Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:40 AM GMT

PDB ID	:	2B63
Title	:	Complete RNA Polymerase II-RNA inhibitor complex
Authors	:	Kettenberger, H.; Eisenfuehr, A.; Brueckner, F.; Theis, M.; Famulok, M.; Cramer, P.
Deposited on	:	2005-09-30
Resolution	:	3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

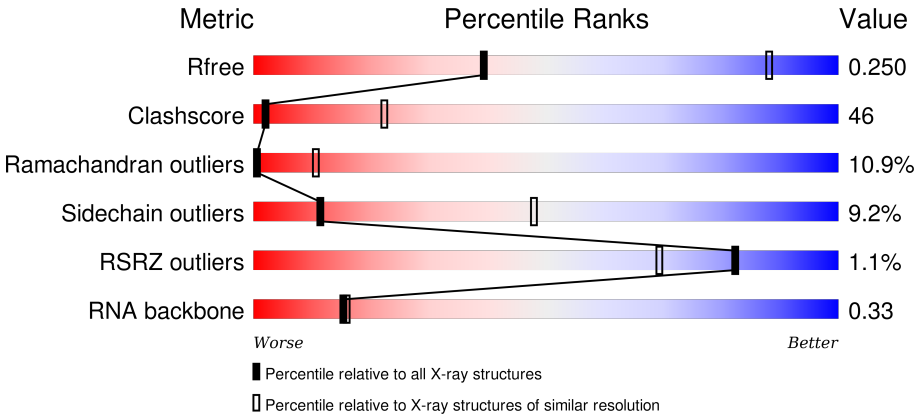
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	R	31	13% 42% 32% 13%
2	A	1733	% 29% 42% 9% • 18%
3	B	1224	% 30% 47% 11% • 9%
4	C	318	27% 45% 12% • 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	221	31% 40% 9% 20%
6	E	215	3% 42% 51% 7%
7	F	155	19% 29% 6% 46%
8	G	171	37% 51% 10%
9	H	146	4% 29% 49% 12% 9%
10	I	122	3% 33% 54% 8%
11	J	70	23% 47% 20% 7%
12	K	120	% 43% 46% 7%
13	L	70	% 16% 36% 13% 34%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31731 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 RNA chain called 31-MER.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	Br	C	N	O	P			
1	R	31	666	4	296	119	217	30	88	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	1416	11140	7021	1946	2111	62	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	1112	8836	5594	1548	1639	55	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 5 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	177	1356	840	241	273	2	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 8 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	115	Total	C	N	O	S	0	0	0
			924	593	157	172	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

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

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

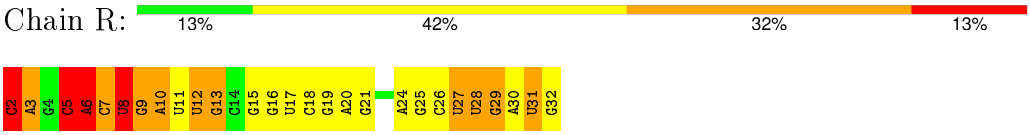
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		

3 Residue-property plots (i)

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

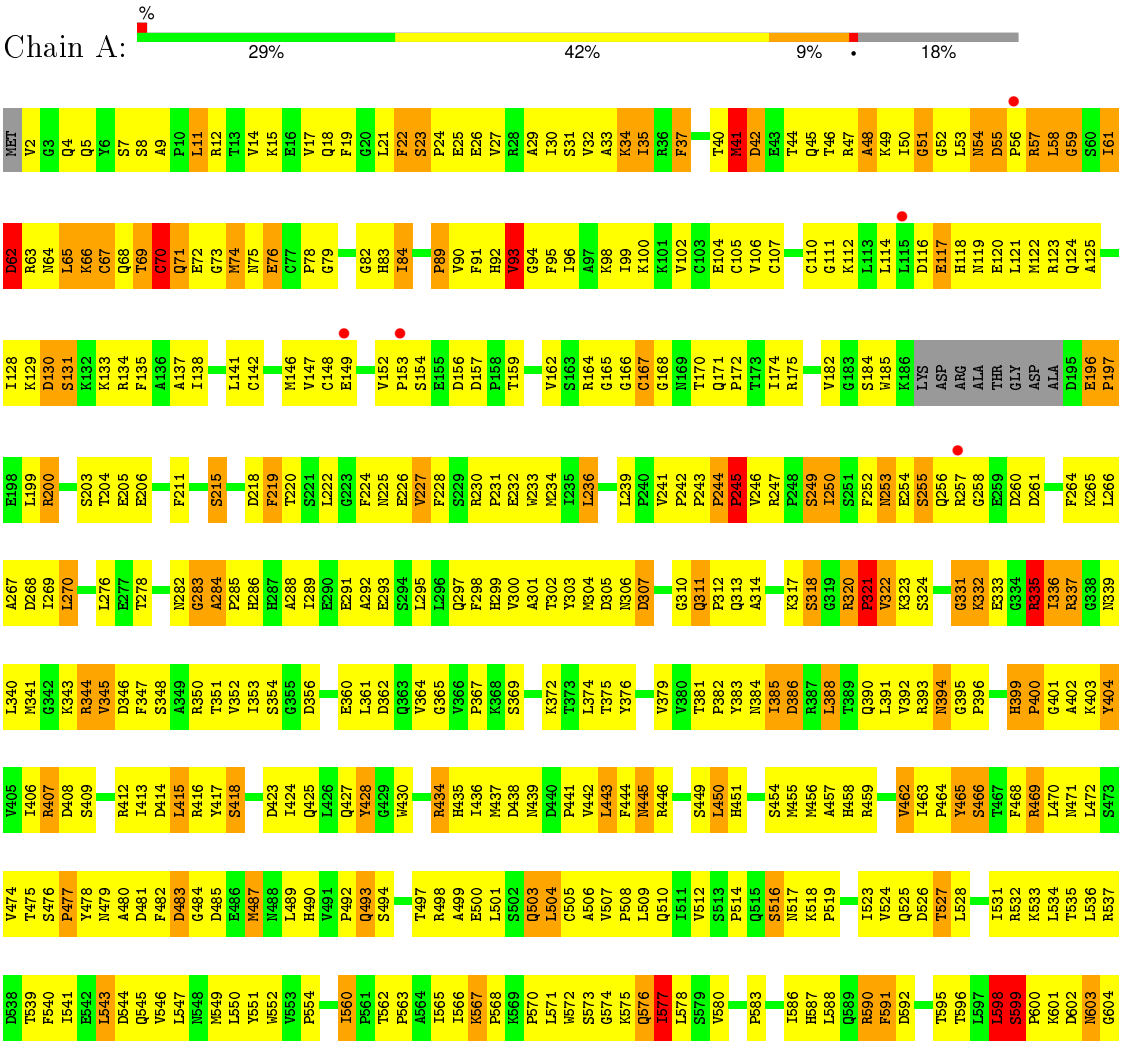
- Molecule 1: 31-MER

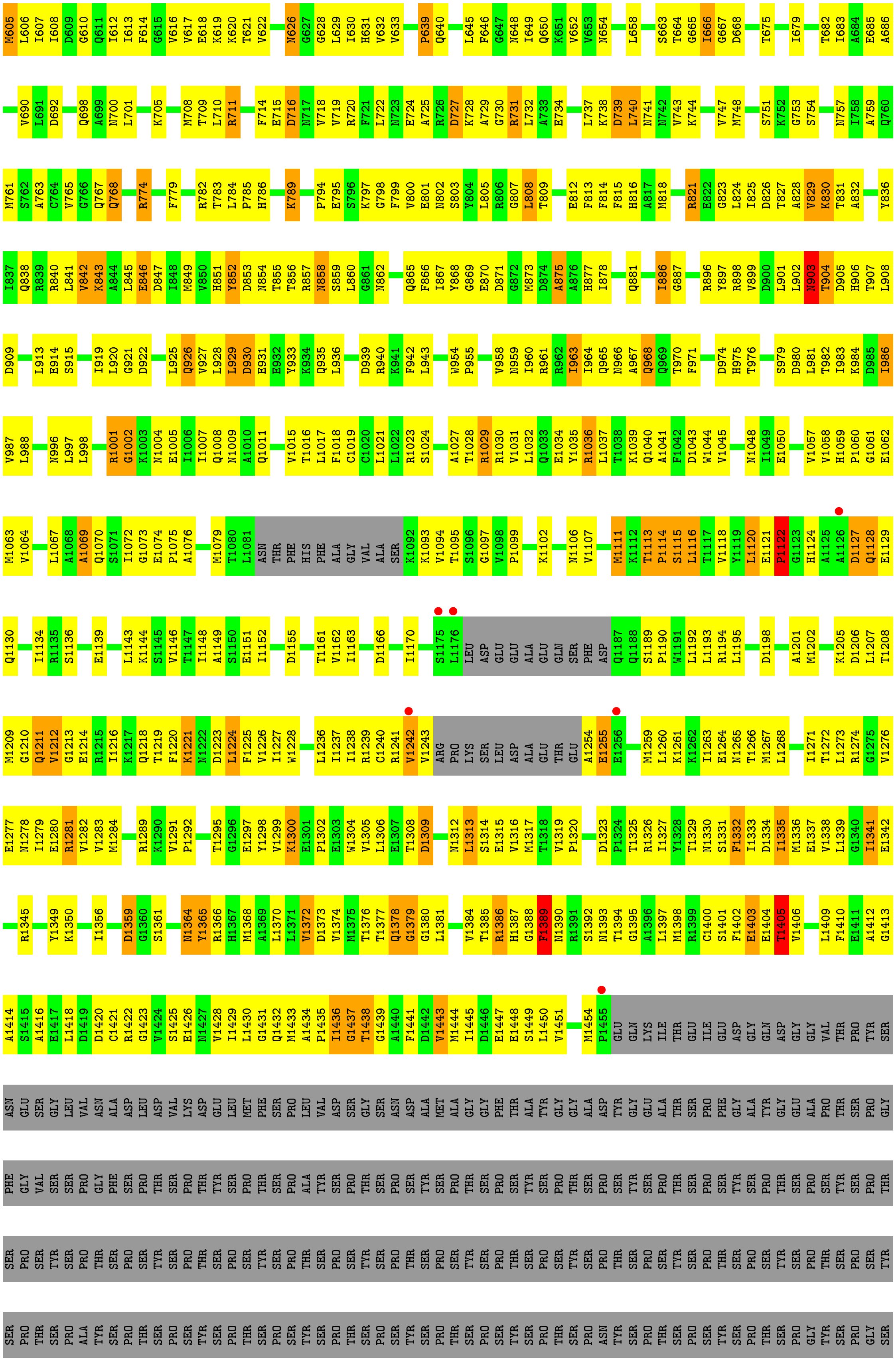
Chain R:



- Molecule 2: DNA-directed RNA polymerase II largest subunit

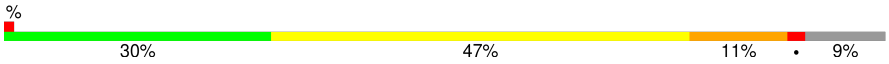
Chain A:

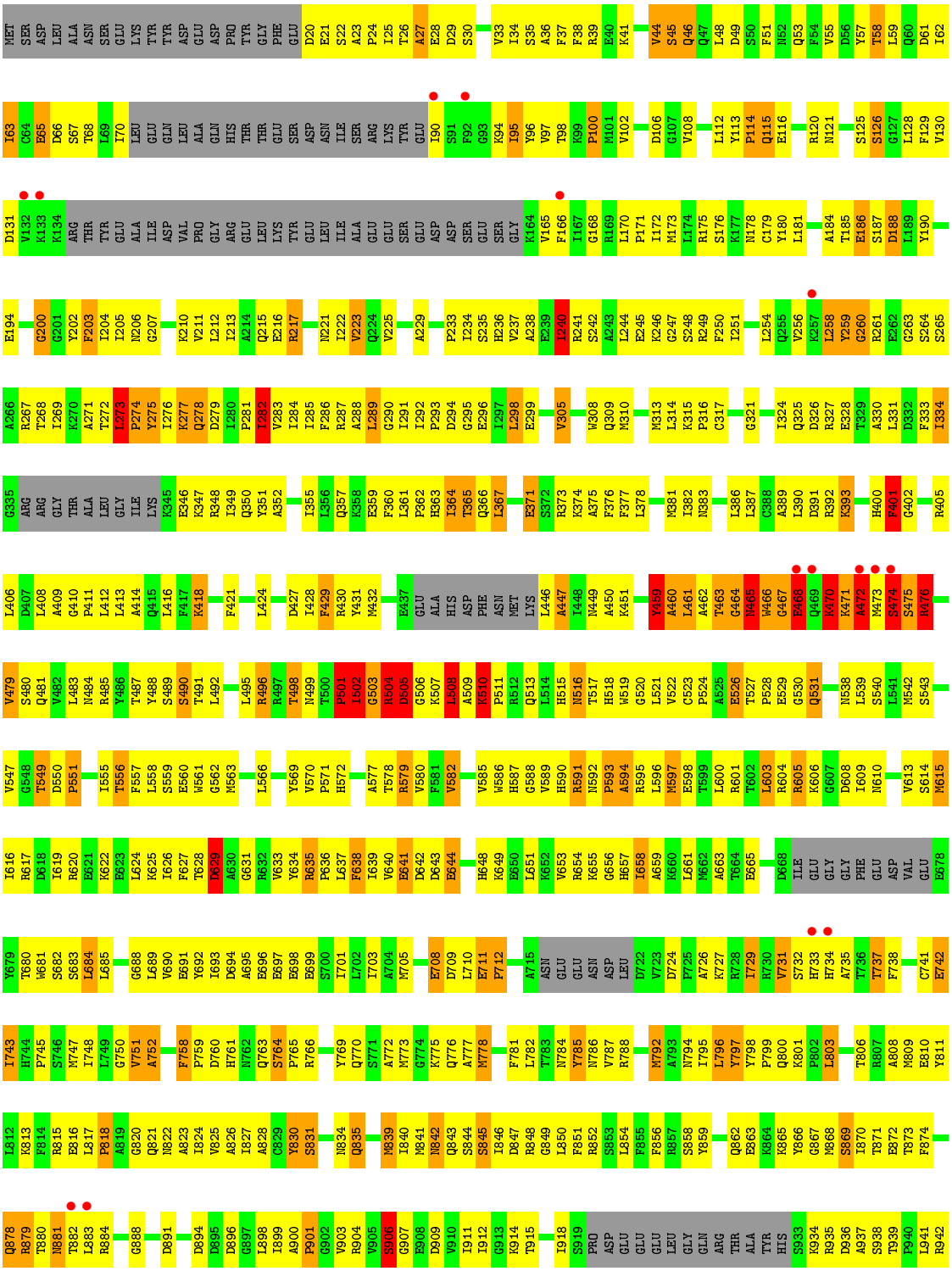


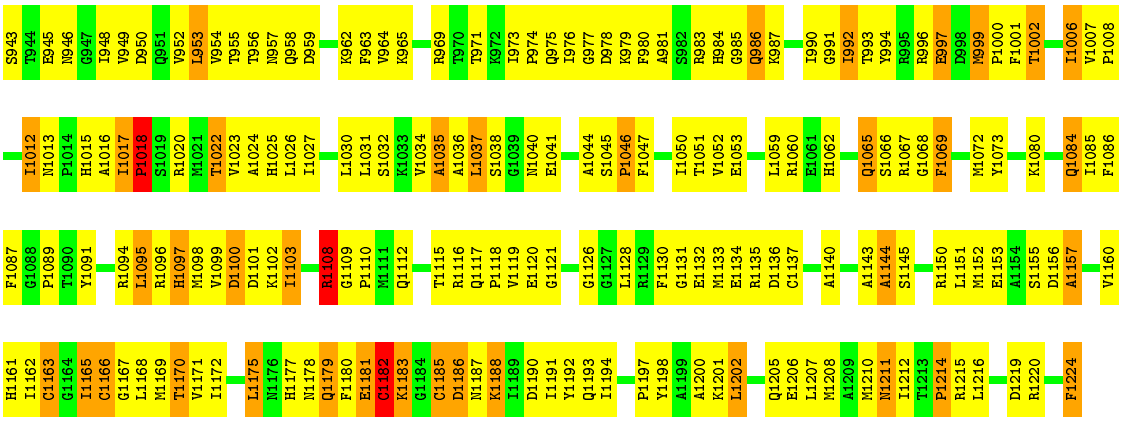

M605 L606 I607 I608 D609 G610 Q611 I612 I613 F614 G615 V616 V617 E618 K619 K620 T621 V622 N626 G627 G628 L629 I630 H631 V632 V633 P639 Q640 L645 F646 G647 N648 I649 Q650 K651 V652 V653 N654 L658 S663 T664 G665 I666 G667 D668 T675 I679 T682 I683 A684 E685 A686
V690 L691 D692 Q698 A699 N700 L701 K705 M708 T709 L710 R711 F714 E715 D716 N717 V718 V719 R720 F721 L722 N723 E724 A725 R726 D727 K728 A729 G730 R731 L732 A733 E734 L737 K738 D739 L740 N741 N742 V743 K744 V747 M748 S751 K752 G753 S754 N757 I758 A759 Q760
M761 S762 A763 C764 V765 G766 Q767 Q768 R774 F779 R782 T783 L784 P785 H786 K789 P794 E795 S796 K797 G798 F799 V800 E801 N802 S803 Y804 L805 R806 G807 L808 T809 E812 F813 F814 F815 H816 A817 M818 R821 E822 G823 L824 I825 D826 T827 A828 V829 K830 T831 A832 Y836
I837 Q838 R839 R840 L841 V842 K843 A844 L845 E846 D847 I848 M849 V850 H851 Y852 D853 N854 T855 T856 R857 N858 S859 L860 G861 N862 Q865 F866 I867 Y868 G869 E870 D871 G872 M873 D874 A875 A876 H877 I878 Q881 I886 G887 R896 Y897 R898 V899 D900 L901 L902 N903 T904 D905 H906 T907 L908
D909 L913 E914 S915 I919 L920 G921 D922 L925 Q926 V927 L928 L929 D930 E931 E932 Y933 K934 Q935 L936 D939 R940 K941 F942 L943 W954 P955 V958 N959 I960 R961 R962 I963 I964 Q965 N966 A967 Q968 Q969 T970 F971 D974 H975 T976 S979 D980 L981 T982 I983 K984 D985 I986
V987 L988 N996 L997 L998 R1001 G1002 K1003 N1004 E1005 I1006 I1007 Q1008 N1009 A1010 Q1011 V1015 T1016 L1017 F1018 C1019 C1020 L1021 L1022 R1023 S1024 A1027 T1028 R1029 R1030 V1031 L1032 Q1033 E1034 Y1035 R1036 L1037 T1038 K1039 Q1040 A1041 F1042 D1043 W1044 V1045 N1048 I1049 E1050 V1057 V1058 H1059 P1060 G1061 E1062
M1063 V1064 L1067 A1068 A1069 Q1070 S1071 I1072 G1073 E1074 P1075 A1076 M1079 T1080 L1081 ASN THR PHE HIS PHE ALA GLY VAL ALA SER K1092 K1093 V1094 T1095 S1096 G1097 V1098 P1099 K1102 N1106 V1107 M1111 K1112 T1113 P1114 S1115 L1116 T1117 V1118 Y1119 L1120 E1121 P1122 G1123 H1124 A1125 A1126 D1127 Q1128 E1129
Q1130 I1134 R1135 S1136 E1139 L1143 K1144 S1145 V1146 T1147 I1148 A1149 S1150 E1151 I1152 D1155 T1161 V1162 I1163 D1166 I1170 S1175 L1176 LEU ASP GLU GLU ALA GLU GLN SER PHE ASP Q1187 Q1188 S1189 P1190 W1191 L1192 L1193 R1194 L1195 D1198 A1201 M1202 K1205 D1206 L1207 T1208
M1209 G1210 Q1211 V1212 G1213 E1214 R1215 I1216 K1217 Q1218 T1219 F1220 K1221 N1222 D1223 L1224 F1225 V1226 I1227 W1228 L1236 T1237 I1238 R1239 C1240 R1241 V1242 V1243 ARG PRO LYS SER LEU ASP ALA GLU THR GLU A1254 E1255 E1256 M1259 L1260 K1261 K1262 I1263 E1264 N1265 T1266 M1267 L1268 I1271 T1272 L1273 R1274 G1275 V1276
E1277 N1278 I1279 E1280 R1281 V1282 V1283 M1284 R1289 K1290 V1291 P1292 T1295 G1296 E1297 Y1298 V1299 K1300 E1301 P1302 E1303 W1304 V1305 L1306 E1307 T1308 D1309 N1312 L1313 S1314 E1315 V1316 M1317 T1318 V1319 P1320 D1323 P1324 T1325 R1326 I1327 Y1328 T1329 N1330 S1331 F1332 I1333 D1334 I1335 M1336 E1337 V1338 L1339 G1340 I1341 E1342
R1345 Y1349 K1350 I1356 D1359 G1360 S1361 N1364 Y1365 R1366 H1367 M1368 A1369 L1370 L1371 V1372 D1373 V1374 M1375 T1376 T1377 Q1378 G1379 G1380 L1381 V1384 T1385 R1386 H1387 G1388 F1389 N1390 R1391 S1392 N1393 T1394 G1395 A1396 L1397 M1398 R1399 C1400 S1401 F1402 E1403 E1404 T1405 V1406 L1409 F1410 E1411 A1412 G1413
A1414 S1415 A1416 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 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 PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR
SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER 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 PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO ASN TYR SER PRO THR SER PRO SER TYR SER PRO GLY TYR SER PRO GLY SER

• Molecule 3: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B:

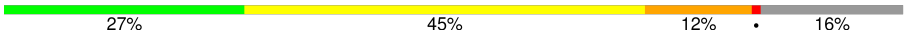


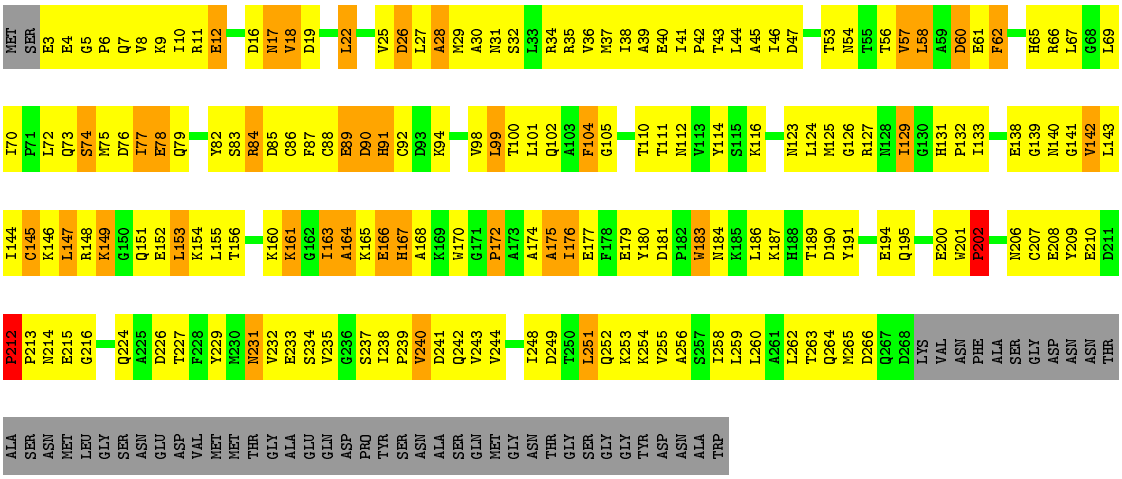




• Molecule 4: DNA-directed RNA polymerase II 45 kDa polypeptide

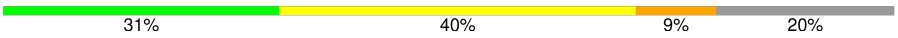
Chain C:

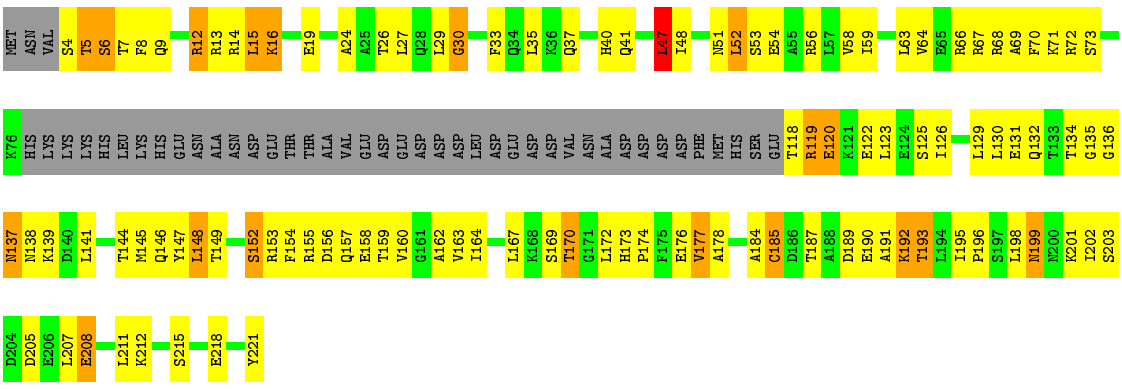




• Molecule 5: DNA-directed RNA polymerase II 32 kDa polypeptide

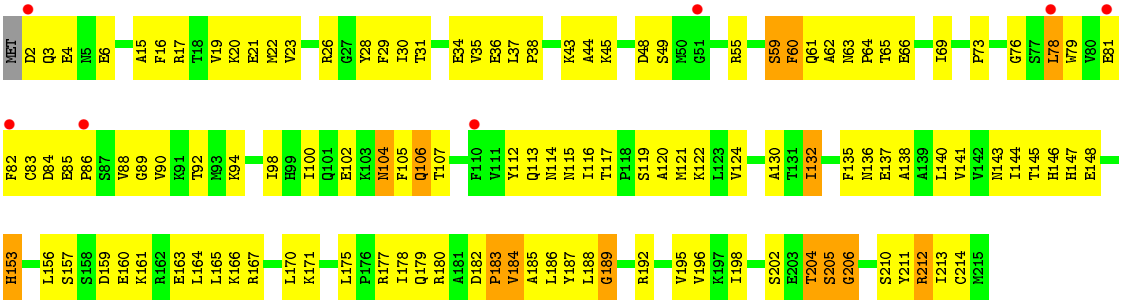
Chain D:



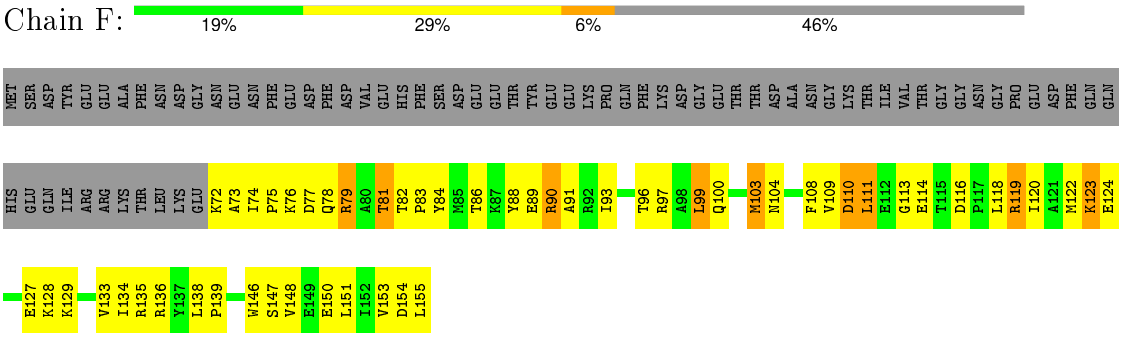


• Molecule 6: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

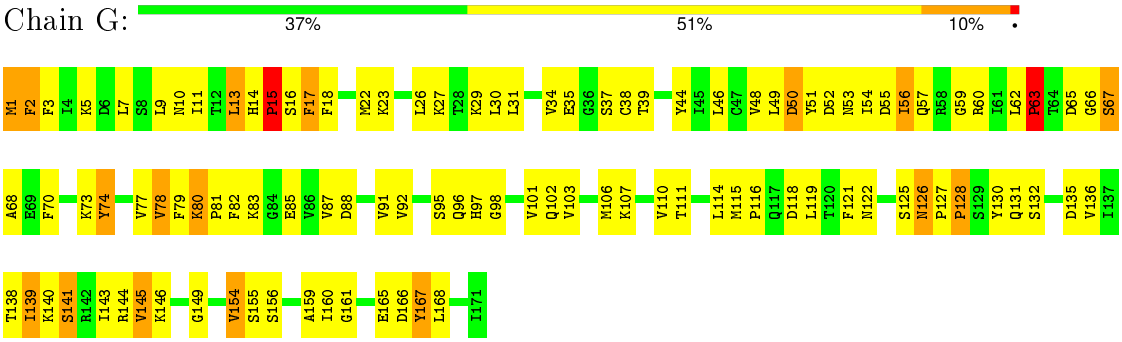
Chain E:



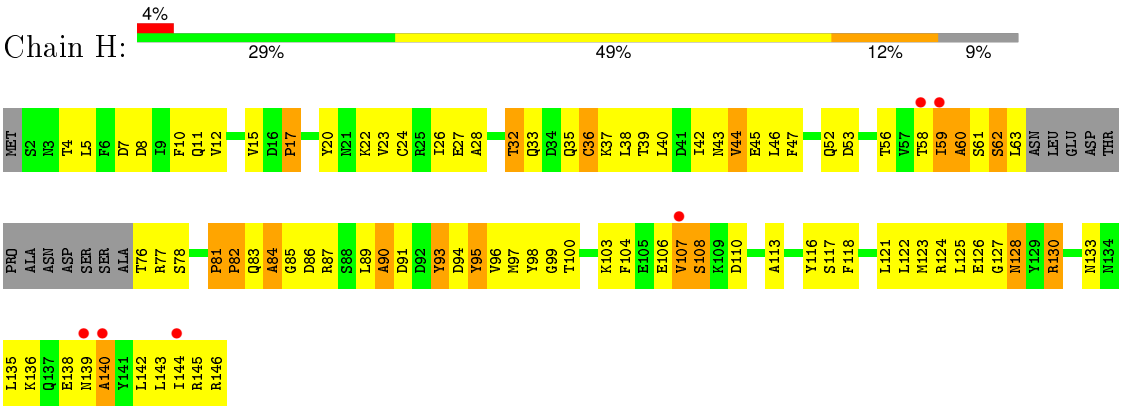
• Molecule 7: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide



• Molecule 8: DNA-directed RNA polymerase II 19 kDa polypeptide

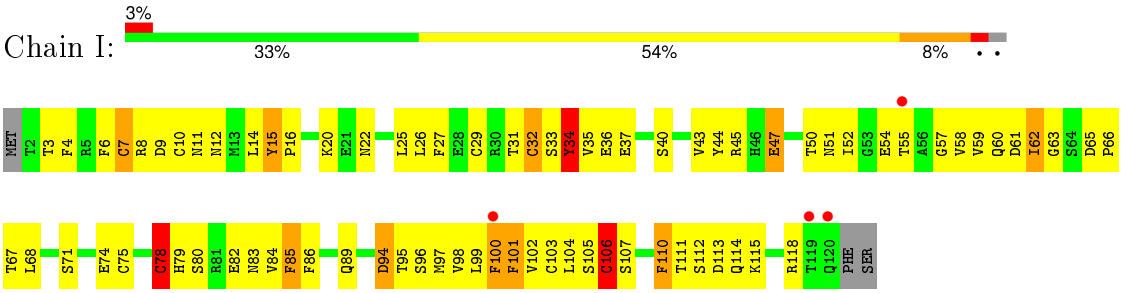


• Molecule 9: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide



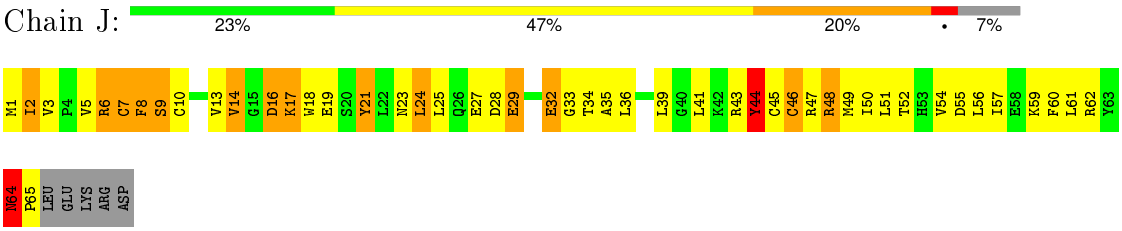
• Molecule 10: DNA-directed RNA polymerase II subunit 9

Chain I:



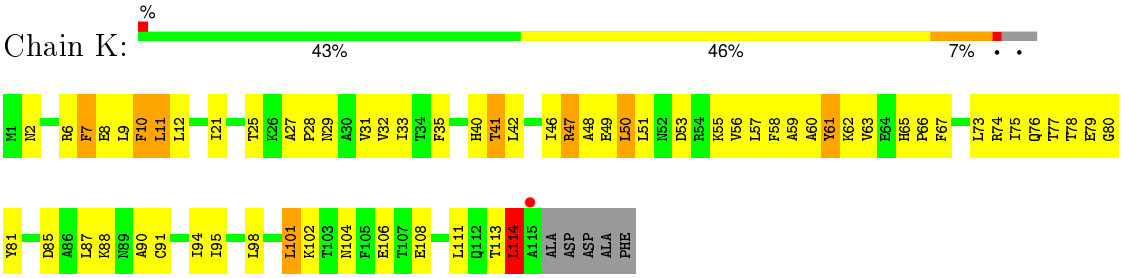
• Molecule 11: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:



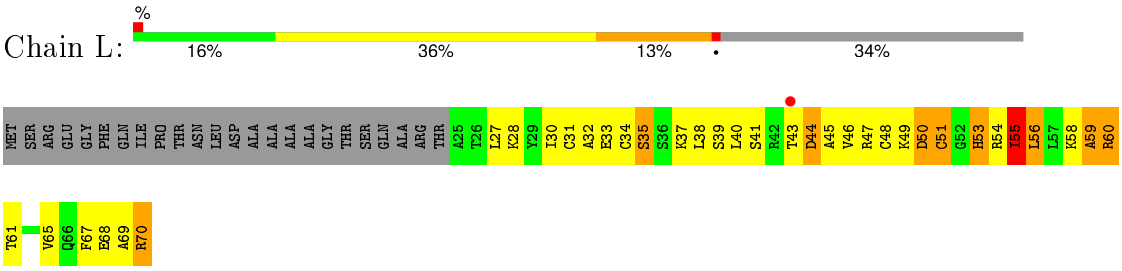
• Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:



• Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	224.59Å 399.81Å 286.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 49.15 – 3.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.80) 99.1 (49.15-3.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.273 0.226 , 0.250	Depositor DCC
R_{free} test set	2527 reflections (2.04%)	DCC
Wilson B-factor (Å^2)	121.4	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 64.6	EDS
Estimated twinning fraction	0.015 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.018 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 248494 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	31731	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5BU, 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	R	0.93	1/652 (0.2%)	1.19	4/1017 (0.4%)
2	A	0.48	0/11339	0.74	5/15334 (0.0%)
3	B	0.47	0/9008	0.78	19/12146 (0.2%)
4	C	0.47	0/2133	0.75	1/2891 (0.0%)
5	D	0.45	0/1365	0.68	0/1837
6	E	0.44	0/1788	0.67	0/2406
7	F	0.56	0/691	0.76	0/933
8	G	0.51	0/1368	0.75	0/1844
9	H	0.39	0/1086	0.64	0/1470
10	I	0.39	0/989	0.70	0/1331
11	J	0.51	0/541	0.82	0/727
12	K	0.46	0/942	0.68	0/1272
13	L	0.53	0/365	0.75	0/485
All	All	0.48	1/32267 (0.0%)	0.76	29/43693 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	R	0	2
11	J	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	2	C	C3'-C2'	5.33	1.58	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	503	GLY	N-CA-C	-10.94	85.76	113.10
3	B	273	LEU	C-N-CD	-9.80	99.03	120.60
1	R	2	C	O4'-C1'-N1	9.55	115.84	108.20
3	B	508	LEU	N-CA-C	-8.97	86.78	111.00
1	R	5	C	C2'-C3'-O3'	7.04	124.98	109.50
3	B	479	VAL	N-CA-C	-6.26	94.11	111.00
3	B	468	GLU	N-CA-C	6.23	127.83	111.00
3	B	471	LYS	N-CA-C	-6.22	94.20	111.00
3	B	470	LYS	N-CA-C	6.16	127.64	111.00
3	B	474	SER	N-CA-C	6.08	127.42	111.00
3	B	472	ALA	N-CA-C	6.04	127.31	111.00
3	B	1185	CYS	CA-CB-SG	6.04	124.87	114.00
3	B	1166	CYS	CA-CB-SG	-5.97	103.25	114.00
2	A	331	GLY	N-CA-C	5.96	128.00	113.10
3	B	275	TYR	N-CA-C	-5.83	95.27	111.00
3	B	473	MET	N-CA-C	-5.82	95.28	111.00
3	B	1185	CYS	N-CA-C	-5.79	95.36	111.00
2	A	344	ARG	N-CA-C	-5.76	95.46	111.00
2	A	311	GLN	N-CA-C	5.43	125.67	111.00
3	B	1182	CYS	N-CA-C	-5.41	96.39	111.00
2	A	1403	GLU	N-CA-C	5.27	125.24	111.00
3	B	1182	CYS	CA-CB-SG	-5.26	104.53	114.00
3	B	464	GLY	N-CA-C	-5.22	100.04	113.10
4	C	183	TRP	N-CA-C	-5.15	97.09	111.00
1	R	8	U	N1-C1'-C2'	5.14	120.68	114.00
3	B	502	ILE	N-CA-C	5.10	124.77	111.00
1	R	6	A	N9-C1'-C2'	5.07	120.59	114.00
2	A	466	SER	N-CA-C	5.05	124.63	111.00
3	B	273	LEU	C-N-CA	5.04	143.15	122.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	J	44	TYR	Sidechain
1	R	2	C	Sidechain
1	R	5	C	Sidechain

5.2 Too-close contacts (i)

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	666	0	331	42	0
2	A	11140	0	11217	1087	0
3	B	8836	0	8871	910	0
4	C	2095	0	2051	242	0
5	D	1356	0	1319	118	0
6	E	1752	0	1776	129	0
7	F	679	0	701	56	0
8	G	1340	0	1357	132	0
9	H	1068	0	1040	123	0
10	I	971	0	928	83	0
11	J	532	0	542	84	0
12	K	924	0	934	78	0
13	L	363	0	386	41	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	31731	0	31453	2875	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 46.

