45
2:B:802:PRO:HG3	2:B:1091:TYR:CE1	2.51	0.45
3:C:248:ILE:HD13	11:K:101:LEU:HD22	1.99	0.45
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.30	0.45
10:J:1:MET:H2	10:J:57:ILE:H	1.62	0.45
11:K:61:TYR:CG	11:K:61:TYR:O	2.69	0.45
1:A:1349:TYR:HE2	1:A:1353:TYR:CD1	2.34	0.45
1:A:135:PHE:CD1	1:A:222:LEU:HD21	2.51	0.45
1:A:203:SER:O	1:A:206:GLU:HB3	2.17	0.45
1:A:46:THR:O	1:A:47:ARG:C	2.55	0.45
1:A:529:CYS:SG	1:A:662:PHE:CZ	3.10	0.45
1:A:528:LEU:CD1	1:A:749:ALA:HB1	2.46	0.45
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.99	0.45
2:B:1058:LEU:O	2:B:1061:GLU:HB2	2.15	0.45
2:B:424:LEU:O	2:B:428:ILE:HG13	2.16	0.45
2:B:515:HIS:CD2	2:B:516:ASN:N	2.83	0.45
2:B:758:PHE:N	2:B:759:PRO:CD	2.80	0.45
2:B:844:SER:O	2:B:848:ARG:HG3	2.15	0.45
3:C:8:VAL:C	3:C:9:LYS:HG3	2.36	0.45
7:G:119:LEU:HA	7:G:132:SER:OG	2.16	0.45
7:G:44:TYR:CE1	7:G:157:ILE:HB	2.51	0.45
8:H:32:THR:HG22	8:H:33:GLN:OE1	2.16	0.45
11:K:30:ALA:HB2	11:K:76:GLN:HG3	1.97	0.45
1:A:1229:SER:HB2	1:A:1230:GLU:H	1.48	0.45
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.00	0.45
1:A:19:PHE:HZ	1:A:1397:LEU:CD2	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ASP:OD2	1:A:261:ASP:N	2.48	0.45
1:A:445:ASN:HA	1:A:478:TYR:CE2	2.51	0.45
1:A:925:LEU:O	1:A:929:LEU:HD23	2.17	0.45
2:B:1016:ALA:CB	2:B:1020:ARG:HE	2.29	0.45
2:B:102:VAL:O	2:B:109:THR:HG23	2.17	0.45
2:B:496:ARG:NH1	2:B:541:LEU:HA	2.31	0.45
2:B:599:THR:HG22	2:B:600:LEU:HD23	1.99	0.45
2:B:797:TYR:HD2	2:B:798:TYR:HE2	1.64	0.45
2:B:841:MET:CE	2:B:1010:LEU:HG	2.46	0.45
2:B:936:ASP:CG	2:B:937:ALA:H	2.19	0.45
4:D:172:LEU:HD11	4:D:202:ILE:HG21	1.97	0.45
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.99	0.45
5:E:139:ALA:O	5:E:140:LEU:HD23	2.17	0.45
6:F:127:GLU:O	6:F:129:LYS:N	2.49	0.45
7:G:119:LEU:HA	7:G:132:SER:HG	1.81	0.45
12:L:38:LEU:CG	12:L:39:SER:H	2.29	0.45
1:A:135:PHE:HD1	1:A:222:LEU:HD21	1.80	0.45
1:A:303:TYR:O	1:A:325:ILE:HG13	2.16	0.45
1:A:403:LYS:C	1:A:415:LEU:HB2	2.36	0.45
1:A:689:LYS:HG2	1:A:689:LYS:O	2.16	0.45
1:A:833:GLU:O	1:A:837:ILE:HG13	2.16	0.45
2:B:1070:GLU:O	2:B:1084:GLN:HB3	2.15	0.45
2:B:1147:LEU:O	2:B:1148:LYS:C	2.53	0.45
2:B:259:TYR:N	2:B:259:TYR:CD1	2.85	0.45
2:B:542:MET:HB3	2:B:636:PRO:HD3	1.98	0.45
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.97	0.45
2:B:912:ILE:HD11	2:B:966:VAL:HG21	1.97	0.45
6:F:125:LEU:O	6:F:128:LYS:N	2.48	0.45
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.99	0.45
2:B:1076:HIS:CD2	11:K:40:HIS:CE1	2.90	0.45
11:K:59:ALA:HA	11:K:74:ARG:O	2.15	0.45
12:L:40:LEU:HD22	12:L:44:ASP:OD1	2.17	0.45
1:A:1129:GLU:O	1:A:1133:LEU:HG	2.16	0.45
1:A:1135:ARG:HG2	1:A:1136:SER:N	2.32	0.45
1:A:1138:ILE:HA	1:A:1275:GLY:HA2	1.99	0.45
1:A:1365:TYR:CD1	5:E:203:GLU:HG2	2.52	0.45
1:A:239:LEU:CD1	1:A:240:PRO:HD2	2.36	0.45
1:A:58:LEU:HD12	1:A:244:PRO:CG	2.47	0.45
1:A:671:ALA:H	1:A:676:MET:CE	2.25	0.45
1:A:929:LEU:N	1:A:929:LEU:CD2	2.79	0.45
2:B:510:LYS:O	2:B:511:PRO:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:602:THR:HA	2:B:605:ARG:HB2	1.98	0.45
2:B:779:GLY:O	2:B:795:ILE:HA	2.17	0.45
3:C:130:GLY:O	3:C:132:PRO:HD3	2.17	0.45
3:C:175:ALA:HB2	10:J:10:CYS:HB2	1.97	0.45
3:C:237:SER:C	3:C:238:ILE:HG13	2.37	0.45
5:E:96:PHE:CZ	5:E:100:ILE:HD11	2.51	0.45
8:H:15:VAL:HG13	8:H:24:CYS:HB3	1.98	0.45
1:A:1004:ASN:HD22	1:A:1007:ILE:HG13	1.82	0.45
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.61	0.45
1:A:1368:MET:HE3	1:A:1368:MET:HB2	1.74	0.45
1:A:1395:GLY:HA3	1:A:1426:GLU:OE2	2.16	0.45
1:A:444:PHE:CE2	1:A:470:LEU:HD13	2.51	0.45
1:A:489:LEU:C	1:A:490:HIS:CD2	2.90	0.45
1:A:590:ARG:O	1:A:591:PHE:CB	2.57	0.45
1:A:741:ASN:ND2	1:A:741:ASN:C	2.67	0.45
2:B:44:VAL:O	2:B:45:SER:C	2.54	0.45
2:B:839:MET:HG3	2:B:1010:LEU:HD21	1.98	0.45
2:B:887:HIS:CD2	2:B:888:GLY:H	2.34	0.45
3:C:58:LEU:HD13	3:C:62:PHE:CD2	2.51	0.45
4:D:54:GLU:CD	4:D:164:ILE:HD11	2.37	0.45
4:D:39:ASN:ND2	4:D:40:HIS:N	2.64	0.45
7:G:1:MET:SD	7:G:79:PHE:CE1	3.10	0.45
8:H:35:GLN:H	8:H:35:GLN:HG3	1.57	0.45
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.34	0.45
8:H:4:THR:HG21	8:H:7:ASP:OD2	2.16	0.45
10:J:17:LYS:HB3	10:J:39:LEU:HD23	1.98	0.45
10:J:56:LEU:O	10:J:60:PHE:CD2	2.70	0.45
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.47	0.45
1:A:252:PHE:O	1:A:253:ASN:CB	2.65	0.45
1:A:73:GLY:O	1:A:74:MET:C	2.55	0.45
1:A:763:ALA:O	1:A:803:SER:HB3	2.17	0.45
2:B:1078:GLY:O	2:B:1079:LYS:C	2.55	0.45
2:B:234:ILE:CG1	2:B:257:LYS:HB3	2.45	0.45
2:B:811:TYR:N	2:B:811:TYR:CD1	2.83	0.45
2:B:918:ILE:HG21	2:B:935:ARG:NH2	2.32	0.45
2:B:878:GLN:N	2:B:934:LYS:HZ3	2.10	0.45
2:B:942:ARG:HA	2:B:942:ARG:HD3	1.67	0.45
2:B:956:THR:HA	2:B:961:LEU:O	2.17	0.45
4:D:126:ILE:C	4:D:128:VAL:N	2.70	0.45
4:D:146:GLN:O	4:D:149:THR:HG22	2.17	0.45
7:G:104:GLY:C	7:G:106:MET:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:14:HIS:HD2	7:G:16:SER:H	1.63	0.45
12:L:39:SER:O	12:L:40:LEU:CG	2.57	0.45
1:A:1279:ILE:HG22	1:A:1282:VAL:CG2	2.47	0.45
1:A:598:LEU:HD13	8:H:115:TYR:HE2	1.81	0.45
1:A:897:TYR:HD2	1:A:936:LEU:CD1	2.30	0.45
2:B:102:VAL:HG23	2:B:112:LEU:HD22	1.97	0.45
4:D:29:LEU:HB3	4:D:33:PHE:HB2	1.98	0.45
4:D:52:LEU:H	4:D:182:SER:HB3	1.82	0.45
7:G:116:PRO:C	7:G:118:ASP:H	2.19	0.45
11:K:47:ARG:NH1	11:K:51:LEU:HD22	2.32	0.45
1:A:1173:HIS:CB	1:A:1227:ILE:HD13	2.47	0.45
1:A:1188:GLN:OE1	1:A:1241:ARG:HD3	2.17	0.45
1:A:16:GLU:CD	2:B:1220:ARG:HA	2.37	0.45
1:A:55:ASP:HB2	1:A:59:GLY:O	2.17	0.45
2:B:291:ILE:HG21	2:B:300:HIS:CD2	2.52	0.45
2:B:398:ARG:NH1	2:B:398:ARG:CB	2.80	0.45
2:B:66:ASP:OD1	2:B:422:LYS:HE2	2.17	0.45
2:B:950:ASP:HB2	2:B:969:ARG:HB3	1.99	0.45
3:C:183:TRP:O	3:C:184:ASN:C	2.55	0.45
3:C:241:ASP:O	3:C:245:VAL:HG23	2.17	0.45
3:C:67:LEU:HA	3:C:70:ILE:HD11	1.97	0.45
4:D:192:LYS:HD2	4:D:199:ASN:HA	1.98	0.45
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.82	0.45
6:F:85:MET:SD	6:F:90:ARG:HB2	2.57	0.45
7:G:106:MET:HG3	7:G:157:ILE:O	2.16	0.45
7:G:79:PHE:HD1	7:G:80:LYS:N	2.14	0.45
10:J:7:CYS:CB	10:J:49:MET:HE3	2.47	0.45
11:K:56:VAL:O	11:K:56:VAL:CG1	2.64	0.45
1:A:709:THR:CG2	1:A:710:LEU:N	2.79	0.45
1:A:899:VAL:CG1	1:A:908:LEU:HD21	2.43	0.45
2:B:1013:ASN:ND2	2:B:1015:HIS:HD2	2.13	0.45
2:B:416:LEU:HD11	2:B:460:ALA:HB3	1.98	0.45
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.98	0.45
2:B:948:ILE:HD12	2:B:969:ARG:HH11	1.81	0.45
4:D:129:LEU:O	4:D:132:GLN:HG3	2.17	0.45
4:D:151:PHE:N	4:D:151:PHE:HD1	2.15	0.45
7:G:129:SER:OG	7:G:130:TYR:N	2.49	0.45
7:G:163:ILE:HG13	7:G:163:ILE:O	2.17	0.45
8:H:82:PRO:C	8:H:84:ALA:N	2.68	0.45
1:A:1132:LYS:HA	1:A:1135:ARG:HB3	1.99	0.44
1:A:1311:VAL:HG11	1:A:1329:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1370:LEU:O	1:A:1371:LEU:C	2.55	0.44
1:A:1445:ILE:CD1	7:G:59:GLY:H	2.29	0.44
1:A:181:LEU:HA	1:A:181:LEU:HD23	1.87	0.44
1:A:58:LEU:HD13	1:A:244:PRO:HD3	1.97	0.44
1:A:814:PHE:CD2	1:A:814:PHE:C	2.90	0.44
1:A:886:ILE:HD11	1:A:943:LEU:O	2.16	0.44
2:B:1037:LEU:HD12	2:B:1037:LEU:N	2.32	0.44
2:B:1073:TYR:OH	3:C:179:GLU:HG3	2.17	0.44
2:B:1109:GLY:HA3	2:B:1110:PRO:HD3	1.80	0.44
2:B:179:CYS:O	2:B:181:LEU:N	2.50	0.44
2:B:360:PHE:CZ	2:B:361:LEU:HD13	2.52	0.44
2:B:219:ALA:HA	2:B:405:ARG:HG2	1.98	0.44
2:B:483:LEU:HG	2:B:485:ARG:HD3	1.98	0.44
4:D:126:ILE:C	4:D:128:VAL:H	2.20	0.44
4:D:185:CYS:HB3	4:D:211:LEU:HD22	1.99	0.44
4:D:35:LEU:HD12	4:D:35:LEU:N	2.25	0.44
5:E:187:TYR:CD2	5:E:188:LEU:HD23	2.50	0.44
6:F:101:ILE:CG2	6:F:117:PRO:HB3	2.46	0.44
11:K:23:PRO:HA	11:K:31:VAL:HG22	1.98	0.44
1:A:1196:GLU:HG3	1:A:1197:LEU:N	2.31	0.44
1:A:1396:ALA:HB2	1:A:1417:GLU:OE1	2.17	0.44
1:A:1424:VAL:O	1:A:1425:SER:C	2.56	0.44
1:A:93:VAL:HG11	1:A:305:ASP:HB3	1.99	0.44
1:A:425:GLN:CD	1:A:425:GLN:N	2.71	0.44
1:A:434:ARG:HH21	1:A:437:MET:H	1.65	0.44
1:A:506:ALA:C	1:A:508:PRO:HD2	2.38	0.44
1:A:69:THR:HG21	2:B:1174:LYS:HZ3	1.82	0.44
1:A:886:ILE:HG13	1:A:943:LEU:HB2	1.98	0.44
2:B:101:MET:HB2	2:B:169:ARG:HH12	1.82	0.44
2:B:241:ARG:HH21	2:B:251:ILE:HD13	1.82	0.44
2:B:785:TYR:C	2:B:787:VAL:H	2.20	0.44
8:H:5:LEU:O	8:H:6:PHE:HB2	2.17	0.44
11:K:63:VAL:O	11:K:63:VAL:CG2	2.61	0.44
1:A:1153:TYR:CZ	1:A:1163:ILE:HD11	2.53	0.44
1:A:1290:LYS:HA	1:A:1299:VAL:O	2.17	0.44
1:A:27:VAL:O	1:A:29:ALA:N	2.50	0.44
1:A:384:ASN:O	1:A:385:ILE:C	2.54	0.44
1:A:434:ARG:HH21	1:A:437:MET:HG3	1.80	0.44
1:A:664:THR:O	1:A:664:THR:CG2	2.64	0.44
1:A:868:TYR:O	1:A:870:GLU:N	2.50	0.44
2:B:244:LEU:HD12	2:B:250:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:LEU:HD22	2:B:361:LEU:CD1	2.47	0.44
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.99	0.44
2:B:750:GLY:H	2:B:753:ALA:HB3	1.80	0.44
2:B:766:ARG:HH21	2:B:1020:ARG:HB3	1.81	0.44
3:C:109:SER:O	3:C:110:THR:C	2.55	0.44
3:C:129:ILE:O	3:C:129:ILE:HG22	2.16	0.44
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.52	0.44
5:E:67:GLU:O	5:E:70:SER:HB3	2.17	0.44
8:H:82:PRO:HB2	8:H:83:GLN:H	1.67	0.44
11:K:114:LEU:O	11:K:114:LEU:HD23	2.17	0.44
2:B:1076:HIS:CD2	11:K:40:HIS:CD2	3.05	0.44
11:K:5:ASP:CB	11:K:7:PHE:CZ	2.96	0.44
1:A:1157:ASP:C	1:A:1159:ARG:H	2.20	0.44
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.98	0.44
1:A:1407:GLU:H	1:A:1407:GLU:CD	2.21	0.44
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.18	0.44
1:A:671:ALA:HB3	1:A:676:MET:HG3	1.99	0.44
2:B:1003:ALA:HB1	3:C:179:GLU:HB2	1.99	0.44
2:B:1185:CYS:SG	4:D:17:LYS:HE3	2.57	0.44
2:B:1204:PHE:CZ	2:B:1216:LEU:HD21	2.52	0.44
2:B:866:TYR:HD2	2:B:870:ILE:HD12	1.82	0.44
2:B:980:PHE:CD1	2:B:980:PHE:N	2.86	0.44
3:C:258:ILE:HG13	11:K:19:LEU:HD11	1.98	0.44
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.99	0.44
4:D:185:CYS:SG	4:D:186:ASP:N	2.90	0.44
4:D:203:SER:OG	4:D:206:GLU:HB2	2.17	0.44
5:E:150:VAL:HG12	5:E:151:PRO:HD2	1.98	0.44
5:E:98:ILE:HA	5:E:101:GLN:HB3	1.99	0.44
12:L:61:THR:HG21	12:L:63:ARG:NH2	2.32	0.44
1:A:100:LYS:O	1:A:104:GLU:HG3	2.18	0.44
1:A:1107:VAL:O	1:A:1107:VAL:CG1	2.64	0.44
1:A:313:GLN:O	1:A:314:ALA:C	2.56	0.44
1:A:523:ILE:HG22	1:A:528:LEU:HB3	1.99	0.44
1:A:598:LEU:HA	8:H:122:LEU:CD1	2.46	0.44
1:A:670:ILE:HG22	1:A:805:LEU:HD21	1.98	0.44
1:A:886:ILE:HD11	1:A:943:LEU:C	2.37	0.44
1:A:88:LYS:HE2	1:A:205:GLU:OE2	2.17	0.44
2:B:362:PRO:O	2:B:366:GLN:HG3	2.17	0.44
2:B:54:PHE:HB2	2:B:410:GLY:HA2	1.99	0.44
3:C:192:TRP:CE3	3:C:192:TRP:O	2.71	0.44
4:D:202:ILE:HD11	4:D:207:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:7:CYS:HB2	10:J:49:MET:HE3	2.00	0.44
2:B:515:HIS:CG	2:B:516:ASN:H	2.34	0.44
4:D:66:ARG:HG3	7:G:51:TYR:CD1	2.53	0.44
7:G:99:PHE:HE1	7:G:101:VAL:HG23	1.82	0.44
8:H:94:ASP:O	8:H:95:TYR:HB2	2.17	0.44
2:B:1076:HIS:CD2	11:K:40:HIS:NE2	2.78	0.44
