Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 03:30 AM EDT

PDB ID	:	3GTP
Title	:	Backtracked RNA polymerase II complex with 24mer RNA
Authors	:	Wang, D.; Bushnell, D.A.; Huang, X.; Westover, K.D.; Levitt, M.; Kornberg, R.D.
Deposited on	:	2009-03-27
Resolution	:	3.90 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

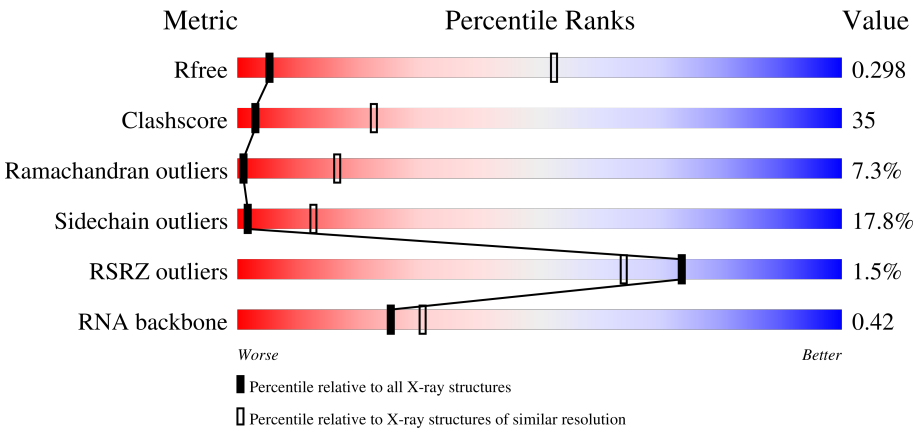
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)
RNA backbone	3102	1040 (4.76-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1733	2% 31% 38% 11% • 20%
2	B	1224	% 34% 44% 10% • 10%
3	C	318	30% 42% 12% • 16%
4	E	215	2% 47% 41% 10% •

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Mol	Chain	Length	Quality of chain
5	F	155	26% 23% 5% 46%
6	H	146	2% 34% 42% 14% 9%
7	I	122	47% 40% 10%
8	J	70	27% 53% 11% 7%
9	K	120	42% 44% 8% 5%
10	L	70	% 26% 24% 14% 34%
11	R	24	8% 17% 17% 12% 46%
12	T	28	14% 61% 25%
13	N	14	7% 21% 57% 21%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ZN	J	101	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 29279 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1395	10969	6917	1923	2068	61	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1106	8792	5568	1538	1631	55	0	0	0

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

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

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

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

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

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

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

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

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 11 is a RNA chain called RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP *UP*GP*CP*AP*GP*AP*CP*GP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
11	R	13	280	126	55	87	12	0	0	0

- Molecule 12 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
12	T	28	566	271	104	164	27	0	0	0

- Molecule 13 is a DNA chain called DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP *GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	N	14	284	137	49	85	13	0	0	0

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

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

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

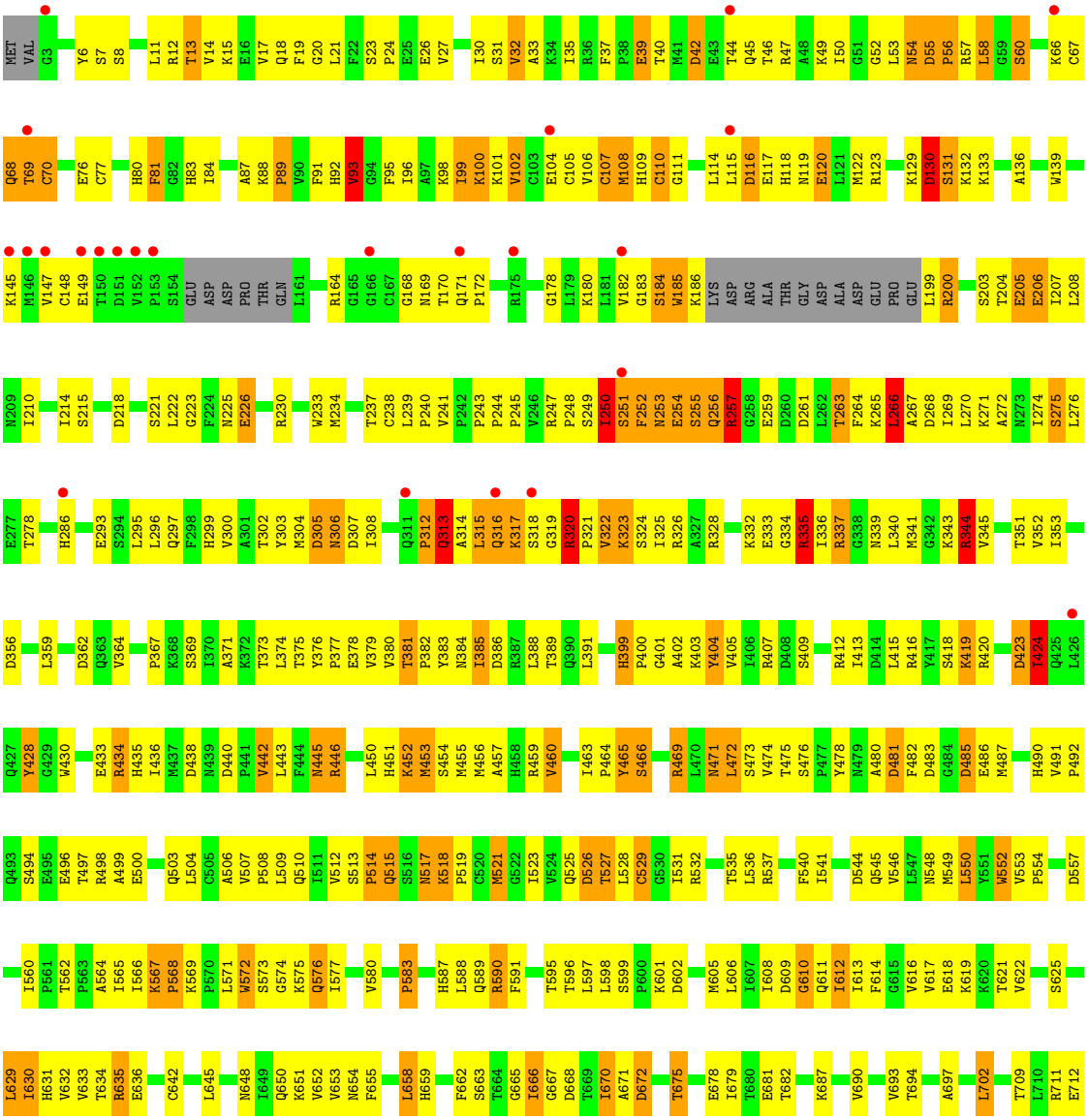
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	A	1	1	1	0	0

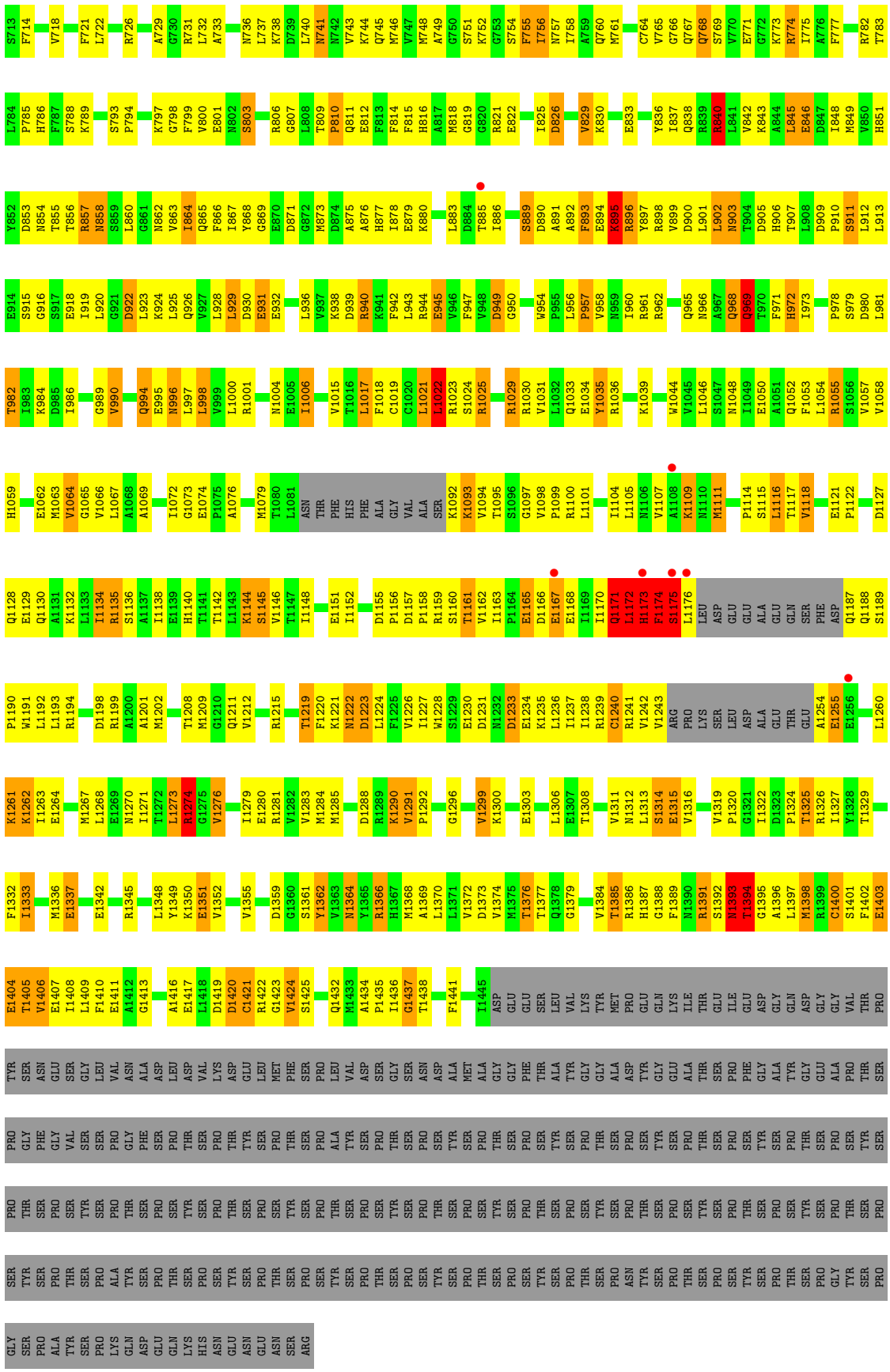
3 Residue-property plots (i)

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

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

Chain A: 2% 31% 38% 11% • 20%

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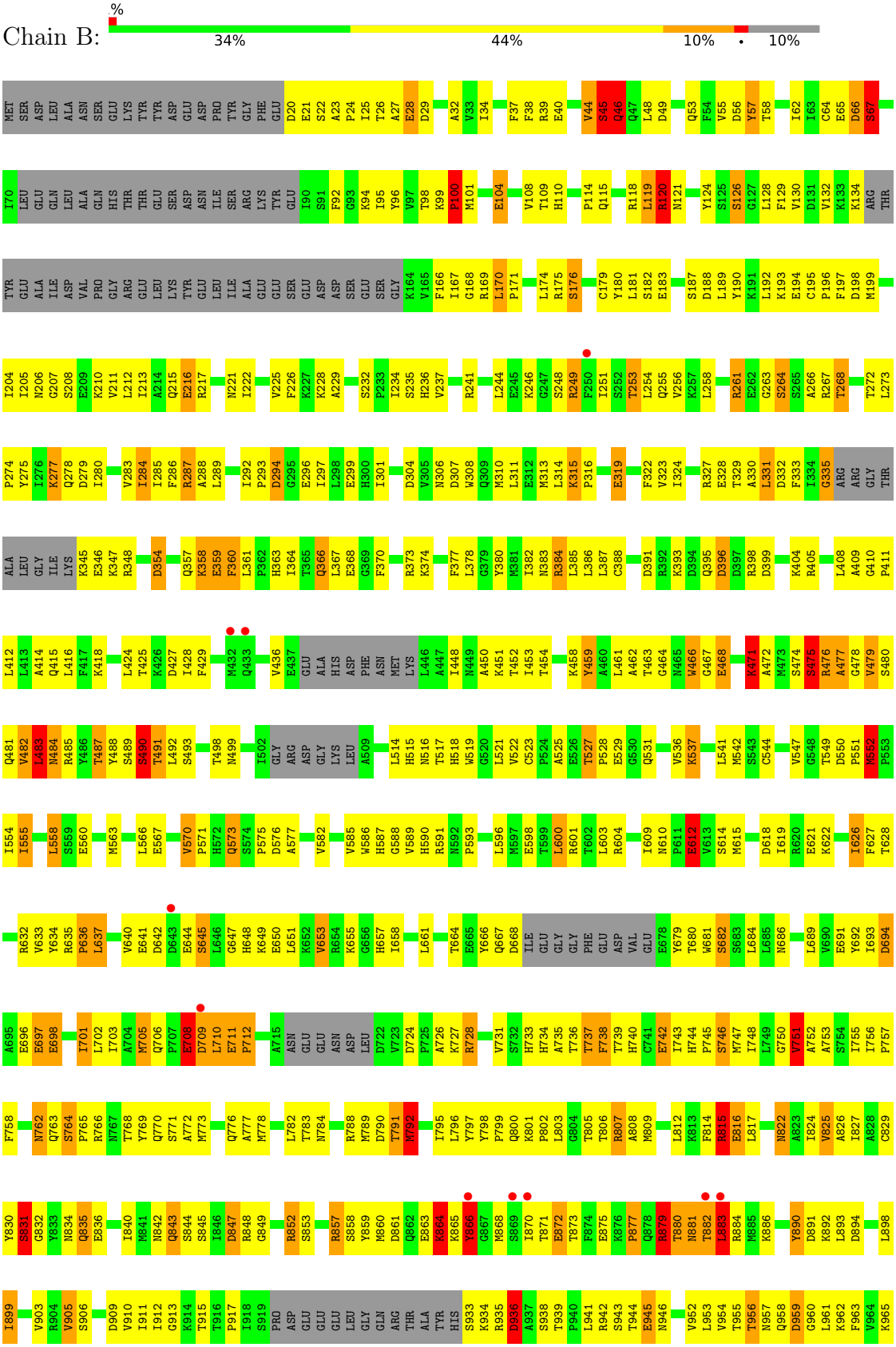
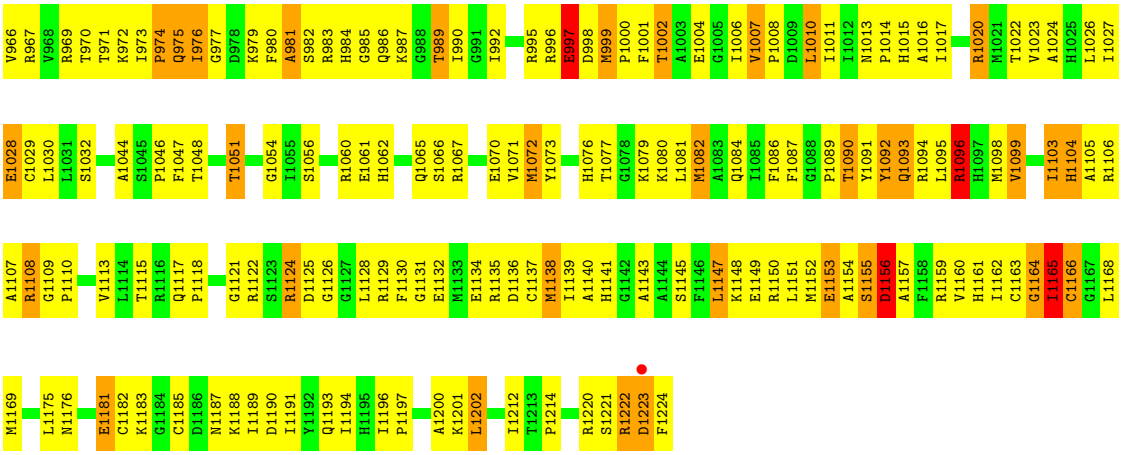
L784 P785 H786 F787 S788 K789 S793 P794 K797 G798 F799 V800 E801 N802 S803 R806 G807 L808 T809 P810 Q811 E812 F813 F814 F815 H816 A817 M818 G819 G820 R821 E822 I825 D826 V829 K830 E833 Y836 I837 Q838 R839 R840 L841 V842 K843 A844 L845 E846 D847 I848 M849 V850 H851
Y852 D853 N854 T855 T856 R857 N858 S859 L860 G861 N862 V863 I864 Q865 F866 I867 Y868 G869 E870 D871 G872 M873 D874 A875 A876 H877 I878 E879 K880 L883 D884 T885 I886 S889 D890 A891 A892 F893 E894 K895 R896 Y897 R898 V899 D900 L901 L902 N903 T904 D905 H906 T907 L908 D909 P910 S911 L912 L913
E914 S915 G916 S917 E918 I919 L920 G921 D922 L923 K924 L925 Q926 V927 L928 L929 D930 E931 E932 L936 V937 K938 D939 R940 K941 F942 L943 R944 E945 V946 F947 V948 D949 G950 W954 P955 L956 P957 V958 N959 I960 R961 R962 Q965 N966 A967 Q968 Q969 T970 F971 H972 I973 P978 S979 D980 L981
T982 I983 K984 D985 I986 G989 V990 Q994 E995 N996 L997 L998 V999 L1000 R1001 N1004 E1005 I1006 V1015 K938 T1016 L1017 F1018 C1019 C1020 L1021 L1022 R1023 S1024 R1025 R1029 R1030 V1031 L1032 Q1033 E1034 Y1035 R1036 K1039 W1044 V1045 L1046 S1047 N1048 I1049 E1050 A1051 Q1052 F1053 L1054 R1055 S1056 V1057 V1058
H1059 E1062 M1063 V1064 G1065 V1066 L1067 A1068 A1069 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 R1100 L1101 I1104 L1105 N1106 V1107 A1108 K1109 N1110 M1111 P1114 S1115 L1116 T1117 V1118 E1121 P1122 D1127
Q1128 E1129 Q1130 A1131 K1132 L1133 I1134 R1135 S1136 A1137 I1138 E1139 H1140 T1141 T1142 L1143 K1144 S1145 V1146 T1147 I1148 E1151 I1152 D1155 P1156 D1157 P1158 R1159 S1160 T1161 V1162 I1163 P1164 E1165 D1166 E1167 E1168 I1169 I1170 Q1171 L1172 H1173 F1174 S1175 L1176 LEU ASP GLU GLU ALA GLU GLN SER PHE ASP Q1187 Q1188 S1189
P1190 W1191 L1192 L1193 R1194 D1198 R1199 A1200 A1201 M1202 T1208 M1209 G1210 Q1211 V1212 R1215 T1219 F1220 K1221 N1222 D1223 L1224 F1225 V1226 V1227 W1228 S1229 E1230 D1231 N1232 D1233 E1234 K1235 L1236 I1237 I1238 R1239 C1240 R1241 V1242 V1243 ARG PRO LYS SER LEU ASP ALA GLU THR GLU A1254 E1255 E1256 L1260
K1261 K1262 I1263 E1264 M1267 L1268 E1259 N1270 I1271 T1272 L1273 R1274 G1275 V1276 I1279 E1280 R1281 V1282 V1283 M1284 M1285 D1288 R1289 K1290 V1291 P1292 G1296 V1299 K1300 E1303 L1306 E1307 T1308 V1311 N1312 L1313 S1314 E1315 V1316 V1319 P1320 G1321 I1322 D1323 P1324 T1325 R1326 I1327 Y1328 T1329
F1332 I1333 M1336 E1337 E1342 R1345 L1348 Y1349 K1350 E1351 V1352 V1355 D1359 G1360 S1361 Y1362 V1363 N1364 Y1365 R1366 H1367 M1368 A1369 L1370 L1371 V1372 D1373 V1374 M1375 T1376 T1377 Q1378 G1379 V1384 T1385 R1386 H1387 G1388 F1389 N1390 R1391 S1392 N1393 T1394 G1395 A1396 L1397 M1398 R1399 C1400 S1401 F1402 E1403
E1404 T1405 V1406 E1407 I1408 L1409 F1410 E1411 A1412 G1413 A1416 E1417 L1418 D1419 D1420 C1421 R1422 G1423 V1424 S1425 Q1432 M1433 A1434 P1435 I1436 G1437 T1438 F1441 I1445 ASP GLU GLU SER LEU VAL LYS TYR MET PRO GLU GLN LYS ILE THR GLU ILE GLU ASP GLY GLN ASP GLY GLY VAL PRO ALA THR
TYR SER ASN GLU SER GLY LEU VAL ASN ALA ASP LEU ASP VAL LEU MET PHE SER PRO LEU VAL ASP SER PRO SER GLY SER ASN ASP ALA MET ALA GLY GLY PHE THR ALA TYR GLY GLY ALA ASP TYR GLY GLU GLU SER THR SER TYR TYR SER PRO SER PHE GLY ALA TYR GLY GLU ALA PRO SER THR
PRO GLY PHE GLY VAL SER SER PRO PRO GLY PHE SER PRO SER PRO THR PRO ALA TYR SER PRO SER TYR SER PRO THR SER PRO SER PRO THR SER PRO THR SER PRO SER TYR SER PRO SER TYR SER PRO THR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TYR SER PRO THR SER PRO SER TY

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

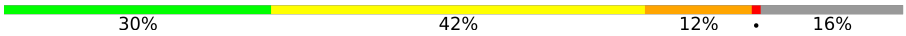
Chain B:

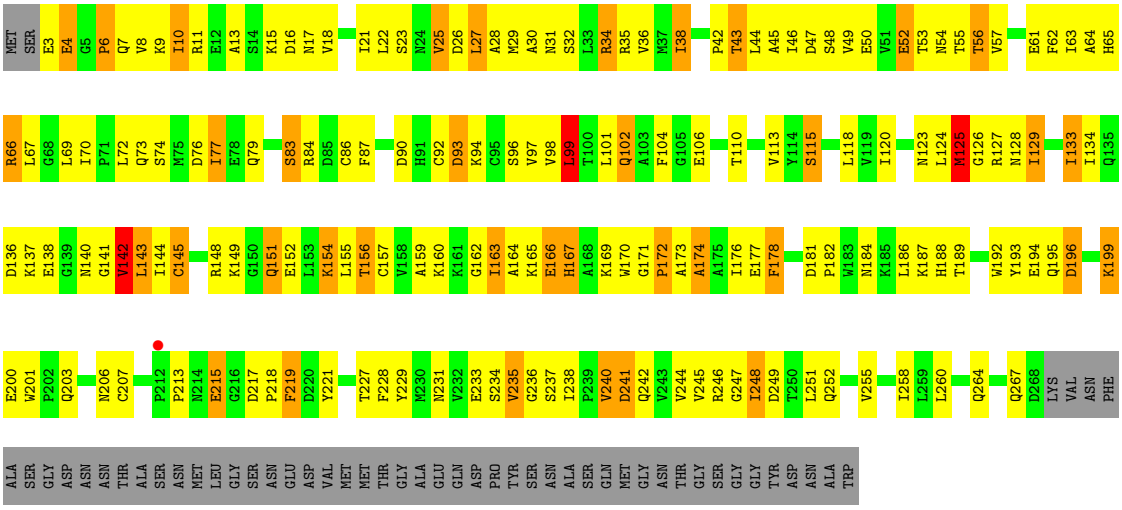




- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

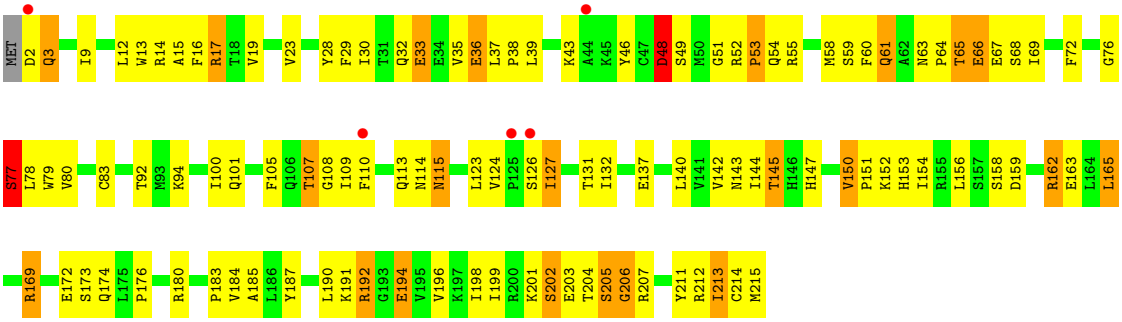
Chain C:





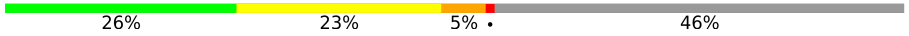
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

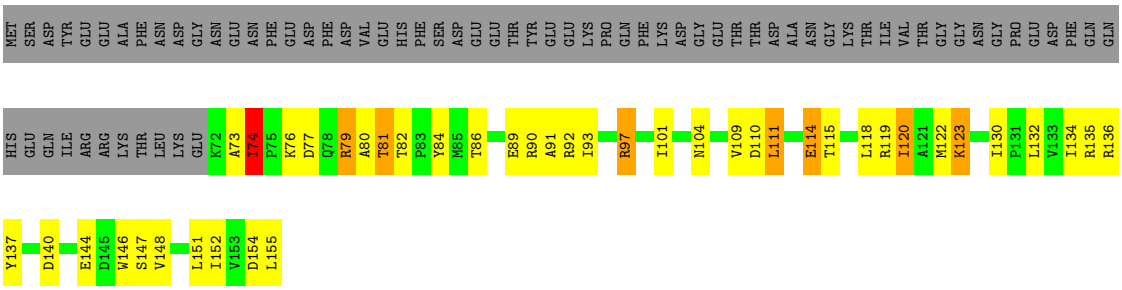
Chain E:



- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

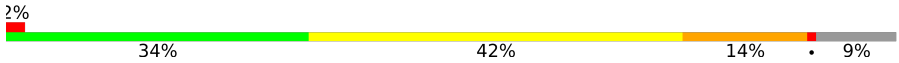
Chain F:

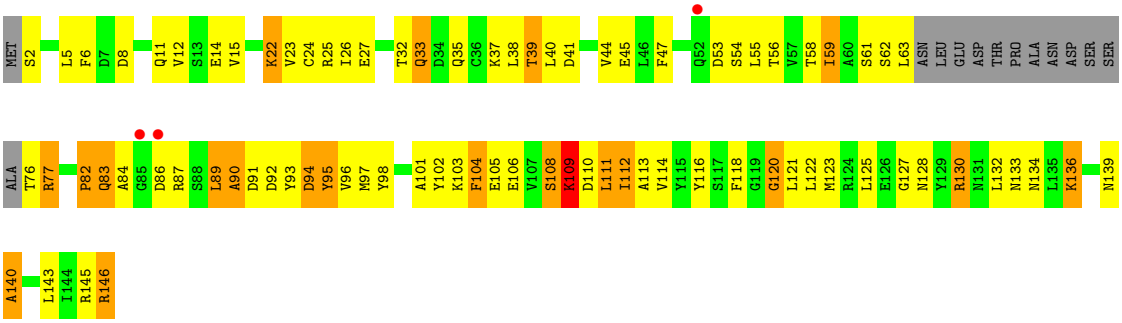




• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

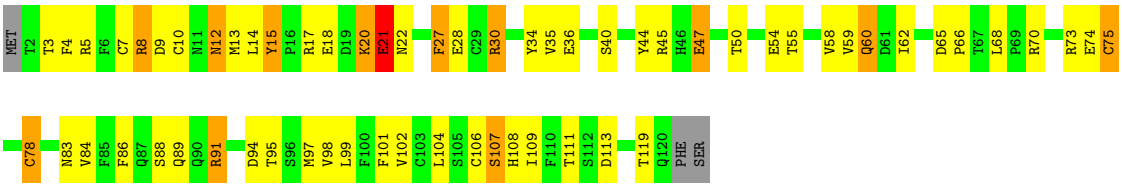
Chain H:





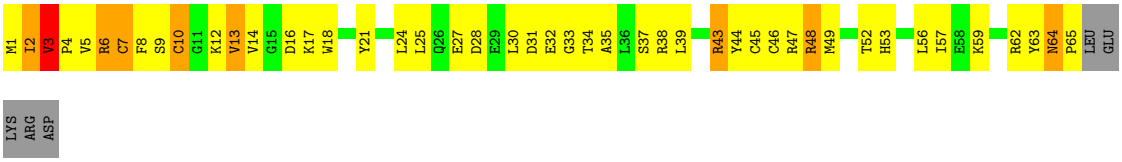
• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I:



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:

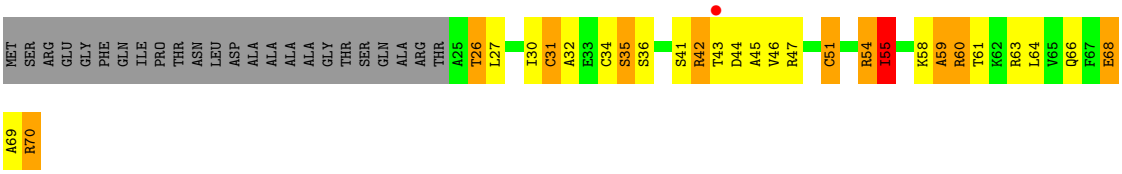


• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:

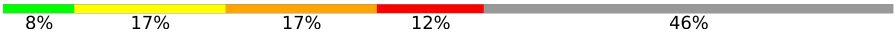
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



• Molecule 11: RNA (5'-R(*AP*UP*CP*GP*AP*GP*AP*GP*GP*AP*UP*GP*CP*AP*GP*AP*CP*GP*UP*UP*UP*UP*UP*U)-3')

Chain R:

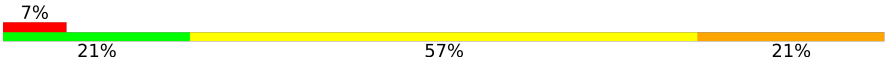


• Molecule 12: DNA (28-MER)

Chain T:

• Molecule 13: DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3')

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	170.78Å 222.11Å 194.85Å 90.00° 102.06° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 43.63 – 3.90	Depositor EDS
% Data completeness (in resolution range)	91.6 (50.00-3.90) 91.7 (43.63-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 3.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.266 , 0.299 0.269 , 0.298	Depositor DCC
R_{free} test set	3001 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	117.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 58.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	29279	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.06	51/11163 (0.5%)	0.84	14/15091 (0.1%)
2	B	1.12	54/8963 (0.6%)	0.86	12/12086 (0.1%)
3	C	1.06	8/2133 (0.4%)	0.85	2/2891 (0.1%)
4	E	1.10	11/1788 (0.6%)	0.77	1/2406 (0.0%)
5	F	1.00	3/691 (0.4%)	0.79	0/933
6	H	1.09	10/1086 (0.9%)	0.82	2/1470 (0.1%)
7	I	1.11	5/989 (0.5%)	0.94	4/1331 (0.3%)
8	J	1.12	1/541 (0.2%)	0.99	2/727 (0.3%)
9	K	1.08	2/937 (0.2%)	0.84	2/1265 (0.2%)
10	L	1.15	2/365 (0.5%)	0.93	0/485
11	R	1.35	3/314 (1.0%)	1.76	6/489 (1.2%)
12	T	2.13	19/634 (3.0%)	1.96	27/975 (2.8%)
13	N	2.23	6/317 (1.9%)	1.73	10/488 (2.0%)
All	All	1.14	175/29921 (0.6%)	0.92	82/40637 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	H	0	1
All	All	0	2

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	12	DT	C5-C7	20.75	1.62	1.50
12	T	3	DA	P-O5'	20.57	1.80	1.59
12	T	3	DA	C4'-O4'	17.05	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	N	12	DT	N3-C4	12.54	1.48	1.38
1	A	833	GLU	CD-OE1	11.61	1.38	1.25
1	A	1129	GLU	CD-OE2	10.83	1.37	1.25
1	A	1230	GLU	CD-OE1	10.35	1.37	1.25
4	E	126	SER	CB-OG	10.25	1.55	1.42
12	T	4	DC	C2-O2	10.16	1.33	1.24
2	B	698	GLU	CD-OE2	10.12	1.36	1.25
12	T	3	DA	C3'-C2'	10.01	1.64	1.52
3	C	52	GLU	CD-OE2	9.90	1.36	1.25
1	A	205	GLU	CD-OE1	9.80	1.36	1.25
12	T	4	DC	N1-C6	9.76	1.43	1.37
9	K	54	ARG	CZ-NH1	9.72	1.45	1.33
1	A	1034	GLU	CD-OE2	9.57	1.36	1.25
2	B	612	GLU	CD-OE1	9.51	1.36	1.25
1	A	1129	GLU	CD-OE1	9.44	1.36	1.25
9	K	93	SER	CB-OG	9.36	1.54	1.42
2	B	708	GLU	CD-OE1	9.25	1.35	1.25
13	N	12	DT	C5-C6	9.07	1.40	1.34
3	C	138	GLU	CD-OE1	9.06	1.35	1.25
1	A	945	GLU	CD-OE2	8.87	1.35	1.25
1	A	840	ARG	CZ-NH1	8.79	1.44	1.33
6	H	14	GLU	CD-OE1	8.62	1.35	1.25
2	B	529	GLU	CD-OE1	8.61	1.35	1.25
2	B	1061	GLU	CD-OE1	8.37	1.34	1.25
6	H	120	GLY	C-O	8.28	1.36	1.23
12	T	3	DA	C5'-C4'	-8.23	1.42	1.51
1	A	879	GLU	CD-OE2	8.22	1.34	1.25
11	R	4	G	P-O5'	8.20	1.68	1.59
13	N	12	DT	N1-C6	8.19	1.44	1.38
2	B	698	GLU	CD-OE1	8.13	1.34	1.25
2	B	697	GLU	CD-OE2	8.11	1.34	1.25
2	B	872	GLU	CD-OE1	8.03	1.34	1.25
2	B	39	ARG	CZ-NH1	7.91	1.43	1.33
4	E	194	GLU	CD-OE1	7.90	1.34	1.25
12	T	4	DC	N3-C4	7.89	1.39	1.33
6	H	105	GLU	CD-OE1	7.83	1.34	1.25
2	B	1061	GLU	CD-OE2	7.76	1.34	1.25
3	C	138	GLU	CD-OE2	7.68	1.34	1.25
6	H	105	GLU	CD-OE2	7.67	1.34	1.25
10	L	36	SER	CB-OG	7.66	1.52	1.42
1	A	1234	GLU	CD-OE2	7.64	1.34	1.25
2	B	346	GLU	CD-OE1	7.61	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1314	SER	CB-OG	7.49	1.51	1.42
1	A	636	GLU	CD-OE2	7.45	1.33	1.25
6	H	54	SER	CB-OG	7.44	1.51	1.42
2	B	335	GLY	C-O	7.37	1.35	1.23
2	B	1070	GLU	CB-CG	7.35	1.66	1.52
12	T	1	DC	N1-C6	7.32	1.41	1.37
12	T	2	DT	N3-C4	7.23	1.44	1.38
1	A	1136	SER	CB-OG	7.22	1.51	1.42
2	B	529	GLU	CG-CD	7.19	1.62	1.51
12	T	3	DA	C3'-O3'	7.15	1.53	1.44
1	A	1234	GLU	CD-OE1	7.11	1.33	1.25
1	A	995	GLU	CD-OE1	7.09	1.33	1.25
7	I	5	ARG	CZ-NH1	7.07	1.42	1.33
1	A	1023	ARG	CZ-NH1	7.06	1.42	1.33
1	A	1121	GLU	CD-OE2	7.04	1.33	1.25
2	B	328	GLU	CD-OE1	7.00	1.33	1.25
6	H	14	GLU	CG-CD	6.90	1.62	1.51
12	T	14	DG	C2-N2	-6.89	1.27	1.34
1	A	496	GLU	CD-OE1	6.84	1.33	1.25
4	E	33	GLU	CD-OE2	6.84	1.33	1.25
1	A	726	ARG	CZ-NH1	6.77	1.41	1.33
2	B	359	GLU	CD-OE2	6.73	1.33	1.25
1	A	205	GLU	CD-OE2	6.72	1.33	1.25
2	B	475	SER	CB-OG	6.65	1.50	1.42
1	A	328	ARG	CZ-NH1	6.57	1.41	1.33
2	B	697	GLU	CD-OE1	6.55	1.32	1.25
7	I	21	GLU	CD-OE2	6.55	1.32	1.25
4	E	48	ASP	CG-OD1	6.52	1.40	1.25
1	A	1230	GLU	CD-OE2	6.51	1.32	1.25
13	N	2	DT	P-O5'	6.48	1.66	1.59
3	C	48	SER	CB-OG	6.45	1.50	1.42
12	T	4	DC	C4-C5	6.44	1.48	1.43
2	B	1224	PHE	C-O	6.40	1.35	1.23
1	A	898	ARG	CZ-NH1	6.37	1.41	1.33
4	E	162	ARG	CZ-NH1	6.32	1.41	1.33
13	N	14	DG	C3'-C2'	6.27	1.59	1.52
2	B	368	GLU	CD-OE1	6.22	1.32	1.25
1	A	995	GLU	CD-OE2	6.18	1.32	1.25
12	T	2	DT	O3'-P	6.14	1.68	1.61
2	B	346	GLU	CD-OE2	6.12	1.32	1.25
2	B	1070	GLU	CG-CD	6.12	1.61	1.51
1	A	1215	ARG	CZ-NH1	6.09	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1337	GLU	CD-OE2	6.07	1.32	1.25
2	B	126	SER	CB-OG	6.07	1.50	1.42
1	A	1361	SER	CB-OG	6.06	1.50	1.42
2	B	872	GLU	CD-OE2	6.04	1.32	1.25
2	B	573	GLN	CD-NE2	5.99	1.47	1.32
5	F	155	LEU	C-OXT	5.98	1.34	1.23
1	A	968	GLN	CD-NE2	5.95	1.47	1.32
12	T	4	DC	N1-C2	5.95	1.46	1.40
2	B	1096	ARG	CZ-NH1	5.94	1.40	1.33
1	A	1062	GLU	CD-OE2	5.92	1.32	1.25
11	R	10	A	P-O5'	5.91	1.65	1.59
8	J	37	SER	CB-OG	5.90	1.50	1.42
6	H	146	ARG	CZ-NH1	5.90	1.40	1.33
4	E	205	SER	CB-OG	5.87	1.49	1.42
3	C	203	GLN	CD-NE2	5.86	1.47	1.32
2	B	120	ARG	CZ-NH1	5.84	1.40	1.33
1	A	369	SER	CB-OG	5.82	1.49	1.42
7	I	40	SER	CB-OG	5.81	1.49	1.42
1	A	1144	LYS	CE-NZ	5.78	1.63	1.49
2	B	358	LYS	CD-CE	5.76	1.65	1.51
2	B	183	GLU	CD-OE1	5.73	1.31	1.25
2	B	39	ARG	NE-CZ	5.73	1.40	1.33
6	H	92	ASP	CG-OD2	5.73	1.38	1.25
1	A	1303	GLU	CD-OE1	5.72	1.31	1.25
4	E	172	GLU	CD-OE1	5.70	1.31	1.25
3	C	106	GLU	CD-OE1	5.65	1.31	1.25
2	B	764	SER	CB-OG	5.64	1.49	1.42
1	A	409	SER	CB-OG	5.62	1.49	1.42
3	C	137	LYS	CD-CE	5.61	1.65	1.51
10	L	60	ARG	CZ-NH1	5.59	1.40	1.33
1	A	789	LYS	CE-NZ	5.59	1.63	1.49
4	E	194	GLU	CD-OE2	5.59	1.31	1.25
1	A	496	GLU	CD-OE2	5.58	1.31	1.25
1	A	1315	GLU	CD-OE1	5.57	1.31	1.25
5	F	114	GLU	CD-OE2	5.57	1.31	1.25
1	A	1055	ARG	CZ-NH1	5.54	1.40	1.33
1	A	811	GLN	CD-NE2	5.51	1.46	1.32
1	A	335	ARG	CZ-NH1	5.51	1.40	1.33
2	B	558	LEU	CG-CD2	5.49	1.72	1.51
1	A	1262	LYS	CE-NZ	5.48	1.62	1.49
1	A	518	LYS	CE-NZ	5.46	1.62	1.49
12	T	2	DT	C5-C7	5.46	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1423	GLY	C-O	5.45	1.32	1.23
2	B	358	LYS	CE-NZ	5.44	1.62	1.49
2	B	708	GLU	CD-OE2	5.43	1.31	1.25
2	B	1164	GLY	C-O	5.42	1.32	1.23
12	T	1	DC	C4-C5	5.41	1.47	1.43
3	C	219	PHE	C-O	5.41	1.33	1.23
12	T	1	DC	N1-C2	5.37	1.45	1.40
2	B	777	ALA	C-O	5.36	1.33	1.23
1	A	879	GLU	CD-OE1	5.35	1.31	1.25
6	H	14	GLU	CB-CG	5.34	1.62	1.52
12	T	1	DC	N3-C4	5.34	1.37	1.33
2	B	696	GLU	CD-OE2	5.30	1.31	1.25
7	I	21	GLU	CD-OE1	5.29	1.31	1.25
6	H	22	LYS	C-O	5.29	1.33	1.23
2	B	890	TYR	CG-CD2	5.28	1.46	1.39
2	B	598	GLU	CD-OE2	5.28	1.31	1.25
1	A	938	LYS	CE-NZ	5.28	1.62	1.49
1	A	1034	GLU	CD-OE1	5.24	1.31	1.25
1	A	133	LYS	CD-CE	5.23	1.64	1.51
2	B	560	GLU	CD-OE1	5.23	1.31	1.25
2	B	1183	LYS	CE-NZ	5.23	1.62	1.49
2	B	368	GLU	CD-OE2	5.22	1.31	1.25
1	A	1215	ARG	NE-CZ	5.21	1.39	1.33
2	B	216	GLU	CG-CD	5.21	1.59	1.51
2	B	816	GLU	CG-CD	5.21	1.59	1.51
2	B	936	ASP	CG-OD2	5.20	1.37	1.25
2	B	183	GLU	CD-OE2	5.19	1.31	1.25
1	A	773	LYS	CE-NZ	5.19	1.62	1.49
1	A	950	GLY	C-O	5.19	1.31	1.23
2	B	267	ARG	CZ-NH1	5.18	1.39	1.33
4	E	172	GLU	CG-CD	5.17	1.59	1.51
2	B	1048	THR	CB-OG1	5.17	1.53	1.43
2	B	560	GLU	CD-OE2	5.17	1.31	1.25
2	B	468	GLU	CG-CD	5.16	1.59	1.51
1	A	994	GLN	CD-NE2	5.15	1.45	1.32
2	B	253	THR	C-O	5.15	1.33	1.23
2	B	890	TYR	CG-CD1	5.14	1.45	1.39
2	B	100	PRO	CB-CG	5.14	1.75	1.50
4	E	173	SER	CB-OG	5.13	1.49	1.42
11	R	4	G	P-OP2	5.12	1.57	1.49
7	I	27	PHE	CE2-CZ	5.10	1.47	1.37
4	E	202	SER	CB-OG	5.08	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1062	GLU	CD-OE1	5.08	1.31	1.25
2	B	890	TYR	CE2-CZ	5.07	1.45	1.38
5	F	92	ARG	CZ-NH2	5.05	1.39	1.33
12	T	2	DT	N1-C2	5.00	1.42	1.38

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1215	ARG	NE-CZ-NH2	-12.59	114.01	120.30
12	T	3	DA	O4'-C4'-C3'	-12.07	98.76	106.00
12	T	16	DC	O4'-C4'-C3'	-11.55	99.07	106.00
11	R	13	C	C1'-O4'-C4'	-10.90	101.18	109.90
2	B	287	ARG	NE-CZ-NH2	-10.47	115.06	120.30
9	K	54	ARG	NE-CZ-NH2	-9.34	115.63	120.30
12	T	27	DA	O4'-C4'-C3'	-9.30	100.42	106.00
1	A	840	ARG	NE-CZ-NH2	-8.60	116.00	120.30
2	B	1222	ARG	NE-CZ-NH2	-8.47	116.06	120.30
12	T	15	DA	P-O3'-C3'	8.28	129.63	119.70
12	T	25	DC	O4'-C1'-N1	8.28	113.79	108.00
13	N	12	DT	N3-C4-O4	7.76	124.56	119.90
13	N	12	DT	C5-C4-O4	-7.76	119.47	124.90
1	A	898	ARG	NE-CZ-NH2	-7.74	116.43	120.30
12	T	15	DA	C1'-O4'-C4'	-7.70	102.40	110.10
12	T	16	DC	O4'-C1'-N1	7.62	113.33	108.00
8	J	10	CYS	CA-CB-SG	7.61	127.69	114.00
7	I	5	ARG	NE-CZ-NH2	-7.55	116.53	120.30
13	N	10	DG	P-O3'-C3'	7.55	128.75	119.70
1	A	898	ARG	NE-CZ-NH1	7.48	124.04	120.30
7	I	70	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	B	331	LEU	CB-CG-CD2	-7.43	98.37	111.00
12	T	1	DC	O4'-C1'-N1	7.35	113.15	108.00
12	T	3	DA	C5'-C4'-C3'	7.31	127.26	114.10
12	T	1	DC	C1'-O4'-C4'	-7.17	102.93	110.10
13	N	9	DC	O4'-C1'-N1	7.04	112.93	108.00
2	B	39	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	1023	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	A	328	ARG	NE-CZ-NH2	-6.74	116.93	120.30
12	T	19	DT	N3-C2-O2	-6.66	118.31	122.30
2	B	1096	ARG	NE-CZ-NH2	-6.63	116.99	120.30
12	T	6	DG	P-O3'-C3'	6.60	127.62	119.70
1	A	1023	ARG	NE-CZ-NH2	-6.32	117.14	120.30
3	C	66	ARG	NE-CZ-NH2	-6.29	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	10	CYS	CA-CB-SG	6.25	125.24	114.00
11	R	13	C	C6-N1-C2	6.24	122.80	120.30
1	A	726	ARG	NE-CZ-NH2	-6.15	117.22	120.30
13	N	12	DT	C4-C5-C6	-6.12	114.33	118.00
12	T	22	DT	C4'-C3'-C2'	-6.05	97.66	103.10
1	A	344	ARG	NE-CZ-NH1	6.03	123.32	120.30
2	B	120	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	1215	ARG	NE-CZ-NH1	6.00	123.30	120.30
4	E	162	ARG	NE-CZ-NH2	-5.95	117.33	120.30
12	T	20	DC	C6-N1-C2	-5.95	117.92	120.30
11	R	10	A	O4'-C1'-N9	-5.91	103.47	108.20
6	H	146	ARG	NE-CZ-NH1	5.85	123.22	120.30
2	B	39	ARG	NE-CZ-NH2	-5.81	117.40	120.30
12	T	27	DA	O4'-C1'-N9	5.80	112.06	108.00
12	T	3	DA	O5'-P-OP2	5.74	117.58	110.70
12	T	7	DA	O4'-C1'-N9	5.71	112.00	108.00
12	T	11	DG	O4'-C1'-N9	5.69	111.98	108.00
6	H	146	ARG	NE-CZ-NH2	-5.60	117.50	120.30
2	B	852	ARG	NE-CZ-NH2	-5.55	117.52	120.30
12	T	1	DC	N1-C2-O2	5.46	122.18	118.90
1	A	305	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	335	ARG	NE-CZ-NH2	-5.44	117.58	120.30
12	T	4	DC	N3-C4-C5	5.42	124.07	121.90
12	T	22	DT	P-O3'-C3'	5.41	126.19	119.70
12	T	12	DC	O4'-C1'-N1	5.38	111.77	108.00
13	N	10	DG	C1'-O4'-C4'	-5.37	104.73	110.10
2	B	476	ARG	NE-CZ-NH2	-5.36	117.62	120.30
13	N	5	DT	O4'-C1'-N1	5.36	111.75	108.00
12	T	4	DC	O4'-C1'-N1	5.35	111.75	108.00
2	B	1096	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	B	476	ARG	NE-CZ-NH1	5.27	122.94	120.30
3	C	99	LEU	CA-CB-CG	5.27	127.42	115.30
12	T	24	DT	N3-C4-O4	5.25	123.05	119.90
13	N	1	DC	O4'-C1'-N1	5.24	111.66	108.00
11	R	10	A	C5-C6-N6	-5.23	119.52	123.70
12	T	24	DT	C5-C4-O4	-5.19	121.27	124.90
12	T	28	DT	C4-C5-C7	5.17	122.10	119.00
2	B	883	LEU	CA-CB-CG	5.15	127.14	115.30
13	N	6	DT	O4'-C1'-N1	5.14	111.60	108.00
11	R	5	A	N9-C1'-C2'	5.13	120.67	114.00
8	J	3	VAL	CB-CA-C	-5.12	101.67	111.40
12	T	2	DT	C4-C5-C7	5.10	122.06	119.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	I	91	ARG	NE-CZ-NH2	-5.09	117.75	120.30
9	K	54	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	936	LEU	CA-CB-CG	5.06	126.94	115.30
11	R	3	C	O4'-C1'-N1	5.05	112.24	108.20
1	A	1116	LEU	CA-CB-CG	5.03	126.87	115.30
13	N	11	DG	C1'-O4'-C4'	-5.01	105.09	110.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	523	ILE	Peptide
6	H	61	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10969	0	11070	870	0
2	B	8792	0	8825	673	0
3	C	2095	0	2051	163	0
4	E	1752	0	1776	90	0
5	F	679	0	701	39	0
6	H	1068	0	1040	97	0
7	I	971	0	928	46	0
8	J	532	0	544	79	0
9	K	919	0	929	71	0
10	L	363	0	387	24	0
11	R	280	0	143	19	0
12	T	566	0	314	20	0
13	N	284	0	161	5	0
14	A	2	0	0	1	0
14	B	1	0	0	1	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	2	0
14	L	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	1	0	0	0	0
All	All	29279	0	28869	2008	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 35.