All (2875) 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)
5:D:40:HIS:HB3	8:G:73:LYS:NZ	1.60	1.16
2:A:1329:THR:HG22	2:A:1331:SER:H	1.01	1.12
3:B:827:ILE:HG12	3:B:1012:ILE:HD11	1.18	1.11
3:B:463:THR:HB	3:B:465:ASN:HB2	1.32	1.10
1:R:3:A:OP2	3:B:531:GLN:HB3	1.50	1.10
3:B:882:THR:HG22	3:B:884:ARG:H	1.14	1.10
9:H:59:ILE:HG22	9:H:60:ALA:H	0.92	1.08
10:I:34:TYR:HD2	10:I:35:VAL:N	1.54	1.06
11:J:5:VAL:HG12	11:J:6:ARG:HG3	1.31	1.05
2:A:53:LEU:HD23	2:A:54:ASN:N	1.71	1.04
2:A:53:LEU:CD2	2:A:54:ASN:H	1.69	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:100:THR:HG23	9:H:138:GLU:HA	1.35	1.04
8:G:13:LEU:HD21	8:G:17:PHE:HB2	1.39	1.04
2:A:779:PHE:CE1	2:A:785:PRO:HD3	1.94	1.03
12:K:47:ARG:HB3	12:K:47:ARG:HH11	1.17	1.03
2:A:61:ILE:HG22	2:A:62:ASP:H	1.22	1.03
2:A:107:CYS:H	2:A:114:LEU:HD21	1.22	1.03
2:A:590:ARG:NH2	2:A:620:LYS:HB3	1.74	1.03
4:C:57:VAL:HG11	11:J:60:PHE:HB3	1.41	1.01
9:H:59:ILE:HG22	9:H:60:ALA:N	1.72	1.01
2:A:1161:THR:HG22	2:A:1163:ILE:H	1.26	1.01
2:A:53:LEU:HD23	2:A:54:ASN:H	0.87	1.01
2:A:826:ASP:O	2:A:830:LYS:HB2	1.61	1.01
3:B:509:ALA:O	3:B:511:PRO:HD3	1.61	1.00
6:E:29:PHE:O	6:E:30:ILE:HG13	1.61	1.00
2:A:225:ASN:ND2	2:A:228:PHE:H	1.60	1.00
8:G:138:THR:HG22	8:G:139:ILE:H	1.25	0.99
3:B:577:ALA:HB1	3:B:589:VAL:HG11	1.45	0.98
11:J:3:VAL:HG21	11:J:18:TRP:HB2	1.43	0.98
11:J:64:ASN:HB3	11:J:65:PRO:CD	1.92	0.98
3:B:505:ASP:CG	3:B:506:GLY:H	1.68	0.97
8:G:143:ILE:HG22	8:G:144:ARG:H	1.28	0.97
3:B:684:LEU:H	3:B:684:LEU:HD12	1.30	0.96
2:A:907:THR:HG22	2:A:908:LEU:H	1.26	0.96
3:B:276:ILE:HD11	3:B:355:ILE:HG21	1.45	0.95
3:B:65:GLU:HG3	3:B:66:ASP:H	1.30	0.95
2:A:767:GLN:HE21	2:A:774:ARG:HB3	1.28	0.95
3:B:365:THR:HG23	3:B:367:LEU:H	1.32	0.94
2:A:249:SER:O	2:A:250:ILE:HG12	1.66	0.94
2:A:1116:LEU:HG	2:A:1308:THR:HG21	1.46	0.94
9:H:59:ILE:CG2	9:H:60:ALA:H	1.79	0.94
6:E:94:LYS:HE2	6:E:98:ILE:HD11	1.49	0.94
3:B:510:LYS:HD2	3:B:510:LYS:H	1.32	0.93
10:I:85:PHE:HD2	10:I:85:PHE:H	1.08	0.93
2:A:858:ASN:ND2	2:A:860:LEU:H	1.67	0.93
2:A:1329:THR:HG22	2:A:1331:SER:N	1.84	0.92
2:A:868:TYR:CE1	2:A:1064:VAL:HG11	2.04	0.92
5:D:40:HIS:HB3	8:G:73:LYS:HZ3	1.18	0.92
3:B:800:GLN:HB3	11:J:52:THR:HG21	1.51	0.92
2:A:783:THR:HG22	2:A:784:LEU:HG	1.51	0.91
12:K:21:ILE:HG12	12:K:33:ILE:HG13	1.52	0.91
2:A:901:LEU:HG	2:A:926:GLN:HE21	1.32	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1017:LEU:HB2	6:E:206:GLY:H	1.33	0.91
9:H:23:VAL:HG22	9:H:43:ASN:HA	1.52	0.90
7:F:93:ILE:HD11	7:F:134:ILE:HD11	1.51	0.90
2:A:225:ASN:HD22	2:A:228:PHE:H	0.98	0.90
2:A:567:LYS:CG	2:A:568:PRO:HD2	2.01	0.90
3:B:1072:MET:CE	3:B:1085:ILE:HB	2.01	0.89
2:A:1094:VAL:HG13	2:A:1113:THR:HG21	1.55	0.89
4:C:17:ASN:HD22	4:C:17:ASN:N	1.70	0.89
3:B:642:ASP:HA	3:B:649:LYS:HA	1.52	0.89
8:G:143:ILE:HG22	8:G:144:ARG:N	1.84	0.89
3:B:589:VAL:HG12	3:B:590:HIS:H	1.36	0.89
7:F:82:THR:HG22	7:F:84:TYR:H	1.36	0.89
2:A:1428:VAL:HG13	3:B:1151:LEU:HD21	1.53	0.88
3:B:271:ALA:HB1	3:B:273:LEU:HD11	1.53	0.88
3:B:1065:GLN:HE21	3:B:1067:ARG:N	1.70	0.88
4:C:47:ASP:HA	13:L:69:ALA:HB3	1.55	0.88
10:I:111:THR:HG22	10:I:113:ASP:H	1.35	0.88
9:H:42:ILE:HG23	9:H:95:TYR:HE1	1.37	0.88
2:A:907:THR:HG22	2:A:908:LEU:N	1.89	0.88
4:C:251:LEU:O	4:C:251:LEU:HD12	1.73	0.88
3:B:953:LEU:HD21	3:B:965:LYS:HB2	1.56	0.87
12:K:47:ARG:HB3	12:K:47:ARG:NH1	1.89	0.87
3:B:705:MET:H	3:B:710:LEU:HD12	1.39	0.87
2:A:369:SER:HB3	12:K:2:ASN:HD21	1.37	0.87
3:B:1007:VAL:HG22	3:B:1008:PRO:HD2	1.54	0.87
3:B:827:ILE:CG1	3:B:1012:ILE:HD11	2.04	0.87
6:E:153:HIS:HB3	6:E:196:VAL:HG11	1.56	0.87
2:A:590:ARG:HH21	2:A:620:LYS:HB3	1.31	0.87
2:A:1242:VAL:HG12	2:A:1243:VAL:H	1.35	0.86
3:B:281:PRO:HG2	3:B:284:ILE:HD13	1.57	0.86
3:B:510:LYS:CD	3:B:510:LYS:H	1.87	0.86
4:C:142:VAL:H	11:J:16:ASP:HB3	1.40	0.86
3:B:846:ILE:HG23	3:B:974:PRO:HG2	1.57	0.86
11:J:64:ASN:HB3	11:J:65:PRO:HD3	1.55	0.86
2:A:1312:ASN:O	2:A:1316:VAL:HG23	1.74	0.86
3:B:821:GLN:HE22	3:B:851:PHE:HA	1.40	0.86
6:E:156:LEU:HD12	6:E:195:VAL:HB	1.57	0.86
2:A:1438:THR:HB	3:B:1144:ALA:HB3	1.55	0.86
3:B:476:ARG:HH11	3:B:476:ARG:HA	1.40	0.86
2:A:1364:ASN:HD22	2:A:1365:TYR:N	1.73	0.85
2:A:399:HIS:HB3	2:A:400:PRO:HD3	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:164:ALA:HA	4:C:167:HIS:O	1.75	0.85
2:A:164:ARG:HG3	2:A:165:GLY:H	1.38	0.85
2:A:821:ARG:HB2	2:A:821:ARG:HH11	1.41	0.85
3:B:800:GLN:HB3	11:J:52:THR:CG2	2.06	0.85
1:R:2:C:O2'	1:R:3:A:OP1	1.95	0.85
2:A:56:PRO:O	2:A:57:ARG:HG3	1.76	0.85
6:E:144:ILE:HD12	6:E:145:THR:N	1.91	0.84
2:A:527:THR:HG21	2:A:650:GLN:HG2	1.57	0.84
8:G:115:MET:HB2	8:G:116:PRO:HD2	1.57	0.84
1:R:29:G:H4'	2:A:1386:ARG:HH12	1.42	0.84
2:A:981:LEU:HD21	2:A:1039:LYS:HA	1.58	0.84
2:A:285:PRO:HG2	2:A:288:ALA:HB3	1.60	0.84
2:A:567:LYS:HG3	2:A:568:PRO:HD2	1.56	0.84
2:A:15:LYS:HB3	3:B:1220:ARG:HH21	1.43	0.83
3:B:980:PHE:HE1	3:B:990:ILE:HD11	1.42	0.83
9:H:126:GLU:C	9:H:130:ARG:HH22	1.82	0.83
2:A:800:VAL:HG22	2:A:812:GLU:HB3	1.60	0.83
2:A:628:GLY:O	2:A:632:VAL:HG23	1.78	0.83
2:A:1394:THR:HG21	2:A:1398:MET:SD	2.19	0.83
10:I:8:ARG:HG3	10:I:34:TYR:HE1	1.43	0.83
2:A:54:ASN:HB3	2:A:247:ARG:HH12	1.44	0.83
2:A:768:GLN:HG2	2:A:816:HIS:HA	1.61	0.83
2:A:147:VAL:N	2:A:171:GLN:HE21	1.75	0.83
3:B:1152:MET:CE	3:B:1157:ALA:HA	2.08	0.82
4:C:167:HIS:HA	12:K:6:ARG:HH12	1.43	0.82
3:B:120:ARG:HG2	3:B:955:THR:HG21	1.59	0.82
3:B:1072:MET:HE3	3:B:1085:ILE:HB	1.61	0.82
2:A:528:LEU:O	2:A:531:ILE:HG22	1.79	0.82
3:B:952:VAL:HG12	3:B:953:LEU:N	1.94	0.82
8:G:145:VAL:HG12	8:G:146:LYS:H	1.43	0.82
2:A:901:LEU:H	2:A:926:GLN:NE2	1.77	0.82
5:D:134:THR:HG22	5:D:136:GLY:H	1.44	0.82
2:A:22:PHE:HB2	3:B:1211:ASN:ND2	1.94	0.82
3:B:273:LEU:N	3:B:273:LEU:HD22	1.93	0.82
5:D:144:THR:HG21	8:G:46:LEU:HD13	1.59	0.81
3:B:463:THR:CB	3:B:465:ASN:HB2	2.08	0.81
8:G:14:HIS:ND1	8:G:15:PRO:HD2	1.95	0.81
3:B:284:ILE:H	3:B:284:ILE:HD12	1.45	0.81
12:K:113:THR:O	12:K:114:LEU:HB2	1.78	0.81
2:A:828:ALA:CB	3:B:530:GLY:HA2	2.09	0.81
3:B:579:ARG:HB2	3:B:586:TRP:NE1	1.95	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:879:ARG:HH11	3:B:883:LEU:HD22	1.46	0.81
4:C:186:LEU:HD21	4:C:224:GLN:O	1.81	0.81
2:A:254:GLU:O	2:A:256:GLN:N	2.13	0.81
3:B:25:ILE:HD11	3:B:653:VAL:O	1.80	0.81
3:B:801:LYS:O	11:J:52:THR:HG23	1.81	0.81
5:D:59:ILE:HD11	8:G:77:VAL:HG11	1.60	0.81
2:A:472:LEU:HD11	3:B:835:GLN:NE2	1.94	0.81
8:G:56:ILE:H	8:G:56:ILE:HD12	1.46	0.81
5:D:202:ILE:HG23	5:D:203:SER:N	1.96	0.81
2:A:1329:THR:CG2	2:A:1331:SER:H	1.89	0.80
13:L:60:ARG:HG2	13:L:61:THR:H	1.46	0.80
2:A:67:CYS:O	2:A:70:CYS:HB3	1.82	0.80
2:A:524:VAL:HG12	2:A:525:GLN:H	1.45	0.80
3:B:1201:LYS:HE2	3:B:1205:GLN:OE1	1.81	0.80
8:G:1:MET:HE3	8:G:80:LYS:H	1.45	0.80
2:A:567:LYS:HZ1	9:H:46:LEU:HB2	1.46	0.80
3:B:918:ILE:HB	3:B:935:ARG:HD2	1.61	0.80
10:I:34:TYR:CD2	10:I:35:VAL:N	2.45	0.80
4:C:16:ASP:C	4:C:17:ASN:HD22	1.85	0.80
3:B:464:GLY:C	3:B:466:TRP:H	1.83	0.80
3:B:516:ASN:N	3:B:516:ASN:HD22	1.77	0.80
8:G:143:ILE:CG2	8:G:144:ARG:H	1.94	0.80
6:E:202:SER:OG	6:E:204:THR:HG22	1.82	0.79
2:A:598:LEU:HA	9:H:122:LEU:HD13	1.62	0.79
10:I:26:LEU:HD23	10:I:37:GLU:HA	1.64	0.79
2:A:798:GLY:HA2	2:A:815:PHE:CD1	2.17	0.79
3:B:501:PRO:HG2	3:B:502:ILE:HG12	1.64	0.79
2:A:49:LYS:NZ	2:A:61:ILE:HG12	1.98	0.79
3:B:589:VAL:HG12	3:B:590:HIS:N	1.97	0.79
5:D:33:PHE:CE2	8:G:80:LYS:NZ	2.50	0.79
3:B:1187:ASN:O	3:B:1188:LYS:HB2	1.81	0.79
4:C:31:ASN:O	4:C:34:ARG:HB3	1.82	0.79
3:B:579:ARG:HB2	3:B:586:TRP:HE1	1.46	0.79
3:B:23:ALA:HB1	3:B:24:PRO:HD2	1.65	0.79
3:B:247:GLY:H	3:B:418:LYS:NZ	1.79	0.79
2:A:907:THR:CG2	2:A:908:LEU:H	1.96	0.79
2:A:351:THR:HG22	3:B:1103:ILE:HA	1.65	0.79
2:A:1189:SER:O	2:A:1241:ARG:HD3	1.82	0.78
3:B:463:THR:C	3:B:465:ASN:H	1.85	0.78
2:A:767:GLN:NE2	2:A:774:ARG:HB3	1.97	0.78
2:A:535:THR:HG21	2:A:616:VAL:HA	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1345:ARG:HG3	2:A:1376:THR:HG21	1.63	0.78
2:A:107:CYS:N	2:A:114:LEU:HD21	1.99	0.78
2:A:1420:ASP:HB3	2:A:1422:ARG:HG3	1.66	0.78
2:A:855:THR:HG23	2:A:857:ARG:HG3	1.63	0.78
3:B:466:TRP:O	3:B:468:GLU:N	2.17	0.78
4:C:172:PRO:O	4:C:235:VAL:HG23	1.83	0.78
2:A:1102:LYS:HG2	2:A:1106:ASN:HD21	1.47	0.78
2:A:728:LYS:HA	2:A:731:ARG:HB2	1.65	0.77
3:B:613:VAL:HG13	3:B:627:PHE:O	1.85	0.77
3:B:293:PRO:HG2	3:B:296:GLU:HB3	1.66	0.77
2:A:877:HIS:C	2:A:878:ILE:HG13	2.03	0.77
3:B:654:ARG:H	3:B:657:HIS:HD2	1.29	0.77
2:A:913:LEU:HD12	2:A:914:GLU:N	1.98	0.77
2:A:56:PRO:HD2	2:A:58:LEU:HG	1.67	0.77
3:B:1172:ILE:N	3:B:1172:ILE:HD12	2.00	0.77
10:I:34:TYR:HD2	10:I:35:VAL:H	1.32	0.77
2:A:146:MET:HA	2:A:171:GLN:HB2	1.65	0.77
2:A:709:THR:HG23	10:I:94:ASP:HA	1.66	0.77
3:B:37:PHE:CD1	3:B:41:LYS:HG3	2.19	0.77
5:D:35:LEU:H	5:D:35:LEU:HD12	1.50	0.77
8:G:122:ASN:ND2	8:G:125:SER:HB3	1.99	0.77
2:A:567:LYS:NZ	9:H:46:LEU:HB2	1.98	0.77
2:A:442:VAL:HB	2:A:489:LEU:HD11	1.67	0.77
3:B:211:VAL:O	3:B:480:SER:HA	1.83	0.77
3:B:472:ALA:C	3:B:474:SER:H	1.87	0.77
3:B:1017:ILE:HB	3:B:1018:PRO:HD3	1.66	0.76
3:B:37:PHE:CE1	3:B:41:LYS:HG3	2.20	0.76
3:B:582:VAL:HG23	3:B:626:ILE:HB	1.65	0.76
2:A:577:ILE:O	2:A:580:VAL:HG23	1.85	0.76
9:H:4:THR:HA	9:H:60:ALA:HB2	1.67	0.76
2:A:1428:VAL:HG13	3:B:1151:LEU:CD2	2.16	0.76
2:A:84:ILE:HG22	2:A:239:LEU:HB3	1.67	0.76
11:J:16:ASP:OD1	11:J:17:LYS:HD2	1.86	0.76
2:A:41:MET:HB3	2:A:49:LYS:HA	1.66	0.76
3:B:955:THR:HG22	3:B:956:THR:N	2.01	0.76
9:H:36:CYS:HA	9:H:126:GLU:O	1.84	0.76
2:A:828:ALA:HB1	3:B:530:GLY:HA2	1.67	0.76
3:B:505:ASP:CG	3:B:506:GLY:N	2.39	0.76
2:A:230:ARG:H	2:A:233:TRP:HE3	1.33	0.76
2:A:24:PRO:HD2	2:A:233:TRP:HE1	1.51	0.76
2:A:438:ASP:O	2:A:439:ASN:HB2	1.86	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1162:ILE:HG22	3:B:1163:CYS:H	1.50	0.76
6:E:116:ILE:HG22	6:E:117:THR:N	2.01	0.76
9:H:23:VAL:HG13	9:H:42:ILE:O	1.85	0.76
2:A:250:ILE:O	2:A:258:GLY:HA3	1.85	0.76
3:B:510:LYS:N	3:B:510:LYS:HD2	1.98	0.76
3:B:205:ILE:N	3:B:205:ILE:HD12	2.00	0.76
2:A:541:ILE:HG21	2:A:549:MET:HE3	1.66	0.75
11:J:3:VAL:HG21	11:J:18:TRP:CB	2.17	0.75
3:B:273:LEU:HD23	3:B:273:LEU:O	1.85	0.75
6:E:22:MET:HE3	6:E:26:ARG:HE	1.49	0.75
2:A:1206:ASP:HB3	2:A:1274:ARG:HH12	1.51	0.75
3:B:996:ARG:HH22	4:C:175:ALA:H	1.33	0.75
3:B:463:THR:HB	3:B:465:ASN:CB	2.15	0.75
3:B:841:MET:HG2	3:B:846:ILE:HD11	1.67	0.75
6:E:19:VAL:O	6:E:23:VAL:HG23	1.86	0.75
2:A:382:PRO:HB3	2:A:428:TYR:HE2	1.51	0.75
11:J:57:ILE:HA	11:J:60:PHE:HD2	1.51	0.75
2:A:1345:ARG:HG2	2:A:1372:VAL:HG13	1.66	0.75
2:A:1063:MET:SD	2:A:1436:ILE:HG13	2.26	0.75
2:A:1370:LEU:O	2:A:1374:VAL:HG23	1.87	0.75
3:B:1182:CYS:SG	3:B:1182:CYS:O	2.45	0.75
2:A:438:ASP:OD1	2:A:462:VAL:HG23	1.86	0.75
3:B:983:ARG:HD2	3:B:1091:TYR:HB3	1.69	0.75
2:A:1444:MET:HG2	8:G:60:ARG:HA	1.69	0.74
2:A:374:LEU:HB3	2:A:436:ILE:HD11	1.69	0.74
2:A:1313:LEU:O	2:A:1315:GLU:N	2.20	0.74
1:R:11:U:H4'	1:R:12:5BU:OP2	1.85	0.74
4:C:32:SER:O	4:C:36:VAL:HG23	1.88	0.74
3:B:580:VAL:HG13	3:B:624:LEU:HB3	1.69	0.74
2:A:339:ASN:HB3	3:B:1117:GLN:HE22	1.51	0.74
4:C:248:ILE:HD12	12:K:101:LEU:HD22	1.69	0.74
4:C:147:LEU:HB2	4:C:151:GLN:HB2	1.68	0.74
3:B:711:GLU:H	3:B:712:PRO:HD2	1.50	0.74
10:I:55:THR:HG22	10:I:58:VAL:HG21	1.69	0.74
9:H:61:SER:O	9:H:62:SER:HB3	1.88	0.74
5:D:63:LEU:HD12	5:D:129:LEU:HG	1.68	0.74
3:B:125:SER:HA	3:B:171:PRO:HA	1.68	0.74
2:A:1107:VAL:HG12	2:A:1107:VAL:O	1.87	0.74
1:R:15:G:OP1	3:B:474:SER:HB3	1.86	0.74
3:B:1096:ARG:O	3:B:1097:HIS:HB2	1.86	0.74
3:B:882:THR:HG22	3:B:884:ARG:N	1.98	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:50:ILE:O	2:A:52:GLY:N	2.19	0.74
2:A:666:ILE:HD12	2:A:667:GLY:H	1.53	0.74
3:B:284:ILE:N	3:B:284:ILE:HD12	2.03	0.74
2:A:93:VAL:HG13	2:A:301:ALA:HB1	1.69	0.74
2:A:1261:LYS:O	2:A:1264:GLU:HB3	1.88	0.74
2:A:14:VAL:H	2:A:1432:GLN:HE22	1.36	0.73
6:E:153:HIS:HB3	6:E:196:VAL:CG1	2.18	0.73
2:A:21:LEU:HD21	2:A:1414:ALA:HA	1.70	0.73
8:G:138:THR:HG22	8:G:139:ILE:N	2.00	0.73
2:A:1057:VAL:HG12	2:A:1058:VAL:N	2.04	0.73
5:D:7:THR:O	5:D:9:GLN:N	2.22	0.73
12:K:56:VAL:HA	12:K:77:THR:HG22	1.68	0.73
8:G:13:LEU:CD2	8:G:17:PHE:HB2	2.18	0.73
2:A:1372:VAL:HG12	2:A:1373:ASP:N	2.03	0.73
2:A:853:ASP:OD1	2:A:855:THR:HB	1.88	0.73
2:A:743:VAL:O	2:A:747:VAL:HG23	1.87	0.73
3:B:834:ASN:HB3	3:B:840:ILE:HG13	1.71	0.73
3:B:978:ASP:OD2	3:B:1098:MET:HG2	1.88	0.73
3:B:1099:VAL:O	3:B:1101:ASP:N	2.21	0.73
6:E:124:VAL:HG13	6:E:132:ILE:HD13	1.70	0.73
11:J:57:ILE:HA	11:J:60:PHE:CD2	2.23	0.73
10:I:111:THR:HG22	10:I:113:ASP:N	2.03	0.73
2:A:567:LYS:CD	2:A:568:PRO:HD2	2.19	0.73
5:D:47:LEU:HD13	5:D:48:ILE:H	1.54	0.73
2:A:1325:THR:HG23	6:E:146:HIS:O	1.88	0.73
4:C:116:LYS:HD3	4:C:140:ASN:HB3	1.70	0.73
3:B:1065:GLN:HE21	3:B:1067:ARG:H	1.37	0.73
2:A:55:ASP:C	2:A:57:ARG:H	1.90	0.73
3:B:952:VAL:HG12	3:B:953:LEU:H	1.54	0.72
8:G:56:ILE:HD12	8:G:56:ILE:N	2.04	0.72
2:A:524:VAL:HG12	2:A:525:GLN:N	2.02	0.72
2:A:710:LEU:H	2:A:710:LEU:HD12	1.53	0.72
3:B:215:GLN:HE22	3:B:499:ASN:HD22	1.36	0.72
3:B:862:GLN:HG2	3:B:963:PHE:HD1	1.54	0.72
4:C:77:ILE:HG12	4:C:161:LYS:HE3	1.71	0.72
3:B:516:ASN:H	3:B:516:ASN:HD22	1.35	0.72
3:B:1007:VAL:HG22	3:B:1008:PRO:CD	2.19	0.72
3:B:509:ALA:O	3:B:511:PRO:CD	2.36	0.72
3:B:1072:MET:HE1	3:B:1085:ILE:HB	1.70	0.72
3:B:616:ILE:N	3:B:616:ILE:HD12	2.04	0.72
4:C:148:ARG:HG2	4:C:149:LYS:H	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:341:MET:HE1	2:A:843:LYS:HZ3	1.54	0.72
12:K:58:PHE:HE2	12:K:74:ARG:HE	1.32	0.72
3:B:622:LYS:HE2	10:I:59:VAL:HG22	1.71	0.72
2:A:1116:LEU:N	2:A:1308:THR:HG22	2.04	0.72
2:A:1444:MET:HE1	7:F:135:ARG:HB2	1.72	0.72
4:C:37:MET:HA	4:C:41:ILE:HD11	1.70	0.72
2:A:70:CYS:O	2:A:72:GLU:HG2	1.90	0.72
2:A:1102:LYS:HG2	2:A:1106:ASN:ND2	2.04	0.72
3:B:1224:PHE:HE2	6:E:171:LYS:HG3	1.55	0.72
2:A:567:LYS:HB3	9:H:96:VAL:H	1.55	0.72
2:A:875:ALA:HA	2:A:878:ILE:HD12	1.72	0.72
6:E:135:PHE:HD2	6:E:140:LEU:HD21	1.52	0.72
2:A:886:ILE:HG22	2:A:887:GLY:N	2.04	0.72
4:C:77:ILE:HA	4:C:129:ILE:HD11	1.71	0.72
9:H:93:TYR:HB3	9:H:144:ILE:O	1.90	0.72
4:C:194:GLU:O	4:C:195:GLN:HG3	1.90	0.72
8:G:143:ILE:CG2	8:G:144:ARG:N	2.53	0.71
5:D:33:PHE:CZ	8:G:80:LYS:NZ	2.59	0.71
4:C:166:GLU:HG3	12:K:10:PHE:HZ	1.55	0.71
13:L:53:HIS:HB3	13:L:55:ILE:HD11	1.71	0.71
2:A:1283:VAL:HG12	2:A:1284:MET:H	1.55	0.71
8:G:1:MET:HE3	8:G:80:LYS:N	2.03	0.71
2:A:23:SER:HA	2:A:233:TRP:NE1	2.05	0.71
2:A:269:ILE:HG12	2:A:299:HIS:HB3	1.72	0.71
1:R:7:C:H3'	1:R:8:U:H5"	1.71	0.71
3:B:1051:THR:HG22	3:B:1052:VAL:N	2.05	0.71
4:C:92:CYS:SG	4:C:94:LYS:HB3	2.29	0.71
3:B:827:ILE:HG12	3:B:1012:ILE:CD1	2.10	0.71
2:A:886:ILE:HD11	2:A:943:LEU:HB3	1.72	0.71
2:A:1329:THR:H	2:A:1335:ILE:HD11	1.55	0.71
3:B:1002:THR:HG21	3:B:1006:ILE:HD12	1.72	0.71
3:B:291:ILE:HD12	3:B:291:ILE:N	2.04	0.71
2:A:93:VAL:HG22	2:A:301:ALA:HA	1.71	0.71
3:B:806:THR:HB	3:B:809:MET:HG3	1.71	0.71
3:B:999:MET:HE3	3:B:999:MET:HA	1.73	0.71
3:B:977:GLY:HA3	3:B:1099:VAL:HG21	1.73	0.71
2:A:1155:ASP:OD2	2:A:1161:THR:HG23	1.90	0.71
4:C:114:TYR:HB3	4:C:140:ASN:O	1.90	0.71
2:A:984:LYS:HB3	2:A:988:LEU:HD12	1.73	0.71
2:A:763:ALA:O	2:A:803:SER:HB3	1.91	0.71
3:B:357:GLN:HA	3:B:374:LYS:NZ	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:195:ILE:O	5:D:195:ILE:HG22	1.91	0.70
9:H:100:THR:OG1	9:H:138:GLU:HG3	1.91	0.70
2:A:225:ASN:HD22	2:A:228:PHE:N	1.82	0.70
3:B:865:LYS:HE2	3:B:871:THR:OG1	1.91	0.70
2:A:35:ILE:HA	2:A:52:GLY:O	1.90	0.70
2:A:1161:THR:HG22	2:A:1163:ILE:N	2.04	0.70
6:E:22:MET:HE3	6:E:26:ARG:NE	2.06	0.70
3:B:859:TYR:OH	3:B:941:LEU:HD12	1.91	0.70
3:B:745:PRO:O	3:B:748:ILE:HG12	1.91	0.70
2:A:768:GLN:CG	2:A:816:HIS:HA	2.21	0.70
2:A:541:ILE:HG21	2:A:549:MET:CE	2.21	0.70
3:B:95:ILE:HG12	3:B:130:VAL:HG22	1.72	0.70
2:A:302:THR:HA	2:A:305:ASP:O	1.90	0.70
4:C:31:ASN:OD1	4:C:34:ARG:HD3	1.92	0.70
8:G:1:MET:SD	8:G:79:PHE:CD1	2.85	0.70
2:A:858:ASN:HD22	2:A:858:ASN:C	1.95	0.70
5:D:59:ILE:O	5:D:63:LEU:HB2	1.91	0.70
4:C:212:PRO:HB3	4:C:213:PRO:HD2	1.74	0.70
2:A:537:ARG:HD2	9:H:20:TYR:CE1	2.26	0.70
8:G:119:LEU:HD12	8:G:131:GLN:O	1.90	0.70
2:A:63:ARG:HA	2:A:74:MET:SD	2.31	0.70
6:E:213:ILE:HG12	6:E:214:CYS:H	1.57	0.70
2:A:134:ARG:HG2	2:A:134:ARG:O	1.90	0.70
3:B:274:PRO:O	3:B:275:TYR:HB2	1.91	0.70
3:B:468:GLU:N	3:B:468:GLU:CD	2.45	0.69
2:A:537:ARG:HD2	9:H:20:TYR:HE1	1.57	0.69
1:R:3:A:H2	1:R:15:G:H21	1.37	0.69
2:A:600:PRO:HG2	2:A:601:LYS:H	1.56	0.69
4:C:258:ILE:HD13	12:K:35:PHE:HE2	1.57	0.69
3:B:1162:ILE:HD11	3:B:1194:ILE:CG1	2.21	0.69
2:A:381:THR:OG1	2:A:382:PRO:HD2	1.91	0.69
2:A:1409:LEU:HD13	3:B:1207:LEU:HD11	1.74	0.69
3:B:782:LEU:HD12	3:B:788:ARG:HH11	1.56	0.69
2:A:306:ASN:HB2	2:A:324:SER:HB3	1.74	0.69
2:A:1279:ILE:HD11	2:A:1316:VAL:HG21	1.73	0.69
3:B:240:ILE:HG22	3:B:254:LEU:HB3	1.73	0.69
3:B:737:THR:HG21	10:I:66:PRO:HA	1.74	0.69
2:A:1116:LEU:H	2:A:1308:THR:HG22	1.57	0.69
10:I:111:THR:HG22	10:I:112:SER:N	2.06	0.69
2:A:164:ARG:HG3	2:A:165:GLY:N	2.07	0.69
2:A:1349:TYR:HB2	2:A:1372:VAL:HG21	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:4:THR:HG22	9:H:5:LEU:H	1.56	0.69
3:B:364:ILE:HG12	3:B:585:VAL:HG13	1.74	0.69
3:B:274:PRO:O	3:B:276:ILE:HD13	1.93	0.69
3:B:980:PHE:CE1	3:B:990:ILE:HD11	2.25	0.69
4:C:124:LEU:O	4:C:127:ARG:HG2	1.93	0.69
10:I:68:LEU:HB3	10:I:84:VAL:HG23	1.74	0.69
2:A:1166:ASP:OD2	2:A:1239:ARG:HD2	1.93	0.69
2:A:90:VAL:HG12	2:A:297:GLN:NE2	2.07	0.69
2:A:68:GLN:C	2:A:70:CYS:H	1.96	0.69
2:A:783:THR:HG21	2:A:815:PHE:CZ	2.28	0.69
3:B:284:ILE:H	3:B:284:ILE:CD1	2.06	0.69
4:C:73:GLN:HB3	4:C:131:HIS:H	1.58	0.69
2:A:567:LYS:HB2	9:H:94:ASP:O	1.93	0.68
3:B:708:GLU:O	3:B:710:LEU:N	2.26	0.68
3:B:847:ASP:HB3	4:C:167:HIS:NE2	2.09	0.68
3:B:1099:VAL:HG13	3:B:1103:ILE:CD1	2.23	0.68
12:K:53:ASP:OD1	12:K:55:LYS:HB2	1.93	0.68
8:G:11:ILE:HG21	8:G:29:LYS:HG2	1.75	0.68
7:F:77:ASP:O	7:F:78:GLN:HB2	1.93	0.68
12:K:12:LEU:HD12	12:K:12:LEU:H	1.58	0.68
6:E:198:ILE:N	6:E:198:ILE:HD12	2.08	0.68
3:B:555:ILE:HD11	3:B:587:HIS:CD2	2.27	0.68
2:A:49:LYS:HZ3	2:A:61:ILE:HG12	1.56	0.68
2:A:61:ILE:HG22	2:A:62:ASP:N	2.03	0.68
9:H:98:TYR:C	9:H:118:PHE:HD2	1.96	0.68
6:E:61:GLN:HB2	6:E:79:TRP:CE3	2.28	0.68
2:A:1441:PHE:CZ	7:F:89:GLU:HA	2.29	0.68
2:A:701:LEU:HD21	10:I:114:GLN:HB2	1.74	0.68
3:B:758:PHE:HB3	3:B:761:HIS:HD2	1.57	0.68
6:E:116:ILE:HG22	6:E:117:THR:H	1.59	0.68
2:A:794:PRO:HG2	2:A:795:GLU:OE2	1.93	0.68
2:A:903:ASN:C	2:A:903:ASN:HD22	1.97	0.68
3:B:378:LEU:O	3:B:382:ILE:HG13	1.93	0.68
2:A:1402:PHE:CE1	2:A:1403:GLU:HG3	2.29	0.68
3:B:797:TYR:CD2	3:B:852:ARG:HB2	2.28	0.68
2:A:1364:ASN:HD22	2:A:1364:ASN:C	1.96	0.68
4:C:43:THR:HG22	4:C:44:LEU:N	2.09	0.68
8:G:74:TYR:HD2	8:G:74:TYR:H	1.39	0.68
2:A:981:LEU:CD2	2:A:1039:LYS:HA	2.24	0.68
3:B:363:HIS:O	3:B:364:ILE:HB	1.94	0.68
2:A:1341:ILE:HD12	2:A:1379:GLY:O	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:244:PRO:O	2:A:246:VAL:N	2.26	0.68
4:C:98:VAL:C	4:C:99:LEU:HD23	2.14	0.68
5:D:144:THR:O	5:D:148:LEU:HB2	1.94	0.68
3:B:1002:THR:HG23	3:B:1006:ILE:HG13	1.76	0.68
2:A:1111:MET:HE2	2:A:1330:ASN:OD1	1.94	0.67
2:A:374:LEU:CB	2:A:436:ILE:HD11	2.24	0.67
9:H:99:GLY:HA3	9:H:118:PHE:HA	1.76	0.67
9:H:81:PRO:CB	9:H:82:PRO:HD2	2.25	0.67
3:B:479:VAL:O	3:B:480:SER:HB3	1.92	0.67
2:A:1148:ILE:HD11	2:A:1198:ASP:HB2	1.76	0.67
2:A:463:ILE:HD13	2:A:469:ARG:HD2	1.77	0.67
2:A:1032:LEU:O	2:A:1036:ARG:HD3	1.93	0.67
8:G:7:LEU:HB2	8:G:74:TYR:CE2	2.29	0.67
3:B:501:PRO:O	3:B:502:ILE:HG13	1.93	0.67
3:B:899:ILE:HD11	3:B:911:ILE:HA	1.76	0.67
3:B:1099:VAL:HG12	3:B:1100:ASP:N	2.07	0.67
12:K:65:HIS:HD2	12:K:67:PHE:H	1.43	0.67
3:B:483:LEU:HD12	3:B:484:ASN:N	2.10	0.67
4:C:148:ARG:CG	4:C:149:LYS:H	2.05	0.67
5:D:192:LYS:NZ	5:D:199:ASN:HA	2.10	0.67
3:B:217:ARG:HE	3:B:405:ARG:HB2	1.60	0.67
2:A:119:ASN:O	2:A:122:MET:HB3	1.95	0.67
5:D:40:HIS:CB	8:G:73:LYS:HZ3	2.02	0.67
3:B:955:THR:CG2	3:B:956:THR:N	2.58	0.67
2:A:1319:VAL:HG13	2:A:1320:PRO:HD2	1.77	0.67
2:A:147:VAL:N	2:A:171:GLN:NE2	2.42	0.67
6:E:132:ILE:N	6:E:132:ILE:HD12	2.10	0.67
3:B:310:MET:O	3:B:313:MET:HB2	1.95	0.67
2:A:474:VAL:O	2:A:477:PRO:HD2	1.95	0.67
9:H:81:PRO:HB3	9:H:82:PRO:HD2	1.76	0.67
3:B:879:ARG:NH1	3:B:883:LEU:HD22	2.10	0.66
2:A:898:ARG:HB2	2:A:933:TYR:CE1	2.30	0.66
2:A:353:ILE:HG21	2:A:487:MET:HE3	1.76	0.66
3:B:260:GLY:O	3:B:267:ARG:HD3	1.95	0.66
2:A:4:GLN:O	2:A:5:GLN:HB2	1.95	0.66
5:D:153:ARG:NH2	5:D:184:ALA:HA	2.10	0.66
4:C:189:THR:HG22	4:C:190:ASP:N	2.09	0.66
2:A:1114:PRO:HG2	2:A:1115:SER:H	1.60	0.66
2:A:845:LEU:HD22	2:A:1374:VAL:HG21	1.78	0.66
2:A:965:GLN:HA	2:A:968:GLN:HG3	1.78	0.66
13:L:31:CYS:SG	13:L:34:CYS:N	2.66	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:996:ARG:NH2	4:C:175:ALA:H	1.92	0.66
5:D:192:LYS:HZ3	5:D:199:ASN:HA	1.60	0.66
2:A:551:TYR:CE2	12:K:62:LYS:HE2	2.30	0.66
2:A:664:THR:HG22	2:A:665:GLY:N	2.09	0.66
3:B:463:THR:C	3:B:465:ASN:N	2.49	0.66
12:K:12:LEU:HD12	12:K:12:LEU:N	2.10	0.66
3:B:515:HIS:H	3:B:518:HIS:HD2	1.44	0.66
2:A:147:VAL:H	2:A:171:GLN:HE21	1.42	0.66
2:A:84:ILE:O	2:A:84:ILE:HG23	1.96	0.66
3:B:696:GLU:O	3:B:699:GLU:HB2	1.95	0.66
2:A:414:ASP:OD1	2:A:416:ARG:HG2	1.96	0.66
2:A:1149:ALA:HB2	10:I:47:GLU:HA	1.77	0.66
2:A:11:LEU:O	2:A:11:LEU:HD23	1.96	0.66
3:B:642:ASP:HB3	3:B:649:LYS:HD2	1.78	0.66
2:A:343:LYS:HE2	3:B:1156:ASP:OD2	1.96	0.66
3:B:918:ILE:HG21	3:B:935:ARG:NH1	2.11	0.66
2:A:903:ASN:ND2	2:A:905:ASP:H	1.92	0.66
3:B:483:LEU:HD12	3:B:484:ASN:H	1.61	0.66
3:B:806:THR:HG22	3:B:808:ALA:N	2.10	0.66
2:A:1028:THR:O	2:A:1032:LEU:HD12	1.96	0.66
8:G:132:SER:HB3	8:G:135:ASP:H	1.61	0.66
10:I:8:ARG:HG3	10:I:34:TYR:CE1	2.29	0.66
6:E:61:GLN:HG2	6:E:62:ALA:N	2.10	0.66
12:K:27:ALA:HB1	12:K:28:PRO:HD2	1.77	0.66
2:A:629:LEU:HD23	2:A:629:LEU:O	1.95	0.66
10:I:62:ILE:HG12	10:I:62:ILE:O	1.96	0.66
3:B:468:GLU:H	3:B:468:GLU:CD	2.00	0.65
2:A:590:ARG:NH1	2:A:590:ARG:HG3	2.09	0.65
2:A:1017:LEU:HB3	6:E:205:SER:HA	1.78	0.65
3:B:1152:MET:HE1	3:B:1157:ALA:HA	1.77	0.65
8:G:145:VAL:HG12	8:G:146:LYS:N	2.10	0.65
2:A:474:VAL:C	2:A:477:PRO:HD2	2.17	0.65
3:B:558:LEU:CD2	3:B:596:LEU:HD11	2.27	0.65
5:D:52:LEU:HD21	5:D:147:TYR:HE2	1.61	0.65
9:H:59:ILE:O	9:H:60:ALA:HB3	1.97	0.65
3:B:390:LEU:O	3:B:392:ARG:HG3	1.96	0.65
3:B:496:ARG:HB3	3:B:496:ARG:HH11	1.61	0.65
3:B:830:TYR:CE2	3:B:1000:PRO:HD3	2.32	0.65
2:A:658:LEU:HD13	3:B:831:SER:HA	1.78	0.65
9:H:12:VAL:HA	9:H:28:ALA:HB2	1.79	0.65
8:G:110:VAL:HG13	8:G:161:GLY:O	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:52:ILE:HG13	10:I:52:ILE:O	1.96	0.65
3:B:274:PRO:HD2	3:B:274:PRO:O	1.96	0.65
3:B:821:GLN:NE2	3:B:851:PHE:HA	2.09	0.65
4:C:35:ARG:HH12	12:K:40:HIS:HB2	1.62	0.65
3:B:1166:CYS:SG	3:B:1166:CYS:O	2.53	0.65
2:A:565:ILE:C	2:A:566:ILE:HD13	2.17	0.65
2:A:117:GLU:H	2:A:117:GLU:CD	1.97	0.65
2:A:42:ASP:HA	2:A:46:THR:O	1.94	0.65
2:A:828:ALA:HB2	3:B:530:GLY:HA2	1.78	0.65
6:E:124:VAL:HG13	6:E:132:ILE:HB	1.77	0.65
3:B:94:LYS:HG2	3:B:95:ILE:N	2.11	0.65
4:C:100:THR:HG22	4:C:101:LEU:H	1.60	0.65
5:D:170:THR:HB	5:D:172:LEU:HG	1.77	0.65
2:A:1242:VAL:HG12	2:A:1243:VAL:N	2.10	0.65
5:D:56:ARG:HB2	5:D:148:LEU:HD22	1.78	0.65
11:J:50:ILE:H	11:J:50:ILE:HD12	1.60	0.65
3:B:464:GLY:C	3:B:466:TRP:N	2.49	0.65
3:B:504:ARG:HB3	3:B:507:LYS:HE2	1.78	0.65
2:A:356:ASP:HB2	2:A:469:ARG:HH11	1.61	0.65
3:B:563:MET:HE1	3:B:580:VAL:HB	1.79	0.65
3:B:948:ILE:HG22	3:B:949:VAL:O	1.96	0.65
2:A:344:ARG:HB2	3:B:1118:PRO:HD2	1.77	0.65
5:D:160:VAL:O	5:D:164:ILE:HG13	1.97	0.65
2:A:203:SER:OG	2:A:206:GLU:HB2	1.97	0.65
2:A:783:THR:HG21	2:A:815:PHE:CE2	2.31	0.65
3:B:850:LEU:HD12	3:B:851:PHE:N	2.12	0.65
2:A:114:LEU:HD13	2:A:171:GLN:OE1	1.97	0.65
2:A:547:LEU:HD22	12:K:58:PHE:CE1	2.32	0.65
2:A:1451:VAL:O	2:A:1454:MET:HG2	1.96	0.65
3:B:210:LYS:HE2	3:B:462:ALA:O	1.97	0.64
3:B:555:ILE:C	3:B:557:PHE:H	2.00	0.64
4:C:8:VAL:HG12	4:C:9:LYS:H	1.61	0.64
4:C:177:GLU:HB2	4:C:231:ASN:HB3	1.78	0.64
2:A:901:LEU:H	2:A:926:GLN:HE21	1.45	0.64
3:B:240:ILE:CG2	3:B:254:LEU:HB3	2.27	0.64
3:B:247:GLY:H	3:B:418:LYS:HZ1	1.46	0.64
9:H:15:VAL:HG22	9:H:26:ILE:HD11	1.78	0.64
6:E:55:ARG:HD2	6:E:83:CYS:O	1.97	0.64
2:A:666:ILE:HD11	3:B:1067:ARG:O	1.97	0.64
13:L:30:ILE:HG22	13:L:31:CYS:O	1.97	0.64
3:B:95:ILE:HG12	3:B:130:VAL:CG2	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:92:HIS:O	2:A:94:GLY:N	2.29	0.64
11:J:23:ASN:C	11:J:25:LEU:H	2.00	0.64
4:C:67:LEU:HD11	4:C:155:LEU:CD1	2.28	0.64
2:A:869:GLY:O	2:A:870:GLU:HB2	1.97	0.64
9:H:40:LEU:HD13	9:H:123:MET:HB2	1.78	0.64
2:A:1373:ASP:HA	2:A:1376:THR:HG22	1.78	0.64
2:A:782:ARG:NH2	3:B:699:GLU:O	2.28	0.64
5:D:52:LEU:HD21	5:D:147:TYR:CE2	2.32	0.64
2:A:1015:VAL:HG12	2:A:1019:CYS:SG	2.37	0.64
4:C:5:GLY:O	4:C:7:GLN:HG3	1.98	0.64
1:R:12:5BU:O2'	1:R:13:G:O5'	2.07	0.64
4:C:166:GLU:O	4:C:167:HIS:HB2	1.97	0.64
2:A:979:SER:OG	2:A:980:ASP:N	2.30	0.64
3:B:1162:ILE:HD11	3:B:1194:ILE:HG13	1.80	0.64
11:J:50:ILE:N	11:J:50:ILE:HD12	2.13	0.64
3:B:758:PHE:HB3	3:B:761:HIS:CD2	2.31	0.64
1:R:3:A:C2	1:R:16:G:H1'	2.33	0.64
1:R:15:G:O2'	1:R:16:G:H5'	1.97	0.64
3:B:1001:PHE:CZ	3:B:1073:TYR:HB2	2.32	0.64
8:G:1:MET:HG3	8:G:85:GLU:OE2	1.98	0.64
4:C:189:THR:HG22	4:C:190:ASP:H	1.60	0.64
3:B:644:GLU:HG2	3:B:654:ARG:HH22	1.61	0.64
3:B:1152:MET:HE3	3:B:1157:ALA:HA	1.79	0.64
3:B:411:PRO:O	3:B:414:ALA:HB3	1.96	0.64
9:H:35:GLN:O	9:H:37:LYS:HG3	1.96	0.64
2:A:340:LEU:HD21	3:B:1200:ALA:N	2.12	0.64
5:D:40:HIS:CB	8:G:73:LYS:NZ	2.52	0.64
2:A:55:ASP:CG	2:A:55:ASP:O	2.33	0.64
2:A:809:THR:HG23	2:A:812:GLU:OE1	1.98	0.64
2:A:709:THR:HG22	2:A:711:ARG:H	1.62	0.64
2:A:1072:ILE:O	2:A:1075:PRO:HG2	1.98	0.64
3:B:701:ILE:HD11	3:B:703:ILE:HD11	1.80	0.64
2:A:32:VAL:HG21	2:A:68:GLN:NE2	2.12	0.64
3:B:799:PRO:HB3	3:B:818:PRO:HG2	1.80	0.64
2:A:69:THR:C	2:A:71:GLN:H	2.02	0.63
3:B:504:ARG:CB	3:B:507:LYS:HE2	2.28	0.63
6:E:161:LYS:HD2	6:E:195:VAL:CG2	2.28	0.63
2:A:166:GLY:O	2:A:167:CYS:SG	2.56	0.63
9:H:44:VAL:HG12	9:H:44:VAL:O	1.98	0.63
3:B:770:GLN:OE1	3:B:983:ARG:HA	1.98	0.63
2:A:1120:LEU:HD12	2:A:1120:LEU:N	2.13	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:55:ASP:N	2:A:56:PRO:HD3	2.13	0.63
3:B:918:ILE:CB	3:B:935:ARG:HD2	2.27	0.63
4:C:148:ARG:H	4:C:151:GLN:HG3	1.63	0.63
2:A:881:GLN:NE2	2:A:959:ASN:HA	2.13	0.63
5:D:130:LEU:C	5:D:132:GLN:H	2.02	0.63
2:A:829:VAL:C	2:A:831:THR:H	1.99	0.63
11:J:1:MET:N	11:J:56:LEU:N	2.47	0.63
1:R:28:5BU:H2'	1:R:29:G:C8	2.33	0.63
3:B:1085:ILE:HD12	3:B:1085:ILE:N	2.13	0.63
3:B:273:LEU:CD2	3:B:273:LEU:N	2.62	0.63
3:B:999:MET:HG3	3:B:1000:PRO:HD2	1.81	0.63
3:B:446:LEU:O	3:B:447:ALA:HB3	1.99	0.63
2:A:172:PRO:HB3	2:A:185:TRP:CE2	2.33	0.63
4:C:18:VAL:O	4:C:18:VAL:HG12	1.97	0.63
5:D:40:HIS:CE1	5:D:41:GLN:HG3	2.33	0.63
4:C:56:THR:HG22	4:C:57:VAL:N	2.12	0.63
4:C:67:LEU:HA	4:C:70:ILE:HD13	1.81	0.63
3:B:842:ASN:ND2	3:B:845:SER:OG	2.29	0.63
2:A:1438:THR:HB	3:B:1144:ALA:CB	2.26	0.63
3:B:1034:VAL:HG12	3:B:1035:ALA:N	2.14	0.63
2:A:332:LYS:HG2	2:A:333:GLU:HG2	1.80	0.63
3:B:1099:VAL:C	3:B:1101:ASP:H	2.00	0.63
4:C:262:LEU:HD11	12:K:87:LEU:HD23	1.81	0.63
3:B:463:THR:HB	3:B:465:ASN:H	1.64	0.63
3:B:952:VAL:CG1	3:B:953:LEU:N	2.62	0.63
2:A:1004:ASN:O	2:A:1008:GLN:HB2	1.98	0.63
3:B:359:GLU:O	3:B:362:PRO:HD3	1.98	0.63
3:B:821:GLN:HE22	3:B:851:PHE:CA	2.09	0.63
4:C:76:ASP:O	4:C:79:GLN:HG2	1.98	0.63
3:B:1119:VAL:HG23	3:B:1126:GLY:HA2	1.80	0.63
1:R:8:U:H2'	1:R:8:U:O2	1.99	0.62
2:A:1102:LYS:O	2:A:1106:ASN:ND2	2.32	0.62
3:B:282:ILE:N	3:B:282:ILE:HD13	2.14	0.62
12:K:63:VAL:HG23	12:K:63:VAL:O	1.98	0.62
7:F:147:SER:OG	7:F:150:GLU:HG3	1.98	0.62
2:A:821:ARG:HB2	2:A:821:ARG:NH1	2.14	0.62
2:A:842:VAL:HG11	3:B:1136:ASP:OD2	1.98	0.62
2:A:563:PRO:HG3	2:A:572:TRP:CZ2	2.34	0.62
2:A:836:TYR:CE2	2:A:840:ARG:HD2	2.34	0.62
3:B:658:ILE:HG22	3:B:659:ALA:N	2.13	0.62
2:A:567:LYS:HD3	9:H:95:TYR:CD2	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:272:THR:O	3:B:273:LEU:HB3	1.99	0.62
2:A:1325:THR:O	6:E:148:GLU:HB2	1.99	0.62
3:B:65:GLU:HG3	3:B:66:ASP:N	2.10	0.62
3:B:1096:ARG:O	3:B:1097:HIS:CB	2.47	0.62
7:F:76:LYS:O	7:F:79:ARG:HD3	1.98	0.62
7:F:109:VAL:HG21	7:F:124:GLU:HA	1.81	0.62
2:A:63:ARG:HG2	2:A:74:MET:SD	2.40	0.62
4:C:166:GLU:HG3	12:K:10:PHE:CZ	2.34	0.62
3:B:1006:ILE:HD13	11:J:44:TYR:CE2	2.34	0.62
2:A:1272:THR:C	2:A:1273:LEU:HD12	2.19	0.62
5:D:185:CYS:HB3	5:D:211:LEU:HD22	1.81	0.62
2:A:856:THR:HB	2:A:865:GLN:HB2	1.82	0.62
7:F:89:GLU:OE2	7:F:134:ILE:HG21	1.99	0.62
5:D:66:ARG:O	5:D:70:PHE:HB2	2.00	0.62
2:A:1313:LEU:HD23	2:A:1338:VAL:HG21	1.81	0.62
9:H:17:PRO:HB3	9:H:24:CYS:SG	2.38	0.62
2:A:401:GLY:C	2:A:435:HIS:HD2	2.03	0.62
3:B:95:ILE:HD13	3:B:96:TYR:N	2.15	0.62
5:D:189:ASP:O	5:D:193:THR:HB	2.00	0.62
2:A:1127:ASP:O	2:A:1130:GLN:HB3	1.99	0.62
3:B:200:GLY:HA2	3:B:202:TYR:CE2	2.35	0.62
2:A:1454:MET:O	2:A:1454:MET:HG3	1.99	0.62
2:A:79:GLY:HA3	2:A:243:PRO:HG3	1.82	0.62
2:A:506:ALA:HB3	2:A:509:LEU:HD12	1.82	0.62
2:A:82:GLY:O	2:A:241:VAL:N	2.26	0.62
6:E:163:GLU:O	6:E:166:LYS:N	2.33	0.62
2:A:1206:ASP:CB	2:A:1274:ARG:HH12	2.11	0.62
2:A:335:ARG:HA	2:A:339:ASN:HD22	1.65	0.62
2:A:295:LEU:O	2:A:298:PHE:HB3	2.00	0.62
2:A:225:ASN:ND2	2:A:227:VAL:H	1.98	0.62
2:A:254:GLU:HB2	3:B:935:ARG:HH22	1.65	0.62
5:D:33:PHE:CE1	8:G:80:LYS:HD2	2.35	0.62
9:H:143:LEU:C	9:H:144:ILE:HG13	2.20	0.62
9:H:84:ALA:HB1	9:H:87:ARG:HB2	1.82	0.62
3:B:526:GLU:HG2	3:B:538:ASN:HD22	1.63	0.62
3:B:27:ALA:O	3:B:29:ASP:N	2.33	0.62
7:F:111:LEU:C	7:F:113:GLY:H	2.03	0.62
5:D:156:ASP:C	5:D:158:GLU:H	2.02	0.62
3:B:1160:VAL:HG11	3:B:1169:MET:SD	2.40	0.61
2:A:129:LYS:O	2:A:130:ASP:HB2	1.99	0.61
3:B:653:VAL:CG2	3:B:689:LEU:HB3	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:446:ARG:HB2	2:A:487:MET:SD	2.40	0.61
6:E:17:ARG:O	6:E:21:GLU:HG3	1.99	0.61
3:B:521:LEU:HB3	3:B:633:VAL:HG11	1.82	0.61
6:E:15:ALA:O	6:E:19:VAL:HG23	2.00	0.61
3:B:1224:PHE:CE2	6:E:171:LYS:HG3	2.34	0.61
3:B:906:SER:HA	3:B:946:ASN:HB2	1.81	0.61
2:A:1130:GLN:NE2	2:A:1134:ILE:HD11	2.15	0.61
13:L:46:VAL:HG12	13:L:46:VAL:O	2.00	0.61
3:B:556:THR:O	3:B:556:THR:HG22	2.00	0.61
3:B:778:MET:HE1	3:B:1094:ARG:HD3	1.81	0.61
13:L:30:ILE:O	13:L:56:LEU:HA	2.00	0.61
3:B:637:LEU:HD12	3:B:693:ILE:HD12	1.82	0.61
3:B:1095:LEU:HD12	3:B:1095:LEU:H	1.65	0.61
2:A:573:SER:O	2:A:576:GLN:HB2	2.00	0.61
3:B:984:HIS:CD2	3:B:1025:HIS:HB2	2.35	0.61
3:B:53:GLN:HG2	3:B:547:VAL:HG22	1.83	0.61
2:A:244:PRO:HB2	2:A:245:PRO:HD3	1.83	0.61
2:A:535:THR:HG21	2:A:617:VAL:H	1.65	0.61
2:A:709:THR:CG2	10:I:94:ASP:HA	2.30	0.61
13:L:39:SER:O	13:L:40:LEU:HG	2.00	0.61
3:B:465:ASN:O	3:B:466:TRP:C	2.38	0.61
9:H:89:LEU:HB3	9:H:91:ASP:OD1	1.99	0.61
1:R:2:C:C2'	1:R:3:A:OP1	2.49	0.61
3:B:240:ILE:HG23	3:B:240:ILE:O	2.00	0.61
3:B:272:THR:C	3:B:273:LEU:HD13	2.21	0.61
8:G:80:LYS:HG2	8:G:80:LYS:O	2.01	0.61
9:H:89:LEU:C	9:H:91:ASP:H	2.02	0.61
2:A:1435:PRO:HA	2:A:1439:GLY:O	2.01	0.61
3:B:1183:LYS:HA	3:B:1186:ASP:HA	1.82	0.61
5:D:195:ILE:HG22	5:D:198:LEU:HG	1.81	0.61
3:B:408:LEU:C	3:B:412:LEU:HD12	2.21	0.61
3:B:168:GLY:H	3:B:450:ALA:HB1	1.66	0.61
3:B:51:PHE:CD2	3:B:173:MET:HB3	2.36	0.61
3:B:640:VAL:HG12	3:B:640:VAL:O	1.99	0.61
2:A:147:VAL:H	2:A:171:GLN:NE2	1.97	0.61
2:A:567:LYS:CG	2:A:568:PRO:CD	2.77	0.61
4:C:31:ASN:O	4:C:34:ARG:N	2.34	0.61
5:D:48:ILE:N	5:D:48:ILE:HD12	2.16	0.61
2:A:384:ASN:CG	2:A:388:LEU:HD12	2.20	0.61
3:B:862:GLN:HG2	3:B:963:PHE:CD1	2.36	0.61
3:B:1051:THR:HG22	3:B:1052:VAL:H	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1004:ASN:ND2	6:E:167:ARG:HD2	2.15	0.61
5:D:138:ASN:OD1	5:D:141:LEU:HB2	2.00	0.61
7:F:81:THR:HB	7:F:136:ARG:NH1	2.16	0.61
4:C:56:THR:HG22	4:C:57:VAL:H	1.64	0.61
2:A:463:ILE:HB	2:A:464:PRO:HD2	1.83	0.61
3:B:293:PRO:HG2	3:B:296:GLU:CB	2.30	0.61
2:A:341:MET:HE1	2:A:843:LYS:NZ	2.15	0.61
3:B:1045:SER:O	3:B:1046:PRO:O	2.19	0.61
12:K:46:ILE:O	12:K:50:LEU:HB2	2.00	0.61
2:A:1447:GLU:OE2	8:G:23:LYS:HB2	2.00	0.61
2:A:925:LEU:O	2:A:927:VAL:N	2.34	0.61
9:H:59:ILE:CG2	9:H:60:ALA:N	2.46	0.60
4:C:66:ARG:NH2	11:J:3:VAL:O	2.34	0.60
2:A:33:ALA:HB1	2:A:56:PRO:HB2	1.82	0.60
2:A:224:PHE:CE2	2:A:231:PRO:HG3	2.36	0.60
3:B:1162:ILE:HG22	3:B:1163:CYS:N	2.16	0.60
2:A:1124:HIS:HB3	2:A:1130:GLN:HG2	1.83	0.60
2:A:427:GLN:HB2	2:A:430:TRP:CD2	2.36	0.60
9:H:100:THR:HG23	9:H:138:GLU:CA	2.21	0.60
8:G:1:MET:SD	8:G:2:PHE:N	2.74	0.60
2:A:321:PRO:O	2:A:322:VAL:HB	2.00	0.60
9:H:40:LEU:CD1	9:H:123:MET:HB2	2.31	0.60
2:A:825:ILE:C	2:A:827:THR:H	2.03	0.60
3:B:825:VAL:CG1	3:B:826:ALA:N	2.63	0.60
4:C:17:ASN:ND2	4:C:17:ASN:N	2.43	0.60
2:A:340:LEU:HD13	2:A:1429:ILE:HG23	1.84	0.60
2:A:1389:PHE:CD1	2:A:1389:PHE:C	2.74	0.60
8:G:138:THR:CG2	8:G:139:ILE:H	2.07	0.60
10:I:26:LEU:CD2	10:I:37:GLU:HA	2.31	0.60
2:A:914:GLU:HB2	2:A:979:SER:O	2.01	0.60
6:E:61:GLN:HB2	6:E:79:TRP:HE3	1.66	0.60
3:B:642:ASP:HB3	3:B:649:LYS:CD	2.31	0.60
3:B:710:LEU:HA	3:B:733:HIS:HB3	1.82	0.60
2:A:464:PRO:HG2	2:A:465:TYR:HD1	1.65	0.60
9:H:38:LEU:HD12	9:H:124:ARG:O	2.00	0.60
2:A:388:LEU:HA	2:A:391:LEU:HD12	1.82	0.60
3:B:557:PHE:CD2	3:B:557:PHE:C	2.75	0.60
3:B:521:LEU:HD13	3:B:633:VAL:HB	1.84	0.60
2:A:148:CYS:HB3	2:A:168:GLY:HA2	1.83	0.60
3:B:33:VAL:HG21	3:B:638:PHE:HZ	1.67	0.60
8:G:91:VAL:HG12	8:G:92:VAL:N	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:387:LEU:H	3:B:387:LEU:HD12	1.66	0.60
3:B:472:ALA:C	3:B:474:SER:N	2.55	0.60
1:R:16:G:C4	1:R:17:5BU:BR	3.10	0.60
2:A:61:ILE:CG2	2:A:62:ASP:H	2.01	0.60
3:B:501:PRO:C	3:B:502:ILE:HG13	2.21	0.60
3:B:865:LYS:HZ2	3:B:869:SER:HA	1.66	0.60
6:E:182:ASP:O	6:E:185:ALA:N	2.35	0.60
3:B:515:HIS:HD2	3:B:517:THR:H	1.50	0.60
2:A:896:ARG:HD3	2:A:897:TYR:CE1	2.37	0.60
10:I:7:CYS:HB3	10:I:14:LEU:HD21	1.84	0.60
2:A:1094:VAL:HG13	2:A:1113:THR:CG2	2.30	0.59
6:E:161:LYS:HD2	6:E:195:VAL:HG23	1.84	0.59
4:C:161:LYS:O	4:C:170:TRP:NE1	2.35	0.59
6:E:178:ILE:HG22	6:E:213:ILE:O	2.02	0.59
2:A:1120:LEU:CD1	2:A:1120:LEU:H	2.14	0.59
10:I:101:PHE:N	10:I:101:PHE:CD1	2.70	0.59
3:B:466:TRP:C	3:B:468:GLU:H	2.04	0.59
8:G:15:PRO:HA	8:G:18:PHE:CD1	2.38	0.59
3:B:1130:PHE:CE1	3:B:1150:ARG:HG3	2.37	0.59
3:B:1162:ILE:HD11	3:B:1194:ILE:HG12	1.83	0.59
4:C:147:LEU:HD23	4:C:147:LEU:N	2.17	0.59
3:B:527:THR:OG1	3:B:528:PRO:HD2	2.02	0.59
2:A:720:ARG:O	2:A:724:GLU:HB2	2.02	0.59
8:G:87:VAL:HG21	8:G:103:VAL:HG11	1.85	0.59
2:A:734:GLU:O	2:A:734:GLU:HG2	2.02	0.59
3:B:882:THR:CG2	3:B:884:ARG:HB2	2.32	0.59
2:A:41:MET:O	2:A:50:ILE:HG13	2.01	0.59
3:B:589:VAL:CG1	3:B:590:HIS:H	2.12	0.59
2:A:475:THR:HG23	2:A:476:SER:N	2.17	0.59
2:A:534:LEU:O	2:A:574:GLY:HA3	2.02	0.59
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.83	0.59
4:C:73:GLN:HE21	4:C:75:MET:H	1.48	0.59
2:A:965:GLN:O	2:A:968:GLN:HB2	2.02	0.59
2:A:92:HIS:HB2	2:A:236:LEU:HD21	1.83	0.59
2:A:252:PHE:O	2:A:253:ASN:HB2	2.03	0.59
11:J:1:MET:H2	11:J:56:LEU:N	1.98	0.59
3:B:952:VAL:CG1	3:B:953:LEU:H	2.15	0.59
2:A:808:LEU:HD23	2:A:812:GLU:C	2.22	0.59
2:A:24:PRO:HD2	2:A:233:TRP:NE1	2.16	0.59
2:A:1209:MET:SD	2:A:1236:LEU:HD22	2.42	0.59
3:B:213:ILE:HD11	3:B:481:GLN:OE1	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:567:LYS:HB3	9:H:95:TYR:HA	1.83	0.59
3:B:1002:THR:HG21	3:B:1006:ILE:CD1	2.31	0.59
3:B:350:GLN:O	3:B:352:ALA:N	2.35	0.59
2:A:317:LYS:O	2:A:318:SER:HB3	2.02	0.59
2:A:84:ILE:HD11	2:A:270:LEU:HD13	1.84	0.59
4:C:133:ILE:CD1	4:C:237:SER:HA	2.32	0.59
11:J:41:LEU:HD13	11:J:50:ILE:HD13	1.83	0.59
3:B:288:ALA:HB2	3:B:330:ALA:HB1	1.83	0.59
8:G:143:ILE:N	8:G:143:ILE:HD12	2.18	0.59
3:B:999:MET:HE2	3:B:1000:PRO:HD2	1.83	0.59
4:C:186:LEU:HD12	4:C:186:LEU:N	2.17	0.59
2:A:388:LEU:O	2:A:392:VAL:HG23	2.02	0.59
2:A:341:MET:HE1	3:B:1135:ARG:NH1	2.18	0.59
4:C:8:VAL:HG12	4:C:9:LYS:N	2.17	0.59
3:B:282:ILE:CD1	3:B:282:ILE:N	2.66	0.59
3:B:521:LEU:HD22	3:B:633:VAL:HG12	1.84	0.59
6:E:157:SER:OG	6:E:160:GLU:HG3	2.02	0.59
3:B:113:TYR:HB3	3:B:114:PRO:HD2	1.85	0.59
2:A:590:ARG:HH11	2:A:590:ARG:HG3	1.67	0.59
10:I:111:THR:CG2	10:I:112:SER:N	2.65	0.59
2:A:666:ILE:CD1	2:A:667:GLY:H	2.16	0.59
9:H:127:GLY:O	9:H:128:ASN:HB2	2.03	0.59
6:E:16:PHE:CE2	6:E:20:LYS:HE2	2.37	0.59
4:C:148:ARG:HG2	4:C:149:LYS:N	2.17	0.59
2:A:30:ILE:HG23	3:B:1170:THR:CG2	2.33	0.59
8:G:15:PRO:HA	8:G:18:PHE:CE1	2.38	0.59
8:G:139:ILE:HG22	8:G:140:LYS:N	2.17	0.59
3:B:276:ILE:O	3:B:276:ILE:HG23	2.02	0.59
2:A:1364:ASN:ND2	2:A:1364:ASN:C	2.56	0.59
2:A:650:GLN:O	2:A:654:ASN:HB2	2.03	0.59
10:I:50:THR:CG2	10:I:52:ILE:HG12	2.33	0.59
3:B:314:LEU:O	3:B:317:CYS:HB3	2.03	0.59
3:B:606:LYS:HD2	3:B:608:ASP:OD2	2.03	0.59
2:A:1332:PHE:H	2:A:1332:PHE:HD2	1.51	0.59
3:B:505:ASP:O	3:B:507:LYS:N	2.35	0.59
2:A:1115:SER:HA	2:A:1308:THR:HG23	1.84	0.59
3:B:579:ARG:HG2	3:B:579:ARG:HH11	1.67	0.59
4:C:22:LEU:HD21	12:K:101:LEU:HD11	1.85	0.59
3:B:1002:THR:CG2	3:B:1006:ILE:HG13	2.32	0.59
3:B:797:TYR:HD2	3:B:852:ARG:HB2	1.66	0.59
2:A:1208:THR:HG22	2:A:1210:GLY:H	1.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:880:THR:O	3:B:881:ASN:HB2	2.02	0.59
10:I:82:GLU:HB3	10:I:104:LEU:HD12	1.85	0.59
3:B:1069:PHE:HD1	3:B:1069:PHE:H	1.51	0.59
2:A:504:LEU:HD12	2:A:504:LEU:N	2.18	0.59
2:A:1212:VAL:O	2:A:1216:ILE:HG13	2.03	0.58
2:A:154:SER:HB3	2:A:162:VAL:HG21	1.84	0.58
3:B:39:ARG:NH2	3:B:665:GLU:HG2	2.18	0.58
4:C:226:ASP:O	4:C:227:THR:HB	2.03	0.58
2:A:1144:LYS:HB2	2:A:1268:LEU:O	2.03	0.58
2:A:858:ASN:HD21	2:A:860:LEU:H	1.46	0.58
1:R:29:G:C4'	2:A:1386:ARG:HH12	2.15	0.58
1:R:19:G:H1	1:R:28:5BU:H3	1.51	0.58
9:H:107:VAL:HG21	9:H:126:GLU:OE2	2.03	0.58
2:A:471:ASN:O	2:A:474:VAL:HG12	2.02	0.58
2:A:219:PHE:O	2:A:222:LEU:O	2.19	0.58
4:C:208:GLU:O	4:C:210:GLU:N	2.36	0.58
2:A:711:ARG:NH1	10:I:95:THR:HB	2.19	0.58
2:A:903:ASN:HD22	2:A:904:THR:N	2.00	0.58
3:B:526:GLU:HG2	3:B:538:ASN:ND2	2.18	0.58
3:B:1023:VAL:O	3:B:1026:LEU:HB2	2.03	0.58
3:B:365:THR:CG2	3:B:367:LEU:H	2.11	0.58
2:A:1102:LYS:CG	2:A:1106:ASN:HD21	2.13	0.58
2:A:1299:VAL:HG12	2:A:1300:LYS:N	2.18	0.58
2:A:1356:ILE:HG22	2:A:1361:SER:HB2	1.84	0.58
1:R:10:A:O2'	1:R:12:5BU:C6	2.51	0.58
8:G:91:VAL:HB	8:G:139:ILE:O	2.03	0.58
2:A:816:HIS:CD2	3:B:764:SER:HB2	2.39	0.58
2:A:351:THR:HB	3:B:1103:ILE:HD12	1.85	0.58
2:A:1198:ASP:O	2:A:1202:MET:HG2	2.03	0.58
2:A:1118:VAL:O	2:A:1305:VAL:HG13	2.03	0.58
2:A:57:ARG:O	2:A:58:LEU:O	2.21	0.58
2:A:567:LYS:HB3	9:H:96:VAL:N	2.18	0.58
2:A:1402:PHE:CD1	2:A:1403:GLU:HG3	2.37	0.58
2:A:22:PHE:CB	3:B:1211:ASN:ND2	2.66	0.58
3:B:1099:VAL:HG13	3:B:1103:ILE:HD13	1.85	0.58
2:A:1224:LEU:HD12	2:A:1241:ARG:O	2.03	0.58
6:E:22:MET:HE1	6:E:26:ARG:NH2	2.19	0.58
2:A:838:GLN:O	2:A:842:VAL:HG23	2.03	0.58
2:A:823:GLY:O	2:A:825:ILE:N	2.37	0.58
10:I:29:CYS:SG	10:I:32:CYS:N	2.64	0.58
3:B:503:GLY:O	3:B:504:ARG:HB2	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1099:VAL:HG13	3:B:1103:ILE:HD11	1.86	0.58
3:B:95:ILE:CG1	3:B:130:VAL:HG22	2.34	0.58
3:B:400:HIS:O	3:B:402:GLY:N	2.37	0.58
11:J:32:GLU:O	11:J:34:THR:N	2.37	0.58
3:B:504:ARG:HB3	3:B:507:LYS:CE	2.33	0.58
2:A:1057:VAL:HG12	2:A:1058:VAL:H	1.68	0.58
9:H:130:ARG:H	9:H:130:ARG:HD2	1.68	0.58
2:A:1372:VAL:CG1	2:A:1373:ASP:N	2.67	0.58
2:A:710:LEU:HD12	2:A:710:LEU:N	2.17	0.58
2:A:135:PHE:C	2:A:137:ALA:H	2.06	0.58
2:A:1206:ASP:O	2:A:1274:ARG:NH1	2.35	0.58
2:A:384:ASN:O	2:A:385:ILE:C	2.41	0.58
4:C:37:MET:HA	4:C:41:ILE:CD1	2.33	0.58
11:J:8:PHE:H	11:J:49:MET:CE	2.17	0.58
3:B:94:LYS:O	3:B:130:VAL:HG13	2.04	0.58
13:L:49:LYS:O	13:L:50:ASP:CB	2.51	0.58
2:A:774:ARG:CZ	2:A:797:LYS:HG3	2.33	0.58
1:R:27:5BU:BR	1:R:28:5BU:BR	3.32	0.58
3:B:955:THR:CG2	3:B:956:THR:H	2.17	0.58
2:A:663:SER:OG	2:A:664:THR:N	2.37	0.58
3:B:866:TYR:O	3:B:868:MET:N	2.37	0.58
2:A:590:ARG:HH11	2:A:590:ARG:CG	2.17	0.57
3:B:254:LEU:HD23	3:B:381:MET:CE	2.33	0.57
3:B:1073:TYR:OH	4:C:179:GLU:HG3	2.04	0.57
2:A:224:PHE:CZ	2:A:231:PRO:HG3	2.39	0.57
2:A:1195:LEU:HD11	2:A:1267:MET:CE	2.34	0.57
3:B:773:MET:SD	3:B:987:LYS:HD3	2.44	0.57
6:E:48:ASP:CG	6:E:49:SER:H	2.06	0.57
5:D:29:LEU:HD22	8:G:82:PHE:CE2	2.39	0.57
2:A:754:SER:H	2:A:757:ASN:HD22	1.52	0.57
10:I:110:PHE:HD2	10:I:110:PHE:H	1.51	0.57
4:C:175:ALA:O	4:C:176:ILE:HG13	2.04	0.57
4:C:6:PRO:HB2	12:K:101:LEU:HD12	1.86	0.57
3:B:309:GLN:OE1	10:I:52:ILE:HD11	2.03	0.57
6:E:165:LEU:HD23	6:E:170:LEU:HB2	1.85	0.57
12:K:47:ARG:CB	12:K:47:ARG:HH11	2.05	0.57
3:B:1065:GLN:NE2	3:B:1066:SER:N	2.53	0.57
2:A:546:VAL:HG13	2:A:577:ILE:HG21	1.86	0.57
7:F:74:ILE:HG23	7:F:75:PRO:HD2	1.86	0.57
10:I:50:THR:HG22	10:I:51:ASN:N	2.19	0.57
3:B:282:ILE:HD13	3:B:283:VAL:H	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:373:ARG:HA	3:B:566:LEU:HD23	1.85	0.57
3:B:210:LYS:HA	3:B:481:GLN:O	2.04	0.57
3:B:504:ARG:HB3	3:B:507:LYS:NZ	2.19	0.57
4:C:43:THR:CG2	4:C:44:LEU:N	2.67	0.57
2:A:1291:VAL:HG13	2:A:1292:PRO:HD2	1.87	0.57
7:F:99:LEU:HD12	7:F:99:LEU:O	2.04	0.57
3:B:466:TRP:C	3:B:468:GLU:N	2.57	0.57
1:R:7:C:N3	3:B:465:ASN:ND2	2.53	0.57
3:B:846:ILE:CG2	3:B:974:PRO:HG2	2.33	0.57
12:K:42:LEU:O	12:K:46:ILE:HG12	2.04	0.57
2:A:858:ASN:ND2	2:A:858:ASN:C	2.58	0.57
3:B:778:MET:CE	3:B:1094:ARG:HD3	2.35	0.57
2:A:1345:ARG:HD2	2:A:1373:ASP:OD1	2.05	0.57
2:A:1378:GLN:O	6:E:177:ARG:HB2	2.04	0.57
7:F:111:LEU:H	7:F:111:LEU:HD12	1.69	0.57
2:A:963:ILE:HD11	2:A:1048:ASN:HB3	1.87	0.57
2:A:89:PRO:HB2	2:A:204:THR:HG22	1.87	0.57
2:A:75:ASN:O	2:A:76:GLU:HB2	2.05	0.57
3:B:274:PRO:CD	3:B:274:PRO:O	2.52	0.57
2:A:868:TYR:CE1	2:A:1064:VAL:CG1	2.83	0.57
9:H:42:ILE:HG23	9:H:95:TYR:CE1	2.29	0.57
3:B:847:ASP:C	3:B:849:GLY:H	2.07	0.57
9:H:123:MET:HE3	9:H:142:LEU:HD22	1.85	0.57
7:F:138:LEU:HB3	7:F:139:PRO:HD2	1.87	0.57
4:C:174:ALA:O	4:C:175:ALA:HB3	2.05	0.57
12:K:58:PHE:HE2	12:K:74:ARG:NE	2.02	0.57
3:B:515:HIS:CD2	3:B:517:THR:H	2.21	0.57
2:A:1094:VAL:CG1	2:A:1113:THR:HG21	2.32	0.57
6:E:163:GLU:O	6:E:164:LEU:C	2.42	0.57
3:B:57:TYR:CD1	3:B:57:TYR:N	2.72	0.57
10:I:16:PRO:HB3	10:I:27:PHE:CE2	2.40	0.57
2:A:1116:LEU:N	2:A:1308:THR:CG2	2.67	0.57
7:F:86:THR:OG1	7:F:89:GLU:HG3	2.05	0.57
2:A:500:GLU:OE2	2:A:1438:THR:HG21	2.05	0.57
3:B:549:THR:H	3:B:628:THR:HG23	1.70	0.57
1:R:7:C:N4	1:R:13:G:H21	2.02	0.57
2:A:645:LEU:O	2:A:646:PHE:C	2.43	0.57
12:K:55:LYS:HB3	12:K:81:TYR:CD1	2.39	0.57
7:F:81:THR:HB	7:F:136:ARG:HH11	1.69	0.57
2:A:1214:GLU:O	2:A:1218:GLN:HG2	2.05	0.57
8:G:53:ASN:HD22	8:G:53:ASN:N	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1385:THR:HG22	2:A:1386:ARG:N	2.20	0.56