12:L:55:ILE:CG1	12:L:56:LEU:H	2.31	0.44
1:A:329:LEU:O	1:A:330:LYS:O	2.36	0.44
2:B:1034:VAL:HA	2:B:1037:LEU:HD12	1.99	0.44
2:B:879:ARG:HE	2:B:879:ARG:CA	2.31	0.44
5:E:117:THR:HB	5:E:120:ALA:CB	2.46	0.44
5:E:184:VAL:O	5:E:187:TYR:HB3	2.18	0.44
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.48	0.44
8:H:81:PRO:O	8:H:82:PRO:O	2.36	0.44
1:A:1163:ILE:HG23	1:A:1164:PRO:HD2	1.99	0.44
1:A:1167:GLU:HA	1:A:1170:ILE:HD12	1.99	0.44
1:A:310:GLY:O	1:A:312:PRO:HD2	2.18	0.44
1:A:595:THR:HG23	1:A:603:ASN:HB2	2.00	0.44
1:A:897:TYR:CD2	1:A:936:LEU:CD1	3.01	0.44
2:B:578:THR:HG23	2:B:622:LYS:C	2.38	0.44
2:B:885:MET:HA	2:B:936:ASP:HB2	2.00	0.44
2:B:911:ILE:HD11	2:B:941:LEU:HB2	2.00	0.44
2:B:1080:LYS:HG3	3:C:180:TYR:OH	2.18	0.44
4:D:173:HIS:C	4:D:175:PHE:N	2.71	0.44
7:G:165:GLU:HG2	7:G:165:GLU:H	1.37	0.44
9:I:7:CYS:HB2	9:I:34:TYR:CD2	2.53	0.44
1:A:1215:ARG:HA	1:A:1215:ARG:HD2	1.80	0.44
1:A:1265:ASN:C	1:A:1267:MET:H	2.21	0.44
1:A:195:ASP:O	1:A:196:GLU:O	2.36	0.44
1:A:254:GLU:O	1:A:255:SER:C	2.56	0.44
1:A:35:ILE:H	1:A:35:ILE:CD1	2.20	0.44
1:A:360:GLU:O	1:A:362:ASP:N	2.51	0.44
1:A:633:VAL:O	1:A:636:GLU:N	2.51	0.44
1:A:809:THR:HG21	2:B:730:ARG:HG3	2.00	0.44
1:A:858:ASN:HD22	1:A:858:ASN:N	2.11	0.44
2:B:1192:TYR:CG	2:B:1218:THR:HG21	2.52	0.44
2:B:121:ASN:HA	2:B:207:GLY:CA	2.48	0.44
2:B:430:ARG:CB	2:B:430:ARG:HH11	2.30	0.44
4:D:178:ALA:O	4:D:181:GLY:N	2.50	0.44
4:D:33:PHE:CE2	7:G:3:PHE:CD1	3.06	0.44
5:E:63:ASN:CB	5:E:64:PRO:HD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:90:VAL:CG2	5:E:90:VAL:O	2.66	0.44
7:G:143:ILE:HG12	7:G:170:ALA:CA	2.43	0.44
7:G:14:HIS:CD2	7:G:15:PRO:CD	3.01	0.44
11:K:35:PHE:N	11:K:35:PHE:HD1	2.15	0.44
12:L:26:THR:CG2	12:L:27:LEU:H	2.23	0.44
1:A:1018:PHE:O	1:A:1019:CYS:C	2.57	0.43
1:A:1162:VAL:HG12	1:A:1162:VAL:O	2.18	0.43
1:A:1170:ILE:HG22	1:A:1174:PHE:HE1	1.81	0.43
1:A:1398:MET:HE3	1:A:1398:MET:HB2	1.94	0.43
1:A:1397:LEU:HA	1:A:1400:CYS:SG	2.58	0.43
1:A:1402:PHE:O	1:A:1404:GLU:N	2.51	0.43
1:A:14:VAL:HA	2:B:1217:TYR:O	2.18	0.43
1:A:211:PHE:HA	1:A:214:ILE:CD1	2.47	0.43
1:A:690:VAL:HG21	1:A:722:LEU:HD11	1.98	0.43
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.18	0.43
1:A:841:LEU:CD2	1:A:845:LEU:HD11	2.48	0.43
1:A:663:SER:HB2	2:B:1085:ILE:HG13	1.99	0.43
2:B:1212:ILE:O	2:B:1212:ILE:CG2	2.66	0.43
2:B:225:VAL:HG22	2:B:396:ASP:OD2	2.18	0.43
2:B:878:GLN:OE1	2:B:879:ARG:HG2	2.18	0.43
2:B:913:GLY:HA2	2:B:938:SER:OG	2.17	0.43
3:C:242:GLN:O	3:C:246:ARG:HG2	2.17	0.43
4:D:66:ARG:HD2	4:D:133:THR:HB	1.99	0.43
7:G:160:ILE:HD12	7:G:160:ILE:N	2.32	0.43
1:A:1106:ASN:O	1:A:1107:VAL:HB	2.18	0.43
1:A:1207:LEU:HD21	1:A:1274:ARG:NE	2.33	0.43
1:A:1223:ASP:HA	1:A:1243:VAL:HG22	1.97	0.43
1:A:92:HIS:CE1	1:A:1410:PHE:HE2	2.33	0.43
1:A:390:GLN:HE21	1:A:394:ASN:ND2	2.16	0.43
1:A:523:ILE:HD13	1:A:622:VAL:HG23	1.99	0.43
2:B:205:ILE:O	2:B:207:GLY:N	2.51	0.43
2:B:276:ILE:HG22	2:B:276:ILE:O	2.18	0.43
2:B:313:MET:HE3	2:B:386:LEU:HD13	2.00	0.43
2:B:360:PHE:CD2	2:B:361:LEU:HB2	2.53	0.43
2:B:619:ILE:CG2	2:B:620:ARG:N	2.80	0.43
2:B:521:LEU:HD11	2:B:695:ALA:HB2	2.00	0.43
2:B:1073:TYR:HE2	3:C:180:TYR:CE2	2.36	0.43
3:C:53:THR:HB	3:C:154:LYS:HB2	1.99	0.43
4:D:48:ILE:CG2	4:D:48:ILE:O	2.66	0.43
5:E:98:ILE:HG22	5:E:102:GLU:OE2	2.19	0.43
5:E:147:HIS:HD2	5:E:148:GLU:N	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:VAL:HG13	5:E:201:LYS:HB3	1.98	0.43
5:E:24:LYS:HG2	5:E:25:ASP:N	2.34	0.43
8:H:5:LEU:HD22	8:H:133:ASN:O	2.18	0.43
8:H:95:TYR:HE2	8:H:97:MET:CG	2.31	0.43
11:K:23:PRO:CA	11:K:31:VAL:HG13	2.46	0.43
1:A:114:LEU:O	1:A:115:LEU:HG	2.18	0.43
1:A:1332:PHE:HD2	1:A:1332:PHE:H	1.66	0.43
1:A:298:PHE:CE2	1:A:314:ALA:HB2	2.53	0.43
1:A:774:ARG:HG3	1:A:797:LYS:HE3	2.00	0.43
1:A:946:VAL:C	1:A:947:PHE:HD2	2.21	0.43
1:A:91:PHE:HE2	1:A:99:ILE:HG21	1.82	0.43
2:B:125:SER:HB2	2:B:169:ARG:HB3	2.00	0.43
2:B:219:ALA:H	2:B:404:LYS:HA	1.84	0.43
2:B:605:ARG:HG2	2:B:688:GLY:CA	2.48	0.43
3:C:130:GLY:O	3:C:132:PRO:CD	2.67	0.43
6:F:103:MET:CE	7:G:66:GLY:H	2.31	0.43
7:G:41:LYS:HD3	7:G:42:PHE:CZ	2.54	0.43
8:H:37:LYS:O	8:H:38:LEU:HB2	2.19	0.43
1:A:1215:ARG:HA	1:A:1218:GLN:HG2	2.00	0.43
1:A:1215:ARG:HH22	1:A:1272:THR:CB	2.31	0.43
1:A:588:LEU:HG	1:A:589:GLN:N	2.32	0.43
1:A:595:THR:HG23	1:A:603:ASN:CB	2.49	0.43
1:A:804:TYR:HH	1:A:816:HIS:HE2	1.66	0.43
1:A:852:TYR:HA	1:A:852:TYR:HD2	1.70	0.43
1:A:337:ARG:HG2	2:B:1132:GLU:OE2	2.19	0.43
2:B:1191:ILE:HG22	2:B:1192:TYR:N	2.34	0.43
2:B:1191:ILE:CG2	2:B:1192:TYR:N	2.82	0.43
2:B:510:LYS:HG3	2:B:511:PRO:CD	2.27	0.43
2:B:530:GLY:O	2:B:533:CYS:HB2	2.19	0.43
2:B:639:ILE:CG2	2:B:641:GLU:HG2	2.48	0.43
1:A:472:LEU:HD11	2:B:835:GLN:NE2	2.33	0.43
2:B:979:LYS:C	2:B:980:PHE:CD1	2.91	0.43
3:C:191:TYR:HD2	3:C:201:TRP:NE1	2.16	0.43
5:E:142:VAL:HG12	5:E:143:ASN:N	2.33	0.43
6:F:124:GLU:HG2	6:F:129:LYS:O	2.19	0.43
7:G:89:GLY:HA3	7:G:103:VAL:CG2	2.48	0.43
7:G:96:GLN:H	7:G:96:GLN:HG3	1.69	0.43
11:K:91:CYS:O	11:K:94:ILE:HB	2.19	0.43
1:A:1114:PRO:O	1:A:1311:VAL:HG23	2.19	0.43
1:A:1256:GLU:C	1:A:1258:HIS:H	2.22	0.43
1:A:37:PHE:CD1	1:A:37:PHE:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:MET:CE	1:A:507:VAL:HG23	2.46	0.43
1:A:993:LEU:O	1:A:994:GLN:C	2.56	0.43
2:B:1130:PHE:CE2	2:B:1150:ARG:HG2	2.54	0.43
1:A:7:SER:HB3	2:B:1193:GLN:NE2	2.33	0.43
2:B:209:GLU:O	2:B:482:VAL:HG12	2.17	0.43
2:B:486:TYR:HD1	2:B:1096:ARG:HH22	1.65	0.43
2:B:516:ASN:ND2	2:B:516:ASN:H	2.16	0.43
2:B:514:LEU:HD12	2:B:518:HIS:CD2	2.53	0.43
2:B:852:ARG:HG2	2:B:973:ILE:HG23	2.00	0.43
3:C:240:VAL:O	3:C:241:ASP:C	2.56	0.43
3:C:259:LEU:O	3:C:262:LEU:HB2	2.19	0.43
3:C:62:PHE:O	3:C:66:ARG:HG2	2.18	0.43
3:C:9:LYS:O	3:C:20:PHE:HB2	2.18	0.43
4:D:163:VAL:O	4:D:166:LEU:HB3	2.19	0.43
4:D:20:GLU:HG2	4:D:20:GLU:O	2.18	0.43
4:D:71:LYS:O	4:D:74:GLN:HB2	2.19	0.43
5:E:138:ALA:HA	5:E:141:VAL:CG2	2.45	0.43
5:E:82:PHE:N	5:E:82:PHE:CD1	2.87	0.43
7:G:1:MET:SD	7:G:79:PHE:CD1	3.12	0.43
11:K:43:GLY:O	11:K:47:ARG:HB2	2.17	0.43
11:K:84:LYS:O	11:K:87:LEU:HB3	2.17	0.43
1:A:1037:LEU:HD13	1:A:1041:ALA:CB	2.49	0.43
1:A:735:VAL:O	1:A:735:VAL:HG12	2.19	0.43
2:B:1023:VAL:HG12	2:B:1027:ILE:CD1	2.46	0.43
2:B:745:PRO:HB2	2:B:1047:PHE:CD1	2.53	0.43
2:B:640:VAL:O	2:B:641:GLU:C	2.57	0.43
2:B:641:GLU:HB2	2:B:643:ASP:OD1	2.19	0.43
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.52	0.43
2:B:798:TYR:HE1	10:J:4:PRO:HA	1.84	0.43
2:B:866:TYR:HB2	2:B:870:ILE:HB	2.01	0.43
3:C:201:TRP:HA	3:C:201:TRP:CE3	2.53	0.43
6:F:83:PRO:HG2	6:F:84:TYR:CD1	2.54	0.43
7:G:106:MET:HG2	7:G:107:LYS:H	1.83	0.43
11:K:45:LEU:HG	11:K:94:ILE:HD13	2.00	0.43
1:A:1152:ILE:CG2	1:A:1260:LEU:HD23	2.45	0.43
1:A:98:LYS:HE2	1:A:224:PHE:HE1	1.83	0.43
1:A:419:LYS:C	1:A:421:ALA:H	2.21	0.43
1:A:499:ALA:O	1:A:500:GLU:C	2.56	0.43
1:A:548:ASN:HD21	11:K:47:ARG:NH2	2.15	0.43
1:A:679:ILE:CG2	1:A:729:ALA:HB1	2.47	0.43
2:B:1026:LEU:HG	2:B:1026:LEU:H	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.49	0.43
2:B:100:PRO:HB2	2:B:180:TYR:HE1	1.84	0.43
2:B:181:LEU:O	2:B:182:SER:C	2.57	0.43
2:B:240:ILE:HD12	2:B:241:ARG:H	1.83	0.43
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.84	0.43
2:B:660:LYS:O	2:B:663:ALA:HB3	2.18	0.43
2:B:796:LEU:HD23	2:B:799:PRO:HA	1.99	0.43
2:B:877:PRO:CA	2:B:934:LYS:HZ3	2.32	0.43
2:B:900:ALA:O	2:B:903:VAL:HG23	2.18	0.43
3:C:100:THR:HB	3:C:119:VAL:HG23	2.01	0.43
4:D:192:LYS:HD2	4:D:199:ASN:N	2.33	0.43
4:D:119:ARG:HB2	4:D:221:TYR:CE1	2.53	0.43
5:E:63:ASN:CB	5:E:64:PRO:CD	2.96	0.43
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.53	0.43
6:F:85:MET:O	6:F:155:LEU:HD21	2.19	0.43
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.54	0.43
7:G:84:GLY:HA2	7:G:146:LYS:HE2	2.00	0.43
1:A:185:TRP:HZ3	1:A:200:ARG:HB3	1.84	0.43
1:A:59:GLY:HA3	1:A:244:PRO:HG2	2.01	0.43
1:A:37:PHE:HB2	1:A:52:GLY:HA3	2.00	0.43
1:A:578:LEU:O	1:A:580:VAL:N	2.52	0.43
1:A:535:THR:HG21	1:A:617:VAL:HG23	2.00	0.43
2:B:1212:ILE:O	2:B:1214:PRO:HD3	2.17	0.43
2:B:533:CYS:C	2:B:535:LEU:N	2.72	0.43
2:B:651:LEU:O	2:B:654:ARG:NE	2.50	0.43
5:E:74:ASP:OD1	5:E:74:ASP:N	2.51	0.43
8:H:6:PHE:CD2	8:H:7:ASP:N	2.87	0.43
11:K:31:VAL:CG1	11:K:32:VAL:N	2.82	0.43
1:A:1219:THR:HG23	1:A:1220:PHE:N	2.33	0.43
1:A:135:PHE:CD1	1:A:222:LEU:CD2	2.98	0.43
1:A:27:VAL:C	1:A:29:ALA:N	2.71	0.43
1:A:338:GLY:HA2	2:B:1129:ARG:NH2	2.34	0.43
1:A:851:HIS:CB	6:F:139:PRO:HG3	2.48	0.43
1:A:985:ASP:O	1:A:986:ILE:C	2.57	0.43
2:B:1033:LYS:O	2:B:1036:ALA:HB3	2.19	0.43
2:B:115:GLN:O	2:B:118:ARG:HB2	2.19	0.43
2:B:333:PHE:CD2	2:B:333:PHE:O	2.72	0.43
2:B:498:THR:O	2:B:536:VAL:HA	2.18	0.43
2:B:557:PHE:O	2:B:561:TRP:HD1	2.02	0.43
2:B:764:SER:N	2:B:765:PRO:CD	2.81	0.43
4:D:175:PHE:O	4:D:176:GLU:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:138:THR:O	7:G:140:LYS:N	2.51	0.43
12:L:63:ARG:O	12:L:64:LEU:C	2.57	0.43
1:A:744:LYS:O	1:A:748:MET:CB	2.65	0.43
1:A:22:PHE:HB3	2:B:1211:ASN:ND2	2.34	0.43
2:B:1167:GLY:HA3	2:B:1215:ARG:HA	2.00	0.43
2:B:222:ILE:C	2:B:240:ILE:HD13	2.39	0.43
2:B:281:PRO:HG2	2:B:284:ILE:HG13	2.00	0.43
2:B:352:ALA:O	2:B:353:LYS:C	2.58	0.43
2:B:541:LEU:HD12	2:B:747:MET:HE1	2.00	0.43
2:B:841:MET:HE3	2:B:1010:LEU:HG	2.00	0.43
2:B:839:MET:CE	2:B:980:PHE:HB2	2.48	0.43
2:B:998:ASP:N	2:B:998:ASP:OD1	2.51	0.43
3:C:46:ILE:HG13	3:C:72:LEU:HD21	2.01	0.43
5:E:190:LEU:HD23	5:E:190:LEU:N	2.33	0.43
7:G:91:VAL:HG12	7:G:92:VAL:N	2.34	0.43
12:L:55:ILE:HG12	12:L:56:LEU:N	2.34	0.43
1:A:15:LYS:HG3	2:B:1219:ASP:HA	2.01	0.42
1:A:42:ASP:HB3	1:A:45:GLN:CA	2.49	0.42
1:A:53:LEU:CD2	1:A:54:ASN:H	2.19	0.42
1:A:34:LYS:NZ	1:A:57:ARG:NH1	2.67	0.42
1:A:853:ASP:OD1	1:A:855:THR:CB	2.67	0.42
2:B:1106:ARG:CZ	2:B:1110:PRO:HD2	2.48	0.42
2:B:59:LEU:HD21	2:B:128:LEU:HD11	2.01	0.42
2:B:215:GLN:HE21	2:B:476:ARG:HH11	1.67	0.42
2:B:724:ASP:HB3	2:B:727:LYS:CG	2.48	0.42
2:B:638:PHE:HB2	2:B:741:CYS:HB3	2.00	0.42
2:B:857:ARG:HG2	2:B:858:SER:H	1.83	0.42
4:D:145:MET:O	4:D:149:THR:HG22	2.18	0.42
4:D:188:ALA:CA	4:D:191:ALA:HB3	2.33	0.42
2:B:294:ASP:OD1	9:I:12:ASN:HA	2.19	0.42
11:K:107:THR:O	11:K:111:LEU:HG	2.19	0.42
11:K:94:ILE:O	11:K:98:LEU:HG	2.18	0.42
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.19	0.42
1:A:224:PHE:HE2	1:A:231:PRO:HA	1.83	0.42
1:A:526:ASP:HB2	2:B:835:GLN:OE1	2.19	0.42
1:A:661:GLY:CA	2:B:1081:LEU:HD22	2.49	0.42
1:A:662:PHE:O	2:B:828:ALA:HA	2.18	0.42
1:A:821:ARG:O	1:A:825:ILE:HG13	2.19	0.42
2:B:1043:ASP:O	2:B:1050:ILE:HD11	2.19	0.42
1:A:343:LYS:HG2	2:B:1151:LEU:HD12	2.02	0.42
2:B:1173:ALA:HB1	2:B:1175:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:736:THR:HA	2:B:738:PHE:CE1	2.54	0.42
2:B:807:ARG:HH11	2:B:807:ARG:HB3	1.84	0.42