All (2008) 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)
6:H:104:PHE:CZ	6:H:136:LYS:HB3	1.37	1.55
7:I:109:ILE:CG1	7:I:109:ILE:CD1	1.84	1.53
2:B:100:PRO:CG	2:B:100:PRO:CB	1.75	1.48
1:A:256:GLN:CA	1:A:257:ARG:HB3	1.42	1.47
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.37	1.35
6:H:109:LYS:HB3	6:H:110:ASP:C	1.43	1.35
1:A:351:THR:HG23	2:B:1103:ILE:CD1	1.64	1.25
1:A:315:LEU:CB	1:A:316:GLN:HA	1.61	1.25
1:A:253:ASN:HB2	1:A:256:GLN:C	1.56	1.24
6:H:109:LYS:HB3	6:H:110:ASP:CA	1.66	1.24
6:H:109:LYS:CA	6:H:110:ASP:HB2	1.66	1.23
2:B:1106:ARG:HD3	2:B:1126:GLY:O	1.36	1.23
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.73	1.21
1:A:315:LEU:HB3	1:A:316:GLN:CA	1.68	1.21
2:B:976:ILE:O	2:B:990:ILE:HB	1.41	1.19
6:H:109:LYS:CB	6:H:110:ASP:HB2	1.74	1.18
6:H:109:LYS:CG	6:H:111:LEU:HD22	1.74	1.18
1:A:900:ASP:O	1:A:906:HIS:O	1.60	1.17
1:A:1116:LEU:HD13	1:A:1329:THR:OG1	1.43	1.17
2:B:757:PRO:HG3	2:B:983:ARG:NH2	1.58	1.16
1:A:256:GLN:CB	1:A:257:ARG:HB3	1.76	1.15
1:A:1391:ARG:O	1:A:1391:ARG:HD3	1.47	1.14
6:H:109:LYS:HA	6:H:110:ASP:HB2	1.27	1.14
1:A:256:GLN:HA	1:A:257:ARG:CB	1.68	1.14
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.17	1.14
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	1.83	1.14
6:H:109:LYS:HB3	6:H:110:ASP:CB	1.77	1.13
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.26	1.13
1:A:253:ASN:HB2	1:A:256:GLN:O	1.48	1.12
1:A:351:THR:CG2	2:B:1103:ILE:HD12	1.78	1.11
6:H:104:PHE:CZ	6:H:136:LYS:CB	2.32	1.11
1:A:257:ARG:O	1:A:257:ARG:HG2	1.44	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:981:ALA:CB	2:B:987:LYS:HA	1.81	1.10
5:F:114:GLU:OE2	5:F:119:ARG:HG2	1.50	1.10
11:R:4:G:H2'	11:R:5:A:H8	1.16	1.10
6:H:109:LYS:CB	6:H:110:ASP:CB	2.30	1.09
1:A:256:GLN:CB	1:A:257:ARG:CD	2.31	1.09
1:A:351:THR:HG22	1:A:352:VAL:H	1.09	1.08
2:B:983:ARG:HG3	2:B:1093:GLN:NE2	1.66	1.08
1:A:119:ASN:O	1:A:123:ARG:HG3	1.53	1.08
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.12	1.07
1:A:256:GLN:CB	1:A:257:ARG:HD2	1.85	1.07
7:I:75:CYS:SG	7:I:78:CYS:HB3	1.94	1.07
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.84	1.06
9:K:113:THR:O	9:K:114:LEU:HB2	1.49	1.06
1:A:256:GLN:HB3	1:A:257:ARG:HD2	1.37	1.05
1:A:351:THR:HG22	1:A:352:VAL:N	1.70	1.05
6:H:109:LYS:HG2	6:H:111:LEU:HD22	1.30	1.05
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.38	1.05
1:A:765:VAL:CG2	1:A:800:VAL:HB	1.86	1.05
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.34	1.05
1:A:256:GLN:CA	1:A:257:ARG:CB	2.30	1.04
2:B:882:THR:HG21	2:B:935:ARG:HA	1.38	1.04
1:A:351:THR:HG23	2:B:1103:ILE:HD12	1.10	1.04
1:A:382:PRO:HD3	1:A:428:TYR:HE2	1.19	1.04
1:A:256:GLN:HB2	1:A:257:ARG:HD3	1.40	1.04
8:J:1:MET:N	8:J:56:LEU:H	1.55	1.03
6:H:109:LYS:HG2	6:H:111:LEU:CD2	1.88	1.03
1:A:256:GLN:HB2	1:A:257:ARG:CD	1.88	1.02
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.90	1.02
1:A:315:LEU:HD12	1:A:318:SER:O	1.58	1.01
3:C:3:GLU:HG3	3:C:4:GLU:H	1.20	1.01
2:B:213:ILE:HD11	2:B:481:GLN:OE1	1.61	1.01
2:B:634:TYR:HE1	2:B:692:TYR:CD1	1.79	1.01
2:B:706:GLN:O	2:B:710:LEU:HB2	1.61	1.01
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.37	1.01
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.41	1.00
1:A:667:GLY:HA2	1:A:670:ILE:HG13	1.44	1.00
1:A:868:TYR:HE1	1:A:1064:VAL:CG1	1.74	1.00
8:J:48:ARG:HH21	8:J:49:MET:HE1	1.26	1.00
11:R:4:G:H2'	11:R:5:A:C8	1.95	1.00
1:A:382:PRO:HD3	1:A:428:TYR:CE2	1.97	1.00
3:C:102:GLN:HG2	3:C:154:LYS:HD3	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:29:PHE:O	4:E:30:ILE:HG13	1.60	0.99
1:A:573:SER:H	1:A:576:GLN:HG3	1.27	0.99
8:J:10:CYS:SG	8:J:43:ARG:HD2	2.03	0.99
1:A:256:GLN:HB3	1:A:257:ARG:CD	1.92	0.99
1:A:855:THR:HG21	1:A:857:ARG:HE	1.26	0.98
1:A:1348:LEU:HD23	1:A:1372:VAL:HG22	1.44	0.98
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.29	0.98
6:H:109:LYS:CB	6:H:110:ASP:C	2.30	0.98
2:B:1076:HIS:ND1	9:K:40:HIS:CD2	2.32	0.98
1:A:39:GLU:O	1:A:53:LEU:HD12	1.62	0.97
1:A:1364:ASN:HD21	1:A:1366:ARG:HG2	1.23	0.97
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.24	0.97
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.43	0.97
2:B:807:ARG:HG3	2:B:807:ARG:HH11	1.25	0.96
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	0.81	0.96
1:A:860:LEU:CD1	1:A:1393:ASN:HD22	1.78	0.96
1:A:1364:ASN:ND2	1:A:1366:ARG:CG	2.27	0.96
1:A:860:LEU:HD13	1:A:1393:ASN:HD22	1.28	0.96
8:J:44:TYR:HA	8:J:47:ARG:HB2	1.47	0.96
1:A:662:PHE:HD2	2:B:829:CYS:HG	1.13	0.96
8:J:35:ALA:O	8:J:39:LEU:HD12	1.64	0.95
8:J:7:CYS:SG	8:J:10:CYS:N	2.38	0.95
1:A:630:ILE:H	1:A:630:ILE:HD12	1.28	0.94
1:A:901:LEU:HA	1:A:907:THR:HG23	1.49	0.94
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.50	0.93
11:R:3:C:H42	12:T:26:DG:H1	1.17	0.93
1:A:1172:LEU:O	1:A:1173:HIS:HB3	1.69	0.93
1:A:256:GLN:HA	1:A:257:ARG:HB3	0.95	0.93
2:B:992:ILE:HD11	9:K:67:PHE:HE2	1.33	0.93
1:A:573:SER:O	1:A:576:GLN:HB2	1.69	0.93
1:A:662:PHE:HD2	2:B:829:CYS:SG	1.92	0.92
6:H:104:PHE:HZ	6:H:136:LYS:HB3	1.12	0.92
1:A:765:VAL:HG23	1:A:800:VAL:HB	1.50	0.92
2:B:64:CYS:HA	2:B:67:SER:HB2	1.50	0.92
2:B:757:PRO:HG3	2:B:983:ARG:HH22	1.26	0.91
1:A:249:SER:C	1:A:250:ILE:HG12	1.91	0.90
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.53	0.90
3:C:66:ARG:NH2	8:J:4:PRO:HA	1.86	0.90
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.35	0.90
2:B:634:TYR:CE1	2:B:692:TYR:CD1	2.59	0.90
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:925:LEU:O	1:A:929:LEU:HB2	1.73	0.89
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.54	0.89
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.38	0.89
1:A:253:ASN:CB	1:A:256:GLN:C	2.41	0.89
6:H:109:LYS:CA	6:H:110:ASP:CB	2.48	0.88
1:A:1156:PRO:O	1:A:1158:PRO:HD3	1.74	0.88
1:A:256:GLN:HB3	1:A:257:ARG:HB3	1.56	0.88
2:B:1032:SER:HB3	2:B:1089:PRO:HG2	1.53	0.88
1:A:382:PRO:CD	1:A:428:TYR:HE2	1.85	0.88
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.56	0.88
7:I:75:CYS:SG	7:I:78:CYS:CB	2.63	0.87
1:A:630:ILE:HD12	1:A:630:ILE:N	1.89	0.87
2:B:1117:GLN:HG2	2:B:1156:ASP:OD2	1.75	0.87
2:B:829:CYS:SG	2:B:1014:PRO:CG	2.63	0.86
2:B:100:PRO:HD3	2:B:126:SER:OG	1.75	0.86
1:A:105:CYS:O	1:A:114:LEU:HG	1.75	0.86
4:E:28:TYR:CE1	4:E:78:LEU:HD13	2.10	0.86
6:H:82:PRO:O	6:H:83:GLN:HB2	1.72	0.86
1:A:351:THR:CG2	1:A:352:VAL:H	1.89	0.86
2:B:770:GLN:NE2	2:B:1093:GLN:HE22	1.73	0.86
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.57	0.86
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.58	0.86
1:A:751:SER:OG	2:B:1015:HIS:HE1	1.57	0.86
2:B:913:GLY:HA2	2:B:938:SER:HB3	1.56	0.85
1:A:276:LEU:HD21	1:A:293:GLU:HG2	1.57	0.85
2:B:955:THR:HG22	2:B:956:THR:H	1.39	0.85
2:B:610:ASN:OD1	2:B:612:GLU:HB2	1.76	0.85
2:B:829:CYS:SG	2:B:1014:PRO:HG3	2.16	0.85
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.56	0.85
6:H:110:ASP:O	6:H:111:LEU:HD13	1.77	0.85
1:A:343:LYS:HD2	2:B:1151:LEU:HG	1.57	0.85
1:A:814:PHE:CE1	2:B:514:LEU:HD21	2.12	0.84
6:H:104:PHE:HD2	6:H:114:VAL:HG12	1.43	0.84
1:A:635:ARG:HE	1:A:877:HIS:HA	1.41	0.84
1:A:507:VAL:HG13	1:A:521:MET:HE1	1.58	0.84
1:A:512:VAL:HA	1:A:519:PRO:HA	1.59	0.84
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.31	0.84
6:H:47:PHE:HB3	6:H:95:TYR:CD1	2.12	0.84
1:A:253:ASN:CB	1:A:257:ARG:N	2.40	0.84
1:A:264:PHE:CZ	1:A:317:LYS:HB2	2.12	0.84
1:A:840:ARG:HE	1:A:1385:THR:HG23	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:65:HIS:HD2	9:K:67:PHE:H	1.26	0.84
1:A:855:THR:CG2	1:A:857:ARG:HE	1.89	0.84
8:J:3:VAL:HG21	8:J:18:TRP:CG	2.12	0.83
2:B:1096:ARG:HG2	2:B:1096:ARG:HH11	1.42	0.83
1:A:1118:VAL:HA	1:A:1327:ILE:HG13	1.57	0.83
1:A:903:ASN:O	1:A:907:THR:OG1	1.95	0.83
2:B:892:LYS:HG2	2:B:903:VAL:HG11	1.61	0.83
2:B:1099:VAL:HG12	2:B:1103:ILE:HD11	1.58	0.83
2:B:1136:ASP:HA	2:B:1139:ILE:HD12	1.61	0.83
2:B:37:PHE:O	2:B:38:PHE:HB2	1.77	0.83
2:B:955:THR:HG22	2:B:956:THR:N	1.93	0.83
4:E:61:GLN:HB3	4:E:79:TRP:HE3	1.43	0.83
3:C:260:LEU:O	3:C:264:GLN:HG3	1.79	0.82
1:A:251:SER:O	1:A:252:PHE:CD2	2.32	0.82
2:B:1032:SER:CB	2:B:1089:PRO:HG2	2.09	0.82
1:A:106:VAL:HG11	1:A:214:ILE:HD11	1.61	0.82
1:A:1407:GLU:CD	1:A:1407:GLU:H	1.83	0.82
2:B:174:LEU:HD22	2:B:204:ILE:HD11	1.60	0.82
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.59	0.82
1:A:909:ASP:OD1	1:A:911:SER:HB3	1.79	0.82
2:B:870:ILE:O	2:B:871:THR:OG1	1.97	0.82
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.60	0.82
1:A:672:ASP:N	1:A:736:ASN:HD21	1.78	0.82
6:H:47:PHE:CB	6:H:95:TYR:HD1	1.93	0.82
1:A:567:LYS:HB3	6:H:96:VAL:H	1.43	0.81
2:B:329:THR:HA	2:B:332:ASP:HB2	1.61	0.81
1:A:889:SER:HB2	1:A:892:ALA:H	1.44	0.81
2:B:986:GLN:NE2	2:B:1016:ALA:HB1	1.95	0.81
1:A:115:LEU:HD22	1:A:119:ASN:HD22	1.45	0.81
1:A:528:LEU:HD23	1:A:751:SER:HA	1.63	0.81
2:B:803:LEU:N	2:B:822:ASN:HD21	1.79	0.81
3:C:70:ILE:HD11	3:C:144:ILE:CD1	2.09	0.81
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.09	0.81
2:B:600:LEU:HD12	2:B:615:MET:SD	2.20	0.81
1:A:120:GLU:OE2	1:A:123:ARG:HD3	1.80	0.81
1:A:675:THR:O	1:A:679:ILE:HD12	1.81	0.80
1:A:110:CYS:SG	1:A:111:GLY:N	2.53	0.80
1:A:630:ILE:H	1:A:630:ILE:CD1	1.93	0.80
2:B:634:TYR:CE1	2:B:692:TYR:HD1	2.00	0.80
2:B:1073:TYR:CE2	2:B:1080:LYS:CG	2.64	0.80
3:C:74:SER:O	3:C:77:ILE:HB	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LYS:HG2	1:A:139:TRP:NE1	1.96	0.80
2:B:1076:HIS:ND1	9:K:40:HIS:HD2	1.79	0.80
3:C:56:THR:HG21	3:C:145:CYS:SG	2.22	0.80
4:E:63:ASN:HB3	4:E:64:PRO:CD	2.12	0.80
4:E:114:ASN:O	4:E:115:ASN:HB3	1.80	0.80
1:A:182:VAL:HG12	1:A:183:GLY:H	1.46	0.80
5:F:81:THR:HB	5:F:136:ARG:HH11	1.46	0.80
2:B:636:PRO:HB3	2:B:743:ILE:CG1	2.11	0.80
1:A:545:GLN:HB3	1:A:549:MET:HE3	1.63	0.79
1:A:98:LYS:O	1:A:102:VAL:HG23	1.82	0.79
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	1.82	0.79
1:A:256:GLN:CB	1:A:257:ARG:CB	2.60	0.79
1:A:909:ASP:O	1:A:911:SER:N	2.15	0.79
2:B:870:ILE:CG2	2:B:871:THR:N	2.45	0.79
2:B:982:SER:O	2:B:1093:GLN:HG3	1.81	0.79
3:C:167:HIS:CE1	10:L:70:ARG:HB3	2.17	0.79
1:A:722:LEU:HD11	1:A:794:PRO:HB3	1.64	0.79
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.48	0.79
1:A:253:ASN:ND2	1:A:257:ARG:HA	1.96	0.79
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	1.82	0.79
3:C:166:GLU:HG3	9:K:10:PHE:HZ	1.48	0.79
3:C:3:GLU:HG3	3:C:4:GLU:N	1.97	0.79
5:F:109:VAL:HG12	5:F:110:ASP:N	1.98	0.79
2:B:636:PRO:HB3	2:B:743:ILE:HG13	1.63	0.78
3:C:70:ILE:CD1	3:C:144:ILE:HD11	2.11	0.78
3:C:102:GLN:HG2	3:C:154:LYS:CD	2.13	0.78
1:A:672:ASP:H	1:A:736:ASN:HD21	1.31	0.78
7:I:35:VAL:HG12	7:I:36:GLU:H	1.47	0.78
3:C:142:VAL:HG13	3:C:143:LEU:N	1.98	0.78
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.64	0.78
5:F:114:GLU:OE2	5:F:119:ARG:CG	2.31	0.78
1:A:1105:LEU:HD23	1:A:1384:VAL:HG21	1.66	0.78
1:A:264:PHE:CZ	1:A:317:LYS:CB	2.67	0.78
1:A:315:LEU:HB3	1:A:316:GLN:HA	0.82	0.78
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.13	0.78
2:B:762:ASN:OD1	2:B:984:HIS:HD2	1.67	0.78
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.66	0.78
5:F:109:VAL:HG12	5:F:110:ASP:H	1.49	0.78
2:B:757:PRO:CG	2:B:983:ARG:NH2	2.45	0.77
2:B:770:GLN:HE22	2:B:1093:GLN:HE22	1.31	0.77
3:C:166:GLU:HG3	9:K:10:PHE:CZ	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:35:ALA:O	8:J:39:LEU:CD1	2.31	0.77
1:A:344:ARG:HG3	1:A:344:ARG:NH1	1.96	0.77
1:A:860:LEU:CD1	1:A:1393:ASN:ND2	2.46	0.77
4:E:61:GLN:HB3	4:E:79:TRP:CE3	2.19	0.77
2:B:635:ARG:CB	2:B:636:PRO:HD2	2.01	0.77
6:H:104:PHE:HZ	6:H:136:LYS:CB	1.84	0.77
6:H:109:LYS:HB2	6:H:111:LEU:HB2	1.66	0.77
8:J:48:ARG:HH21	8:J:49:MET:CE	1.97	0.77
1:A:253:ASN:CB	1:A:256:GLN:O	2.30	0.77
2:B:363:HIS:O	2:B:364:ILE:HB	1.83	0.77
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.65	0.77
5:F:76:LYS:O	5:F:79:ARG:HD2	1.85	0.77
1:A:552:TRP:NE1	1:A:655:PHE:CD1	2.53	0.77
2:B:807:ARG:HH11	2:B:807:ARG:CG	1.97	0.77
3:C:167:HIS:HD2	3:C:169:LYS:H	1.33	0.77
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.65	0.77
1:A:401:GLY:C	1:A:435:HIS:CD2	2.58	0.77
1:A:452:LYS:HB2	2:B:1141:HIS:CE1	2.20	0.77
1:A:1172:LEU:O	1:A:1173:HIS:CB	2.31	0.77
1:A:250:ILE:O	1:A:251:SER:CB	2.33	0.77
1:A:351:THR:CG2	2:B:1103:ILE:CD1	2.49	0.76
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.64	0.76
8:J:1:MET:N	8:J:56:LEU:N	2.33	0.76
2:B:522:VAL:HG11	2:B:537:LYS:HB3	1.67	0.76
1:A:1025:ARG:HG2	1:A:1025:ARG:HH11	1.50	0.76
2:B:796:LEU:HB3	2:B:799:PRO:HD3	1.66	0.76
2:B:996:ARG:NH2	3:C:38:ILE:HD13	2.00	0.76
2:B:1073:TYR:CD2	2:B:1080:LYS:HG3	2.21	0.76
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.20	0.76
4:E:28:TYR:HE1	4:E:78:LEU:HD13	1.51	0.76
8:J:5:VAL:HG12	8:J:6:ARG:HG3	1.67	0.76
2:B:293:PRO:O	2:B:297:ILE:HG12	1.86	0.76
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.49	0.76
2:B:981:ALA:HB2	2:B:987:LYS:CA	2.14	0.75
1:A:1394:THR:HG22	1:A:1398:MET:HE3	1.67	0.75
3:C:258:ILE:HD11	9:K:42:LEU:HD21	1.66	0.75
1:A:1222:ASN:O	1:A:1223:ASP:HB3	1.86	0.75
6:H:47:PHE:HB3	6:H:95:TYR:HD1	1.50	0.75
9:K:57:LEU:HD12	9:K:76:GLN:HG2	1.68	0.75
1:A:19:PHE:HE1	1:A:1396:ALA:HB3	1.50	0.75
1:A:257:ARG:HH11	1:A:257:ARG:CG	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:VAL:HG12	1:A:459:ARG:O	1.87	0.75
2:B:976:ILE:HD11	2:B:992:ILE:HD12	1.68	0.75
2:B:825:VAL:HG23	2:B:1010:LEU:HG	1.69	0.75
5:F:111:LEU:HD13	5:F:111:LEU:H	1.51	0.75
7:I:7:CYS:SG	7:I:8:ARG:O	2.44	0.75
1:A:253:ASN:HB2	1:A:257:ARG:N	1.98	0.75
2:B:899:ILE:HD11	2:B:911:ILE:HG23	1.68	0.75
2:B:1154:ALA:O	2:B:1155:SER:CB	2.35	0.75
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.67	0.75
1:A:15:LYS:HE2	2:B:1220:ARG:HG2	1.69	0.75
1:A:252:PHE:CG	1:A:252:PHE:O	2.39	0.75
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.51	0.74
1:A:482:PHE:O	2:B:989:THR:HG23	1.88	0.74
1:A:671:ALA:HB1	1:A:736:ASN:ND2	2.02	0.74
1:A:853:ASP:OD1	1:A:855:THR:HG22	1.86	0.74
2:B:628:THR:O	2:B:628:THR:HG22	1.87	0.74
3:C:252:GLN:HG3	9:K:95:ILE:HG23	1.69	0.74
7:I:35:VAL:HG12	7:I:36:GLU:N	2.02	0.74
2:B:64:CYS:HA	2:B:67:SER:CB	2.16	0.74
8:J:1:MET:H1	8:J:56:LEU:H	1.34	0.74
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.22	0.74
1:A:507:VAL:HG13	1:A:521:MET:CE	2.18	0.74
1:A:535:THR:HG21	1:A:617:VAL:H	1.50	0.74
12:T:15:DA:H2"	12:T:16:DC:O5'	1.87	0.74
2:B:549:THR:HG22	2:B:550:ASP:H	1.53	0.74
1:A:567:LYS:NZ	6:H:97:MET:HG2	2.03	0.74
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.68	0.74
2:B:789:MET:CE	2:B:965:LYS:HB3	2.18	0.74
6:H:111:LEU:HD12	6:H:127:GLY:O	1.87	0.73
5:F:101:ILE:HD13	5:F:120:ILE:HG22	1.69	0.73
2:B:373:ARG:HA	2:B:566:LEU:CD2	2.15	0.73
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.86	0.73
1:A:667:GLY:HA2	1:A:670:ILE:CG1	2.19	0.73
1:A:250:ILE:O	1:A:251:SER:HB3	1.89	0.73
1:A:1173:HIS:ND1	1:A:1174:PHE:N	2.36	0.73
12:T:26:DG:N3	12:T:27:DA:H1'	2.03	0.73
1:A:7:SER:HB3	2:B:1193:GLN:OE1	1.89	0.73
1:A:1175:SER:OG	1:A:1176:LEU:N	2.21	0.73
2:B:992:ILE:HD11	9:K:67:PHE:CE2	2.22	0.73
10:L:42:ARG:O	10:L:44:ASP:N	2.22	0.73
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:ARG:CG	2:B:1093:GLN:NE2	2.51	0.72
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.23	0.72
1:A:940:ARG:CZ	1:A:944:ARG:HH21	2.02	0.72
2:B:287:ARG:NH1	2:B:324:ILE:O	2.22	0.72
1:A:67:CYS:HB3	1:A:70:CYS:SG	2.29	0.72
2:B:1164:GLY:HA3	2:B:1190:ASP:HB3	1.70	0.72
1:A:100:LYS:HD3	1:A:104:GLU:OE1	1.90	0.72
1:A:269:ILE:HG13	1:A:299:HIS:HB3	1.70	0.72
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.70	0.72
1:A:148:CYS:HB3	1:A:168:GLY:HA2	1.71	0.72
2:B:980:PHE:O	2:B:981:ALA:HB3	1.90	0.72
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.71	0.72
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.47	0.72
1:A:107:CYS:SG	1:A:108:MET:N	2.62	0.71
1:A:312:PRO:O	1:A:313:GLN:HB2	1.90	0.71
1:A:261:ASP:HB3	1:A:323:LYS:HD2	1.73	0.71
1:A:351:THR:HG23	2:B:1103:ILE:HD13	1.71	0.71
2:B:636:PRO:HB2	2:B:637:LEU:HB3	1.70	0.71
1:A:629:LEU:HD23	1:A:633:VAL:HG23	1.70	0.71
6:H:109:LYS:HG3	6:H:111:LEU:HD22	1.70	0.71
1:A:256:GLN:HB3	1:A:257:ARG:CB	2.20	0.71
1:A:402:ALA:HB2	1:A:434:ARG:HA	1.70	0.71
1:A:1424:VAL:HG13	1:A:1436:ILE:HD11	1.71	0.71
2:B:778:MET:CE	2:B:853:SER:HB3	2.21	0.71
3:C:166:GLU:O	3:C:167:HIS:HB2	1.90	0.71
1:A:423:ASP:C	1:A:424:ILE:HG13	2.11	0.71
2:B:762:ASN:OD1	2:B:984:HIS:CD2	2.43	0.71
1:A:252:PHE:O	1:A:252:PHE:CD1	2.43	0.71
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.90	0.71
2:B:880:THR:O	2:B:881:ASN:HB2	1.89	0.71
9:K:102:LYS:O	9:K:106:GLU:HG2	1.91	0.71
1:A:129:LYS:O	1:A:130:ASP:HB2	1.91	0.71
1:A:1025:ARG:HG2	1:A:1025:ARG:NH1	2.02	0.71
2:B:292:ILE:HD11	2:B:327:ARG:HG2	1.71	0.71
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.73	0.71
6:H:58:THR:HG22	6:H:59:ILE:N	2.06	0.71
1:A:68:GLN:O	1:A:70:CYS:N	2.24	0.70
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.72	0.70
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.57	0.70
10:L:46:VAL:HG12	10:L:47:ARG:H	1.56	0.70
1:A:901:LEU:H	1:A:926:GLN:NE2	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:589:VAL:HG12	2:B:590:HIS:N	2.05	0.70
2:B:744:HIS:HD2	2:B:746:SER:OG	1.73	0.70
2:B:1163:CYS:HB3	2:B:1166:CYS:O	1.90	0.70
1:A:326:ARG:HG2	1:A:1406:VAL:HG21	1.71	0.70
2:B:870:ILE:HG23	2:B:871:THR:H	1.56	0.70
8:J:45:CYS:SG	8:J:46:CYS:N	2.64	0.70
1:A:1273:LEU:O	1:A:1274:ARG:HB3	1.91	0.70
2:B:1096:ARG:HG2	2:B:1096:ARG:NH1	2.05	0.70
6:H:104:PHE:CE1	6:H:136:LYS:HB3	2.22	0.70
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.73	0.70
3:C:148:ARG:NH1	8:J:64:ASN:HA	2.07	0.70
1:A:445:ASN:HB2	1:A:454:SER:O	1.92	0.69
1:A:1391:ARG:HD3	1:A:1391:ARG:C	2.12	0.69
2:B:975:GLN:HG2	2:B:976:ILE:H	1.56	0.69
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.23	0.69
5:F:135:ARG:HG2	5:F:137:TYR:CE1	2.27	0.69
1:A:629:LEU:HD23	1:A:633:VAL:CG2	2.21	0.69
1:A:1404:GLU:O	1:A:1408:ILE:HG12	1.92	0.69
2:B:211:VAL:O	2:B:480:SER:HA	1.92	0.69
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	1.92	0.69
1:A:1116:LEU:H	1:A:1308:THR:HB	1.57	0.69
2:B:682:SER:O	2:B:686:ASN:ND2	2.25	0.69
3:C:66:ARG:HH22	8:J:4:PRO:HA	1.56	0.69
1:A:367:PRO:HB3	1:A:466:SER:HA	1.74	0.69
1:A:765:VAL:CG2	1:A:800:VAL:CB	2.68	0.69
2:B:1051:THR:HB	2:B:1054:GLY:H	1.58	0.69
1:A:1025:ARG:HH11	1:A:1025:ARG:CG	2.06	0.69
1:A:1111:MET:HG2	1:A:1114:PRO:HG3	1.73	0.69
2:B:475:SER:C	2:B:477:ALA:N	2.45	0.69
2:B:589:VAL:HG12	2:B:590:HIS:H	1.56	0.69
2:B:636:PRO:CB	2:B:637:LEU:HA	2.22	0.69
2:B:852:ARG:NH2	10:L:70:ARG:O	2.26	0.69
2:B:976:ILE:O	2:B:990:ILE:CB	2.34	0.69
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.74	0.69
1:A:264:PHE:HZ	1:A:317:LYS:CB	2.05	0.69
2:B:373:ARG:HD3	2:B:566:LEU:CD2	2.22	0.69
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.91	0.68
1:A:37:PHE:HB2	1:A:52:GLY:CA	2.23	0.68
1:A:1222:ASN:O	1:A:1223:ASP:CB	2.41	0.68
2:B:986:GLN:HE22	2:B:1016:ALA:HB1	1.56	0.68
1:A:116:ASP:C	1:A:118:HIS:H	1.97	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:LEU:HD11	2:B:285:ILE:HD11	1.75	0.68
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.75	0.68
9:K:65:HIS:CD2	9:K:67:PHE:HB2	2.28	0.68
1:A:265:LYS:C	1:A:267:ALA:H	1.96	0.68
2:B:637:LEU:HD11	2:B:693:ILE:HG13	1.76	0.68
1:A:845:LEU:O	1:A:848:ILE:HG12	1.94	0.68
1:A:1021:LEU:O	1:A:1024:SER:N	2.27	0.68
1:A:731:ARG:HG3	1:A:755:PHE:CZ	2.28	0.68
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.34	0.68
2:B:475:SER:C	2:B:477:ALA:H	1.95	0.68
6:H:109:LYS:CG	6:H:110:ASP:HB2	2.24	0.68
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.76	0.67
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.58	0.67
5:F:111:LEU:H	5:F:111:LEU:CD1	2.06	0.67
2:B:32:ALA:HB3	2:B:658:ILE:HD11	1.76	0.67
4:E:19:VAL:O	4:E:23:VAL:HG23	1.94	0.67
1:A:855:THR:HG21	1:A:857:ARG:NE	2.04	0.67
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.76	0.67
1:A:504:LEU:HD11	5:F:91:ALA:CB	2.24	0.67
2:B:487:THR:O	2:B:490:SER:HB3	1.93	0.67
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.27	0.67
1:A:814:PHE:HE1	2:B:514:LEU:HD21	1.60	0.67
1:A:1101:LEU:O	1:A:1105:LEU:HD12	1.95	0.67
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.75	0.67
1:A:19:PHE:CE1	1:A:1396:ALA:HB3	2.30	0.67
1:A:264:PHE:HZ	1:A:317:LYS:HB3	1.59	0.67
1:A:332:LYS:C	1:A:334:GLY:H	1.98	0.67
1:A:883:LEU:HD11	1:A:1017:LEU:HD21	1.77	0.67
2:B:955:THR:CG2	2:B:956:THR:H	2.07	0.67
1:A:1116:LEU:HD13	1:A:1329:THR:HG1	1.60	0.67
2:B:221:ASN:N	2:B:241:ARG:O	2.21	0.67
6:H:89:LEU:O	6:H:91:ASP:N	2.27	0.67
8:J:6:ARG:H	8:J:14:VAL:H	1.43	0.67
8:J:7:CYS:HB2	8:J:49:MET:HE3	1.75	0.67
2:B:603:LEU:HB3	2:B:609:ILE:HG12	1.76	0.66
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.77	0.66
2:B:213:ILE:CD1	2:B:481:GLN:OE1	2.40	0.66
8:J:45:CYS:HG	14:J:101:ZN:ZN	1.07	0.66
1:A:527:THR:HG22	1:A:653:VAL:HB	1.78	0.66
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.59	0.66
2:B:615:MET:HG2	2:B:626:ILE:HG23	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:956:THR:HA	2:B:961:LEU:O	1.96	0.66
1:A:344:ARG:HH11	1:A:344:ARG:CG	2.05	0.66
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.95	0.66
2:B:847:ASP:N	2:B:847:ASP:OD1	2.28	0.66
1:A:1434:ALA:O	1:A:1436:ILE:N	2.29	0.66
1:A:577:ILE:O	1:A:580:VAL:HG23	1.95	0.66
2:B:1181:GLU:HG2	2:B:1188:LYS:HG2	1.77	0.66
3:C:165:LYS:O	9:K:6:ARG:NH1	2.29	0.66
10:L:42:ARG:C	10:L:44:ASP:H	1.99	0.66
2:B:471:LYS:HG3	2:B:472:ALA:N	2.09	0.66
1:A:119:ASN:O	1:A:123:ARG:CG	2.40	0.66
1:A:567:LYS:HZ1	6:H:97:MET:HG2	1.60	0.66
3:C:124:LEU:O	3:C:127:ARG:HG2	1.96	0.66
1:A:256:GLN:HB3	1:A:257:ARG:CG	2.26	0.66
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.76	0.66
1:A:751:SER:HG	2:B:1015:HIS:HE1	1.43	0.66
2:B:635:ARG:O	2:B:636:PRO:O	2.14	0.66
2:B:1166:CYS:SG	14:B:1307:ZN:ZN	1.84	0.66
1:A:252:PHE:HE2	12:T:27:DA:H61	1.43	0.65
2:B:980:PHE:CE1	2:B:990:ILE:HG13	2.31	0.65
1:A:185:TRP:O	1:A:186:LYS:HB2	1.96	0.65
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.78	0.65
1:A:892:ALA:HA	1:A:895:LYS:HE3	1.78	0.65
2:B:384:ARG:HH22	2:B:621:GLU:CG	2.08	0.65
2:B:567:GLU:H	2:B:567:GLU:CD	1.99	0.65
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	1.77	0.65
2:B:830:TYR:O	2:B:831:SER:C	2.33	0.65
1:A:907:THR:HG21	1:A:920:LEU:HG	1.78	0.65
2:B:129:PHE:CE2	2:B:166:PHE:HB2	2.31	0.65
2:B:999:MET:HG2	2:B:1008:PRO:HD2	1.78	0.65
5:F:84:TYR:CE1	5:F:152:ILE:HD12	2.32	0.65
6:H:104:PHE:CE2	6:H:136:LYS:HB3	2.24	0.65
1:A:77:CYS:SG	14:A:1735:ZN:ZN	1.85	0.65
2:B:345:LYS:O	2:B:348:ARG:HG2	1.96	0.65
2:B:980:PHE:CE1	2:B:990:ILE:HD11	2.31	0.65
1:A:115:LEU:HD11	1:A:145:LYS:HE3	1.79	0.65
1:A:575:LYS:HB3	1:A:612:ILE:HG12	1.78	0.65
2:B:549:THR:HG22	2:B:550:ASP:N	2.11	0.65
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.77	0.65
3:C:3:GLU:HB3	9:K:104:ASN:OD1	1.96	0.65
1:A:1130:GLN:HG3	1:A:1134:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.78	0.65
1:A:503:GLN:HB2	1:A:504:LEU:HD12	1.78	0.65
8:J:45:CYS:SG	14:J:101:ZN:ZN	1.85	0.65
2:B:1094:ARG:HH22	2:B:1098:MET:HG2	1.62	0.64
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.32	0.64
6:H:109:LYS:CB	6:H:111:LEU:N	2.60	0.64
2:B:370:PHE:HD2	2:B:373:ARG:HG3	1.62	0.64
2:B:864:LYS:HB3	2:B:872:GLU:H	1.60	0.64
1:A:1134:ILE:O	1:A:1138:ILE:HG12	1.97	0.64
2:B:778:MET:HE3	2:B:853:SER:HB3	1.80	0.64
6:H:93:TYR:HA	6:H:145:ARG:HB3	1.79	0.64
1:A:401:GLY:O	1:A:435:HIS:CD2	2.50	0.64
1:A:1319:VAL:HG13	1:A:1320:PRO:HD2	1.77	0.64
6:H:130:ARG:HB3	6:H:134:ASN:HD22	1.63	0.64
1:A:455:MET:HE1	2:B:1130:PHE:HE1	1.63	0.64
1:A:567:LYS:O	1:A:569:LYS:N	2.30	0.64
1:A:900:ASP:HB3	1:A:906:HIS:O	1.98	0.64
2:B:62:ILE:HD12	2:B:418:LYS:HG3	1.80	0.64
1:A:525:GLN:O	1:A:526:ASP:C	2.36	0.64
1:A:809:THR:HB	1:A:810:PRO:HD2	1.79	0.64
2:B:803:LEU:H	2:B:822:ASN:HD21	1.45	0.64
4:E:63:ASN:HB3	4:E:64:PRO:HD3	1.79	0.64
4:E:66:GLU:O	4:E:68:SER:N	2.31	0.64
1:A:380:VAL:HG21	1:A:430:TRP:HB2	1.78	0.64
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.80	0.64
4:E:185:ALA:HA	4:E:190:LEU:HD23	1.80	0.64
8:J:1:MET:H2	8:J:56:LEU:H	1.43	0.64
9:K:57:LEU:HD12	9:K:76:GLN:CG	2.27	0.64
1:A:343:LYS:NZ	2:B:1197:PRO:HB3	2.12	0.64
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.78	0.64
11:R:4:G:C2'	11:R:5:A:H8	2.04	0.64
2:B:378:LEU:O	2:B:382:ILE:HG12	1.99	0.63
6:H:97:MET:HB2	6:H:118:PHE:CD2	2.32	0.63
1:A:532:ARG:HH22	1:A:745:GLN:HE21	1.46	0.63
1:A:535:THR:CG2	1:A:616:VAL:HA	2.28	0.63
2:B:955:THR:HG23	10:L:54:ARG:O	1.98	0.63
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.62	0.63
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.81	0.63
1:A:1312:ASN:O	1:A:1316:VAL:HG23	1.99	0.63
2:B:636:PRO:HB2	2:B:637:LEU:CA	2.28	0.63
5:F:135:ARG:HG2	5:F:137:TYR:HE1	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:GLY:H	1:A:435:HIS:HD2	1.44	0.63
2:B:45:SER:OG	2:B:46:GLN:N	2.29	0.63
6:H:23:VAL:HG21	6:H:121:LEU:HD21	1.81	0.63
1:A:500:GLU:HG2	2:B:1143:ALA:HB1	1.81	0.63
1:A:810:PRO:HD3	2:B:1047:PHE:CD2	2.33	0.63
6:H:104:PHE:CD2	6:H:114:VAL:HG12	2.31	0.63
1:A:206:GLU:O	1:A:210:ILE:HG12	1.99	0.63
1:A:315:LEU:CB	1:A:316:GLN:CA	2.46	0.63
1:A:401:GLY:N	1:A:435:HIS:HD2	1.97	0.63
1:A:1342:GLU:HG2	4:E:212:ARG:HH11	1.64	0.63
2:B:763:GLN:O	2:B:766:ARG:HB2	1.97	0.63
12:T:13:DA:H61	13:N:2:DT:C7	2.12	0.63
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.79	0.63
1:A:1394:THR:HG22	1:A:1398:MET:CE	2.28	0.63
2:B:784:ASN:CG	2:B:788:ARG:HD2	2.20	0.63
2:B:824:ILE:HG12	8:J:48:ARG:NH1	2.14	0.63
1:A:261:ASP:HB3	1:A:323:LYS:CD	2.29	0.62
1:A:451:HIS:HB3	1:A:453:MET:H	1.64	0.62
1:A:1189:SER:OG	1:A:1190:PRO:HD2	1.99	0.62
1:A:767:GLN:OE1	1:A:767:GLN:HA	1.99	0.62
2:B:783:THR:HG21	8:J:59:LYS:HB3	1.81	0.62
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.81	0.62
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.46	0.62
1:A:352:VAL:HG12	1:A:353:ILE:N	2.13	0.62
1:A:1393:ASN:N	1:A:1393:ASN:OD1	2.32	0.62
8:J:45:CYS:O	8:J:48:ARG:HG3	1.99	0.62
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	2.15	0.62
2:B:711:GLU:H	2:B:712:PRO:HD3	1.63	0.62
2:B:980:PHE:CE1	2:B:990:ILE:CD1	2.83	0.62
6:H:109:LYS:HG2	6:H:111:LEU:HD23	1.81	0.62
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.29	0.62
10:L:51:CYS:SG	14:L:105:ZN:ZN	1.89	0.62
1:A:315:LEU:CD1	1:A:318:SER:O	2.40	0.62
2:B:622:LYS:HE3	7:I:59:VAL:HG22	1.82	0.62
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.64	0.62
5:F:74:ILE:HG21	5:F:144:GLU:HG2	1.80	0.62
6:H:47:PHE:CB	6:H:95:TYR:CD1	2.75	0.62
3:C:144:ILE:HG22	3:C:145:CYS:HB3	1.80	0.62
2:B:273:LEU:HD11	2:B:285:ILE:CD1	2.30	0.62
2:B:636:PRO:HB3	2:B:743:ILE:HG12	1.81	0.62
2:B:807:ARG:HG3	2:B:807:ARG:NH1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:955:THR:CG2	2:B:956:THR:N	2.63	0.62
8:J:6:ARG:HG2	8:J:13:VAL:HA	1.81	0.62
7:I:111:THR:HG22	7:I:113:ASP:H	1.63	0.62
3:C:102:GLN:CG	3:C:154:LYS:HD3	2.26	0.62
9:K:92:ASN:HA	9:K:95:ILE:HD12	1.81	0.62
1:A:1392:SER:O	1:A:1393:ASN:C	2.38	0.62
2:B:474:SER:C	2:B:476:ARG:H	2.03	0.62
3:C:45:ALA:HA	3:C:72:LEU:CD1	2.23	0.62
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.12	0.61
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.40	0.61
1:A:869:GLY:O	4:E:204:THR:HG21	2.00	0.61
1:A:709:THR:HB	1:A:712:GLU:H	1.65	0.61
1:A:826:ASP:O	1:A:830:LYS:N	2.27	0.61
1:A:900:ASP:O	1:A:907:THR:HA	2.00	0.61
2:B:636:PRO:HB2	2:B:637:LEU:CB	2.29	0.61
2:B:982:SER:OG	2:B:983:ARG:N	2.30	0.61
6:H:108:SER:OG	6:H:109:LYS:N	2.33	0.61
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.81	0.61
2:B:490:SER:O	2:B:493:SER:N	2.33	0.61
3:C:248:ILE:HG12	9:K:101:LEU:HD13	1.83	0.61
4:E:61:GLN:CB	4:E:79:TRP:HE3	2.11	0.61
1:A:302:THR:HG21	1:A:313:GLN:NE2	2.16	0.61
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.30	0.61
2:B:830:TYR:O	2:B:832:GLY:N	2.34	0.61
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.81	0.61
1:A:116:ASP:O	1:A:118:HIS:N	2.34	0.61
1:A:860:LEU:HD11	1:A:1393:ASN:ND2	2.15	0.61
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.83	0.61
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.32	0.61
3:C:49:VAL:HG12	3:C:155:LEU:HD22	1.83	0.61
1:A:335:ARG:NH1	2:B:1202:LEU:HD12	2.16	0.61
1:A:336:ILE:HA	1:A:340:LEU:HD12	1.83	0.61
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.23	0.61
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.82	0.61
2:B:981:ALA:HB1	2:B:987:LYS:HA	1.80	0.61
9:K:70:ARG:O	9:K:71:PHE:HB3	2.01	0.61
1:A:203:SER:O	1:A:207:ILE:HD12	2.01	0.61
1:A:315:LEU:HD13	1:A:319:GLY:O	2.01	0.61
3:C:182:PRO:HB2	3:C:207:CYS:SG	2.41	0.61
5:F:81:THR:HB	5:F:136:ARG:NH1	2.14	0.61
1:A:809:THR:H	1:A:812:GLU:HB2	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.83	0.60
1:A:253:ASN:HD22	1:A:257:ARG:HA	1.66	0.60
1:A:351:THR:HG21	1:A:466:SER:O	2.01	0.60
1:A:553:VAL:HG23	1:A:652:VAL:CG2	2.30	0.60
1:A:1134:ILE:O	1:A:1138:ILE:CG1	2.49	0.60
2:B:980:PHE:CD1	2:B:990:ILE:HG13	2.36	0.60
3:C:143:LEU:C	3:C:143:LEU:HD12	2.20	0.60
6:H:96:VAL:HG13	6:H:143:LEU:HG	1.82	0.60
1:A:913:LEU:HG	1:A:915:SER:H	1.67	0.60
1:A:648:ASN:O	1:A:652:VAL:HG23	2.01	0.60
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.15	0.60
2:B:957:ASN:HB3	2:B:961:LEU:HB2	1.83	0.60
4:E:29:PHE:O	4:E:30:ILE:CG1	2.45	0.60
6:H:109:LYS:HA	6:H:110:ASP:CB	2.16	0.60
8:J:1:MET:H2	8:J:56:LEU:N	1.99	0.60
10:L:41:SER:O	10:L:42:ARG:O	2.18	0.60
1:A:899:VAL:HG23	1:A:1029:ARG:HG3	1.84	0.60
3:C:93:ASP:O	3:C:127:ARG:NH2	2.35	0.60
1:A:553:VAL:HG23	1:A:652:VAL:HG22	1.83	0.60
2:B:770:GLN:HG2	2:B:983:ARG:O	2.01	0.60
2:B:1104:HIS:HB2	2:B:1122:ARG:HD2	1.84	0.60
3:C:173:ALA:O	3:C:174:ALA:HB2	2.02	0.60
8:J:2:ILE:HG23	8:J:2:ILE:O	2.02	0.60
1:A:535:THR:HG22	1:A:616:VAL:HA	1.84	0.60
1:A:490:HIS:HB3	2:B:1150:ARG:CZ	2.32	0.60
1:A:1333:ILE:O	1:A:1333:ILE:HD13	2.02	0.60
2:B:870:ILE:HG22	2:B:871:THR:N	2.16	0.60
1:A:93:VAL:HG21	1:A:304:MET:HB3	1.82	0.60
3:C:76:ASP:OD2	3:C:128:ASN:HB3	2.01	0.60
1:A:380:VAL:HG23	1:A:430:TRP:O	2.02	0.59
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.84	0.59
1:A:956:LEU:HD11	1:A:1017:LEU:HD22	1.84	0.59
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.83	0.59
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.83	0.59
2:B:322:PHE:HZ	7:I:30:ARG:HH11	1.47	0.59
2:B:383:ASN:O	2:B:387:LEU:HB2	2.01	0.59
8:J:3:VAL:HG22	8:J:53:HIS:CE1	2.38	0.59
1:A:105:CYS:O	1:A:114:LEU:CG	2.48	0.59
2:B:373:ARG:HD3	2:B:566:LEU:HD23	1.82	0.59
1:A:253:ASN:ND2	1:A:257:ARG:CA	2.66	0.59
1:A:257:ARG:O	1:A:257:ARG:CG	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:ASN:HD22	1:A:744:LYS:H	1.49	0.59
3:C:184:ASN:ND2	3:C:187:LYS:HA	2.17	0.59
6:H:108:SER:OG	6:H:109:LYS:HE2	2.02	0.59
1:A:68:GLN:C	1:A:70:CYS:H	2.06	0.59
1:A:100:LYS:O	1:A:104:GLU:HG3	2.03	0.59
1:A:264:PHE:CZ	1:A:317:LYS:HB3	2.35	0.59
1:A:741:ASN:ND2	1:A:744:LYS:H	2.00	0.59
2:B:515:HIS:H	2:B:518:HIS:CD2	2.20	0.59
3:C:115:SER:HB3	3:C:142:VAL:HG12	1.83	0.59
8:J:7:CYS:HB2	8:J:49:MET:CE	2.31	0.59
1:A:95:PHE:O	1:A:99:ILE:HG13	2.01	0.59
