Full wwPDB X-ray Structure Validation Report (i)

Sep 7, 2023 – 10:58 AM EDT

PDB ID	:	4G7O
Title	:	Crystal structure of Thermus thermophilus transcription initiation complex containing 2 nt of RNA
Authors	:	Zhang, Y.; Ebright, R.H.
Deposited on	:	2012-07-20
Resolution	:	2.99 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:

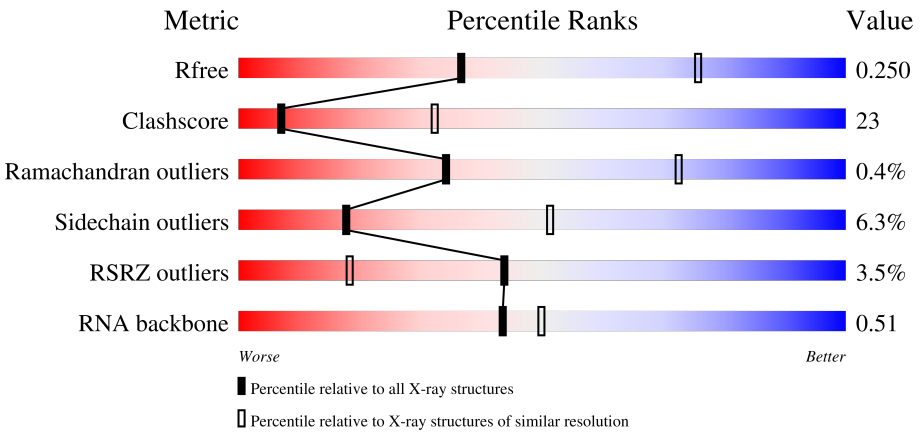
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	315	44% 26% • 28%
1	B	315	% 41% 26% • 30%
1	K	315	48% 23% • 28%
1	L	315	% 43% 26% • 29%

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Mol	Chain	Length	Quality of chain
2	C	1119	3% 59% 38%
2	M	1119	7% 56% 40%
3	D	1524	3% 59% 34%
3	N	1524	4% 56% 38%
4	E	99	3% 68% 25% 5%
4	O	99	3% 71% 23% 5%
5	F	443	% 51% 25% 22%
5	P	443	4% 46% 28% 22%
6	G	21	48% 19% 10% 24%
6	Q	21	33% 43% 24%
7	H	27	52% 33% 11%
7	R	27	52% 37% 11%
8	I	2	100%
8	S	2	100%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 57231 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	226	1782	1138	310	332	2	0	0	0
1	B	222	1750	1118	304	326	2	0	0	0
1	K	226	1782	1138	310	332	2	0	0	0
1	L	225	1773	1133	308	330	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1111	8770	5548	1564	1634	24	0	0	0
2	M	1111	8770	5548	1564	1634	24	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1482	11704	7421	2059	2189	35	0	0	0
3	N	1489	11746	7446	2066	2198	36	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	94	761	486	132	139	4	0	0	0
4	O	94	761	486	132	139	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	346	2807	1770	509	524	4	0	0	0
			Total	C	N	O	S			
5	P	347	2814	1774	510	526	4	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1
P	-19	MET	-	expression tag	UNP Q5SKW1
P	-18	GLY	-	expression tag	UNP Q5SKW1
P	-17	SER	-	expression tag	UNP Q5SKW1
P	-16	SER	-	expression tag	UNP Q5SKW1
P	-15	HIS	-	expression tag	UNP Q5SKW1
P	-14	HIS	-	expression tag	UNP Q5SKW1
P	-13	HIS	-	expression tag	UNP Q5SKW1
P	-12	HIS	-	expression tag	UNP Q5SKW1
P	-11	HIS	-	expression tag	UNP Q5SKW1
P	-10	HIS	-	expression tag	UNP Q5SKW1
P	-9	SER	-	expression tag	UNP Q5SKW1
P	-8	SER	-	expression tag	UNP Q5SKW1
P	-7	GLY	-	expression tag	UNP Q5SKW1
P	-6	LEU	-	expression tag	UNP Q5SKW1

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Chain	Residue	Modelled	Actual	Comment	Reference
P	-5	VAL	-	expression tag	UNP Q5SKW1
P	-4	PRO	-	expression tag	UNP Q5SKW1
P	-3	ARG	-	expression tag	UNP Q5SKW1
P	-2	GLY	-	expression tag	UNP Q5SKW1
P	-1	SER	-	expression tag	UNP Q5SKW1
P	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
6	G	16	328	156	63	94	15	0	0	0
			Total	C	N	O	P			
6	Q	16	328	156	63	94	15	0	0	0

- Molecule 7 is a DNA chain called 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
7	H	24	495	236	94	142	23	0	0	0
			Total	C	N	O	P			
7	R	24	495	236	94	142	23	0	0	0

- Molecule 8 is a RNA chain called 5'-R(*GP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
8	I	2	42	20	10	11	1	0	0	0
			Total	C	N	O	P			
8	S	2	42	20	10	11	1	0	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
9	D	2	2	2	0	0
			Total	Zn		
9	N	2	2	2	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
10	D	2	2	2	0	0
			Total	Mg		
10	K	1	1	1	0	0
			Total	Mg		
10	N	2	2	2	0	0

- Molecule 11 is water.

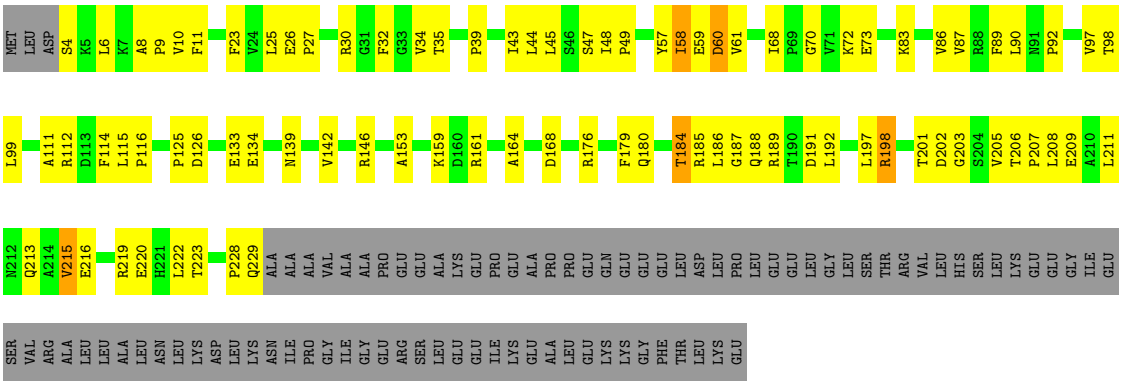
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	14	14	14	0	0
			Total	O		
11	B	3	3	3	0	0
			Total	O		
11	C	53	53	53	0	0
			Total	O		
11	D	58	58	58	0	0
			Total	O		
11	E	8	8	8	0	0
			Total	O		
11	F	10	10	10	0	0
			Total	O		
11	G	5	5	5	0	0
			Total	O		
11	H	2	2	2	0	0
			Total	O		
11	K	4	4	4	0	0
			Total	O		
11	L	3	3	3	0	0
			Total	O		
11	M	33	33	33	0	0
			Total	O		
11	N	52	52	52	0	0
			Total	O		
11	O	5	5	5	0	0
			Total	O		
11	P	16	16	16	0	0
			Total	O		
11	Q	2	2	2	0	0
			Total	O		
11	R	3	3	3	0	0
			Total	O		
11	S	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.

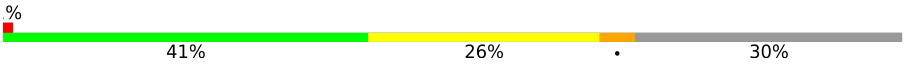
• Molecule 1: DNA-directed RNA polymerase subunit alpha

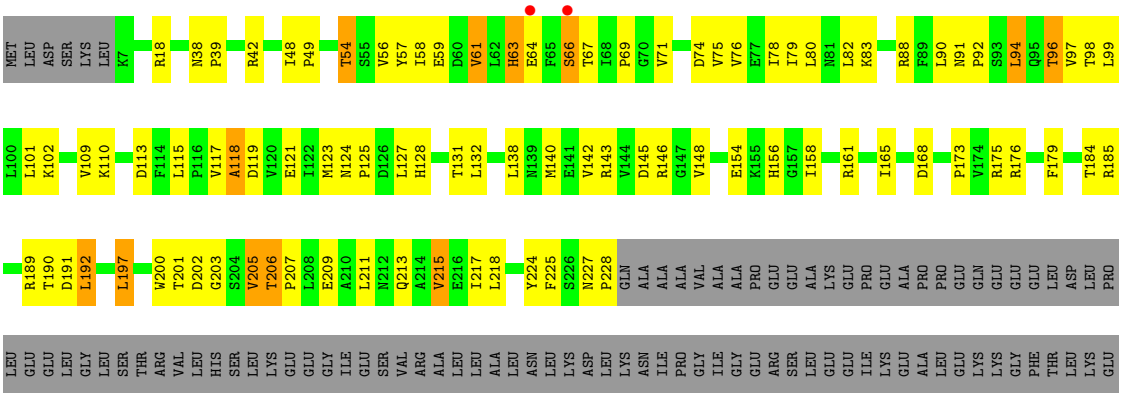
Chain A:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

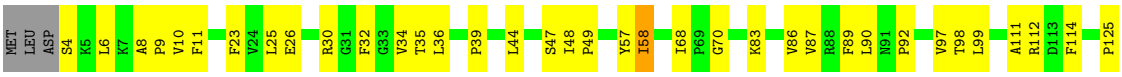
Chain B:

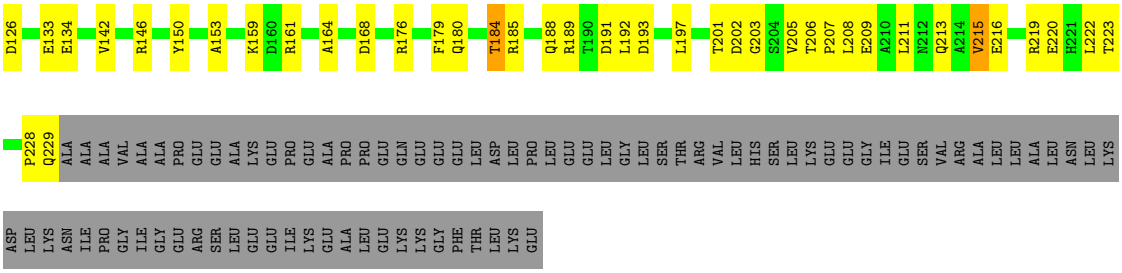




• Molecule 1: DNA-directed RNA polymerase subunit alpha

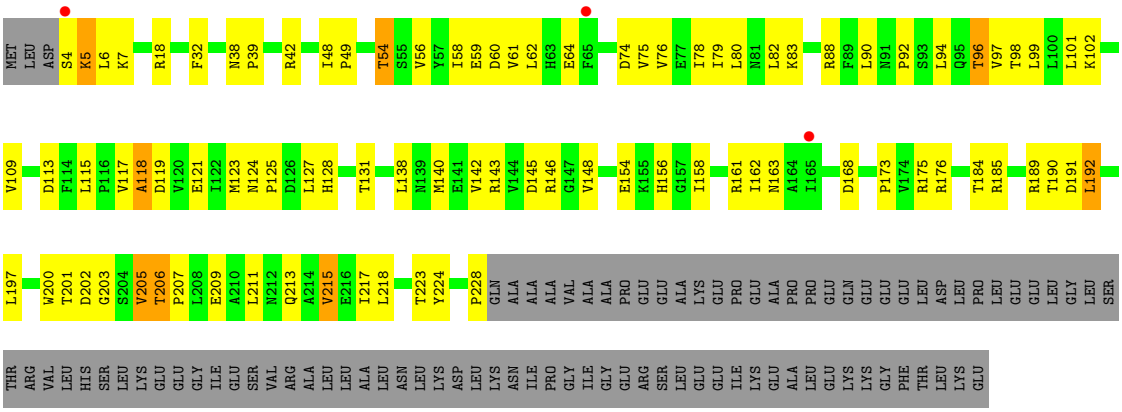
Chain K:





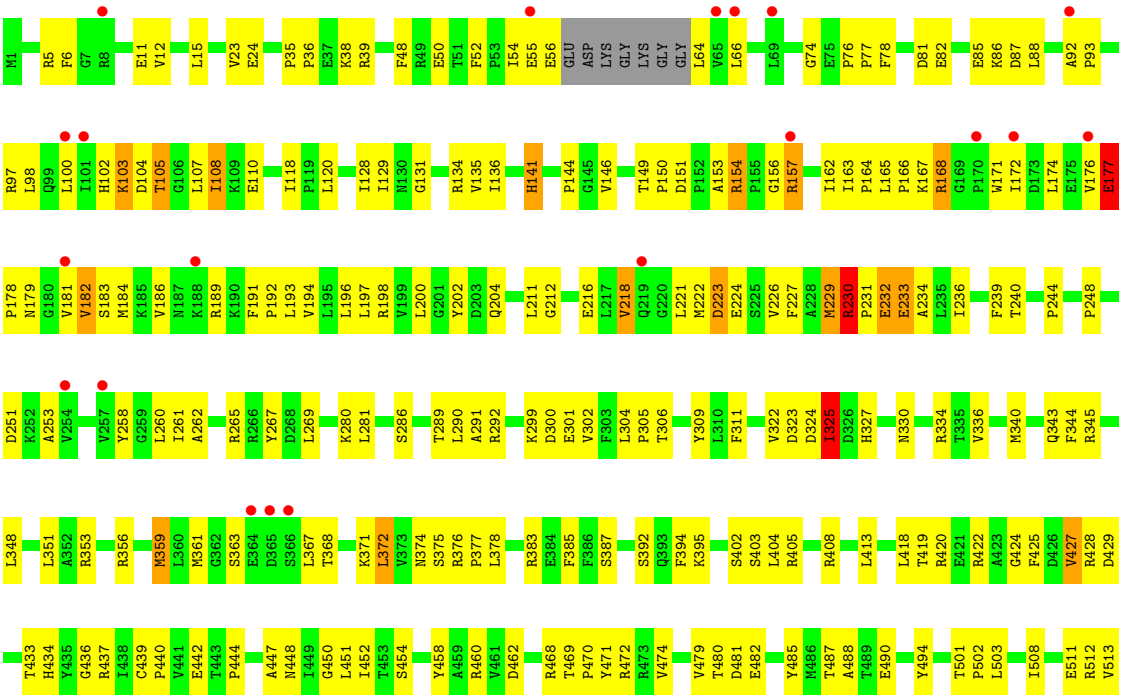
- Molecule 1: DNA-directed RNA polymerase subunit alpha

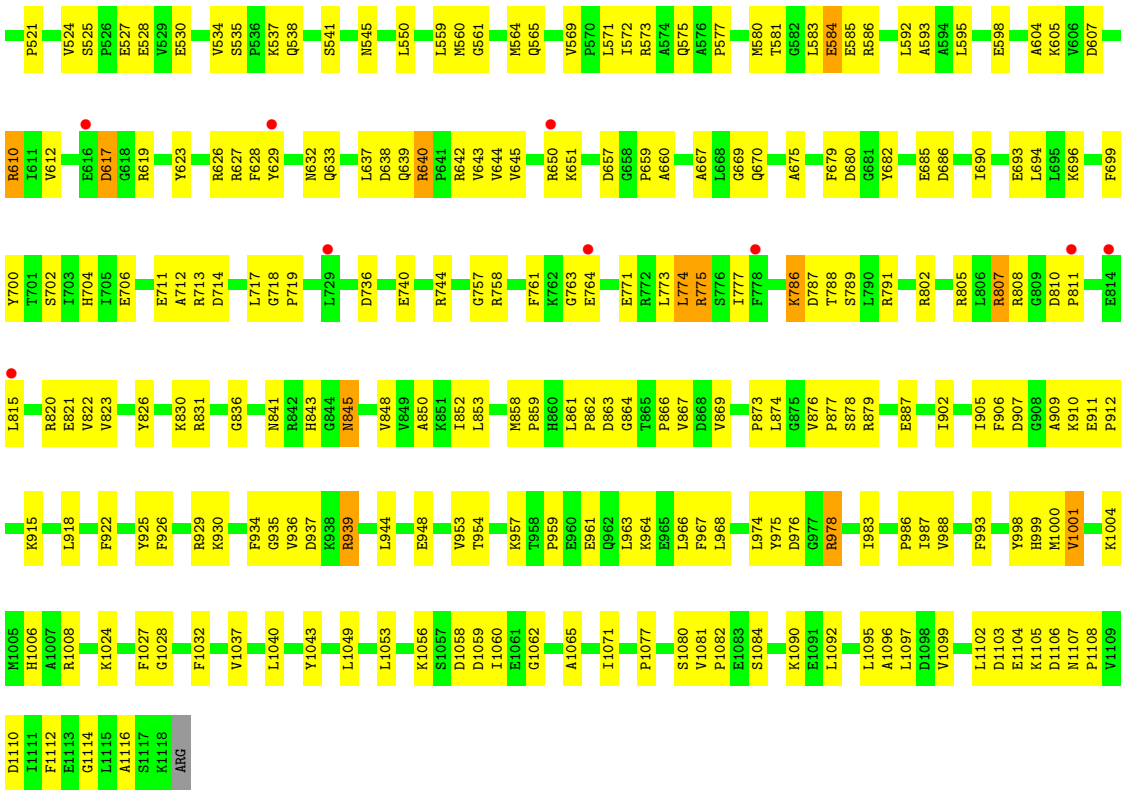
Chain L:



- Molecule 2: DNA-directed RNA polymerase subunit beta

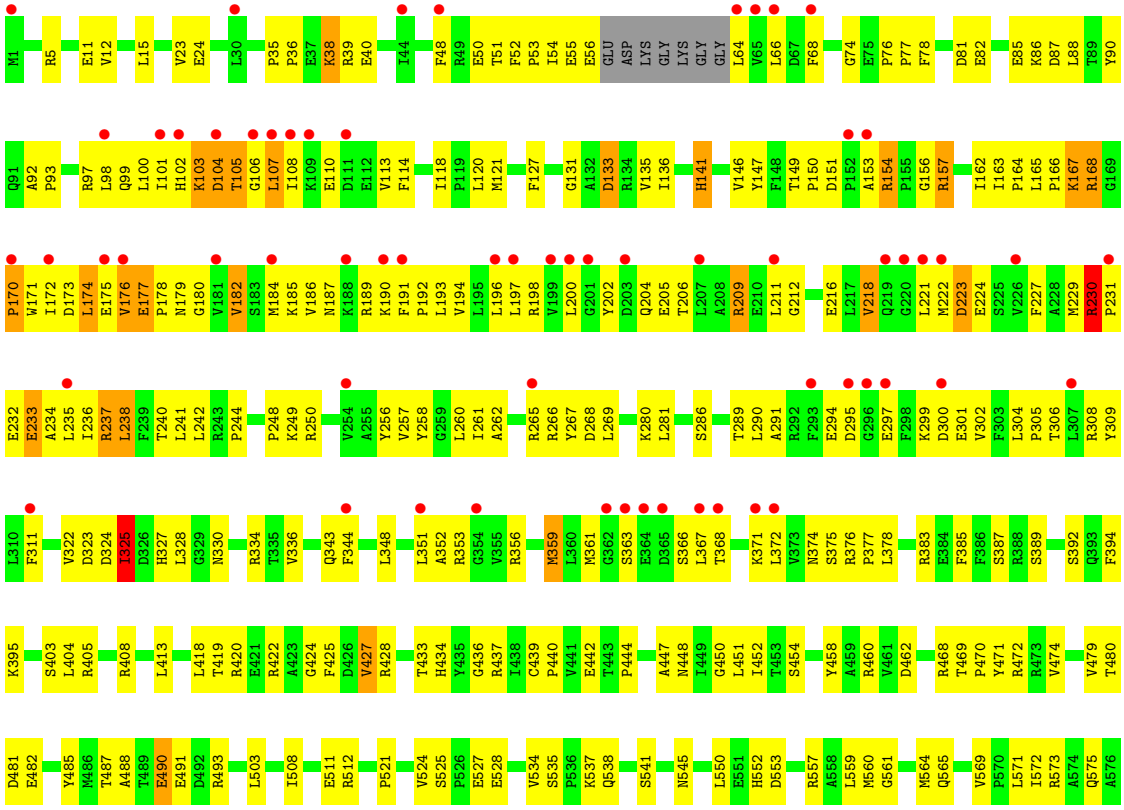
Chain C:

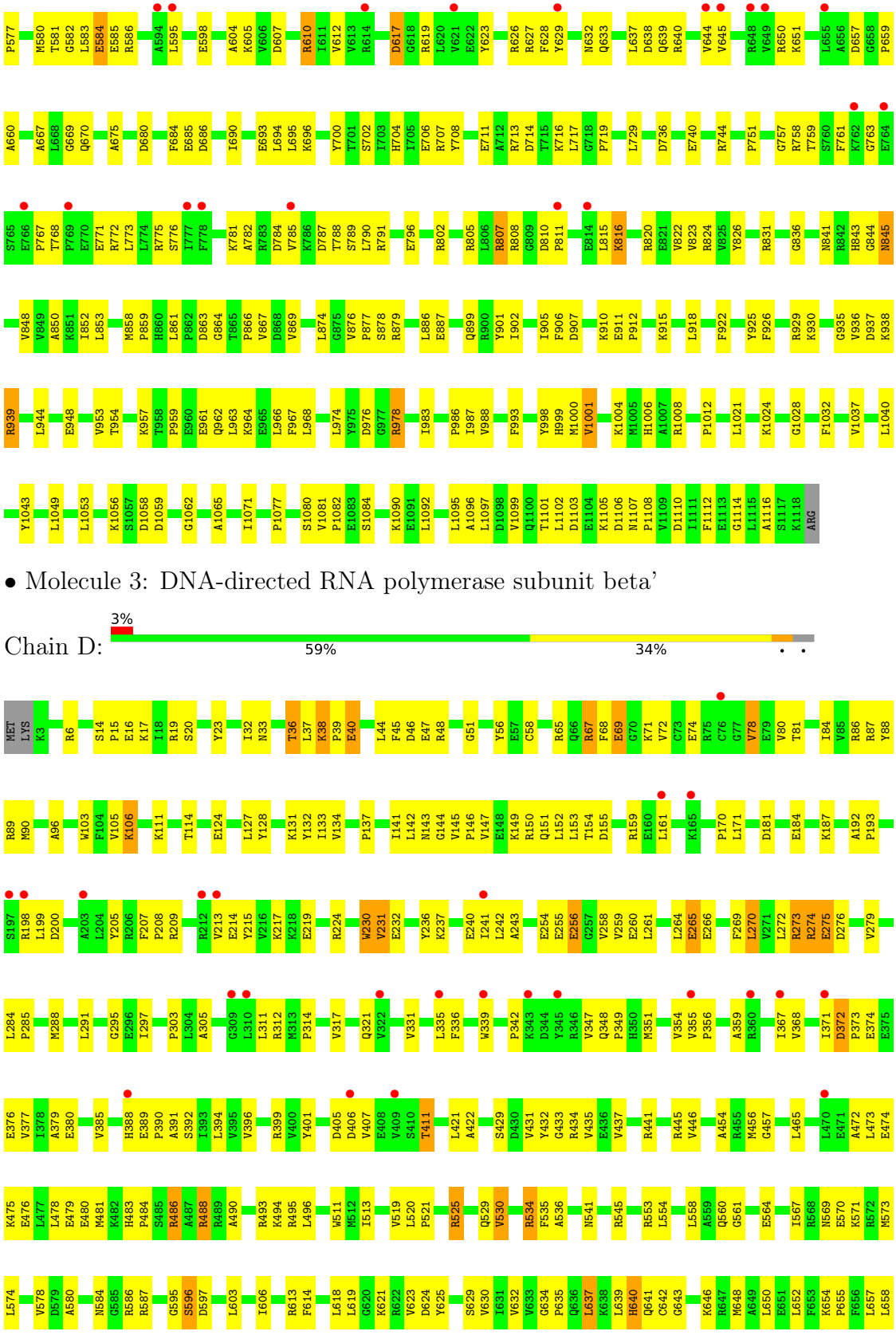




- Molecule 2: DNA-directed RNA polymerase subunit beta

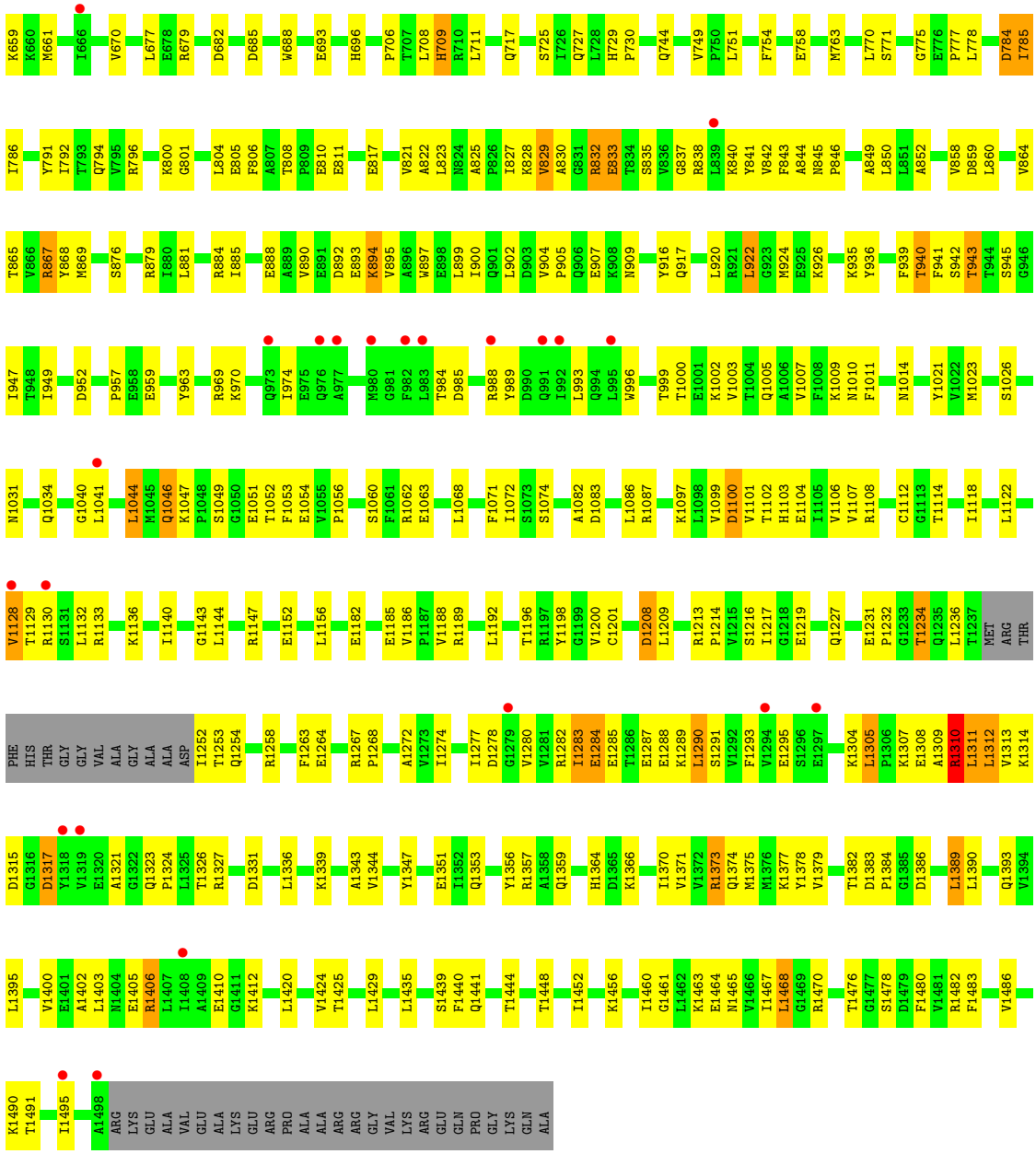
Chain M:





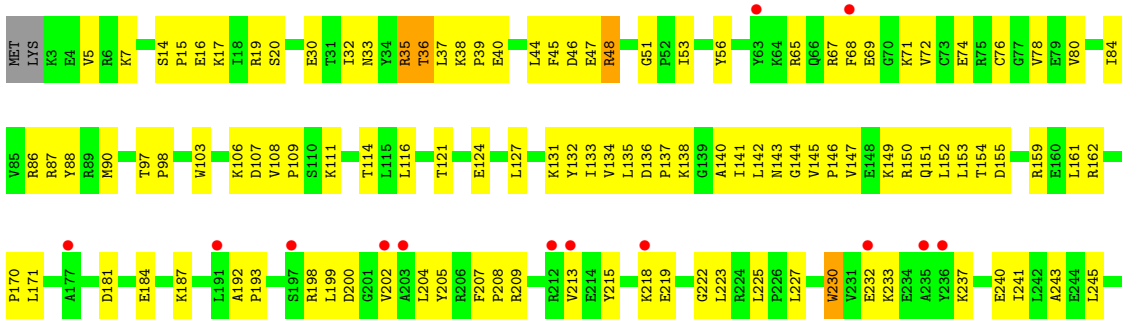
• Molecule 3: DNA-directed RNA polymerase subunit beta'

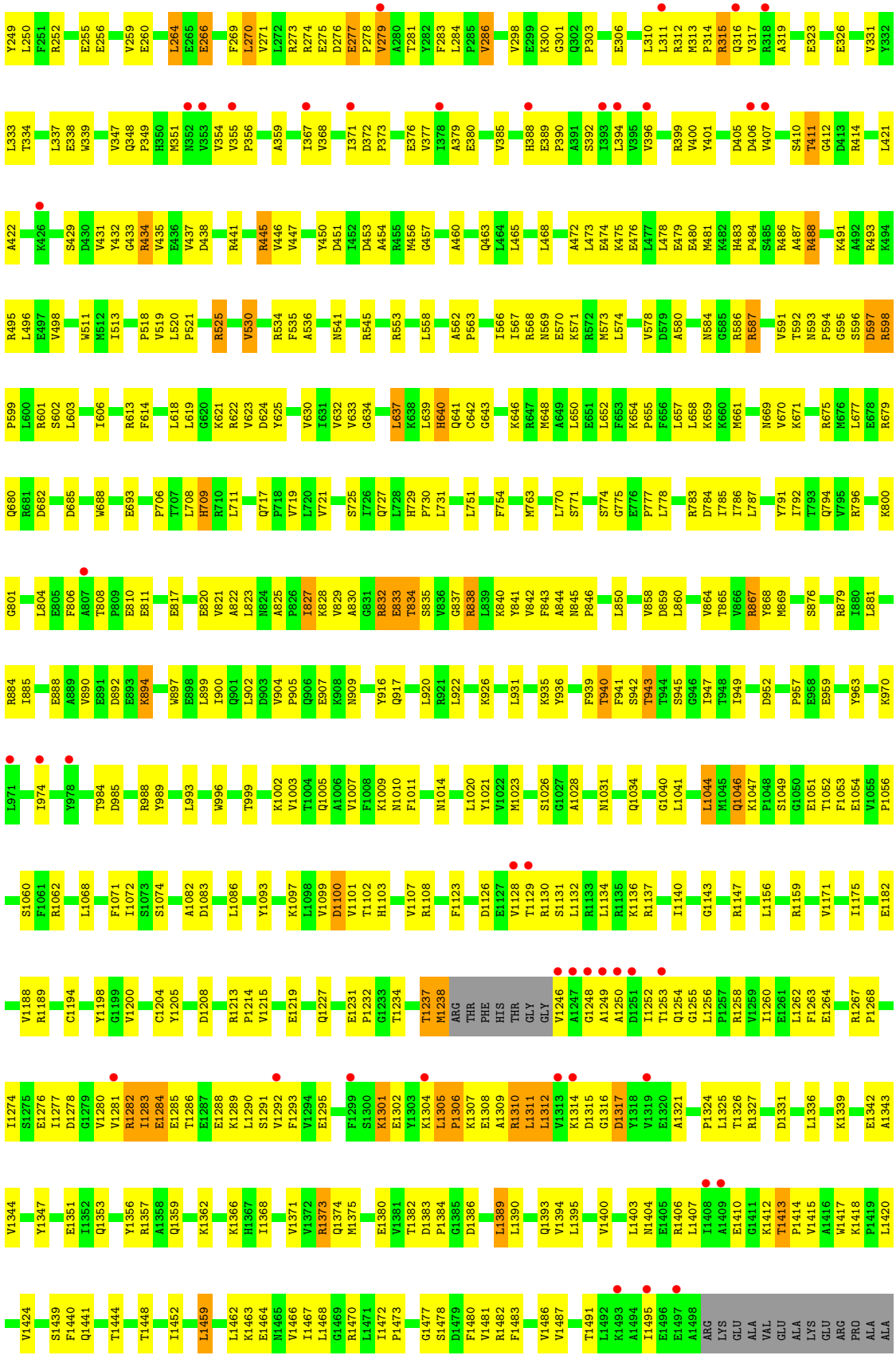
Chain D:



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

Chain N:




Y249 L250 F251 R252 E255 E256 V259 E260 L264 E265 E266 F269 L270 V271 L272 R273 R274 E275 D276 E277 P278 V279 A280 T281 Y282 F283 L284 P285 V286 V298 E299 K300 G301 Q302 P303 E306 L310 L311 R312 M313 P314 R315 Q316 V317 R318 A319 E323 E326 V331 Y332
L333 T334 L337 E338 W339 V347 Q348 P349 H350 M351 M352 V353 V354 V355 P356 A359 I367 V368 I371 D372 P373 E376 V377 I378 A379 E380 V385 H388 E389 P390 A391 S392 I393 L394 V395 V396 R399 V400 Y401 D405 D406 V407 S410 T411 G412 D413 R414 L421
A422 K426 S429 D430 V431 Y432 G433 R434 V435 E436 V437 D438 R441 R445 V446 V447 Y450 D451 I452 D453 A454 R455 M456 G457 A460 Q463 L464 L465 L468 A472 L473 E474 K475 E476 L477 L478 E479 E480 M481 K482 H483 P484 S485 R486 A487 R488 K491 A492 R493 K494
R495 L496 E497 V498 W511 M512 I513 P518 V519 L520 P521 R525 V530 R534 F535 A536 N541 R545 R553 L558 A562 P563 I566 I567 R568 N569 E570 K571 R572 M573 L574 V578 D579 A580 N584 G585 R586 R587 V591 T592 N593 P594 G595 S596 D597 R598
P599 L600 R601 S602 L603 I606 R613 F614 L618 L619 G620 K621 R622 V623 D624 Y625 V630 I631 V632 V633 G634 L637 K638 L639 H640 Q641 C642 G643 K646 R647 M648 A649 L650 E651 L652 F653 K654 P655 F656 L657 L658 K659 K660 M661 N669 V670 K671 R675 M676 L677 E678 R679
Q680 R681 D682 D685 W688 E693 P706 T707 L708 H709 R710 L711 Q717 P718 V719 L720 V721 S725 I726 Q727 L728 H729 P730 L731 L751 F754 M763 L770 S771 S774 G775 E776 P777 L778 R783 D784 I785 I786 L787 Y791 I792 T793 Q794 V795 R796 K800
G801 L804 E805 F806 A807 T808 P809 E810 E811 E817 E820 V821 A822 L823 N824 A825 P826 I827 K828 V829 A830 G831 R832 E833 T834 S835 V836 G837 R838 L839 K840 Y841 V842 F843 A844 N845 P846 L850 V858 D859 L860 V864 T865 V866 R867 Y868 M869 S876 R879 I880 L881
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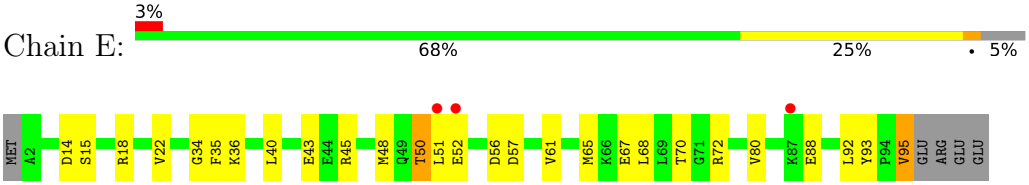
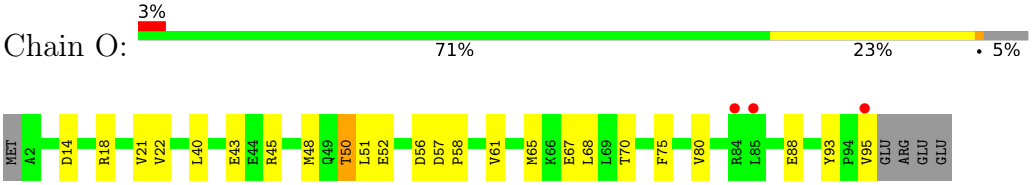
L971 I974 Y978 T984 D985 R988 Y989 L993 W996 T999 K1002 V1003 T1004 Q1005 A1006 V1007 F1008 K1009 N1010 F1011 N1014 L1020 Y1021 V1022 M1023 S1026 G1027 A1028 N1031 Q1034 G1040 L1041 L1044 M1045 Q1046 K1047 P1048 S1049 G1050 E1051 T1052 F1053 E1054 V1055 P1056
S1060 F1061 R1062 L1068 F1071 I1072 S1073 S1074 A1082 D1083 L1086 Y1093 K1097 L1098 V1099 D1100 V1101 T1102 H1103 V1107 R1108 F1123 D1126 E1127 V1128 T1129 R1130 S1131 L1132 R1133 L1134 R1135 K1136 R1137 I1140 G1143 R1147 L1156 R1159 V1171 I1175 E1182
V1188 R1189 C1194 Y1198 G1199 V1200 C1204 Y1205 D1208 R1213 P1214 V1215 E1219 Q1227 E1231 P1232 G1233 T1234 T1237 M1238 ARG THR PHE HIS THR GLY GLY V1246 A1247 G1248 A1249 A1250 D1251 I1252 T1253 Q1254 G1255 L1256 P1257 R1258 V1259 I1260 E1261 L1262 F1263 E1264 R1267 P1268
I1274 S1275 E1276 I1277 D1278 G1279 V1280 V1281 R1282 I1283 E1284 E1285 T1286 E1287 E1288 K1289 L1290 S1291 V1292 F1293 V1294 E1295 F1299 S1300 K1301 E1302 Y1303 K1304 L1305 P1306 K1307 E1308 A1309 R1310 L1311 L1312 V1313 K1314 D1315 G1316 D1317 Y1318 V1319 E1320 A1321 P1324 L1325 T1326 R1327 D1331 L1336 K1339 E1342 A1343
V1344 Y1347 E1351 I1352 Q1353 Y1356 R1357 A1358 Q1359 K1362 K1366 H1367 I1368 V1371 V1372 R1373 Q1374 M1375 E1380 V1381 T1382 D1383 P1384 G1385 D1386 L1389 L1390 Q1393 V1394 L1395 V1400 L1403 N1404 E1405 R1406 L1407 I1408 A1409 E1410 G1411 K1412 T1413 P1414 V1415 A1416 W1417 K1418 P1419 L1420
V1424 S1439 F1440 Q1441 T1444 T1448 I1452 L1459 L1462 K1463 E1464 N1465 V1466 I1467 L1468 G1469 R1470 L1471 I1472 P1473 G1477 S1478 D1479 F1480 V1481 R1482 F1483 V1486 V1487 T1491 L1492 K1493 A1494 I1495 E1496 E1497 A1498 ARG LYS GLU ALA VAL GLU ALA LYS GLU ARG PRO ALA ALA

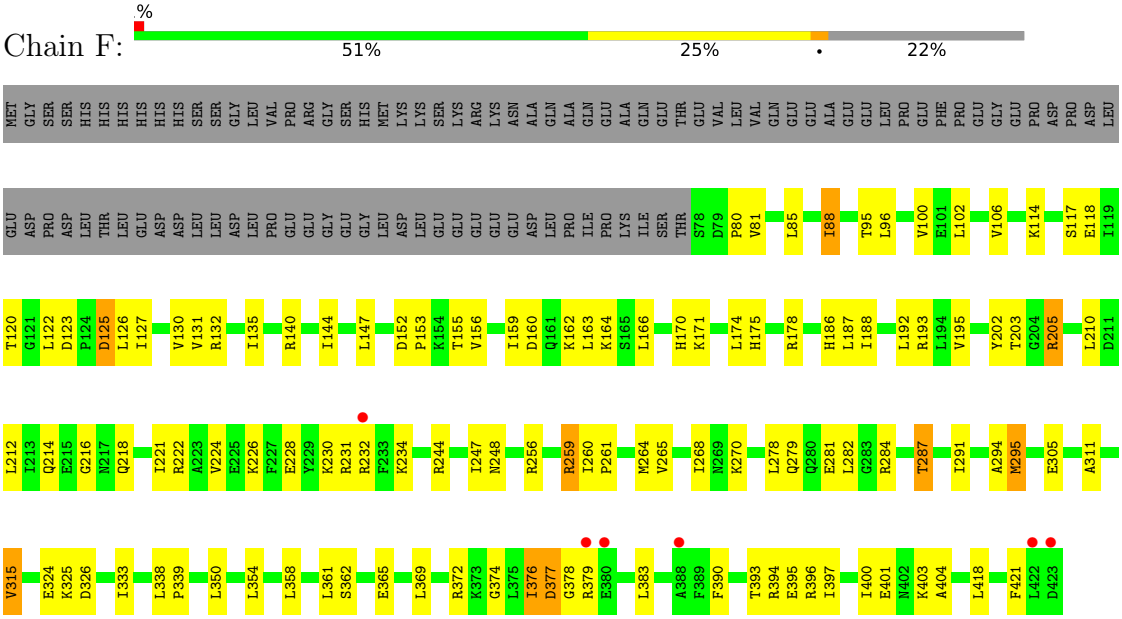
• Molecule 4: DNA-directed RNA polymerase subunit omega



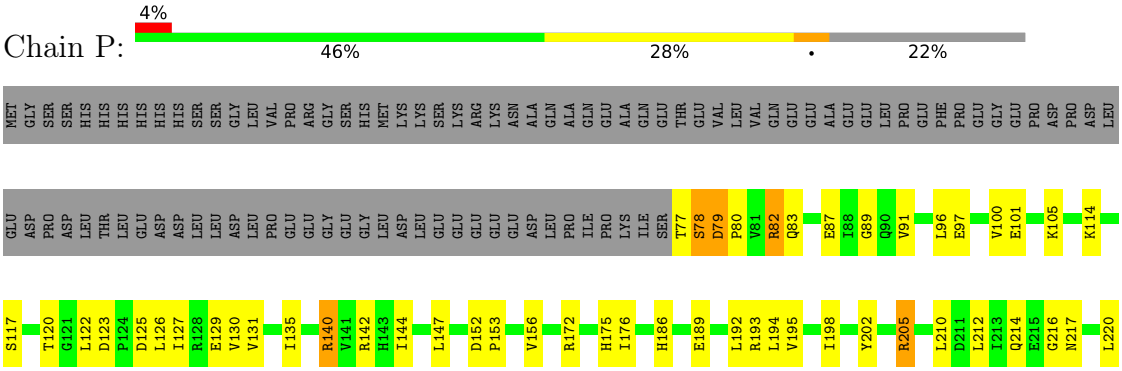
• Molecule 4: DNA-directed RNA polymerase subunit omega

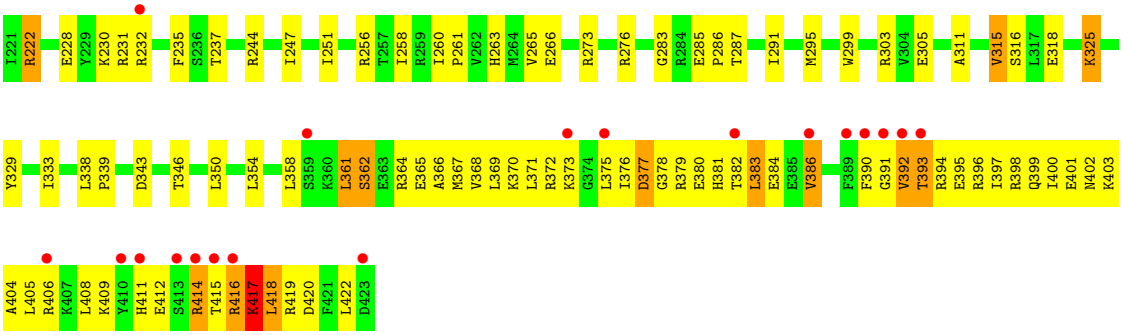


• Molecule 5: RNA polymerase sigma factor



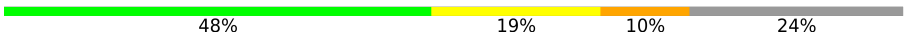
• Molecule 5: RNA polymerase sigma factor





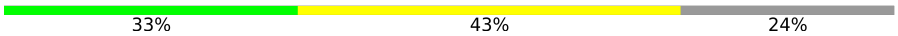
• Molecule 6: 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'

Chain G:



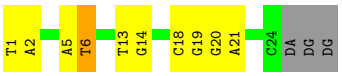
• Molecule 6: 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'

Chain Q:



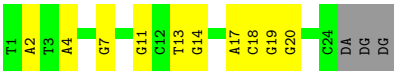
• Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain H:



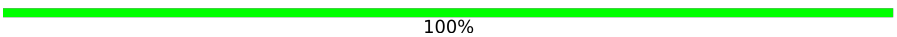
• Molecule 7: 5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*GP*CP*AP*GP*G)-3'

Chain R:



• Molecule 8: 5'-R(*GP*A)-3'

Chain I:



There are no outlier residues recorded for this chain.

• Molecule 8: 5'-R(*GP*A)-3'

Chain S: 100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	185.48Å 103.88Å 297.34Å 90.00° 98.23° 90.00°	Depositor
Resolution (Å)	46.61 – 2.99 49.59 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.61-2.99) 95.5 (49.59-2.99)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.205 , 0.247 0.207 , 0.250	Depositor DCC
R_{free} test set	1946 reflections (0.88%)	wwPDB-VP
Wilson B-factor (Å^2)	65.4	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	57231	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0787e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.29	0/1814	0.50	0/2466
1	B	0.27	0/1782	0.49	0/2424
1	K	0.27	0/1814	0.49	0/2466
1	L	0.28	0/1805	0.51	0/2454
2	C	0.30	0/8937	0.49	0/12087
2	M	0.31	0/8937	0.50	0/12087
3	D	0.31	1/11910 (0.0%)	0.49	0/16105
3	N	0.31	1/11952 (0.0%)	0.50	0/16162
4	E	0.28	0/775	0.44	0/1045
4	O	0.26	0/775	0.44	0/1045
5	F	0.28	0/2852	0.46	0/3837
5	P	0.28	0/2859	0.45	0/3847
6	G	0.55	0/368	1.09	2/567 (0.4%)
6	Q	0.47	0/368	1.05	0/567
7	H	0.51	0/556	1.26	3/858 (0.3%)
7	R	0.52	0/556	1.23	2/858 (0.2%)
8	I	0.35	0/47	0.68	0/72
8	S	0.25	0/47	0.55	0/72
All	All	0.31	2/58154 (0.0%)	0.53	7/79019 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	1
5	P	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	599	PRO	C-N	5.34	1.46	1.34
3	D	105	VAL	C-N	5.13	1.45	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	17	DA	O4'-C1'-N9	6.77	112.74	108.00
7	H	6	DT	O4'-C1'-N1	-6.45	103.49	108.00
7	H	20	DG	C1'-O4'-C4'	-6.17	103.93	110.10
6	G	16	DC	O4'-C4'-C3'	-5.77	102.19	104.50
7	R	20	DG	C1'-O4'-C4'	-5.40	104.70	110.10
6	G	15	DT	O4'-C4'-C3'	-5.27	102.39	104.50
7	H	21	DA	O4'-C1'-N9	5.21	111.65	108.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	104	ASP	Peptide
5	P	82	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1782	0	1834	81	0
1	B	1750	0	1797	92	0
1	K	1782	0	1834	60	0
1	L	1773	0	1826	76	0
2	C	8770	0	8872	436	0
2	M	8770	0	8871	518	2
3	D	11704	0	11934	544	1
3	N	11746	0	11974	664	0
4	E	761	0	778	26	0
4	O	761	0	778	25	0
5	F	2807	0	2882	111	0
5	P	2814	0	2888	168	1
6	G	328	0	181	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	328	0	181	6	0
7	H	495	0	272	8	0
7	R	495	0	272	14	0
8	I	42	0	23	0	0
8	S	42	0	23	0	0
9	D	2	0	0	0	0
9	N	2	0	0	0	0
10	D	2	0	0	0	0
10	K	1	0	0	0	0
10	N	2	0	0	0	0
11	A	14	0	0	0	0
11	B	3	0	0	0	0
11	C	53	0	0	0	0
11	D	58	0	0	0	0
11	E	8	0	0	0	0
11	F	10	0	0	0	0
11	G	5	0	0	0	0
11	H	2	0	0	0	0
11	K	4	0	0	0	0
11	L	3	0	0	0	0
11	M	33	0	0	1	0
11	N	52	0	0	1	0
11	O	5	0	0	0	0
11	P	16	0	0	0	0
11	Q	2	0	0	0	0
11	R	3	0	0	0	0
11	S	1	0	0	0	0
All	All	57231	0	57220	2617	2

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 23.