3:C:45:ALA:HA	3:C:72:LEU:HD13	2.00	0.42
3:C:70:ILE:HG22	3:C:71:PRO:CD	2.48	0.42
4:D:56:ARG:CD	4:D:149:THR:HA	2.43	0.42
4:D:198:LEU:N	4:D:198:LEU:HD23	2.34	0.42
5:E:185:ALA:CA	5:E:190:LEU:HG	2.49	0.42
5:E:92:THR:O	5:E:95:THR:HB	2.19	0.42
6:F:87:LYS:HG3	6:F:88:TYR:CE1	2.52	0.42
12:L:31:CYS:O	12:L:35:SER:HA	2.19	0.42
1:A:1025:ARG:O	1:A:1035:TYR:HE1	2.02	0.42
1:A:1100:ARG:HA	1:A:1103:GLU:OE1	2.20	0.42
1:A:1109:LYS:HD2	1:A:1109:LYS:HA	1.71	0.42
1:A:1161:THR:H	1:A:1170:ILE:HD13	1.84	0.42
1:A:1362:TYR:CE1	1:A:1363:VAL:O	2.72	0.42
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.54	0.42
1:A:619:LYS:O	1:A:623:GLY:HA3	2.19	0.42
1:A:783:THR:HG21	1:A:796:SER:O	2.19	0.42
1:A:845:LEU:O	1:A:846:GLU:C	2.58	0.42
2:B:281:PRO:O	2:B:283:VAL:N	2.53	0.42
2:B:459:TYR:O	2:B:463:THR:OG1	2.38	0.42
2:B:522:VAL:HG12	2:B:523:CYS:H	1.78	0.42
2:B:610:ASN:HA	2:B:611:PRO:HD3	1.92	0.42
2:B:70:ILE:HG13	2:B:429:PHE:HZ	1.84	0.42
1:A:1325:THR:O	5:E:148:GLU:HB3	2.20	0.42
5:E:167:ARG:O	5:E:168:TYR:CG	2.72	0.42
10:J:17:LYS:O	10:J:18:TRP:C	2.56	0.42
11:K:30:ALA:HB2	11:K:76:GLN:CG	2.49	0.42
3:C:167:HIS:HA	11:K:6:ARG:HH12	1.84	0.42
1:A:1397:LEU:N	1:A:1397:LEU:HD23	2.35	0.42
1:A:109:HIS:NE2	1:A:169:ASN:ND2	2.67	0.42
1:A:41:MET:O	1:A:42:ASP:O	2.37	0.42
1:A:474:VAL:HG23	1:A:521:MET:CE	2.47	0.42
1:A:446:ARG:HB2	1:A:487:MET:CE	2.49	0.42
1:A:809:THR:HG23	1:A:812:GLU:OE1	2.19	0.42
2:B:566:LEU:HD22	2:B:586:TRP:O	2.20	0.42
2:B:641:GLU:HB2	2:B:643:ASP:OD2	2.19	0.42
2:B:707:PRO:HB3	2:B:741:CYS:SG	2.58	0.42
4:D:173:HIS:O	4:D:175:PHE:N	2.53	0.42
3:C:69:LEU:O	10:J:6:ARG:NH1	2.52	0.42
1:A:1095:THR:HB	1:A:1100:ARG:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:ILE:HG13	9:I:44:TYR:CD2	2.54	0.42
1:A:92:HIS:CE1	1:A:1410:PHE:CE2	3.06	0.42
1:A:1450:LEU:HD21	7:G:19:GLY:O	2.19	0.42
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.55	0.42
1:A:571:LEU:HD22	8:H:46:LEU:HD11	2.01	0.42
1:A:848:ILE:HA	1:A:857:ARG:O	2.20	0.42
1:A:904:THR:HG22	1:A:904:THR:O	2.19	0.42
2:B:1040:ASN:O	2:B:1041:GLU:C	2.57	0.42
2:B:378:LEU:O	2:B:378:LEU:HD12	2.19	0.42
2:B:498:THR:O	2:B:536:VAL:HG13	2.19	0.42
2:B:627:PHE:CE1	2:B:696:GLU:HG2	2.55	0.42
2:B:830:TYR:HB3	2:B:831:SER:H	1.44	0.42
4:D:167:LEU:C	4:D:169:SER:N	2.70	0.42
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.83	0.42
6:F:88:TYR:CD1	6:F:88:TYR:N	2.86	0.42
10:J:9:SER:HB2	10:J:45:CYS:CB	2.50	0.42
12:L:55:ILE:HG12	12:L:56:LEU:H	1.85	0.42
1:A:1211:GLN:O	1:A:1214:GLU:HB2	2.19	0.42
1:A:59:GLY:O	1:A:244:PRO:HG2	2.19	0.42
1:A:41:MET:HA	1:A:49:LYS:HA	2.01	0.42
1:A:647:GLY:O	1:A:648:ASN:C	2.57	0.42
1:A:661:GLY:O	1:A:662:PHE:HB2	2.19	0.42
1:A:919:ILE:HD11	1:A:925:LEU:CD1	2.49	0.42
1:A:907:THR:HG21	1:A:920:LEU:HD21	2.01	0.42
2:B:205:ILE:O	2:B:206:ASN:C	2.57	0.42
2:B:817:LEU:N	2:B:818:PRO:CD	2.81	0.42
2:B:916:THR:HA	2:B:917:PRO:HD3	1.82	0.42
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.40	0.42
5:E:116:ILE:HG22	5:E:120:ALA:HB3	2.01	0.42
5:E:162:ARG:HB3	5:E:162:ARG:NH1	2.34	0.42
8:H:130:ARG:HD3	8:H:130:ARG:N	2.35	0.42
1:A:548:ASN:ND2	11:K:47:ARG:HH21	2.15	0.42
1:A:1291:VAL:CG2	1:A:1292:PRO:HD2	2.49	0.42
1:A:151:ASP:OD1	1:A:163:SER:HB3	2.19	0.42
1:A:424:ILE:HG22	1:A:425:GLN:O	2.19	0.42
1:A:532:ARG:C	1:A:534:LEU:H	2.22	0.42
1:A:914:GLU:HB2	1:A:979:SER:O	2.19	0.42
1:A:946:VAL:HG22	5:E:201:LYS:CD	2.44	0.42
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.02	0.42
2:B:129:PHE:CD2	2:B:166:PHE:HB2	2.54	0.42
2:B:286:PHE:CE1	2:B:378:LEU:HG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:PRO:O	2:B:747:MET:N	2.53	0.42
3:C:47:ASP:OD2	3:C:170:TRP:HH2	2.02	0.42
3:C:187:LYS:HA	3:C:187:LYS:HD3	1.77	0.42
4:D:146:GLN:HA	4:D:149:THR:HG22	2.02	0.42
4:D:53:SER:O	4:D:54:GLU:C	2.57	0.42
5:E:17:ARG:O	5:E:21:GLU:HG3	2.19	0.42
6:F:82:THR:CG2	6:F:83:PRO:HD2	2.50	0.42
7:G:79:PHE:CE2	7:G:105:PRO:HD2	2.55	0.42
3:C:167:HIS:CD2	12:L:70:ARG:CG	3.03	0.42
1:A:1163:ILE:CG2	1:A:1164:PRO:HD2	2.50	0.42
1:A:1284:MET:CA	1:A:1306:LEU:HD23	2.50	0.42
1:A:555:ASP:OD2	1:A:644:LYS:HE2	2.20	0.42
1:A:779:PHE:CZ	2:B:517:THR:HA	2.55	0.42
1:A:811:GLN:CD	1:A:811:GLN:H	2.23	0.42
1:A:851:HIS:HB3	6:F:139:PRO:HG3	2.02	0.42
1:A:89:PRO:HD2	1:A:205:GLU:HG3	2.02	0.42
2:B:1130:PHE:HD2	2:B:1151:LEU:HD11	1.85	0.42
2:B:1166:CYS:C	2:B:1168:LEU:N	2.73	0.42
2:B:277:LYS:N	2:B:277:LYS:HD3	2.35	0.42
2:B:514:LEU:HA	2:B:514:LEU:HD12	1.91	0.42
2:B:792:MET:O	2:B:793:ALA:HB2	2.20	0.42
2:B:877:PRO:C	2:B:878:GLN:HG3	2.40	0.42
3:C:77:ILE:HD12	3:C:77:ILE:O	2.19	0.42
1:A:522:GLY:HA2	1:A:630:ILE:CD1	2.50	0.42
1:A:607:ILE:HG12	1:A:612:ILE:HA	2.02	0.42
2:B:1174:LYS:O	2:B:1176:ASN:N	2.44	0.42
2:B:123:THR:C	2:B:125:SER:H	2.23	0.42
2:B:335:GLY:HA2	2:B:348:ARG:HB2	2.01	0.42
2:B:461:LEU:HD12	2:B:461:LEU:HA	1.85	0.42
2:B:597:MET:HE2	2:B:597:MET:HA	2.00	0.42
2:B:405:ARG:HA	2:B:631:GLY:O	2.19	0.42
2:B:650:GLU:HG3	2:B:651:LEU:H	1.84	0.42
3:C:136:ASP:OD2	3:C:137:LYS:N	2.53	0.42
6:F:146:TRP:HB3	6:F:151:LEU:CD1	2.49	0.42
10:J:31:ASP:OD1	10:J:34:THR:HB	2.20	0.42
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.35	0.42
1:A:1035:TYR:O	1:A:1036:ARG:CB	2.58	0.42
1:A:1156:PRO:HA	1:A:1190:PRO:CB	2.35	0.42
1:A:101:LYS:HG2	1:A:139:TRP:CE2	2.55	0.42
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.51	0.42
1:A:225:ASN:HD22	1:A:227:VAL:H	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:PRO:O	1:A:397:ASN:CG	2.58	0.42
1:A:442:VAL:HG12	1:A:490:HIS:O	2.20	0.42
1:A:565:ILE:O	1:A:570:PRO:HA	2.20	0.42
1:A:61:ILE:HG22	1:A:62:ASP:H	1.84	0.42
1:A:670:ILE:HG22	1:A:805:LEU:HD11	2.01	0.42
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.48	0.42
2:B:1074:ASN:OD1	2:B:1075:GLY:N	2.53	0.42
2:B:467:GLY:HA3	2:B:475:SER:HB3	2.01	0.42
2:B:515:HIS:CG	2:B:516:ASN:N	2.88	0.42
2:B:515:HIS:O	2:B:518:HIS:HB2	2.20	0.42
2:B:641:GLU:HB2	2:B:643:ASP:CG	2.40	0.42
1:A:802:ASN:ND2	2:B:728:ARG:HB2	2.35	0.42
2:B:840:ILE:HG21	2:B:1011:ILE:HD12	2.02	0.42
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.42	0.42
5:E:100:ILE:HG23	5:E:105:PHE:HB2	2.01	0.42
5:E:54:GLN:O	5:E:57:MET:HB3	2.20	0.42
6:F:125:LEU:HA	6:F:130:ILE:HD11	2.01	0.42
6:F:127:GLU:O	6:F:128:LYS:C	2.57	0.42
7:G:79:PHE:HD2	7:G:105:PRO:HD2	1.85	0.42
2:B:785:TYR:CE2	10:J:60:PHE:HE1	2.37	0.42
1:A:1099:PRO:HG2	1:A:1100:ARG:H	1.85	0.41
1:A:1102:LYS:O	1:A:1103:GLU:C	2.57	0.41
1:A:1215:ARG:O	1:A:1216:ILE:C	2.58	0.41
1:A:1242:VAL:O	1:A:1243:VAL:CG1	2.67	0.41
1:A:1264:GLU:HG3	1:A:1265:ASN:OD1	2.20	0.41
1:A:1300:LYS:C	1:A:1302:PRO:HD3	2.40	0.41
1:A:1317:MET:HE1	1:A:1338:VAL:HG11	2.01	0.41
1:A:316:GLN:O	1:A:317:LYS:C	2.58	0.41
1:A:335:ARG:HA	1:A:339:ASN:ND2	2.27	0.41
1:A:403:LYS:HB3	1:A:404:TYR:CD1	2.54	0.41
1:A:425:GLN:NE2	1:A:425:GLN:N	2.54	0.41
1:A:451:HIS:O	1:A:452:LYS:C	2.57	0.41
1:A:503:GLN:HA	1:A:503:GLN:OE1	2.20	0.41
1:A:61:ILE:HG22	1:A:62:ASP:N	2.35	0.41
1:A:795:GLU:CD	1:A:795:GLU:N	2.71	0.41
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.36	0.41
2:B:278:GLN:HB3	2:B:279:ASP:H	1.69	0.41
2:B:563:MET:HE1	2:B:580:VAL:HG11	2.02	0.41
2:B:651:LEU:C	2:B:653:VAL:H	2.24	0.41
2:B:860:MET:HG3	2:B:965:LYS:HG2	2.01	0.41
2:B:900:ALA:HA	2:B:901:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:245:VAL:O	3:C:246:ARG:C	2.58	0.41
5:E:152:LYS:HD2	5:E:152:LYS:HA	1.86	0.41
7:G:146:LYS:HB2	7:G:168:LEU:HD11	2.02	0.41
7:G:160:ILE:CG2	7:G:161:GLY:N	2.81	0.41
7:G:163:ILE:HA	7:G:168:LEU:HD13	2.02	0.41
11:K:55:LYS:HB2	11:K:81:TYR:CE1	2.55	0.41
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.19	0.41
1:A:162:VAL:HG12	1:A:163:SER:H	1.85	0.41
1:A:284:ALA:HB1	1:A:289:ILE:HD11	2.03	0.41
1:A:399:HIS:O	1:A:435:HIS:HD2	2.04	0.41
1:A:475:THR:HG23	1:A:476:SER:N	2.35	0.41
1:A:474:VAL:HG23	1:A:477:PRO:HG2	2.02	0.41
1:A:541:ILE:HD12	1:A:577:ILE:CD1	2.49	0.41
1:A:580:VAL:HG12	1:A:580:VAL:O	2.19	0.41
1:A:654:ASN:O	1:A:657:LEU:HB3	2.20	0.41
1:A:767:GLN:HE21	1:A:774:ARG:HB2	1.81	0.41
2:B:1051:THR:HB	2:B:1054:GLY:H	1.84	0.41
2:B:565:PRO:C	2:B:567:GLU:N	2.73	0.41
2:B:68:THR:HG22	2:B:91:SER:CA	2.50	0.41
2:B:778:MET:SD	2:B:794:ASN:HB3	2.59	0.41
2:B:781:PHE:CD1	2:B:782:LEU:HG	2.54	0.41
3:C:124:LEU:HD23	3:C:126:GLY:HA2	2.02	0.41
3:C:77:ILE:CA	3:C:129:ILE:HD11	2.49	0.41
3:C:16:ASP:HA	3:C:240:VAL:HG13	2.02	0.41
3:C:93:ASP:O	3:C:127:ARG:NH2	2.52	0.41
4:D:213:GLU:O	4:D:216:ASN:HB2	2.20	0.41
5:E:131:THR:C	5:E:132:ILE:HG13	2.41	0.41
9:I:15:TYR:N	9:I:15:TYR:HD1	2.16	0.41
11:K:99:GLY:O	11:K:102:LYS:HB3	2.20	0.41
11:K:5:ASP:O	11:K:6:ARG:C	2.59	0.41
1:A:1396:ALA:HA	1:A:1399:ARG:CZ	2.49	0.41
1:A:389:THR:N	1:A:426:LEU:HD11	2.35	0.41
1:A:501:LEU:HA	1:A:505:CYS:SG	2.60	0.41
2:B:487:THR:O	2:B:490:SER:N	2.53	0.41
2:B:549:THR:CG2	2:B:550:ASP:H	2.32	0.41
2:B:846:ILE:HG23	2:B:974:PRO:HG2	2.02	0.41
4:D:123:LEU:HD22	4:D:149:THR:HG21	2.02	0.41
4:D:216:ASN:C	4:D:218:GLU:N	2.73	0.41
5:E:121:MET:C	5:E:123:LEU:H	2.23	0.41
2:B:1038:SER:O	10:J:33:GLY:HA3	2.20	0.41
1:A:1097:GLY:O	1:A:1098:VAL:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLY:O	1:A:259:GLU:O	2.39	0.41
1:A:528:LEU:CG	1:A:529:CYS:N	2.81	0.41
1:A:562:THR:CG2	1:A:563:PRO:HD2	2.50	0.41
1:A:690:VAL:HG23	1:A:721:PHE:HD1	1.85	0.41
1:A:829:VAL:HG11	2:B:508:LEU:HD13	2.03	0.41
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.18	0.41
2:B:21:GLU:HG3	2:B:21:GLU:O	2.21	0.41
2:B:248:SER:O	2:B:249:ARG:C	2.59	0.41
2:B:519:TRP:HE1	2:B:635:ARG:NH2	2.18	0.41
2:B:754:SER:HB2	2:B:812:LEU:CD1	2.49	0.41
2:B:778:MET:HE2	2:B:1094:ARG:HG2	2.03	0.41
3:C:114:TYR:C	3:C:116:LYS:H	2.24	0.41
4:D:198:LEU:O	4:D:199:ASN:HB2	2.20	0.41
4:D:48:ILE:HG21	7:G:4:ILE:HB	2.01	0.41
5:E:45:LYS:HB3	5:E:46:TYR:CE1	2.54	0.41
6:F:152:ILE:HG22	6:F:153:VAL:H	1.85	0.41
9:I:17:ARG:CG	9:I:18:GLU:H	2.31	0.41
11:K:11:LEU:HA	11:K:11:LEU:HD22	1.65	0.41
1:A:1006:ILE:HD12	5:E:167:ARG:HB2	2.01	0.41
1:A:1011:GLN:HE22	1:A:1015:VAL:CG2	2.32	0.41
1:A:1280:GLU:O	1:A:1281:ARG:C	2.58	0.41
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.21	0.41
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.87	0.41
1:A:35:ILE:HG13	1:A:52:GLY:O	2.21	0.41
1:A:767:GLN:HE22	1:A:797:LYS:CB	2.34	0.41
1:A:784:LEU:O	1:A:786:HIS:N	2.53	0.41
2:B:179:CYS:C	2:B:181:LEU:N	2.74	0.41
2:B:596:LEU:HD21	2:B:624:LEU:HD22	2.03	0.41
2:B:706:GLN:C	2:B:708:GLU:H	2.24	0.41
3:C:124:LEU:C	3:C:126:GLY:N	2.73	0.41
4:D:194:LEU:CD2	4:D:194:LEU:N	2.82	0.41
5:E:213:ILE:CG1	5:E:214:CYS:N	2.81	0.41
6:F:96:THR:HG22	6:F:100:GLN:OE1	2.20	0.41
1:A:1120:LEU:HD12	1:A:1120:LEU:N	2.35	0.41
1:A:1166:ASP:O	1:A:1170:ILE:HG13	2.21	0.41
1:A:1263:ILE:HG13	1:A:1263:ILE:H	1.43	0.41