1:A:583:PRO:O	1:A:610:GLY:HA2	2.02	0.59
1:A:840:ARG:HG3	1:A:1402:PHE:HZ	1.67	0.59
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.84	0.59
1:A:922:ASP:OD1	1:A:923:LEU:N	2.34	0.59
2:B:190:TYR:CZ	2:B:196:PRO:HG2	2.37	0.59
2:B:308:TRP:HA	2:B:311:LEU:HD12	1.84	0.59
9:K:24:ASP:OD2	9:K:74:ARG:HD2	2.02	0.59
2:B:210:LYS:NZ	2:B:482:VAL:HG13	2.17	0.59
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.32	0.59
3:C:167:HIS:ND1	10:L:70:ARG:HB3	2.18	0.59
4:E:176:PRO:O	4:E:212:ARG:HA	2.02	0.59
6:H:109:LYS:CG	6:H:110:ASP:CB	2.81	0.59
6:H:139:ASN:O	6:H:140:ALA:HB2	2.02	0.59
12:T:27:DA:H2'	12:T:27:DA:N3	2.17	0.59
1:A:565:ILE:HG12	1:A:567:LYS:NZ	2.18	0.59
2:B:515:HIS:CD2	2:B:517:THR:H	2.20	0.59
2:B:636:PRO:CB	2:B:637:LEU:CA	2.80	0.59
2:B:870:ILE:HG23	2:B:871:THR:N	2.14	0.59
2:B:980:PHE:HE1	2:B:990:ILE:CD1	2.16	0.59
1:A:107:CYS:SG	1:A:108:MET:O	2.60	0.59
1:A:341:MET:HE2	1:A:1401:SER:HB2	1.84	0.59
1:A:517:ASN:HD22	1:A:1364:ASN:HB2	1.66	0.59
1:A:1168:GLU:HG2	1:A:1168:GLU:O	2.03	0.59
2:B:179:CYS:SG	2:B:180:TYR:N	2.75	0.59
3:C:247:GLY:O	3:C:248:ILE:C	2.39	0.59
6:H:89:LEU:HB2	6:H:91:ASP:OD1	2.03	0.59
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.84	0.58
2:B:708:GLU:O	2:B:710:LEU:N	2.35	0.58
1:A:1276:VAL:HB	1:A:1279:ILE:HD13	1.86	0.58
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:NE2	3:C:237:SER:O	2.36	0.58
5:F:111:LEU:CD1	5:F:111:LEU:N	2.67	0.58
6:H:58:THR:HG22	6:H:59:ILE:H	1.68	0.58
1:A:341:MET:CE	1:A:1401:SER:HB2	2.34	0.58
1:A:1400:CYS:O	1:A:1405:THR:HG23	2.04	0.58
2:B:745:PRO:O	2:B:747:MET:N	2.36	0.58
1:A:1116:LEU:HD22	1:A:1311:VAL:HG22	1.85	0.58
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.33	0.58
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.85	0.58
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.86	0.58
1:A:256:GLN:CB	1:A:257:ARG:HD3	2.10	0.58
1:A:1152:ILE:HD12	7:I:44:TYR:HD2	1.68	0.58
1:A:1220:PHE:CD1	1:A:1224:LEU:CD2	2.86	0.58
2:B:770:GLN:HB2	2:B:983:ARG:O	2.04	0.58
2:B:1154:ALA:O	2:B:1155:SER:HB2	2.03	0.58
3:C:134:ILE:HD12	3:C:141:GLY:H	1.68	0.58
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.86	0.58
1:A:596:THR:C	1:A:598:LEU:H	2.06	0.58
1:A:1019:CYS:O	1:A:1022:LEU:HB3	2.03	0.58
1:A:58:LEU:HD22	1:A:244:PRO:HD2	1.85	0.58
1:A:251:SER:O	1:A:252:PHE:HD2	1.86	0.58
1:A:1025:ARG:HG3	1:A:1030:ARG:NH1	2.18	0.58
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.86	0.58
4:E:77:SER:HB3	4:E:105:PHE:HD2	1.68	0.58
1:A:55:ASP:H	1:A:56:PRO:HD2	1.69	0.58
1:A:58:LEU:HD21	1:A:243:PRO:HB3	1.86	0.58
1:A:253:ASN:HD22	1:A:257:ARG:CA	2.17	0.58
2:B:976:ILE:HG23	2:B:977:GLY:N	2.18	0.58
8:J:7:CYS:CB	8:J:49:MET:HE3	2.34	0.58
1:A:265:LYS:HD3	1:A:302:THR:HG22	1.86	0.57
1:A:335:ARG:O	1:A:339:ASN:HB2	2.04	0.57
1:A:527:THR:HG21	1:A:650:GLN:HA	1.86	0.57
6:H:5:LEU:HD22	6:H:133:ASN:O	2.04	0.57
1:A:567:LYS:CB	1:A:568:PRO:CD	2.57	0.57
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.86	0.57
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.34	0.57
2:B:913:GLY:HA2	2:B:938:SER:CB	2.31	0.57
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.85	0.57
5:F:109:VAL:CG1	5:F:110:ASP:H	2.16	0.57
1:A:55:ASP:O	1:A:58:LEU:N	2.37	0.57
1:A:446:ARG:HD3	1:A:478:TYR:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:O	1:A:57:ARG:N	2.37	0.57
1:A:381:THR:HG22	1:A:384:ASN:ND2	2.19	0.57
1:A:690:VAL:HG13	1:A:718:VAL:HG22	1.86	0.57
1:A:840:ARG:HG3	1:A:1402:PHE:CZ	2.39	0.57
2:B:120:ARG:HE	2:B:955:THR:CG2	2.17	0.57
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.34	0.57
4:E:190:LEU:HD12	4:E:194:GLU:O	2.03	0.57
6:H:47:PHE:HB2	6:H:95:TYR:HD1	1.68	0.57
12:T:26:DG:C2	12:T:27:DA:H1'	2.39	0.57
1:A:54:ASN:O	1:A:55:ASP:HB2	2.04	0.57
1:A:675:THR:C	1:A:679:ILE:HD12	2.25	0.57
1:A:709:THR:HG23	7:I:94:ASP:HA	1.86	0.57
1:A:909:ASP:C	1:A:911:SER:N	2.56	0.57
2:B:865:LYS:O	2:B:866:TYR:C	2.43	0.57
2:B:957:ASN:HD22	2:B:959:ASP:H	1.52	0.57
9:K:46:ILE:O	9:K:50:LEU:HB2	2.04	0.57
1:A:535:THR:HG21	1:A:617:VAL:N	2.19	0.57
1:A:635:ARG:NE	1:A:877:HIS:HA	2.16	0.57
2:B:357:GLN:HA	2:B:374:LYS:NZ	2.19	0.57
7:I:84:VAL:HG13	7:I:84:VAL:O	2.04	0.57
12:T:18:DA:C2	12:T:19:DT:N3	2.72	0.57
1:A:659:HIS:O	2:B:1081:LEU:HD23	2.03	0.57
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.87	0.57
1:A:1073:GLY:O	1:A:1076:ALA:HB3	2.05	0.57
2:B:384:ARG:HH22	2:B:621:GLU:HG3	1.68	0.57
6:H:38:LEU:CD1	6:H:125:LEU:HD13	2.33	0.57
1:A:1151:GLU:OE2	7:I:45:ARG:NH1	2.38	0.57
1:A:1173:HIS:ND1	1:A:1173:HIS:C	2.58	0.57
2:B:115:GLN:O	2:B:119:LEU:HD12	2.05	0.57
2:B:235:SER:OG	2:B:236:HIS:HD2	1.88	0.57
5:F:109:VAL:CG1	5:F:110:ASP:N	2.67	0.57
2:B:211:VAL:HG23	2:B:483:LEU:HA	1.87	0.56
1:A:99:ILE:HG12	1:A:234:MET:SD	2.45	0.56
1:A:378:GLU:OE1	1:A:434:ARG:HD3	2.05	0.56
2:B:120:ARG:HE	2:B:955:THR:HG21	1.69	0.56
2:B:1106:ARG:CD	2:B:1126:GLY:O	2.30	0.56
4:E:213:ILE:HG12	4:E:214:CYS:H	1.69	0.56
2:B:322:PHE:CD1	2:B:322:PHE:O	2.58	0.56
2:B:552:MET:HA	2:B:555:ILE:HB	1.86	0.56
2:B:733:HIS:O	2:B:735:ALA:N	2.30	0.56
2:B:801:LYS:O	8:J:52:THR:CG2	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.19	0.56
2:B:1149:GLU:HG3	2:B:1153:GLU:HB2	1.86	0.56
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.21	0.56
6:H:41:ASP:O	6:H:121:LEU:HD13	2.06	0.56
9:K:63:VAL:HG23	9:K:63:VAL:O	2.04	0.56
1:A:356:ASP:OD2	9:K:65:HIS:HE1	1.88	0.56
2:B:750:GLY:O	2:B:752:ALA:N	2.39	0.56
2:B:806:THR:H	2:B:809:MET:HG3	1.71	0.56
2:B:815:ARG:HB2	2:B:816:GLU:OE1	2.05	0.56
2:B:980:PHE:O	2:B:981:ALA:CB	2.53	0.56
4:E:29:PHE:HD1	4:E:65:THR:HB	1.69	0.56
1:A:404:TYR:HA	1:A:413:ILE:O	2.06	0.56
2:B:277:LYS:NZ	2:B:335:GLY:HA2	2.20	0.56
9:K:47:ARG:HB3	9:K:47:ARG:HH11	1.71	0.56
1:A:13:THR:HG22	1:A:1432:GLN:NE2	2.20	0.56
1:A:722:LEU:HD13	1:A:799:PHE:CD1	2.41	0.56
1:A:1017:LEU:HB2	4:E:205:SER:HA	1.88	0.56
1:A:1025:ARG:NH1	1:A:1025:ARG:CG	2.68	0.56
1:A:1319:VAL:CG1	1:A:1320:PRO:HD2	2.35	0.56
2:B:100:PRO:HD3	2:B:126:SER:HG	1.70	0.56
3:C:98:VAL:C	3:C:99:LEU:HD23	2.25	0.56
3:C:173:ALA:O	3:C:235:VAL:HG22	2.05	0.56
1:A:451:HIS:HB3	1:A:453:MET:N	2.19	0.56
1:A:678:GLU:HA	1:A:681:GLU:HG2	1.87	0.56
1:A:751:SER:HG	2:B:1015:HIS:CE1	2.20	0.56
2:B:797:TYR:HH	2:B:971:THR:HG1	1.54	0.56
5:F:76:LYS:O	5:F:79:ARG:CD	2.54	0.56
3:C:148:ARG:HG2	3:C:149:LYS:H	1.70	0.56
6:H:82:PRO:O	6:H:83:GLN:CB	2.48	0.56
1:A:694:THR:HA	1:A:714:PHE:CE1	2.40	0.56
2:B:801:LYS:O	8:J:52:THR:HG23	2.05	0.56
1:A:451:HIS:CE1	1:A:1074:GLU:HG3	2.41	0.56
2:B:288:ALA:N	2:B:330:ALA:HB1	2.21	0.56
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.88	0.56
11:R:3:C:N4	12:T:26:DG:H1	1.95	0.56
1:A:253:ASN:HB3	1:A:257:ARG:N	2.21	0.55
2:B:115:GLN:OE1	2:B:115:GLN:HA	2.06	0.55
2:B:745:PRO:C	2:B:747:MET:H	2.09	0.55
2:B:1166:CYS:HB3	2:B:1185:CYS:SG	2.46	0.55
1:A:598:LEU:HB3	6:H:25:ARG:HH12	1.72	0.55
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.88	0.55
2:B:881:ASN:HB2	2:B:933:SER:N	2.21	0.55
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.88	0.55
1:A:483:ASP:OD1	11:R:11:U:OP1	2.25	0.55
1:A:876:ALA:HB3	1:A:877:HIS:CD2	2.40	0.55
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.71	0.55
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.07	0.55
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.88	0.55
2:B:983:ARG:HG3	2:B:1093:GLN:HE21	1.64	0.55
3:C:42:PRO:HA	3:C:163:ILE:HG23	1.87	0.55
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.89	0.55
9:K:37:LYS:O	9:K:38:GLU:HG2	2.06	0.55
1:A:500:GLU:HG2	2:B:1143:ALA:CB	2.37	0.55
1:A:911:SER:O	1:A:978:PRO:HB3	2.06	0.55
2:B:744:HIS:CD2	2:B:746:SER:OG	2.57	0.55
2:B:753:ALA:HA	2:B:756:ILE:HD12	1.88	0.55
2:B:274:PRO:HB2	2:B:359:GLU:HB3	1.87	0.55
8:J:48:ARG:NH2	8:J:49:MET:CE	2.68	0.55
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.72	0.55
2:B:34:ILE:HD13	2:B:542:MET:CE	2.37	0.55
4:E:77:SER:CB	4:E:105:PHE:HA	2.37	0.55
8:J:44:TYR:CA	8:J:47:ARG:HB2	2.29	0.55
1:A:119:ASN:HB3	1:A:122:MET:HB3	1.88	0.55
1:A:464:PRO:HG2	9:K:67:PHE:CD1	2.42	0.55
1:A:485:ASP:OD1	1:A:485:ASP:N	2.33	0.55
1:A:525:GLN:O	1:A:528:LEU:N	2.38	0.55
1:A:765:VAL:HG23	1:A:766:GLY:H	1.71	0.55
2:B:644:GLU:HB3	2:B:647:GLY:O	2.06	0.55
3:C:66:ARG:HH21	8:J:4:PRO:HA	1.68	0.55
6:H:109:LYS:N	6:H:109:LYS:HD3	2.20	0.55
2:B:637:LEU:H	2:B:637:LEU:HD12	1.72	0.55
1:A:104:GLU:O	1:A:171:GLN:OE1	2.26	0.54
1:A:344:ARG:HB3	2:B:1118:PRO:HD2	1.89	0.54
1:A:507:VAL:CG1	1:A:521:MET:HE1	2.34	0.54
1:A:851:HIS:HD2	1:A:857:ARG:HG3	1.70	0.54
1:A:896:ARG:HH11	1:A:897:TYR:HE1	1.54	0.54
2:B:980:PHE:CE1	2:B:990:ILE:CG1	2.90	0.54
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.88	0.54
1:A:272:ALA:HA	1:A:275:SER:HB3	1.89	0.54
1:A:751:SER:CB	2:B:1015:HIS:HE1	2.19	0.54
2:B:62:ILE:HD12	2:B:418:LYS:CG	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:LYS:HG3	3:C:21:ILE:HB	1.89	0.54
4:E:191:LYS:H	4:E:194:GLU:HB2	1.72	0.54
8:J:48:ARG:NH2	8:J:49:MET:HE1	2.09	0.54
1:A:1384:VAL:HA	1:A:1389:PHE:HD2	1.73	0.54
2:B:814:PHE:C	2:B:816:GLU:H	2.09	0.54
1:A:120:GLU:OE2	1:A:120:GLU:HA	2.07	0.54
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.07	0.54
1:A:913:LEU:HD23	1:A:915:SER:HB2	1.88	0.54
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.72	0.54
1:A:253:ASN:HB3	1:A:257:ARG:H	1.73	0.54
1:A:947:PHE:CD2	1:A:954:TRP:CE2	2.96	0.54
9:K:6:ARG:O	9:K:8:GLU:N	2.41	0.54
1:A:919:ILE:HG23	1:A:925:LEU:HD12	1.90	0.54
2:B:708:GLU:HG3	2:B:709:ASP:H	1.73	0.54
2:B:917:PRO:HA	2:B:934:LYS:HA	1.90	0.54
3:C:148:ARG:HH12	8:J:64:ASN:HA	1.72	0.54
7:I:109:ILE:CD1	7:I:109:ILE:CB	2.80	0.54
1:A:67:CYS:CB	1:A:70:CYS:SG	2.96	0.54
1:A:98:LYS:O	1:A:102:VAL:CG2	2.54	0.54
1:A:101:LYS:HG2	1:A:139:TRP:HE1	1.72	0.54
1:A:535:THR:O	1:A:575:LYS:HE2	2.08	0.54
1:A:605:MET:HE3	1:A:606:LEU:H	1.73	0.54
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	2.96	0.54
1:A:1220:PHE:CD1	1:A:1224:LEU:HD22	2.42	0.54
2:B:1128:LEU:HD23	12:T:21:DC:OP1	2.08	0.54
1:A:265:LYS:C	1:A:267:ALA:N	2.60	0.54
1:A:391:LEU:HB3	1:A:401:GLY:HA2	1.90	0.54
1:A:996:ASN:HA	1:A:998:LEU:HD23	1.88	0.54
2:B:980:PHE:O	2:B:1095:LEU:CD1	2.56	0.54
3:C:22:LEU:HD23	3:C:25:VAL:CG2	2.38	0.54
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.22	0.54
1:A:116:ASP:C	1:A:118:HIS:N	2.61	0.54
1:A:265:LYS:NZ	1:A:323:LYS:HE2	2.23	0.54
1:A:928:LEU:O	1:A:931:GLU:HB3	2.07	0.54
1:A:1170:ILE:O	1:A:1171:GLN:O	2.26	0.54
2:B:176:SER:O	2:B:182:SER:HB2	2.08	0.54
3:C:8:VAL:HG11	9:K:105:PHE:HD1	1.73	0.54
1:A:1224:LEU:O	1:A:1226:VAL:HG23	2.08	0.54
1:A:1349:TYR:HB2	1:A:1372:VAL:HG21	1.90	0.54
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.43	0.54
3:C:22:LEU:HD23	3:C:25:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:61:TYR:HA	9:K:72:LYS:O	2.08	0.54
1:A:257:ARG:CG	1:A:257:ARG:NH1	2.62	0.53
1:A:947:PHE:HE2	1:A:954:TRP:CD2	2.26	0.53
2:B:464:GLY:HA2	2:B:479:VAL:O	2.08	0.53
4:E:61:GLN:HG2	4:E:79:TRP:HE3	1.73	0.53
6:H:109:LYS:CB	6:H:111:LEU:HD22	2.37	0.53
8:J:12:LYS:NZ	8:J:17:LYS:NZ	2.56	0.53
1:A:786:HIS:ND1	2:B:703:ILE:HB	2.23	0.53
2:B:778:MET:HE1	2:B:853:SER:HB3	1.91	0.53
2:B:1175:LEU:O	2:B:1176:ASN:HB3	2.09	0.53
8:J:7:CYS:CA	8:J:49:MET:HE3	2.38	0.53
1:A:532:ARG:O	1:A:535:THR:N	2.40	0.53
1:A:889:SER:HB2	1:A:892:ALA:N	2.19	0.53
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.43	0.53
1:A:249:SER:O	1:A:250:ILE:HG12	2.06	0.53
1:A:871:ASP:HB3	4:E:204:THR:HG22	1.89	0.53
1:A:1173:HIS:O	1:A:1175:SER:N	2.41	0.53
1:A:1191:TRP:HB3	1:A:1260:LEU:HD22	1.90	0.53
3:C:124:LEU:C	3:C:126:GLY:N	2.61	0.53
1:A:37:PHE:HB2	1:A:52:GLY:HA2	1.91	0.53
2:B:25:ILE:CD1	2:B:653:VAL:HB	2.38	0.53
2:B:204:ILE:O	2:B:205:ILE:HD13	2.08	0.53
2:B:736:THR:O	2:B:736:THR:HG22	2.09	0.53
4:E:52:ARG:HB3	4:E:53:PRO:CD	2.38	0.53
10:L:42:ARG:C	10:L:44:ASP:N	2.61	0.53
1:A:1116:LEU:CD2	1:A:1311:VAL:HA	2.39	0.53
1:A:1364:ASN:ND2	1:A:1366:ARG:H	2.06	0.53
2:B:614:SER:H	2:B:632:ARG:HH12	1.57	0.53
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.91	0.53
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.73	0.53
4:E:66:GLU:C	4:E:68:SER:N	2.61	0.53
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.39	0.53
1:A:940:ARG:CZ	1:A:944:ARG:NH2	2.69	0.53
2:B:653:VAL:HG13	2:B:689:LEU:HD13	1.89	0.53
2:B:702:LEU:HD23	2:B:738:PHE:N	2.22	0.53
2:B:784:ASN:OD1	2:B:788:ARG:HD2	2.09	0.53
1:A:445:ASN:CB	1:A:455:MET:HG2	2.38	0.53
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.09	0.53
4:E:14:ARG:HH12	4:E:142:VAL:HG22	1.74	0.53
6:H:23:VAL:CG2	6:H:121:LEU:HD21	2.38	0.53
10:L:32:ALA:HB3	10:L:55:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.39	0.53
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.91	0.53
1:A:909:ASP:C	1:A:911:SER:H	2.10	0.53
4:E:2:ASP:O	4:E:3:GLN:HB3	2.09	0.53
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.90	0.53
1:A:119:ASN:HB3	1:A:122:MET:CB	2.39	0.53
1:A:809:THR:CB	1:A:810:PRO:HD2	2.38	0.53
1:A:863:VAL:HG11	1:A:866:PHE:CE2	2.43	0.53
2:B:451:LYS:O	2:B:452:THR:C	2.48	0.53
2:B:498:THR:O	2:B:536:VAL:HA	2.09	0.53
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.44	0.53
7:I:75:CYS:SG	7:I:78:CYS:HB2	2.48	0.53
8:J:43:ARG:HB3	8:J:43:ARG:HH11	1.74	0.53
9:K:53:ASP:OD1	9:K:56:VAL:HG23	2.08	0.53
1:A:754:SER:H	1:A:757:ASN:ND2	2.07	0.52
1:A:1161:THR:HG22	1:A:1162:VAL:H	1.74	0.52
2:B:770:GLN:CG	2:B:983:ARG:O	2.57	0.52
2:B:1072:MET:O	2:B:1081:LEU:HB2	2.08	0.52
2:B:1162:ILE:HD13	2:B:1168:LEU:O	2.08	0.52
1:A:755:PHE:O	1:A:758:ILE:N	2.42	0.52
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.63	0.52
1:A:913:LEU:HD11	1:A:981:LEU:O	2.09	0.52
2:B:516:ASN:HD22	2:B:516:ASN:H	1.57	0.52
3:C:16:ASP:O	3:C:233:GLU:HA	2.10	0.52
4:E:69:ILE:O	4:E:69:ILE:HG22	2.09	0.52
1:A:27:VAL:O	1:A:30:ILE:HG22	2.10	0.52
1:A:863:VAL:HG11	1:A:866:PHE:CD2	2.43	0.52
1:A:1394:THR:CG2	1:A:1398:MET:CE	2.88	0.52
2:B:635:ARG:O	2:B:636:PRO:C	2.46	0.52
2:B:1148:LYS:O	2:B:1152:MET:HB2	2.09	0.52
4:E:66:GLU:C	4:E:68:SER:H	2.13	0.52
7:I:35:VAL:CG1	7:I:36:GLU:N	2.72	0.52
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.92	0.52
1:A:642:CYS:O	1:A:645:LEU:HB3	2.08	0.52
2:B:476:ARG:O	2:B:478:GLY:N	2.43	0.52
1:A:498:ARG:O	1:A:499:ALA:C	2.48	0.52
1:A:856:THR:O	1:A:864:ILE:HG12	2.10	0.52
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.74	0.52
1:A:1261:LYS:C	1:A:1263:ILE:H	2.12	0.52
2:B:482:VAL:HG11	12:T:25:DC:H5"	1.91	0.52
1:A:332:LYS:O	1:A:334:GLY:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:LYS:HE2	13:N:3:DG:OP2	2.09	0.52
1:A:1170:ILE:O	1:A:1171:GLN:C	2.47	0.52
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.39	0.52
2:B:358:LYS:HA	2:B:366:GLN:HG2	1.91	0.52
2:B:981:ALA:O	2:B:1092:TYR:CD2	2.63	0.52
2:B:1084:GLN:NE2	3:C:192:TRP:HB2	2.25	0.52
3:C:49:VAL:CG1	3:C:155:LEU:HD22	2.39	0.52
3:C:167:HIS:CD2	3:C:169:LYS:HG2	2.45	0.52
6:H:109:LYS:CB	6:H:110:ASP:CA	2.49	0.52
7:I:55:THR:HG23	7:I:58:VAL:CG2	2.40	0.52
8:J:7:CYS:HA	8:J:49:MET:HG2	1.92	0.52
1:A:249:SER:C	1:A:250:ILE:CG1	2.72	0.52
1:A:320:ARG:HD3	2:B:471:LYS:HG2	1.91	0.52
2:B:208:SER:OG	2:B:210:LYS:HE2	2.10	0.52
2:B:483:LEU:HD22	2:B:484:ASN:H	1.75	0.52
2:B:825:VAL:HG12	2:B:1090:THR:OG1	2.09	0.52
7:I:35:VAL:CG1	7:I:36:GLU:H	2.19	0.52
8:J:44:TYR:HA	8:J:47:ARG:CB	2.31	0.52
2:B:65:GLU:OE1	2:B:65:GLU:N	2.43	0.52
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.91	0.52
3:C:57:VAL:CG2	8:J:57:ILE:HD11	2.40	0.52
1:A:541:ILE:HD11	1:A:574:GLY:HA2	1.91	0.52
1:A:575:LYS:HG2	1:A:612:ILE:HD11	1.90	0.52
1:A:731:ARG:HG3	1:A:755:PHE:CE1	2.44	0.52
1:A:901:LEU:CG	1:A:926:GLN:HE21	2.23	0.52
2:B:249:ARG:HA	2:B:249:ARG:HE	1.75	0.52
2:B:549:THR:CG2	2:B:550:ASP:H	2.22	0.52
2:B:879:ARG:H	2:B:879:ARG:CZ	2.23	0.52
2:B:915:THR:HB	2:B:934:LYS:HB3	1.92	0.52
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.75	0.52
1:A:19:PHE:HB3	1:A:1413:GLY:HA2	1.91	0.52
1:A:352:VAL:CG1	1:A:353:ILE:N	2.72	0.52
1:A:504:LEU:HD11	5:F:91:ALA:HB1	1.91	0.52
1:A:573:SER:N	1:A:576:GLN:HG3	2.10	0.52
1:A:754:SER:H	1:A:757:ASN:HD22	1.58	0.52
1:A:830:LYS:HD3	1:A:1079:MET:O	2.10	0.52
1:A:1267:MET:O	1:A:1271:ILE:HB	2.09	0.52
1:A:1420:ASP:O	1:A:1421:CYS:CB	2.57	0.52
2:B:770:GLN:HE22	2:B:1093:GLN:NE2	2.03	0.52
2:B:859:TYR:OH	2:B:941:LEU:HD22	2.09	0.52
3:C:142:VAL:CG1	3:C:143:LEU:N	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:61:GLN:HG2	4:E:79:TRP:CE3	2.45	0.52
11:R:12:G:O2'	11:R:13:C:O5'	2.23	0.52
1:A:268:ASP:O	1:A:299:HIS:ND1	2.43	0.51
2:B:474:SER:C	2:B:476:ARG:N	2.63	0.51
2:B:791:THR:HA	2:B:858:SER:HB2	1.91	0.51
2:B:905:VAL:HG12	2:B:909:ASP:HB2	1.92	0.51
3:C:241:ASP:O	3:C:245:VAL:HG23	2.10	0.51
5:F:132:LEU:O	5:F:148:VAL:HG23	2.10	0.51
6:H:58:THR:CG2	6:H:59:ILE:N	2.73	0.51
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.92	0.51
3:C:31:ASN:O	3:C:34:ARG:N	2.42	0.51
1:A:120:GLU:OE2	1:A:123:ARG:CD	2.55	0.51
1:A:401:GLY:C	1:A:435:HIS:HD2	2.11	0.51
1:A:474:VAL:O	1:A:478:TYR:HD1	1.94	0.51
1:A:815:PHE:O	1:A:818:MET:N	2.43	0.51
1:A:226:GLU:O	1:A:230:ARG:HD2	2.10	0.51
2:B:373:ARG:HD3	2:B:566:LEU:HD22	1.92	0.51
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.92	0.51
1:A:765:VAL:HG21	1:A:800:VAL:CG1	2.41	0.51
1:A:1166:ASP:OD1	1:A:1237:ILE:HD13	2.10	0.51
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.63	0.51
2:B:329:THR:HA	2:B:332:ASP:CB	2.35	0.51
3:C:193:TYR:HA	3:C:200:GLU:OE1	2.11	0.51
1:A:755:PHE:O	1:A:757:ASN:N	2.44	0.51
1:A:903:ASN:ND2	1:A:906:HIS:HB2	2.26	0.51
1:A:1116:LEU:CD1	1:A:1329:THR:OG1	2.36	0.51
2:B:92:PHE:HD2	2:B:132:VAL:HG22	1.76	0.51
10:L:34:CYS:O	10:L:35:SER:HB2	2.11	0.51
1:A:568:PRO:HD3	6:H:94:ASP:O	2.09	0.51
1:A:765:VAL:HG21	1:A:800:VAL:HG11	1.92	0.51
1:A:919:ILE:HD12	1:A:925:LEU:CD1	2.41	0.51
2:B:299:GLU:OE2	2:B:571:PRO:HG2	2.10	0.51
2:B:525:ALA:O	2:B:527:THR:HG22	2.09	0.51
1:A:343:LYS:HZ1	2:B:1197:PRO:HB3	1.74	0.51
1:A:1021:LEU:O	1:A:1022:LEU:C	2.48	0.51
2:B:114:PRO:HG3	2:B:181:LEU:HD21	1.93	0.51
2:B:589:VAL:CG1	2:B:590:HIS:N	2.74	0.51
2:B:893:LEU:HD11	2:B:910:VAL:HG12	1.92	0.51
4:E:29:PHE:C	4:E:30:ILE:HG13	2.30	0.51
1:A:587:HIS:HE2	1:A:969:GLN:HG2	1.76	0.51
2:B:1137:CYS:HA	2:B:1140:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:94:LYS:HE3	4:E:123:LEU:HD11	1.92	0.51
1:A:343:LYS:NZ	2:B:1156:ASP:HB2	2.25	0.51
1:A:979:SER:OG	1:A:980:ASP:N	2.44	0.51
1:A:1189:SER:O	1:A:1241:ARG:HD3	2.11	0.51
2:B:1154:ALA:O	2:B:1155:SER:HB3	2.09	0.51
6:H:109:LYS:HB2	6:H:111:LEU:N	2.26	0.51
1:A:567:LYS:HZ1	6:H:97:MET:CG	2.24	0.50
1:A:860:LEU:HD21	1:A:1394:THR:H	1.75	0.50
1:A:1173:HIS:C	1:A:1175:SER:H	2.13	0.50
1:A:1192:LEU:HD11	1:A:1239:ARG:HB3	1.93	0.50
2:B:840:ILE:HG23	2:B:992:ILE:HG22	1.93	0.50
2:B:842:ASN:O	2:B:843:GLN:C	2.47	0.50
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.12	0.50
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.93	0.50
3:C:178:PHE:C	3:C:178:PHE:CD2	2.83	0.50
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.93	0.50
2:B:212:LEU:HD12	2:B:409:ALA:HB1	1.92	0.50
2:B:286:PHE:HB3	2:B:297:ILE:HD12	1.93	0.50
2:B:770:GLN:NE2	2:B:1093:GLN:NE2	2.53	0.50
2:B:879:ARG:H	2:B:879:ARG:NE	2.09	0.50
2:B:1032:SER:HB3	2:B:1089:PRO:CG	2.35	0.50
1:A:1239:ARG:C	1:A:1240:CYS:SG	2.89	0.50
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.44	0.50
2:B:490:SER:O	2:B:491:THR:C	2.49	0.50
11:R:13:C:O4'	11:R:13:C:OP2	2.30	0.50
1:A:296:LEU:O	1:A:300:VAL:HG23	2.11	0.50
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.93	0.50
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.77	0.50
2:B:45:SER:O	2:B:46:GLN:C	2.50	0.50
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.12	0.50
2:B:215:GLN:OE1	2:B:479:VAL:HG13	2.11	0.50
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.93	0.50
4:E:213:ILE:HG12	4:E:214:CYS:N	2.25	0.50
1:A:532:ARG:HG3	1:A:616:VAL:HG11	1.94	0.50
2:B:34:ILE:HD13	2:B:542:MET:HE3	1.93	0.50
2:B:1071:VAL:HG11	2:B:1080:LYS:HE2	1.94	0.50
3:C:35:ARG:NH1	9:K:41:THR:H	2.09	0.50
7:I:58:VAL:O	7:I:58:VAL:HG12	2.11	0.50
1:A:1436:ILE:O	1:A:1437:GLY:C	2.49	0.50
2:B:212:LEU:HD21	2:B:461:LEU:CD1	2.41	0.50
2:B:604:ARG:HA	2:B:609:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:ASP:HB3	9:K:109:TRP:CZ2	2.46	0.50
1:A:265:LYS:O	1:A:267:ALA:N	2.44	0.50
1:A:383:TYR:HB3	5:F:115:THR:HB	1.94	0.50
1:A:537:ARG:HG3	1:A:602:ASP:OD2	2.11	0.50
1:A:629:LEU:O	1:A:633:VAL:HG23	2.12	0.50
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.52	0.50
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.77	0.50
2:B:1106:ARG:HG3	2:B:1107:ALA:N	2.27	0.50
1:A:1140:HIS:HB3	1:A:1279:ILE:O	2.12	0.50
1:A:1393:ASN:O	1:A:1394:THR:O	2.30	0.50
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.45	0.50
2:B:128:LEU:HB2	2:B:167:ILE:O	2.11	0.50
2:B:745:PRO:C	2:B:747:MET:N	2.62	0.50
1:A:596:THR:O	1:A:598:LEU:N	2.45	0.50
2:B:942:ARG:HB2	2:B:945:GLU:HB2	1.94	0.50
2:B:954:VAL:O	10:L:55:ILE:O	2.29	0.50
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.11	0.50
4:E:144:ILE:HG13	4:E:145:THR:N	2.27	0.50
1:A:402:ALA:CB	1:A:434:ARG:HA	2.42	0.49
1:A:860:LEU:HD13	1:A:1393:ASN:ND2	2.10	0.49
2:B:315:LYS:N	2:B:316:PRO:HD2	2.27	0.49
2:B:884:ARG:O	2:B:936:ASP:HB3	2.11	0.49
2:B:1004:GLU:O	3:C:177:GLU:HG2	2.13	0.49
3:C:167:HIS:CD2	3:C:169:LYS:H	2.20	0.49
1:A:313:GLN:HB3	1:A:322:VAL:CG1	2.41	0.49
1:A:1006:ILE:HD11	4:E:163:GLU:HG3	1.93	0.49
1:A:1174:PHE:O	1:A:1175:SER:O	2.30	0.49
2:B:20:ASP:N	2:B:655:LYS:HZ3	2.10	0.49
2:B:34:ILE:HD11	2:B:743:ILE:HG22	1.94	0.49
2:B:235:SER:CB	2:B:236:HIS:HD2	2.25	0.49
3:C:22:LEU:HD21	3:C:25:VAL:HG21	1.93	0.49
3:C:62:PHE:O	3:C:65:HIS:HB3	2.12	0.49
1:A:407:ARG:HD3	1:A:413:ILE:CD1	2.43	0.49
1:A:471:ASN:O	1:A:472:LEU:C	2.50	0.49
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.47	0.49
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.27	0.49
2:B:636:PRO:HB3	2:B:637:LEU:HA	1.91	0.49
2:B:983:ARG:HG3	2:B:1093:GLN:CD	2.32	0.49
2:B:1077:THR:HG23	2:B:1079:LYS:N	2.27	0.49
4:E:46:TYR:CE2	4:E:58:MET:HA	2.47	0.49
6:H:109:LYS:CD	6:H:110:ASP:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.47	0.49
1:A:757:ASN:O	1:A:761:MET:HG3	2.12	0.49
1:A:1222:ASN:O	1:A:1223:ASP:OD1	2.30	0.49
1:A:1313:LEU:C	1:A:1315:GLU:H	2.16	0.49
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.95	0.49
4:E:48:ASP:OD2	4:E:49:SER:N	2.45	0.49
7:I:7:CYS:HB2	7:I:14:LEU:HD21	1.94	0.49
1:A:108:MET:O	1:A:110:CYS:N	2.41	0.49
1:A:1152:ILE:HD12	7:I:44:TYR:CD2	2.47	0.49
1:A:1173:HIS:C	1:A:1175:SER:N	2.65	0.49
1:A:1191:TRP:CE3	1:A:1191:TRP:HA	2.46	0.49
1:A:1392:SER:O	1:A:1393:ASN:O	2.30	0.49
2:B:701:ILE:HG12	2:B:702:LEU:N	2.26	0.49
2:B:890:TYR:CD2	2:B:910:VAL:HG11	2.48	0.49
5:F:97:ARG:HD2	5:F:101:ILE:HG13	1.93	0.49
6:H:98:TYR:CE1	6:H:139:ASN:OD1	2.65	0.49
10:L:68:GLU:OE1	10:L:68:GLU:O	2.30	0.49
1:A:738:LYS:NZ	3:C:194:GLU:HA	2.28	0.49
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.28	0.49
2:B:57:TYR:CD1	2:B:57:TYR:N	2.81	0.49
2:B:783:THR:CG2	8:J:59:LYS:HB3	2.41	0.49
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.77	0.49
3:C:186:LEU:HB3	3:C:188:HIS:HD2	1.77	0.49
1:A:1364:ASN:HD22	1:A:1366:ARG:CG	2.10	0.49
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.94	0.49
2:B:666:TYR:CD1	2:B:666:TYR:O	2.66	0.49
2:B:953:LEU:HB3	2:B:965:LYS:HB2	1.94	0.49
3:C:57:VAL:HG23	8:J:57:ILE:HD11	1.95	0.49
4:E:61:GLN:CG	4:E:79:TRP:HE3	2.25	0.49
7:I:106:CYS:O	7:I:107:SER:C	2.51	0.49
8:J:3:VAL:CG2	8:J:18:TRP:CG	2.90	0.49
8:J:12:LYS:NZ	8:J:17:LYS:HZ1	2.11	0.49
1:A:1132:LYS:O	1:A:1135:ARG:HB3	2.13	0.49
1:A:1400:CYS:SG	1:A:1409:LEU:HG	2.53	0.49
1:A:1402:PHE:CD2	1:A:1403:GLU:HB2	2.48	0.49
3:C:178:PHE:C	3:C:178:PHE:HD2	2.16	0.49
4:E:94:LYS:HE3	4:E:123:LEU:CD1	2.43	0.49
5:F:81:THR:O	5:F:82:THR:C	2.51	0.49
1:A:483:ASP:OD1	11:R:11:U:P	2.71	0.49
2:B:644:GLU:CB	2:B:647:GLY:O	2.60	0.49
2:B:848:ARG:HH22	2:B:996:ARG:NH1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:77:SER:HB3	4:E:105:PHE:HA	1.94	0.49
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.48	0.49
12:T:13:DA:C2	12:T:14:DG:N3	2.81	0.49
1:A:106:VAL:HG12	1:A:107:CYS:N	2.28	0.48
1:A:782:ARG:NH1	1:A:785:PRO:HA	2.28	0.48
1:A:840:ARG:CG	1:A:1402:PHE:HZ	2.26	0.48
1:A:1006:ILE:HD11	4:E:163:GLU:CG	2.42	0.48
1:A:1167:GLU:O	1:A:1167:GLU:HG2	2.12	0.48
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.76	0.48
2:B:844:SER:OG	2:B:996:ARG:N	2.39	0.48
2:B:1082:MET:HA	3:C:189:THR:HA	1.94	0.48
5:F:136:ARG:HD2	5:F:146:TRP:CD1	2.48	0.48
1:A:20:GLY:O	1:A:21:LEU:HD23	2.13	0.48
1:A:101:LYS:HD3	1:A:139:TRP:CE2	2.48	0.48
1:A:108:MET:C	1:A:110:CYS:H	2.16	0.48
1:A:591:PHE:HA	1:A:595:THR:HG21	1.94	0.48
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.79	0.48
1:A:815:PHE:O	1:A:818:MET:HB2	2.12	0.48
1:A:962:ARG:HA	1:A:965:GLN:HE21	1.77	0.48
1:A:1406:VAL:HG13	1:A:1410:PHE:CE1	2.49	0.48
2:B:197:PHE:HE1	8:J:59:LYS:HD3	1.78	0.48
2:B:976:ILE:HG23	2:B:977:GLY:H	1.78	0.48
3:C:251:LEU:O	3:C:255:VAL:HG23	2.13	0.48
6:H:109:LYS:HB3	6:H:110:ASP:O	2.05	0.48
12:T:13:DA:H61	13:N:2:DT:H73	1.76	0.48
1:A:335:ARG:HH11	2:B:1202:LEU:HD12	1.78	0.48
1:A:913:LEU:CD2	1:A:915:SER:HB2	2.43	0.48
1:A:1053:PHE:O	1:A:1055:ARG:N	2.47	0.48
2:B:120:ARG:HH21	2:B:956:THR:HG23	1.77	0.48
2:B:234:ILE:HG21	2:B:237:VAL:HG22	1.93	0.48
2:B:310:MET:O	2:B:313:MET:HB2	2.13	0.48
2:B:316:PRO:HA	2:B:319:GLU:HG3	1.95	0.48
2:B:661:LEU:HD23	2:B:679:TYR:O	2.13	0.48
2:B:772:ALA:O	2:B:776:GLN:NE2	2.46	0.48
9:K:49:GLU:HG3	9:K:94:ILE:HD11	1.94	0.48
1:A:380:VAL:HG11	1:A:428:TYR:H	1.78	0.48
1:A:491:VAL:H	2:B:1150:ARG:NH2	2.11	0.48
1:A:765:VAL:HG23	1:A:766:GLY:N	2.27	0.48
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.13	0.48
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.77	0.48
3:C:124:LEU:C	3:C:126:GLY:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:48:ASP:HB3	4:E:54:GLN:HB2	1.94	0.48
1:A:130:ASP:C	1:A:132:LYS:H	2.17	0.48
1:A:388:LEU:O	1:A:391:LEU:N	2.46	0.48
1:A:544:ASP:HB2	9:K:47:ARG:HH21	1.77	0.48
1:A:569:LYS:HE3	3:C:221:TYR:O	2.14	0.48
1:A:1146:VAL:HG12	1:A:1201:ALA:HB1	1.94	0.48
1:A:1311:VAL:HG11	1:A:1329:THR:HG21	1.94	0.48
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.95	0.48
2:B:898:LEU:HD13	2:B:952:VAL:HG11	1.94	0.48
4:E:16:PHE:O	4:E:19:VAL:N	2.42	0.48
1:A:56:PRO:O	1:A:57:ARG:HB2	2.13	0.48
1:A:313:GLN:HB3	1:A:322:VAL:HG11	1.96	0.48
1:A:319:GLY:CA	1:A:320:ARG:HH11	2.27	0.48
1:A:388:LEU:O	1:A:389:THR:C	2.52	0.48
1:A:860:LEU:HD11	1:A:1393:ASN:HB2	1.94	0.48
2:B:459:TYR:C	2:B:459:TYR:CD2	2.87	0.48
2:B:980:PHE:O	2:B:1095:LEU:HG	2.13	0.48
4:E:201:LYS:HE2	4:E:207:ARG:HD3	1.96	0.48
10:L:34:CYS:O	10:L:35:SER:CB	2.62	0.48
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.46	0.48
2:B:266:ALA:O	2:B:268:THR:HG22	2.13	0.48
2:B:515:HIS:HD2	2:B:517:THR:H	1.62	0.48
1:A:91:PHE:HB3	1:A:96:ILE:HD11	1.96	0.48
1:A:568:PRO:HB3	3:C:221:TYR:CZ	2.49	0.48
1:A:760:GLN:HE21	1:A:765:VAL:HA	1.78	0.48
2:B:314:LEU:O	2:B:315:LYS:C	2.52	0.48
2:B:593:PRO:HA	2:B:596:LEU:HB3	1.94	0.48
2:B:1084:GLN:HE21	3:C:192:TRP:HB2	1.79	0.48
3:C:43:THR:HG23	3:C:44:LEU:N	2.29	0.48
7:I:8:ARG:O	7:I:9:ASP:HB2	2.13	0.48
1:A:115:LEU:HD13	1:A:119:ASN:ND2	2.28	0.48
1:A:351:THR:HG21	2:B:1103:ILE:HD12	1.82	0.48
1:A:452:LYS:HB2	2:B:1141:HIS:HE1	1.74	0.48
1:A:473:SER:O	1:A:521:MET:HB3	2.14	0.48
1:A:575:LYS:HB3	1:A:612:ILE:CG1	2.43	0.48
1:A:1030:ARG:O	1:A:1031:VAL:C	2.52	0.48
1:A:1101:LEU:HD13	1:A:1355:VAL:HG11	1.96	0.48
1:A:1397:LEU:O	1:A:1400:CYS:HB2	2.14	0.48
2:B:44:VAL:O	2:B:45:SER:C	2.52	0.48
2:B:640:VAL:O	2:B:640:VAL:HG12	2.13	0.48
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:63:LEU:C	6:H:90:ALA:HB3	2.34	0.48
6:H:120:GLY:O	6:H:122:LEU:HG	2.14	0.48
9:K:18:LYS:O	9:K:19:LEU:HD23	2.14	0.48
1:A:919:ILE:HD12	1:A:925:LEU:HD11	1.94	0.48
1:A:982:THR:C	1:A:984:LYS:H	2.17	0.48
1:A:1337:GLU:O	4:E:183:PRO:HG3	2.14	0.48
2:B:1138:MET:HA	2:B:1138:MET:HE3	1.95	0.48
12:T:26:DG:N2	12:T:27:DA:H1'	2.29	0.48
1:A:249:SER:O	1:A:250:ILE:CG1	2.62	0.47
1:A:1376:THR:HG23	1:A:1376:THR:O	2.14	0.47
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.96	0.47
2:B:589:VAL:CG1	2:B:590:HIS:H	2.25	0.47
2:B:857:ARG:O	2:B:967:ARG:HG3	2.14	0.47
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.14	0.47
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.49	0.47
7:I:17:ARG:HG2	7:I:18:GLU:H	1.78	0.47
1:A:265:LYS:HZ1	1:A:323:LYS:HE2	1.79	0.47
2:B:55:VAL:HG12	2:B:56:ASP:N	2.29	0.47
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.95	0.47
3:C:29:MET:O	3:C:32:SER:N	2.47	0.47
1:A:440:ASP:H	1:A:460:VAL:HG23	1.79	0.47
1:A:1362:TYR:CD1	1:A:1362:TYR:C	2.86	0.47
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.96	0.47
2:B:263:GLY:O	2:B:264:SER:C	2.52	0.47
2:B:1153:GLU:OE2	2:B:1153:GLU:N	2.47	0.47
4:E:15:ALA:HA	4:E:140:LEU:O	2.13	0.47
4:E:199:ILE:O	4:E:199:ILE:HG22	2.14	0.47
12:T:5:DC:H2"	12:T:6:DG:O5'	2.14	0.47
1:A:15:LYS:HD2	2:B:1220:ARG:NH1	2.29	0.47
1:A:438:ASP:HA	1:A:460:VAL:O	2.13	0.47
2:B:254:LEU:HD22	2:B:361:LEU:HD11	1.96	0.47
2:B:395:GLN:HG2	2:B:396:ASP:H	1.78	0.47
4:E:205:SER:O	4:E:207:ARG:N	2.47	0.47
5:F:90:ARG:O	5:F:91:ALA:C	2.52	0.47
5:F:93:ILE:HG23	5:F:132:LEU:HD12	1.95	0.47
1:A:253:ASN:ND2	1:A:257:ARG:N	2.63	0.47
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.95	0.47
1:A:767:GLN:NE2	1:A:774:ARG:HE	2.12	0.47
1:A:855:THR:HG23	1:A:857:ARG:HG2	1.97	0.47
1:A:982:THR:C	1:A:984:LYS:N	2.67	0.47
2:B:681:TRP:O	2:B:684:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:875:GLU:O	2:B:877:PRO:HD3	2.14	0.47
8:J:16:ASP:OD1	8:J:17:LYS:HG3	2.14	0.47
9:K:5:ASP:O	9:K:6:ARG:C	2.52	0.47
1:A:848:ILE:HD13	1:A:858:ASN:HB3	1.97	0.47
2:B:573:GLN:O	2:B:575:PRO:HD3	2.13	0.47
2:B:757:PRO:HG3	2:B:983:ARG:CZ	2.36	0.47
2:B:972:LYS:HD3	2:B:1098:MET:SD	2.54	0.47
3:C:43:THR:CG2	3:C:44:LEU:N	2.77	0.47
8:J:56:LEU:O	8:J:57:ILE:C	2.53	0.47
9:K:60:ALA:O	9:K:73:LEU:HA	2.14	0.47
11:R:5:A:C2	11:R:6:G:C5	3.03	0.47
1:A:256:GLN:CB	1:A:257:ARG:CG	2.90	0.47
1:A:332:LYS:C	1:A:334:GLY:N	2.67	0.47
1:A:464:PRO:CG	9:K:67:PHE:CD1	2.98	0.47
1:A:557:ASP:HA	9:K:26:LYS:HE3	1.96	0.47
1:A:894:GLU:C	1:A:896:ARG:H	2.17	0.47
1:A:949:ASP:OD1	1:A:949:ASP:N	2.38	0.47
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.97	0.47
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.15	0.47
2:B:479:VAL:O	2:B:480:SER:HB3	2.15	0.47
2:B:765:PRO:O	2:B:769:TYR:CD1	2.68	0.47
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.63	0.47
3:C:142:VAL:HG13	3:C:143:LEU:H	1.78	0.47
3:C:186:LEU:CB	3:C:188:HIS:HD2	2.28	0.47
8:J:25:LEU:HD21	8:J:32:GLU:HG3	1.96	0.47
1:A:182:VAL:HG12	1:A:183:GLY:N	2.23	0.47
1:A:375:THR:OG1	1:A:433:GLU:HB3	2.15	0.47
1:A:382:PRO:N	1:A:428:TYR:HE2	2.12	0.47
1:A:463:ILE:CB	1:A:464:PRO:HD2	2.44	0.47
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.50	0.47
1:A:608:ILE:HG12	1:A:613:ILE:HG13	1.97	0.47
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.58	0.47