3:B:563:MET:CE	3:B:580:VAL:HB	2.34	0.56
2:A:1420:ASP:O	2:A:1421:CYS:HB2	2.05	0.56
6:E:116:ILE:CG2	6:E:117:THR:H	2.18	0.56
6:E:116:ILE:CG2	6:E:117:THR:N	2.67	0.56
4:C:47:ASP:HA	13:L:69:ALA:CB	2.31	0.56
4:C:249:ASP:O	4:C:252:GLN:HB3	2.06	0.56
3:B:408:LEU:O	3:B:411:PRO:HD2	2.04	0.56
3:B:1120:GLU:HG2	3:B:1121:GLY:N	2.19	0.56
2:A:499:ALA:O	2:A:503:GLN:HB2	2.04	0.56
8:G:7:LEU:O	8:G:73:LYS:HD2	2.06	0.56
2:A:1114:PRO:O	2:A:1115:SER:O	2.23	0.56
2:A:369:SER:HB3	12:K:2:ASN:ND2	2.16	0.56
4:C:167:HIS:CD2	4:C:168:ALA:H	2.23	0.56
9:H:126:GLU:C	9:H:130:ARG:NH2	2.57	0.56
5:D:134:THR:HG22	5:D:135:GLY:N	2.18	0.56
2:A:855:THR:HG21	2:A:857:ARG:HE	1.69	0.56
2:A:445:ASN:HB2	2:A:455:MET:HG2	1.88	0.56
2:A:1323:ASP:OD1	2:A:1325:THR:HB	2.04	0.56
2:A:586:ILE:CD1	2:A:633:VAL:HG22	2.34	0.56
2:A:336:ILE:HG22	2:A:337:ARG:N	2.20	0.56
2:A:919:ILE:HG23	2:A:925:LEU:HD12	1.85	0.56
5:D:47:LEU:C	5:D:48:ILE:HD12	2.25	0.56
2:A:498:ARG:O	2:A:501:LEU:N	2.38	0.56
3:B:1115:THR:O	3:B:1116:ARG:HB2	2.05	0.56
2:A:805:LEU:HD11	3:B:1052:VAL:HG21	1.87	0.56
3:B:185:THR:H	3:B:188:ASP:HB2	1.70	0.56
2:A:935:GLN:HE21	2:A:1023:ARG:NH1	2.04	0.56
2:A:67:CYS:O	2:A:68:GLN:HB2	2.05	0.56
3:B:828:ALA:HB2	3:B:1085:ILE:HG23	1.87	0.56
3:B:299:GLU:OE2	3:B:572:HIS:HE1	1.88	0.56
6:E:85:GLU:HB2	6:E:88:VAL:HG22	1.86	0.56
3:B:357:GLN:O	3:B:366:GLN:HA	2.06	0.56
2:A:1425:SER:O	2:A:1426:GLU:C	2.44	0.56
2:A:1450:LEU:O	2:A:1450:LEU:HG	2.05	0.56
2:A:289:ILE:C	2:A:291:GLU:H	2.08	0.56
4:C:184:ASN:ND2	4:C:187:LYS:HA	2.21	0.56
11:J:27:GLU:C	11:J:29:GLU:H	2.09	0.56
2:A:361:LEU:HA	2:A:471:ASN:HD22	1.70	0.56
7:F:103:MET:CE	8:G:66:GLY:H	2.19	0.56
5:D:155:ARG:O	5:D:155:ARG:HG2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:34:VAL:HG11	8:G:74:TYR:HE1	1.71	0.56
2:A:146:MET:CA	2:A:171:GLN:HB2	2.34	0.56
3:B:504:ARG:HB3	3:B:507:LYS:HZ1	1.71	0.56
3:B:569:TYR:CE1	3:B:589:VAL:HG21	2.41	0.56
2:A:384:ASN:OD1	2:A:388:LEU:HD12	2.06	0.56
3:B:777:ALA:HA	3:B:1095:LEU:HA	1.87	0.56
3:B:803:LEU:HD12	3:B:1032:SER:HB3	1.87	0.56
4:C:29:MET:HE1	12:K:98:LEU:HG	1.88	0.56
11:J:1:MET:N	11:J:56:LEU:H	2.03	0.56
2:A:1116:LEU:HD12	2:A:1116:LEU:C	2.25	0.56
2:A:849:MET:CE	2:A:1061:GLY:HA2	2.36	0.56
2:A:547:LEU:HD22	12:K:58:PHE:CD1	2.41	0.56
3:B:758:PHE:CE1	3:B:1027:ILE:HG22	2.41	0.56
5:D:170:THR:CG2	5:D:172:LEU:HG	2.36	0.56
3:B:401:PHE:CE2	3:B:633:VAL:HG21	2.39	0.56
10:I:75:CYS:SG	10:I:103:CYS:SG	3.03	0.56
2:A:567:LYS:NZ	9:H:47:PHE:HB2	2.20	0.56
3:B:1000:PRO:O	3:B:1007:VAL:HG23	2.06	0.56
3:B:284:ILE:HD11	3:B:321:GLY:HA2	1.88	0.56
2:A:1444:MET:O	7:F:133:VAL:N	2.38	0.56
2:A:1120:LEU:HD12	2:A:1120:LEU:H	1.70	0.56
3:B:464:GLY:O	3:B:466:TRP:N	2.39	0.56
2:A:399:HIS:CB	2:A:400:PRO:HD3	2.33	0.56
3:B:1182:CYS:O	3:B:1186:ASP:N	2.39	0.56
4:C:237:SER:C	4:C:238:ILE:HD12	2.25	0.56
3:B:467:GLY:O	3:B:470:LYS:HG3	2.06	0.55
10:I:7:CYS:HB2	10:I:34:TYR:CD1	2.41	0.55
4:C:66:ARG:O	4:C:69:LEU:N	2.39	0.55
8:G:128:PRO:O	8:G:138:THR:HG23	2.05	0.55
3:B:822:ASN:ND2	11:J:52:THR:HG21	2.21	0.55
3:B:254:LEU:HD23	3:B:381:MET:HE3	1.88	0.55
2:A:524:VAL:HG12	2:A:525:GLN:HG2	1.88	0.55
2:A:1334:ASP:O	2:A:1336:MET:N	2.38	0.55
2:A:626:ASN:O	2:A:631:HIS:CD2	2.58	0.55
9:H:22:LYS:O	9:H:23:VAL:HG23	2.05	0.55
4:C:36:VAL:HG21	4:C:251:LEU:HD22	1.88	0.55
2:A:629:LEU:C	2:A:629:LEU:HD23	2.27	0.55
7:F:103:MET:O	7:F:104:ASN:HB2	2.06	0.55
2:A:1094:VAL:HG22	2:A:1113:THR:HG21	1.88	0.55
2:A:855:THR:HG21	2:A:857:ARG:NE	2.22	0.55
3:B:1172:ILE:N	3:B:1172:ILE:CD1	2.68	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:843:LYS:HD3	2:A:846:GLU:OE2	2.06	0.55
3:B:591:ARG:O	3:B:593:PRO:HD3	2.06	0.55
5:D:51:ASN:O	5:D:54:GLU:HB3	2.06	0.55
3:B:44:VAL:O	3:B:45:SER:C	2.45	0.55
7:F:119:ARG:HG3	7:F:119:ARG:HH11	1.71	0.55
2:A:72:GLU:OE2	3:B:1175:LEU:HB2	2.07	0.55
5:D:134:THR:HG22	5:D:136:GLY:N	2.19	0.55
4:C:74:SER:O	4:C:238:ILE:HD11	2.07	0.55
2:A:964:ILE:HD13	2:A:1045:VAL:HG21	1.89	0.55
9:H:58:THR:C	9:H:59:ILE:HD12	2.26	0.55
2:A:590:ARG:O	2:A:591:PHE:HB2	2.05	0.55
4:C:86:CYS:O	4:C:88:CYS:N	2.39	0.55
4:C:88:CYS:SG	4:C:92:CYS:HB3	2.46	0.55
2:A:1410:PHE:HA	3:B:1212:ILE:HD11	1.88	0.55
3:B:428:ILE:O	3:B:432:MET:HE2	2.07	0.55
2:A:321:PRO:O	2:A:322:VAL:CB	2.54	0.55
2:A:503:GLN:HE21	7:F:90:ARG:HH21	1.53	0.55
2:A:741:ASN:HD22	2:A:744:LYS:H	1.54	0.55
4:C:69:LEU:HD12	4:C:69:LEU:N	2.20	0.55
3:B:503:GLY:O	3:B:507:LYS:HG3	2.06	0.55
2:A:901:LEU:HG	2:A:926:GLN:NE2	2.11	0.55
3:B:839:MET:CE	3:B:980:PHE:HB2	2.37	0.55
3:B:1202:LEU:O	3:B:1206:GLU:HG3	2.06	0.55
2:A:1334:ASP:C	2:A:1336:MET:N	2.58	0.55
2:A:1121:GLU:CG	2:A:1122:PRO:HD2	2.37	0.55
2:A:929:LEU:HD23	2:A:983:ILE:HG21	1.88	0.55
3:B:681:TRP:HA	3:B:684:LEU:HD13	1.88	0.55
2:A:583:PRO:HG2	2:A:586:ILE:HD11	1.88	0.55
8:G:154:VAL:HG12	8:G:155:SER:N	2.22	0.55
2:A:55:ASP:H	2:A:56:PRO:HD3	1.71	0.55
2:A:1093:LYS:O	2:A:1094:VAL:HG23	2.06	0.55
8:G:1:MET:CE	8:G:80:LYS:H	2.16	0.55
3:B:217:ARG:C	3:B:217:ARG:HD2	2.27	0.55
2:A:722:LEU:O	2:A:725:ALA:HB3	2.06	0.55
2:A:196:GLU:HG2	2:A:197:PRO:HD2	1.88	0.55
3:B:365:THR:HG23	3:B:367:LEU:N	2.12	0.55
3:B:831:SER:CB	3:B:994:TYR:OH	2.54	0.55
2:A:93:VAL:CG2	2:A:301:ALA:HA	2.37	0.55
3:B:130:VAL:HG12	3:B:131:ASP:N	2.21	0.55
3:B:1110:PRO:O	3:B:1119:VAL:HG22	2.07	0.55
3:B:233:PRO:HG2	3:B:234:ILE:CD1	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:7:SER:C	2:A:9:ALA:H	2.10	0.55
3:B:223:VAL:HG11	3:B:381:MET:HG2	1.87	0.55
3:B:844:SER:O	3:B:847:ASP:HB2	2.07	0.55
3:B:558:LEU:O	3:B:560:GLU:N	2.40	0.55
9:H:15:VAL:HG22	9:H:26:ILE:CD1	2.36	0.55
2:A:317:LYS:O	2:A:318:SER:CB	2.54	0.55
3:B:346:GLU:CA	3:B:349:ILE:HD13	2.37	0.55
3:B:465:ASN:O	3:B:466:TRP:O	2.25	0.54
2:A:225:ASN:ND2	2:A:228:PHE:N	2.43	0.54
2:A:90:VAL:CG1	2:A:297:GLN:NE2	2.70	0.54
3:B:1166:CYS:O	3:B:1168:LEU:N	2.36	0.54
2:A:613:ILE:HG22	2:A:614:PHE:HD2	1.72	0.54
2:A:639:PRO:CD	2:A:640:GLN:H	2.19	0.54
5:D:37:GLN:OE1	8:G:5:LYS:NZ	2.34	0.54
3:B:642:ASP:O	3:B:644:GLU:N	2.40	0.54
3:B:850:LEU:HD12	3:B:851:PHE:H	1.70	0.54
1:R:29:G:H4'	2:A:1386:ARG:NH1	2.17	0.54
2:A:630:ILE:HD13	2:A:645:LEU:HD23	1.88	0.54
5:D:47:LEU:HD13	5:D:48:ILE:N	2.21	0.54
3:B:1187:ASN:O	3:B:1188:LYS:CB	2.53	0.54
3:B:34:ILE:O	3:B:37:PHE:HB3	2.07	0.54
6:E:88:VAL:HG12	6:E:89:GLY:N	2.20	0.54
3:B:1023:VAL:O	3:B:1026:LEU:N	2.39	0.54
3:B:373:ARG:HG2	3:B:566:LEU:HD23	1.89	0.54
2:A:675:THR:O	2:A:679:ILE:HG12	2.08	0.54
1:R:7:C:H41	1:R:13:G:H21	1.53	0.54
2:A:40:THR:HG23	2:A:54:ASN:HD21	1.71	0.54
2:A:869:GLY:O	6:E:204:THR:HG21	2.07	0.54
2:A:567:LYS:CB	2:A:568:PRO:CD	2.84	0.54
9:H:56:THR:O	9:H:144:ILE:HA	2.08	0.54
3:B:247:GLY:H	3:B:418:LYS:HZ3	1.55	0.54
2:A:577:ILE:HD13	2:A:577:ILE:N	2.22	0.54
2:A:518:LYS:HG3	2:A:519:PRO:O	2.08	0.54
3:B:798:TYR:HE2	4:C:62:PHE:CZ	2.25	0.54
6:E:114:ASN:O	6:E:115:ASN:HB3	2.08	0.54
2:A:49:LYS:HD3	2:A:55:ASP:HB3	1.88	0.54
3:B:254:LEU:HD11	3:B:273:LEU:HG	1.88	0.54
9:H:142:LEU:C	9:H:143:LEU:HD12	2.28	0.54
2:A:269:ILE:HD11	2:A:300:VAL:HA	1.89	0.54
4:C:73:GLN:NE2	4:C:75:MET:H	2.05	0.54
3:B:949:VAL:HG12	3:B:950:ASP:N	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:126:ASN:HD22	8:G:127:PRO:HA	1.70	0.54
11:J:51:LEU:O	11:J:51:LEU:HD12	2.08	0.54
2:A:650:GLN:O	2:A:654:ASN:ND2	2.37	0.54
3:B:945:GLU:O	3:B:946:ASN:HB3	2.08	0.54
2:A:1341:ILE:HB	6:E:182:ASP:OD2	2.08	0.54
2:A:130:ASP:O	2:A:131:SER:C	2.45	0.54
3:B:114:PRO:HG2	3:B:115:GLN:H	1.71	0.54
2:A:588:LEU:O	2:A:606:LEU:HA	2.07	0.54
3:B:274:PRO:HD2	3:B:276:ILE:HD13	1.89	0.54
10:I:85:PHE:N	10:I:85:PHE:CD2	2.61	0.54
2:A:598:LEU:O	2:A:599:SER:C	2.46	0.54
2:A:12:ARG:O	3:B:1194:ILE:HG22	2.08	0.54
2:A:382:PRO:CB	2:A:428:TYR:HE2	2.18	0.54
5:D:52:LEU:O	5:D:54:GLU:N	2.37	0.54
3:B:387:LEU:H	3:B:387:LEU:CD1	2.21	0.54
3:B:258:LEU:O	3:B:258:LEU:HG	2.07	0.54
4:C:253:LYS:O	4:C:256:ALA:HB3	2.07	0.54
3:B:1156:ASP:O	3:B:1157:ALA:O	2.26	0.54
3:B:954:VAL:O	13:L:55:ILE:O	2.25	0.54
3:B:94:LYS:HG2	3:B:95:ILE:H	1.73	0.54
2:A:1341:ILE:CG2	2:A:1342:GLU:N	2.71	0.54
5:D:208:GLU:O	5:D:212:LYS:HG3	2.07	0.54
8:G:91:VAL:CG2	8:G:143:ILE:HD13	2.37	0.54
2:A:866:PHE:C	2:A:867:ILE:HG13	2.28	0.54
3:B:1065:GLN:HG3	3:B:1067:ARG:H	1.71	0.54
2:A:1420:ASP:CB	2:A:1422:ARG:HG3	2.37	0.54
2:A:541:ILE:N	2:A:541:ILE:HD12	2.23	0.54
5:D:130:LEU:O	5:D:132:GLN:N	2.41	0.54
2:A:1265:ASN:HD21	3:B:265:SER:HB3	1.73	0.54
7:F:90:ARG:HG3	7:F:91:ALA:N	2.23	0.54
2:A:1001:ARG:O	2:A:1002:GLY:O	2.26	0.54
7:F:128:LYS:HE2	7:F:151:LEU:O	2.08	0.54
2:A:492:PRO:O	2:A:493:GLN:NE2	2.41	0.54
3:B:272:THR:O	3:B:273:LEU:CB	2.55	0.54
4:C:167:HIS:HA	12:K:6:ARG:NH1	2.19	0.54
3:B:1208:MET:O	3:B:1211:ASN:N	2.31	0.54
8:G:1:MET:O	8:G:3:PHE:CE1	2.61	0.54
2:A:441:PRO:HD2	2:A:498:ARG:NH2	2.22	0.54
6:E:177:ARG:C	6:E:212:ARG:HD3	2.28	0.54
2:A:37:PHE:CD1	2:A:37:PHE:N	2.76	0.54
4:C:66:ARG:NH1	11:J:2:ILE:HG21	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:70:CYS:O	2:A:70:CYS:SG	2.65	0.54
12:K:31:VAL:HG12	12:K:32:VAL:N	2.23	0.54
3:B:918:ILE:CG1	3:B:935:ARG:HD2	2.38	0.54
5:D:64:VAL:O	5:D:67:ARG:N	2.41	0.54
2:A:853:ASP:OD1	2:A:855:THR:CB	2.56	0.54
2:A:352:VAL:HG12	2:A:353:ILE:N	2.23	0.54
2:A:563:PRO:HB3	2:A:571:LEU:O	2.08	0.54
2:A:407:ARG:HA	2:A:430:TRP:CD1	2.43	0.54
3:B:1022:THR:HG23	3:B:1022:THR:O	2.08	0.54
5:D:122:GLU:HA	5:D:125:SER:OG	2.09	0.54
1:R:2:C:H1'	1:R:3:A:OP1	2.08	0.53
9:H:4:THR:HG22	9:H:5:LEU:N	2.22	0.53
3:B:508:LEU:N	3:B:508:LEU:HD13	2.23	0.53
2:A:1116:LEU:O	2:A:1308:THR:HG22	2.07	0.53
3:B:953:LEU:O	3:B:953:LEU:HD23	2.08	0.53
3:B:563:MET:HE2	3:B:588:GLY:N	2.23	0.53
2:A:535:THR:CG2	2:A:616:VAL:HA	2.37	0.53
2:A:490:HIS:HB3	3:B:1150:ARG:NH1	2.23	0.53
3:B:90:ILE:HD11	3:B:432:MET:SD	2.48	0.53
2:A:322:VAL:HG12	2:A:323:LYS:N	2.23	0.53
3:B:258:LEU:CG	3:B:258:LEU:O	2.56	0.53
12:K:90:ALA:O	12:K:94:ILE:HG12	2.08	0.53
10:I:43:VAL:O	10:I:43:VAL:HG12	2.07	0.53
9:H:58:THR:O	9:H:59:ILE:HD12	2.09	0.53
11:J:2:ILE:HG22	11:J:3:VAL:O	2.08	0.53
2:A:1017:LEU:CB	6:E:205:SER:HA	2.38	0.53
3:B:1065:GLN:NE2	3:B:1067:ARG:HG2	2.23	0.53
3:B:287:ARG:NH1	3:B:324:ILE:O	2.40	0.53
3:B:282:ILE:HD11	3:B:317:CYS:SG	2.47	0.53
2:A:1195:LEU:HD11	2:A:1267:MET:HE3	1.90	0.53
2:A:1118:VAL:CG2	2:A:1306:LEU:HB2	2.38	0.53
2:A:450:LEU:O	2:A:1070:GLN:HB3	2.08	0.53
9:H:59:ILE:O	9:H:60:ALA:CB	2.56	0.53
2:A:50:ILE:C	2:A:52:GLY:N	2.61	0.53
6:E:29:PHE:C	6:E:30:ILE:HG13	2.25	0.53
2:A:1116:LEU:HD12	2:A:1116:LEU:O	2.09	0.53
2:A:751:SER:OG	3:B:1015:HIS:CE1	2.61	0.53
9:H:56:THR:HB	9:H:145:ARG:HG2	1.91	0.53
3:B:1031:LEU:CD2	3:B:1044:ALA:HB2	2.39	0.53
2:A:427:GLN:HG3	2:A:430:TRP:CZ2	2.43	0.53
3:B:259:TYR:H	3:B:259:TYR:HD1	1.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:146:GLN:O	5:D:149:THR:HG22	2.08	0.53
3:B:360:PHE:O	3:B:361:LEU:C	2.45	0.53
2:A:1027:ALA:O	2:A:1031:VAL:HG23	2.07	0.53
2:A:1030:ARG:HG3	2:A:1034:GLU:OE2	2.07	0.53
3:B:269:ILE:N	3:B:269:ILE:HD12	2.23	0.53
2:A:1057:VAL:CG1	2:A:1058:VAL:N	2.70	0.53
4:C:237:SER:O	4:C:238:ILE:HD12	2.08	0.53
2:A:563:PRO:HG3	2:A:572:TRP:CE2	2.43	0.53
2:A:1265:ASN:ND2	3:B:265:SER:HB3	2.23	0.53
2:A:1291:VAL:HG13	2:A:1292:PRO:CD	2.39	0.53
3:B:1060:ARG:CZ	4:C:202:PRO:HG3	2.38	0.53
4:C:260:LEU:O	4:C:264:GLN:HG3	2.08	0.53
3:B:120:ARG:CG	3:B:955:THR:HG21	2.34	0.53
2:A:645:LEU:HG	2:A:649:ILE:HD12	1.90	0.53
3:B:1115:THR:HG22	3:B:1117:GLN:HG3	1.91	0.53
2:A:269:ILE:HD13	2:A:300:VAL:HG22	1.90	0.53
2:A:265:LYS:HE2	2:A:302:THR:CG2	2.38	0.53
2:A:629:LEU:HD23	2:A:633:VAL:HG23	1.91	0.53
2:A:345:VAL:HG23	2:A:346:ASP:O	2.09	0.53
3:B:35:SER:O	3:B:39:ARG:HG3	2.08	0.53
2:A:1334:ASP:C	2:A:1336:MET:H	2.11	0.53
7:F:118:LEU:O	7:F:122:MET:HG3	2.09	0.53
3:B:562:GLY:HA3	3:B:590:HIS:CE1	2.43	0.53
2:A:808:LEU:HD23	2:A:813:PHE:N	2.23	0.53
2:A:903:ASN:C	2:A:903:ASN:ND2	2.61	0.53
2:A:1031:VAL:HG12	2:A:1031:VAL:O	2.08	0.53
2:A:683:ILE:HG21	2:A:801:GLU:HG3	1.90	0.53
3:B:245:GLU:O	3:B:246:LYS:HG3	2.08	0.53
8:G:149:GLY:O	8:G:159:ALA:HB1	2.08	0.53
9:H:27:GLU:HG2	9:H:39:THR:HG23	1.91	0.53
11:J:21:TYR:HB2	11:J:39:LEU:CD1	2.39	0.53
2:A:41:MET:O	2:A:42:ASP:C	2.47	0.53
2:A:56:PRO:O	2:A:57:ARG:CG	2.53	0.53
2:A:456:MET:HB2	2:A:478:TYR:OH	2.08	0.53
5:D:202:ILE:CG2	5:D:203:SER:N	2.68	0.53
3:B:121:ASN:HA	3:B:207:GLY:HA3	1.91	0.53
2:A:1207:LEU:HA	2:A:1211:GLN:OE1	2.09	0.53
2:A:382:PRO:HB3	2:A:428:TYR:CE2	2.38	0.53
11:J:44:TYR:HD2	11:J:44:TYR:H	1.57	0.53
2:A:963:ILE:HD11	2:A:1048:ASN:CB	2.39	0.53
2:A:50:ILE:C	2:A:52:GLY:H	2.10	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:68:GLN:O	2:A:70:CYS:N	2.36	0.53
2:A:730:GLY:C	2:A:732:LEU:H	2.12	0.53
3:B:293:PRO:C	3:B:294:ASP:O	2.45	0.53
2:A:1283:VAL:HG12	2:A:1284:MET:N	2.22	0.53
4:C:179:GLU:HG2	4:C:180:TYR:N	2.24	0.53
4:C:167:HIS:CD2	4:C:168:ALA:N	2.77	0.53
2:A:466:SER:HB3	3:B:1103:ILE:HG12	1.91	0.53
3:B:979:LYS:HG2	3:B:1095:LEU:HD13	1.90	0.53
3:B:640:VAL:O	3:B:641:GLU:C	2.48	0.53
2:A:322:VAL:CG1	2:A:323:LYS:N	2.71	0.53
3:B:880:THR:HB	3:B:934:LYS:HE3	1.91	0.53
2:A:686:ALA:O	2:A:690:VAL:HG23	2.09	0.53
5:D:14:ARG:O	5:D:16:LYS:N	2.42	0.53
2:A:1339:LEU:HD13	6:E:147:HIS:CD2	2.44	0.53
1:R:17:5BU:O2'	1:R:18:C:H5'	2.09	0.53
2:A:49:LYS:HZ1	2:A:61:ILE:H	1.55	0.53
2:A:71:GLN:HG3	2:A:72:GLU:N	2.24	0.53
2:A:2:VAL:HG21	3:B:1157:ALA:HB1	1.89	0.53
3:B:973:ILE:HG23	3:B:974:PRO:HD2	1.90	0.53
3:B:62:ILE:HG23	3:B:418:LYS:HG2	1.91	0.53
3:B:593:PRO:O	3:B:596:LEU:N	2.42	0.53
9:H:32:THR:HG22	9:H:33:GLN:OE1	2.09	0.53
3:B:387:LEU:N	3:B:387:LEU:HD12	2.24	0.53
4:C:184:ASN:HD21	4:C:187:LYS:HA	1.72	0.53
9:H:110:ASP:O	9:H:128:ASN:ND2	2.42	0.52
2:A:1398:MET:C	2:A:1400:CYS:H	2.11	0.52
3:B:58:THR:O	3:B:62:ILE:HG12	2.09	0.52
2:A:84:ILE:CG2	2:A:239:LEU:HB3	2.37	0.52
3:B:421:PHE:O	3:B:424:LEU:HB3	2.09	0.52
3:B:1178:ASN:O	3:B:1179:GLN:C	2.48	0.52
2:A:1280:GLU:O	2:A:1282:VAL:HG23	2.08	0.52
3:B:997:GLU:H	3:B:997:GLU:CD	2.10	0.52
2:A:49:LYS:HZ1	2:A:61:ILE:N	2.07	0.52
2:A:567:LYS:HB2	2:A:568:PRO:CD	2.39	0.52
3:B:1073:TYR:CE2	3:B:1080:LYS:HG2	2.44	0.52
3:B:516:ASN:ND2	3:B:516:ASN:N	2.50	0.52
2:A:1373:ASP:O	2:A:1376:THR:HG22	2.09	0.52
5:D:167:LEU:O	5:D:170:THR:OG1	2.28	0.52
10:I:83:ASN:HA	10:I:102:VAL:O	2.09	0.52
2:A:590:ARG:HH21	2:A:620:LYS:CB	2.13	0.52
2:A:590:ARG:NH1	2:A:590:ARG:CG	2.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1094:VAL:CG1	2:A:1095:THR:N	2.72	0.52
3:B:847:ASP:HB3	4:C:167:HIS:CD2	2.44	0.52
13:L:32:ALA:HB2	13:L:55:ILE:HG13	1.91	0.52
3:B:287:ARG:HA	3:B:291:ILE:O	2.09	0.52
3:B:203:PHE:CB	3:B:205:ILE:HD11	2.39	0.52
2:A:586:ILE:HD13	2:A:633:VAL:HG22	1.91	0.52
2:A:340:LEU:HD13	2:A:1429:ILE:CG2	2.38	0.52
3:B:185:THR:O	3:B:186:GLU:C	2.47	0.52
2:A:512:VAL:HA	2:A:519:PRO:HA	1.90	0.52
6:E:2:ASP:O	6:E:3:GLN:HG2	2.09	0.52
3:B:603:LEU:HB3	3:B:609:ILE:HG13	1.91	0.52
6:E:112:TYR:CE1	6:E:136:ASN:HA	2.44	0.52
2:A:276:LEU:HG	2:A:276:LEU:O	2.09	0.52
2:A:590:ARG:HG2	2:A:591:PHE:N	2.23	0.52
6:E:145:THR:HG21	6:E:187:TYR:CD2	2.44	0.52
2:A:442:VAL:O	2:A:457:ALA:HA	2.10	0.52
3:B:285:ILE:HG21	3:B:378:LEU:CD2	2.39	0.52
3:B:984:HIS:NE2	3:B:1025:HIS:HA	2.24	0.52
4:C:259:LEU:HD13	12:K:91:CYS:HB2	1.91	0.52
3:B:843:GLN:HA	3:B:846:ILE:HD13	1.91	0.52
2:A:877:HIS:O	2:A:878:ILE:HG13	2.09	0.52
5:D:156:ASP:HB2	5:D:159:THR:HG23	1.91	0.52
13:L:27:LEU:HD13	13:L:37:LYS:HE2	1.92	0.52
2:A:1254:ALA:O	2:A:1255:GLU:HB2	2.10	0.52
8:G:35:GLU:OE2	8:G:48:VAL:HG23	2.09	0.52
3:B:251:ILE:O	3:B:251:ILE:HG22	2.10	0.52
3:B:840:ILE:HG22	3:B:841:MET:N	2.25	0.52
2:A:857:ARG:NH1	7:F:139:PRO:HB2	2.25	0.52
2:A:710:LEU:H	2:A:710:LEU:CD1	2.19	0.52
3:B:582:VAL:CG2	3:B:626:ILE:HB	2.36	0.52
3:B:1183:LYS:HE3	3:B:1183:LYS:O	2.09	0.52
4:C:244:VAL:O	4:C:248:ILE:HG12	2.10	0.52
3:B:1051:THR:CG2	3:B:1052:VAL:N	2.72	0.52
3:B:349:ILE:HD12	3:B:349:ILE:N	2.25	0.52
3:B:969:ARG:NH1	4:C:61:GLU:OE1	2.43	0.52
3:B:235:SER:OG	3:B:236:HIS:CD2	2.62	0.52
2:A:69:THR:O	2:A:71:GLN:N	2.43	0.52
4:C:191:TYR:HB3	4:C:201:TRP:CD1	2.45	0.52
2:A:524:VAL:CG1	2:A:525:GLN:N	2.72	0.52
8:G:101:VAL:CG1	8:G:102:GLN:N	2.73	0.52
3:B:309:GLN:HG3	10:I:52:ILE:CD1	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1074:GLU:N	2:A:1075:PRO:HD2	2.24	0.52
2:A:986:ILE:HG22	2:A:987:VAL:N	2.23	0.52
2:A:244:PRO:HG2	2:A:245:PRO:CD	2.38	0.52
2:A:465:TYR:CD2	3:B:976:ILE:HG13	2.44	0.52
9:H:98:TYR:C	9:H:118:PHE:CD2	2.80	0.52
2:A:1345:ARG:HG2	2:A:1372:VAL:CG1	2.39	0.52
3:B:899:ILE:CD1	3:B:911:ILE:HA	2.40	0.52
2:A:134:ARG:O	2:A:138:ILE:HG12	2.08	0.52
7:F:75:PRO:O	7:F:77:ASP:O	2.27	0.52
3:B:796:LEU:HD12	3:B:797:TYR:N	2.24	0.52
3:B:558:LEU:C	3:B:560:GLU:H	2.13	0.52
2:A:1237:ILE:HG22	2:A:1238:ILE:N	2.25	0.52
1:R:20:A:H2'	1:R:21:G:C8	2.45	0.52
3:B:810:GLU:HB2	3:B:815:ARG:HH22	1.75	0.52
2:A:765:VAL:HG23	2:A:802:ASN:O	2.10	0.52
4:C:235:VAL:HG13	11:J:13:VAL:HG23	1.91	0.52
2:A:55:ASP:C	2:A:57:ARG:N	2.58	0.52
2:A:446:ARG:CD	2:A:480:ALA:HB2	2.40	0.52
5:D:153:ARG:HB3	5:D:154:PHE:CE1	2.45	0.52
2:A:829:VAL:O	2:A:831:THR:N	2.38	0.52
2:A:899:VAL:HB	2:A:929:LEU:HD11	1.91	0.52
3:B:842:ASN:HB2	3:B:1008:PRO:O	2.10	0.52
5:D:144:THR:O	5:D:144:THR:HG22	2.10	0.52
2:A:1072:ILE:HD11	2:A:1368:MET:HG2	1.91	0.52
7:F:79:ARG:HH21	7:F:146:TRP:HA	1.75	0.52
3:B:172:ILE:HG22	3:B:173:MET:N	2.23	0.52
2:A:98:LYS:O	2:A:102:VAL:HG23	2.10	0.52
3:B:237:VAL:HG12	3:B:238:ALA:N	2.24	0.52
1:R:15:G:H2'	1:R:16:G:H8	1.75	0.51
2:A:35:ILE:HG12	2:A:56:PRO:HG2	1.91	0.51
8:G:91:VAL:HG23	8:G:143:ILE:HD13	1.91	0.51
2:A:709:THR:HG22	2:A:710:LEU:N	2.25	0.51
2:A:1315:GLU:C	2:A:1317:MET:H	2.13	0.51
2:A:982:THR:HG22	2:A:984:LYS:H	1.75	0.51
4:C:73:GLN:NE2	4:C:75:MET:N	2.58	0.51
4:C:101:LEU:HD12	4:C:102:GLN:N	2.25	0.51
3:B:880:THR:O	3:B:934:LYS:HG3	2.09	0.51
7:F:103:MET:HE3	8:G:66:GLY:H	1.75	0.51
2:A:1193:LEU:HB2	2:A:1260:LEU:HD11	1.92	0.51
7:F:127:GLU:O	7:F:129:LYS:HG3	2.09	0.51
3:B:999:MET:HA	3:B:999:MET:CE	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1313:LEU:C	2:A:1315:GLU:H	2.13	0.51
2:A:339:ASN:HB3	3:B:1117:GLN:NE2	2.23	0.51
3:B:824:ILE:HG12	11:J:48:ARG:HH12	1.74	0.51
7:F:109:VAL:HG11	7:F:123:LYS:HG2	1.92	0.51
3:B:112:LEU:HG	3:B:113:TYR:N	2.25	0.51
2:A:73:GLY:O	2:A:75:ASN:N	2.43	0.51
3:B:57:TYR:O	3:B:59:LEU:N	2.43	0.51
13:L:43:THR:O	13:L:43:THR:HG22	2.10	0.51
8:G:15:PRO:HD3	8:G:67:SER:HA	1.91	0.51
4:C:181:ASP:CG	4:C:186:LEU:HD13	2.30	0.51
3:B:865:LYS:NZ	3:B:869:SER:HA	2.24	0.51
5:D:156:ASP:O	5:D:158:GLU:N	2.43	0.51
2:A:939:ASP:OD1	2:A:1023:ARG:NH1	2.43	0.51
12:K:91:CYS:O	12:K:95:ILE:HG12	2.11	0.51
4:C:27:LEU:O	4:C:30:ALA:HB3	2.10	0.51
2:A:53:LEU:O	2:A:54:ASN:C	2.48	0.51
2:A:69:THR:C	2:A:71:GLN:N	2.63	0.51
9:H:47:PHE:CD2	9:H:47:PHE:O	2.63	0.51
4:C:167:HIS:HD2	4:C:168:ALA:H	1.58	0.51
2:A:1313:LEU:HD23	2:A:1338:VAL:CG2	2.40	0.51
11:J:8:PHE:H	11:J:49:MET:HE1	1.74	0.51
3:B:1045:SER:HB3	3:B:1046:PRO:HD2	1.91	0.51
5:D:137:ASN:C	5:D:137:ASN:HD22	2.13	0.51
3:B:1068:GLY:O	3:B:1069:PHE:O	2.28	0.51
13:L:48:CYS:SG	13:L:49:LYS:N	2.84	0.51
2:A:450:LEU:N	2:A:450:LEU:HD12	2.25	0.51
3:B:936:ASP:OD1	3:B:937:ALA:N	2.43	0.51
2:A:997:LEU:HD13	2:A:1018:PHE:HE2	1.76	0.51
3:B:464:GLY:HA3	3:B:479:VAL:O	2.11	0.51
3:B:240:ILE:C	3:B:240:ILE:HD13	2.31	0.51
4:C:31:ASN:HA	4:C:34:ARG:HB3	1.91	0.51
4:C:31:ASN:O	4:C:32:SER:C	2.48	0.51
2:A:401:GLY:O	2:A:435:HIS:CD2	2.63	0.51
8:G:102:GLN:HG3	8:G:106:MET:O	2.10	0.51
2:A:21:LEU:HD21	2:A:1414:ALA:CA	2.40	0.51
3:B:428:ILE:HG22	3:B:432:MET:HE1	1.92	0.51
3:B:383:ASN:O	3:B:387:LEU:HD13	2.09	0.51
3:B:601:ARG:O	3:B:605:ARG:HG3	2.09	0.51
2:A:1227:ILE:HG22	2:A:1228:TRP:N	2.24	0.51
2:A:1398:MET:C	2:A:1400:CYS:N	2.62	0.51
8:G:106:MET:CG	8:G:107:LYS:N	2.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:91:ASP:C	9:H:93:TYR:H	2.13	0.51
2:A:1437:GLY:O	2:A:1439:GLY:N	2.44	0.51
3:B:1183:LYS:N	3:B:1183:LYS:CE	2.74	0.51
2:A:1149:ALA:CB	10:I:47:GLU:HA	2.41	0.51
5:D:170:THR:CB	5:D:172:LEU:HG	2.40	0.51
4:C:18:VAL:HG23	4:C:240:VAL:CG1	2.40	0.51
10:I:61:ASP:C	10:I:63:GLY:H	2.13	0.51
11:J:2:ILE:HD11	11:J:57:ILE:HD13	1.92	0.51
3:B:614:SER:C	3:B:615:MET:HG3	2.30	0.51
3:B:1183:LYS:H	3:B:1183:LYS:CE	2.24	0.51
3:B:558:LEU:HD22	3:B:596:LEU:HD11	1.93	0.51
2:A:196:GLU:CG	2:A:197:PRO:HD2	2.41	0.51
3:B:233:PRO:HG2	3:B:234:ILE:HD12	1.92	0.51
8:G:9:LEU:HG	8:G:10:ASN:N	2.26	0.51
2:A:42:ASP:O	2:A:44:THR:N	2.44	0.51
9:H:42:ILE:CG2	9:H:43:ASN:N	2.73	0.51
7:F:82:THR:HG22	7:F:84:TYR:N	2.17	0.51
2:A:768:GLN:HG2	2:A:816:HIS:CA	2.38	0.51
3:B:635:ARG:NH2	3:B:742:GLU:OE2	2.44	0.51
6:E:23:VAL:HG13	6:E:28:TYR:HD1	1.76	0.51
3:B:661:LEU:C	3:B:663:ALA:H	2.14	0.51
3:B:48:LEU:O	3:B:51:PHE:N	2.43	0.51
3:B:798:TYR:HE2	4:C:62:PHE:HZ	1.59	0.51
4:C:26:ASP:O	4:C:27:LEU:C	2.49	0.51
2:A:996:ASN:HB3	2:A:1050:GLU:OE2	2.09	0.51
2:A:738:LYS:C	2:A:740:LEU:H	2.14	0.51
3:B:393:LYS:HE3	3:B:393:LYS:HA	1.92	0.51
3:B:305:VAL:HG12	3:B:305:VAL:O	2.10	0.51
2:A:54:ASN:CB	2:A:247:ARG:HH12	2.19	0.51
2:A:567:LYS:CE	9:H:46:LEU:HB2	2.41	0.51
3:B:616:ILE:HG13	3:B:697:GLU:HG3	1.91	0.51
4:C:38:ILE:HD11	4:C:176:ILE:HD12	1.92	0.51
2:A:757:ASN:O	2:A:761:MET:HG3	2.11	0.51
2:A:1450:LEU:HD11	7:F:108:PHE:CZ	2.45	0.51
4:C:91:HIS:O	4:C:91:HIS:CD2	2.64	0.51
2:A:34:LYS:CD	2:A:34:LYS:N	2.74	0.51
13:L:53:HIS:HB3	13:L:55:ILE:CD1	2.41	0.51
5:D:202:ILE:HG21	5:D:207:LEU:HB2	1.93	0.51
9:H:143:LEU:O	9:H:144:ILE:HG13	2.11	0.51
2:A:120:GLU:C	2:A:122:MET:H	2.15	0.51
2:A:1430:LEU:O	3:B:1197:PRO:HD2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:638:PHE:HB2	3:B:741:CYS:O	2.11	0.51
3:B:1017:ILE:HB	3:B:1018:PRO:CD	2.39	0.50
8:G:101:VAL:HG12	8:G:102:GLN:N	2.26	0.50
8:G:81:PRO:HG3	8:G:106:MET:SD	2.51	0.50
5:D:51:ASN:O	5:D:52:LEU:O	2.28	0.50
2:A:587:HIS:O	2:A:588:LEU:HB2	2.11	0.50
2:A:1027:ALA:HB3	2:A:1030:ARG:HB2	1.93	0.50
2:A:116:ASP:O	2:A:118:HIS:N	2.44	0.50
3:B:276:ILE:CG2	3:B:276:ILE:O	2.59	0.50
2:A:567:LYS:CB	9:H:95:TYR:HA	2.40	0.50
4:C:36:VAL:HG21	4:C:251:LEU:HB2	1.92	0.50
12:K:6:ARG:O	12:K:9:LEU:HG	2.11	0.50
3:B:292:ILE:N	3:B:293:PRO:HD2	2.26	0.50
2:A:231:PRO:C	2:A:233:TRP:H	2.14	0.50
4:C:35:ARG:HA	4:C:38:ILE:HG12	1.93	0.50
2:A:1436:ILE:O	2:A:1436:ILE:HG22	2.11	0.50
11:J:23:ASN:C	11:J:25:LEU:N	2.65	0.50
2:A:307:ASP:N	2:A:307:ASP:OD2	2.44	0.50
3:B:212:LEU:HD23	3:B:480:SER:HB2	1.93	0.50
2:A:907:THR:CG2	2:A:908:LEU:N	2.58	0.50
13:L:53:HIS:O	13:L:55:ILE:HG12	2.11	0.50
2:A:524:VAL:CG1	2:A:525:GLN:H	2.17	0.50
6:E:23:VAL:O	6:E:28:TYR:HB2	2.11	0.50
2:A:1127:ASP:HB3	2:A:1130:GLN:CB	2.42	0.50
3:B:957:ASN:O	3:B:959:ASP:N	2.45	0.50
2:A:543:LEU:C	2:A:545:GLN:H	2.15	0.50
2:A:244:PRO:CB	2:A:245:PRO:HD3	2.42	0.50
2:A:666:ILE:N	2:A:666:ILE:HD12	2.26	0.50
13:L:59:ALA:O	13:L:60:ARG:O	2.29	0.50
2:A:84:ILE:O	2:A:84:ILE:CG2	2.59	0.50
2:A:1443:VAL:C	2:A:1444:MET:HG3	2.31	0.50
3:B:1133:MET:O	3:B:1136:ASP:HB2	2.11	0.50
11:J:44:TYR:N	11:J:44:TYR:CD2	2.80	0.50
3:B:496:ARG:NH1	3:B:539:LEU:HB2	2.26	0.50
2:A:1120:LEU:CD1	2:A:1120:LEU:N	2.73	0.50
2:A:823:GLY:C	2:A:825:ILE:H	2.15	0.50
12:K:48:ALA:O	12:K:51:LEU:N	2.40	0.50
2:A:106:VAL:HG13	2:A:112:LYS:O	2.12	0.50
2:A:567:LYS:HZ2	9:H:47:PHE:HB2	1.76	0.50
4:C:84:ARG:NE	12:K:11:LEU:HD11	2.27	0.50
4:C:38:ILE:CD1	4:C:176:ILE:HD12	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:133:ILE:HD11	4:C:237:SER:HA	1.93	0.50
3:B:1006:ILE:HD13	11:J:44:TYR:HE2	1.77	0.50
9:H:15:VAL:HG22	9:H:26:ILE:CG1	2.40	0.50
3:B:57:TYR:HD1	3:B:57:TYR:N	2.10	0.50
2:A:1213:GLY:O	2:A:1214:GLU:C	2.49	0.50
2:A:1336:MET:CE	2:A:1381:LEU:HG	2.41	0.50
2:A:622:VAL:O	2:A:622:VAL:HG13	2.12	0.50
3:B:470:LYS:HE2	3:B:471:LYS:H	1.77	0.50
4:C:67:LEU:HD11	4:C:155:LEU:HD12	1.93	0.50
3:B:590:HIS:NE2	3:B:592:ASN:O	2.44	0.50
2:A:767:GLN:NE2	2:A:774:ARG:HD2	2.26	0.50
3:B:272:THR:O	3:B:273:LEU:HD13	2.12	0.50
3:B:955:THR:HG22	3:B:956:THR:O	2.12	0.50
9:H:139:ASN:O	9:H:140:ALA:HB2	2.12	0.50
3:B:204:ILE:C	3:B:205:ILE:HD12	2.32	0.50
4:C:239:PRO:HB2	4:C:241:ASP:OD1	2.12	0.50
2:A:1409:LEU:HD13	3:B:1207:LEU:CD1	2.41	0.50
2:A:332:LYS:HB2	2:A:337:ARG:CZ	2.42	0.50
2:A:337:ARG:HD3	3:B:1132:GLU:OE2	2.11	0.50
8:G:15:PRO:O	8:G:16:SER:C	2.50	0.50
3:B:800:GLN:HB3	11:J:52:THR:HG22	1.89	0.50
2:A:1094:VAL:HG12	2:A:1095:THR:N	2.26	0.50
3:B:839:MET:HE1	3:B:980:PHE:HB2	1.94	0.50
3:B:1099:VAL:C	3:B:1101:ASP:N	2.65	0.50
2:A:218:ASP:O	2:A:219:PHE:C	2.50	0.50
3:B:776:GLN:O	3:B:1095:LEU:HB3	2.11	0.50
5:D:5:THR:O	5:D:6:SER:O	2.29	0.50
8:G:136:VAL:HG12	8:G:136:VAL:O	2.10	0.50
7:F:86:THR:HG23	7:F:89:GLU:OE1	2.12	0.50
3:B:648:HIS:CG	3:B:649:LYS:N	2.79	0.50
4:C:82:TYR:O	4:C:83:SER:C	2.49	0.50
2:A:401:GLY:C	2:A:435:HIS:CD2	2.83	0.50
2:A:853:ASP:C	2:A:853:ASP:OD1	2.49	0.50
4:C:175:ALA:HB1	11:J:43:ARG:HH12	1.76	0.50
2:A:236:LEU:HD23	2:A:236:LEU:N	2.26	0.50
2:A:507:VAL:N	2:A:508:PRO:CD	2.75	0.50
2:A:503:GLN:HE21	7:F:90:ARG:NH2	2.09	0.50
3:B:295:GLY:H	3:B:298:LEU:HD23	1.77	0.50
2:A:971:PHE:CE2	2:A:1040:GLN:HG2	2.47	0.50
2:A:868:TYR:CD1	2:A:1064:VAL:HG11	2.47	0.50
2:A:356:ASP:HB2	2:A:469:ARG:NH1	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:841:MET:CG	3:B:846:ILE:HD11	2.41	0.50
13:L:60:ARG:HG2	13:L:61:THR:N	2.21	0.50
2:A:1436:ILE:O	2:A:1437:GLY:C	2.49	0.50
4:C:147:LEU:HD12	4:C:151:GLN:O	2.11	0.50
6:E:213:ILE:HG12	6:E:214:CYS:N	2.25	0.50
2:A:1356:ILE:CG2	2:A:1361:SER:HB2	2.41	0.50
3:B:695:ALA:O	3:B:698:GLU:HB3	2.12	0.50
3:B:190:TYR:CE2	11:J:62:ARG:HB3	2.46	0.50
3:B:487:THR:CG2	3:B:488:TYR:N	2.75	0.50
3:B:460:ALA:O	3:B:462:ALA:N	2.45	0.49
4:C:56:THR:HG22	4:C:58:LEU:H	1.76	0.49
4:C:70:ILE:HD12	4:C:70:ILE:H	1.76	0.49
2:A:51:GLY:HA2	2:A:56:PRO:HA	1.94	0.49
3:B:508:LEU:HD22	3:B:508:LEU:H	1.76	0.49
3:B:653:VAL:HG22	3:B:689:LEU:HB3	1.94	0.49
5:D:134:THR:CG2	5:D:135:GLY:N	2.75	0.49
2:A:546:VAL:O	2:A:550:LEU:HG	2.12	0.49
6:E:16:PHE:CZ	6:E:20:LYS:HE2	2.47	0.49
4:C:243:VAL:HG12	4:C:243:VAL:O	2.12	0.49
9:H:82:PRO:C	9:H:84:ALA:H	2.15	0.49
10:I:50:THR:HG22	10:I:52:ILE:H	1.77	0.49
10:I:16:PRO:HB3	10:I:27:PHE:CD2	2.46	0.49
4:C:70:ILE:HD12	4:C:70:ILE:N	2.27	0.49
2:A:1279:ILE:HG23	2:A:1308:THR:OG1	2.13	0.49
3:B:705:MET:N	3:B:710:LEU:HD12	2.19	0.49
2:A:215:SER:HG	2:A:218:ASP:CG	2.16	0.49
11:J:44:TYR:HD2	11:J:44:TYR:N	2.11	0.49
6:E:79:TRP:CD1	6:E:100:ILE:HD11	2.47	0.49
2:A:1148:ILE:HD11	2:A:1198:ASP:CB	2.41	0.49
3:B:315:LYS:N	3:B:316:PRO:HD2	2.26	0.49
5:D:137:ASN:HD22	5:D:138:ASN:N	2.10	0.49
5:D:120:GLU:HA	5:D:123:LEU:HD12	1.94	0.49
11:J:21:TYR:HA	11:J:39:LEU:HD11	1.94	0.49
3:B:97:VAL:HG12	3:B:178:ASN:HD21	1.77	0.49
12:K:10:PHE:N	12:K:10:PHE:CD2	2.79	0.49
4:C:60:ASP:OD2	13:L:60:ARG:NH2	2.45	0.49
3:B:1183:LYS:HE2	3:B:1183:LYS:H	1.78	0.49
5:D:198:LEU:O	5:D:199:ASN:C	2.50	0.49
2:A:1130:GLN:HE21	2:A:1134:ILE:HD11	1.76	0.49
3:B:234:ILE:N	3:B:234:ILE:HD12	2.27	0.49
2:A:942:PHE:C	2:A:942:PHE:CD2	2.86	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:821:GLN:HE22	3:B:851:PHE:N	2.11	0.49
3:B:34:ILE:O	3:B:37:PHE:N	2.44	0.49
4:C:241:ASP:CG	4:C:242:GLN:N	2.65	0.49
3:B:363:HIS:CD2	3:B:585:VAL:HG22	2.47	0.49
3:B:761:HIS:HB2	3:B:1024:ALA:HB2	1.94	0.49
10:I:50:THR:HG23	10:I:52:ILE:HG12	1.94	0.49
6:E:165:LEU:HD22	6:E:170:LEU:O	2.12	0.49
2:A:1005:GLU:O	2:A:1009:ASN:HB2	2.12	0.49
2:A:1007:ILE:C	2:A:1009:ASN:H	2.15	0.49
6:E:136:ASN:OD1	6:E:137:GLU:N	2.45	0.49
2:A:1227:ILE:HG22	2:A:1228:TRP:H	1.75	0.49
9:H:76:THR:HG22	9:H:76:THR:O	2.12	0.49
11:J:5:VAL:O	11:J:6:ARG:O	2.30	0.49
3:B:503:GLY:O	3:B:504:ARG:CB	2.59	0.49
3:B:506:GLY:O	3:B:508:LEU:HD22	2.13	0.49
3:B:684:LEU:N	3:B:684:LEU:HD12	2.13	0.49
2:A:401:GLY:O	2:A:435:HIS:HD2	1.94	0.49
2:A:381:THR:HG23	2:A:383:TYR:H	1.76	0.49
2:A:1444:MET:HG2	8:G:60:ARG:CA	2.39	0.49
2:A:335:ARG:NH1	3:B:1202:LEU:HD13	2.27	0.49
3:B:515:HIS:O	3:B:518:HIS:HB2	2.12	0.49
3:B:558:LEU:C	3:B:560:GLU:N	2.66	0.49
2:A:96:ILE:H	2:A:96:ILE:HD12	1.76	0.49
2:A:1359:ASP:C	2:A:1361:SER:H	2.15	0.49
2:A:1121:GLU:HG3	2:A:1122:PRO:HD2	1.95	0.49
3:B:798:TYR:CE2	4:C:62:PHE:CZ	3.00	0.49
3:B:971:THR:OG1	4:C:61:GLU:HG3	2.12	0.49
5:D:162:ALA:O	5:D:163:VAL:C	2.51	0.49
3:B:1214:PRO:HG2	3:B:1214:PRO:O	2.13	0.49
1:R:16:G:C5	1:R:17:5BU:BR	3.20	0.49
3:B:555:ILE:C	3:B:557:PHE:N	2.65	0.49
2:A:1336:MET:HE2	2:A:1381:LEU:HG	1.94	0.49
3:B:180:TYR:HD1	3:B:180:TYR:H	1.59	0.49
3:B:653:VAL:HG22	3:B:689:LEU:HD22	1.93	0.49
6:E:202:SER:C	6:E:204:THR:H	2.16	0.49
2:A:921:GLY:O	2:A:922:ASP:C	2.50	0.49
10:I:25:LEU:HD12	10:I:26:LEU:H	1.76	0.49
2:A:455:MET:HE3	3:B:1134:GLU:HG3	1.95	0.49
2:A:1011:GLN:NE2	2:A:1015:VAL:HG21	2.27	0.49
4:C:27:LEU:O	4:C:30:ALA:N	2.46	0.49
2:A:157:ASP:C	2:A:159:THR:H	2.15	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:65:THR:O	6:E:69:ILE:HG13	2.12	0.49
2:A:1327:ILE:HG22	6:E:147:HIS:CE1	2.48	0.49
2:A:147:VAL:C	2:A:171:GLN:HE21	2.16	0.49
2:A:399:HIS:O	2:A:401:GLY:N	2.46	0.49
6:E:22:MET:HE1	6:E:26:ARG:HH21	1.77	0.49
2:A:269:ILE:CG1	2:A:299:HIS:HB3	2.42	0.49
3:B:781:PHE:O	3:B:782:LEU:HG	2.13	0.49
6:E:198:ILE:N	6:E:210:SER:O	2.44	0.49
2:A:1304:TRP:O	2:A:1305:VAL:HG23	2.13	0.49
3:B:185:THR:H	3:B:188:ASP:CB	2.24	0.49
2:A:1059:HIS:ND1	7:F:86:THR:HA	2.27	0.49
2:A:567:LYS:HD3	9:H:95:TYR:CG	2.48	0.49
2:A:472:LEU:HD11	3:B:835:GLN:CD	2.33	0.49
4:C:239:PRO:O	4:C:241:ASP:N	2.46	0.49
11:J:23:ASN:O	11:J:25:LEU:N	2.46	0.49
3:B:38:PHE:HD1	3:B:811:TYR:CD2	2.31	0.49
11:J:14:VAL:CG1	11:J:14:VAL:O	2.61	0.49
2:A:71:GLN:HG3	2:A:72:GLU:H	1.78	0.49
3:B:990:ILE:HG22	3:B:991:GLY:N	2.28	0.49
5:D:56:ARG:HA	5:D:148:LEU:HD13	1.95	0.49
3:B:363:HIS:O	3:B:364:ILE:CB	2.61	0.49
13:L:38:LEU:O	13:L:39:SER:HB3	2.13	0.49
5:D:69:ALA:HA	5:D:72:ARG:HG3	1.94	0.49
5:D:190:GLU:HG3	8:G:167:TYR:CD2	2.48	0.49
2:A:768:GLN:NE2	2:A:816:HIS:ND1	2.61	0.48
2:A:877:HIS:C	2:A:878:ILE:CG1	2.80	0.48
3:B:203:PHE:N	3:B:203:PHE:CD1	2.81	0.48
2:A:1206:ASP:CB	2:A:1274:ARG:NH1	2.76	0.48
4:C:6:PRO:HB3	4:C:25:VAL:HG12	1.95	0.48
5:D:54:GLU:O	5:D:58:VAL:HG23	2.13	0.48
2:A:96:ILE:H	2:A:96:ILE:CD1	2.27	0.48
3:B:33:VAL:O	3:B:36:ALA:HB3	2.13	0.48
2:A:1265:ASN:O	2:A:1267:MET:N	2.46	0.48
13:L:44:ASP:O	13:L:45:ALA:HB3	2.13	0.48
2:A:100:LYS:O	2:A:104:GLU:HG3	2.12	0.48
2:A:40:THR:HG22	2:A:41:MET:CG	2.42	0.48
2:A:376:TYR:OH	2:A:498:ARG:HD2	2.13	0.48
4:C:238:ILE:HG22	4:C:243:VAL:HG23	1.94	0.48
2:A:829:VAL:C	2:A:831:THR:N	2.66	0.48
13:L:28:LYS:HB2	13:L:39:SER:HA	1.95	0.48
4:C:226:ASP:O	4:C:227:THR:CB	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1118:VAL:HG23	2:A:1306:LEU:HB2	1.95	0.48
3:B:550:ASP:OD1	3:B:551:PRO:HD2	2.13	0.48
3:B:20:ASP:O	3:B:22:SER:N	2.37	0.48
2:A:1329:THR:CG2	2:A:1330:ASN:N	2.76	0.48
8:G:1:MET:SD	8:G:79:PHE:CE1	3.06	0.48
9:H:116:TYR:HB2	9:H:123:MET:HB3	1.95	0.48
3:B:582:VAL:O	3:B:582:VAL:HG12	2.13	0.48
3:B:205:ILE:O	3:B:207:GLY:N	2.46	0.48
3:B:129:PHE:CD2	3:B:166:PHE:HA	2.49	0.48
3:B:796:LEU:HD12	3:B:797:TYR:H	1.77	0.48
3:B:785:TYR:C	3:B:785:TYR:CD1	2.87	0.48
3:B:1219:ASP:O	3:B:1219:ASP:OD1	2.31	0.48
3:B:507:LYS:HD3	3:B:507:LYS:HA	1.53	0.48
2:A:475:THR:CG2	2:A:476:SER:N	2.77	0.48
8:G:26:LEU:HD12	8:G:56:ILE:HG21	1.93	0.48
6:E:117:THR:HG22	6:E:119:SER:H	1.77	0.48
6:E:28:TYR:CE1	6:E:78:LEU:HD13	2.49	0.48
12:K:57:LEU:N	12:K:76:GLN:O	2.38	0.48
2:A:664:THR:CG2	2:A:665:GLY:N	2.76	0.48
5:D:185:CYS:HB3	5:D:211:LEU:CD2	2.43	0.48
6:E:180:ARG:HH21	6:E:192:ARG:HB2	1.78	0.48
4:C:10:ILE:HG13	12:K:108:GLU:HB3	1.95	0.48
2:A:482:PHE:C	2:A:484:GLY:H	2.16	0.48
9:H:10:PHE:CD1	9:H:10:PHE:N	2.81	0.48
5:D:40:HIS:HB3	8:G:73:LYS:HZ2	1.65	0.48
3:B:648:HIS:CG	3:B:649:LYS:H	2.32	0.48
4:C:35:ARG:NH1	12:K:41:THR:H	2.12	0.48
6:E:179:GLN:HB2	6:E:182:ASP:HB2	1.96	0.48
3:B:405:ARG:HA	3:B:631:GLY:O	2.13	0.48
5:D:51:ASN:OD1	5:D:52:LEU:O	2.32	0.48
6:E:55:ARG:NH1	6:E:113:GLN:NE2	2.61	0.48
3:B:33:VAL:HG21	3:B:638:PHE:CZ	2.48	0.48
3:B:1177:HIS:HB2	3:B:1179:GLN:HE21	1.77	0.48
10:I:100:PHE:N	10:I:100:PHE:CD1	2.81	0.48
2:A:1384:VAL:HG12	2:A:1384:VAL:O	2.13	0.48
4:C:53:THR:O	4:C:153:LEU:HA	2.14	0.48
4:C:66:ARG:NH2	11:J:5:VAL:HG23	2.29	0.48
2:A:901:LEU:CG	2:A:926:GLN:HE21	2.17	0.48
6:E:205:SER:O	6:E:206:GLY:C	2.52	0.48
4:C:179:GLU:HG2	4:C:180:TYR:H	1.78	0.48
3:B:992:ILE:HG13	3:B:993:THR:N	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:58:LYS:O	13:L:59:ALA:O	2.32	0.48
6:E:120:ALA:O	6:E:122:LYS:N	2.46	0.48
4:C:146:LYS:C	4:C:147:LEU:HD23	2.34	0.48
3:B:515:HIS:HB3	3:B:518:HIS:CD2	2.48	0.48
2:A:825:ILE:C	2:A:827:THR:N	2.65	0.48
8:G:31:LEU:CD2	8:G:48:VAL:HG21	2.44	0.48
2:A:17:VAL:HA	3:B:1215:ARG:O	2.13	0.48
3:B:1180:PHE:O	3:B:1181:GLU:HB2	2.13	0.48
5:D:40:HIS:CG	5:D:41:GLN:N	2.82	0.48
11:J:2:ILE:HD11	11:J:57:ILE:CD1	2.44	0.48
2:A:1116:LEU:HG	2:A:1308:THR:CG2	2.32	0.48
2:A:867:ILE:O	2:A:868:TYR:C	2.51	0.48
3:B:642:ASP:CA	3:B:649:LYS:HA	2.35	0.48
4:C:47:ASP:CA	13:L:69:ALA:HB3	2.37	0.48
9:H:128:ASN:O	9:H:128:ASN:OD1	2.31	0.48
2:A:1259:MET:C	2:A:1261:LYS:H	2.17	0.48
2:A:1341:ILE:HG23	2:A:1342:GLU:N	2.27	0.48
5:D:153:ARG:C	5:D:154:PHE:CD1	2.87	0.48
2:A:831:THR:HG23	2:A:832:ALA:N	2.28	0.48
3:B:773:MET:C	3:B:775:LYS:H	2.17	0.48
2:A:450:LEU:HD12	2:A:450:LEU:H	1.78	0.48
10:I:100:PHE:N	10:I:100:PHE:HD1	2.11	0.48
3:B:863:GLU:HG3	3:B:962:LYS:HB2	1.96	0.48
2:A:591:PHE:HA	2:A:595:THR:HG21	1.95	0.48
11:J:64:ASN:HB3	11:J:65:PRO:HD2	1.91	0.48
2:A:858:ASN:ND2	2:A:859:SER:N	2.61	0.48
2:A:1242:VAL:CG1	2:A:1243:VAL:H	2.18	0.48
3:B:980:PHE:CE2	3:B:1094:ARG:HG3	2.49	0.48
2:A:664:THR:HG22	2:A:665:GLY:H	1.75	0.48
3:B:1197:PRO:O	3:B:1200:ALA:N	2.47	0.48
2:A:831:THR:CG2	2:A:832:ALA:N	2.76	0.48
2:A:1127:ASP:HB3	2:A:1130:GLN:HB2	1.96	0.48
2:A:929:LEU:HD23	2:A:983:ILE:CG2	2.44	0.48
3:B:1060:ARG:NE	4:C:202:PRO:HG3	2.29	0.48
2:A:1021:LEU:O	2:A:1024:SER:HB3	2.14	0.48
2:A:774:ARG:HB2	2:A:797:LYS:O	2.13	0.48
3:B:843:GLN:O	3:B:844:SER:C	2.51	0.48
6:E:198:ILE:H	6:E:198:ILE:HD12	1.78	0.48
2:A:566:ILE:HD13	2:A:566:ILE:N	2.29	0.48
9:H:15:VAL:HG22	9:H:26:ILE:HG12	1.96	0.48
3:B:327:ARG:O	3:B:330:ALA:HB3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1450:LEU:O	2:A:1450:LEU:CG	2.61	0.48
2:A:744:LYS:HG2	2:A:748:MET:HE2	1.96	0.48
2:A:1007:ILE:C	2:A:1009:ASN:N	2.67	0.48
2:A:543:LEU:O	2:A:545:GLN:N	2.46	0.48
4:C:183:TRP:CZ2	4:C:207:CYS:HB3	2.49	0.48
2:A:1128:GLN:HG3	2:A:1129:GLU:N	2.29	0.48
3:B:731:VAL:HG12	3:B:732:SER:N	2.29	0.48
4:C:39:ALA:HA	4:C:164:ALA:HB3	1.95	0.48
3:B:476:ARG:NH1	3:B:476:ARG:HA	2.19	0.48
2:A:26:GLU:O	2:A:29:ALA:N	2.46	0.48
2:A:269:ILE:CD1	2:A:300:VAL:HA	2.43	0.48
3:B:806:THR:CG2	3:B:808:ALA:HB3	2.44	0.48
2:A:583:PRO:HG2	2:A:586:ILE:CD1	2.43	0.48
2:A:313:GLN:O	2:A:314:ALA:HB3	2.14	0.48
9:H:83:GLN:C	9:H:85:GLY:H	2.16	0.48
8:G:59:GLY:HA3	8:G:70:PHE:CE2	2.49	0.48
4:C:263:THR:C	4:C:265:MET:H	2.17	0.48
11:J:1:MET:H1	11:J:56:LEU:H	1.62	0.47
2:A:567:LYS:HZ2	9:H:46:LEU:C	2.17	0.47
2:A:372:LYS:HA	2:A:435:HIS:ND1	2.28	0.47
3:B:1102:LYS:O	3:B:1103:ILE:C	2.51	0.47
3:B:1183:LYS:HE3	3:B:1183:LYS:N	2.29	0.47
4:C:148:ARG:CG	4:C:149:LYS:N	2.75	0.47
2:A:166:GLY:O	2:A:167:CYS:CB	2.62	0.47
2:A:1002:GLY:HA3	2:A:1007:ILE:HG21	1.96	0.47
2:A:276:LEU:HD21	2:A:293:GLU:HG3	1.95	0.47
3:B:878:GLN:O	3:B:878:GLN:OE1	2.33	0.47
2:A:249:SER:O	2:A:250:ILE:CG1	2.52	0.47
3:B:272:THR:N	3:B:273:LEU:HD13	2.28	0.47
3:B:1001:PHE:CD2	4:C:34:ARG:NH2	2.82	0.47
3:B:955:THR:HG23	13:L:54:ARG:O	2.13	0.47
3:B:955:THR:OG1	13:L:55:ILE:HA	2.14	0.47
3:B:977:GLY:HA3	3:B:1099:VAL:CG2	2.43	0.47
2:A:14:VAL:HG21	3:B:1216:LEU:HD12	1.96	0.47
4:C:79:GLN:O	4:C:127:ARG:NH1	2.47	0.47
4:C:73:GLN:N	4:C:131:HIS:O	2.47	0.47
4:C:7:GLN:HG2	12:K:104:ASN:HD22	1.78	0.47
5:D:185:CYS:CB	5:D:211:LEU:HD22	2.44	0.47
6:E:3:GLN:HG3	6:E:4:GLU:N	2.29	0.47
2:A:1226:VAL:HG12	2:A:1227:ILE:N	2.29	0.47
4:C:206:ASN:OD1	4:C:229:TYR:CD2	2.67	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:117:SER:HA	9:H:121:LEU:O	2.14	0.47
2:A:920:LEU:HD23	2:A:920:LEU:C	2.34	0.47
2:A:62:ASP:HB3	2:A:64:ASN:ND2	2.29	0.47
2:A:873:MET:C	2:A:1058:VAL:HG23	2.34	0.47
4:C:114:TYR:OH	11:J:19:GLU:OE2	2.32	0.47
10:I:68:LEU:HB3	10:I:84:VAL:CG2	2.43	0.47
3:B:285:ILE:O	3:B:289:LEU:HB2	2.14	0.47
3:B:429:PHE:C	3:B:431:TYR:H	2.18	0.47
3:B:446:LEU:O	3:B:447:ALA:CB	2.62	0.47
2:A:1423:GLY:HA3	2:A:1426:GLU:HG2	1.95	0.47
3:B:466:TRP:O	3:B:467:GLY:C	2.52	0.47
4:C:65:HIS:O	4:C:69:LEU:HD13	2.13	0.47
2:A:61:ILE:O	2:A:63:ARG:N	2.48	0.47
2:A:68:GLN:C	2:A:70:CYS:N	2.67	0.47
2:A:774:ARG:NH2	2:A:797:LYS:HG3	2.30	0.47
3:B:1072:MET:CE	3:B:1087:PHE:HD1	2.27	0.47
3:B:831:SER:HB3	3:B:994:TYR:OH	2.14	0.47
4:C:83:SER:C	4:C:85:ASP:H	2.18	0.47
2:A:527:THR:CG2	2:A:650:GLN:HA	2.45	0.47
2:A:1385:THR:O	2:A:1387:HIS:N	2.48	0.47
3:B:763:GLN:HG2	3:B:765:PRO:HD2	1.96	0.47
2:A:472:LEU:O	2:A:475:THR:HG22	2.15	0.47
3:B:205:ILE:CD1	3:B:205:ILE:N	2.71	0.47
12:K:55:LYS:HB2	12:K:81:TYR:CE1	2.49	0.47
12:K:50:LEU:HD13	12:K:75:ILE:HD11	1.96	0.47
12:K:65:HIS:CD2	12:K:67:PHE:H	2.26	0.47
2:A:1074:GLU:C	2:A:1076:ALA:H	2.18	0.47
5:D:185:CYS:SG	5:D:191:ALA:HB2	2.55	0.47
8:G:95:SER:C	8:G:97:HIS:H	2.17	0.47
2:A:1143:LEU:HB2	2:A:1271:ILE:CG2	2.44	0.47
2:A:347:PHE:HE2	2:A:375:THR:HG22	1.78	0.47
2:A:364:VAL:HG13	2:A:364:VAL:O	2.14	0.47
2:A:567:LYS:HG3	2:A:568:PRO:CD	2.35	0.47
3:B:1007:VAL:CG2	3:B:1008:PRO:HD2	2.35	0.47
3:B:821:GLN:HE22	3:B:851:PHE:H	1.62	0.47
2:A:15:LYS:HB3	3:B:1220:ARG:NH2	2.21	0.47
8:G:106:MET:HG2	8:G:107:LYS:N	2.28	0.47
3:B:1050:ILE:HG22	3:B:1051:THR:N	2.28	0.47
12:K:42:LEU:HD23	12:K:46:ILE:HG13	1.96	0.47
2:A:1403:GLU:O	2:A:1404:GLU:HG3	2.14	0.47
11:J:34:THR:O	11:J:35:ALA:C	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:89:PRO:HB2	2:A:204:THR:CG2	2.44	0.47
1:R:30:A:H2'	1:R:31:U:O4'	2.15	0.47
5:D:118:THR:O	5:D:119:ARG:C	2.53	0.47
3:B:644:GLU:HG2	3:B:654:ARG:NH2	2.26	0.47
8:G:115:MET:HB2	8:G:116:PRO:CD	2.36	0.47
13:L:60:ARG:CG	13:L:61:THR:H	2.23	0.47
2:A:382:PRO:HD3	2:A:428:TYR:CD2	2.49	0.47
5:D:195:ILE:O	5:D:198:LEU:HG	2.14	0.47
9:H:81:PRO:CB	9:H:82:PRO:CD	2.91	0.47
4:C:189:THR:CG2	4:C:190:ASP:H	2.27	0.47
2:A:96:ILE:N	2:A:96:ILE:HD12	2.28	0.47
3:B:410:GLY:O	3:B:413:LEU:N	2.47	0.47
3:B:1110:PRO:HG2	3:B:1119:VAL:CG2	2.45	0.47
5:D:191:ALA:C	5:D:193:THR:H	2.17	0.47
5:D:156:ASP:C	5:D:158:GLU:N	2.67	0.47
2:A:427:GLN:HB2	2:A:430:TRP:CE2	2.50	0.47
3:B:773:MET:CE	3:B:985:GLY:HA2	2.44	0.47
4:C:255:VAL:HG21	12:K:94:ILE:HG21	1.97	0.47
1:R:20:A:H2'	1:R:21:G:H8	1.79	0.47
2:A:19:PHE:HB3	2:A:1413:GLY:HA2	1.95	0.47
2:A:698:GLN:HA	10:I:97:MET:O	2.15	0.47
2:A:184:SER:HB3	2:A:199:LEU:HD23	1.96	0.47
3:B:529:GLU:O	3:B:531:GLN:HG2	2.15	0.47
2:A:1057:VAL:CG1	2:A:1058:VAL:H	2.28	0.47
4:C:16:ASP:C	4:C:17:ASN:ND2	2.63	0.47
3:B:579:ARG:CB	3:B:586:TRP:HE1	2.22	0.47
3:B:1201:LYS:HE2	3:B:1205:GLN:CD	2.33	0.47
9:H:93:TYR:CD1	9:H:93:TYR:N	2.82	0.47
2:A:1189:SER:OG	2:A:1190:PRO:HD2	2.15	0.47
2:A:501:LEU:HA	2:A:505:CYS:HB2	1.96	0.47
6:E:88:VAL:CG1	6:E:89:GLY:N	2.78	0.47
12:K:40:HIS:ND1	12:K:61:TYR:OH	2.29	0.47
7:F:109:VAL:HG23	7:F:124:GLU:HG2	1.97	0.47
3:B:825:VAL:HG13	3:B:826:ALA:N	2.30	0.47
2:A:897:TYR:HB3	2:A:936:LEU:HD12	1.95	0.47
3:B:184:ALA:HB1	3:B:188:ASP:HB3	1.97	0.47
2:A:516:SER:O	2:A:518:LYS:N	2.47	0.47
2:A:276:LEU:HD13	2:A:292:ALA:C	2.35	0.47
3:B:386:LEU:O	3:B:389:ALA:N	2.48	0.47
3:B:487:THR:HG22	3:B:488:TYR:N	2.29	0.47
2:A:578:LEU:HD23	2:A:612:ILE:CD1	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:896:ASP:OD1	3:B:898:LEU:HG	2.14	0.47
2:A:532:ARG:O	2:A:533:LYS:C	2.52	0.47
3:B:882:THR:HG21	3:B:884:ARG:HB2	1.96	0.47
8:G:13:LEU:HD21	8:G:17:PHE:CB	2.27	0.47
2:A:595:THR:O	2:A:596:THR:HG23	2.15	0.47
3:B:842:ASN:ND2	3:B:845:SER:H	2.13	0.47
3:B:615:MET:C	3:B:616:ILE:HD12	2.35	0.47
2:A:1434:ALA:O	2:A:1436:ILE:N	2.44	0.47
3:B:244:LEU:HD21	3:B:366:GLN:NE2	2.29	0.47
8:G:27:LYS:O	8:G:30:LEU:HB3	2.15	0.47
3:B:225:VAL:HA	3:B:237:VAL:O	2.14	0.47
2:A:1445:ILE:HD13	8:G:18:PHE:CE2	2.50	0.47
12:K:21:ILE:HG23	12:K:31:VAL:HG11	1.97	0.47
3:B:1156:ASP:HB3	3:B:1198:TYR:N	2.30	0.47
3:B:271:ALA:HB1	3:B:273:LEU:CD1	2.34	0.47
3:B:635:ARG:HH11	3:B:635:ARG:HG3	1.80	0.47
4:C:112:ASN:HB2	4:C:114:TYR:HE1	1.80	0.47
9:H:24:CYS:HB2	9:H:44:VAL:HG21	1.97	0.47
3:B:658:ILE:O	3:B:661:LEU:HB2	2.14	0.47
3:B:526:GLU:O	3:B:526:GLU:HG2	2.14	0.47
2:A:1152:ILE:HG23	2:A:1192:LEU:O	2.14	0.47
5:D:4:SER:O	5:D:5:THR:CB	2.62	0.47
4:C:144:ILE:HG22	4:C:145:CYS:HB3	1.95	0.47
4:C:70:ILE:HG13	4:C:142:VAL:HG11	1.96	0.47
11:J:14:VAL:HG12	11:J:14:VAL:O	2.13	0.47
2:A:476:SER:N	2:A:477:PRO:CD	2.78	0.47
9:H:143:LEU:N	9:H:143:LEU:HD12	2.30	0.47
4:C:213:PRO:O	4:C:214:ASN:HB2	2.14	0.47
2:A:1073:GLY:O	2:A:1076:ALA:HB3	2.14	0.47
8:G:53:ASN:ND2	8:G:53:ASN:N	2.62	0.47
3:B:361:LEU:HD21	3:B:377:PHE:CD2	2.50	0.47
3:B:63:ILE:HD13	3:B:63:ILE:O	2.15	0.47
3:B:912:ILE:O	3:B:938:SER:HB3	2.16	0.47
2:A:997:LEU:HD13	2:A:1018:PHE:CE2	2.50	0.47
6:E:35:VAL:C	6:E:37:LEU:H	2.18	0.47
4:C:234:SER:OG	4:C:235:VAL:N	2.47	0.46
2:A:474:VAL:HG22	2:A:474:VAL:O	2.15	0.46
9:H:99:GLY:N	9:H:118:PHE:CD2	2.84	0.46
2:A:853:ASP:O	2:A:854:ASN:HB2	2.13	0.46
2:A:730:GLY:O	2:A:732:LEU:N	2.48	0.46
3:B:635:ARG:NH1	3:B:635:ARG:HG3	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:203:PHE:HB2	3:B:205:ILE:HD11	1.98	0.46
6:E:23:VAL:HG13	6:E:78:LEU:HD13	1.97	0.46
11:J:48:ARG:HD2	11:J:48:ARG:C	2.36	0.46
3:B:185:THR:O	3:B:188:ASP:N	2.48	0.46
10:I:71:SER:OG	10:I:83:ASN:HB2	2.15	0.46
2:A:1329:THR:HG22	2:A:1330:ASN:N	2.29	0.46
1:R:7:C:H41	1:R:13:G:N2	2.12	0.46
4:C:235:VAL:HG13	11:J:13:VAL:CG2	2.45	0.46
2:A:42:ASP:HB3	2:A:45:GLN:H	1.81	0.46
3:B:653:VAL:HG22	3:B:689:LEU:HD13	1.97	0.46
2:A:867:ILE:O	2:A:870:GLU:N	2.42	0.46
2:A:1017:LEU:HB2	6:E:206:GLY:N	2.15	0.46
3:B:999:MET:HB3	3:B:1007:VAL:HG21	1.96	0.46
2:A:808:LEU:CD2	2:A:813:PHE:HA	2.45	0.46
6:E:20:LYS:O	6:E:23:VAL:N	2.47	0.46
3:B:899:ILE:HG22	3:B:900:ALA:N	2.30	0.46
3:B:593:PRO:O	3:B:595:ARG:N	2.48	0.46
12:K:85:ASP:O	12:K:88:LYS:HB2	2.14	0.46
2:A:852:TYR:CZ	7:F:136:ARG:HG2	2.51	0.46
3:B:896:ASP:C	3:B:896:ASP:OD1	2.54	0.46
2:A:1041:ALA:O	2:A:1044:TRP:HB3	2.16	0.46
11:J:6:ARG:HG2	11:J:13:VAL:HA	1.97	0.46
4:C:238:ILE:HG22	4:C:243:VAL:CG2	2.45	0.46
9:H:62:SER:O	9:H:63:LEU:C	2.53	0.46
6:E:124:VAL:HG13	6:E:132:ILE:CD1	2.41	0.46