All (2617) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:157:ARG:NH1	2:M:176:VAL:HG11	1.23	1.47
2:C:64:LEU:N	2:C:103:LYS:NZ	1.61	1.47
2:M:64:LEU:N	2:M:103:LYS:NZ	1.64	1.45
2:M:107:LEU:HD12	2:M:108:ILE:N	1.11	1.40
2:M:740:GLU:OE1	2:M:805:ARG:NH1	1.57	1.36
1:B:58:ILE:HB	1:B:61:VAL:CG1	1.56	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:219:GLU:CG	3:D:339:TRP:HH2	1.41	1.34
2:M:157:ARG:NH1	2:M:176:VAL:CG1	1.88	1.33
3:D:33:ASN:OD1	3:D:36:THR:HG22	1.26	1.32
3:N:1283:ILE:CG2	3:N:1315:ASP:OD1	1.84	1.25
2:C:157:ARG:NH1	2:C:176:VAL:HG11	1.52	1.24
2:C:229:MET:O	2:C:230:ARG:CG	1.84	1.23
2:M:157:ARG:HH11	2:M:176:VAL:CG1	1.45	1.23
3:N:219:GLU:CB	3:N:339:TRP:HH2	1.50	1.22
3:N:219:GLU:CG	3:N:339:TRP:HH2	1.51	1.22
2:C:740:GLU:OE1	2:C:805:ARG:NH1	1.73	1.21
2:M:229:MET:HE3	2:M:233:GLU:O	1.07	1.21
2:C:64:LEU:N	2:C:103:LYS:HZ2	1.21	1.20
3:N:835:SER:HB3	3:N:838:ARG:NE	1.55	1.20
3:N:835:SER:CB	3:N:838:ARG:HE	1.55	1.20
3:N:1283:ILE:HG23	3:N:1315:ASP:CG	1.60	1.20
2:M:231:PRO:HG2	2:M:232:GLU:OE2	1.44	1.18
2:M:229:MET:CE	2:M:233:GLU:O	1.90	1.18
3:N:1290:LEU:CG	3:N:1307:LYS:HE2	1.73	1.17
2:C:108:ILE:HD12	2:C:108:ILE:O	1.45	1.17
3:D:256:GLU:O	3:D:274:ARG:NH1	1.77	1.17
3:N:1283:ILE:HG23	3:N:1315:ASP:OD1	1.39	1.17
2:M:105:THR:CG2	2:M:107:LEU:HB3	1.74	1.17
3:D:894:LYS:HD2	3:D:894:LYS:N	1.49	1.16
3:D:1305:LEU:HD23	3:D:1305:LEU:N	1.55	1.16
1:A:4:SER:O	1:A:189:ARG:NH2	1.79	1.16
3:N:1305:LEU:N	3:N:1305:LEU:HD23	1.56	1.15
2:M:229:MET:CE	2:M:233:GLU:C	2.15	1.15
2:M:107:LEU:CD1	2:M:108:ILE:N	2.08	1.15
2:C:229:MET:O	2:C:230:ARG:HG2	0.99	1.14
2:M:182:VAL:CG2	2:M:193:LEU:HB3	1.75	1.14
3:N:219:GLU:CG	3:N:339:TRP:CH2	2.31	1.14
3:D:219:GLU:HG3	3:D:339:TRP:HH2	1.11	1.13
3:N:1283:ILE:CG2	3:N:1315:ASP:CG	2.16	1.13
2:M:105:THR:HG21	2:M:107:LEU:HB3	1.29	1.12
2:C:182:VAL:CG2	2:C:193:LEU:HB3	1.79	1.12
2:M:64:LEU:N	2:M:103:LYS:HZ2	1.25	1.12
2:M:172:ILE:HG13	2:M:186:VAL:HG22	1.21	1.11
1:B:58:ILE:HB	1:B:61:VAL:HG13	1.19	1.11
3:D:1283:ILE:H	3:D:1283:ILE:CD1	1.54	1.11
3:N:219:GLU:HB2	3:N:339:TRP:CH2	1.86	1.11
3:D:219:GLU:CG	3:D:339:TRP:CH2	2.34	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:416:ARG:O	5:P:417:LYS:HB3	1.44	1.10
3:N:1310:ARG:HD3	3:N:1327:ARG:NH1	1.65	1.10
2:M:198:ARG:HE	2:M:230:ARG:HA	1.13	1.10
3:N:1283:ILE:O	3:N:1283:ILE:HD13	1.49	1.10
5:F:205:ARG:HH11	5:F:205:ARG:CG	1.64	1.09
2:M:229:MET:O	2:M:230:ARG:HG2	1.51	1.09
2:M:182:VAL:HG21	2:M:193:LEU:HB3	1.32	1.09
2:M:229:MET:HE3	2:M:233:GLU:C	1.72	1.08
3:N:32:ILE:CG1	5:P:258:ILE:HD13	1.82	1.08
3:N:894:LYS:H	3:N:894:LYS:HD2	1.14	1.08
2:C:157:ARG:NH1	2:C:176:VAL:CG1	2.16	1.08
3:N:1290:LEU:HG	3:N:1307:LYS:HE2	1.13	1.08
3:N:1310:ARG:CD	3:N:1327:ARG:HH11	1.67	1.08
5:F:205:ARG:HH11	5:F:205:ARG:HG2	0.96	1.07
1:B:58:ILE:CB	1:B:61:VAL:CG1	2.32	1.07
3:D:890:VAL:HB	3:D:922:LEU:CD1	1.84	1.07
2:M:105:THR:HG22	2:M:107:LEU:H	0.94	1.07
3:N:1238:MET:C	3:N:1253:THR:OG1	1.92	1.07
3:N:124:GLU:OE2	3:N:587:ARG:NH2	1.89	1.06
2:C:182:VAL:HG21	2:C:193:LEU:HB3	1.38	1.06
2:M:229:MET:HG2	2:M:233:GLU:HG2	1.35	1.06
3:D:1283:ILE:HD12	3:D:1283:ILE:N	1.55	1.06
5:P:417:LYS:HG3	5:P:418:LEU:H	1.02	1.05
5:P:231:ARG:O	5:P:232:ARG:HG3	1.53	1.05
2:M:64:LEU:HD22	2:M:100:LEU:HD11	1.33	1.05
3:D:274:ARG:HH11	3:D:274:ARG:HG3	0.92	1.05
3:D:894:LYS:H	3:D:894:LYS:CD	1.62	1.05
2:M:172:ILE:HG13	2:M:186:VAL:CG2	1.86	1.05
2:M:167:LYS:O	2:M:168:ARG:HD2	1.57	1.05
3:N:219:GLU:CB	3:N:339:TRP:CH2	2.38	1.04
3:N:32:ILE:HG13	5:P:258:ILE:HD13	1.33	1.04
3:D:219:GLU:HG3	3:D:339:TRP:CH2	1.92	1.04
3:D:1304:LYS:C	3:D:1305:LEU:HD23	1.77	1.04
5:P:417:LYS:HG3	5:P:418:LEU:N	1.71	1.04
3:D:67:ARG:NH1	3:D:67:ARG:HB2	1.71	1.03
3:D:1310:ARG:C	3:D:1311:LEU:HD23	1.78	1.03
3:N:46:ASP:OD1	3:N:48:ARG:N	1.91	1.03
1:A:57:TYR:CD1	1:A:161:ARG:HD2	1.94	1.03
3:D:33:ASN:OD1	3:D:36:THR:CG2	2.05	1.03
3:N:835:SER:HB3	3:N:838:ARG:HE	0.88	1.02
1:B:58:ILE:HB	1:B:61:VAL:HG11	1.38	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:260:GLU:OE1	3:N:273:ARG:NH1	1.92	1.02
3:N:890:VAL:HB	3:N:922:LEU:HD13	1.40	1.02
2:C:230:ARG:HB2	2:C:231:PRO:HD2	1.39	1.01
2:M:179:ASN:OD1	2:M:180:GLY:N	1.93	1.01
2:C:154:ARG:HH11	2:C:154:ARG:HG2	0.84	1.00
1:K:201:THR:HG22	1:K:203:GLY:H	1.27	1.00
2:C:154:ARG:HG2	2:C:154:ARG:NH1	1.65	1.00
2:M:154:ARG:HG2	2:M:154:ARG:HH11	0.84	1.00
3:D:1312:LEU:CD2	3:D:1327:ARG:HG2	1.92	0.99
5:F:281:GLU:HG2	5:F:282:LEU:HD23	1.40	0.99
1:B:58:ILE:CB	1:B:61:VAL:HG11	1.91	0.99
5:F:205:ARG:HG2	5:F:205:ARG:NH1	1.70	0.99
2:M:105:THR:HG22	2:M:107:LEU:N	1.78	0.99
3:D:1311:LEU:HD23	3:D:1311:LEU:N	1.78	0.99
2:M:628:PHE:H	2:M:638:ASP:HB3	1.26	0.98
2:C:108:ILE:HD12	2:C:108:ILE:C	1.83	0.98
3:N:595:GLY:O	3:N:597:ASP:OD2	1.80	0.98
2:C:164:PRO:HD2	2:C:171:TRP:CD1	1.99	0.98
1:A:201:THR:HG22	1:A:203:GLY:H	1.26	0.98
1:A:184:THR:HG22	1:A:192:LEU:CB	1.94	0.98
3:N:1254:GLN:HB3	3:N:1258:ARG:HB2	1.46	0.98
2:M:167:LYS:C	2:M:168:ARG:HD2	1.83	0.97
3:D:124:GLU:OE2	3:D:587:ARG:NH2	1.96	0.97
3:N:1290:LEU:HG	3:N:1307:LYS:CE	1.94	0.97
2:C:154:ARG:HH11	2:C:154:ARG:CG	1.76	0.97
1:B:110:LYS:HZ2	1:B:128:HIS:HB2	1.27	0.97
2:M:154:ARG:HH11	2:M:154:ARG:CG	1.76	0.97
5:P:414:ARG:HG2	5:P:414:ARG:HH11	1.29	0.97
3:N:411:THR:HA	3:N:435:VAL:CG1	1.95	0.96
3:D:67:ARG:HH11	3:D:67:ARG:CG	1.76	0.96
1:B:201:THR:HG22	1:B:203:GLY:H	1.25	0.96
3:D:219:GLU:HG2	3:D:339:TRP:HH2	1.30	0.96
3:N:1310:ARG:HD3	3:N:1327:ARG:HH11	0.81	0.96
1:L:162:ILE:O	1:L:163:ASN:HB2	1.66	0.96
2:M:154:ARG:HG2	2:M:154:ARG:NH1	1.65	0.96
2:M:229:MET:CB	2:M:233:GLU:HB3	1.96	0.96
5:P:91:VAL:O	5:P:193:ARG:NH2	1.97	0.96
1:L:201:THR:HG22	1:L:203:GLY:H	1.25	0.95
3:N:438:ASP:OD1	3:N:441:ARG:HD2	1.65	0.95
2:C:628:PHE:H	2:C:638:ASP:HB3	1.27	0.95
2:M:107:LEU:HD12	2:M:107:LEU:C	1.80	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:229:MET:O	2:M:233:GLU:HB2	1.65	0.95
2:M:198:ARG:NE	2:M:230:ARG:HA	1.81	0.95
1:K:4:SER:O	1:K:189:ARG:NH2	2.00	0.94
2:M:229:MET:HE2	2:M:233:GLU:C	1.86	0.94
3:N:1305:LEU:N	3:N:1305:LEU:CD2	2.30	0.94
2:M:177:GLU:OE1	2:M:190:LYS:NZ	1.99	0.94
1:B:58:ILE:CB	1:B:61:VAL:HG13	1.95	0.94
2:M:521:PRO:HB3	3:N:1068:LEU:HD21	1.48	0.94
3:D:274:ARG:NH1	3:D:274:ARG:HG3	1.72	0.93
1:L:206:THR:HG22	1:L:209:GLU:H	1.33	0.93
3:D:1309:ALA:O	3:D:1310:ARG:HB3	1.68	0.93
2:M:229:MET:HE2	2:M:234:ALA:N	1.84	0.93
1:A:184:THR:HG22	1:A:192:LEU:HB3	1.50	0.93
1:B:206:THR:HG22	1:B:209:GLU:H	1.32	0.93
3:D:274:ARG:HH11	3:D:274:ARG:CG	1.80	0.93
3:D:1305:LEU:N	3:D:1305:LEU:CD2	2.30	0.93
2:C:102:HIS:HB3	2:C:105:THR:CG2	1.99	0.93
3:D:67:ARG:NH1	3:D:67:ARG:CB	2.30	0.93
2:M:229:MET:HE1	2:M:234:ALA:HA	1.51	0.93
3:N:209:ARG:N	3:N:389:GLU:O	2.01	0.93
3:D:45:PHE:O	3:D:86:ARG:NH2	2.01	0.93
3:N:46:ASP:OD2	3:N:48:ARG:HG3	1.69	0.93
3:N:1283:ILE:HG21	3:N:1315:ASP:OD1	1.66	0.93
3:N:890:VAL:HB	3:N:922:LEU:CD1	1.98	0.92
5:P:417:LYS:CG	5:P:418:LEU:N	2.30	0.92
2:M:198:ARG:HE	2:M:230:ARG:CA	1.82	0.92
5:F:231:ARG:C	5:F:232:ARG:HG3	1.89	0.92
3:N:1290:LEU:CD2	3:N:1307:LYS:HE2	1.98	0.92
3:D:894:LYS:HD2	3:D:894:LYS:H	1.01	0.92
1:B:58:ILE:CG2	1:B:61:VAL:CG1	2.48	0.92
3:D:890:VAL:HB	3:D:922:LEU:HD12	1.49	0.91
2:M:229:MET:HG2	2:M:233:GLU:CG	1.99	0.91
3:D:1283:ILE:HG13	3:D:1315:ASP:CG	1.91	0.91
2:M:230:ARG:HB2	2:M:231:PRO:HD2	1.53	0.91
3:D:892:ASP:OD1	3:D:894:LYS:CD	2.18	0.91
3:N:45:PHE:O	3:N:86:ARG:NH2	2.04	0.91
2:M:172:ILE:CG1	2:M:186:VAL:CG2	2.48	0.91
2:M:107:LEU:CD1	2:M:108:ILE:H	1.77	0.91
5:P:231:ARG:C	5:P:232:ARG:HG3	1.87	0.91
2:C:102:HIS:HB3	2:C:105:THR:HG22	1.53	0.91
2:M:229:MET:CG	2:M:233:GLU:HB3	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:414:ARG:HG2	5:P:414:ARG:NH1	1.85	0.90
3:D:1284:GLU:HG2	3:D:1291:SER:HB3	1.51	0.90
2:M:229:MET:CE	2:M:234:ALA:HA	2.02	0.90
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.51	0.90
1:K:206:THR:HB	1:K:209:GLU:HG3	1.52	0.90
2:M:237:ARG:O	2:M:241:LEU:HG	1.71	0.90
1:A:206:THR:HB	1:A:209:GLU:HG3	1.52	0.90
3:N:219:GLU:HG3	3:N:339:TRP:CH2	2.06	0.90
2:C:324:ASP:C	2:C:325:ILE:HG23	1.91	0.90
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.53	0.90
2:C:418:LEU:HD11	2:C:427:VAL:HG11	1.54	0.90
3:N:32:ILE:CG1	5:P:258:ILE:CD1	2.50	0.89
3:N:894:LYS:HD2	3:N:894:LYS:N	1.86	0.89
3:D:821:VAL:HG11	3:D:827:ILE:HD11	1.51	0.89
2:C:168:ARG:NH2	2:C:265:ARG:O	2.05	0.89
2:M:324:ASP:C	2:M:325:ILE:HG23	1.91	0.89
3:N:1237:THR:HG22	3:N:1238:MET:N	1.86	0.89
2:C:172:ILE:HG12	2:C:186:VAL:CG2	2.01	0.89
3:N:227:LEU:HG	3:N:331:VAL:HG13	1.55	0.89
2:C:198:ARG:HE	2:C:230:ARG:HA	1.38	0.88
3:D:1285:GLU:OE1	3:D:1307:LYS:HE2	1.74	0.88
5:P:417:LYS:CG	5:P:418:LEU:H	1.80	0.88
3:D:67:ARG:HH11	3:D:67:ARG:HG3	1.36	0.88
3:D:892:ASP:OD1	3:D:894:LYS:HD3	1.74	0.88
3:N:894:LYS:H	3:N:894:LYS:CD	1.84	0.88
1:A:59:GLU:O	1:A:60:ASP:HB2	1.71	0.88
2:C:405:ARG:HD2	2:C:442:GLU:OE2	1.72	0.88
1:B:66:SER:O	1:B:75:VAL:HG23	1.73	0.88
3:D:209:ARG:N	3:D:389:GLU:O	2.07	0.88
2:M:105:THR:CG2	2:M:107:LEU:H	1.85	0.88
3:D:219:GLU:HG2	3:D:339:TRP:CH2	2.07	0.87
2:M:487:THR:HG22	2:M:490:GLU:HB2	1.55	0.87
3:N:411:THR:HA	3:N:435:VAL:HG12	1.56	0.87
1:A:57:TYR:CE1	1:A:161:ARG:HD2	2.08	0.87
3:D:1312:LEU:CD2	3:D:1327:ARG:CG	2.53	0.87
2:M:405:ARG:HD2	2:M:442:GLU:OE2	1.73	0.87
3:N:1486:VAL:HG21	4:O:22:VAL:HG13	1.54	0.87
2:M:229:MET:HG2	2:M:233:GLU:HB3	1.57	0.86
3:D:821:VAL:HG11	3:D:827:ILE:CD1	2.05	0.86