2:B:701:ILE:HD11	2:B:703:ILE:CD1	2.43	0.47
3:C:69:LEU:H	3:C:69:LEU:CD2	2.27	0.47
4:E:127:ILE:HD13	4:E:127:ILE:H	1.80	0.47
4:E:180:ARG:HB2	4:E:215:MET:OXT	2.15	0.47
6:H:15:VAL:HA	6:H:26:ILE:HD12	1.96	0.47
12:T:8:DT:H3	13:N:7:DA:H61	1.63	0.47
1:A:321:PRO:O	1:A:322:VAL:HG22	2.14	0.47
1:A:849:MET:HG3	1:A:849:MET:O	2.13	0.47
1:A:1004:ASN:OD1	1:A:1006:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:HIS:CD2	1:A:1227:ILE:HG12	2.49	0.47
2:B:384:ARG:O	2:B:385:LEU:C	2.52	0.47
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.62	0.47
3:C:56:THR:CG2	3:C:145:CYS:SG	3.00	0.47
3:C:124:LEU:O	3:C:126:GLY:N	2.48	0.47
6:H:145:ARG:HG3	6:H:146:ARG:HG3	1.96	0.47
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.96	0.47
1:A:239:LEU:HD12	1:A:240:PRO:CD	2.37	0.47
1:A:252:PHE:CD1	1:A:252:PHE:C	2.87	0.47
1:A:1165:GLU:O	1:A:1166:ASP:OD1	2.33	0.47
1:A:1395:GLY:O	1:A:1398:MET:HB3	2.15	0.47
2:B:241:ARG:HA	2:B:253:THR:HG22	1.96	0.47
2:B:1006:ILE:HD11	8:J:43:ARG:HB2	1.97	0.47
2:B:1106:ARG:NH1	2:B:1110:PRO:HD2	2.29	0.47
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.48	0.46
1:A:475:THR:HG22	1:A:476:SER:N	2.29	0.46
1:A:998:LEU:HG	1:A:1001:ARG:NH1	2.30	0.46
2:B:981:ALA:CB	2:B:987:LYS:CA	2.72	0.46
2:B:1155:SER:O	2:B:1156:ASP:OD2	2.33	0.46
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.97	0.46
3:C:133:ILE:HD13	3:C:236:GLY:O	2.15	0.46
1:A:694:THR:HA	1:A:714:PHE:HE1	1.81	0.46
1:A:947:PHE:HD2	1:A:954:TRP:CE2	2.31	0.46
1:A:1406:VAL:HG12	1:A:1407:GLU:N	2.30	0.46
3:C:69:LEU:H	3:C:69:LEU:HD22	1.80	0.46
7:I:109:ILE:H	7:I:109:ILE:HD12	1.79	0.46
1:A:317:LYS:HD2	1:A:317:LYS:HA	1.43	0.46
1:A:465:TYR:HD2	2:B:976:ILE:HB	1.81	0.46
2:B:278:GLN:HG2	2:B:279:ASP:H	1.79	0.46
3:C:50:GLU:HB2	3:C:156:THR:HB	1.97	0.46
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.97	0.46
3:C:206:ASN:ND2	3:C:229:TYR:CB	2.79	0.46
10:L:59:ALA:O	10:L:60:ARG:HB2	2.14	0.46
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.98	0.46
1:A:893:PHE:C	1:A:893:PHE:CD2	2.89	0.46
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.96	0.46
2:B:523:CYS:SG	2:B:750:GLY:N	2.88	0.46
2:B:655:LYS:O	2:B:658:ILE:HG22	2.16	0.46
2:B:999:MET:CG	2:B:1008:PRO:HD2	2.43	0.46
3:C:10:ILE:HG21	3:C:13:ALA:HB2	1.96	0.46
3:C:142:VAL:H	8:J:16:ASP:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:24:LEU:O	8:J:30:LEU:HB2	2.16	0.46
1:A:1161:THR:HG22	1:A:1162:VAL:N	2.30	0.46
2:B:174:LEU:HD12	2:B:174:LEU:HA	1.59	0.46
1:A:266:LEU:HD23	1:A:303:TYR:CE1	2.50	0.46
1:A:653:VAL:O	1:A:654:ASN:C	2.53	0.46
1:A:666:ILE:CD1	2:B:1030:LEU:HD13	2.39	0.46
1:A:711:ARG:NH2	7:I:91:ARG:HH12	2.14	0.46
1:A:765:VAL:CG2	1:A:800:VAL:CG1	2.94	0.46
1:A:840:ARG:NE	1:A:1385:THR:HG23	2.22	0.46
2:B:411:PRO:HA	2:B:414:ALA:HB3	1.96	0.46
2:B:1094:ARG:HH22	2:B:1098:MET:CG	2.28	0.46
2:B:1121:GLY:O	2:B:1126:GLY:HA3	2.16	0.46
3:C:134:ILE:HG22	3:C:136:ASP:HB3	1.98	0.46
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.98	0.46
1:A:185:TRP:HZ3	1:A:200:ARG:HB3	1.80	0.46
1:A:315:LEU:HB2	1:A:316:GLN:HA	1.79	0.46
1:A:401:GLY:CA	1:A:435:HIS:HD2	2.29	0.46
1:A:821:ARG:O	1:A:825:ILE:HG12	2.16	0.46
1:A:893:PHE:O	1:A:896:ARG:HB2	2.16	0.46
2:B:882:THR:HG22	2:B:884:ARG:H	1.80	0.46
2:B:952:VAL:HG13	2:B:966:VAL:HG22	1.98	0.46
1:A:658:LEU:HD13	2:B:831:SER:N	2.30	0.46
1:A:1220:PHE:CD1	1:A:1224:LEU:HD23	2.51	0.46
2:B:248:SER:HB3	2:B:249:ARG:H	1.49	0.46
2:B:377:PHE:O	2:B:380:TYR:N	2.48	0.46
2:B:1007:VAL:HG13	2:B:1008:PRO:N	2.30	0.46
2:B:1084:GLN:HE21	3:C:192:TRP:CB	2.29	0.46
3:C:64:ALA:HA	3:C:67:LEU:HD12	1.98	0.46
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.98	0.46
6:H:104:PHE:HD2	6:H:114:VAL:CG1	2.22	0.46
7:I:15:TYR:N	7:I:15:TYR:CD1	2.83	0.46
10:L:30:ILE:HG22	10:L:31:CYS:O	2.16	0.46
1:A:359:LEU:HD23	1:A:359:LEU:HA	1.81	0.46
1:A:481:ASP:OD1	1:A:483:ASP:OD2	2.34	0.46
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.16	0.46
1:A:837:ILE:HD13	1:A:840:ARG:HH12	1.81	0.46
2:B:228:LYS:HE2	2:B:228:LYS:HB3	1.79	0.46
3:C:66:ARG:HH22	8:J:4:PRO:CA	2.27	0.46
3:C:67:LEU:HD11	3:C:155:LEU:HD13	1.98	0.46
4:E:165:LEU:HD22	4:E:165:LEU:HA	1.82	0.46
9:K:56:VAL:HG13	9:K:77:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:ILE:O	1:A:1065:GLY:N	2.46	0.46
1:A:901:LEU:O	1:A:907:THR:OG1	2.34	0.46
1:A:1100:ARG:HH12	1:A:1111:MET:HE2	1.81	0.46
2:B:550:ASP:OD1	2:B:551:PRO:CD	2.64	0.46
8:J:21:TYR:CZ	8:J:25:LEU:HD11	2.50	0.46
8:J:30:LEU:HD11	8:J:38:ARG:HH12	1.81	0.46
1:A:15:LYS:O	1:A:1420:ASP:O	2.32	0.45
1:A:19:PHE:O	1:A:1416:ALA:HA	2.16	0.45
1:A:971:PHE:O	1:A:972:HIS:O	2.34	0.45
1:A:1104:ILE:HG21	1:A:1352:VAL:HG22	1.97	0.45
1:A:1434:ALA:HB3	1:A:1436:ILE:HD12	1.98	0.45
1:A:553:VAL:HG13	1:A:554:PRO:HD2	1.97	0.45
2:B:363:HIS:O	2:B:364:ILE:CB	2.59	0.45
3:C:246:ARG:HA	3:C:249:ASP:HB2	1.98	0.45
4:E:108:GLY:HA3	4:E:132:ILE:HG12	1.99	0.45
1:A:356:ASP:HB2	1:A:469:ARG:HH11	1.81	0.45
1:A:961:ARG:HB2	1:A:1025:ARG:HH12	1.81	0.45
1:A:1290:LYS:HA	1:A:1299:VAL:O	2.17	0.45
2:B:48:LEU:HD22	2:B:176:SER:HA	1.99	0.45
2:B:205:ILE:C	2:B:207:GLY:H	2.20	0.45
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.85	0.45
2:B:458:LYS:O	2:B:462:ALA:CB	2.65	0.45
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.97	0.45
2:B:792:MET:HE1	2:B:857:ARG:NH2	2.31	0.45
4:E:202:SER:OG	4:E:204:THR:HB	2.16	0.45
10:L:41:SER:C	10:L:42:ARG:O	2.55	0.45
11:R:13:C:O2	11:R:13:C:O2'	2.30	0.45
1:A:512:VAL:HG23	1:A:519:PRO:N	2.31	0.45
1:A:665:GLY:O	1:A:668:ASP:HB2	2.16	0.45
2:B:1002:THR:HG22	2:B:1006:ILE:HB	1.99	0.45
4:E:63:ASN:CB	4:E:64:PRO:HD3	2.44	0.45
5:F:130:ILE:HG22	5:F:132:LEU:HG	1.98	0.45
13:N:11:DG:H2"	13:N:12:DT:O4'	2.16	0.45
1:A:172:PRO:HB3	1:A:183:GLY:HA3	1.98	0.45
1:A:1396:ALA:HB2	1:A:1417:GLU:OE1	2.16	0.45
2:B:370:PHE:CD2	2:B:373:ARG:HG3	2.46	0.45
3:C:21:ILE:HD12	3:C:229:TYR:CE2	2.52	0.45
6:H:22:LYS:O	6:H:23:VAL:HG23	2.15	0.45
6:H:111:LEU:O	6:H:112:ILE:HB	2.15	0.45
11:R:6:G:H2'	11:R:7:A:H8	1.80	0.45
1:A:53:LEU:O	1:A:56:PRO:HD2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:PRO:O	1:A:515:GLN:C	2.55	0.45
2:B:99:LYS:O	2:B:100:PRO:O	2.34	0.45
2:B:542:MET:HB3	2:B:636:PRO:HD3	1.98	0.45
2:B:981:ALA:CA	2:B:987:LYS:HA	2.41	0.45
4:E:80:VAL:HG13	4:E:109:ILE:HG21	1.97	0.45
5:F:147:SER:O	5:F:151:LEU:HD12	2.16	0.45
8:J:7:CYS:HA	8:J:49:MET:HE3	1.97	0.45
1:A:253:ASN:HD22	1:A:257:ARG:N	2.14	0.45
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.31	0.45
2:B:40:GLU:HG3	2:B:681:TRP:HB3	1.99	0.45
2:B:65:GLU:CD	2:B:66:ASP:H	2.20	0.45
2:B:515:HIS:H	2:B:518:HIS:HD2	1.63	0.45
2:B:542:MET:HE1	2:B:743:ILE:HG21	1.98	0.45
2:B:770:GLN:CB	2:B:983:ARG:O	2.64	0.45
2:B:879:ARG:HB2	2:B:880:THR:H	1.48	0.45
2:B:1073:TYR:OH	2:B:1080:LYS:HE3	2.17	0.45
3:C:35:ARG:HH11	9:K:41:THR:N	2.15	0.45
4:E:13:TRP:CZ3	4:E:39:LEU:HB2	2.51	0.45
5:F:86:THR:OG1	5:F:89:GLU:HG3	2.16	0.45
11:R:13:C:O2	11:R:13:C:C2'	2.61	0.45
1:A:302:THR:HA	1:A:305:ASP:O	2.17	0.45
1:A:323:LYS:HD3	1:A:323:LYS:N	2.32	0.45
1:A:492:PRO:HB3	1:A:497:THR:HG22	1.98	0.45
1:A:658:LEU:HD22	2:B:831:SER:HA	1.99	0.45
1:A:807:GLY:HA3	2:B:728:ARG:NH1	2.31	0.45
1:A:1109:LYS:HB2	1:A:1109:LYS:HE3	1.56	0.45
2:B:210:LYS:HZ3	2:B:482:VAL:HG13	1.80	0.45
2:B:522:VAL:HG12	2:B:523:CYS:N	2.32	0.45
2:B:768:THR:O	2:B:771:SER:HB2	2.17	0.45
2:B:1084:GLN:H	2:B:1084:GLN:CD	2.20	0.45
2:B:1124:ARG:O	2:B:1125:ASP:C	2.53	0.45
6:H:93:TYR:HA	6:H:145:ARG:CB	2.47	0.45
6:H:113:ALA:HA	6:H:125:LEU:O	2.17	0.45
2:B:248:SER:H	2:B:418:LYS:NZ	2.15	0.45
2:B:1175:LEU:HD23	2:B:1176:ASN:N	2.32	0.45
3:C:134:ILE:CG2	3:C:136:ASP:HB3	2.46	0.45
12:T:14:DG:H2'	12:T:15:DA:C8	2.52	0.45
1:A:765:VAL:HG21	1:A:800:VAL:CB	2.44	0.45
1:A:866:PHE:CZ	4:E:211:TYR:HB2	2.52	0.45
1:A:1261:LYS:C	1:A:1263:ILE:N	2.70	0.45
2:B:128:LEU:HD21	2:B:170:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:LYS:HZ2	2:B:335:GLY:CA	2.30	0.45
2:B:1104:HIS:ND1	2:B:1105:ALA:N	2.65	0.45
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.51	0.45
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.60	0.44
1:A:172:PRO:HA	1:A:184:SER:O	2.15	0.44
1:A:531:ILE:HG21	1:A:622:VAL:HG11	1.98	0.44
1:A:606:LEU:HB2	1:A:614:PHE:CE2	2.52	0.44
1:A:899:VAL:O	1:A:929:LEU:HD12	2.17	0.44
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.47	0.44
4:E:100:ILE:HG12	4:E:105:PHE:HD1	1.82	0.44
4:E:143:ASN:OD1	4:E:187:TYR:HE1	2.00	0.44
5:F:80:ALA:O	5:F:81:THR:C	2.55	0.44
6:H:89:LEU:C	6:H:91:ASP:H	2.18	0.44
7:I:45:ARG:HE	7:I:47:GLU:HG3	1.82	0.44
7:I:106:CYS:O	7:I:108:HIS:N	2.50	0.44
8:J:6:ARG:CG	8:J:13:VAL:HA	2.46	0.44
1:A:17:VAL:HB	1:A:1419:ASP:HB3	1.98	0.44
1:A:147:VAL:HG23	1:A:149:GLU:HG3	1.99	0.44
1:A:251:SER:O	1:A:252:PHE:CG	2.70	0.44
1:A:302:THR:HG21	1:A:313:GLN:HE22	1.83	0.44
1:A:565:ILE:HG12	1:A:567:LYS:HZ2	1.80	0.44
1:A:966:ASN:O	1:A:1044:TRP:CH2	2.70	0.44
1:A:1117:THR:O	1:A:1117:THR:HG22	2.17	0.44
1:A:1209:MET:O	1:A:1212:VAL:HB	2.17	0.44
2:B:205:ILE:O	2:B:206:ASN:HB2	2.16	0.44
2:B:216:GLU:HB3	2:B:499:ASN:O	2.18	0.44
2:B:277:LYS:HZ2	2:B:335:GLY:HA2	1.82	0.44
3:C:92:CYS:O	3:C:96:SER:N	2.45	0.44
4:E:12:LEU:HD13	4:E:55:ARG:HH21	1.81	0.44
1:A:66:LYS:C	1:A:68:GLN:H	2.20	0.44
1:A:482:PHE:HD1	2:B:835:GLN:O	2.00	0.44
2:B:255:GLN:HB2	2:B:272:THR:HB	2.00	0.44
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.53	0.44
3:C:120:ILE:H	3:C:120:ILE:HG12	1.62	0.44
4:E:108:GLY:O	4:E:132:ILE:HG23	2.17	0.44
4:E:113:GLN:HB3	4:E:137:GLU:OE1	2.17	0.44
9:K:55:LYS:HB2	9:K:81:TYR:CE1	2.52	0.44
1:A:11:LEU:HA	2:B:1193:GLN:O	2.18	0.44
1:A:88:LYS:HE2	1:A:205:GLU:OE2	2.18	0.44
1:A:344:ARG:CZ	2:B:1129:ARG:HB2	2.47	0.44
1:A:599:SER:C	1:A:601:LYS:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:PHE:CD2	2:B:829:CYS:SG	2.83	0.44
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.82	0.44
2:B:101:MET:HE3	2:B:169:ARG:HH22	1.83	0.44
2:B:711:GLU:H	2:B:712:PRO:CD	2.30	0.44
2:B:852:ARG:HG2	2:B:973:ILE:HG23	1.98	0.44
2:B:864:LYS:HD2	2:B:865:LYS:O	2.18	0.44
8:J:30:LEU:HD11	8:J:38:ARG:NH1	2.32	0.44
8:J:45:CYS:HG	8:J:46:CYS:N	2.16	0.44
1:A:23:SER:O	1:A:27:VAL:HG23	2.18	0.44
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.32	0.44
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.30	0.44
1:A:1152:ILE:HG12	1:A:1260:LEU:HD23	1.99	0.44
1:A:1313:LEU:O	1:A:1315:GLU:N	2.51	0.44
2:B:808:ALA:O	2:B:812:LEU:HG	2.18	0.44
2:B:864:LYS:N	2:B:872:GLU:OE1	2.44	0.44
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.38	0.44
5:F:134:ILE:HG22	5:F:136:ARG:HG3	1.98	0.44
1:A:930:ASP:O	1:A:931:GLU:C	2.56	0.44
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.98	0.44
2:B:905:VAL:HG12	2:B:909:ASP:CB	2.48	0.44
2:B:1138:MET:HA	2:B:1138:MET:CE	2.47	0.44
2:B:1152:MET:O	2:B:1153:GLU:C	2.55	0.44
3:C:84:ARG:HD3	9:K:11:LEU:HD21	1.99	0.44
1:A:14:VAL:HB	1:A:1432:GLN:HE22	1.82	0.44
1:A:380:VAL:HG23	1:A:430:TRP:C	2.38	0.44
1:A:540:PHE:CB	1:A:571:LEU:HD23	2.48	0.44
1:A:777:PHE:HD2	1:A:782:ARG:C	2.20	0.44
2:B:48:LEU:O	2:B:49:ASP:C	2.56	0.44
2:B:354:ASP:O	2:B:357:GLN:N	2.48	0.44
2:B:650:GLU:HG3	2:B:651:LEU:N	2.33	0.44
2:B:766:ARG:HA	2:B:769:TYR:HD1	1.82	0.44
2:B:806:THR:HG22	2:B:808:ALA:H	1.82	0.44
2:B:829:CYS:SG	2:B:1014:PRO:HG2	2.52	0.44
6:H:26:ILE:N	6:H:40:LEU:O	2.49	0.44
7:I:21:GLU:H	7:I:21:GLU:HG3	1.45	0.44
9:K:55:LYS:HB2	9:K:81:TYR:HE1	1.82	0.44
10:L:27:LEU:HD23	10:L:27:LEU:H	1.83	0.44
1:A:650:GLN:O	1:A:651:LYS:C	2.56	0.44
1:A:756:ILE:O	1:A:760:GLN:HG2	2.18	0.44
1:A:793:SER:HB2	1:A:794:PRO:CD	2.39	0.44
1:A:947:PHE:CE2	1:A:954:TRP:CD2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:ARG:O	2:B:175:ARG:HG2	2.18	0.44
2:B:739:THR:OG1	2:B:740:HIS:N	2.50	0.44
2:B:783:THR:HG22	8:J:63:TYR:HE1	1.82	0.44
3:C:148:ARG:O	3:C:151:GLN:HG3	2.18	0.44
4:E:35:VAL:C	4:E:37:LEU:H	2.21	0.44
6:H:109:LYS:HD3	6:H:109:LYS:H	1.82	0.44
1:A:405:VAL:HG23	1:A:415:LEU:HD11	1.99	0.44
1:A:412:ARG:NH2	1:A:433:GLU:OE2	2.51	0.44
1:A:1222:ASN:HD22	1:A:1222:ASN:HA	1.63	0.44
2:B:120:ARG:NE	2:B:955:THR:HG21	2.33	0.44
2:B:586:TRP:NE1	2:B:588:GLY:O	2.51	0.44
2:B:980:PHE:O	2:B:1095:LEU:HD12	2.17	0.44
2:B:1131:GLY:O	2:B:1134:GLU:N	2.50	0.44
12:T:26:DG:C2	12:T:27:DA:C8	3.06	0.44
1:A:343:LYS:HZ3	2:B:1197:PRO:HB3	1.82	0.43
1:A:353:ILE:HD12	1:A:482:PHE:HD2	1.83	0.43
1:A:545:GLN:O	1:A:546:VAL:C	2.56	0.43
1:A:865:GLN:NE2	1:A:1370:LEU:HA	2.33	0.43
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.58	0.43
1:A:1066:VAL:HG11	2:B:1136:ASP:O	2.18	0.43
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.58	0.43
1:A:1393:ASN:HB2	1:A:1394:THR:H	1.52	0.43
1:A:1406:VAL:CG1	1:A:1410:PHE:CE1	3.01	0.43
1:A:1420:ASP:HB3	1:A:1422:ARG:HG2	1.99	0.43
2:B:235:SER:OG	2:B:236:HIS:N	2.51	0.43
2:B:322:PHE:CZ	7:I:30:ARG:HD2	2.52	0.43
2:B:384:ARG:HA	2:B:384:ARG:HD2	1.59	0.43
2:B:490:SER:OG	2:B:491:THR:N	2.47	0.43
2:B:842:ASN:O	2:B:845:SER:N	2.51	0.43
2:B:890:TYR:O	2:B:892:LYS:N	2.51	0.43
4:E:63:ASN:HB3	4:E:64:PRO:HD2	1.99	0.43
4:E:144:ILE:HG13	4:E:145:THR:H	1.82	0.43
7:I:68:LEU:HB3	7:I:84:VAL:HG22	2.00	0.43
1:A:819:GLY:O	1:A:822:GLU:N	2.50	0.43
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.33	0.43
1:A:1132:LYS:CG	1:A:1135:ARG:HH12	2.30	0.43
2:B:25:ILE:HG22	2:B:26:THR:N	2.32	0.43
2:B:57:TYR:N	2:B:57:TYR:HD1	2.16	0.43
2:B:96:TYR:N	2:B:129:PHE:O	2.44	0.43
2:B:522:VAL:HG11	2:B:537:LYS:CB	2.43	0.43
4:E:36:GLU:O	4:E:38:PRO:HD3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:4:PHE:H	7:I:4:PHE:HD2	1.64	0.43
1:A:371:ALA:O	1:A:435:HIS:HB3	2.18	0.43
1:A:947:PHE:CZ	4:E:203:GLU:HA	2.54	0.43
2:B:99:LYS:HA	2:B:100:PRO:HD2	1.70	0.43
2:B:168:GLY:H	2:B:450:ALA:HB1	1.83	0.43
2:B:301:ILE:HD13	2:B:382:ILE:HG21	2.01	0.43
2:B:814:PHE:C	2:B:816:GLU:N	2.72	0.43
2:B:1076:HIS:CG	9:K:40:HIS:CD2	3.04	0.43
4:E:61:GLN:CB	4:E:79:TRP:HA	2.48	0.43
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.99	0.43
1:A:108:MET:N	1:A:108:MET:SD	2.92	0.43
1:A:332:LYS:H	1:A:337:ARG:HB3	1.83	0.43
1:A:1171:GLN:HB3	1:A:1172:LEU:H	1.68	0.43
2:B:189:LEU:O	2:B:192:LEU:N	2.51	0.43
2:B:277:LYS:NZ	2:B:335:GLY:CA	2.81	0.43
2:B:633:VAL:O	2:B:694:ASP:HB2	2.19	0.43
1:A:24:PRO:HB3	1:A:237:THR:HB	2.00	0.43
1:A:33:ALA:HB1	1:A:35:ILE:HD11	2.00	0.43
1:A:253:ASN:O	1:A:254:GLU:HB2	2.16	0.43
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.17	0.43
1:A:535:THR:O	1:A:536:LEU:C	2.57	0.43
1:A:919:ILE:O	1:A:922:ASP:HB2	2.19	0.43
1:A:981:LEU:HD21	1:A:1039:LYS:HA	2.01	0.43
1:A:1104:ILE:CD1	1:A:1351:GLU:HB3	2.48	0.43
1:A:1332:PHE:CE1	1:A:1348:LEU:HD12	2.53	0.43
2:B:493:SER:HB2	2:B:751:VAL:HG11	2.00	0.43
2:B:582:VAL:HB	2:B:587:HIS:CD2	2.53	0.43
2:B:755:ILE:O	2:B:755:ILE:CG2	2.66	0.43
2:B:826:ALA:O	2:B:1011:ILE:HA	2.19	0.43
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.48	0.43
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.34	0.43
3:C:83:SER:OG	3:C:160:LYS:HB3	2.18	0.43
3:C:171:GLY:HA2	3:C:172:PRO:HD3	1.81	0.43
9:K:57:LEU:HB2	9:K:76:GLN:HG2	2.01	0.43
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.84	0.43
1:A:261:ASP:CB	1:A:323:LYS:HD2	2.46	0.43
1:A:800:VAL:HG13	1:A:812:GLU:HB3	2.01	0.43
1:A:862:ASN:HA	4:E:174:GLN:HB3	2.00	0.43
1:A:939:ASP:O	1:A:942:PHE:N	2.51	0.43
1:A:1407:GLU:O	1:A:1411:GLU:HG2	2.18	0.43
2:B:226:PHE:O	2:B:228:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:635:ARG:HH12	2:B:742:GLU:CD	2.22	0.43
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.83	0.43
3:C:196:ASP:HB3	3:C:199:LYS:HB2	2.00	0.43
9:K:94:ILE:O	9:K:95:ILE:C	2.54	0.43
11:R:9:G:C2'	11:R:10:A:H5'	2.49	0.43
1:A:319:GLY:CA	1:A:320:ARG:NH1	2.81	0.43
1:A:379:VAL:HG12	1:A:380:VAL:N	2.34	0.43
1:A:1161:THR:HG23	1:A:1239:ARG:NH2	2.33	0.43
1:A:1208:THR:OG1	1:A:1211:GLN:HB2	2.19	0.43
2:B:274:PRO:O	2:B:275:TYR:HB2	2.19	0.43
2:B:428:ILE:HD11	2:B:448:ILE:HD13	1.99	0.43
2:B:575:PRO:HD2	2:B:576:ASP:H	1.84	0.43
2:B:802:PRO:HA	2:B:1091:TYR:CD1	2.54	0.43
2:B:1027:ILE:O	2:B:1029:CYS:N	2.51	0.43
3:C:79:GLN:HE21	3:C:127:ARG:HB3	1.84	0.43
1:A:407:ARG:HD3	1:A:413:ILE:HD13	2.01	0.43
1:A:609:ASP:CG	1:A:610:GLY:H	2.22	0.43
1:A:1142:THR:O	1:A:1145:SER:OG	2.29	0.43
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.19	0.43
2:B:115:GLN:HG2	2:B:193:LYS:HB2	2.01	0.43
2:B:519:TRP:O	2:B:519:TRP:CD1	2.72	0.43
2:B:766:ARG:NH2	11:R:13:C:H5'	2.34	0.43
2:B:870:ILE:C	2:B:871:THR:OG1	2.56	0.43
2:B:981:ALA:HB2	2:B:987:LYS:CB	2.48	0.43
3:C:3:GLU:CG	3:C:4:GLU:N	2.73	0.43
3:C:144:ILE:HD13	3:C:144:ILE:HA	1.93	0.43
9:K:44:ASN:HA	9:K:61:TYR:CE2	2.54	0.43
1:A:254:GLU:HA	1:A:255:SER:HA	1.63	0.43
1:A:384:ASN:O	1:A:385:ILE:C	2.57	0.43
1:A:385:ILE:H	1:A:385:ILE:HG13	1.65	0.43
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.83	0.43
1:A:1219:THR:HG21	1:A:1271:ILE:CD1	2.49	0.43
2:B:292:ILE:N	2:B:293:PRO:CD	2.82	0.43
2:B:541:LEU:CB	2:B:747:MET:HE3	2.48	0.43
2:B:766:ARG:HH21	2:B:1020:ARG:HB3	1.83	0.43
2:B:1013:ASN:C	2:B:1015:HIS:H	2.21	0.43
3:C:176:ILE:O	3:C:176:ILE:HG22	2.19	0.43
6:H:41:ASP:HB3	6:H:121:LEU:HD22	2.01	0.43
1:A:996:ASN:C	1:A:998:LEU:N	2.72	0.43
1:A:1384:VAL:HA	1:A:1389:PHE:CD2	2.51	0.43
3:C:99:LEU:HD23	3:C:99:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:8:ARG:O	7:I:9:ASP:CB	2.67	0.43
1:A:588:LEU:HD13	1:A:632:VAL:HG21	2.01	0.42
1:A:629:LEU:CD2	1:A:633:VAL:HG21	2.49	0.42
1:A:900:ASP:HB3	1:A:906:HIS:HB3	2.00	0.42
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.39	0.42
1:A:1377:THR:C	1:A:1379:GLY:H	2.22	0.42
2:B:261:ARG:N	2:B:264:SER:HB2	2.34	0.42
2:B:973:ILE:HG22	2:B:974:PRO:HD2	2.00	0.42
7:I:20:LYS:HB2	7:I:21:GLU:H	1.49	0.42
8:J:9:SER:OG	8:J:45:CYS:HB2	2.19	0.42
9:K:47:ARG:O	9:K:50:LEU:N	2.52	0.42
1:A:53:LEU:HB3	1:A:54:ASN:H	1.50	0.42
1:A:472:LEU:O	1:A:475:THR:CB	2.67	0.42
1:A:491:VAL:H	2:B:1150:ARG:HH22	1.67	0.42
1:A:526:ASP:O	1:A:529:CYS:N	2.52	0.42
1:A:567:LYS:NZ	6:H:97:MET:SD	2.92	0.42
1:A:1025:ARG:O	1:A:1035:TYR:OH	2.34	0.42
1:A:1369:ALA:O	1:A:1370:LEU:C	2.54	0.42
2:B:170:LEU:HG	2:B:171:PRO:O	2.18	0.42
2:B:408:LEU:O	2:B:412:LEU:HG	2.19	0.42
2:B:412:LEU:CD1	2:B:479:VAL:HG11	2.48	0.42
2:B:702:LEU:HG	2:B:738:PHE:HD2	1.83	0.42
2:B:898:LEU:HD12	10:L:58:LYS:HD2	2.01	0.42
2:B:997:GLU:H	2:B:997:GLU:HG3	1.65	0.42
2:B:1006:ILE:HG22	2:B:1087:PHE:HZ	1.84	0.42
3:C:163:ILE:O	3:C:166:GLU:N	2.31	0.42
5:F:118:LEU:O	5:F:122:MET:HG3	2.19	0.42
8:J:56:LEU:O	8:J:59:LYS:N	2.40	0.42
1:A:256:GLN:HB2	1:A:257:ARG:HD2	1.66	0.42
1:A:440:ASP:O	1:A:460:VAL:HG23	2.18	0.42
1:A:532:ARG:HG3	1:A:616:VAL:CG1	2.50	0.42
1:A:550:LEU:HD13	1:A:550:LEU:HA	1.69	0.42
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.67	0.42
1:A:1325:THR:HA	4:E:147:HIS:HA	2.01	0.42
1:A:1349:TYR:CA	1:A:1372:VAL:HG21	2.49	0.42
2:B:306:ASN:O	2:B:308:TRP:N	2.50	0.42
2:B:515:HIS:CD2	2:B:517:THR:OG1	2.73	0.42
2:B:684:LEU:HD23	2:B:689:LEU:HD12	2.01	0.42
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.55	0.42
2:B:782:LEU:HB3	2:B:784:ASN:OD1	2.19	0.42
2:B:1106:ARG:NH2	2:B:1109:GLY:H	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:ASN:O	3:C:54:ASN:CG	2.57	0.42
6:H:39:THR:O	6:H:123:MET:HA	2.19	0.42
7:I:60:GLN:NE2	7:I:107:SER:OG	2.52	0.42
1:A:532:ARG:HH22	1:A:745:GLN:HG2	1.84	0.42
1:A:1092:LYS:O	1:A:1093:LYS:HG3	2.19	0.42
2:B:124:TYR:OH	2:B:179:CYS:SG	2.59	0.42
2:B:814:PHE:O	2:B:816:GLU:N	2.52	0.42
2:B:840:ILE:HB	2:B:1011:ILE:HD12	2.02	0.42
6:H:97:MET:SD	6:H:121:LEU:HD12	2.59	0.42
9:K:46:ILE:HG21	9:K:73:LEU:HD22	2.01	0.42
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.54	0.42
1:A:528:LEU:HD21	1:A:749:ALA:O	2.19	0.42
1:A:670:ILE:H	1:A:670:ILE:HG12	1.63	0.42
1:A:1130:GLN:O	1:A:1134:ILE:HG13	2.19	0.42
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.85	0.42
1:A:1385:THR:O	1:A:1387:HIS:N	2.51	0.42
2:B:195:CYS:HA	2:B:196:PRO:HD3	1.79	0.42
2:B:549:THR:CG2	2:B:550:ASP:N	2.78	0.42
3:C:97:VAL:HG21	3:C:129:ILE:CG2	2.48	0.42
3:C:217:ASP:HA	3:C:218:PRO:HD3	1.89	0.42
11:R:2:U:H2'	11:R:3:C:C6	2.54	0.42
1:A:544:ASP:HB2	9:K:47:ARG:NH2	2.35	0.42
1:A:858:ASN:ND2	1:A:858:ASN:H	2.17	0.42
1:A:965:GLN:HA	1:A:968:GLN:HG2	2.01	0.42
1:A:1151:GLU:O	1:A:1193:LEU:HA	2.20	0.42
1:A:1364:ASN:HD21	1:A:1366:ARG:CG	2.09	0.42
3:C:69:LEU:HD22	3:C:69:LEU:N	2.33	0.42
5:F:82:THR:HG22	5:F:84:TYR:HB2	2.01	0.42
1:A:32:VAL:HB	1:A:57:ARG:CB	2.50	0.42
1:A:442:VAL:O	1:A:457:ALA:HA	2.20	0.42
1:A:899:VAL:HG23	1:A:1029:ARG:CG	2.49	0.42
1:A:997:LEU:O	1:A:1053:PHE:CE2	2.73	0.42
2:B:25:ILE:CG2	2:B:26:THR:N	2.83	0.42
2:B:299:GLU:CD	2:B:571:PRO:HG2	2.39	0.42
2:B:519:TRP:CD1	2:B:519:TRP:C	2.93	0.42
2:B:1027:ILE:O	2:B:1030:LEU:N	2.52	0.42
2:B:1139:ILE:H	2:B:1139:ILE:HG13	1.64	0.42
3:C:13:ALA:HA	3:C:17:ASN:O	2.20	0.42
3:C:219:PHE:CB	6:H:45:GLU:HG2	2.50	0.42
7:I:98:VAL:HG11	7:I:113:ASP:HB2	2.01	0.42
8:J:7:CYS:SG	8:J:7:CYS:O	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:VAL:HG11	1:A:428:TYR:N	2.35	0.42
1:A:1407:GLU:CD	1:A:1407:GLU:N	2.63	0.42
2:B:795:ILE:HG22	2:B:796:LEU:N	2.34	0.42
2:B:863:GLU:HG3	2:B:962:LYS:HB3	2.01	0.42
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.54	0.42
4:E:143:ASN:OD1	4:E:187:TYR:CE1	2.73	0.42
6:H:6:PHE:CZ	6:H:8:ASP:HB2	2.55	0.42
9:K:7:PHE:HA	9:K:10:PHE:CE2	2.55	0.42
1:A:42:ASP:HA	1:A:46:THR:O	2.19	0.42
1:A:571:LEU:C	1:A:572:TRP:CE3	2.93	0.42
1:A:919:ILE:O	1:A:920:LEU:C	2.58	0.42
1:A:947:PHE:CE2	1:A:954:TRP:CE2	3.07	0.42
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.40	0.42
2:B:20:ASP:O	2:B:22:SER:N	2.51	0.42
2:B:95:ILE:HD12	2:B:130:VAL:HG22	2.02	0.42
2:B:386:LEU:C	2:B:388:CYS:H	2.23	0.42
2:B:708:GLU:HG3	2:B:709:ASP:N	2.35	0.42
2:B:796:LEU:HD12	2:B:796:LEU:HA	1.74	0.42
2:B:956:THR:HG22	10:L:46:VAL:HG21	2.01	0.42
2:B:1104:HIS:CG	2:B:1122:ARG:HB2	2.55	0.42
5:F:109:VAL:HG11	5:F:123:LYS:HG2	2.01	0.42
8:J:1:MET:H1	8:J:56:LEU:CB	2.33	0.42
1:A:564:ALA:O	6:H:97:MET:HB3	2.19	0.42
1:A:567:LYS:C	1:A:569:LYS:H	2.22	0.42
1:A:809:THR:HB	1:A:810:PRO:CD	2.47	0.42
2:B:582:VAL:HA	2:B:626:ILE:O	2.20	0.42
3:C:142:VAL:CG2	8:J:5:VAL:HG13	2.50	0.42
4:E:66:GLU:O	4:E:69:ILE:N	2.51	0.42
4:E:153:HIS:O	4:E:154:ILE:HD13	2.19	0.42
6:H:76:THR:O	6:H:77:ARG:O	2.37	0.42
6:H:98:TYR:HE1	6:H:139:ASN:HA	1.84	0.42
9:K:3:ALA:HA	9:K:4:PRO:HD3	1.79	0.42
1:A:376:TYR:CE2	1:A:377:PRO:O	2.73	0.41
1:A:733:ALA:O	1:A:737:LEU:HG	2.19	0.41
2:B:120:ARG:HA	2:B:963:PHE:CE2	2.54	0.41
2:B:451:LYS:HA	2:B:454:THR:HB	2.02	0.41
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.19	0.41
2:B:975:GLN:HG2	2:B:976:ILE:N	2.27	0.41
2:B:992:ILE:HD12	2:B:992:ILE:HA	1.82	0.41
4:E:169:ARG:HG3	5:F:140:ASP:HB3	2.01	0.41
6:H:12:VAL:HG21	6:H:53:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:82:ASP:HA	9:K:83:PRO:HD2	1.75	0.41
1:A:171:GLN:HE21	1:A:171:GLN:HB3	1.72	0.41
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.90	0.41
1:A:943:LEU:C	1:A:945:GLU:N	2.74	0.41
2:B:653:VAL:HA	2:B:657:HIS:HD2	1.85	0.41
2:B:906:SER:HB3	2:B:946:ASN:CB	2.50	0.41
2:B:1094:ARG:NH2	2:B:1098:MET:HG2	2.33	0.41
3:C:101:LEU:HD21	3:C:113:VAL:CG1	2.49	0.41
3:C:133:ILE:HD13	3:C:237:SER:HA	2.02	0.41
4:E:78:LEU:HD12	4:E:107:THR:HB	2.02	0.41
1:A:843:LYS:HZ1	2:B:1135:ARG:NH2	2.18	0.41
2:B:977:GLY:O	2:B:989:THR:HB	2.21	0.41
2:B:984:HIS:NE2	2:B:1024:ALA:HB3	2.36	0.41
3:C:118:LEU:HD23	3:C:118:LEU:HA	1.89	0.41
7:I:15:TYR:O	7:I:27:PHE:HA	2.21	0.41
8:J:6:ARG:HA	8:J:12:LYS:O	2.20	0.41
1:A:31:SER:HB2	1:A:81:PHE:O	2.21	0.41
1:A:66:LYS:C	1:A:68:GLN:N	2.74	0.41
1:A:399:HIS:O	1:A:400:PRO:C	2.56	0.41
1:A:989:GLY:O	1:A:990:VAL:C	2.59	0.41
1:A:1396:ALA:O	1:A:1397:LEU:C	2.58	0.41
2:B:217:ARG:NH2	2:B:405:ARG:HG3	2.35	0.41
2:B:284:ILE:H	2:B:284:ILE:HG12	1.74	0.41
2:B:323:VAL:O	2:B:324:ILE:HG13	2.20	0.41
3:C:104:PHE:CD1	3:C:152:GLU:HG3	2.55	0.41
3:C:167:HIS:HD2	3:C:169:LYS:N	2.08	0.41
3:C:242:GLN:HA	3:C:245:VAL:HB	2.03	0.41
4:E:29:PHE:C	4:E:30:ILE:CG1	2.87	0.41
5:F:89:GLU:O	5:F:93:ILE:HG12	2.20	0.41
9:K:65:HIS:CD2	9:K:67:PHE:H	2.18	0.41
10:L:26:THR:O	10:L:26:THR:HG22	2.20	0.41
1:A:508:PRO:C	1:A:510:GLN:H	2.23	0.41
1:A:743:VAL:HA	1:A:746:MET:HE2	2.02	0.41
2:B:279:ASP:O	2:B:280:ILE:HD13	2.20	0.41
2:B:697:GLU:O	2:B:698:GLU:C	2.59	0.41
2:B:816:GLU:O	2:B:817:LEU:HD12	2.20	0.41
2:B:860:MET:SD	2:B:861:ASP:N	2.94	0.41
2:B:1168:LEU:HD21	2:B:1214:PRO:HD2	2.02	0.41
8:J:6:ARG:N	8:J:14:VAL:HG22	2.35	0.41
11:R:3:C:H2'	11:R:4:G:H8	1.85	0.41
1:A:49:LYS:NZ	1:A:60:SER:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:CD2	1:A:92:HIS:C	2.94	0.41
1:A:374:LEU:C	1:A:436:ILE:HD13	2.41	0.41
1:A:446:ARG:HG3	1:A:487:MET:HG2	2.01	0.41
1:A:560:ILE:H	1:A:560:ILE:HG12	1.67	0.41
1:A:658:LEU:HD12	1:A:658:LEU:O	2.21	0.41
1:A:1194:ARG:HG3	1:A:1237:ILE:CG2	2.51	0.41
2:B:26:THR:O	2:B:27:ALA:C	2.59	0.41
2:B:757:PRO:CB	2:B:1044:ALA:HB1	2.51	0.41
2:B:789:MET:HE2	2:B:965:LYS:HB3	2.01	0.41
2:B:890:TYR:CD2	2:B:910:VAL:HG21	2.55	0.41
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.56	0.41
4:E:184:VAL:O	4:E:187:TYR:HB3	2.20	0.41
7:I:102:VAL:O	7:I:104:LEU:HD23	2.21	0.41
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.20	0.41
1:A:491:VAL:N	2:B:1150:ARG:NH2	2.68	0.41
1:A:697:ALA:HA	1:A:702:LEU:HB2	2.01	0.41
1:A:741:ASN:O	1:A:745:GLN:HG3	2.20	0.41
1:A:1313:LEU:C	1:A:1315:GLU:N	2.74	0.41
2:B:360:PHE:O	2:B:361:LEU:C	2.59	0.41
2:B:544:CYS:HB2	2:B:634:TYR:CZ	2.55	0.41
2:B:737:THR:O	2:B:738:PHE:C	2.58	0.41
2:B:1147:LEU:O	2:B:1147:LEU:HD22	2.21	0.41
3:C:46:ILE:HA	3:C:159:ALA:HA	2.03	0.41
3:C:53:THR:O	3:C:154:LYS:N	2.42	0.41
3:C:57:VAL:HG23	8:J:57:ILE:CD1	2.51	0.41
9:K:4:PRO:O	9:K:5:ASP:C	2.59	0.41
1:A:44:THR:O	1:A:45:GLN:HB2	2.20	0.41
1:A:250:ILE:HB	1:A:251:SER:H	1.77	0.41
1:A:306:ASN:HD22	1:A:306:ASN:N	2.18	0.41
1:A:472:LEU:CD2	2:B:835:GLN:HB3	2.51	0.41
1:A:535:THR:HG21	1:A:616:VAL:HA	2.00	0.41
1:A:565:ILE:HG23	1:A:567:LYS:HG2	2.03	0.41
1:A:588:LEU:HA	1:A:588:LEU:HD12	1.82	0.41
2:B:474:SER:O	2:B:476:ARG:N	2.53	0.41
2:B:570:VAL:HG21	2:B:573:GLN:OE1	2.21	0.41
2:B:619:ILE:HG13	7:I:65:ASP:HB2	2.02	0.41
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.56	0.41
2:B:834:ASN:CG	2:B:1013:ASN:HB2	2.41	0.41
2:B:1165:ILE:HB	2:B:1166:CYS:H	1.63	0.41
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.86	0.41
3:C:31:ASN:ND2	3:C:35:ARG:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:7:PHE:CD1	9:K:7:PHE:C	2.94	0.41
9:K:105:PHE:O	9:K:106:GLU:C	2.59	0.41
11:R:3:C:H2'	11:R:4:G:C8	2.55	0.41
12:T:26:DG:H21	12:T:27:DA:H1'	1.84	0.41
1:A:215:SER:O	1:A:218:ASP:HB2	2.20	0.41
1:A:525:GLN:HB2	2:B:835:GLN:OE1	2.21	0.41
1:A:545:GLN:O	1:A:548:ASN:N	2.53	0.41
1:A:777:PHE:HD2	1:A:782:ARG:CA	2.33	0.41
1:A:803:SER:OG	1:A:806:ARG:HG3	2.21	0.41
2:B:56:ASP:C	2:B:57:TYR:CD1	2.94	0.41
2:B:92:PHE:CD2	2:B:132:VAL:HG22	2.54	0.41
2:B:104:GLU:H	2:B:104:GLU:HG2	1.55	0.41
2:B:288:ALA:HA	2:B:331:LEU:HD12	2.02	0.41
2:B:450:ALA:O	2:B:453:ILE:N	2.53	0.41
2:B:864:LYS:N	2:B:872:GLU:HB2	2.35	0.41
3:C:3:GLU:HB3	9:K:104:ASN:CG	2.41	0.41
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.56	0.41
3:C:244:VAL:HG21	9:K:105:PHE:CE1	2.56	0.41
8:J:64:ASN:HB3	8:J:65:PRO:HD3	2.03	0.41
9:K:10:PHE:CD1	9:K:11:LEU:CD1	3.04	0.41
1:A:68:GLN:C	1:A:70:CYS:N	2.73	0.41
2:B:27:ALA:O	2:B:28:GLU:C	2.60	0.41
2:B:205:ILE:C	2:B:207:GLY:N	2.74	0.41
2:B:488:TYR:O	2:B:490:SER:N	2.54	0.41
2:B:492:LEU:HB3	2:B:751:VAL:HG21	2.03	0.41
2:B:554:ILE:HG22	2:B:558:LEU:HD11	2.02	0.41
2:B:604:ARG:HD3	2:B:691:GLU:HG2	2.02	0.41
7:I:101:PHE:N	7:I:101:PHE:CD1	2.89	0.41
1:A:384:ASN:O	1:A:386:ASP:N	2.54	0.40
1:A:1194:ARG:HH21	1:A:1237:ILE:HD13	1.86	0.40
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	2.21	0.40
2:B:458:LYS:O	2:B:462:ALA:HB2	2.21	0.40
2:B:1076:HIS:ND1	9:K:40:HIS:NE2	2.67	0.40
2:B:1200:ALA:O	2:B:1201:LYS:C	2.59	0.40
3:C:35:ARG:HH11	9:K:41:THR:H	1.69	0.40
4:E:16:PHE:O	4:E:17:ARG:C	2.59	0.40
6:H:58:THR:CG2	6:H:59:ILE:H	2.30	0.40
1:A:101:LYS:HG2	1:A:139:TRP:CE2	2.55	0.40
1:A:391:LEU:HD22	1:A:400:PRO:C	2.41	0.40
1:A:609:ASP:C	1:A:611:GLN:H	2.24	0.40
1:A:737:LEU:HA	1:A:737:LEU:HD23	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:MET:CE	2:B:169:ARG:HH22	2.34	0.40
2:B:1168:LEU:HB3	2:B:1169:MET:H	1.70	0.40
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.61	0.40
2:B:1190:ASP:O	2:B:1191:ILE:HG13	2.21	0.40
4:E:77:SER:HB2	4:E:105:PHE:HA	2.04	0.40
4:E:150:VAL:HA	4:E:151:PRO:HD3	1.94	0.40
6:H:33:GLN:H	6:H:33:GLN:HG2	1.64	0.40
8:J:1:MET:H1	8:J:56:LEU:HB2	1.86	0.40
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.51	0.40
1:A:381:THR:OG1	1:A:382:PRO:HD2	2.22	0.40
1:A:587:HIS:CE1	1:A:609:ASP:H	2.40	0.40
1:A:709:THR:HG22	1:A:711:ARG:H	1.87	0.40
1:A:909:ASP:O	1:A:912:LEU:N	2.51	0.40
1:A:973:ILE:HD12	1:A:973:ILE:HA	1.92	0.40
1:A:1271:ILE:HD13	1:A:1271:ILE:HA	1.89	0.40
2:B:550:ASP:HA	2:B:551:PRO:HD3	1.83	0.40
2:B:829:CYS:SG	2:B:1014:PRO:CD	3.09	0.40
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	2.02	0.40
11:R:2:U:H2'	11:R:3:C:H6	1.87	0.40
1:A:131:SER:HB3	1:A:223:GLY:HA2	2.03	0.40
1:A:251:SER:O	1:A:252:PHE:CB	2.70	0.40
1:A:321:PRO:HG3	2:B:471:LYS:NZ	2.37	0.40
1:A:322:VAL:HA	1:A:323:LYS:HD3	2.04	0.40
1:A:744:LYS:O	1:A:748:MET:HG3	2.21	0.40
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	2.02	0.40
1:A:947:PHE:N	1:A:947:PHE:CD1	2.89	0.40
2:B:176:SER:O	2:B:182:SER:CB	2.69	0.40
2:B:273:LEU:HA	2:B:274:PRO:HD2	1.67	0.40
2:B:313:MET:O	2:B:316:PRO:HD2	2.22	0.40
2:B:450:ALA:O	2:B:451:LYS:C	2.60	0.40
3:C:31:ASN:HD21	3:C:35:ARG:HD2	1.86	0.40
4:E:191:LYS:O	4:E:214:CYS:HB3	2.22	0.40
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.76	0.40
8:J:12:LYS:HZ2	8:J:17:LYS:HZ3	1.70	0.40
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.36	0.40
1:A:344:ARG:NH2	12:T:21:DC:OP2	2.52	0.40
1:A:380:VAL:CG2	1:A:430:TRP:HB2	2.47	0.40
1:A:602:ASP:HB3	1:A:616:VAL:HG23	2.04	0.40
1:A:629:LEU:HD23	1:A:633:VAL:HG21	2.00	0.40
1:A:803:SER:OG	1:A:806:ARG:HD2	2.21	0.40
1:A:890:ASP:O	1:A:893:PHE:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:ARG:HG2	1:A:1366:ARG:H	1.71	0.40
2:B:542:MET:SD	2:B:636:PRO:HG3	2.62	0.40
2:B:658:ILE:HD12	2:B:658:ILE:HA	1.83	0.40
2:B:1027:ILE:O	2:B:1028:GLU:C	2.59	0.40
4:E:58:MET:O	4:E:60:PHE:N	2.55	0.40
6:H:44:VAL:O	6:H:44:VAL:CG1	2.69	0.40
7:I:73:ARG:HB3	7:I:74:GLU:H	1.60	0.40
7:I:98:VAL:CG1	7:I:99:LEU:N	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1383/1733 (80%)	1027 (74%)	248 (18%)	108 (8%)	1 15
2	B	1088/1224 (89%)	823 (76%)	195 (18%)	70 (6%)	1 19
3	C	264/318 (83%)	195 (74%)	51 (19%)	18 (7%)	1 18
4	E	212/215 (99%)	163 (77%)	35 (16%)	14 (7%)	1 19
5	F	82/155 (53%)	62 (76%)	15 (18%)	5 (6%)	1 20
6	H	129/146 (88%)	94 (73%)	24 (19%)	11 (8%)	1 13
7	I	117/122 (96%)	83 (71%)	23 (20%)	11 (9%)	0 12
8	J	63/70 (90%)	50 (79%)	9 (14%)	4 (6%)	1 19
9	K	112/120 (93%)	86 (77%)	21 (19%)	5 (4%)	2 25
10	L	44/70 (63%)	20 (46%)	16 (36%)	8 (18%)	0 2
All	All	3494/4173 (84%)	2603 (74%)	637 (18%)	254 (7%)	1 16