4:C:112:ASN:CB	4:C:114:TYR:CE1	2.98	0.46
2:A:898:ARG:HD3	2:A:933:TYR:CD1	2.50	0.46
2:A:79:GLY:HA3	2:A:243:PRO:CG	2.43	0.46
2:A:196:GLU:HG2	2:A:197:PRO:CD	2.44	0.46
2:A:605:MET:HE2	2:A:606:LEU:N	2.29	0.46
9:H:11:GLN:HA	9:H:53:ASP:O	2.15	0.46
2:A:1115:SER:OG	2:A:1116:LEU:N	2.49	0.46
12:K:33:ILE:N	12:K:33:ILE:HD12	2.30	0.46
3:B:205:ILE:C	3:B:207:GLY:N	2.69	0.46
4:C:241:ASP:CG	4:C:242:GLN:H	2.18	0.46
2:A:120:GLU:C	2:A:122:MET:N	2.69	0.46
2:A:344:ARG:C	2:A:345:VAL:CG1	2.84	0.46
3:B:114:PRO:O	3:B:116:GLU:N	2.47	0.46
2:A:89:PRO:C	2:A:204:THR:HG21	2.36	0.46
3:B:903:VAL:HG12	3:B:904:ARG:N	2.30	0.46
4:C:3:GLU:HG2	4:C:4:GLU:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:274:PRO:C	3:B:276:ILE:N	2.66	0.46
2:A:913:LEU:HD11	2:A:915:SER:OG	2.15	0.46
3:B:1051:THR:HG22	3:B:1053:GLU:H	1.81	0.46
3:B:95:ILE:HA	3:B:129:PHE:O	2.14	0.46
3:B:496:ARG:HH12	3:B:539:LEU:HB2	1.79	0.46
2:A:532:ARG:NH1	2:A:532:ARG:HG2	2.30	0.46
2:A:1151:GLU:HA	10:I:44:TYR:O	2.16	0.46
3:B:179:CYS:SG	3:B:181:LEU:HB2	2.55	0.46
3:B:331:LEU:N	3:B:331:LEU:HD12	2.31	0.46
3:B:466:TRP:CD1	3:B:468:GLU:OE2	2.69	0.46
2:A:244:PRO:HG2	2:A:245:PRO:HD2	1.98	0.46
2:A:49:LYS:CD	2:A:55:ASP:HB3	2.44	0.46
2:A:871:ASP:OD2	2:A:873:MET:HB2	2.16	0.46
9:H:43:ASN:OD1	9:H:46:LEU:HG	2.16	0.46
3:B:654:ARG:O	3:B:656:GLY:N	2.49	0.46
5:D:144:THR:O	5:D:144:THR:CG2	2.64	0.46
3:B:1163:CYS:SG	3:B:1165:ILE:N	2.74	0.46
2:A:381:THR:HG23	2:A:383:TYR:N	2.31	0.46
2:A:537:ARG:O	2:A:540:PHE:CE1	2.69	0.46
2:A:539:THR:C	2:A:540:PHE:CD1	2.89	0.46
2:A:1036:ARG:HH11	2:A:1036:ARG:HG2	1.80	0.46
2:A:898:ARG:HB2	2:A:933:TYR:HE1	1.77	0.46
3:B:489:SER:OG	3:B:490:SER:N	2.49	0.46
6:E:186:LEU:C	6:E:189:GLY:H	2.18	0.46
3:B:816:GLU:O	3:B:817:LEU:HD23	2.16	0.46
10:I:54:GLU:OE2	10:I:118:ARG:NH1	2.48	0.46
3:B:729:ILE:O	3:B:729:ILE:HG22	2.15	0.46
1:R:5:C:H4'	1:R:6:A:OP1	2.14	0.46
4:C:46:ILE:HD12	4:C:67:LEU:HB3	1.97	0.46
3:B:822:ASN:HD22	11:J:52:THR:HG21	1.80	0.46
6:E:143:ASN:OD1	6:E:187:TYR:CE1	2.69	0.46
2:A:809:THR:H	2:A:812:GLU:HB2	1.81	0.46
2:A:133:LYS:C	2:A:135:PHE:H	2.19	0.46
2:A:219:PHE:CE2	2:A:231:PRO:HD2	2.51	0.46
6:E:78:LEU:HB2	6:E:107:THR:HB	1.98	0.46
3:B:911:ILE:HD11	3:B:941:LEU:HD13	1.98	0.46
7:F:114:GLU:OE2	7:F:119:ARG:HG2	2.16	0.46
2:A:605:MET:HE2	2:A:607:ILE:HG13	1.97	0.46
2:A:174:ILE:HG23	2:A:182:VAL:O	2.16	0.46
8:G:111:THR:HB	8:G:114:LEU:HB2	1.96	0.46
4:C:58:LEU:N	4:C:58:LEU:HD22	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:767:GLN:HE21	2:A:774:ARG:HD2	1.81	0.46
2:A:860:LEU:HB3	2:A:862:ASN:OD1	2.16	0.46
6:E:153:HIS:ND1	6:E:153:HIS:N	2.64	0.46
2:A:463:ILE:HD12	2:A:464:PRO:O	2.16	0.46
2:A:385:ILE:HG22	2:A:386:ASP:N	2.31	0.46
4:C:112:ASN:HB3	4:C:114:TYR:CE1	2.51	0.46
4:C:43:THR:CG2	4:C:44:LEU:H	2.29	0.46
4:C:86:CYS:C	4:C:88:CYS:H	2.19	0.46
3:B:94:LYS:O	3:B:130:VAL:HA	2.15	0.46
2:A:1409:LEU:CD1	3:B:1207:LEU:HD11	2.44	0.46
2:A:90:VAL:HG12	2:A:297:GLN:HE22	1.77	0.46
2:A:353:ILE:HD13	2:A:487:MET:HE2	1.98	0.46
2:A:836:TYR:CZ	2:A:840:ARG:HD2	2.51	0.46
6:E:157:SER:C	6:E:159:ASP:H	2.19	0.46
6:E:157:SER:HG	6:E:160:GLU:HG3	1.80	0.46
2:A:608:ILE:HD12	2:A:613:ILE:HG13	1.98	0.46
5:D:215:SER:HA	5:D:218:GLU:HB2	1.98	0.46
3:B:639:ILE:HD13	3:B:690:VAL:HA	1.97	0.46
2:A:1327:ILE:HG22	6:E:147:HIS:HE1	1.81	0.46
2:A:1155:ASP:OD2	2:A:1162:VAL:N	2.39	0.46
2:A:913:LEU:HD12	2:A:913:LEU:C	2.36	0.46
6:E:100:ILE:HG23	6:E:105:PHE:HB2	1.98	0.46
2:A:1273:LEU:N	2:A:1273:LEU:HD12	2.31	0.46
3:B:773:MET:C	3:B:775:LYS:N	2.70	0.46
3:B:680:THR:O	3:B:683:SER:OG	2.32	0.46
3:B:644:GLU:CG	3:B:654:ARG:HH22	2.28	0.46
3:B:240:ILE:CG2	3:B:240:ILE:O	2.64	0.46
2:A:399:HIS:CB	2:A:400:PRO:CD	2.94	0.46
3:B:980:PHE:HD2	3:B:1094:ARG:HA	1.81	0.46
2:A:23:SER:HA	2:A:233:TRP:CD1	2.51	0.46
2:A:437:MET:O	2:A:438:ASP:C	2.54	0.46
3:B:1031:LEU:HD23	3:B:1044:ALA:HB2	1.98	0.46
2:A:346:ASP:CG	3:B:1108:ARG:HA	2.37	0.46
2:A:897:TYR:HB3	2:A:936:LEU:CD1	2.46	0.46
2:A:626:ASN:O	2:A:631:HIS:HD2	1.98	0.46
2:A:1021:LEU:O	2:A:1021:LEU:HD12	2.16	0.46
4:C:104:PHE:HD2	4:C:105:GLY:N	2.13	0.46
11:J:24:LEU:HD23	11:J:24:LEU:N	2.30	0.46
1:R:9:G:H5'	1:R:10:A:OP1	2.14	0.45
3:B:508:LEU:O	3:B:509:ALA:C	2.50	0.45
10:I:99:LEU:O	10:I:111:THR:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:42:ILE:CG2	9:H:95:TYR:HE1	2.19	0.45
2:A:350:ARG:O	2:A:351:THR:HG22	2.16	0.45
3:B:296:GLU:O	3:B:299:GLU:HB2	2.16	0.45
3:B:542:MET:HB3	3:B:636:PRO:HD2	1.98	0.45
3:B:203:PHE:HB3	3:B:205:ILE:HD11	1.97	0.45
3:B:806:THR:HA	3:B:1045:SER:OG	2.16	0.45
5:D:123:LEU:HD23	5:D:149:THR:HG21	1.98	0.45
2:A:1333:ILE:O	2:A:1337:GLU:HG3	2.16	0.45
2:A:618:GLU:O	2:A:619:LYS:C	2.54	0.45
3:B:333:PHE:C	3:B:334:ILE:HG12	2.35	0.45
2:A:57:ARG:O	2:A:68:GLN:NE2	2.48	0.45
2:A:908:LEU:O	2:A:909:ASP:C	2.54	0.45
2:A:463:ILE:HD13	2:A:469:ARG:CD	2.46	0.45
3:B:376:PHE:HB3	3:B:586:TRP:CZ3	2.51	0.45
2:A:442:VAL:CB	2:A:489:LEU:HD11	2.42	0.45
3:B:1131:GLY:N	3:B:1134:GLU:OE1	2.48	0.45
2:A:84:ILE:HD11	2:A:270:LEU:HD22	1.98	0.45
3:B:125:SER:O	3:B:126:SER:HB3	2.17	0.45
12:K:53:ASP:HB3	12:K:56:VAL:HG23	1.99	0.45
4:C:77:ILE:CG2	4:C:78:GLU:N	2.79	0.45
3:B:865:LYS:HD3	3:B:870:ILE:O	2.16	0.45
2:A:807:GLY:HA2	3:B:760:ASP:O	2.16	0.45
5:D:51:ASN:O	5:D:52:LEU:C	2.53	0.45
3:B:661:LEU:C	3:B:663:ALA:N	2.69	0.45
7:F:109:VAL:HG12	7:F:110:ASP:N	2.32	0.45
8:G:121:PHE:HB2	8:G:130:TYR:CE2	2.51	0.45
13:L:33:GLU:C	13:L:35:SER:H	2.19	0.45
7:F:96:THR:O	7:F:100:GLN:HG3	2.16	0.45
9:H:113:ALA:HA	9:H:125:LEU:O	2.16	0.45
2:A:737:LEU:HD23	2:A:737:LEU:HA	1.65	0.45
10:I:34:TYR:O	10:I:35:VAL:HG23	2.17	0.45
2:A:244:PRO:CB	2:A:245:PRO:CD	2.94	0.45
2:A:1064:VAL:O	2:A:1064:VAL:HG12	2.15	0.45
3:B:846:ILE:HG23	3:B:974:PRO:CG	2.38	0.45
2:A:523:ILE:HG22	2:A:528:LEU:HB2	1.99	0.45
2:A:1211:GLN:O	2:A:1212:VAL:C	2.55	0.45
2:A:93:VAL:HG23	2:A:304:MET:HE3	1.98	0.45
3:B:797:TYR:CD2	3:B:852:ARG:CB	2.99	0.45
3:B:593:PRO:HG2	3:B:617:ARG:NH2	2.31	0.45
2:A:1431:GLY:HA3	3:B:1197:PRO:HD3	1.98	0.45
2:A:897:TYR:N	2:A:897:TYR:CD1	2.84	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:29:LEU:O	5:D:30:GLY:O	2.35	0.45
5:D:37:GLN:HE22	8:G:5:LYS:HD2	1.79	0.45
4:C:40:GLU:OE1	4:C:254:LYS:NZ	2.49	0.45
8:G:160:ILE:H	8:G:160:ILE:HD12	1.82	0.45
2:A:1170:ILE:HG13	2:A:1170:ILE:H	1.60	0.45
2:A:70:CYS:O	2:A:71:GLN:C	2.53	0.45
3:B:240:ILE:HD13	3:B:241:ARG:N	2.32	0.45
3:B:1169:MET:HE1	3:B:1201:LYS:HA	1.99	0.45
3:B:37:PHE:HE2	3:B:542:MET:HA	1.82	0.45
3:B:616:ILE:CD1	3:B:616:ILE:N	2.74	0.45
2:A:1409:LEU:O	2:A:1412:ALA:HB3	2.16	0.45
2:A:1342:GLU:OE2	6:E:212:ARG:NH1	2.43	0.45
2:A:92:HIS:O	2:A:95:PHE:N	2.46	0.45
3:B:556:THR:O	3:B:556:THR:CG2	2.63	0.45
3:B:604:ARG:O	3:B:606:LYS:N	2.50	0.45
13:L:49:LYS:O	13:L:50:ASP:HB2	2.17	0.45
2:A:98:LYS:O	2:A:102:VAL:N	2.47	0.45
6:E:59:SER:HB3	6:E:81:GLU:HA	1.99	0.45
2:A:494:SER:O	2:A:497:THR:N	2.48	0.45
10:I:8:ARG:O	10:I:10:CYS:N	2.49	0.45
12:K:31:VAL:CG1	12:K:32:VAL:N	2.79	0.45
6:E:144:ILE:HD12	6:E:145:THR:H	1.78	0.45
9:H:127:GLY:N	9:H:130:ARG:HH22	2.12	0.45
2:A:1394:THR:CG2	2:A:1398:MET:SD	2.98	0.45
3:B:1015:HIS:C	3:B:1017:ILE:H	2.20	0.45
2:A:875:ALA:HA	2:A:878:ILE:CD1	2.44	0.45
4:C:35:ARG:NH1	12:K:40:HIS:HB2	2.30	0.45
6:E:78:LEU:C	6:E:78:LEU:HD23	2.36	0.45
4:C:41:ILE:HD12	4:C:41:ILE:N	2.30	0.45
2:A:840:ARG:O	2:A:841:LEU:C	2.54	0.45
3:B:44:VAL:O	3:B:46:GLN:HG3	2.17	0.45
2:A:1263:ILE:O	2:A:1267:MET:HG3	2.16	0.45
3:B:981:ALA:HB2	3:B:987:LYS:HA	1.98	0.45
3:B:872:GLU:HA	3:B:915:THR:O	2.17	0.45
3:B:873:THR:O	3:B:914:LYS:HA	2.16	0.45
3:B:467:GLY:O	3:B:470:LYS:CG	2.64	0.45
8:G:88:ASP:HB3	8:G:144:ARG:HG3	1.99	0.45
11:J:64:ASN:CB	11:J:65:PRO:CD	2.80	0.45
2:A:1385:THR:HG22	2:A:1386:ARG:H	1.80	0.45
3:B:778:MET:HE1	3:B:1094:ARG:CD	2.46	0.45
2:A:22:PHE:CB	3:B:1211:ASN:HD21	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:350:ARG:O	2:A:351:THR:CG2	2.64	0.45
2:A:443:LEU:HD23	2:A:501:LEU:HD22	1.99	0.45
3:B:820:GLY:N	3:B:1091:TYR:OH	2.50	0.45
2:A:264:PHE:O	2:A:267:ALA:N	2.49	0.45
4:C:258:ILE:HD13	12:K:35:PHE:CE2	2.46	0.45
2:A:236:LEU:CD2	2:A:236:LEU:N	2.79	0.45
3:B:903:VAL:CG1	3:B:904:ARG:N	2.80	0.45
3:B:347:LYS:HG3	3:B:348:ARG:H	1.81	0.45
7:F:97:ARG:HA	7:F:97:ARG:HD2	1.69	0.45
2:A:970:THR:O	2:A:970:THR:HG22	2.16	0.45
6:E:92:THR:HG22	6:E:92:THR:O	2.17	0.45
3:B:801:LYS:N	11:J:52:THR:CG2	2.79	0.45
3:B:953:LEU:CD2	3:B:965:LYS:HB2	2.35	0.45
2:A:283:GLY:O	2:A:285:PRO:CD	2.65	0.45
3:B:1013:ASN:OD1	3:B:1015:HIS:N	2.47	0.45
2:A:26:GLU:O	2:A:27:VAL:C	2.54	0.45
2:A:335:ARG:NH1	3:B:1206:GLU:OE2	2.50	0.45
4:C:6:PRO:HB3	4:C:25:VAL:CG1	2.47	0.45
12:K:56:VAL:HG22	12:K:77:THR:HG22	1.99	0.45
2:A:268:ASP:HB3	2:A:299:HIS:CE1	2.52	0.45
2:A:123:ARG:O	2:A:125:ALA:N	2.50	0.45
5:D:153:ARG:HB3	5:D:154:PHE:CD1	2.52	0.45
2:A:881:GLN:HE22	2:A:960:ILE:H	1.64	0.45
3:B:26:THR:O	3:B:29:ASP:HB2	2.16	0.45
3:B:327:ARG:HH22	3:B:371:GLU:HG2	1.82	0.45
3:B:113:TYR:CB	3:B:114:PRO:HD2	2.46	0.45
3:B:258:LEU:O	3:B:259:TYR:O	2.35	0.45
8:G:17:PHE:CD2	8:G:17:PHE:N	2.85	0.45
2:A:901:LEU:N	2:A:926:GLN:NE2	2.58	0.45
3:B:840:ILE:HD13	3:B:994:TYR:HE1	1.81	0.45
4:C:242:GLN:C	4:C:244:VAL:H	2.19	0.45
9:H:63:LEU:C	9:H:90:ALA:HB3	2.37	0.45
4:C:37:MET:SD	4:C:232:VAL:HG21	2.56	0.45
12:K:49:GLU:HG3	12:K:94:ILE:HG12	1.99	0.45
3:B:238:ALA:HB3	3:B:256:VAL:HB	1.99	0.45
3:B:20:ASP:C	3:B:22:SER:H	2.16	0.45
2:A:532:ARG:HG2	2:A:532:ARG:HH11	1.82	0.45
3:B:248:SER:O	3:B:249:ARG:HB2	2.16	0.45
10:I:6:PHE:HB3	10:I:12:ASN:O	2.16	0.45
2:A:1388:GLY:O	2:A:1390:ASN:N	2.50	0.45
7:F:72:LYS:O	7:F:73:ALA:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:459:TYR:CD2	3:B:459:TYR:C	2.90	0.45
8:G:34:VAL:HG11	8:G:74:TYR:CE1	2.52	0.45
2:A:1330:ASN:OD1	2:A:1330:ASN:C	2.55	0.45
2:A:58:LEU:O	2:A:59:GLY:O	2.35	0.45
3:B:843:GLN:O	3:B:846:ILE:N	2.49	0.45
3:B:821:GLN:NE2	3:B:851:PHE:CD2	2.85	0.45
2:A:1364:ASN:O	2:A:1365:TYR:C	2.55	0.45
8:G:1:MET:O	8:G:3:PHE:CD1	2.70	0.45
4:C:77:ILE:HA	4:C:129:ILE:CD1	2.44	0.45
12:K:42:LEU:HD23	12:K:46:ILE:CG1	2.46	0.45
5:D:52:LEU:C	5:D:54:GLU:H	2.19	0.45
3:B:429:PHE:HA	3:B:432:MET:CE	2.47	0.45
2:A:89:PRO:O	2:A:204:THR:HG21	2.17	0.45
4:C:123:ASN:ND2	4:C:125:MET:SD	2.90	0.45
2:A:1433:MET:CE	8:G:63:PRO:HB2	2.46	0.45
10:I:34:TYR:C	10:I:34:TYR:CD2	2.87	0.45
2:A:343:LYS:NZ	3:B:1151:LEU:O	2.30	0.45
2:A:808:LEU:HD22	2:A:813:PHE:HA	1.98	0.45
2:A:1345:ARG:CG	2:A:1372:VAL:HG13	2.43	0.45
3:B:324:ILE:CG2	3:B:325:GLN:N	2.80	0.45
4:C:175:ALA:HB1	11:J:43:ARG:NH1	2.31	0.45
3:B:726:ALA:HB1	3:B:1051:THR:HG21	1.99	0.45
2:A:446:ARG:HD2	2:A:480:ALA:HB2	1.99	0.45
2:A:1076:ALA:HA	2:A:1079:MET:HE3	1.99	0.45
2:A:1299:VAL:HG12	2:A:1300:LYS:H	1.81	0.45
2:A:1291:VAL:HG13	2:A:1292:PRO:N	2.32	0.45
6:E:136:ASN:OD1	6:E:138:ALA:N	2.49	0.45
2:A:738:LYS:HB2	2:A:740:LEU:CD2	2.46	0.45
2:A:40:THR:HG22	2:A:41:MET:HG2	1.98	0.44
2:A:783:THR:CG2	2:A:815:PHE:CE2	2.99	0.44
3:B:1065:GLN:HB2	4:C:201:TRP:CZ3	2.52	0.44
2:A:728:LYS:O	2:A:732:LEU:HG	2.17	0.44
12:K:61:TYR:C	12:K:61:TYR:CD2	2.90	0.44
3:B:289:LEU:HD13	3:B:375:ALA:HB2	1.99	0.44
3:B:313:MET:O	3:B:316:PRO:HD2	2.17	0.44
2:A:565:ILE:O	2:A:570:PRO:HA	2.17	0.44
10:I:101:PHE:HD1	10:I:101:PHE:N	2.15	0.44
7:F:90:ARG:HD3	7:F:155:LEU:CD1	2.47	0.44
2:A:605:MET:CE	2:A:606:LEU:H	2.29	0.44
5:D:205:ASP:O	5:D:208:GLU:N	2.50	0.44
2:A:1278:ASN:O	2:A:1280:GLU:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:104:PHE:CZ	9:H:136:LYS:HG2	2.53	0.44
10:I:7:CYS:SG	10:I:8:ARG:O	2.75	0.44
11:J:3:VAL:HG21	11:J:18:TRP:CG	2.52	0.44
2:A:244:PRO:O	2:A:247:ARG:N	2.40	0.44
8:G:88:ASP:HB3	8:G:144:ARG:CB	2.47	0.44
3:B:800:GLN:CB	11:J:52:THR:HG22	2.47	0.44
9:H:89:LEU:C	9:H:91:ASP:N	2.69	0.44
3:B:292:ILE:HD12	3:B:326:ASP:HA	1.99	0.44
3:B:1051:THR:CG2	3:B:1052:VAL:H	2.29	0.44
3:B:520:GLY:HA2	3:B:748:ILE:HG22	2.00	0.44
4:C:99:LEU:HD23	4:C:99:LEU:N	2.32	0.44
4:C:101:LEU:C	4:C:101:LEU:HD12	2.38	0.44
2:A:92:HIS:HB2	2:A:236:LEU:CD2	2.48	0.44
10:I:32:CYS:HB2	10:I:33:SER:H	1.46	0.44
3:B:549:THR:HG22	3:B:550:ASP:H	1.82	0.44
10:I:74:GLU:HA	10:I:80:SER:O	2.18	0.44
5:D:126:ILE:HD13	5:D:126:ILE:HA	1.87	0.44
8:G:140:LYS:O	8:G:141:SER:C	2.56	0.44
2:A:1372:VAL:HG12	2:A:1373:ASP:H	1.81	0.44
2:A:877:HIS:O	2:A:878:ILE:CG1	2.65	0.44
2:A:1315:GLU:C	2:A:1317:MET:N	2.70	0.44
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.99	0.44
2:A:836:TYR:O	2:A:840:ARG:HD3	2.17	0.44
3:B:350:GLN:C	3:B:352:ALA:N	2.69	0.44
10:I:74:GLU:HB2	10:I:79:HIS:HA	2.00	0.44
3:B:792:MET:HA	3:B:856:PHE:O	2.18	0.44
3:B:766:ARG:HH22	3:B:1020:ARG:HH11	1.65	0.44
2:A:1058:VAL:CG1	2:A:1059:HIS:N	2.81	0.44
9:H:42:ILE:HG23	9:H:43:ASN:N	2.32	0.44
2:A:474:VAL:HG22	2:A:478:TYR:CE1	2.52	0.44
5:D:47:LEU:HD11	8:G:3:PHE:CD2	2.52	0.44
5:D:47:LEU:HD11	8:G:3:PHE:CE2	2.51	0.44
2:A:599:SER:HA	2:A:600:PRO:HD2	1.84	0.44
7:F:74:ILE:CG2	7:F:75:PRO:HD2	2.46	0.44
6:E:84:ASP:O	6:E:86:PRO:HD3	2.18	0.44
3:B:1120:GLU:CG	3:B:1121:GLY:N	2.79	0.44
2:A:608:ILE:C	2:A:610:GLY:N	2.71	0.44
2:A:1260:LEU:O	2:A:1260:LEU:HG	2.16	0.44
3:B:766:ARG:HD3	3:B:766:ARG:HA	1.83	0.44
2:A:404:TYR:N	2:A:415:LEU:HD12	2.33	0.44
4:C:89:GLU:O	4:C:90:ASP:CB	2.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:365:GLY:O	2:A:468:PHE:HA	2.18	0.44
4:C:163:ILE:C	4:C:165:LYS:H	2.21	0.44
8:G:51:TYR:C	8:G:51:TYR:CD2	2.91	0.44
5:D:177:VAL:HG12	5:D:177:VAL:O	2.18	0.44
1:R:6:A:OP1	3:B:210:LYS:HE3	2.17	0.44
3:B:681:TRP:C	3:B:683:SER:N	2.71	0.44
3:B:654:ARG:HH11	3:B:654:ARG:HG3	1.82	0.44
9:H:56:THR:HG21	9:H:145:ARG:HE	1.81	0.44
3:B:98:THR:O	3:B:126:SER:HB2	2.18	0.44
5:D:192:LYS:NZ	5:D:192:LYS:HB3	2.32	0.44
3:B:859:TYR:CZ	3:B:941:LEU:HD12	2.53	0.44
3:B:737:THR:HG22	10:I:66:PRO:HB3	2.00	0.44
2:A:925:LEU:C	2:A:927:VAL:H	2.21	0.44
2:A:289:ILE:C	2:A:291:GLU:N	2.71	0.44
2:A:668:ASP:HA	2:A:741:ASN:OD1	2.17	0.44
2:A:608:ILE:C	2:A:610:GLY:H	2.21	0.44
9:H:4:THR:HA	9:H:60:ALA:CB	2.44	0.44
3:B:801:LYS:O	11:J:52:THR:CG2	2.60	0.44
2:A:255:SER:OG	3:B:918:ILE:HG23	2.18	0.44
4:C:60:ASP:HB3	13:L:67:PHE:CZ	2.53	0.44
9:H:98:TYR:HE1	9:H:139:ASN:HA	1.83	0.44
3:B:287:ARG:HG2	3:B:292:ILE:HA	1.99	0.44
4:C:174:ALA:O	4:C:175:ALA:CB	2.66	0.44
12:K:55:LYS:CB	12:K:81:TYR:CE1	3.01	0.44
2:A:117:GLU:N	2:A:117:GLU:CD	2.69	0.44
2:A:91:PHE:HD2	2:A:96:ILE:HG13	1.82	0.44
3:B:408:LEU:HA	3:B:408:LEU:HD12	1.82	0.44
2:A:1130:GLN:O	2:A:1134:ILE:HG12	2.18	0.44
7:F:103:MET:HE1	8:G:65:ASP:HB2	2.00	0.44
3:B:97:VAL:HG12	3:B:178:ASN:ND2	2.32	0.44
3:B:794:ASN:O	3:B:795:ILE:HD12	2.17	0.44
1:R:2:C:C1'	1:R:3:A:OP1	2.65	0.44
8:G:13:LEU:O	8:G:67:SER:HA	2.17	0.44
10:I:111:THR:CG2	10:I:112:SER:H	2.31	0.44
3:B:800:GLN:CA	11:J:52:THR:HG22	2.48	0.44
8:G:80:LYS:HA	8:G:81:PRO:HD2	1.78	0.44
3:B:635:ARG:HB2	3:B:636:PRO:HD2	1.99	0.44
4:C:44:LEU:HB2	4:C:77:ILE:HD12	2.00	0.44
4:C:77:ILE:HG23	4:C:78:GLU:N	2.32	0.44
2:A:1410:PHE:C	2:A:1412:ALA:H	2.20	0.44
6:E:61:GLN:HB2	6:E:79:TRP:CZ3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:120:GLU:O	2:A:122:MET:N	2.51	0.44
2:A:899:VAL:CG2	2:A:1029:ARG:HG2	2.48	0.44
2:A:899:VAL:HB	2:A:929:LEU:CD1	2.48	0.44
12:K:79:GLU:HG2	12:K:80:GLY:N	2.31	0.44
2:A:1329:THR:HB	2:A:1335:ILE:HD11	1.99	0.44
2:A:779:PHE:HE1	2:A:785:PRO:HD3	1.66	0.44
2:A:767:GLN:OE1	2:A:799:PHE:HB2	2.18	0.44
3:B:579:ARG:HB2	3:B:586:TRP:CE2	2.53	0.44
9:H:89:LEU:O	9:H:91:ASP:N	2.49	0.44
2:A:374:LEU:HB2	2:A:436:ILE:CD1	2.48	0.44
4:C:29:MET:CE	12:K:98:LEU:HG	2.46	0.44
2:A:964:ILE:CD1	2:A:1045:VAL:HG21	2.48	0.44
3:B:221:ASN:OD1	3:B:242:SER:HA	2.18	0.44
10:I:15:TYR:CD1	10:I:15:TYR:N	2.86	0.44
4:C:56:THR:CG2	4:C:57:VAL:N	2.80	0.44
2:A:868:TYR:OH	2:A:1366:ARG:HD3	2.18	0.44
2:A:567:LYS:NZ	9:H:47:PHE:CB	2.81	0.44
2:A:23:SER:O	2:A:26:GLU:N	2.50	0.44
3:B:758:PHE:CE1	3:B:1044:ALA:HB1	2.53	0.44
3:B:405:ARG:HE	3:B:629:ASP:HB3	1.82	0.44
3:B:51:PHE:O	3:B:55:VAL:HG23	2.17	0.44
2:A:75:ASN:O	2:A:76:GLU:CB	2.66	0.44
6:E:138:ALA:HA	6:E:141:VAL:HG23	2.00	0.44
2:A:1192:LEU:HG	2:A:1193:LEU:N	2.33	0.44
3:B:763:GLN:O	3:B:764:SER:C	2.57	0.43
6:E:89:GLY:HA2	6:E:117:THR:OG1	2.17	0.43
11:J:7:CYS:CA	11:J:49:MET:HE3	2.48	0.43
3:B:560:GLU:O	3:B:561:TRP:CD1	2.71	0.43
5:D:130:LEU:C	5:D:132:GLN:N	2.69	0.43
5:D:176:GLU:C	5:D:178:ALA:H	2.21	0.43
2:A:700:ASN:HB2	10:I:98:VAL:HG22	2.00	0.43
3:B:620:ARG:NH2	10:I:89:GLN:NE2	2.66	0.43
3:B:578:THR:O	3:B:578:THR:HG22	2.17	0.43
2:A:1220:PHE:O	2:A:1221:LYS:HB2	2.17	0.43
3:B:491:THR:O	3:B:492:LEU:C	2.55	0.43
2:A:1162:VAL:HG12	2:A:1162:VAL:O	2.18	0.43
2:A:500:GLU:OE1	3:B:1143:ALA:C	2.56	0.43
2:A:443:LEU:HD11	2:A:455:MET:HB3	2.00	0.43
4:C:44:LEU:HB2	4:C:77:ILE:CD1	2.48	0.43
3:B:129:PHE:CE2	3:B:166:PHE:HA	2.52	0.43
3:B:558:LEU:O	3:B:561:TRP:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:593:PRO:O	3:B:594:ALA:C	2.55	0.43
2:A:852:TYR:HA	2:A:1060:PRO:HB3	2.00	0.43
8:G:87:VAL:CG2	8:G:103:VAL:HG11	2.48	0.43
3:B:102:VAL:HG23	3:B:112:LEU:HB2	1.99	0.43
7:F:90:ARG:HD3	7:F:155:LEU:HD12	1.98	0.43
2:A:587:HIS:HA	2:A:607:ILE:O	2.18	0.43
3:B:225:VAL:HG12	3:B:238:ALA:HA	2.01	0.43
4:C:152:GLU:HG2	4:C:153:LEU:H	1.82	0.43
2:A:1276:VAL:HG12	2:A:1277:GLU:N	2.33	0.43
13:L:70:ARG:HG2	13:L:70:ARG:HH11	1.83	0.43
2:A:774:ARG:H	2:A:774:ARG:HG2	1.55	0.43
2:A:343:LYS:HZ2	3:B:1151:LEU:HG	1.83	0.43
3:B:847:ASP:C	3:B:849:GLY:N	2.72	0.43
1:R:28:5BU:H2'	1:R:29:G:H8	1.81	0.43
2:A:751:SER:OG	3:B:1015:HIS:HE1	2.00	0.43
9:H:116:TYR:O	9:H:122:LEU:HA	2.18	0.43
11:J:49:MET:HB3	11:J:50:ILE:HD12	2.00	0.43
3:B:96:TYR:N	3:B:129:PHE:O	2.40	0.43
2:A:264:PHE:O	2:A:265:LYS:C	2.56	0.43
3:B:496:ARG:HB3	3:B:496:ARG:NH1	2.29	0.43
2:A:964:ILE:HD13	2:A:1045:VAL:CG2	2.48	0.43
11:J:36:LEU:O	11:J:39:LEU:N	2.51	0.43
4:C:27:LEU:O	4:C:28:ALA:C	2.57	0.43
10:I:60:GLN:NE2	10:I:107:SER:OG	2.51	0.43
6:E:6:GLU:O	6:E:6:GLU:HG3	2.18	0.43
2:A:966:ASN:O	2:A:967:ALA:C	2.57	0.43
4:C:58:LEU:N	4:C:58:LEU:CD2	2.81	0.43
9:H:47:PHE:CD2	9:H:95:TYR:HD1	2.36	0.43
3:B:272:THR:OG1	3:B:279:ASP:OD1	2.36	0.43
2:A:464:PRO:HG2	2:A:465:TYR:CD1	2.50	0.43
12:K:7:PHE:HA	12:K:10:PHE:CE2	2.54	0.43
5:D:64:VAL:C	5:D:66:ARG:N	2.72	0.43
9:H:123:MET:HE3	9:H:142:LEU:CD2	2.49	0.43
2:A:1376:THR:HA	2:A:1380:GLY:O	2.19	0.43
2:A:443:LEU:O	2:A:489:LEU:HD12	2.19	0.43
3:B:515:HIS:H	3:B:518:HIS:CD2	2.31	0.43
2:A:344:ARG:O	2:A:345:VAL:HG12	2.18	0.43
7:F:81:THR:HG21	7:F:136:ARG:HD3	1.99	0.43
4:C:183:TRP:CE2	4:C:207:CYS:HB3	2.53	0.43
2:A:19:PHE:O	2:A:1416:ALA:HA	2.18	0.43
3:B:221:ASN:O	3:B:222:ILE:HD13	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:954:TRP:HB3	2:A:955:PRO:HD2	2.00	0.43
3:B:619:ILE:HD12	10:I:65:ASP:HB2	1.99	0.43
2:A:510:GLN:HA	2:A:510:GLN:OE1	2.19	0.43
3:B:743:ILE:HG12	3:B:743:ILE:H	1.49	0.43
11:J:13:VAL:O	11:J:14:VAL:HG23	2.18	0.43
2:A:244:PRO:HG2	2:A:245:PRO:HD3	2.01	0.43
3:B:273:LEU:CD2	3:B:273:LEU:O	2.63	0.43
13:L:51:CYS:HB2	13:L:53:HIS:HD2	1.82	0.43
3:B:215:GLN:NE2	3:B:499:ASN:HD22	2.11	0.43
2:A:353:ILE:HD13	2:A:487:MET:CE	2.48	0.43
2:A:1076:ALA:HA	2:A:1079:MET:CE	2.48	0.43
3:B:45:SER:O	3:B:48:LEU:HB2	2.19	0.43
2:A:1332:PHE:N	2:A:1332:PHE:CD2	2.84	0.43
4:C:254:LYS:O	4:C:256:ALA:N	2.52	0.43
3:B:639:ILE:HD11	3:B:691:GLU:HB2	2.00	0.43
3:B:464:GLY:CA	3:B:479:VAL:O	2.67	0.43
11:J:1:MET:N	11:J:54:VAL:O	2.51	0.43
3:B:684:LEU:HA	3:B:689:LEU:HD12	2.00	0.43
3:B:365:THR:HG23	3:B:367:LEU:CB	2.48	0.43
8:G:78:VAL:HG12	8:G:79:PHE:H	1.84	0.43
3:B:290:GLY:C	3:B:291:ILE:HD12	2.39	0.43
5:D:26:THR:O	5:D:27:LEU:HB2	2.19	0.43
4:C:242:GLN:C	4:C:244:VAL:N	2.72	0.43
4:C:131:HIS:HA	4:C:132:PRO:HD3	1.86	0.43
12:K:87:LEU:O	12:K:88:LYS:C	2.56	0.43
3:B:526:GLU:HB2	3:B:752:ALA:HB3	2.01	0.43
7:F:111:LEU:C	7:F:113:GLY:N	2.68	0.43
4:C:229:TYR:CD1	4:C:229:TYR:N	2.86	0.43
3:B:1030:LEU:HD12	3:B:1030:LEU:HA	1.80	0.43
1:R:2:C:N3	1:R:16:G:C2	2.87	0.43
4:C:186:LEU:CD1	4:C:186:LEU:N	2.81	0.43
13:L:30:ILE:HD11	13:L:59:ALA:HB2	2.00	0.43
2:A:23:SER:O	2:A:25:GLU:N	2.52	0.43
2:A:1434:ALA:HA	2:A:1435:PRO:HD3	1.91	0.43
11:J:47:ARG:C	11:J:49:MET:N	2.72	0.43
7:F:74:ILE:HG22	7:F:75:PRO:N	2.34	0.43
3:B:758:PHE:O	3:B:760:ASP:N	2.51	0.43
4:C:19:ASP:HA	4:C:231:ASN:HA	2.00	0.43
3:B:1026:LEU:HD23	3:B:1086:PHE:CE2	2.54	0.43
6:E:31:THR:O	6:E:35:VAL:HG23	2.18	0.43
1:R:13:G:H4'	2:A:320:ARG:HD3	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:1:MET:HA	11:J:57:ILE:H	1.83	0.43
8:G:49:LEU:HD21	8:G:77:VAL:HG23	1.99	0.43
2:A:902:LEU:O	2:A:903:ASN:HB2	2.19	0.43
2:A:1265:ASN:C	2:A:1267:MET:N	2.70	0.43
2:A:939:ASP:O	2:A:940:ARG:C	2.54	0.43
3:B:1178:ASN:O	3:B:1179:GLN:O	2.36	0.43
3:B:634:TYR:CD1	3:B:692:TYR:HB3	2.53	0.43
1:R:11:U:HO2'	1:R:12:5BU:P	2.42	0.43
4:C:83:SER:O	4:C:85:ASP:N	2.47	0.43
3:B:1208:MET:C	3:B:1210:MET:H	2.22	0.43
8:G:1:MET:HE3	8:G:80:LYS:O	2.19	0.43
2:A:1206:ASP:O	2:A:1207:LEU:HG	2.19	0.43
2:A:265:LYS:HG2	2:A:303:TYR:HA	2.00	0.43
3:B:737:THR:CG2	10:I:66:PRO:HA	2.44	0.43
2:A:1401:SER:O	2:A:1402:PHE:HB2	2.18	0.43
3:B:595:ARG:O	3:B:596:LEU:C	2.57	0.43
2:A:348:SER:HB2	3:B:1128:LEU:HD12	1.99	0.43
2:A:1289:ARG:NH1	2:A:1326:ARG:NH1	2.66	0.43
3:B:449:ASN:ND2	3:B:451:LYS:HB3	2.34	0.43
3:B:1190:ASP:O	3:B:1191:ILE:HD12	2.18	0.43
10:I:8:ARG:H	10:I:34:TYR:HE1	1.66	0.43
3:B:1066:SER:O	3:B:1067:ARG:HD3	2.18	0.43
6:E:164:LEU:HD11	6:E:211:TYR:CE1	2.54	0.43
3:B:1097:HIS:H	3:B:1098:MET:HE2	1.82	0.43
3:B:501:PRO:C	3:B:502:ILE:CG1	2.87	0.43
2:A:714:PHE:O	2:A:718:VAL:HG23	2.19	0.43
6:E:90:VAL:HA	6:E:120:ALA:HB2	2.01	0.43
3:B:983:ARG:CD	3:B:1091:TYR:HB3	2.45	0.43
3:B:806:THR:CG2	3:B:808:ALA:H	2.32	0.43
3:B:782:LEU:HB3	3:B:784:ASN:OD1	2.18	0.43
2:A:586:ILE:HD11	2:A:633:VAL:HG22	2.01	0.43
3:B:431:TYR:CE1	3:B:447:ALA:HB2	2.54	0.43
3:B:27:ALA:C	3:B:29:ASP:N	2.73	0.43
2:A:925:LEU:C	2:A:927:VAL:N	2.72	0.43
2:A:1151:GLU:OE2	10:I:45:ARG:NH1	2.52	0.43
6:E:186:LEU:C	6:E:188:LEU:N	2.71	0.43
3:B:277:LYS:HB2	3:B:278:GLN:H	1.58	0.43
2:A:648:ASN:OD1	2:A:648:ASN:N	2.52	0.43
2:A:901:LEU:O	2:A:921:GLY:N	2.42	0.42
9:H:107:VAL:O	9:H:108:SER:O	2.38	0.42
9:H:116:TYR:HE2	9:H:140:ALA:CB	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:123:MET:HG2	9:H:124:ARG:N	2.32	0.42
4:C:160:LYS:O	4:C:161:LYS:O	2.36	0.42
2:A:960:ILE:O	2:A:961:ARG:C	2.57	0.42
2:A:1007:ILE:O	2:A:1009:ASN:N	2.52	0.42
2:A:276:LEU:HD13	2:A:292:ALA:O	2.19	0.42
2:A:1226:VAL:C	2:A:1227:ILE:HG13	2.39	0.42
2:A:971:PHE:HE2	2:A:1040:GLN:HG2	1.84	0.42
3:B:522:VAL:HG12	3:B:523:CYS:N	2.33	0.42
2:A:682:THR:HA	2:A:685:GLU:HG2	2.00	0.42
6:E:34:GLU:HG2	6:E:34:GLU:O	2.19	0.42
2:A:1161:THR:C	2:A:1163:ILE:H	2.22	0.42
2:A:600:PRO:C	2:A:602:ASP:H	2.22	0.42
10:I:95:THR:HG22	10:I:96:SER:N	2.34	0.42
2:A:135:PHE:CE1	2:A:222:LEU:HD22	2.53	0.42
3:B:121:ASN:HA	3:B:207:GLY:CA	2.49	0.42
11:J:7:CYS:CB	11:J:46:CYS:HB3	2.49	0.42
3:B:95:ILE:CB	3:B:130:VAL:HG22	2.48	0.42
2:A:629:LEU:C	2:A:629:LEU:CD2	2.87	0.42
2:A:332:LYS:O	2:A:333:GLU:HB2	2.19	0.42
13:L:38:LEU:HD12	13:L:38:LEU:C	2.40	0.42
2:A:823:GLY:C	2:A:825:ILE:N	2.71	0.42
3:B:609:ILE:O	3:B:610:ASN:C	2.56	0.42
3:B:236:HIS:CE1	3:B:389:ALA:HA	2.55	0.42
3:B:487:THR:HB	3:B:490:SER:HB3	2.00	0.42
3:B:785:TYR:CD1	3:B:786:ASN:N	2.87	0.42
2:A:578:LEU:HD23	2:A:612:ILE:HD11	2.02	0.42
12:K:102:LYS:O	12:K:106:GLU:HG3	2.18	0.42
2:A:814:PHE:O	2:A:818:MET:HG3	2.19	0.42
1:R:7:C:H3'	1:R:8:U:C5'	2.46	0.42
3:B:510:LYS:HB3	3:B:513:GLN:HB2	2.01	0.42
2:A:870:GLU:HB2	6:E:204:THR:HG21	2.01	0.42
8:G:81:PRO:HB3	8:G:106:MET:HE1	2.01	0.42
9:H:145:ARG:O	9:H:146:ARG:HB2	2.18	0.42
2:A:374:LEU:HB2	2:A:436:ILE:HD11	2.01	0.42
3:B:806:THR:HG21	3:B:808:ALA:HB3	2.01	0.42
3:B:899:ILE:HD12	3:B:911:ILE:HG23	2.02	0.42
4:C:258:ILE:CD1	12:K:42:LEU:HD21	2.48	0.42
9:H:82:PRO:O	9:H:84:ALA:N	2.41	0.42
2:A:481:ASP:OD1	2:A:485:ASP:OD2	2.37	0.42
3:B:1034:VAL:O	3:B:1036:ALA:N	2.52	0.42
2:A:1195:LEU:HD11	2:A:1267:MET:HE1	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1445:ILE:HD11	8:G:68:ALA:HB2	2.01	0.42
3:B:1001:PHE:CE2	3:B:1073:TYR:HB2	2.54	0.42
2:A:630:ILE:CD1	2:A:645:LEU:HD23	2.49	0.42
2:A:523:ILE:CD1	2:A:649:ILE:HG21	2.50	0.42
3:B:1135:ARG:O	3:B:1136:ASP:C	2.56	0.42
11:J:7:CYS:CB	11:J:49:MET:HE3	2.50	0.42
3:B:797:TYR:HE1	3:B:854:LEU:HD21	1.84	0.42
3:B:558:LEU:HD21	3:B:596:LEU:HD11	2.01	0.42
2:A:95:PHE:O	2:A:96:ILE:C	2.56	0.42
9:H:33:GLN:C	9:H:35:GLN:H	2.23	0.42
8:G:22:MET:O	8:G:23:LYS:C	2.57	0.42
12:K:60:ALA:O	12:K:73:LEU:HD12	2.19	0.42
2:A:362:ASP:OD1	2:A:459:ARG:HD2	2.19	0.42
2:A:1335:ILE:HG23	2:A:1339:LEU:HD12	2.00	0.42
3:B:882:THR:O	3:B:883:LEU:CB	2.67	0.42
3:B:683:SER:OG	3:B:684:LEU:HD12	2.19	0.42
3:B:276:ILE:HD11	3:B:355:ILE:HD13	2.02	0.42
2:A:1279:ILE:CD1	2:A:1316:VAL:HG21	2.45	0.42
4:C:191:TYR:CD2	4:C:201:TRP:CD1	3.07	0.42
3:B:501:PRO:HB2	3:B:502:ILE:H	1.64	0.42
2:A:1349:TYR:CB	2:A:1372:VAL:HG21	2.46	0.42
2:A:728:LYS:O	2:A:729:ALA:C	2.56	0.42
2:A:845:LEU:CD2	2:A:1374:VAL:HG21	2.46	0.42
3:B:1115:THR:CG2	3:B:1117:GLN:HG3	2.49	0.42
4:C:143:LEU:HD21	4:C:146:LYS:HE2	2.01	0.42
2:A:352:VAL:HG13	2:A:485:ASP:O	2.20	0.42
2:A:1449:SER:C	2:A:1451:VAL:H	2.22	0.42
4:C:208:GLU:C	4:C:210:GLU:H	2.23	0.42
3:B:186:GLU:HB3	3:B:187:SER:H	1.68	0.42
2:A:37:PHE:HD1	2:A:37:PHE:N	2.17	0.42
3:B:492:LEU:O	3:B:495:LEU:N	2.48	0.42
2:A:715:GLU:O	2:A:716:ASP:C	2.57	0.42
2:A:282:ASN:O	2:A:284:ALA:N	2.53	0.42
6:E:60:PHE:C	6:E:60:PHE:CD2	2.92	0.42
2:A:1329:THR:N	2:A:1335:ILE:HD11	2.28	0.42
2:A:63:ARG:HA	2:A:74:MET:CE	2.50	0.42
2:A:283:GLY:O	2:A:285:PRO:HD2	2.20	0.42
3:B:975:GLN:O	3:B:990:ILE:HG13	2.20	0.42
3:B:615:MET:HA	3:B:625:LYS:O	2.20	0.42
4:C:248:ILE:O	4:C:252:GLN:HB2	2.19	0.42
12:K:50:LEU:HD13	12:K:75:ILE:CD1	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:VAL:CG1	2:A:297:GLN:HA	2.48	0.42
6:E:198:ILE:N	6:E:198:ILE:CD1	2.77	0.42
3:B:555:ILE:O	3:B:557:PHE:N	2.52	0.42
13:L:47:ARG:HG3	13:L:47:ARG:HH11	1.84	0.42
5:D:145:MET:O	5:D:149:THR:N	2.53	0.42
3:B:794:ASN:C	3:B:795:ILE:HD12	2.40	0.42
3:B:823:ALA:O	3:B:1089:PRO:HA	2.20	0.42
5:D:40:HIS:NE2	5:D:41:GLN:HG3	2.34	0.42
1:R:2:C:H1'	1:R:3:A:P	2.60	0.42
2:A:826:ASP:HB2	2:A:830:LYS:HD3	2.02	0.42
3:B:653:VAL:CG2	3:B:689:LEU:HD22	2.50	0.42
5:D:63:LEU:O	5:D:66:ARG:HB3	2.20	0.42
2:A:1373:ASP:CA	2:A:1376:THR:HG22	2.48	0.42
10:I:95:THR:HG22	10:I:96:SER:O	2.20	0.42
5:D:35:LEU:HD21	5:D:173:HIS:HB3	2.02	0.42
3:B:996:ARG:HH12	4:C:174:ALA:HA	1.85	0.42
2:A:134:ARG:NH1	2:A:220:THR:O	2.52	0.42
8:G:98:GLY:HA3	8:G:110:VAL:O	2.19	0.42
3:B:408:LEU:O	3:B:410:GLY:N	2.53	0.42
3:B:48:LEU:O	3:B:49:ASP:C	2.58	0.42
4:C:254:LYS:C	4:C:256:ALA:N	2.73	0.42
5:D:146:GLN:O	5:D:149:THR:N	2.48	0.42
3:B:1060:ARG:C	3:B:1062:HIS:H	2.23	0.42
3:B:936:ASP:OD1	3:B:938:SER:N	2.46	0.42
2:A:818:MET:HE2	2:A:818:MET:HB3	1.91	0.42
3:B:1038:SER:C	3:B:1040:ASN:H	2.22	0.42
3:B:597:MET:O	3:B:600:LEU:N	2.52	0.42
5:D:71:LYS:C	5:D:73:SER:N	2.73	0.42
2:A:393:ARG:O	2:A:395:GLY:N	2.53	0.42
2:A:1225:PHE:O	2:A:1240:CYS:HA	2.18	0.42
8:G:125:SER:OG	8:G:128:PRO:HA	2.18	0.42
2:A:1308:THR:HG23	2:A:1309:ASP:N	2.34	0.42
3:B:763:GLN:C	3:B:765:PRO:HD2	2.40	0.42
3:B:1165:ILE:HG22	5:D:15:LEU:HA	2.01	0.42
2:A:122:MET:O	2:A:123:ARG:C	2.58	0.42
3:B:190:TYR:CD2	11:J:62:ARG:HB3	2.55	0.42
3:B:873:THR:HG22	3:B:874:PHE:N	2.35	0.42
3:B:750:GLY:O	3:B:751:VAL:C	2.58	0.42
3:B:460:ALA:O	3:B:461:LEU:C	2.59	0.42
2:A:590:ARG:HD3	2:A:604:GLY:HA2	2.02	0.42
2:A:860:LEU:HA	2:A:860:LEU:HD23	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:285:PRO:CG	2:A:288:ALA:HB3	2.39	0.42
2:A:730:GLY:C	2:A:732:LEU:N	2.73	0.42
4:C:102:GLN:HG2	4:C:154:LYS:HG2	2.01	0.42
2:A:1004:ASN:C	2:A:1004:ASN:OD1	2.58	0.42
2:A:1214:GLU:C	2:A:1218:GLN:HE21	2.23	0.42
3:B:258:LEU:HD12	3:B:258:LEU:C	2.40	0.42
3:B:63:ILE:HD13	3:B:421:PHE:CZ	2.55	0.42
2:A:974:ASP:C	2:A:976:THR:H	2.23	0.42
2:A:552:TRP:O	2:A:554:PRO:HD3	2.19	0.42
3:B:878:GLN:O	3:B:879:ARG:C	2.57	0.42
2:A:784:LEU:C	2:A:786:HIS:H	2.22	0.42
3:B:843:GLN:N	3:B:994:TYR:O	2.43	0.42
4:C:166:GLU:O	4:C:167:HIS:CB	2.66	0.42
5:D:63:LEU:CD1	5:D:129:LEU:HG	2.45	0.42
2:A:135:PHE:C	2:A:137:ALA:N	2.70	0.42
2:A:23:SER:HB3	2:A:233:TRP:CZ2	2.55	0.42
11:J:47:ARG:HH11	11:J:47:ARG:HG2	1.85	0.42
2:A:789:LYS:HE3	10:I:67:THR:OG1	2.20	0.42
2:A:1062:GLU:OE2	7:F:88:TYR:OH	2.34	0.42
2:A:44:THR:O	2:A:45:GLN:HB2	2.20	0.41
2:A:55:ASP:O	2:A:55:ASP:OD2	2.37	0.41
2:A:500:GLU:OE2	3:B:1145:SER:HB2	2.20	0.41
8:G:145:VAL:CG1	8:G:146:LYS:H	2.23	0.41
2:A:47:ARG:HH12	2:A:254:GLU:HG2	1.84	0.41
3:B:170:LEU:HA	3:B:171:PRO:HD2	1.94	0.41
4:C:77:ILE:C	4:C:79:GLN:H	2.23	0.41
3:B:1034:VAL:HG23	3:B:1059:LEU:HD13	2.02	0.41
2:A:896:ARG:HB3	2:A:897:TYR:CD1	2.55	0.41
2:A:76:GLU:O	2:A:78:PRO:HD3	2.20	0.41
8:G:9:LEU:CG	8:G:10:ASN:N	2.83	0.41
2:A:18:GLN:HG2	2:A:1418:LEU:HD13	2.01	0.41
8:G:166:ASP:C	8:G:168:LEU:H	2.24	0.41
3:B:263:GLY:O	3:B:264:SER:C	2.58	0.41
4:C:11:ARG:O	4:C:12:GLU:C	2.58	0.41
2:A:560:ILE:HG13	9:H:78:SER:HB2	2.02	0.41
8:G:50:ASP:OD1	8:G:50:ASP:O	2.38	0.41
4:C:56:THR:CG2	4:C:57:VAL:H	2.32	0.41
2:A:53:LEU:CD2	2:A:54:ASN:N	2.53	0.41
3:B:276:ILE:CD1	3:B:355:ILE:HG21	2.33	0.41
12:K:6:ARG:O	12:K:8:GLU:N	2.53	0.41
11:J:48:ARG:HE	11:J:49:MET:HE2	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:911:ILE:HD11	3:B:941:LEU:HB2	2.02	0.41
8:G:119:LEU:HD12	8:G:131:GLN:C	2.41	0.41
2:A:185:TRP:CZ3	2:A:200:ARG:HG2	2.55	0.41
3:B:63:ILE:CD1	3:B:421:PHE:CZ	3.03	0.41
2:A:403:LYS:O	2:A:404:TYR:CG	2.73	0.41
2:A:444:PHE:HB3	2:A:458:HIS:CD2	2.55	0.41
2:A:1097:GLY:C	2:A:1099:PRO:HD2	2.41	0.41
3:B:70:ILE:O	3:B:70:ILE:HG22	2.19	0.41
3:B:519:TRP:CD1	3:B:519:TRP:C	2.93	0.41
3:B:769:TYR:O	3:B:772:ALA:N	2.53	0.41
8:G:122:ASN:HD22	8:G:125:SER:HB3	1.80	0.41
2:A:926:GLN:O	2:A:930:ASP:HB2	2.20	0.41
8:G:44:TYR:O	8:G:78:VAL:CG1	2.68	0.41
2:A:600:PRO:CG	2:A:601:LYS:H	2.29	0.41
4:C:44:LEU:HD23	4:C:44:LEU:C	2.41	0.41
5:D:198:LEU:O	5:D:201:LYS:HB2	2.20	0.41
6:E:61:GLN:HG2	6:E:62:ALA:H	1.80	0.41
4:C:189:THR:CG2	4:C:190:ASP:N	2.77	0.41
12:K:27:ALA:HB1	12:K:28:PRO:CD	2.45	0.41
3:B:773:MET:O	3:B:775:LYS:N	2.53	0.41
2:A:744:LYS:HG2	2:A:748:MET:CE	2.51	0.41
3:B:523:CYS:SG	3:B:524:PRO:HD2	2.59	0.41
3:B:1137:CYS:O	3:B:1140:ALA:HB3	2.20	0.41
2:A:260:ASP:O	2:A:261:ASP:C	2.57	0.41
1:R:5:C:O2'	3:B:463:THR:HA	2.21	0.41
12:K:10:PHE:CD1	12:K:11:LEU:CD2	3.04	0.41
3:B:1171:VAL:C	3:B:1172:ILE:HD12	2.39	0.41
3:B:542:MET:HG2	3:B:747:MET:HB3	2.02	0.41
2:A:541:ILE:HG22	2:A:546:VAL:HG23	2.01	0.41
2:A:23:SER:O	2:A:24:PRO:C	2.58	0.41
2:A:1205:LYS:O	2:A:1206:ASP:C	2.59	0.41
2:A:1216:ILE:HA	2:A:1219:THR:OG1	2.19	0.41
2:A:1435:PRO:O	2:A:1436:ILE:HD12	2.20	0.41
4:C:148:ARG:O	4:C:149:LYS:C	2.59	0.41
2:A:242:PRO:HA	2:A:243:PRO:HD2	1.86	0.41
8:G:23:LYS:HE2	8:G:27:LYS:NZ	2.34	0.41
8:G:51:TYR:O	8:G:54:ILE:HG13	2.21	0.41
5:D:176:GLU:O	5:D:178:ALA:N	2.53	0.41
3:B:498:THR:HG22	3:B:498:THR:O	2.21	0.41
4:C:66:ARG:O	4:C:67:LEU:C	2.58	0.41
2:A:779:PHE:CD1	2:A:785:PRO:HD3	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:774:ARG:NE	2:A:797:LYS:CB	2.83	0.41
3:B:801:LYS:N	11:J:52:THR:HG22	2.35	0.41
9:H:43:ASN:C	9:H:45:GLU:H	2.23	0.41
3:B:579:ARG:HD2	3:B:586:TRP:CZ2	2.56	0.41
3:B:1160:VAL:HG12	3:B:1161:HIS:H	1.86	0.41
2:A:913:LEU:HD12	2:A:914:GLU:H	1.81	0.41
2:A:489:LEU:HD12	2:A:490:HIS:N	2.35	0.41
3:B:202:TYR:CE1	3:B:204:ILE:HD11	2.56	0.41
2:A:90:VAL:HG13	2:A:297:GLN:CD	2.41	0.41
10:I:50:THR:CG2	10:I:51:ASN:N	2.82	0.41
2:A:1015:VAL:CG1	2:A:1019:CYS:SG	3.08	0.41
3:B:1109:GLY:HA3	3:B:1110:PRO:HD2	1.80	0.41
2:A:1265:ASN:O	2:A:1268:LEU:N	2.53	0.41
2:A:1359:ASP:C	2:A:1361:SER:N	2.74	0.41
7:F:103:MET:CE	8:G:65:ASP:HB2	2.50	0.41
3:B:798:TYR:CE2	4:C:62:PHE:HZ	2.36	0.41
5:D:12:ARG:O	5:D:14:ARG:N	2.54	0.41
2:A:34:LYS:HD3	2:A:34:LYS:H	1.84	0.41
9:H:76:THR:O	9:H:77:ARG:HB2	2.20	0.41
2:A:18:GLN:O	3:B:1215:ARG:HG2	2.20	0.41
8:G:59:GLY:HA3	8:G:70:PHE:CD2	2.55	0.41
2:A:1143:LEU:HB2	2:A:1271:ILE:HG21	2.01	0.41
9:H:103:LYS:HG2	9:H:104:PHE:N	2.35	0.41
6:E:63:ASN:HA	6:E:64:PRO:HD3	1.87	0.41
3:B:274:PRO:N	3:B:276:ILE:HB	2.36	0.41
3:B:980:PHE:CD2	3:B:1094:ARG:HA	2.55	0.41
9:H:93:TYR:CD2	9:H:143:LEU:HB3	2.55	0.41
2:A:381:THR:HG22	2:A:384:ASN:ND2	2.36	0.41
2:A:341:MET:CE	2:A:843:LYS:NZ	2.82	0.41
4:C:41:ILE:HA	4:C:42:PRO:HD3	1.82	0.41
3:B:95:ILE:C	3:B:95:ILE:HD13	2.41	0.41
12:K:65:HIS:CD2	12:K:66:PRO:HD2	2.56	0.41
2:A:506:ALA:HB1	2:A:508:PRO:HD2	2.03	0.41
13:L:40:LEU:HB3	13:L:41:SER:H	1.72	0.41
3:B:45:SER:O	3:B:48:LEU:N	2.50	0.41
10:I:78:CYS:SG	10:I:103:CYS:SG	3.12	0.41
8:G:126:ASN:HA	8:G:126:ASN:HD22	1.56	0.41
5:D:53:SER:CB	5:D:152:SER:HB3	2.50	0.41
3:B:1084:GLN:H	3:B:1084:GLN:NE2	2.19	0.41
2:A:402:ALA:HA	2:A:434:ARG:HA	2.01	0.41
2:A:1405:THR:HB	2:A:1406:VAL:H	1.76	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:504:ARG:HB2	3:B:507:LYS:HE2	2.03	0.41
3:B:976:ILE:CD1	3:B:992:ILE:HA	2.51	0.41
3:B:1096:ARG:HG2	3:B:1096:ARG:HH11	1.85	0.41
3:B:918:ILE:HG21	3:B:935:ARG:HH11	1.81	0.41
2:A:851:HIS:O	2:A:854:ASN:N	2.44	0.41
3:B:582:VAL:O	3:B:582:VAL:CG1	2.67	0.41
3:B:616:ILE:CG1	3:B:697:GLU:HA	2.51	0.41
2:A:1261:LYS:C	2:A:1264:GLU:H	2.23	0.41
6:E:132:ILE:CD1	6:E:132:ILE:N	2.78	0.41
3:B:378:LEU:O	3:B:378:LEU:HD12	2.20	0.41
3:B:314:LEU:O	3:B:317:CYS:CB	2.68	0.41
3:B:172:ILE:CG2	3:B:173:MET:N	2.83	0.41
6:E:157:SER:C	6:E:159:ASP:N	2.73	0.41
2:A:639:PRO:CD	2:A:640:GLN:N	2.84	0.41
13:L:27:LEU:HD23	13:L:27:LEU:N	2.35	0.41
6:E:66:GLU:HA	6:E:69:ILE:HD12	2.01	0.41
6:E:81:GLU:C	6:E:82:PHE:HD1	2.24	0.41
2:A:152:VAL:HG13	2:A:153:PRO:HD2	2.03	0.41
2:A:390:GLN:O	2:A:394:ASN:ND2	2.53	0.41
9:H:7:ASP:O	9:H:8:ASP:HB2	2.21	0.41
2:A:406:ILE:HG22	2:A:412:ARG:HA	2.03	0.41
3:B:683:SER:O	3:B:685:LEU:N	2.54	0.41
3:B:275:TYR:C	3:B:276:ILE:HD12	2.41	0.41
2:A:463:ILE:HB	2:A:464:PRO:CD	2.50	0.41
9:H:127:GLY:N	9:H:130:ARG:NH2	2.68	0.41
3:B:580:VAL:O	3:B:586:TRP:HD1	2.04	0.41
2:A:478:TYR:O	2:A:479:ASN:HB3	2.21	0.41
6:E:78:LEU:HA	6:E:107:THR:HB	2.03	0.41
3:B:130:VAL:CG1	3:B:131:ASP:N	2.83	0.41
9:H:12:VAL:HA	9:H:28:ALA:CB	2.50	0.41
4:C:100:THR:HG22	4:C:101:LEU:N	2.29	0.41
2:A:605:MET:CE	2:A:607:ILE:HG13	2.50	0.41
2:A:606:LEU:HD23	2:A:614:PHE:CE2	2.55	0.41
3:B:798:TYR:CE2	4:C:62:PHE:CE2	3.09	0.41
5:D:24:ALA:HA	8:G:83:LYS:O	2.20	0.41
4:C:45:ALA:HA	4:C:72:LEU:HD12	2.02	0.41
2:A:99:ILE:HG23	2:A:211:PHE:CZ	2.56	0.41
2:A:65:LEU:O	2:A:66:LYS:C	2.59	0.41
3:B:1012:ILE:N	3:B:1012:ILE:HD13	2.35	0.41
3:B:882:THR:O	3:B:883:LEU:HB2	2.21	0.41
10:I:8:ARG:HB2	10:I:8:ARG:HE	1.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:7:SER:C	2:A:9:ALA:N	2.73	0.41
2:A:7:SER:O	2:A:9:ALA:N	2.54	0.41
2:A:1279:ILE:HD11	2:A:1316:VAL:CG2	2.45	0.41
10:I:85:PHE:HD1	10:I:99:LEU:HD13	1.86	0.41
2:A:1059:HIS:O	2:A:1061:GLY:N	2.54	0.41
2:A:666:ILE:HD12	2:A:667:GLY:N	2.29	0.41
2:A:1242:VAL:O	2:A:1243:VAL:HB	2.21	0.41
3:B:840:ILE:HG23	3:B:992:ILE:HG23	2.03	0.41
2:A:464:PRO:O	2:A:465:TYR:O	2.39	0.41
6:E:161:LYS:C	6:E:163:GLU:N	2.72	0.41
2:A:528:LEU:HD23	2:A:751:SER:HA	2.03	0.41
3:B:918:ILE:HG13	3:B:935:ARG:HD2	2.02	0.41
13:L:60:ARG:HH21	13:L:65:VAL:HG21	1.85	0.41
2:A:711:ARG:O	2:A:714:PHE:N	2.53	0.41
3:B:615:MET:HB3	3:B:626:ILE:HG12	2.03	0.41
2:A:12:ARG:CZ	3:B:1192:TYR:HE2	2.34	0.41
6:E:117:THR:O	6:E:120:ALA:HB3	2.21	0.41
3:B:129:PHE:HA	3:B:165:VAL:O	2.20	0.41
6:E:105:PHE:O	6:E:106:GLN:HB2	2.21	0.41
2:A:481:ASP:OD1	2:A:483:ASP:OD2	2.38	0.41
5:D:51:ASN:C	5:D:52:LEU:O	2.58	0.41
3:B:496:ARG:CB	3:B:496:ARG:HH11	2.31	0.41
3:B:948:ILE:N	3:B:948:ILE:HD12	2.36	0.41
3:B:949:VAL:HG12	3:B:950:ASP:H	1.84	0.41
6:E:55:ARG:H	6:E:84:ASP:CG	2.22	0.41
3:B:1034:VAL:HA	3:B:1037:LEU:HD12	2.03	0.41
3:B:400:HIS:O	3:B:401:PHE:C	2.58	0.41
2:A:575:LYS:O	2:A:576:GLN:O	2.38	0.41
3:B:53:GLN:HG2	3:B:547:VAL:CG2	2.50	0.41
2:A:407:ARG:HD2	2:A:413:ILE:HD11	2.03	0.41
3:B:773:MET:HE1	3:B:985:GLY:HA2	2.03	0.41
2:A:1397:LEU:HB2	2:A:1426:GLU:OE1	2.20	0.41
7:F:103:MET:O	7:F:104:ASN:CB	2.68	0.41
6:E:112:TYR:CE1	6:E:136:ASN:HB2	2.56	0.41
6:E:138:ALA:HA	6:E:141:VAL:CG2	2.51	0.41
2:A:18:GLN:HB2	3:B:1215:ARG:HB2	2.02	0.41
8:G:51:TYR:O	8:G:51:TYR:CD2	2.74	0.41
2:A:417:TYR:O	2:A:418:SER:C	2.59	0.41
6:E:102:GLU:C	6:E:104:ASN:N	2.73	0.41
2:A:226:GLU:O	2:A:226:GLU:HG2	2.21	0.41
2:A:705:LYS:HB2	2:A:708:MET:HE3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:621:THR:HG22	2:A:621:THR:O	2.21	0.41
2:A:603:ASN:HB3	2:A:604:GLY:H	1.62	0.41
2:A:1094:VAL:HG13	2:A:1113:THR:CB	2.51	0.41
3:B:654:ARG:H	3:B:657:HIS:CD2	2.20	0.41
7:F:82:THR:HA	7:F:83:PRO:HD3	1.80	0.41
3:B:1152:MET:HE3	3:B:1157:ALA:CA	2.49	0.41
2:A:514:PRO:CB	2:A:875:ALA:HB3	2.51	0.41
5:D:27:LEU:HD13	5:D:173:HIS:HD2	1.86	0.41
3:B:1045:SER:HB3	3:B:1046:PRO:CD	2.50	0.41
2:A:1198:ASP:HB3	2:A:1201:ALA:HB3	2.03	0.41
3:B:1086:PHE:CG	3:B:1086:PHE:O	2.71	0.41
4:C:163:ILE:O	4:C:165:LYS:N	2.54	0.41
3:B:216:GLU:HA	3:B:406:LEU:HD23	2.03	0.41
3:B:734:HIS:O	3:B:735:ALA:HB2	2.21	0.41
7:F:116:ASP:O	7:F:120:ILE:HG13	2.21	0.41
2:A:310:GLY:O	2:A:312:PRO:HD2	2.21	0.41
4:C:142:VAL:N	11:J:16:ASP:HB3	2.21	0.40
2:A:41:MET:HB3	2:A:48:ALA:O	2.21	0.40
2:A:7:SER:HA	3:B:1175:LEU:HD22	2.02	0.40
2:A:871:ASP:HB3	6:E:204:THR:HG23	2.03	0.40
3:B:976:ILE:O	3:B:976:ILE:HG22	2.20	0.40
3:B:1208:MET:C	3:B:1210:MET:N	2.74	0.40
5:D:48:ILE:N	5:D:48:ILE:CD1	2.84	0.40
2:A:1443:VAL:O	2:A:1444:MET:HG3	2.21	0.40
4:C:238:ILE:HA	4:C:239:PRO:HD3	1.91	0.40
4:C:77:ILE:O	4:C:79:GLN:N	2.54	0.40
3:B:1110:PRO:HG2	3:B:1119:VAL:HG21	2.02	0.40
8:G:83:LYS:HG2	8:G:149:GLY:HA2	2.03	0.40
6:E:184:VAL:C	6:E:186:LEU:H	2.24	0.40
2:A:928:LEU:O	2:A:931:GLU:N	2.55	0.40
9:H:5:LEU:HD22	9:H:133:ASN:O	2.22	0.40
2:A:40:THR:HG22	2:A:41:MET:HG3	2.03	0.40
3:B:680:THR:HB	3:B:681:TRP:H	1.59	0.40
9:H:95:TYR:CE2	9:H:97:MET:HG3	2.56	0.40
3:B:952:VAL:O	3:B:953:LEU:HB3	2.21	0.40
9:H:106:GLU:O	9:H:108:SER:N	2.52	0.40
2:A:255:SER:O	2:A:256:GLN:HG3	2.21	0.40
6:E:23:VAL:CG1	6:E:28:TYR:HD1	2.34	0.40
4:C:111:THR:C	4:C:112:ASN:HD22	2.24	0.40
4:C:114:TYR:C	4:C:116:LYS:H	2.23	0.40
4:C:94:LYS:HB2	4:C:94:LYS:HE3	1.80	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:91:PHE:N	2:A:91:PHE:CD1	2.90	0.40
3:B:640:VAL:HG22	3:B:651:LEU:HD23	2.03	0.40
3:B:346:GLU:N	3:B:349:ILE:HD13	2.36	0.40
3:B:986:GLN:HE22	3:B:1022:THR:HG21	1.85	0.40
4:C:200:GLU:O	4:C:202:PRO:HD3	2.22	0.40
8:G:149:GLY:O	8:G:159:ALA:CB	2.69	0.40
2:A:1280:GLU:O	2:A:1281:ARG:C	2.59	0.40
8:G:95:SER:O	8:G:97:HIS:N	2.54	0.40
2:A:184:SER:HB3	2:A:199:LEU:CD2	2.51	0.40
11:J:59:LYS:HG2	11:J:59:LYS:H	1.62	0.40
2:A:278:THR:O	2:A:278:THR:HG22	2.21	0.40
2:A:1194:ARG:HG2	2:A:1194:ARG:HH11	1.87	0.40
2:A:32:VAL:HG21	2:A:68:GLN:HE22	1.84	0.40
3:B:1094:ARG:HH21	3:B:1098:MET:HG2	1.86	0.40
9:H:128:ASN:CG	9:H:128:ASN:O	2.59	0.40
2:A:489:LEU:HD12	2:A:490:HIS:H	1.87	0.40
3:B:205:ILE:C	3:B:207:GLY:H	2.24	0.40
4:C:143:LEU:HD21	4:C:146:LYS:CE	2.51	0.40
3:B:215:GLN:NE2	3:B:215:GLN:HA	2.36	0.40
3:B:824:ILE:HG22	3:B:824:ILE:O	2.22	0.40
11:J:45:CYS:O	11:J:48:ARG:HG3	2.20	0.40
3:B:911:ILE:O	3:B:911:ILE:HG22	2.21	0.40
2:A:470:LEU:HD21	2:A:487:MET:HE3	2.03	0.40
8:G:87:VAL:HG23	8:G:103:VAL:HG21	2.03	0.40
2:A:30:ILE:HG23	3:B:1170:THR:HG23	2.02	0.40
11:J:21:TYR:HB2	11:J:39:LEU:HD13	2.04	0.40
2:A:174:ILE:HG22	2:A:175:ARG:N	2.36	0.40
1:R:8:U:O2	1:R:8:U:C2'	2.69	0.40
10:I:34:TYR:HE2	10:I:36:GLU:HB3	1.85	0.40
2:A:246:VAL:HG12	2:A:246:VAL:O	2.19	0.40
12:K:47:ARG:HD3	12:K:59:ALA:O	2.22	0.40
2:A:2:VAL:HG21	3:B:1157:ALA:CB	2.50	0.40
2:A:367:PRO:HB3	2:A:465:TYR:O	2.20	0.40
4:C:84:ARG:O	4:C:85:ASP:OD1	2.40	0.40
2:A:1039:LYS:HE3	2:A:1043:ASP:OD2	2.22	0.40
2:A:1349:TYR:O	2:A:1350:LYS:C	2.60	0.40
2:A:442:VAL:HB	2:A:489:LEU:CD1	2.45	0.40
4:C:35:ARG:NH1	12:K:41:THR:N	2.68	0.40
4:C:112:ASN:N	4:C:112:ASN:HD22	2.17	0.40
5:D:195:ILE:O	5:D:195:ILE:CG2	2.62	0.40
2:A:266:LEU:HD21	2:A:303:TYR:CZ	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:212:PRO:CB	4:C:213:PRO:HD2	2.41	0.40
2:A:352:VAL:CG1	2:A:353:ILE:N	2.84	0.40
3:B:53:GLN:HB2	3:B:547:VAL:HG21	2.03	0.40
13:L:28:LYS:HB2	13:L:39:SER:CA	2.52	0.40
8:G:126:ASN:ND2	8:G:127:PRO:HA	2.35	0.40
2:A:1069:ALA:O	2:A:1070:GLN:C	2.58	0.40
6:E:136:ASN:OD1	6:E:136:ASN:C	2.60	0.40
2:A:543:LEU:C	2:A:545:GLN:N	2.74	0.40
3:B:308:TRP:CH2	10:I:45:ARG:HD3	2.56	0.40
2:A:1390:ASN:O	2:A:1390:ASN:ND2	2.55	0.40
2:A:444:PHE:HB3	2:A:458:HIS:HD2	1.87	0.40
10:I:105:SER:O	10:I:106:CYS:HB3	2.19	0.40
2:A:1335:ILE:O	2:A:1335:ILE:HG22	2.22	0.40
8:G:143:ILE:N	8:G:143:ILE:CD1	2.85	0.40
3:B:254:LEU:HG	3:B:273:LEU:HD12	2.03	0.40
2:A:809:THR:OG1	2:A:812:GLU:HG3	2.22	0.40
3:B:1017:ILE:CB	3:B:1018:PRO:CD	3.00	0.40
2:A:254:GLU:HB2	3:B:935:ARG:NH2	2.35	0.40
2:A:574:GLY:O	2:A:577:ILE:HD13	2.22	0.40
10:I:55:THR:HG22	10:I:58:VAL:CG2	2.43	0.40
3:B:906:SER:O	3:B:941:LEU:HD23	2.22	0.40
3:B:1207:LEU:HA	3:B:1207:LEU:HD23	1.85	0.40
3:B:557:PHE:O	3:B:557:PHE:CD2	2.75	0.40
3:B:283:VAL:O	3:B:286:PHE:HB2	2.20	0.40
2:A:562:THR:HA	2:A:563:PRO:HD3	1.82	0.40
2:A:298:PHE:CZ	2:A:314:ALA:HB2	2.56	0.40
2:A:1299:VAL:CG1	2:A:1300:LYS:N	2.84	0.40
13:L:47:ARG:HB3	13:L:48:CYS:H	1.80	0.40
10:I:110:PHE:CD2	10:I:110:PHE:N	2.83	0.40
7:F:99:LEU:HD12	7:F:99:LEU:C	2.41	0.40
2:A:613:ILE:HG22	2:A:614:PHE:CD2	2.55	0.40
2:A:106:VAL:HG13	2:A:112:LYS:H	1.86	0.40
3:B:190:TYR:HD2	11:J:62:ARG:O	2.05	0.40
8:G:114:LEU:HA	8:G:114:LEU:HD12	1.88	0.40
2:A:141:LEU:O	2:A:142:CYS:SG	2.71	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
2	A	1406/1733 (81%)	973 (69%)	278 (20%)	155 (11%)	0 10
3	B	1096/1224 (90%)	754 (69%)	214 (20%)	128 (12%)	0 9
4	C	264/318 (83%)	172 (65%)	62 (24%)	30 (11%)	0 9
5	D	173/221 (78%)	116 (67%)	36 (21%)	21 (12%)	0 8
6	E	212/215 (99%)	155 (73%)	42 (20%)	15 (7%)	1 23
7	F	82/155 (53%)	72 (88%)	9 (11%)	1 (1%)	16 63
8	G	169/171 (99%)	133 (79%)	19 (11%)	17 (10%)	1 13
9	H	129/146 (88%)	89 (69%)	23 (18%)	17 (13%)	0 6
10	I	117/122 (96%)	83 (71%)	23 (20%)	11 (9%)	1 15
11	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0 1
12	K	113/120 (94%)	83 (74%)	25 (22%)	5 (4%)	3 35
13	L	44/70 (63%)	19 (43%)	16 (36%)	9 (20%)	0 2
All	All	3868/4565 (85%)	2684 (69%)	761 (20%)	423 (11%)	0 11