3:N:1311:LEU:CD2	3:N:1311:LEU:N	2.37	0.86
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.56	0.86
2:M:757:GLY:HA2	2:M:789:SER:HB3	1.58	0.86
2:C:502:PRO:O	2:C:503:LEU:HD23	1.75	0.86
3:N:32:ILE:HD11	5:P:258:ILE:HD11	1.57	0.85
3:N:520:LEU:O	3:N:525:ARG:NH1	2.08	0.85
3:D:520:LEU:O	3:D:525:ARG:NH1	2.09	0.85
3:N:1310:ARG:HD3	3:N:1327:ARG:HD2	1.57	0.85
3:D:47:GLU:HB3	3:D:78:VAL:HG21	1.58	0.85
5:F:281:GLU:HG2	5:F:282:LEU:CD2	2.07	0.85
2:M:229:MET:HB3	2:M:233:GLU:HB3	1.58	0.85
2:M:230:ARG:CB	2:M:231:PRO:HD2	2.06	0.85
3:N:1282:ARG:CD	3:N:1295:GLU:OE2	2.25	0.85
5:P:273:ARG:HG2	5:P:276:ARG:HH12	1.40	0.84
2:C:503:LEU:HD22	2:C:508:ILE:HA	1.60	0.84
3:D:1283:ILE:HG13	3:D:1315:ASP:CB	2.06	0.84
3:N:1283:ILE:CG2	3:N:1315:ASP:CB	2.55	0.84
3:D:274:ARG:NH2	3:D:279:VAL:HG21	1.91	0.84
1:K:201:THR:HG21	1:K:205:VAL:O	1.77	0.84
3:D:1283:ILE:HG13	3:D:1315:ASP:HB2	1.56	0.84
5:P:361:LEU:HD12	5:P:362:SER:H	1.41	0.84
2:C:177:GLU:OE2	2:C:183:SER:HB3	1.77	0.84
3:D:864:VAL:HG12	3:D:865:THR:N	1.92	0.84
3:N:1108:ARG:NH2	3:N:1198:TYR:O	2.11	0.84
1:A:201:THR:HG21	1:A:205:VAL:O	1.77	0.84
2:C:163:ILE:HG23	2:C:171:TRP:NE1	1.93	0.84
2:M:324:ASP:O	2:M:325:ILE:HG23	1.76	0.84
2:M:182:VAL:CG2	2:M:193:LEU:CB	2.55	0.84
1:B:110:LYS:NZ	1:B:128:HIS:HB2	1.92	0.83
2:C:324:ASP:O	2:C:325:ILE:HG23	1.76	0.83
3:N:218:LYS:HG2	3:N:338:GLU:HG2	1.60	0.83
2:C:503:LEU:HD21	2:C:508:ILE:HD13	1.61	0.83
2:C:714:ASP:OD1	2:C:820:ARG:NH2	2.11	0.83
2:M:157:ARG:HH12	2:M:176:VAL:CG1	1.87	0.83
3:N:1237:THR:HG22	3:N:1238:MET:H	1.42	0.83
1:L:90:LEU:HB2	1:L:119:ASP:HB3	1.59	0.83
2:M:224:GLU:H	2:M:224:GLU:CD	1.78	0.83
3:N:864:VAL:HG12	3:N:865:THR:N	1.93	0.83
1:A:188:GLN:HG2	1:A:189:ARG:HG3	1.60	0.82
3:D:1283:ILE:H	3:D:1283:ILE:HD12	0.69	0.82
2:M:105:THR:CG2	2:M:107:LEU:CB	2.56	0.82
3:N:46:ASP:OD1	3:N:47:GLU:N	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:835:SER:HB3	3:N:838:ARG:CG	2.07	0.82
2:M:107:LEU:HD12	2:M:108:ILE:H	1.00	0.82
3:N:1305:LEU:HD23	3:N:1305:LEU:H	1.40	0.82
2:M:171:TRP:CZ3	7:R:13:DT:H2"	2.15	0.82
2:C:224:GLU:H	2:C:224:GLU:CD	1.78	0.82
2:M:418:LEU:HD11	2:M:427:VAL:HG11	1.62	0.82
2:C:231:PRO:HG2	2:C:232:GLU:OE2	1.79	0.82
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.61	0.82
4:O:95:VAL:O	4:O:95:VAL:HG23	1.78	0.82
3:D:785:ILE:HD13	3:D:935:LYS:HA	1.61	0.82
3:D:1312:LEU:HD21	3:D:1327:ARG:HG2	1.61	0.82
3:N:32:ILE:HG13	5:P:258:ILE:CD1	2.10	0.82
3:D:347:VAL:HG13	3:D:351:MET:HG3	1.61	0.82
2:M:428:ARG:NH2	2:M:447:ALA:O	2.12	0.82
3:N:1282:ARG:HD2	3:N:1295:GLU:OE2	1.80	0.82
2:C:103:LYS:O	2:C:104:ASP:HB2	1.80	0.81
3:N:347:VAL:HG13	3:N:351:MET:HG3	1.61	0.81
1:B:90:LEU:HB2	1:B:119:ASP:HB3	1.60	0.81
2:M:437:ARG:NH1	2:M:491:GLU:OE2	2.12	0.81
2:M:103:LYS:O	2:M:104:ASP:HB2	1.80	0.81
3:N:1495:ILE:HG12	4:O:88:GLU:HG3	1.62	0.81
1:B:58:ILE:CG2	1:B:61:VAL:HG11	2.09	0.81
3:D:67:ARG:HH11	3:D:67:ARG:CB	1.89	0.81
2:M:229:MET:HG2	2:M:233:GLU:CB	2.11	0.81
3:N:1312:LEU:CD2	3:N:1327:ARG:HG2	2.10	0.81
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.11	0.81
3:N:1282:ARG:HD2	3:N:1295:GLU:CD	2.01	0.81
3:N:32:ILE:HD11	5:P:258:ILE:CD1	2.10	0.81
3:D:835:SER:OG	3:D:838:ARG:HG3	1.80	0.81
3:N:411:THR:HB	3:N:437:VAL:H	1.45	0.81
2:M:78:PHE:HB3	2:M:82:GLU:HG2	1.63	0.81
2:C:164:PRO:HD2	2:C:171:TRP:HD1	1.45	0.80
3:D:411:THR:HB	3:D:437:VAL:H	1.44	0.80
3:N:219:GLU:HG3	3:N:339:TRP:CZ2	2.17	0.80
5:F:231:ARG:O	5:F:232:ARG:HG3	1.80	0.80
3:D:1439:SER:HB2	3:D:1463:LYS:NZ	1.97	0.80
3:N:1283:ILE:CG2	3:N:1315:ASP:HB2	2.09	0.80
3:N:1311:LEU:N	3:N:1311:LEU:HD22	1.96	0.80
2:M:419:THR:H	2:M:422:ARG:HG3	1.45	0.80
2:C:182:VAL:CG2	2:C:193:LEU:CB	2.60	0.79
3:N:1444:THR:O	3:N:1448:THR:HG23	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:172:ILE:CG1	2:M:186:VAL:HG22	2.08	0.79
2:M:229:MET:O	2:M:230:ARG:CG	2.30	0.79
3:D:821:VAL:CG1	3:D:827:ILE:HD11	2.13	0.79
2:C:419:THR:H	2:C:422:ARG:HG3	1.45	0.79
3:D:835:SER:OG	3:D:838:ARG:CG	2.31	0.79
3:D:1304:LYS:C	3:D:1305:LEU:CD2	2.50	0.79
3:D:1314:LYS:O	3:D:1317:ASP:HB2	1.81	0.79
2:C:78:PHE:HB3	2:C:82:GLU:HG2	1.64	0.79
2:M:717:LEU:HD23	2:M:763:GLY:HA3	1.64	0.79
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.64	0.79
2:M:487:THR:CG2	2:M:490:GLU:HB2	2.12	0.79
2:M:154:ARG:HH21	2:M:177:GLU:C	1.86	0.79
3:D:1444:THR:O	3:D:1448:THR:HG23	1.81	0.78
3:D:1384:PRO:HB3	3:D:1389:LEU:O	1.82	0.78
3:N:277:GLU:OE1	3:N:277:GLU:HA	1.83	0.78
5:P:414:ARG:HH11	5:P:414:ARG:CG	1.96	0.78
2:M:343:GLN:HG3	2:M:385:PHE:HB2	1.63	0.78
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.64	0.78
3:D:1156:LEU:HD23	3:D:1182:GLU:OE2	1.82	0.78
3:N:277:GLU:OE1	3:N:277:GLU:CA	2.31	0.78
3:N:796:ARG:HH12	3:N:859:ASP:HB2	1.48	0.78
3:N:1310:ARG:HH21	3:N:1310:ARG:HG3	1.47	0.78
3:D:1312:LEU:HD23	3:D:1327:ARG:HG3	1.64	0.78
3:N:823:LEU:HD11	3:N:837:GLY:HA2	1.64	0.78
3:N:1093:TYR:OH	3:N:1441:GLN:NE2	2.15	0.78
3:N:1283:ILE:O	3:N:1283:ILE:CD1	2.30	0.78
3:N:1284:GLU:OE1	3:N:1285:GLU:N	2.16	0.78
2:C:157:ARG:HH12	2:C:176:VAL:CG1	1.95	0.78
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.65	0.77
2:M:205:GLU:O	2:M:209:ARG:HG3	1.83	0.77
3:N:843:PHE:CE1	3:N:864:VAL:HG11	2.19	0.77
3:D:796:ARG:HH12	3:D:859:ASP:HB2	1.48	0.77
2:M:102:HIS:O	2:M:106:GLY:N	2.17	0.77
3:N:864:VAL:HG12	3:N:865:THR:H	1.48	0.77
2:C:151:ASP:HB3	2:C:157:ARG:O	1.84	0.77
2:M:1106:ASP:OD1	3:N:7:LYS:NZ	2.15	0.77
3:N:480:GLU:OE2	3:N:488:ARG:NH2	2.17	0.77
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.20	0.77
3:N:821:VAL:HG11	3:N:827:ILE:HD11	1.66	0.77
3:N:1395:LEU:HD11	3:N:1400:VAL:HB	1.66	0.77
3:N:675:ARG:NH1	5:P:420:ASP:OD1	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:717:LEU:HD23	2:C:763:GLY:HA2	1.65	0.77
2:M:182:VAL:HG23	2:M:193:LEU:HB3	1.67	0.77
5:P:231:ARG:O	5:P:232:ARG:CG	2.30	0.77
3:N:33:ASN:HB3	3:N:36:THR:HG23	1.66	0.76
2:C:198:ARG:NE	2:C:230:ARG:HA	2.01	0.76
2:C:503:LEU:CD2	2:C:508:ILE:HA	2.15	0.76
2:C:771:GLU:OE2	2:C:775:ARG:NH2	2.18	0.76
3:D:36:THR:O	3:D:37:LEU:HB2	1.85	0.76
2:M:151:ASP:HB3	2:M:157:ARG:O	1.84	0.76
2:M:1116:ALA:HB2	3:N:88:TYR:HB3	1.67	0.76
3:N:314:PRO:HG2	3:N:317:VAL:CG1	2.15	0.76
3:N:1282:ARG:HD2	3:N:1295:GLU:OE1	1.86	0.76
3:D:67:ARG:HB2	3:D:67:ARG:HH11	1.46	0.76
3:D:480:GLU:OE2	3:D:488:ARG:NH2	2.17	0.76
3:D:806:PHE:HB2	3:D:829:VAL:CG2	2.16	0.76
3:D:864:VAL:HG12	3:D:865:THR:H	1.50	0.76
2:C:108:ILE:O	2:C:108:ILE:CD1	2.30	0.76
2:M:189:ARG:HH12	2:M:244:PRO:HD3	1.50	0.76
2:M:773:LEU:HD23	5:P:354:LEU:HD13	1.65	0.76
2:M:157:ARG:HH11	2:M:157:ARG:HG3	1.50	0.76
2:M:166:PRO:O	2:M:167:LYS:HB2	1.83	0.76
5:P:383:LEU:HD23	5:P:383:LEU:H	1.50	0.76
2:M:487:THR:HG23	2:M:490:GLU:H	1.51	0.76
2:M:157:ARG:HH11	2:M:176:VAL:HG12	1.50	0.76
2:M:238:LEU:CD1	2:M:242:LEU:HD23	2.16	0.76
3:N:835:SER:HB3	3:N:838:ARG:CD	2.14	0.76
2:C:198:ARG:HE	2:C:230:ARG:CA	1.98	0.76
2:M:853:LEU:HB2	2:M:858:MET:HE1	1.67	0.76
2:M:775:ARG:HD3	2:M:782:ALA:HB2	1.66	0.75
3:N:1304:LYS:C	3:N:1305:LEU:HD23	2.06	0.75
2:M:182:VAL:HG23	2:M:193:LEU:CB	2.14	0.75
3:N:1237:THR:HG21	3:N:1246:VAL:HG13	1.67	0.75
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.67	0.75
2:C:757:GLY:HA2	2:C:789:SER:HB3	1.68	0.75
2:M:176:VAL:O	2:M:177:GLU:HB2	1.87	0.75
3:N:1237:THR:CG2	3:N:1246:VAL:HG13	2.16	0.75
3:N:1293:PHE:CZ	3:N:1302:GLU:HG3	2.21	0.75
3:D:411:THR:HA	3:D:435:VAL:HG12	1.67	0.75
1:K:179:PHE:HB3	1:K:197:LEU:HD23	1.68	0.75
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.69	0.74
3:D:1040:GLY:O	3:D:1060:SER:HB3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLU:OE1	1:A:139:ASN:ND2	2.20	0.74
2:C:157:ARG:HH11	2:C:157:ARG:HG3	1.50	0.74
2:M:229:MET:CE	2:M:234:ALA:CA	2.64	0.74
3:N:1040:GLY:O	3:N:1060:SER:HB3	1.88	0.74
1:A:184:THR:HG22	1:A:192:LEU:HB2	1.69	0.74
2:M:154:ARG:NH2	2:M:177:GLU:C	2.41	0.74
1:B:201:THR:HG21	1:B:205:VAL:O	1.86	0.74
2:M:711:GLU:HG2	2:M:822:VAL:HG22	1.69	0.74
3:N:219:GLU:H	3:N:339:TRP:HZ3	1.36	0.74
3:D:32:ILE:HG23	3:D:37:LEU:O	1.88	0.74
3:D:693:GLU:HA	4:E:48:MET:HE1	1.69	0.74
2:M:147:TYR:HA	2:M:323:ASP:OD2	1.88	0.74
5:P:416:ARG:O	5:P:417:LYS:CB	2.30	0.74
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.70	0.74
5:F:397:ILE:HD12	5:F:400:ILE:HD11	1.70	0.74
2:M:157:ARG:HH11	2:M:176:VAL:HG11	0.88	0.74
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.20	0.73
3:D:893:GLU:H	3:D:894:LYS:HE2	1.53	0.73
3:N:1283:ILE:HG21	3:N:1315:ASP:HB2	1.68	0.73
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.70	0.73
3:N:213:VAL:HG21	3:N:367:ILE:HD13	1.70	0.73
2:M:850:ALA:HA	3:N:632:VAL:CG2	2.18	0.73
3:N:274:ARG:NH1	3:N:279:VAL:HG21	2.03	0.73
1:A:83:LYS:HE3	1:A:168:ASP:HB2	1.70	0.73
5:F:202:TYR:OH	5:F:244:ARG:HG2	1.88	0.73
3:N:219:GLU:HG2	3:N:339:TRP:CH2	2.21	0.73
2:C:157:ARG:HH11	2:C:176:VAL:CG1	1.98	0.73
2:M:776:SER:OG	5:P:373:LYS:NZ	2.21	0.73
2:C:850:ALA:HA	3:D:632:VAL:CG2	2.19	0.73
3:D:371:ILE:HD12	5:F:230:LYS:HA	1.70	0.73
3:D:373:PRO:O	3:D:376:GLU:HG2	1.89	0.73
2:C:230:ARG:HB2	2:C:231:PRO:CD	2.14	0.73
3:N:1311:LEU:CD2	3:N:1311:LEU:H	1.99	0.73
2:C:182:VAL:HG23	2:C:193:LEU:CB	2.18	0.73
2:C:324:ASP:C	2:C:325:ILE:CG2	2.57	0.73
3:N:1283:ILE:HG21	3:N:1315:ASP:CB	2.18	0.73
2:C:1116:ALA:HB2	3:D:88:TYR:HB3	1.71	0.72
3:N:65:ARG:NH1	5:P:378:GLY:O	2.22	0.72
3:N:890:VAL:CB	3:N:922:LEU:CD1	2.67	0.72
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.04	0.72