1:A:1259:MET:HG3	1:A:1263:ILE:HD11	2.03	0.41
1:A:512:VAL:HG12	1:A:512:VAL:O	2.20	0.41
1:A:531:ILE:CG1	1:A:578:LEU:HD21	2.51	0.41
1:A:578:LEU:C	1:A:580:VAL:N	2.74	0.41
2:B:119:LEU:HD23	2:B:953:LEU:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ARG:HG2	2:B:955:THR:HG21	2.01	0.41
2:B:121:ASN:HD22	2:B:121:ASN:N	2.19	0.41
2:B:547:VAL:HG12	2:B:612:GLU:OE2	2.20	0.41
2:B:650:GLU:CG	2:B:651:LEU:N	2.82	0.41
2:B:637:LEU:HD13	2:B:740:HIS:HB2	2.01	0.41
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.36	0.41
3:C:53:THR:CG2	3:C:152:GLU:HB3	2.51	0.41
4:D:180:LEU:HD11	4:D:198:LEU:HD11	2.01	0.41
5:E:30:ILE:HG23	5:E:34:GLU:HB3	2.01	0.41
10:J:18:TRP:CH2	10:J:22:LEU:HD11	2.55	0.41
2:B:850:LEU:HA	10:J:8:PHE:HE1	1.84	0.41
12:L:67:PHE:N	12:L:67:PHE:CD1	2.89	0.41
1:A:1068:ALA:HB1	1:A:1367:HIS:HA	2.03	0.41
1:A:125:ALA:HA	1:A:128:ILE:CD1	2.51	0.41
1:A:1265:ASN:C	1:A:1267:MET:N	2.73	0.41
1:A:1437:GLY:C	1:A:1439:GLY:H	2.23	0.41
1:A:285:PRO:O	1:A:288:ALA:N	2.53	0.41
1:A:284:ALA:CB	1:A:289:ILE:HD11	2.50	0.41
1:A:75:ASN:O	1:A:76:GLU:HB2	2.20	0.41
1:A:919:ILE:HD11	1:A:925:LEU:HD11	2.02	0.41
1:A:952:ALA:C	1:A:954:TRP:HD1	2.23	0.41
2:B:114:PRO:O	2:B:115:GLN:C	2.57	0.41
2:B:243:ALA:HA	2:B:250:PHE:O	2.19	0.41
2:B:976:ILE:HA	2:B:976:ILE:HD13	1.85	0.41
3:C:73:GLN:O	3:C:129:ILE:HA	2.20	0.41
3:C:148:ARG:H	3:C:151:GLN:CG	2.26	0.41
3:C:37:MET:HB2	3:C:37:MET:HE2	1.65	0.41
4:D:202:ILE:HG12	4:D:207:LEU:HB2	2.02	0.41
6:F:85:MET:HA	6:F:151:LEU:HD23	2.02	0.41
7:G:21:ARG:O	7:G:22:MET:C	2.59	0.41
1:A:1025:ARG:HA	1:A:1030:ARG:CD	2.51	0.41
1:A:1293:SER:OG	1:A:1295:THR:HG22	2.21	0.41
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	2.02	0.41
1:A:243:PRO:O	1:A:246:VAL:HG23	2.21	0.41
1:A:335:ARG:HA	1:A:335:ARG:HD3	1.82	0.41
1:A:445:ASN:HB2	1:A:455:MET:HA	2.03	0.41
1:A:954:TRP:HA	1:A:955:PRO:HD3	1.97	0.41
2:B:1007:VAL:CG2	2:B:1008:PRO:N	2.83	0.41
2:B:1034:VAL:HA	2:B:1037:LEU:HD11	2.03	0.41
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.86	0.41
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:SER:CB	2:B:236:HIS:HD2	2.33	0.41
2:B:430:ARG:NH1	2:B:430:ARG:CG	2.63	0.41
2:B:877:PRO:HA	2:B:934:LYS:HZ3	1.84	0.41
3:C:167:HIS:ND1	3:C:167:HIS:C	2.74	0.41
3:C:58:LEU:HD13	3:C:62:PHE:CE2	2.56	0.41
5:E:12:LEU:HA	5:E:12:LEU:HD13	1.82	0.41
5:E:136:ASN:OD1	5:E:138:ALA:N	2.54	0.41
5:E:13:TRP:O	5:E:16:PHE:HB3	2.21	0.41
1:A:1061:GLY:O	1:A:1062:GLU:C	2.59	0.41
1:A:1213:GLY:O	1:A:1217:LYS:HB2	2.21	0.41
1:A:1216:ILE:H	1:A:1216:ILE:HG13	1.71	0.41
1:A:1365:TYR:HA	1:A:1368:MET:HE1	2.02	0.41
1:A:385:ILE:CG1	1:A:428:TYR:HE2	2.33	0.41
1:A:445:ASN:O	1:A:487:MET:HE3	2.20	0.41
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.35	0.41
2:B:167:ILE:HD12	2:B:167:ILE:N	2.36	0.41
2:B:205:ILE:HG22	2:B:206:ASN:N	2.35	0.41
2:B:435:THR:C	2:B:437:GLU:H	2.24	0.41
2:B:512:ARG:O	2:B:513:GLN:O	2.39	0.41
2:B:56:ASP:HB3	2:B:57:TYR:CE1	2.55	0.41
1:A:809:THR:CG2	2:B:730:ARG:HG3	2.51	0.41
2:B:841:MET:O	2:B:993:THR:HA	2.21	0.41
3:C:180:TYR:O	3:C:181:ASP:C	2.59	0.41
6:F:76:LYS:HA	6:F:79:ARG:CD	2.51	0.41
7:G:94:CYS:SG	7:G:130:TYR:HE1	2.43	0.41
8:H:102:TYR:HE2	8:H:116:TYR:N	2.19	0.41
9:I:7:CYS:O	9:I:11:ASN:HA	2.21	0.41
1:A:830:LYS:HE2	1:A:1081:LEU:HB2	2.03	0.41
1:A:1153:TYR:CB	1:A:1192:LEU:HD23	2.47	0.41
1:A:120:GLU:HG3	1:A:123:ARG:NH1	2.36	0.41
1:A:446:ARG:HB3	1:A:478:TYR:HB3	2.01	0.41
1:A:545:GLN:O	1:A:546:VAL:C	2.59	0.41
1:A:710:LEU:H	1:A:710:LEU:HD12	1.85	0.41
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.78	0.41
2:B:822:ASN:ND2	2:B:822:ASN:N	2.69	0.41
2:B:874:PHE:HD1	2:B:962:LYS:HD3	1.85	0.41
3:C:258:ILE:HA	3:C:258:ILE:HD12	1.85	0.41
3:C:70:ILE:HA	3:C:71:PRO:HD3	1.86	0.41
5:E:147:HIS:O	5:E:150:VAL:HG23	2.20	0.41
8:H:106:GLU:HG2	8:H:112:ILE:CD1	2.50	0.41
10:J:54:VAL:HG12	10:J:56:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:44:ASN:O	11:K:48:ALA:HB2	2.20	0.41
1:A:204:THR:O	1:A:206:GLU:N	2.54	0.41
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.85	0.41
1:A:311:GLN:O	1:A:313:GLN:N	2.53	0.41
1:A:33:ALA:HA	1:A:57:ARG:NH1	2.36	0.41
1:A:391:LEU:O	1:A:392:VAL:C	2.60	0.41
1:A:54:ASN:N	1:A:54:ASN:HD22	2.17	0.41
1:A:627:GLY:O	1:A:628:GLY:C	2.60	0.41
1:A:766:GLY:HA2	1:A:799:PHE:CE1	2.55	0.41
1:A:808:LEU:HD23	1:A:812:GLU:C	2.42	0.41
1:A:836:TYR:CE2	1:A:840:ARG:CD	3.04	0.41
1:A:857:ARG:HA	1:A:864:ILE:CD1	2.51	0.41
2:B:1065:GLN:CD	2:B:1066:SER:H	2.23	0.41
2:B:294:ASP:C	2:B:296:GLU:N	2.74	0.41
2:B:407:ASP:HB3	2:B:412:LEU:HD21	2.03	0.41
2:B:420:LEU:HD23	2:B:420:LEU:HA	1.94	0.41
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.35	0.41
2:B:92:PHE:CE1	2:B:421:PHE:HZ	2.38	0.41
2:B:941:LEU:HG	2:B:942:ARG:H	1.86	0.41
3:C:221:TYR:CZ	3:C:222:LYS:HE3	2.56	0.41
3:C:259:LEU:HD12	3:C:259:LEU:HA	1.87	0.41
3:C:88:CYS:O	3:C:89:GLU:C	2.58	0.41
4:D:13:ARG:O	4:D:15:LEU:N	2.54	0.41
4:D:8:PHE:CE1	4:D:37:GLN:HB2	2.55	0.41
2:B:1224:PHE:CZ	5:E:171:LYS:HE3	2.56	0.41
5:E:178:ILE:O	5:E:179:GLN:O	2.39	0.41
5:E:188:LEU:HB2	5:E:190:LEU:HD21	2.03	0.41
6:F:74:ILE:HD12	6:F:144:GLU:CG	2.50	0.41
7:G:12:THR:HG22	7:G:13:LEU:N	2.36	0.41
10:J:41:LEU:HD23	10:J:41:LEU:H	1.86	0.41
1:A:25:GLU:OE2	1:A:25:GLU:N	2.54	0.40
1:A:265:LYS:CD	1:A:322:VAL:HG21	2.37	0.40
1:A:35:ILE:HD12	1:A:35:ILE:N	2.22	0.40
1:A:49:LYS:CE	1:A:61:ILE:HG13	2.51	0.40
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.55	0.40
1:A:900:ASP:HB3	1:A:906:HIS:HB3	2.03	0.40
2:B:243:ALA:O	2:B:244:LEU:C	2.59	0.40
2:B:254:LEU:HD12	2:B:272:THR:O	2.21	0.40
2:B:27:ALA:O	2:B:28:GLU:C	2.59	0.40
2:B:640:VAL:CG1	2:B:640:VAL:O	2.69	0.40
2:B:639:ILE:HD11	2:B:691:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:821:GLN:NE2	2:B:851:PHE:H	2.18	0.40
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.84	0.40
2:B:996:ARG:HG3	2:B:996:ARG:H	1.39	0.40
3:C:115:SER:HB3	3:C:142:VAL:HB	2.03	0.40
5:E:13:TRP:HA	5:E:42:PHE:CE2	2.56	0.40
1:A:1445:ILE:HD11	7:G:59:GLY:N	2.37	0.40
10:J:48:ARG:NH1	10:J:48:ARG:CG	2.78	0.40
12:L:36:SER:O	12:L:37:LYS:C	2.60	0.40
1:A:1004:ASN:HD21	1:A:1006:ILE:HB	1.86	0.40
1:A:1313:LEU:O	1:A:1314:SER:C	2.59	0.40
1:A:195:ASP:OD1	1:A:195:ASP:N	2.54	0.40
1:A:323:LYS:HD2	1:A:323:LYS:N	2.36	0.40
1:A:325:ILE:C	1:A:327:ALA:N	2.75	0.40
1:A:380:VAL:HG23	1:A:430:TRP:C	2.41	0.40
1:A:391:LEU:O	1:A:394:ASN:N	2.55	0.40
1:A:441:PRO:O	1:A:492:PRO:CG	2.70	0.40
1:A:507:VAL:HG22	1:A:521:MET:HE1	2.02	0.40
1:A:477:PRO:CG	1:A:521:MET:HE2	2.51	0.40
1:A:741:ASN:HD21	1:A:743:VAL:H	1.70	0.40
2:B:1108:ARG:HG2	2:B:1109:GLY:H	1.85	0.40
2:B:189:LEU:HD13	2:B:196:PRO:HA	2.03	0.40
2:B:522:VAL:CG1	2:B:523:CYS:H	2.31	0.40
2:B:526:GLU:HG2	2:B:538:ASN:HB2	2.03	0.40
2:B:563:MET:O	2:B:565:PRO:HD3	2.21	0.40
3:C:121:VAL:O	3:C:122:SER:C	2.59	0.40
3:C:37:MET:CE	3:C:176:ILE:HD13	2.51	0.40
3:C:263:THR:O	3:C:266:ASP:HB2	2.21	0.40
3:C:8:VAL:CG1	3:C:9:LYS:N	2.85	0.40
5:E:127:ILE:N	5:E:128:PRO:HD3	2.36	0.40
5:E:171:LYS:H	5:E:171:LYS:HG2	1.51	0.40
6:F:131:PRO:O	6:F:132:LEU:HD23	2.21	0.40
7:G:21:ARG:HD3	7:G:21:ARG:HA	1.89	0.40
7:G:79:PHE:C	7:G:79:PHE:HD1	2.22	0.40
7:G:80:LYS:HG2	7:G:82:PHE:CE2	2.56	0.40
10:J:24:LEU:HD23	10:J:24:LEU:HA	1.87	0.40
10:J:9:SER:HB2	10:J:45:CYS:SG	2.61	0.40
1:A:1266:THR:O	1:A:1266:THR:HG22	2.21	0.40
1:A:1279:ILE:HG22	1:A:1282:VAL:HG21	2.03	0.40
1:A:305:ASP:OD1	1:A:306:ASN:N	2.55	0.40
1:A:379:VAL:HG12	1:A:380:VAL:N	2.36	0.40
1:A:490:HIS:HB3	2:B:1150:ARG:CZ	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ILE:HG12	1:A:578:LEU:HD21	2.03	0.40
1:A:829:VAL:C	1:A:831:THR:N	2.74	0.40
2:B:1076:HIS:HD2	11:K:40:HIS:CD2	2.39	0.40
2:B:1114:LEU:HA	2:B:1114:LEU:HD12	1.78	0.40
2:B:221:ASN:HA	2:B:241:ARG:O	2.21	0.40
2:B:276:ILE:O	2:B:276:ILE:CG2	2.68	0.40
2:B:312:GLU:O	2:B:313:MET:C	2.60	0.40
2:B:216:GLU:CA	2:B:406:LEU:HD23	2.45	0.40
2:B:38:PHE:CD2	2:B:43:LEU:CD2	3.05	0.40
2:B:508:LEU:HA	2:B:512:ARG:HE	1.86	0.40
2:B:589:VAL:HG12	2:B:590:HIS:N	2.35	0.40
2:B:529:GLU:OE1	2:B:769:TYR:HE2	2.04	0.40
2:B:773:MET:O	2:B:776:GLN:HB2	2.22	0.40
2:B:789:MET:CE	2:B:965:LYS:HB3	2.51	0.40
3:C:136:ASP:HB2	3:C:141:GLY:CA	2.51	0.40
3:C:13:ALA:HA	3:C:18:VAL:HA	2.03	0.40
5:E:124:VAL:O	5:E:132:ILE:CD1	2.69	0.40
5:E:52:ARG:HA	5:E:53:PRO:HD3	1.79	0.40
7:G:91:VAL:CG1	7:G:92:VAL:N	2.85	0.40
10:J:8:PHE:CD2	10:J:49:MET:SD	3.15	0.40
10:J:5:VAL:HA	10:J:15:GLY:N	2.34	0.40
11:K:38:GLU:HB3	11:K:71:PHE:HE2	1.86	0.40
1:A:1398:MET:CE	1:A:1424:VAL:HG23	2.51	0.40
1:A:670:ILE:O	1:A:670:ILE:HG12	2.21	0.40
1:A:68:GLN:O	1:A:68:GLN:CD	2.59	0.40
1:A:868:TYR:O	1:A:869:GLY:C	2.59	0.40
1:A:98:LYS:HE2	1:A:224:PHE:CE1	2.56	0.40
2:B:1030:LEU:HA	2:B:1030:LEU:HD12	1.89	0.40
2:B:1109:GLY:H	2:B:1111:MET:CE	2.35	0.40
2:B:259:TYR:HB2	2:B:268:THR:HG23	2.03	0.40
2:B:347:LYS:H	2:B:347:LYS:HG2	1.71	0.40
2:B:666:TYR:C	2:B:668:ASP:H	2.25	0.40
2:B:780:VAL:HG11	10:J:56:LEU:HD12	2.02	0.40
2:B:796:LEU:HD11	2:B:821:GLN:HE21	1.86	0.40
3:C:260:LEU:HG	3:C:264:GLN:NE2	2.37	0.40
5:E:18:THR:O	5:E:19:VAL:C	2.59	0.40
6:F:82:THR:HA	6:F:83:PRO:HD3	1.99	0.40
7:G:132:SER:O	7:G:133:SER:C	2.58	0.40
10:J:1:MET:H2	10:J:56:LEU:N	2.19	0.40
1:A:1189:SER:C	1:A:1191:TRP:H	2.25	0.40
1:A:127:ALA:O	1:A:129:LYS:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1351:GLU:C	1:A:1353:TYR:N	2.75	0.40
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.86	0.40
2:B:1138:MET:HB3	2:B:1147:LEU:HD21	2.00	0.40
2:B:421:PHE:O	2:B:424:LEU:HB3	2.22	0.40
2:B:213:ILE:H	2:B:479:VAL:HG12	1.86	0.40
2:B:542:MET:HE2	2:B:747:MET:HE2	2.04	0.40
2:B:636:PRO:HG2	2:B:743:ILE:HD11	2.03	0.40
2:B:990:ILE:HG22	2:B:992:ILE:N	2.34	0.40
3:C:59:ALA:O	3:C:60:ASP:C	2.59	0.40
4:D:124:GLU:O	4:D:128:VAL:HG23	2.21	0.40
8:H:38:LEU:HD13	8:H:125:LEU:CD1	2.52	0.40
11:K:5:ASP:HB2	11:K:7:PHE:CE2	2.54	0.40
12:L:53:HIS:HB3	12:L:55:ILE:HD11	2.00	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	1406/1733 (81%)	974 (69%)	284 (20%)	148 (10%)	0 8
2	B	1081/1224 (88%)	754 (70%)	232 (22%)	95 (9%)	1 12
3	C	264/318 (83%)	187 (71%)	48 (18%)	29 (11%)	0 8
4	D	174/219 (80%)	116 (67%)	43 (25%)	15 (9%)	1 13
5	E	212/215 (99%)	156 (74%)	41 (19%)	15 (7%)	1 16
6	F	85/155 (55%)	61 (72%)	19 (22%)	5 (6%)	1 20
7	G	169/171 (99%)	120 (71%)	43 (25%)	6 (4%)	3 28
8	H	130/146 (89%)	90 (69%)	29 (22%)	11 (8%)	1 13
9	I	45/133 (34%)	31 (69%)	10 (22%)	4 (9%)	1 12
10	J	63/70 (90%)	43 (68%)	14 (22%)	6 (10%)	0 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
11	K	112/120 (93%)	79 (70%)	24 (21%)	9 (8%)	1 14
12	L	44/70 (63%)	21 (48%)	8 (18%)	15 (34%)	0 0
All	All	3785/4574 (83%)	2632 (70%)	795 (21%)	358 (10%)	0 11