All (423) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	31	SER
2	A	48	ALA
2	A	55	ASP
2	A	57	ARG
2	A	58	LEU
2	A	62	ASP
2	A	65	LEU
2	A	66	LYS
2	A	71	GLN
2	A	74	MET
2	A	93	VAL
2	A	128	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	130	ASP
2	A	167	CYS
2	A	170	THR
2	A	250	ILE
2	A	255	SER
2	A	286	HIS
2	A	311	GLN
2	A	318	SER
2	A	321	PRO
2	A	322	VAL
2	A	336	ILE
2	A	418	SER
2	A	423	ASP
2	A	517	ASN
2	A	536	LEU
2	A	567	LYS
2	A	576	GLN
2	A	1002	GLY
2	A	1115	SER
2	A	1314	SER
2	A	1365	TYR
2	A	1377	THR
2	A	1392	SER
2	A	1405	THR
3	B	21	GLU
3	B	27	ALA
3	B	28	GLU
3	B	45	SER
3	B	58	THR
3	B	100	PRO
3	B	186	GLU
3	B	259	TYR
3	B	274	PRO
3	B	351	TYR
3	B	364	ILE
3	B	401	PHE
3	B	466	TRP
3	B	467	GLY
3	B	468	GLU
3	B	470	LYS
3	B	472	ALA
3	B	474	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	502	ILE
3	B	504	ARG
3	B	510	LYS
3	B	571	PRO
3	B	643	ASP
3	B	709	ASP
3	B	727	LYS
3	B	731	VAL
3	B	751	VAL
3	B	867	GLY
3	B	943	SER
3	B	958	GLN
3	B	1046	PRO
3	B	1069	PHE
3	B	1097	HIS
3	B	1100	ASP
3	B	1157	ALA
3	B	1186	ASP
4	C	87	PHE
4	C	141	GLY
4	C	149	LYS
4	C	161	LYS
4	C	167	HIS
4	C	209	TYR
4	C	212	PRO
4	C	231	ASN
5	D	5	THR
5	D	6	SER
5	D	8	PHE
5	D	15	LEU
5	D	19	GLU
5	D	30	GLY
5	D	169	SER
5	D	199	ASN
6	E	59	SER
6	E	106	GLN
6	E	206	GLY
8	G	2	PHE
8	G	62	LEU
8	G	63	PRO
8	G	139	ILE
9	H	36	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	H	62	SER
9	H	82	PRO
9	H	108	SER
9	H	128	ASN
10	I	9	ASP
10	I	47	GLU
10	I	106	CYS
11	J	6	ARG
11	J	32	GLU
11	J	33	GLY
11	J	55	ASP
11	J	64	ASN
12	K	114	LEU
13	L	50	ASP
13	L	56	LEU
13	L	59	ALA
13	L	60	ARG
2	A	42	ASP
2	A	54	ASN
2	A	59	GLY
2	A	69	THR
2	A	70	CYS
2	A	76	GLU
2	A	111	GLY
2	A	117	GLU
2	A	124	GLN
2	A	131	SER
2	A	149	GLU
2	A	156	ASP
2	A	245	PRO
2	A	249	SER
2	A	257	ARG
2	A	331	GLY
2	A	332	LYS
2	A	335	ARG
2	A	415	LEU
2	A	424	ILE
2	A	544	ASP
2	A	626	ASN
2	A	731	ARG
2	A	789	LYS
2	A	808	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	824	LEU
2	A	875	ALA
2	A	926	GLN
2	A	975	HIS
2	A	1016	THR
2	A	1036	ARG
2	A	1120	LEU
2	A	1122	PRO
2	A	1128	GLN
2	A	1136	SER
2	A	1223	ASP
2	A	1266	THR
2	A	1297	GLU
2	A	1378	GLN
2	A	1386	ARG
2	A	1389	PHE
2	A	1438	THR
2	A	1448	GLU
3	B	108	VAL
3	B	114	PRO
3	B	126	SER
3	B	176	SER
3	B	206	ASN
3	B	282	ILE
3	B	334	ILE
3	B	409	ALA
3	B	430	ARG
3	B	460	ALA
3	B	461	LEU
3	B	475	SER
3	B	476	ARG
3	B	543	SER
3	B	591	ARG
3	B	594	ALA
3	B	605	ARG
3	B	629	ASP
3	B	655	LYS
3	B	688	GLY
3	B	708	GLU
3	B	842	ASN
3	B	881	ASN
3	B	888	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	891	ASP
3	B	901	PRO
3	B	907	GLY
3	B	1016	ALA
3	B	1167	GLY
3	B	1175	LEU
3	B	1179	GLN
3	B	1188	LYS
4	C	78	GLU
4	C	84	ARG
4	C	90	ASP
4	C	240	VAL
5	D	12	ARG
5	D	13	ARG
5	D	16	LYS
5	D	47	LEU
5	D	52	LEU
5	D	131	GLU
5	D	157	GLN
6	E	36	GLU
6	E	38	PRO
6	E	45	LYS
6	E	121	MET
6	E	189	GLY
7	F	154	ASP
8	G	50	ASP
8	G	67	SER
8	G	96	GLN
8	G	154	VAL
8	G	167	TYR
9	H	81	PRO
9	H	140	ALA
10	I	57	GLY
11	J	2	ILE
11	J	8	PHE
11	J	9	SER
11	J	17	LYS
11	J	24	LEU
11	J	28	ASP
11	J	29	GLU
12	K	7	PHE
13	L	35	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	L	53	HIS
2	A	8	SER
2	A	253	ASN
2	A	283	GLY
2	A	360	GLU
2	A	394	ASN
2	A	409	SER
2	A	465	TYR
2	A	516	SER
2	A	592	ASP
2	A	598	LEU
2	A	603	ASN
2	A	716	ASP
2	A	739	ASP
2	A	830	LYS
2	A	846	GLU
2	A	852	TYR
2	A	903	ASN
2	A	968	GLN
2	A	1114	PRO
2	A	1139	GLU
2	A	1224	LEU
2	A	1255	GLU
3	B	65	GLU
3	B	115	GLN
3	B	258	LEU
3	B	278	GLN
3	B	328	GLU
3	B	418	LYS
3	B	465	ASN
3	B	501	PRO
3	B	526	GLU
3	B	540	SER
3	B	556	THR
3	B	559	SER
3	B	641	GLU
3	B	711	GLU
3	B	764	SER
3	B	792	MET
3	B	818	PRO
3	B	869	SER
3	B	1017	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	1035	ALA
3	B	1065	GLN
3	B	1108	ARG
3	B	1153	GLU
3	B	1155	SER
4	C	28	ALA
4	C	77	ILE
4	C	153	LEU
4	C	156	THR
4	C	215	GLU
4	C	216	GLY
5	D	68	ARG
5	D	119	ARG
5	D	120	GLU
6	E	43	LYS
6	E	73	PRO
6	E	205	SER
8	G	17	PHE
8	G	118	ASP
8	G	141	SER
9	H	32	THR
9	H	60	ALA
9	H	84	ALA
9	H	135	LEU
10	I	3	THR
10	I	11	ASN
13	L	51	CYS
2	A	89	PRO
2	A	197	PRO
2	A	219	PHE
2	A	483	ASP
2	A	526	ASP
2	A	543	LEU
2	A	577	ILE
2	A	591	PHE
2	A	605	MET
2	A	639	PRO
2	A	719	VAL
2	A	727	ASP
2	A	759	ALA
2	A	843	LYS
2	A	847	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	958	VAL
2	A	1211	GLN
2	A	1221	LYS
2	A	1281	ARG
2	A	1309	ASP
2	A	1313	LEU
2	A	1395	GLY
3	B	67	SER
3	B	229	ALA
3	B	367	LEU
3	B	447	ALA
3	B	505	ASP
3	B	579	ARG
3	B	597	MET
3	B	712	PRO
3	B	738	PHE
3	B	752	ALA
3	B	758	PHE
3	B	879	ARG
3	B	906	SER
3	B	1144	ALA
3	B	1181	GLU
4	C	110	THR
4	C	142	VAL
4	C	164	ALA
5	D	174	PRO
6	E	44	ALA
8	G	57	GLN
8	G	156	SER
8	G	165	GLU
9	H	17	PRO
9	H	52	GLN
9	H	90	ALA
9	H	107	VAL
10	I	78	CYS
12	K	29	ASN
12	K	41	THR
13	L	44	ASP
2	A	41	MET
2	A	84	ILE
2	A	121	LEU
2	A	386	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	428	TYR
2	A	829	VAL
2	A	842	VAL
2	A	904	THR
2	A	1069	ALA
2	A	1335	ILE
2	A	1341	ILE
2	A	1379	GLY
2	A	1437	GLY
3	B	68	THR
3	B	240	ILE
3	B	260	GLY
3	B	459	TYR
3	B	593	PRO
3	B	598	GLU
3	B	803	LEU
3	B	813	LYS
3	B	848	ARG
3	B	1018	PRO
3	B	1041	GLU
4	C	12	GLU
4	C	18	VAL
4	C	60	ASP
4	C	172	PRO
4	C	175	ALA
6	E	130	ALA
6	E	183	PRO
9	H	59	ILE
10	I	20	LYS
10	I	34	TYR
11	J	14	VAL
11	J	61	LEU
12	K	111	LEU
2	A	232	GLU
2	A	244	PRO
2	A	399	HIS
2	A	599	SER
2	A	1242	VAL
3	B	200	GLY
3	B	305	VAL
3	B	391	ASP
3	B	759	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	942	ARG
3	B	992	ILE
4	C	126	GLY
4	C	176	ILE
5	D	177	VAL
6	E	76	GLY
10	I	62	ILE
10	I	115	LYS
2	A	196	GLU
3	B	729	ILE
4	C	202	PRO
5	D	196	PRO
8	G	15	PRO
9	H	44	VAL
2	A	35	ILE
2	A	51	GLY
2	A	284	ALA
2	A	385	ILE
2	A	1212	VAL
13	L	55	ILE
2	A	396	PRO
2	A	400	PRO
2	A	753	GLY
2	A	986	ILE
8	G	128	PRO
2	A	477	PRO
2	A	652	VAL
2	A	1302	PRO
3	B	551	PRO
2	A	61	ILE
3	B	658	ILE
3	B	1165	ILE
4	C	139	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	1239/1520 (82%)	1146 (92%)	93 (8%)	17 57
3	B	964/1061 (91%)	854 (89%)	110 (11%)	7 37
4	C	234/274 (85%)	211 (90%)	23 (10%)	10 44
5	D	140/200 (70%)	128 (91%)	12 (9%)	13 51
6	E	196/197 (100%)	186 (95%)	10 (5%)	29 69
7	F	74/137 (54%)	63 (85%)	11 (15%)	4 26
8	G	152/152 (100%)	137 (90%)	15 (10%)	10 44
9	H	117/128 (91%)	113 (97%)	4 (3%)	44 79
10	I	113/116 (97%)	97 (86%)	16 (14%)	4 29
11	J	60/65 (92%)	51 (85%)	9 (15%)	3 26
12	K	99/102 (97%)	90 (91%)	9 (9%)	12 48
13	L	40/57 (70%)	37 (92%)	3 (8%)	17 57
All	All	3428/4009 (86%)	3113 (91%)	315 (9%)	11 48