3:D:1144:LEU:O	3:D:1147:ARG:HG3	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:83:LYS:HE3	1:K:168:ASP:HB2	1.71	0.72
2:M:204:GLN:HG3	2:M:222:MET:SD	2.30	0.72
3:N:255:GLU:OE1	3:N:274:ARG:NH2	2.19	0.72
3:N:843:PHE:HE1	3:N:864:VAL:HG11	1.55	0.72
3:N:892:ASP:OD1	3:N:894:LYS:CD	2.38	0.72
3:N:1263:PHE:HD2	3:N:1375:MET:CE	2.03	0.72
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.25	0.72
2:M:324:ASP:C	2:M:325:ILE:CG2	2.57	0.72
3:N:256:GLU:HG3	3:N:274:ARG:HE	1.54	0.72
3:N:821:VAL:HG11	3:N:827:ILE:CD1	2.19	0.72
2:M:577:PRO:HG2	2:M:580:MET:HG2	1.71	0.72
3:D:711:LEU:HD13	3:D:778:LEU:HD12	1.70	0.72
3:D:1285:GLU:OE1	3:D:1307:LYS:CE	2.37	0.72
3:D:1486:VAL:HG21	4:E:22:VAL:HG13	1.72	0.72
1:L:201:THR:HG21	1:L:205:VAL:O	1.89	0.72
2:M:238:LEU:HD12	2:M:242:LEU:HD23	1.71	0.72
2:C:229:MET:C	2:C:230:ARG:HG2	2.02	0.72
2:M:48:PHE:O	2:M:52:PHE:HD2	1.72	0.72
2:M:607:ASP:HB2	2:M:610:ARG:NH1	2.04	0.72
5:P:411:HIS:O	5:P:415:THR:HB	1.89	0.72
1:B:110:LYS:HZ2	1:B:128:HIS:CB	2.03	0.72
5:F:281:GLU:CG	5:F:282:LEU:HD23	2.17	0.72
2:M:714:ASP:OD1	2:M:820:ARG:NH2	2.23	0.71
3:N:162:ARG:O	3:N:414:ARG:NH1	2.21	0.71
2:C:419:THR:H	2:C:422:ARG:CG	2.03	0.71
2:M:617:ASP:HB2	2:M:619:ARG:HG2	1.72	0.71
3:N:658:LEU:HA	3:N:661:MET:HE3	1.72	0.71
2:M:206:THR:HA	2:M:209:ARG:HD2	1.72	0.71
2:M:859:PRO:O	2:M:867:VAL:HG22	1.90	0.71
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.25	0.71
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.72	0.71
5:F:205:ARG:CG	5:F:205:ARG:NH1	2.37	0.71
1:K:176:ARG:NH1	2:M:863:ASP:O	2.23	0.71
3:N:1071:PHE:O	3:N:1074:SER:OG	2.09	0.71
5:P:231:ARG:C	5:P:232:ARG:CG	2.59	0.71
3:D:1312:LEU:HD23	3:D:1327:ARG:CG	2.18	0.71
3:N:1310:ARG:HG3	3:N:1310:ARG:NH2	2.05	0.71
3:D:284:LEU:HD22	3:D:288:MET:HE2	1.72	0.71
2:M:64:LEU:CD2	2:M:100:LEU:HD11	2.16	0.71
2:M:419:THR:H	2:M:422:ARG:CG	2.03	0.71
3:N:32:ILE:CD1	5:P:258:ILE:CD1	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:905:ILE:HG22	2:M:906:PHE:CD2	2.26	0.71
3:N:56:TYR:HE1	3:N:69:GLU:HG3	1.54	0.71
3:D:1277:ILE:HG22	3:D:1278:ASP:H	1.55	0.70
2:C:177:GLU:HB2	2:C:181:VAL:O	1.90	0.70
2:C:204:GLN:HG3	2:C:222:MET:SD	2.31	0.70
3:D:596:SER:O	3:D:597:ASP:CG	2.30	0.70
2:M:230:ARG:HB2	2:M:231:PRO:CD	2.21	0.70
2:C:302:VAL:O	2:C:306:THR:HG23	1.91	0.70
2:M:874:LEU:HD12	3:N:784:ASP:OD2	1.90	0.70
3:N:864:VAL:CG1	3:N:865:THR:H	2.05	0.70
2:C:1008:ARG:HH11	2:C:1028:GLY:HA2	1.56	0.70
1:K:39:PRO:HG3	1:L:39:PRO:HG3	1.74	0.70
2:M:628:PHE:H	2:M:638:ASP:CB	2.04	0.70
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.55	0.70
3:N:1284:GLU:OE1	3:N:1284:GLU:C	2.30	0.70
2:C:418:LEU:CD1	2:C:427:VAL:HG11	2.21	0.70
2:C:905:ILE:HG22	2:C:906:PHE:CD2	2.27	0.70
3:D:864:VAL:CG1	3:D:865:THR:H	2.05	0.70
3:N:1044:LEU:H	3:N:1044:LEU:HD12	1.57	0.70
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.73	0.70
3:D:784:ASP:HB2	3:D:939:PHE:HE2	1.57	0.70
3:N:643:GLY:HA3	3:N:727:GLN:HB2	1.74	0.70
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.27	0.69
2:M:1008:ARG:O	3:N:625:TYR:HA	1.92	0.69
3:N:596:SER:C	3:N:597:ASP:OD2	2.30	0.69
3:D:1071:PHE:O	3:D:1074:SER:OG	2.10	0.69
3:N:711:LEU:HD13	3:N:778:LEU:HD12	1.73	0.69
2:C:163:ILE:HG23	2:C:171:TRP:CE2	2.27	0.69
2:M:74:GLY:HA3	2:M:93:PRO:HG2	1.74	0.69
2:M:230:ARG:CB	2:M:231:PRO:CD	2.71	0.69
3:N:266:GLU:OE2	3:N:315:ARG:NH2	2.26	0.69
5:P:415:THR:HG22	5:P:416:ARG:HG2	1.72	0.69
1:B:88:ARG:HB3	1:B:121:GLU:HB2	1.75	0.69
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.75	0.69
2:M:231:PRO:CG	2:M:232:GLU:OE2	2.33	0.69
2:C:1008:ARG:O	3:D:625:TYR:HA	1.91	0.69
3:D:47:GLU:CB	3:D:78:VAL:HG21	2.23	0.69
3:D:493:ARG:HG3	3:D:1390:LEU:HD11	1.73	0.69
3:D:1100:ASP:CG	3:D:1440:PHE:HB2	2.12	0.69
3:D:1118:ILE:HD12	3:D:1192:LEU:HD12	1.73	0.69
2:M:107:LEU:HD12	2:M:108:ILE:CA	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:596:SER:O	3:N:597:ASP:CG	2.30	0.69
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.74	0.69
3:D:493:ARG:HG3	3:D:1390:LEU:CD1	2.23	0.69
3:N:71:LYS:NZ	3:N:74:GLU:OE2	2.21	0.69
3:N:1136:LYS:O	3:N:1140:ILE:HG13	1.92	0.69
3:D:1044:LEU:H	3:D:1044:LEU:HD12	1.58	0.69
3:D:1310:ARG:HD2	3:D:1327:ARG:HB2	1.75	0.69
2:C:628:PHE:H	2:C:638:ASP:CB	2.05	0.69
1:L:88:ARG:HB3	1:L:121:GLU:HB2	1.75	0.68
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.26	0.68
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.75	0.68
2:M:238:LEU:HD12	2:M:238:LEU:O	1.92	0.68
3:N:108:VAL:HB	3:N:109:PRO:HD3	1.75	0.68
3:N:1282:ARG:HH11	3:N:1282:ARG:CG	2.05	0.68
3:N:1282:ARG:HD3	3:N:1295:GLU:OE2	1.92	0.68
2:M:200:LEU:HD13	2:M:300:ASP:HB2	1.75	0.68
2:M:787:ASP:OD2	2:M:791:ARG:NH2	2.27	0.68
2:M:1008:ARG:HH11	2:M:1028:GLY:HA2	1.57	0.68
5:F:231:ARG:O	5:F:232:ARG:CG	2.41	0.68
2:M:262:ALA:HA	2:M:291:ALA:O	1.93	0.68
2:M:302:VAL:O	2:M:306:THR:HG23	1.93	0.68
3:N:963:TYR:CE2	3:N:1002:LYS:HD3	2.28	0.68
2:C:229:MET:HE1	2:C:234:ALA:HA	1.75	0.68
2:C:262:ALA:HA	2:C:289:THR:HG21	1.76	0.68
3:D:823:LEU:HD11	3:D:837:GLY:HA2	1.75	0.68
2:M:286:SER:OG	2:M:301:GLU:OE2	2.10	0.68
3:N:675:ARG:HH12	5:P:420:ASP:HB3	1.59	0.68
2:C:261:ILE:HG23	2:C:290:LEU:HB2	1.74	0.68
3:D:864:VAL:CG1	3:D:865:THR:N	2.57	0.68
3:D:1395:LEU:HD11	3:D:1400:VAL:HB	1.74	0.68
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.26	0.68
2:C:229:MET:HB3	2:C:233:GLU:HB3	1.75	0.68
3:D:1336:LEU:HD13	3:D:1344:VAL:HG21	1.75	0.68
2:M:230:ARG:CG	2:M:231:PRO:HD2	2.23	0.68
1:B:64:GLU:O	1:B:75:VAL:HB	1.94	0.68
3:D:1263:PHE:HD2	3:D:1375:MET:HE1	1.59	0.68
3:D:1311:LEU:N	3:D:1311:LEU:CD2	2.52	0.67
2:M:165:LEU:O	2:M:168:ARG:HB2	1.94	0.67
5:P:384:GLU:HB3	5:P:394:ARG:HD2	1.74	0.67
2:C:157:ARG:NH1	2:C:176:VAL:HG12	2.07	0.67
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:658:LEU:HA	3:D:661:MET:HE3	1.76	0.67
1:A:27:PRO:HB3	1:A:184:THR:HG21	1.76	0.67
5:P:368:VAL:HG12	5:P:390:PHE:CE1	2.30	0.67
2:C:859:PRO:O	2:C:867:VAL:HG22	1.95	0.67
5:F:80:PRO:HB2	5:F:210:LEU:HD11	1.76	0.67
2:M:261:ILE:HG23	2:M:290:LEU:HB2	1.76	0.67
2:C:786:LYS:NZ	2:C:786:LYS:CB	2.57	0.67
2:M:171:TRP:CE3	7:R:13:DT:H2"	2.30	0.67
2:M:758:ARG:HH21	2:M:788:THR:HB	1.60	0.67
3:N:219:GLU:N	3:N:339:TRP:CZ3	2.63	0.67
3:N:864:VAL:CG1	3:N:865:THR:N	2.58	0.67
5:P:364:ARG:O	5:P:368:VAL:HG13	1.95	0.67
2:M:262:ALA:HA	2:M:289:THR:HG21	1.77	0.67
2:M:853:LEU:HB2	2:M:858:MET:CE	2.25	0.67
3:N:1292:VAL:CG2	3:N:1305:LEU:HD11	2.25	0.67
3:D:46:ASP:OD1	3:D:47:GLU:N	2.28	0.66
3:N:892:ASP:OD1	3:N:894:LYS:HD3	1.95	0.66
3:D:142:LEU:HD13	3:D:161:LEU:HD11	1.77	0.66
1:K:57:TYR:CD1	1:K:161:ARG:HD2	2.30	0.66
5:P:127:ILE:O	5:P:131:VAL:HG23	1.95	0.66
2:C:229:MET:CE	2:C:234:ALA:HA	2.25	0.66
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.78	0.66
3:N:1237:THR:HG21	3:N:1246:VAL:HG22	1.76	0.66
1:L:5:LYS:HA	1:L:5:LYS:HE3	1.77	0.66
3:N:1468:LEU:HB3	3:N:1470:ARG:HG3	1.77	0.66
2:M:1058:ASP:OD1	3:N:621:LYS:HE2	1.95	0.66
3:N:988:ARG:NH2	3:N:1054:GLU:OE2	2.29	0.66
5:P:386:VAL:HG12	5:P:397:ILE:HG21	1.76	0.66
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.31	0.66
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.77	0.66
3:D:1482:ARG:HH21	3:D:1483:PHE:HZ	1.43	0.66
5:F:126:LEU:O	5:F:130:VAL:HG23	1.96	0.66
3:N:832:ARG:HH21	3:N:833:GLU:HG3	1.60	0.66
2:C:286:SER:OG	2:C:301:GLU:OE2	2.10	0.66
3:D:832:ARG:HH21	3:D:833:GLU:HG3	1.60	0.66
1:L:6:LEU:HD12	1:L:7:LYS:H	1.60	0.66
2:M:628:PHE:N	2:M:638:ASP:HB3	2.07	0.66
2:M:261:ILE:CG2	2:M:291:ALA:HB3	2.26	0.66
3:N:562:ALA:O	5:P:140:ARG:NH2	2.27	0.66
3:N:1310:ARG:CD	3:N:1327:ARG:HD2	2.25	0.66
5:P:78:SER:O	5:P:80:PRO:CD	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:421:LEU:HD11	3:N:429:SER:HB2	1.77	0.66
3:N:1277:ILE:HG22	3:N:1278:ASP:H	1.61	0.66
2:C:628:PHE:N	2:C:638:ASP:HB3	2.08	0.65
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.29	0.65
3:D:213:VAL:HG21	3:D:367:ILE:HD13	1.78	0.65
3:N:1311:LEU:H	3:N:1311:LEU:HD23	1.59	0.65
2:C:166:PRO:O	2:C:167:LYS:HB2	1.95	0.65
2:C:428:ARG:NH2	2:C:447:ALA:O	2.28	0.65
3:D:348:GLN:HB3	3:D:349:PRO:HD2	1.79	0.65
3:D:1304:LYS:CA	3:D:1305:LEU:HD23	2.27	0.65
2:M:229:MET:HE2	2:M:234:ALA:CA	2.26	0.65
3:N:142:LEU:HD13	3:N:161:LEU:HD11	1.78	0.65
2:M:425:PHE:CE2	3:N:1086:LEU:HD12	2.31	0.65
2:M:874:LEU:CD1	3:N:784:ASP:OD2	2.45	0.65
2:C:680:ASP:OD1	3:D:943:THR:HG21	1.96	0.65
3:D:47:GLU:HB3	3:D:78:VAL:CG2	2.26	0.65
3:D:530:VAL:HG12	5:F:333:ILE:HD12	1.79	0.65
2:M:229:MET:CE	2:M:234:ALA:N	2.48	0.65
2:M:915:LYS:NZ	3:N:952:ASP:OD2	2.29	0.65
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.29	0.65
2:C:1058:ASP:OD1	3:D:621:LYS:HE2	1.95	0.65
2:M:172:ILE:HG12	2:M:186:VAL:CG2	2.27	0.65
3:D:1100:ASP:OD1	3:D:1440:PHE:HB2	1.96	0.65
1:L:49:PRO:HA	1:L:148:VAL:HG12	1.78	0.65
3:D:1283:ILE:CG1	3:D:1315:ASP:CG	2.65	0.65
1:K:228:PRO:O	1:K:229:GLN:HG3	1.96	0.65
2:M:12:VAL:HG21	2:M:472:ARG:HD3	1.77	0.65
2:M:437:ARG:NH2	2:M:491:GLU:OE2	2.29	0.65
3:N:952:ASP:HA	3:N:1062:ARG:HH21	1.62	0.65
2:C:368:THR:H	2:C:371:LYS:HD2	1.62	0.65
3:D:890:VAL:CB	3:D:922:LEU:CD1	2.70	0.65
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.79	0.65
2:M:51:THR:O	2:M:265:ARG:NH2	2.29	0.65
3:D:1310:ARG:C	3:D:1311:LEU:CD2	2.63	0.64
2:M:36:PRO:HA	2:M:39:ARG:HG3	1.79	0.64
2:M:198:ARG:CZ	2:M:230:ARG:HA	2.27	0.64
4:O:52:GLU:OE1	4:O:52:GLU:N	2.27	0.64