All (358) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	42	ASP
1	A	48	ALA
1	A	54	ASN
1	A	57	ARG
1	A	67	CYS
1	A	68	GLN
1	A	74	MET
1	A	119	ASN
1	A	128	ILE
1	A	130	ASP
1	A	167	CYS
1	A	257	ARG
1	A	259	GLU
1	A	286	HIS
1	A	318	SER
1	A	330	LYS
1	A	332	LYS
1	A	361	LEU
1	A	424	ILE
1	A	439	ASN
1	A	465	TYR
1	A	525	GLN
1	A	527	THR
1	A	536	LEU
1	A	557	ASP
1	A	567	LYS
1	A	591	PHE
1	A	597	LEU
1	A	598	LEU
1	A	666	ILE
1	A	790	ASP
1	A	868	TYR
1	A	986	ILE

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Mol	Chain	Res	Type
1	A	1002	GLY
1	A	1036	ARG
1	A	1098	VAL
1	A	1139	GLU
1	A	1223	ASP
1	A	1229	SER
1	A	1232	ASN
1	A	1255	GLU
1	A	1270	ASN
1	A	1339	LEU
1	A	1365	TYR
1	A	1392	SER
1	A	1394	THR
1	A	1405	THR
1	A	1424	VAL
2	B	108	VAL
2	B	184	ALA
2	B	206	ASN
2	B	258	LEU
2	B	364	ILE
2	B	367	LEU
2	B	509	ALA
2	B	732	SER
2	B	735	ALA
2	B	738	PHE
2	B	1036	ALA
2	B	1046	PRO
2	B	1096	ARG
2	B	1103	ILE
2	B	1132	GLU
2	B	1155	SER
2	B	1156	ASP
2	B	1183	LYS
3	C	110	THR
3	C	121	VAL
3	C	128	ASN
3	C	137	LYS
3	C	184	ASN
3	C	227	THR
4	D	19	GLU
4	D	119	ARG
5	E	45	LYS