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	11	LEU
2	A	22	PHE
2	A	23	SER
2	A	34	LYS
2	A	37	PHE
2	A	41	MET
2	A	62	ASP
2	A	67	CYS
2	A	70	CYS
2	A	83	HIS
2	A	93	VAL
2	A	105	CYS
2	A	110	CYS
2	A	200	ARG
2	A	205	GLU
2	A	215	SER
2	A	227	VAL
2	A	234	MET
2	A	236	LEU
2	A	245	PRO
2	A	270	LEU
2	A	307	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	320	ARG
2	A	321	PRO
2	A	335	ARG
2	A	337	ARG
2	A	345	VAL
2	A	354	SER
2	A	379	VAL
2	A	388	LEU
2	A	404	TYR
2	A	407	ARG
2	A	408	ASP
2	A	425	GLN
2	A	434	ARG
2	A	443	LEU
2	A	445	ASN
2	A	449	SER
2	A	450	LEU
2	A	451	HIS
2	A	454	SER
2	A	462	VAL
2	A	469	ARG
2	A	487	MET
2	A	493	GLN
2	A	503	GLN
2	A	504	LEU
2	A	527	THR
2	A	560	ILE
2	A	577	ILE
2	A	590	ARG
2	A	598	LEU
2	A	599	SER
2	A	666	ILE
2	A	692	ASP
2	A	711	ARG
2	A	727	ASP
2	A	739	ASP
2	A	740	LEU
2	A	768	GLN
2	A	774	ARG
2	A	821	ARG
2	A	858	ASN
2	A	886	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	903	ASN
2	A	906	HIS
2	A	929	LEU
2	A	930	ASP
2	A	963	ILE
2	A	998	LEU
2	A	1001	ARG
2	A	1029	ARG
2	A	1035	TYR
2	A	1037	LEU
2	A	1067	LEU
2	A	1111	MET
2	A	1113	THR
2	A	1116	LEU
2	A	1122	PRO
2	A	1127	ASP
2	A	1146	VAL
2	A	1295	THR
2	A	1298	TYR
2	A	1300	LYS
2	A	1332	PHE
2	A	1359	ASP
2	A	1364	ASN
2	A	1372	VAL
2	A	1389	PHE
2	A	1393	ASN
2	A	1405	THR
2	A	1436	ILE
2	A	1443	VAL
3	B	30	SER
3	B	44	VAL
3	B	46	GLN
3	B	61	ASP
3	B	63	ILE
3	B	95	ILE
3	B	100	PRO
3	B	106	ASP
3	B	128	LEU
3	B	175	ARG
3	B	188	ASP
3	B	194	GLU
3	B	203	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	217	ARG
3	B	223	VAL
3	B	240	ILE
3	B	250	PHE
3	B	261	ARG
3	B	268	THR
3	B	273	LEU
3	B	277	LYS
3	B	282	ILE
3	B	289	LEU
3	B	298	LEU
3	B	365	THR
3	B	371	GLU
3	B	393	LYS
3	B	401	PHE
3	B	416	LEU
3	B	427	ASP
3	B	429	PHE
3	B	459	TYR
3	B	463	THR
3	B	465	ASN
3	B	468	GLU
3	B	474	SER
3	B	475	SER
3	B	476	ARG
3	B	485	ARG
3	B	490	SER
3	B	496	ARG
3	B	498	THR
3	B	501	PRO
3	B	502	ILE
3	B	504	ARG
3	B	505	ASP
3	B	508	LEU
3	B	510	LYS
3	B	516	ASN
3	B	531	GLN
3	B	549	THR
3	B	570	VAL
3	B	582	VAL
3	B	603	LEU
3	B	615	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	629	ASP
3	B	635	ARG
3	B	638	PHE
3	B	644	GLU
3	B	682	SER
3	B	684	LEU
3	B	694	ASP
3	B	724	ASP
3	B	737	THR
3	B	742	GLU
3	B	743	ILE
3	B	778	MET
3	B	785	TYR
3	B	787	VAL
3	B	796	LEU
3	B	797	TYR
3	B	830	TYR
3	B	831	SER
3	B	835	GLN
3	B	839	MET
3	B	845	SER
3	B	858	SER
3	B	878	GLN
3	B	894	ASP
3	B	901	PRO
3	B	906	SER
3	B	909	ASP
3	B	939	THR
3	B	953	LEU
3	B	964	VAL
3	B	986	GLN
3	B	997	GLU
3	B	999	MET
3	B	1002	THR
3	B	1006	ILE
3	B	1012	ILE
3	B	1018	PRO
3	B	1022	THR
3	B	1037	LEU
3	B	1047	PHE
3	B	1084	GLN
3	B	1095	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	1103	ILE
3	B	1108	ARG
3	B	1112	GLN
3	B	1163	CYS
3	B	1170	THR
3	B	1182	CYS
3	B	1183	LYS
3	B	1185	CYS
3	B	1193	GLN
3	B	1202	LEU
3	B	1211	ASN
3	B	1214	PRO
3	B	1224	PHE
4	C	17	ASN
4	C	22	LEU
4	C	26	ASP
4	C	54	ASN
4	C	57	VAL
4	C	58	LEU
4	C	62	PHE
4	C	74	SER
4	C	89	GLU
4	C	91	HIS
4	C	99	LEU
4	C	104	PHE
4	C	129	ILE
4	C	138	GLU
4	C	145	CYS
4	C	147	LEU
4	C	163	ILE
4	C	166	GLU
4	C	202	PRO
4	C	212	PRO
4	C	233	GLU
4	C	251	LEU
4	C	266	ASP
5	D	47	LEU
5	D	137	ASN
5	D	139	LYS
5	D	148	LEU
5	D	152	SER
5	D	170	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	D	185	CYS
5	D	187	THR
5	D	192	LYS
5	D	193	THR
5	D	208	GLU
5	D	221	TYR
6	E	60	PHE
6	E	78	LEU
6	E	104	ASN
6	E	132	ILE
6	E	153	HIS
6	E	175	LEU
6	E	183	PRO
6	E	184	VAL
6	E	204	THR
6	E	212	ARG
7	F	79	ARG
7	F	81	THR
7	F	90	ARG
7	F	99	LEU
7	F	103	MET
7	F	110	ASP
7	F	111	LEU
7	F	119	ARG
7	F	123	LYS
7	F	148	VAL
7	F	153	VAL
8	G	1	MET
8	G	13	LEU
8	G	15	PRO
8	G	37	SER
8	G	38	CYS
8	G	39	THR
8	G	52	ASP
8	G	55	ASP
8	G	56	ILE
8	G	63	PRO
8	G	74	TYR
8	G	78	VAL
8	G	80	LYS
8	G	126	ASN
8	G	145	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	H	86	ASP
9	H	93	TYR
9	H	95	TYR
9	H	130	ARG
10	I	4	PHE
10	I	7	CYS
10	I	15	TYR
10	I	22	ASN
10	I	31	THR
10	I	32	CYS
10	I	34	TYR
10	I	40	SER
10	I	78	CYS
10	I	85	PHE
10	I	86	PHE
10	I	94	ASP
10	I	100	PHE
10	I	101	PHE
10	I	106	CYS
10	I	110	PHE
11	J	7	CYS
11	J	9	SER
11	J	10	CYS
11	J	16	ASP
11	J	21	TYR
11	J	44	TYR
11	J	46	CYS
11	J	48	ARG
11	J	64	ASN
12	K	10	PHE
12	K	11	LEU
12	K	25	THR
12	K	47	ARG
12	K	50	LEU
12	K	61	TYR
12	K	78	THR
12	K	101	LEU
12	K	114	LEU
13	L	55	ILE
13	L	68	GLU
13	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such