All (254) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	55	ASP
1	A	68	GLN
1	A	69	THR
1	A	117	GLU
1	A	226	GLU
1	A	248	PRO
1	A	250	ILE
1	A	251	SER
1	A	257	ARG
1	A	266	LEU
1	A	286	HIS
1	A	312	PRO
1	A	315	LEU
1	A	322	VAL
1	A	399	HIS
1	A	428	TYR
1	A	567	LYS
1	A	568	PRO
1	A	755	PHE
1	A	756	ILE
1	A	846	GLU
1	A	972	HIS
1	A	998	LEU
1	A	1036	ARG
1	A	1171	GLN
1	A	1173	HIS
1	A	1175	SER
1	A	1223	ASP
1	A	1255	GLU
1	A	1274	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1421	CYS
2	B	45	SER
2	B	46	GLN
2	B	58	THR
2	B	67	SER
2	B	100	PRO
2	B	176	SER
2	B	229	ALA
2	B	436	VAL
2	B	466	TRP

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Mol	Chain	Res	Type
2	B	475	SER
2	B	477	ALA
2	B	531	GLN
2	B	636	PRO
2	B	709	ASP
2	B	731	VAL
2	B	734	HIS
2	B	751	VAL
2	B	831	SER
2	B	864	LYS
2	B	879	ARG
2	B	1046	PRO
2	B	1103	ILE
2	B	1181	GLU
2	B	1223	ASP
3	C	142	VAL
3	C	174	ALA
4	E	3	GLN
4	E	59	SER
5	F	74	ILE
5	F	81	THR
6	H	32	THR
6	H	77	ARG
6	H	82	PRO
6	H	90	ALA
6	H	140	ALA
7	I	20	LYS
7	I	54	GLU
7	I	107	SER
8	J	2	ILE
8	J	6	ARG
9	K	71	PHE
9	K	81	TYR
10	L	35	SER
10	L	42	ARG
10	L	43	THR
1	A	42	ASP
1	A	50	ILE
1	A	76	GLU
1	A	93	VAL
1	A	130	ASP
1	A	178	GLY