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Mol	Chain	Res	Type
5	E	105	PHE
5	E	168	TYR
5	E	179	GLN
6	F	128	LYS
6	F	139	PRO
6	F	140	ASP
7	G	41	LYS
7	G	139	ILE
8	H	82	PRO
8	H	128	ASN
8	H	140	ALA
10	J	2	ILE
10	J	42	LYS
10	J	64	ASN
11	K	28	PRO
11	K	64	GLU
12	L	35	SER
12	L	39	SER
12	L	46	VAL
12	L	50	ASP
12	L	59	ALA
12	L	60	ARG
12	L	63	ARG
1	A	52	GLY
1	A	66	LYS
1	A	76	GLU
1	A	166	GLY
1	A	204	THR
1	A	253	ASN
1	A	308	ILE
1	A	310	GLY
1	A	314	ALA
1	A	322	VAL
1	A	418	SER
1	A	421	ALA
1	A	438	ASP
1	A	592	ASP
1	A	605	MET
1	A	628	GLY
1	A	636	GLU
1	A	653	VAL
1	A	693	VAL

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Mol	Chain	Res	Type
1	A	780	VAL
1	A	875	ALA
1	A	912	LEU
1	A	985	ASP
1	A	999	VAL
1	A	1067	LEU
1	A	1120	LEU
1	A	1140	HIS
1	A	1188	GLN
1	A	1206	ASP
1	A	1221	LYS
1	A	1233	ASP
1	A	1242	VAL
1	A	1314	SER
1	A	1316	VAL
1	A	1367	HIS
1	A	1437	GLY
2	B	28	GLU
2	B	65	GLU
2	B	68	THR
2	B	369	GLY
2	B	435	THR
2	B	447	ALA
2	B	449	ASN
2	B	483	LEU
2	B	513	GLN
2	B	591	ARG
2	B	731	VAL
2	B	751	VAL
2	B	777	ALA
2	B	786	ASN
2	B	838	SER
2	B	887	HIS
2	B	937	ALA
2	B	938	SER
2	B	1041	GLU
2	B	1079	LYS
2	B	1108	ARG
2	B	1112	GLN
2	B	1157	ALA
2	B	1158	PHE
2	B	1167	GLY