sidechains are listed below:

Mol	Chain	Res	Type
2	A	54	ASN
2	A	64	ASN
2	A	92	HIS
2	A	171	GLN
2	A	225	ASN
2	A	256	GLN
2	A	299	HIS
2	A	306	ASN
2	A	339	ASN
2	A	394	ASN
2	A	435	HIS
2	A	493	GLN
2	A	503	GLN
2	A	631	HIS
2	A	757	ASN
2	A	768	GLN
2	A	786	HIS
2	A	858	ASN
2	A	881	GLN
2	A	903	ASN
2	A	926	GLN
2	A	935	GLN
2	A	994	GLN
2	A	1106	ASN
2	A	1130	GLN
2	A	1218	GLN
2	A	1265	ASN
2	A	1364	ASN
2	A	1393	ASN
2	A	1432	GLN
3	B	46	GLN
3	B	60	GLN
3	B	121	ASN
3	B	178	ASN
3	B	215	GLN
3	B	236	HIS
3	B	363	HIS
3	B	366	GLN
3	B	449	ASN
3	B	469	GLN
3	B	513	GLN
3	B	515	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	516	ASN
3	B	518	HIS
3	B	531	GLN
3	B	538	ASN
3	B	587	HIS
3	B	686	ASN
3	B	821	GLN
3	B	842	ASN
3	B	975	GLN
3	B	1015	HIS
3	B	1065	GLN
3	B	1117	GLN
3	B	1179	GLN
3	B	1193	GLN
3	B	1211	ASN
4	C	17	ASN
4	C	65	HIS
4	C	73	GLN
4	C	112	ASN
4	C	123	ASN
4	C	167	HIS
5	D	39	ASN
5	D	40	HIS
5	D	137	ASN
5	D	173	HIS
5	D	179	GLN
5	D	216	ASN
6	E	8	ASN
6	E	32	GLN
6	E	101	GLN
6	E	104	ASN
6	E	114	ASN
6	E	147	HIS
8	G	53	ASN
8	G	126	ASN
9	H	133	ASN
10	I	12	ASN
10	I	60	GLN
10	I	89	GLN
11	J	64	ASN
12	K	29	ASN
12	K	65	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	L	53	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	31/31 (100%)	16 (51%)	3 (9%)