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Mol	Chain	Res	Type
1	A	313	GLN
1	A	325	ILE
1	A	509	LEU
1	A	526	ASP
1	A	583	PRO
1	A	829	VAL
1	A	910	PRO
1	A	916	GLY
1	A	922	ASP
1	A	931	GLU
1	A	986	ILE
1	A	994	GLN
1	A	1022	LEU
1	A	1054	LEU
1	A	1172	LEU
1	A	1270	ASN
1	A	1314	SER
1	A	1386	ARG
1	A	1388	GLY
1	A	1435	PRO
1	A	1438	THR
2	B	21	GLU
2	B	307	ASP
2	B	333	PHE
2	B	708	GLU
2	B	711	GLU
2	B	738	PHE
2	B	746	SER
2	B	866	TYR
2	B	883	LEU
2	B	891	ASP
2	B	981	ALA
2	B	997	GLU
2	B	1155	SER
3	C	86	CYS
3	C	110	THR
3	C	125	MET
3	C	167	HIS
4	E	67	GLU
4	E	77	SER
4	E	192	ARG
4	E	206	GLY

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Mol	Chain	Res	Type
6	H	83	GLN
6	H	109	LYS
7	I	86	PHE
9	K	7	PHE
10	L	26	THR
10	L	45	ALA
10	L	55	ILE
1	A	56	PRO
1	A	109	HIS
1	A	131	SER
1	A	253	ASN
1	A	333	GLU
1	A	472	LEU
1	A	515	GLN
1	A	597	LEU
1	A	891	ALA
1	A	895	LYS
1	A	958	VAL
1	A	990	VAL
1	A	1157	ASP
1	A	1174	PHE
1	A	1188	GLN
1	A	1221	LYS
1	A	1233	ASP
1	A	1261	LYS
1	A	1424	VAL
2	B	367	LEU
2	B	468	GLU
2	B	471	LYS
2	B	483	LEU
2	B	712	PRO
2	B	815	ARG
2	B	881	ASN
2	B	958	GLN
2	B	1157	ALA
3	C	30	ALA
3	C	227	THR
4	E	17	ARG
4	E	36	GLU
4	E	145	THR
5	F	154	ASP
6	H	62	SER