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Mol	Chain	Res	Type
3	C	5	GLY
3	C	11	ARG
3	C	126	GLY
3	C	141	GLY
3	C	149	LYS
3	C	168	ALA
3	C	213	PRO
3	C	240	VAL
4	D	5	THR
4	D	14	ARG
4	D	16	LYS
4	D	168	LYS
4	D	171	GLY
5	E	3	GLN
5	E	75	MET
5	E	106	GLN
6	F	112	GLU
7	G	154	VAL
8	H	95	TYR
8	H	109	LYS
9	I	3	THR
9	I	8	ARG
10	J	6	ARG
11	K	68	PHE
12	L	26	THR
12	L	47	ARG
12	L	48	CYS
12	L	55	ILE
12	L	56	LEU
1	A	28	ARG
1	A	59	GLY
1	A	169	ASN
1	A	219	PHE
1	A	255	SER
1	A	312	PRO
1	A	317	LYS
1	A	382	PRO
1	A	556	TRP
1	A	596	THR
1	A	785	PRO
1	A	869	GLY
1	A	910	PRO

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Mol	Chain	Res	Type
1	A	1062	GLU
1	A	1114	PRO
1	A	1388	GLY
1	A	1403	GLU
1	A	1422	ARG
1	A	1448	GLU
2	B	27	ALA
2	B	45	SER
2	B	171	PRO
2	B	180	TYR
2	B	249	ARG
2	B	250	PHE
2	B	291	ILE
2	B	409	ALA
2	B	468	GLU
2	B	562	GLY
2	B	575	PRO
2	B	746	SER
2	B	760	ASP
2	B	775	LYS
2	B	802	PRO
2	B	834	ASN
2	B	907	GLY
2	B	959	ASP
2	B	1175	LEU
2	B	1176	ASN
2	B	1223	ASP
3	C	90	ASP
3	C	122	SER
3	C	142	VAL
3	C	167	HIS
3	C	214	ASN
3	C	241	ASP
4	D	31	GLN
4	D	134	THR
4	D	191	ALA
4	D	198	LEU
5	E	73	PRO
5	E	76	GLY
5	E	130	ALA
5	E	151	PRO
7	G	28	THR

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Mol	Chain	Res	Type
7	G	67	SER
8	H	59	ILE
8	H	60	ALA
8	H	81	PRO
9	I	47	GLU
11	K	8	GLU
12	L	45	ALA
12	L	64	LEU
1	A	170	THR
1	A	196	GLU
1	A	420	ARG
1	A	649	ILE
1	A	654	ASN
1	A	958	VAL
1	A	1016	THR
1	A	1124	HIS
1	A	1266	THR
1	A	1377	THR
1	A	1435	PRO
2	B	106	ASP
2	B	186	GLU
2	B	459	TYR
2	B	510	LYS
2	B	524	PRO
2	B	566	LEU
2	B	711	GLU
2	B	906	SER
2	B	1017	ILE
2	B	1169	MET
3	C	13	ALA
3	C	25	VAL
3	C	174	ALA
3	C	224	GLN
5	E	97	VAL
6	F	141	GLY
8	H	83	GLN
10	J	13	VAL
11	K	54	ARG
12	L	40	LEU
1	A	45	GLN
1	A	62	ASP
1	A	75	ASN

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Mol	Chain	Res	Type
1	A	155	GLU
1	A	205	GLU
1	A	396	PRO
1	A	579	SER
1	A	583	PRO
1	A	602	ASP
1	A	647	GLY
1	A	920	LEU
1	A	1080	THR
1	A	1345	ARG
2	B	46	GLN
2	B	124	TYR
2	B	304	ASP
2	B	636	PRO
2	B	707	PRO
2	B	758	PHE
2	B	889	THR
2	B	974	PRO
2	B	987	LYS
2	B	996	ARG
3	C	127	ARG
3	C	132	PRO
4	D	218	GLU
8	H	107	VAL
9	I	9	ASP
10	J	14	VAL
11	K	7	PHE
11	K	10	PHE
11	K	83	PRO
1	A	4	GLN
1	A	492	PRO
1	A	533	LYS
1	A	662	PHE
1	A	976	THR
1	A	1302	PRO
1	A	1428	VAL
2	B	218	SER
2	B	219	ALA
2	B	463	THR
2	B	902	GLY
3	C	175	ALA
4	D	9	GLN

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Mol	Chain	Res	Type
4	D	52	LEU
5	E	118	PRO
5	E	124	VAL
7	G	84	GLY
1	A	311	GLN
1	A	410	GLY
1	A	730	GLY
2	B	323	VAL
2	B	478	GLY
3	C	216	GLY
4	D	18	VAL
8	H	17	PRO
1	A	258	GLY
1	A	385	ILE
1	A	1107	VAL
2	B	24	PRO
1	A	197	PRO
1	A	392	VAL
2	B	100	PRO
2	B	260	GLY
1	A	250	ILE
1	A	800	VAL
1	A	937	VAL
1	A	1122	PRO
3	C	172	PRO
1	A	1190	PRO
2	B	114	PRO
2	B	1014	PRO
11	K	66	PRO
5	E	129	PRO

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	1239/1520 (82%)	1031 (83%)	208 (17%)	2 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	957/1061 (90%)	800 (84%)	157 (16%)	2 14
3	C	234/274 (85%)	200 (86%)	34 (14%)	3 18
4	D	160/198 (81%)	127 (79%)	33 (21%)	1 7
5	E	196/197 (100%)	170 (87%)	26 (13%)	4 20
6	F	77/137 (56%)	65 (84%)	12 (16%)	2 16
7	G	152/152 (100%)	124 (82%)	28 (18%)	1 11
8	H	118/128 (92%)	98 (83%)	20 (17%)	2 13
9	I	45/122 (37%)	35 (78%)	10 (22%)	1 6
10	J	60/65 (92%)	50 (83%)	10 (17%)	2 14
11	K	99/102 (97%)	76 (77%)	23 (23%)	1 5
12	L	40/57 (70%)	29 (72%)	11 (28%)	0 3
All	All	3377/4013 (84%)	2805 (83%)	572 (17%)	2 13

All (572) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	8	SER
1	A	11	LEU
1	A	22	PHE
1	A	32	VAL
1	A	34	LYS
1	A	40	THR
1	A	54	ASN
1	A	58	LEU
1	A	60	SER
1	A	62	ASP
1	A	64	ASN
1	A	68	GLN
1	A	83	HIS
1	A	84	ILE
1	A	96	ILE
1	A	107	CYS
1	A	109	HIS
1	A	110	CYS
1	A	121	LEU
1	A	126	LEU
1	A	145	LYS

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Mol	Chain	Res	Type
1	A	151	ASP
1	A	160	GLN
1	A	162	VAL
1	A	169	ASN
1	A	186	LYS
1	A	195	ASP
1	A	215	SER
1	A	216	VAL
1	A	222	LEU
1	A	225	ASN
1	A	232	GLU
1	A	236	LEU
1	A	249	SER
1	A	261	ASP
1	A	262	LEU
1	A	263	THR
1	A	264	PHE
1	A	265	LYS
1	A	278	THR
1	A	302	THR
1	A	303	TYR
1	A	304	MET
1	A	308	ILE
1	A	316	GLN
1	A	320	ARG
1	A	322	VAL
1	A	337	ARG
1	A	344	ARG
1	A	351	THR
1	A	353	ILE
1	A	359	LEU
1	A	368	LYS
1	A	370	ILE
1	A	375	THR
1	A	383	TYR
1	A	386	ASP
1	A	399	HIS
1	A	404	TYR
1	A	414	ASP
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG

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Mol	Chain	Res	Type
1	A	438	ASP
1	A	440	ASP
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	451	HIS
1	A	455	MET
1	A	468	PHE
1	A	485	ASP
1	A	491	VAL
1	A	493	GLN
1	A	494	SER
1	A	507	VAL
1	A	509	LEU
1	A	512	VAL
1	A	513	SER
1	A	516	SER
1	A	524	VAL
1	A	528	LEU
1	A	533	LYS
1	A	538	ASP
1	A	542	GLU
1	A	577	ILE
1	A	578	LEU
1	A	587	HIS
1	A	595	THR
1	A	596	THR
1	A	598	LEU
1	A	602	ASP
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	630	ILE
1	A	631	HIS
1	A	635	ARG
1	A	640	GLN
1	A	652	VAL
1	A	657	LEU
1	A	670	ILE
1	A	680	THR
1	A	690	VAL
1	A	727	ASP

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Mol	Chain	Res	Type
1	A	738	LYS
1	A	739	ASP
1	A	741	ASN
1	A	742	ASN
1	A	743	VAL
1	A	745	GLN
1	A	774	ARG
1	A	805	LEU
1	A	814	PHE
1	A	827	THR
1	A	831	THR
1	A	833	GLU
1	A	838	GLN
1	A	841	LEU
1	A	845	LEU
1	A	852	TYR
1	A	858	ASN
1	A	860	LEU
1	A	886	ILE
1	A	899	VAL
1	A	902	LEU
1	A	903	ASN
1	A	906	HIS
1	A	919	ILE
1	A	933	TYR
1	A	936	LEU
1	A	939	ASP
1	A	969	GLN
1	A	970	THR
1	A	976	THR
1	A	987	VAL
1	A	988	LEU
1	A	992	ASP
1	A	999	VAL
1	A	1001	ARG
1	A	1017	LEU
1	A	1029	ARG
1	A	1033	GLN
1	A	1036	ARG
1	A	1037	LEU
1	A	1067	LEU
1	A	1072	ILE

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Mol	Chain	Res	Type
1	A	1078	GLN
1	A	1095	THR
1	A	1103	GLU
1	A	1110	ASN
1	A	1111	MET
1	A	1116	LEU
1	A	1120	LEU
1	A	1121	GLU
1	A	1124	HIS
1	A	1134	ILE
1	A	1142	THR
1	A	1159	ARG
1	A	1171	GLN
1	A	1217	LYS
1	A	1219	THR
1	A	1223	ASP
1	A	1228	TRP
1	A	1229	SER
1	A	1241	ARG
1	A	1255	GLU
1	A	1259	MET
1	A	1263	ILE
1	A	1264	GLU
1	A	1271	ILE
1	A	1272	THR
1	A	1274	ARG
1	A	1280	GLU
1	A	1284	MET
1	A	1289	ARG
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1308	THR
1	A	1309	ASP
1	A	1325	THR
1	A	1329	THR
1	A	1331	SER
1	A	1333	ILE
1	A	1336	MET
1	A	1349	TYR
1	A	1362	TYR
1	A	1368	MET

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Mol	Chain	Res	Type
1	A	1370	LEU
1	A	1373	ASP
1	A	1377	THR
1	A	1378	GLN
1	A	1382	THR
1	A	1384	VAL
1	A	1385	THR
1	A	1397	LEU
1	A	1401	SER
1	A	1402	PHE
1	A	1403	GLU
1	A	1405	THR
1	A	1411	GLU
1	A	1424	VAL
1	A	1426	GLU
1	A	1429	ILE
1	A	1442	ASP
1	A	1451	VAL
2	B	29	ASP
2	B	44	VAL
2	B	46	GLN
2	B	47	GLN
2	B	57	TYR
2	B	61	ASP
2	B	63	ILE
2	B	90	ILE
2	B	95	ILE
2	B	102	VAL
2	B	115	GLN
2	B	165	VAL
2	B	181	LEU
2	B	185	THR
2	B	188	ASP
2	B	194	GLU
2	B	202	TYR
2	B	217	ARG
2	B	218	SER
2	B	225	VAL
2	B	249	ARG
2	B	259	TYR
2	B	261	ARG
2	B	276	ILE

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Mol	Chain	Res	Type
2	B	283	VAL
2	B	286	PHE
2	B	289	LEU
2	B	294	ASP
2	B	324	ILE
2	B	328	GLU
2	B	329	THR
2	B	363	HIS
2	B	365	THR
2	B	371	GLU
2	B	378	LEU
2	B	387	LEU
2	B	401	PHE
2	B	413	LEU
2	B	416	LEU
2	B	427	ASP
2	B	429	PHE
2	B	430	ARG
2	B	463	THR
2	B	466	TRP
2	B	473	MET
2	B	476	ARG
2	B	479	VAL
2	B	482	VAL
2	B	485	ARG
2	B	489	SER
2	B	496	ARG
2	B	516	ASN
2	B	531	GLN
2	B	538	ASN
2	B	539	LEU
2	B	552	MET
2	B	557	PHE
2	B	558	LEU
2	B	559	SER
2	B	563	MET
2	B	568	ASP
2	B	570	VAL
2	B	576	ASP
2	B	580	VAL
2	B	597	MET
2	B	602	THR