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	3	A
1	R	6	A
1	R	7	C
1	R	8	U
1	R	9	G
1	R	10	A
1	R	12	5BU
1	R	13	G
1	R	24	A
1	R	25	G
1	R	26	C
1	R	27	5BU
1	R	28	5BU
1	R	29	G
1	R	31	U
1	R	32	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	2	C
1	R	5	C
1	R	6	A

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5BU	R	12	1	13,22,23	2.24	4 (30%)	14,32,35	4.74	5 (35%)
1	5BU	R	17	1	13,22,23	1.65	2 (15%)	14,32,35	4.47	3 (21%)
1	5BU	R	27	1	13,22,23	2.09	2 (15%)	14,32,35	4.48	3 (21%)
1	5BU	R	28	1	13,22,23	2.88	4 (30%)	14,32,35	4.74	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5BU	R	12	1	-	0/3/25/26	0/2/2/2
1	5BU	R	17	1	-	0/3/25/26	0/2/2/2
1	5BU	R	27	1	-	0/3/25/26	0/2/2/2
1	5BU	R	28	1	-	0/3/25/26	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	12	5BU	C4-N3	2.18	1.37	1.33
1	R	28	5BU	C4-N3	2.71	1.38	1.33
1	R	17	5BU	C4-N3	2.87	1.38	1.33
1	R	12	5BU	C6-N1	2.92	1.39	1.35
1	R	27	5BU	C4-N3	3.42	1.39	1.33
1	R	12	5BU	BR-C5	3.72	1.99	1.90
1	R	28	5BU	C6-N1	3.97	1.40	1.35
1	R	17	5BU	C4-C5	4.44	1.44	1.38
1	R	12	5BU	C4-C5	5.89	1.46	1.38
1	R	28	5BU	BR-C5	6.03	2.06	1.90
1	R	27	5BU	C4-C5	6.07	1.46	1.38
1	R	28	5BU	C4-C5	6.70	1.47	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	17	5BU	C5-C4-N3	-8.99	114.40	124.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	27	5BU	C5-C4-N3	-8.50	114.92	124.00
1	R	12	5BU	C5-C4-N3	-8.23	115.21	124.00
1	R	28	5BU	C5-C4-N3	-7.86	115.61	124.00
1	R	12	5BU	BR-C5-C4	-2.05	118.03	121.48
1	R	17	5BU	C5-C6-N1	2.05	123.81	119.79
1	R	27	5BU	C5-C6-N1	2.41	124.51	119.79
1	R	12	5BU	O3'-C3'-C2'	2.48	119.88	111.83
1	R	12	5BU	O4'-C1'-N1	2.91	114.22	108.08
1	R	28	5BU	O3'-C3'-C2'	4.03	124.92	111.83
1	R	17	5BU	C4-N3-C2	13.75	127.13	115.25
1	R	27	5BU	C4-N3-C2	14.02	127.37	115.25
1	R	12	5BU	C4-N3-C2	14.65	127.91	115.25
1	R	28	5BU	C4-N3-C2	14.99	128.20	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	R	12	5BU	4	0
1	R	17	5BU	3	0
1	R	27	5BU	1	0
1	R	28	5BU	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 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	R	23/31 (74%)	0.22	0 100 100	86, 105, 133, 157	0
2	A	1416/1733 (81%)	-0.35	11 (0%) 87 77	22, 86, 159, 180	0
3	B	1112/1224 (90%)	-0.25	15 (1%) 79 65	26, 95, 168, 180	0
4	C	266/318 (83%)	-0.42	0 100 100	47, 82, 139, 156	0
5	D	177/221 (80%)	-0.33	0 100 100	56, 108, 156, 177	0
6	E	214/215 (99%)	-0.09	7 (3%) 50 34	56, 141, 179, 180	0
7	F	84/155 (54%)	-0.52	0 100 100	28, 59, 98, 122	0
8	G	171/171 (100%)	-0.32	0 100 100	54, 82, 124, 133	0
9	H	133/146 (91%)	0.27	6 (4%) 37 24	105, 144, 178, 180	0
10	I	119/122 (97%)	0.02	4 (3%) 49 34	82, 135, 166, 180	0
11	J	65/70 (92%)	-0.53	0 100 100	48, 78, 125, 133	0
12	K	115/120 (95%)	-0.40	1 (0%) 85 74	45, 83, 113, 143	0
13	L	46/70 (65%)	-0.07	1 (2%) 65 50	73, 139, 174, 179	0
All	All	3941/4596 (85%)	-0.28	45 (1%) 82 69	22, 92, 168, 180	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1176	LEU	5.0
3	B	882	THR	4.4
2	A	149	GLU	3.8
3	B	883	LEU	3.6
6	E	51	GLY	3.5
12	K	115	ALA	3.5
3	B	132	VAL	3.5
10	I	119	THR	3.4
2	A	1455	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	56	PRO	3.3
9	H	139	ASN	3.1
9	H	107	VAL	3.1
10	I	120	GLN	3.0
6	E	110	PHE	3.0
3	B	133	LYS	2.9
6	E	2	ASP	2.9
3	B	733	HIS	2.8
9	H	140	ALA	2.7
2	A	257	ARG	2.7
6	E	82	PHE	2.7
3	B	92	PHE	2.7
3	B	473	MET	2.6
3	B	469	GLN	2.6
2	A	115	LEU	2.6
6	E	81	GLU	2.5
2	A	153	PRO	2.5
9	H	59	ILE	2.4
3	B	734	HIS	2.4
9	H	58	THR	2.4
2	A	1126	ALA	2.4
3	B	472	ALA	2.4
10	I	55	THR	2.3
6	E	86	PRO	2.3
3	B	166	PHE	2.3
10	I	100	PHE	2.3
2	A	1256	GLU	2.2
3	B	468	GLU	2.2
3	B	90	ILE	2.1
9	H	144	ILE	2.1
2	A	1175	SER	2.1
6	E	78	LEU	2.1
3	B	474	SER	2.1
13	L	43	THR	2.0
3	B	257	LYS	2.0
2	A	1242	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	5BU	R	17	21/22	0.90	0.18	-	88,105,129,149	0
1	5BU	R	12	21/22	0.88	0.18	-	96,112,134,153	0
1	5BU	R	28	21/22	0.78	0.25	-	130,138,155,167	0
1	5BU	R	27	21/22	0.76	0.24	-	140,148,161,171	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
14	ZN	I	1121	1/1	0.99	0.14	0.21	85,85,85,85	0
14	ZN	A	2456	1/1	0.97	0.11	-0.84	73,73,73,73	0
14	ZN	B	2225	1/1	0.99	0.13	-1.16	66,66,66,66	0
14	ZN	I	1122	1/1	0.99	0.08	-1.27	176,176,176,176	0
14	ZN	L	1071	1/1	0.97	0.05	-1.33	114,114,114,114	0
14	ZN	C	1269	1/1	0.98	0.07	-1.41	48,48,48,48	0
14	ZN	A	2457	1/1	0.99	0.10	-1.59	46,46,46,46	0
14	ZN	J	1066	1/1	0.99	0.13	-2.45	65,65,65,65	0
15	MG	A	2458	1/1	0.98	0.35	-	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.