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.63	0.64
3:D:1143:GLY:O	3:D:1147:ARG:HD2	1.96	0.64
3:N:1143:GLY:O	3:N:1147:ARG:HD2	1.97	0.64
5:P:382:THR:HG23	5:P:384:GLU:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:VAL:O	2:C:177:GLU:HB2	1.97	0.64
4:E:52:GLU:OE1	4:E:52:GLU:N	2.28	0.64
2:M:1103:ASP:HB3	2:M:1105:LYS:H	1.62	0.64
3:N:348:GLN:HB3	3:N:349:PRO:HD2	1.79	0.64
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.78	0.64
3:D:835:SER:OG	3:D:838:ARG:NE	2.30	0.64
5:F:88:ILE:HD11	5:F:192:LEU:HD13	1.79	0.64
2:M:368:THR:H	2:M:371:LYS:HD2	1.62	0.64
3:N:569:ASN:O	3:N:573:MET:HG3	1.98	0.64
3:N:1237:THR:O	3:N:1238:MET:C	2.34	0.64
2:C:232:GLU:OE2	2:C:232:GLU:N	2.30	0.64
1:L:56:VAL:HG22	1:L:142:VAL:HG12	1.78	0.64
2:M:462:ASP:HB3	2:M:468:ARG:HD2	1.79	0.64
5:P:205:ARG:CG	5:P:205:ARG:HH11	2.11	0.64
1:A:11:PHE:O	1:B:228:PRO:HA	1.96	0.64
2:C:198:ARG:HH11	2:C:230:ARG:HA	1.63	0.64
2:C:292:ARG:HG3	2:C:299:LYS:HB2	1.78	0.64
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.79	0.64
3:D:1486:VAL:CG2	4:E:22:VAL:HG13	2.28	0.64
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.78	0.64
3:N:808:THR:HG22	3:N:810:GLU:H	1.63	0.64
3:N:1252:ILE:HG23	3:N:1253:THR:HG23	1.79	0.64
3:D:17:LYS:O	3:D:20:SER:HB3	1.98	0.64
3:D:421:LEU:HD11	3:D:429:SER:HB2	1.79	0.64
3:D:711:LEU:HD13	3:D:778:LEU:CD1	2.27	0.64
1:K:11:PHE:O	1:L:228:PRO:HA	1.98	0.64
1:K:222:LEU:HD21	1:L:218:LEU:HD23	1.80	0.64
2:M:266:ARG:NH1	7:R:11:DG:O6	2.31	0.64
3:N:1315:ASP:OD2	3:N:1316:GLY:N	2.31	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.80	0.64
3:N:1309:ALA:O	3:N:1310:ARG:CB	2.46	0.64
5:P:78:SER:O	5:P:80:PRO:N	2.31	0.64
5:F:212:LEU:HD22	5:F:247:ILE:HG23	1.79	0.63
3:N:46:ASP:OD1	3:N:46:ASP:C	2.35	0.63
3:N:1486:VAL:CG2	4:O:22:VAL:HG13	2.26	0.63
3:N:1495:ILE:HD13	4:O:80:VAL:HG21	1.78	0.63
4:O:95:VAL:O	4:O:95:VAL:CG2	2.46	0.63
1:B:58:ILE:HG21	1:B:61:VAL:HG11	1.78	0.63
2:C:853:LEU:HB2	2:C:858:MET:CE	2.28	0.63
2:C:911:GLU:O	2:C:915:LYS:HG2	1.99	0.63
2:C:1103:ASP:HB3	2:C:1105:LYS:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:134:VAL:HG12	3:N:454:ALA:HB2	1.80	0.63
3:N:1326:THR:HG22	3:N:1327:ARG:H	1.62	0.63
3:D:1370:ILE:O	3:D:1373:ARG:HG2	1.99	0.63
2:C:356:ARG:HA	2:C:359:MET:HG3	1.81	0.63
3:N:639:LEU:HA	3:N:729:HIS:CD2	2.32	0.63
3:D:111:LYS:HG3	3:D:1452:ILE:HD11	1.81	0.63
1:L:162:ILE:O	1:L:163:ASN:CB	2.43	0.63
2:M:413:LEU:HD21	2:M:451:LEU:HD13	1.79	0.63
2:M:595:LEU:HD21	2:M:623:TYR:HB3	1.80	0.63
3:N:786:ILE:HG22	3:N:1026:SER:HB2	1.81	0.63
3:N:894:LYS:N	3:N:894:LYS:CD	2.54	0.63
3:D:1314:LYS:HG3	3:D:1317:ASP:CG	2.18	0.63
2:M:627:ARG:HA	2:M:638:ASP:HB2	1.80	0.63
3:N:711:LEU:HD13	3:N:778:LEU:CD1	2.29	0.63
2:C:230:ARG:CB	2:C:231:PRO:HD2	2.20	0.63
2:C:262:ALA:HA	2:C:289:THR:CG2	2.28	0.63
2:C:786:LYS:NZ	2:C:786:LYS:HB2	2.14	0.63
3:D:808:THR:HG22	3:D:810:GLU:H	1.63	0.63
3:N:56:TYR:HB3	3:N:65:ARG:O	1.98	0.63
3:N:137:PRO:HB3	3:N:147:VAL:HG12	1.81	0.63
2:C:154:ARG:NH1	2:C:154:ARG:CG	2.45	0.63
1:L:56:VAL:HG21	1:L:82:LEU:HD13	1.80	0.63
3:N:996:TRP:CD2	3:N:1056:PRO:HG3	2.33	0.63
2:M:168:ARG:HG3	2:M:168:ARG:NH1	2.14	0.63
2:M:911:GLU:O	2:M:915:LYS:HG2	1.99	0.63
1:A:228:PRO:O	1:A:229:GLN:HG3	1.98	0.62
2:C:503:LEU:CD2	2:C:508:ILE:HD13	2.28	0.62
2:C:773:LEU:O	2:C:777:ILE:HG13	1.99	0.62
3:D:1283:ILE:HG13	3:D:1315:ASP:OD2	1.99	0.62
5:P:78:SER:O	5:P:80:PRO:HD3	1.99	0.62
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.80	0.62
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.33	0.62
2:M:232:GLU:OE2	2:M:232:GLU:N	2.30	0.62
2:M:262:ALA:HA	2:M:289:THR:CG2	2.28	0.62
2:M:874:LEU:O	11:M:1229:HOH:O	2.16	0.62
3:N:493:ARG:HG3	3:N:1390:LEU:CD1	2.29	0.62
4:O:45:ARG:NH1	4:O:56:ASP:OD2	2.32	0.62
5:P:392:VAL:HG21	5:P:397:ILE:HD13	1.80	0.62
3:N:32:ILE:HG12	5:P:258:ILE:HD13	1.74	0.62
3:N:1205:TYR:CE1	3:N:1366:LYS:HD3	2.35	0.62
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1236:LEU:HA	3:D:1359:GLN:HG2	1.81	0.62
3:N:493:ARG:HG3	3:N:1390:LEU:HD11	1.82	0.62
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.81	0.62
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.80	0.62
3:D:1122:LEU:HD12	3:D:1185:GLU:HA	1.80	0.62
3:D:1310:ARG:CA	3:D:1311:LEU:HD23	2.29	0.62
2:C:179:ASN:OD1	2:C:181:VAL:N	2.23	0.62
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.34	0.62
1:K:216:GLU:OE2	1:K:219:ARG:NH2	2.32	0.62
2:M:356:ARG:HA	2:M:359:MET:HG3	1.82	0.62
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.81	0.62
2:C:108:ILE:C	2:C:108:ILE:CD1	2.57	0.62
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.81	0.62
3:D:569:ASN:O	3:D:573:MET:HG3	2.00	0.62
3:D:657:LEU:HG	3:D:661:MET:HE2	1.81	0.62
2:M:171:TRP:CZ3	7:R:14:DG:OP1	2.53	0.62
5:P:96:LEU:O	5:P:100:VAL:HG23	2.00	0.62
1:A:176:ARG:NH1	2:C:863:ASP:O	2.32	0.62
3:D:541:ASN:O	3:D:545:ARG:HG3	2.00	0.62
3:D:786:ILE:HG22	3:D:1026:SER:HB2	1.82	0.62
3:N:276:ASP:C	3:N:277:GLU:OE1	2.38	0.62
3:N:675:ARG:HH12	5:P:420:ASP:CB	2.13	0.62
2:C:136:ILE:HB	2:C:336:VAL:HG12	1.81	0.62
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.14	0.62
2:C:957:LYS:HG2	2:C:961:GLU:OE1	1.99	0.62
3:D:890:VAL:CB	3:D:922:LEU:HD12	2.26	0.62
2:M:874:LEU:HD21	3:N:787:LEU:HD22	1.80	0.62
3:N:237:LYS:O	3:N:240:GLU:HB3	2.00	0.62
1:B:63:HIS:ND1	1:B:66:SER:OG	2.31	0.61
3:D:137:PRO:HB3	3:D:147:VAL:HG12	1.82	0.61
1:L:176:ARG:NH2	3:N:888:GLU:OE1	2.33	0.61
2:M:168:ARG:NH2	2:M:265:ARG:O	2.33	0.61
3:N:657:LEU:HG	3:N:661:MET:HE2	1.80	0.61
5:F:152:ASP:HB2	5:F:153:PRO:HD2	1.81	0.61
2:M:168:ARG:HG3	2:M:168:ARG:HH11	1.64	0.61
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.83	0.61
3:D:67:ARG:CB	3:D:67:ARG:CZ	2.76	0.61
5:F:120:THR:HG22	5:F:122:LEU:HD13	1.82	0.61
1:L:213:GLN:O	1:L:217:ILE:HG13	1.99	0.61
2:M:1006:HIS:HB2	2:M:1024:LYS:HG3	1.82	0.61
3:N:592:THR:OG1	3:N:596:SER:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:717:LEU:CD2	2:M:763:GLY:HA3	2.31	0.61
2:M:1102:LEU:HD23	2:M:1108:PRO:HA	1.82	0.61
3:N:371:ILE:HD12	5:P:230:LYS:HA	1.81	0.61
3:N:1274:ILE:HG22	3:N:1324:PRO:HA	1.81	0.61
3:N:1400:VAL:HG21	3:N:1417:TRP:CD1	2.36	0.61
1:A:184:THR:CG2	1:A:192:LEU:HB3	2.29	0.61
3:D:274:ARG:NH1	3:D:274:ARG:CG	2.48	0.61
2:M:261:ILE:HG21	2:M:291:ALA:HB3	1.83	0.61
2:M:716:LYS:HE3	3:N:35:ARG:O	2.01	0.61
3:N:1311:LEU:HB2	3:N:1325:LEU:O	2.01	0.61
2:C:1090:LYS:HE2	3:D:88:TYR:O	1.99	0.61
3:N:658:LEU:HD23	3:N:661:MET:HE1	1.81	0.61
5:P:361:LEU:HD13	5:P:365:GLU:HB2	1.81	0.61
2:M:198:ARG:HH11	2:M:230:ARG:HA	1.64	0.61
2:M:198:ARG:NH1	2:M:230:ARG:HA	2.15	0.61
2:M:418:LEU:CD1	2:M:427:VAL:HG11	2.31	0.61
2:M:503:LEU:HD21	2:M:508:ILE:HD13	1.83	0.61
3:N:541:ASN:O	3:N:545:ARG:HG3	2.01	0.61
3:N:1101:VAL:HG21	3:N:1424:VAL:HB	1.82	0.61
1:A:10:VAL:HG22	1:A:26:GLU:O	2.00	0.61
2:C:15:LEU:O	2:C:586:ARG:NH2	2.28	0.61
3:D:1410:GLU:O	3:D:1410:GLU:HG2	1.99	0.61
2:M:173:ASP:C	2:M:174:LEU:HD12	2.20	0.61
3:N:373:PRO:O	3:N:376:GLU:HG2	2.00	0.61
3:N:1097:LYS:O	3:N:1101:VAL:HG23	2.01	0.61
3:N:1290:LEU:HD21	3:N:1307:LYS:HE2	1.81	0.61
1:A:57:TYR:CE1	1:A:161:ARG:CD	2.84	0.61
3:D:321:GLN:HB2	3:D:336:PHE:CD2	2.36	0.61
5:F:362:SER:OG	5:F:365:GLU:HG2	2.01	0.61
3:N:473:LEU:HD21	3:N:495:ARG:HH21	1.65	0.61
3:D:321:GLN:HB2	3:D:336:PHE:HD2	1.66	0.60
3:D:473:LEU:HD21	3:D:495:ARG:HH21	1.66	0.60
3:D:963:TYR:HE2	3:D:1002:LYS:HD3	1.66	0.60
3:D:1283:ILE:CD1	3:D:1283:ILE:N	2.30	0.60
2:M:136:ILE:HB	2:M:336:VAL:HG12	1.83	0.60
2:M:480:THR:HG22	2:M:482:GLU:H	1.66	0.60
2:M:957:LYS:HG2	2:M:961:GLU:OE1	2.01	0.60
5:P:205:ARG:NH1	5:P:205:ARG:HG2	2.16	0.60
3:D:33:ASN:O	3:D:37:LEU:HA	2.01	0.60
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.36	0.60
3:N:783:ARG:NH1	3:N:1028:ALA:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.81	0.60
1:B:213:GLN:O	1:B:217:ILE:HG13	2.01	0.60
2:C:383:ARG:O	2:C:387:SER:HB2	2.01	0.60
2:C:480:THR:HG22	2:C:482:GLU:H	1.66	0.60
2:C:595:LEU:HD21	2:C:623:TYR:HB3	1.82	0.60
3:N:355:VAL:HG11	3:N:385:VAL:HG21	1.84	0.60
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.83	0.60
2:M:802:ARG:HB2	2:M:826:TYR:HB2	1.82	0.60
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.82	0.60
2:C:988:VAL:HG21	3:D:949:ILE:O	2.01	0.60
3:N:596:SER:C	3:N:597:ASP:CG	2.60	0.60
2:C:802:ARG:HB2	2:C:826:TYR:HB2	1.81	0.60
3:D:893:GLU:N	3:D:894:LYS:HE2	2.16	0.60
3:N:15:PRO:O	3:N:19:ARG:HG3	2.02	0.60
3:N:586:ARG:HH12	6:Q:10:DG:H5”	1.67	0.60
5:P:329:TYR:CE2	5:P:333:ILE:HD11	2.37	0.60
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.37	0.60
3:D:1309:ALA:O	3:D:1310:ARG:CB	2.46	0.60
6:G:15:DT:H2’	6:G:16:DC:C6	2.37	0.60
2:M:626:ARG:HG3	2:M:629:TYR:CD1	2.37	0.60
3:N:90:MET:HG2	3:N:521:PRO:HD3	1.82	0.60
1:A:184:THR:O	1:A:192:LEU:HB2	2.02	0.60
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.35	0.60
2:M:569:VAL:HG21	2:M:1000:MET:CE	2.32	0.60
2:C:177:GLU:OE2	2:C:183:SER:CB	2.48	0.60
2:C:626:ARG:HG3	2:C:629:TYR:CD1	2.37	0.60
3:D:132:TYR:HB2	3:D:153:LEU:HD12	1.83	0.60
3:D:1490:LYS:HD2	4:E:93:TYR:OH	2.01	0.60
3:N:67:ARG:HH11	3:N:67:ARG:HG3	1.67	0.60
1:A:206:THR:HG23	1:A:207:PRO:HD2	1.84	0.60
1:A:219:ARG:HG3	1:A:220:GLU:N	2.17	0.60
2:C:669:GLY:H	2:C:993:PHE:HZ	1.47	0.59
3:D:1263:PHE:O	3:D:1375:MET:HE2	2.03	0.59
2:M:172:ILE:HG23	2:M:184:MET:HG2	1.83	0.59
2:M:773:LEU:HD22	5:P:375:LEU:HD12	1.84	0.59
2:C:976:ASP:OD1	2:C:978:ARG:HD3	2.02	0.59