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Mol	Chain	Res	Type
2	B	615	MET
2	B	616	ILE
2	B	619	ILE
2	B	626	ILE
2	B	628	THR
2	B	635	ARG
2	B	641	GLU
2	B	646	LEU
2	B	648	HIS
2	B	678	GLU
2	B	684	LEU
2	B	708	GLU
2	B	709	ASP
2	B	737	THR
2	B	739	THR
2	B	743	ILE
2	B	748	ILE
2	B	773	MET
2	B	780	VAL
2	B	786	ASN
2	B	791	THR
2	B	797	TYR
2	B	815	ARG
2	B	816	GLU
2	B	830	TYR
2	B	841	MET
2	B	842	ASN
2	B	844	SER
2	B	856	PHE
2	B	859	TYR
2	B	868	MET
2	B	869	SER
2	B	878	GLN
2	B	879	ARG
2	B	885	MET
2	B	890	TYR
2	B	895	ASP
2	B	904	ARG
2	B	914	LYS
2	B	942	ARG
2	B	944	THR
2	B	946	ASN

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Mol	Chain	Res	Type
2	B	953	LEU
2	B	957	ASN
2	B	959	ASP
2	B	969	ARG
2	B	980	PHE
2	B	983	ARG
2	B	987	LYS
2	B	989	THR
2	B	996	ARG
2	B	998	ASP
2	B	999	MET
2	B	1006	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1012	ILE
2	B	1020	ARG
2	B	1026	LEU
2	B	1029	CYS
2	B	1037	LEU
2	B	1051	THR
2	B	1076	HIS
2	B	1084	GLN
2	B	1087	PHE
2	B	1092	TYR
2	B	1095	LEU
2	B	1112	GLN
2	B	1113	VAL
2	B	1115	THR
2	B	1122	ARG
2	B	1135	ARG
2	B	1147	LEU
2	B	1149	GLU
2	B	1150	ARG
2	B	1156	ASP
2	B	1159	ARG
2	B	1162	ILE
2	B	1170	THR
2	B	1176	ASN
2	B	1177	HIS
2	B	1182	CYS
2	B	1183	LYS
2	B	1185	CYS

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Mol	Chain	Res	Type
2	B	1194	ILE
2	B	1196	ILE
2	B	1210	MET
2	B	1212	ILE
2	B	1216	LEU
2	B	1218	THR
2	B	1223	ASP
3	C	7	GLN
3	C	25	VAL
3	C	43	THR
3	C	48	SER
3	C	56	THR
3	C	63	ILE
3	C	77	ILE
3	C	83	SER
3	C	89	GLU
3	C	93	ASP
3	C	100	THR
3	C	104	PHE
3	C	106	GLU
3	C	112	ASN
3	C	118	LEU
3	C	119	VAL
3	C	123	ASN
3	C	124	LEU
3	C	143	LEU
3	C	145	CYS
3	C	147	LEU
3	C	166	GLU
3	C	178	PHE
3	C	190	ASP
3	C	193	TYR
3	C	201	TRP
3	C	231	ASN
3	C	232	VAL
3	C	235	VAL
3	C	240	VAL
3	C	249	ASP
3	C	254	LYS
3	C	258	ILE
3	C	259	LEU
4	D	5	THR

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Mol	Chain	Res	Type
4	D	11	ARG
4	D	13	ARG
4	D	16	LYS
4	D	17	LYS
4	D	18	VAL
4	D	20	GLU
4	D	22	GLU
4	D	23	ASN
4	D	29	LEU
4	D	34	GLN
4	D	40	HIS
4	D	47	LEU
4	D	50	LEU
4	D	51	ASN
4	D	59	ILE
4	D	65	GLU
4	D	70	PHE
4	D	118	THR
4	D	120	GLU
4	D	123	LEU
4	D	132	GLN
4	D	151	PHE
4	D	156	ASP
4	D	180	LEU
4	D	183	LEU
4	D	194	LEU
4	D	198	LEU
4	D	200	ASN
4	D	202	ILE
4	D	214	LEU
4	D	220	LEU
4	D	221	TYR
5	E	7	ARG
5	E	12	LEU
5	E	17	ARG
5	E	29	PHE
5	E	37	LEU
5	E	41	ASP
5	E	72	PHE
5	E	74	ASP
5	E	84	ASP
5	E	85	GLU

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Mol	Chain	Res	Type
5	E	106	GLN
5	E	114	ASN
5	E	115	ASN
5	E	132	ILE
5	E	144	ILE
5	E	150	VAL
5	E	153	HIS
5	E	165	LEU
5	E	168	TYR
5	E	171	LYS
5	E	173	SER
5	E	175	LEU
5	E	188	LEU
5	E	191	LYS
5	E	192	ARG
5	E	214	CYS
6	F	71	GLU
6	F	79	ARG
6	F	86	THR
6	F	93	ILE
6	F	101	ILE
6	F	107	VAL
6	F	112	GLU
6	F	120	ILE
6	F	138	LEU
6	F	140	ASP
6	F	147	SER
6	F	152	ILE
7	G	1	MET
7	G	7	LEU
7	G	13	LEU
7	G	21	ARG
7	G	42	PHE
7	G	45	ILE
7	G	48	VAL
7	G	51	TYR
7	G	53	ASN
7	G	56	ILE
7	G	67	SER
7	G	74	TYR
7	G	75	ARG
7	G	79	PHE

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Mol	Chain	Res	Type
7	G	87	VAL
7	G	88	ASP
7	G	96	GLN
7	G	97	HIS
7	G	111	THR
7	G	113	HIS
7	G	114	LEU
7	G	126	ASN
7	G	132	SER
7	G	138	THR
7	G	139	ILE
7	G	162	SER
7	G	165	GLU
7	G	168	LEU
8	H	7	ASP
8	H	27	GLU
8	H	33	GLN
8	H	35	GLN
8	H	38	LEU
8	H	53	ASP
8	H	57	VAL
8	H	61	SER
8	H	64	ASN
8	H	80	ARG
8	H	89	LEU
8	H	95	TYR
8	H	102	TYR
8	H	128	ASN
8	H	129	TYR
8	H	130	ARG
8	H	134	ASN
8	H	135	LEU
8	H	138	GLU
8	H	146	ARG
9	I	2	THR
9	I	6	PHE
9	I	8	ARG
9	I	10	CYS
9	I	15	TYR
9	I	19	ASP
9	I	21	GLU
9	I	26	LEU

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Mol	Chain	Res	Type
9	I	28	GLU
9	I	46	HIS
10	J	7	CYS
10	J	8	PHE
10	J	26	GLN
10	J	28	ASP
10	J	41	LEU
10	J	43	ARG
10	J	44	TYR
10	J	48	ARG
10	J	55	ASP
10	J	64	ASN
11	K	2	ASN
11	K	5	ASP
11	K	11	LEU
11	K	32	VAL
11	K	34	THR
11	K	35	PHE
11	K	41	THR
11	K	42	LEU
11	K	47	ARG
11	K	50	LEU
11	K	51	LEU
11	K	53	ASP
11	K	54	ARG
11	K	56	VAL
11	K	57	LEU
11	K	61	TYR
11	K	65	HIS
11	K	68	PHE
11	K	74	ARG
11	K	75	ILE
11	K	81	TYR
11	K	111	LEU
11	K	114	LEU
12	L	27	LEU
12	L	38	LEU
12	L	46	VAL
12	L	47	ARG
12	L	48	CYS
12	L	54	ARG
12	L	55	ILE

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Mol	Chain	Res	Type
12	L	61	THR
12	L	64	LEU
12	L	65	VAL
12	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	68	GLN
1	A	75	ASN
1	A	92	HIS
1	A	171	GLN
1	A	225	ASN
1	A	282	ASN
1	A	297	GLN
1	A	311	GLN
1	A	339	ASN
1	A	358	ASN
1	A	390	GLN
1	A	425	GLN
1	A	435	HIS
1	A	445	ASN
1	A	451	HIS
1	A	471	ASN
1	A	479	ASN
1	A	493	GLN
1	A	515	GLN
1	A	517	ASN
1	A	548	ASN
1	A	603	ASN
1	A	631	HIS
1	A	640	GLN
1	A	706	HIS
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	760	GLN
1	A	767	GLN
1	A	786	HIS

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Mol	Chain	Res	Type
1	A	851	HIS
1	A	858	ASN
1	A	877	HIS
1	A	903	ASN
1	A	926	GLN
1	A	965	GLN
1	A	966	ASN
1	A	972	HIS
1	A	1004	ASN
1	A	1011	GLN
1	A	1078	GLN
1	A	1106	ASN
1	A	1110	ASN
1	A	1124	HIS
1	A	1140	HIS
1	A	1173	HIS
1	A	1211	GLN
1	A	1432	GLN
2	B	47	GLN
2	B	60	GLN
2	B	121	ASN
2	B	178	ASN
2	B	236	HIS
2	B	395	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	531	GLN
2	B	538	ASN
2	B	734	HIS
2	B	744	HIS
2	B	761	HIS
2	B	821	GLN
2	B	842	ASN
2	B	862	GLN
2	B	887	HIS
2	B	946	ASN
2	B	957	ASN
2	B	975	GLN
2	B	984	HIS
2	B	1015	HIS

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Mol	Chain	Res	Type
2	B	1025	HIS
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1097	HIS
2	B	1161	HIS
2	B	1176	ASN
2	B	1193	GLN
2	B	1211	ASN
3	C	7	GLN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	112	ASN
3	C	131	HIS
3	C	203	GLN
3	C	242	GLN
3	C	252	GLN
4	D	39	ASN
4	D	51	ASN
4	D	132	GLN
4	D	157	GLN
4	D	179	GLN
5	E	3	GLN
5	E	101	GLN
5	E	104	ASN
5	E	106	GLN
5	E	143	ASN
5	E	147	HIS
5	E	153	HIS
7	G	14	HIS
7	G	53	ASN
7	G	97	HIS
7	G	113	HIS
7	G	126	ASN
7	G	158	HIS
8	H	128	ASN
8	H	131	ASN
9	I	12	ASN
9	I	22	ASN
11	K	65	HIS
11	K	89	ASN

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Mol	Chain	Res	Type
12	L	53	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1416/1733 (81%)	-0.32	14 (0%) 82 74	31, 133, 223, 314	0
2	B	1103/1224 (90%)	-0.26	11 (0%) 82 74	23, 141, 230, 357	0
3	C	266/318 (83%)	-0.32	0 100 100	58, 139, 209, 281	0
4	D	178/219 (81%)	-0.43	0 100 100	64, 146, 212, 263	0
5	E	214/215 (99%)	-0.35	1 (0%) 91 86	71, 165, 246, 367	0
6	F	87/155 (56%)	-0.36	0 100 100	48, 95, 156, 221	0
7	G	171/171 (100%)	-0.37	0 100 100	43, 121, 199, 230	0
8	H	134/146 (91%)	0.05	4 (2%) 50 39	115, 185, 250, 406	0
9	I	47/133 (35%)	-0.26	0 100 100	93, 163, 204, 221	0
10	J	65/70 (92%)	-0.35	0 100 100	80, 147, 210, 261	0
11	K	114/120 (95%)	-0.36	0 100 100	63, 128, 194, 254	0
12	L	46/70 (65%)	-0.28	0 100 100	93, 159, 240, 306	0
All	All	3841/4574 (83%)	-0.30	30 (0%) 86 79	23, 140, 227, 406	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	134	LYS	3.5
8	H	139	ASN	3.5
1	A	257	ARG	3.4
2	B	472	ALA	3.1
2	B	469	GLN	3.1
8	H	134	ASN	3.0
1	A	255	SER	3.0
2	B	678	GLU	2.8
1	A	1455	PRO	2.8
1	A	114	LEU	2.8
2	B	468	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	164	ARG	2.7
2	B	25	ILE	2.6
1	A	702	LEU	2.6
8	H	86	ASP	2.6
1	A	699	ALA	2.5
1	A	145	LYS	2.5
5	E	93	MET	2.4
2	B	641	GLU	2.3
2	B	919	SER	2.3
8	H	84	ALA	2.2
1	A	251	SER	2.2
1	A	179	LEU	2.2
1	A	700	ASN	2.2
2	B	263	GLY	2.1
2	B	267	ARG	2.1
2	B	21	GLU	2.1
1	A	660	ASN	2.0
1	A	1234	GLU	2.0
1	A	173	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	MG	A	3009	1/1	0.85	0.97	89,89,89,89	0
13	ZN	A	3006	1/1	0.89	0.07	274,274,274,274	0
13	ZN	A	3008	1/1	0.96	0.13	97,97,97,97	0
13	ZN	L	3005	1/1	0.97	0.08	229,229,229,229	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	ZN	C	3002	1/1	0.98	0.11	129,129,129,129	0
13	ZN	J	3001	1/1	0.98	0.29	153,153,153,153	0
13	ZN	B	3007	1/1	0.99	0.20	116,116,116,116	0
13	ZN	I	3003	1/1	1.00	0.12	133,133,133,133	0

6.5 Other polymers (i)

There are no such residues in this entry.