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Mol	Chain	Res	Type
6	H	128	ASN
7	I	21	GLU
7	I	34	TYR
7	I	47	GLU
7	I	88	SER
10	L	54	ARG
1	A	39	GLU
1	A	87	ALA
1	A	314	ALA
1	A	320	ARG
1	A	418	SER
1	A	423	ASP
1	A	424	ILE
1	A	465	TYR
1	A	517	ASN
1	A	576	GLN
1	A	903	ASN
1	A	969	GLN
2	B	251	ILE
2	B	294	ASP
2	B	484	ASN
2	B	490	SER
2	B	491	THR
2	B	645	SER
2	B	648	HIS
2	B	836	GLU
2	B	974	PRO
2	B	1108	ARG
2	B	1165	ILE
2	B	1222	ARG
3	C	28	ALA
3	C	90	ASP
3	C	164	ALA
3	C	172	PRO
3	C	215	GLU
4	E	115	ASN
5	F	73	ALA
5	F	104	ASN
7	I	3	THR
7	I	60	GLN
7	I	89	GLN
1	A	89	PRO

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Mol	Chain	Res	Type
1	A	136	ALA
1	A	335	ARG
1	A	404	TYR
1	A	810	PRO
1	A	1021	LEU
2	B	552	MET
2	B	960	GLY
2	B	1166	CYS
3	C	87	PHE
3	C	213	PRO
4	E	53	PRO
4	E	124	VAL
8	J	3	VAL
9	K	4	PRO
10	L	59	ALA
1	A	324	SER
1	A	932	GLU
1	A	1107	VAL
2	B	489	SER
2	B	792	MET
2	B	976	ILE
2	B	1156	ASP
3	C	6	PRO
4	E	76	GLY
9	K	39	ASP
1	A	1148	ILE
1	A	1437	GLY
2	B	467	GLY
2	B	1017	ILE
1	A	514	PRO
2	B	410	GLY
3	C	240	VAL
3	C	248	ILE
4	E	51	GLY
6	H	112	ILE
8	J	33	GLY
1	A	957	PRO
6	H	59	ILE
1	A	274	ILE
1	A	1122	PRO
2	B	555	ILE
2	B	877	PRO

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Mol	Chain	Res	Type
1	A	610	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1218/1520 (80%)	976 (80%)	242 (20%)	1 9
2	B	960/1061 (90%)	797 (83%)	163 (17%)	2 14
3	C	234/274 (85%)	191 (82%)	43 (18%)	1 11
4	E	196/197 (100%)	168 (86%)	28 (14%)	3 20
5	F	74/137 (54%)	67 (90%)	7 (10%)	8 33
6	H	117/128 (91%)	93 (80%)	24 (20%)	1 8
7	I	113/116 (97%)	97 (86%)	16 (14%)	3 20
8	J	60/65 (92%)	49 (82%)	11 (18%)	1 11
9	K	99/102 (97%)	88 (89%)	11 (11%)	6 27
10	L	40/57 (70%)	32 (80%)	8 (20%)	1 8
All	All	3111/3657 (85%)	2558 (82%)	553 (18%)	2 12

All (553) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	8	SER
1	A	12	ARG
1	A	13	THR
1	A	18	GLN
1	A	26	GLU
1	A	32	VAL
1	A	47	ARG
1	A	58	LEU
1	A	60	SER
1	A	69	THR
1	A	70	CYS

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Mol	Chain	Res	Type
1	A	80	HIS
1	A	81	PHE
1	A	83	HIS
1	A	84	ILE
1	A	93	VAL
1	A	99	ILE
1	A	100	LYS
1	A	102	VAL
1	A	107	CYS
1	A	108	MET
1	A	110	CYS
1	A	116	ASP
1	A	120	GLU
1	A	130	ASP
1	A	164	ARG
1	A	169	ASN
1	A	170	THR
1	A	180	LYS
1	A	184	SER
1	A	185	TRP
1	A	199	LEU
1	A	200	ARG
1	A	204	THR
1	A	206	GLU
1	A	208	LEU
1	A	221	SER
1	A	222	LEU
1	A	225	ASN
1	A	238	CYS
1	A	250	ILE
1	A	252	PHE
1	A	254	GLU
1	A	255	SER
1	A	256	GLN
1	A	257	ARG
1	A	263	THR
1	A	266	LEU
1	A	270	LEU
1	A	271	LYS
1	A	275	SER
1	A	278	THR
1	A	295	LEU

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Mol	Chain	Res	Type
1	A	297	GLN
1	A	306	ASN
1	A	307	ASP
1	A	308	ILE
1	A	313	GLN
1	A	316	GLN
1	A	317	LYS
1	A	320	ARG
1	A	323	LYS
1	A	337	ARG
1	A	344	ARG
1	A	373	THR
1	A	381	THR
1	A	385	ILE
1	A	403	LYS
1	A	416	ARG
1	A	419	LYS
1	A	424	ILE
1	A	434	ARG
1	A	442	VAL
1	A	443	LEU
1	A	445	ASN
1	A	446	ARG
1	A	450	LEU
1	A	452	LYS
1	A	453	MET
1	A	456	MET
1	A	460	VAL
1	A	466	SER
1	A	469	ARG
1	A	471	ASN
1	A	481	ASP
1	A	485	ASP
1	A	486	GLU
1	A	494	SER
1	A	513	SER
1	A	521	MET
1	A	527	THR
1	A	529	CYS
1	A	550	LEU
1	A	552	TRP
1	A	562	THR

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Mol	Chain	Res	Type
1	A	566	ILE
1	A	572	TRP
1	A	589	GLN
1	A	590	ARG
1	A	612	ILE
1	A	618	GLU
1	A	619	LYS
1	A	621	THR
1	A	625	SER
1	A	629	LEU
1	A	630	ILE
1	A	631	HIS
1	A	634	THR
1	A	635	ARG
1	A	658	LEU
1	A	663	SER
1	A	666	ILE
1	A	670	ILE
1	A	672	ASP
1	A	675	THR
1	A	682	THR
1	A	687	LYS
1	A	702	LEU
1	A	732	LEU
1	A	740	LEU
1	A	741	ASN
1	A	752	LYS
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	771	GLU
1	A	774	ARG
1	A	783	THR
1	A	788	SER
1	A	797	LYS
1	A	801	GLU
1	A	803	SER
1	A	826	ASP
1	A	829	VAL
1	A	838	GLN
1	A	840	ARG
1	A	845	LEU

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Mol	Chain	Res	Type
1	A	854	ASN
1	A	857	ARG
1	A	858	ASN
1	A	864	ILE
1	A	867	ILE
1	A	880	LYS
1	A	885	THR
1	A	886	ILE
1	A	889	SER
1	A	893	PHE
1	A	895	LYS
1	A	896	ARG
1	A	902	LEU
1	A	905	ASP
1	A	911	SER
1	A	918	GLU
1	A	924	LYS
1	A	929	LEU
1	A	940	ARG
1	A	949	ASP
1	A	960	ILE
1	A	969	GLN
1	A	982	THR
1	A	996	ASN
1	A	1000	LEU
1	A	1006	ILE
1	A	1017	LEU
1	A	1022	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1033	GLN
1	A	1035	TYR
1	A	1046	LEU
1	A	1048	ASN
1	A	1050	GLU
1	A	1052	GLN
1	A	1057	VAL
1	A	1058	VAL
1	A	1064	VAL
1	A	1067	LEU
1	A	1093	LYS
1	A	1094	VAL

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Mol	Chain	Res	Type
1	A	1095	THR
1	A	1109	LYS
1	A	1111	MET
1	A	1115	SER
1	A	1118	VAL
1	A	1128	GLN
1	A	1134	ILE
1	A	1135	ARG
1	A	1145	SER
1	A	1159	ARG
1	A	1160	SER
1	A	1161	THR
1	A	1165	GLU
1	A	1167	GLU
1	A	1171	GLN
1	A	1172	LEU
1	A	1173	HIS
1	A	1174	PHE
1	A	1175	SER
1	A	1187	GLN
1	A	1199	ARG
1	A	1219	THR
1	A	1222	ASN
1	A	1231	ASP
1	A	1233	ASP
1	A	1235	LYS
1	A	1240	CYS
1	A	1262	LYS
1	A	1264	GLU
1	A	1273	LEU
1	A	1274	ARG
1	A	1276	VAL
1	A	1280	GLU
1	A	1281	ARG
1	A	1285	MET
1	A	1288	ASP
1	A	1290	LYS
1	A	1291	VAL
1	A	1299	VAL
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE

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Mol	Chain	Res	Type
1	A	1336	MET
1	A	1350	LYS
1	A	1351	GLU
1	A	1359	ASP
1	A	1362	TYR
1	A	1364	ASN
1	A	1366	ARG
1	A	1376	THR
1	A	1385	THR
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET
1	A	1400	CYS
1	A	1403	GLU
1	A	1404	GLU
1	A	1405	THR
1	A	1406	VAL
1	A	1420	ASP
1	A	1425	SER
2	B	28	GLU
2	B	44	VAL
2	B	45	SER
2	B	46	GLN
2	B	57	TYR
2	B	66	ASP
2	B	67	SER
2	B	94	LYS
2	B	98	THR
2	B	104	GLU
2	B	108	VAL
2	B	109	THR
2	B	110	HIS
2	B	119	LEU
2	B	120	ARG
2	B	134	LYS
2	B	170	LEU
2	B	187	SER
2	B	188	ASP
2	B	199	MET
2	B	222	ILE
2	B	225	VAL

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Mol	Chain	Res	Type
2	B	232	SER
2	B	244	LEU
2	B	246	LYS
2	B	249	ARG
2	B	261	ARG
2	B	264	SER
2	B	268	THR
2	B	277	LYS
2	B	283	VAL
2	B	284	ILE
2	B	304	ASP
2	B	315	LYS
2	B	319	GLU
2	B	347	LYS
2	B	354	ASP
2	B	360	PHE
2	B	366	GLN
2	B	384	ARG
2	B	391	ASP
2	B	393	LYS
2	B	396	ASP
2	B	398	ARG
2	B	399	ASP
2	B	404	LYS
2	B	415	GLN
2	B	416	LEU
2	B	424	LEU
2	B	425	THR
2	B	427	ASP
2	B	429	PHE
2	B	459	TYR
2	B	463	THR
2	B	471	LYS
2	B	479	VAL
2	B	482	VAL
2	B	483	LEU
2	B	487	THR
2	B	490	SER
2	B	527	THR
2	B	537	LYS
2	B	552	MET
2	B	563	MET

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Mol	Chain	Res	Type
2	B	570	VAL
2	B	591	ARG
2	B	600	LEU
2	B	601	ARG
2	B	612	GLU
2	B	618	ASP
2	B	626	ILE
2	B	627	PHE
2	B	637	LEU
2	B	641	GLU
2	B	645	SER
2	B	653	VAL
2	B	664	THR
2	B	667	GLN
2	B	668	ASP
2	B	680	THR
2	B	682	SER
2	B	694	ASP
2	B	701	ILE
2	B	705	MET
2	B	710	LEU
2	B	728	ARG
2	B	737	THR
2	B	742	GLU
2	B	748	ILE
2	B	751	VAL
2	B	762	ASN
2	B	764	SER
2	B	790	ASP
2	B	791	THR
2	B	792	MET
2	B	805	THR
2	B	807	ARG
2	B	815	ARG
2	B	822	ASN
2	B	825	VAL
2	B	831	SER
2	B	835	GLN
2	B	843	GLN
2	B	847	ASP
2	B	857	ARG
2	B	864	LYS

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Mol	Chain	Res	Type
2	B	866	TYR
2	B	868	MET
2	B	873	THR
2	B	879	ARG
2	B	880	THR
2	B	882	THR
2	B	883	LEU
2	B	886	LYS
2	B	894	ASP
2	B	899	ILE
2	B	905	VAL
2	B	936	ASP
2	B	939	THR
2	B	943	SER
2	B	944	THR
2	B	945	GLU
2	B	956	THR
2	B	959	ASP
2	B	970	THR
2	B	975	GLN
2	B	979	LYS
2	B	989	THR
2	B	997	GLU
2	B	998	ASP
2	B	999	MET
2	B	1002	THR
2	B	1007	VAL
2	B	1010	LEU
2	B	1020	ARG
2	B	1022	THR
2	B	1028	GLU
2	B	1051	THR
2	B	1060	ARG
2	B	1062	HIS
2	B	1072	MET
2	B	1082	MET
2	B	1090	THR
2	B	1092	TYR
2	B	1093	GLN
2	B	1096	ARG
2	B	1099	VAL
2	B	1104	HIS

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Mol	Chain	Res	Type
2	B	1113	VAL
2	B	1115	THR
2	B	1124	ARG
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1153	GLU
2	B	1156	ASP
2	B	1165	ILE
2	B	1189	ILE
2	B	1194	ILE
2	B	1196	ILE
2	B	1202	LEU
2	B	1221	SER
2	B	1223	ASP
3	C	4	GLU
3	C	6	PRO
3	C	10	ILE
3	C	11	ARG
3	C	15	LYS
3	C	18	VAL
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	34	ARG
3	C	36	VAL
3	C	38	ILE
3	C	43	THR
3	C	55	THR
3	C	56	THR
3	C	77	ILE
3	C	83	SER
3	C	93	ASP
3	C	99	LEU
3	C	102	GLN
3	C	115	SER
3	C	125	MET
3	C	129	ILE
3	C	133	ILE
3	C	140	ASN
3	C	142	VAL
3	C	143	LEU

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Mol	Chain	Res	Type
3	C	145	CYS
3	C	151	GLN
3	C	154	LYS
3	C	156	THR
3	C	163	ILE
3	C	166	GLU
3	C	178	PHE
3	C	195	GLN
3	C	196	ASP
3	C	199	LYS
3	C	215	GLU
3	C	234	SER
3	C	235	VAL
3	C	240	VAL
3	C	241	ASP
3	C	267	GLN
4	E	9	ILE
4	E	32	GLN
4	E	33	GLU
4	E	43	LYS
4	E	48	ASP
4	E	61	GLN
4	E	65	THR
4	E	66	GLU
4	E	72	PHE
4	E	77	SER
4	E	83	CYS
4	E	92	THR
4	E	101	GLN
4	E	107	THR
4	E	110	PHE
4	E	127	ILE
4	E	131	THR
4	E	150	VAL
4	E	152	LYS
4	E	156	LEU
4	E	158	SER
4	E	159	ASP
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG
4	E	192	ARG

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Mol	Chain	Res	Type
4	E	196	VAL
4	E	213	ILE
5	F	74	ILE
5	F	77	ASP
5	F	79	ARG
5	F	97	ARG
5	F	111	LEU
5	F	120	ILE
5	F	123	LYS
6	H	2	SER
6	H	11	GLN
6	H	24	CYS
6	H	27	GLU
6	H	33	GLN
6	H	35	GLN
6	H	37	LYS
6	H	39	THR
6	H	55	LEU
6	H	56	THR
6	H	86	ASP
6	H	89	LEU
6	H	94	ASP
6	H	95	TYR
6	H	102	TYR
6	H	103	LYS
6	H	104	PHE
6	H	106	GLU
6	H	108	SER
6	H	109	LYS
6	H	111	LEU
6	H	130	ARG
6	H	132	LEU
6	H	136	LYS
7	I	8	ARG
7	I	12	ASN
7	I	13	MET
7	I	15	TYR
7	I	21	GLU
7	I	22	ASN
7	I	28	GLU
7	I	30	ARG
7	I	50	THR

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Mol	Chain	Res	Type
7	I	62	ILE
7	I	75	CYS
7	I	78	CYS
7	I	83	ASN
7	I	95	THR
7	I	97	MET
7	I	119	THR
8	J	7	CYS
8	J	8	PHE
8	J	13	VAL
8	J	27	GLU
8	J	28	ASP
8	J	31	ASP
8	J	34	THR
8	J	43	ARG
8	J	48	ARG
8	J	62	ARG
8	J	64	ASN
9	K	20	LYS
9	K	33	ILE
9	K	47	ARG
9	K	50	LEU
9	K	51	LEU
9	K	71	PHE
9	K	75	ILE
9	K	101	LEU
9	K	107	THR
9	K	113	THR
9	K	114	LEU
10	L	31	CYS
10	L	51	CYS
10	L	55	ILE
10	L	61	THR
10	L	63	ARG
10	L	66	GLN
10	L	68	GLU
10	L	70	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN

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Mol	Chain	Res	Type
1	A	92	HIS
1	A	169	ASN
1	A	171	GLN
1	A	253	ASN
1	A	313	GLN
1	A	316	GLN
1	A	435	HIS
1	A	447	GLN
1	A	451	HIS
1	A	515	GLN
1	A	517	ASN
1	A	545	GLN
1	A	654	ASN
1	A	700	ASN
1	A	736	ASN
1	A	741	ASN
1	A	742	ASN
1	A	745	GLN
1	A	757	ASN
1	A	760	GLN
1	A	851	HIS
1	A	858	ASN
1	A	877	HIS
1	A	926	GLN
1	A	965	GLN
1	A	968	GLN
1	A	994	GLN
1	A	1008	GLN
1	A	1124	HIS
1	A	1222	ASN
1	A	1278	ASN
1	A	1312	ASN
1	A	1364	ASN
1	A	1390	ASN
1	A	1393	ASN
1	A	1432	GLN
2	B	121	ASN
2	B	236	HIS
2	B	366	GLN
2	B	433	GLN
2	B	465	ASN
2	B	484	ASN

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Mol	Chain	Res	Type
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	734	HIS
2	B	744	HIS
2	B	794	ASN
2	B	822	ASN
2	B	842	ASN
2	B	843	GLN
2	B	862	GLN
2	B	957	ASN
2	B	975	GLN
2	B	984	HIS
2	B	1015	HIS
2	B	1040	ASN
2	B	1065	GLN
2	B	1084	GLN
2	B	1093	GLN
2	B	1097	HIS
2	B	1179	GLN
2	B	1195	HIS
2	B	1211	ASN
3	C	31	ASN
3	C	73	GLN
3	C	79	GLN
3	C	123	ASN
3	C	167	HIS
3	C	203	GLN
3	C	206	ASN
3	C	231	ASN
4	E	32	GLN
4	E	61	GLN
4	E	143	ASN
4	E	147	HIS
6	H	11	GLN
6	H	33	GLN
6	H	134	ASN
7	I	60	GLN
7	I	83	ASN
9	K	40	HIS
9	K	65	HIS

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Mol	Chain	Res	Type
9	K	92	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	R	12/24 (50%)	5 (41%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
11	R	4	G
11	R	10	A
11	R	11	U
11	R	12	G
11	R	13	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1395/1733 (80%)	-0.19	31 (2%)	62	51	80, 126, 198, 230	0
2	B	1106/1224 (90%)	-0.21	11 (0%)	82	75	79, 120, 169, 188	0
3	C	266/318 (83%)	-0.33	1 (0%)	92	87	89, 116, 158, 167	0
4	E	214/215 (99%)	-0.22	5 (2%)	60	50	113, 165, 202, 206	0
5	F	84/155 (54%)	-0.49	0	100	100	110, 133, 152, 159	0
6	H	133/146 (91%)	-0.08	3 (2%)	60	50	137, 155, 178, 180	0
7	I	119/122 (97%)	-0.29	0	100	100	126, 147, 167, 181	0
8	J	65/70 (92%)	-0.35	0	100	100	86, 105, 134, 141	0
9	K	114/120 (95%)	-0.36	0	100	100	96, 118, 135, 139	0
10	L	46/70 (65%)	-0.15	1 (2%)	62	51	118, 175, 189, 193	0
11	R	13/24 (54%)	-0.32	0	100	100	97, 128, 191, 203	0
12	T	28/28 (100%)	-0.13	0	100	100	111, 219, 343, 346	0
13	N	14/14 (100%)	0.16	1 (7%)	16	11	308, 330, 332, 333	0
All	All	3597/4239 (84%)	-0.22	53 (1%)	73	64	79, 127, 194, 346	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	126	SER	4.8
1	A	1176	LEU	4.6
2	B	869	SER	4.5
13	N	1	DC	4.2
2	B	643	ASP	3.9
2	B	1223	ASP	3.9
4	E	125	PRO	3.9
2	B	250	PHE	3.5
1	A	44	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	150	THR	3.3
1	A	69	THR	3.3
1	A	149	GLU	3.2
1	A	286	HIS	3.2
2	B	870	ILE	3.1
1	A	175	ARG	3.1
1	A	153	PRO	3.0
3	C	212	PRO	3.0
6	H	86	ASP	2.9
1	A	318	SER	2.9
2	B	882	THR	2.9
2	B	866	TYR	2.8
1	A	146	MET	2.8
1	A	171	GLN	2.7
1	A	311	GLN	2.6
1	A	426	LEU	2.6
1	A	1175	SER	2.6
1	A	1108	ALA	2.6
4	E	2	ASP	2.5
1	A	147	VAL	2.5
1	A	152	VAL	2.5
2	B	433	GLN	2.5
1	A	182	VAL	2.5
1	A	251	SER	2.4
1	A	316	GLN	2.4
2	B	883	LEU	2.4
1	A	166	GLY	2.3
1	A	1167	GLU	2.3
1	A	115	LEU	2.3
1	A	1256	GLU	2.3
1	A	66	LYS	2.2
1	A	145	LYS	2.2
10	L	43	THR	2.2
4	E	44	ALA	2.2
4	E	110	PHE	2.2
1	A	885	THR	2.1
1	A	1173	HIS	2.1
1	A	151	ASP	2.1
1	A	3	GLY	2.1
1	A	104	GLU	2.1
2	B	432	MET	2.1
6	H	85	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	709	ASP	2.0
6	H	52	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	A	1736	1/1	0.89	0.11	97,97,97,97	0
14	ZN	A	1735	1/1	0.94	0.08	177,177,177,177	0
14	ZN	L	105	1/1	0.97	0.09	183,183,183,183	0
14	ZN	A	1734	1/1	0.97	0.08	181,181,181,181	0
14	ZN	I	204	1/1	0.98	0.04	148,148,148,148	0
14	ZN	I	203	1/1	0.99	0.10	139,139,139,139	0
14	ZN	B	1307	1/1	0.99	0.06	156,156,156,156	0
14	ZN	C	319	1/1	1.00	0.07	107,107,107,107	0
14	ZN	J	101	1/1	1.00	0.13	109,109,109,109	0

6.5 Other polymers (i)

There are no such residues in this entry.