3:D:32:ILE:HD13	3:D:39:PRO:HA	1.83	0.59
3:D:693:GLU:HA	4:E:48:MET:CE	2.32	0.59
3:D:1087:ARG:NH1	3:D:1234:THR:O	2.35	0.59
3:N:127:LEU:HA	3:N:457:GLY:HA2	1.84	0.59
3:N:131:LYS:O	3:N:456:MET:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:412:GLY:H	3:N:435:VAL:HG12	1.66	0.59
3:N:618:LEU:HG	3:N:1467:ILE:HG23	1.84	0.59
1:K:206:THR:HG23	1:K:207:PRO:HD2	1.83	0.59
1:K:219:ARG:HG3	1:K:220:GLU:N	2.17	0.59
3:N:132:TYR:HB2	3:N:153:LEU:HD12	1.83	0.59
3:N:181:ASP:HB2	3:N:205:TYR:CD1	2.37	0.59
3:D:844:ALA:O	3:D:867:ARG:HB3	2.02	0.59
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.37	0.59
3:N:14:SER:HB3	3:N:511:TRP:CE2	2.38	0.59
3:N:774:SER:HB3	3:N:1362:LYS:O	2.03	0.59
3:N:1010:ASN:OD1	3:N:1014:ASN:ND2	2.36	0.59
1:A:70:GLY:N	2:C:607:ASP:OD1	2.36	0.59
2:C:189:ARG:HH12	2:C:244:PRO:HD3	1.67	0.59
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.85	0.59
3:D:1285:GLU:OE1	3:D:1307:LYS:NZ	2.36	0.59
2:M:154:ARG:CG	2:M:154:ARG:NH1	2.45	0.59
3:N:603:LEU:HA	3:N:606:ILE:HD12	1.84	0.59
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.84	0.59
2:C:151:ASP:CB	2:C:157:ARG:O	2.50	0.59
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.85	0.59
3:D:603:LEU:HA	3:D:606:ILE:HD12	1.84	0.59
2:M:15:LEU:O	2:M:586:ARG:NH2	2.29	0.59
5:P:194:LEU:O	5:P:198:ILE:HG13	2.02	0.59
3:D:1435:LEU:O	3:D:1439:SER:OG	2.13	0.59
1:K:206:THR:HG22	1:K:208:LEU:H	1.67	0.59
3:N:845:ASN:HB2	3:N:846:PRO:HD2	1.85	0.59
3:N:1189:ARG:HB3	3:N:1204:CYS:HA	1.84	0.59
3:N:1205:TYR:CZ	3:N:1366:LYS:HD3	2.38	0.59
2:C:157:ARG:HD3	2:C:157:ARG:N	2.18	0.59
3:D:67:ARG:NH1	5:F:379:ARG:HB2	2.18	0.59
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.85	0.59
3:D:388:HIS:O	3:D:390:PRO:HD3	2.02	0.59
3:D:580:ALA:O	3:D:584:ASN:HB2	2.03	0.59
3:D:1478:SER:O	3:D:1482:ARG:HB2	2.03	0.59
5:F:230:LYS:O	5:F:232:ARG:HG3	2.02	0.59
1:L:115:LEU:O	1:L:117:VAL:HG23	2.02	0.59
3:N:844:ALA:O	3:N:867:ARG:HB3	2.03	0.59
3:N:963:TYR:HE2	3:N:1002:LYS:HD3	1.68	0.59
1:A:9:PRO:HD2	1:B:224:TYR:CD2	2.38	0.59
1:B:115:LEU:O	1:B:117:VAL:HG23	2.02	0.59
2:C:134:ARG:NH1	2:C:392:SER:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:482:GLU:HG3	2:C:482:GLU:O	2.01	0.59
3:D:1101:VAL:HG21	3:D:1424:VAL:HB	1.85	0.59
3:D:1439:SER:HB2	3:D:1463:LYS:HZ3	1.67	0.59
2:M:383:ARG:O	2:M:387:SER:HB2	2.03	0.59
2:M:482:GLU:HG3	2:M:482:GLU:O	2.03	0.59
2:M:976:ASP:OD1	2:M:978:ARG:HD3	2.01	0.59
3:N:171:LEU:HD22	3:N:390:PRO:HG2	1.85	0.59
3:N:202:VAL:HG21	3:N:400:VAL:HG13	1.83	0.59
6:Q:15:DT:H2'	6:Q:16:DC:C6	2.38	0.59
2:C:102:HIS:CB	2:C:105:THR:CG2	2.78	0.58
2:C:420:ARG:NH2	2:C:448:ASN:OD1	2.33	0.58
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.36	0.58
3:D:876:SER:OG	3:D:879:ARG:HG3	2.02	0.58
1:K:10:VAL:HG22	1:K:26:GLU:O	2.03	0.58
2:M:858:MET:HG3	2:M:867:VAL:HG23	1.85	0.58
3:N:260:GLU:OE1	3:N:273:ARG:CZ	2.51	0.58
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.38	0.58
2:C:105:THR:O	2:C:105:THR:HG23	2.03	0.58
2:C:157:ARG:HH11	2:C:157:ARG:CG	2.15	0.58
2:M:936:VAL:HG11	2:M:959:PRO:HB2	1.85	0.58
3:N:1286:THR:HG22	3:N:1288:GLU:H	1.68	0.58
4:O:50:THR:HG22	4:O:51:LEU:H	1.67	0.58
1:A:97:VAL:HG12	1:A:99:LEU:HD12	1.86	0.58
3:D:56:TYR:HB3	3:D:65:ARG:O	2.01	0.58
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.84	0.58
3:N:1047:LYS:HG2	3:N:1053:PHE:CZ	2.38	0.58
2:C:487:THR:HG23	2:C:490:GLU:H	1.68	0.58
3:D:33:ASN:HB3	3:D:36:THR:HG23	1.84	0.58
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.44	0.58
2:M:302:VAL:O	2:M:305:PRO:HD2	2.03	0.58
3:N:1384:PRO:HB3	3:N:1389:LEU:O	2.04	0.58
5:P:382:THR:CG2	5:P:384:GLU:HG2	2.33	0.58
2:C:198:ARG:NH1	2:C:230:ARG:HA	2.17	0.58
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.36	0.58
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.39	0.58
5:F:187:LEU:HD23	5:F:224:VAL:HG13	1.84	0.58
2:M:167:LYS:O	2:M:168:ARG:CD	2.44	0.58
2:M:772:ARG:HH22	5:P:380:GLU:HB3	1.69	0.58
3:N:658:LEU:HD23	3:N:661:MET:CE	2.33	0.58
5:P:228:GLU:OE2	5:P:231:ARG:NE	2.37	0.58
5:P:394:ARG:HG2	5:P:395:GLU:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:O	1:A:215:VAL:HG23	2.03	0.58
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.02	0.58
1:K:30:ARG:CD	1:K:191:ASP:OD1	2.51	0.58
1:K:97:VAL:HG12	1:K:99:LEU:HD12	1.86	0.58
1:L:80:LEU:HB3	3:N:867:ARG:NH2	2.18	0.58
3:N:37:LEU:HD13	3:N:535:PHE:CZ	2.39	0.58
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.69	0.58
1:L:94:LEU:HD11	1:L:96:THR:O	2.03	0.58
3:N:149:LYS:O	3:N:150:ARG:HB2	2.03	0.58
3:N:233:LYS:HD2	3:N:240:GLU:OE2	2.03	0.58
3:N:437:VAL:HG11	5:P:175:HIS:CD2	2.39	0.58
2:M:235:LEU:CD1	2:M:257:VAL:HG21	2.34	0.58
2:M:1090:LYS:HE2	3:N:88:TYR:O	2.04	0.58
3:N:317:VAL:HG23	3:N:339:TRP:HB3	1.86	0.58
2:C:714:ASP:OD2	2:C:808:ARG:NH1	2.31	0.58
3:N:876:SER:OG	3:N:879:ARG:HG3	2.02	0.58
2:C:786:LYS:HB2	2:C:786:LYS:HZ2	1.69	0.58
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.38	0.58
3:D:264:LEU:HD12	3:D:264:LEU:O	2.04	0.57
3:D:490:ALA:O	3:D:494:LYS:HG3	2.04	0.57
2:M:420:ARG:NH2	2:M:448:ASN:OD1	2.36	0.57
3:D:433:GLY:HA3	3:D:446:VAL:CG1	2.33	0.57
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.87	0.57
5:F:202:TYR:HE2	5:F:248:ASN:OD1	1.87	0.57
3:N:36:THR:O	3:N:37:LEU:HB2	2.03	0.57
3:N:835:SER:HB3	3:N:838:ARG:HG2	1.85	0.57
3:N:1194:CYS:O	3:N:1373:ARG:NH2	2.37	0.57
3:N:1258:ARG:HH21	3:N:1351:GLU:CG	2.17	0.57
1:B:76:VAL:O	1:B:79:ILE:HG12	2.04	0.57
2:C:327:HIS:CD2	2:C:433:THR:HG21	2.39	0.57
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.86	0.57
3:D:1274:ILE:HG22	3:D:1324:PRO:HA	1.85	0.57
2:M:114:PHE:CD2	5:P:283:GLY:HA2	2.39	0.57
2:M:157:ARG:HD3	2:M:157:ARG:N	2.17	0.57
3:N:259:VAL:HG13	3:N:270:LEU:HD11	1.85	0.57
3:N:276:ASP:O	3:N:277:GLU:OE1	2.22	0.57
5:P:376:ILE:HD12	5:P:377:ASP:HB3	1.86	0.57
3:D:890:VAL:HB	3:D:922:LEU:HD11	1.82	0.57
2:M:127:PHE:O	2:M:133:ASP:HA	2.03	0.57
2:M:146:VAL:HG22	2:M:162:ILE:HG12	1.86	0.57
2:M:179:ASN:OD1	2:M:179:ASN:C	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ALA:O	1:A:114:PHE:HD1	1.87	0.57
1:A:206:THR:HG22	1:A:208:LEU:H	1.70	0.57
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.85	0.57
5:F:202:TYR:O	5:F:205:ARG:HD3	2.04	0.57
2:M:151:ASP:CB	2:M:157:ARG:O	2.50	0.57
3:N:558:LEU:HD13	5:P:142:ARG:HD2	1.86	0.57
3:N:1277:ILE:HG22	3:N:1278:ASP:N	2.19	0.57
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.86	0.57
2:C:327:HIS:NE2	2:C:433:THR:HG21	2.19	0.57
3:D:808:THR:HB	3:D:811:GLU:HG3	1.87	0.57
4:E:50:THR:HG22	4:E:51:LEU:H	1.68	0.57
2:M:157:ARG:HG3	2:M:176:VAL:CG1	2.35	0.57
2:M:690:ILE:HB	2:M:852:ILE:HD13	1.86	0.57
2:M:983:ILE:HG21	2:M:987:ILE:HD11	1.86	0.57
5:P:256:ARG:NH2	5:P:311:ALA:O	2.37	0.57
1:A:57:TYR:CD1	1:A:161:ARG:CD	2.80	0.57
2:C:617:ASP:N	2:C:617:ASP:OD1	2.37	0.57
2:M:182:VAL:HG23	2:M:193:LEU:HB2	1.86	0.57
3:N:388:HIS:O	3:N:390:PRO:HD3	2.04	0.57
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.40	0.57
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.85	0.57
2:M:238:LEU:HD11	2:M:242:LEU:HD23	1.86	0.57
5:P:397:ILE:O	5:P:400:ILE:HG22	2.05	0.57
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.04	0.57
1:K:211:LEU:O	1:K:215:VAL:HG23	2.05	0.57
1:L:76:VAL:O	1:L:79:ILE:HG12	2.05	0.57
2:M:150:PRO:HD3	2:M:322:VAL:CG1	2.35	0.57
3:N:103:TRP:CE2	3:N:1444:THR:HG22	2.40	0.57
3:N:1282:ARG:HH11	3:N:1282:ARG:HG3	1.67	0.57
2:C:171:TRP:CZ3	7:H:13:DT:H2"	2.40	0.57
2:C:174:LEU:HD11	2:C:184:MET:HG3	1.86	0.57
3:D:1010:ASN:OD1	3:D:1014:ASN:ND2	2.37	0.57
5:F:287:THR:O	5:F:291:ILE:HG13	2.05	0.57
3:N:47:GLU:CD	3:N:53:ILE:HG12	2.26	0.57
3:N:563:PRO:HB3	5:P:189:GLU:HG3	1.86	0.57
3:D:784:ASP:HB2	3:D:939:PHE:CE2	2.40	0.56
3:D:1264:GLU:OE1	3:D:1264:GLU:HA	2.05	0.56
3:N:808:THR:HB	3:N:811:GLU:HG3	1.87	0.56
5:P:222:ARG:HD2	5:P:222:ARG:N	2.18	0.56
2:C:157:ARG:HH11	2:C:176:VAL:HG11	1.52	0.56
3:D:15:PRO:O	3:D:19:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:58:ILE:HB	1:L:61:VAL:HB	1.87	0.56
2:M:150:PRO:HD3	2:M:322:VAL:HG13	1.87	0.56
2:M:617:ASP:N	2:M:617:ASP:OD1	2.37	0.56
1:A:30:ARG:HD3	1:A:191:ASP:OD2	2.06	0.56
2:C:302:VAL:O	2:C:305:PRO:HD2	2.06	0.56
2:C:363:SER:O	2:C:367:LEU:HD21	2.04	0.56
3:D:1231:GLU:N	3:D:1232:PRO:HD2	2.21	0.56
1:K:111:ALA:O	1:K:114:PHE:HD1	1.89	0.56
3:N:1276:GLU:OE2	3:N:1301:LYS:HE3	2.04	0.56
5:P:383:LEU:HD12	5:P:398:ARG:HD2	1.87	0.56
2:C:861:LEU:HD23	2:C:974:LEU:CD1	2.35	0.56
3:N:273:ARG:HG3	3:N:278:PRO:HA	1.87	0.56
3:N:1237:THR:CG2	3:N:1238:MET:H	2.09	0.56
3:N:1290:LEU:HG	3:N:1307:LYS:CD	2.35	0.56
3:N:1439:SER:HB2	3:N:1463:LYS:NZ	2.20	0.56
5:P:409:LYS:C	5:P:409:LYS:HD3	2.25	0.56
2:M:105:THR:HG22	2:M:107:LEU:HB3	1.79	0.56
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.39	0.56
5:F:377:ASP:OD1	5:F:379:ARG:N	2.38	0.56
3:N:207:PHE:CZ	5:P:101:GLU:OE2	2.59	0.56
2:C:690:ILE:CD1	2:C:869:VAL:HG22	2.36	0.56
2:C:758:ARG:HH21	2:C:788:THR:HB	1.70	0.56
3:D:127:LEU:HA	3:D:457:GLY:HA2	1.87	0.56
3:D:128:TYR:CZ	3:D:587:ARG:CD	2.88	0.56
2:M:176:VAL:HG12	2:M:177:GLU:N	2.21	0.56
3:N:16:GLU:OE2	3:N:16:GLU:N	2.26	0.56
3:N:835:SER:O	3:N:838:ARG:HG3	2.06	0.56
2:M:524:VAL:CG1	2:M:528:GLU:HB2	2.35	0.56
3:N:573:MET:HE1	5:P:214:GLN:HG3	1.88	0.56
3:N:1311:LEU:CB	3:N:1325:LEU:O	2.54	0.56
5:P:358:LEU:O	5:P:366:ALA:HB2	2.05	0.56
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.06	0.56
2:M:118:ILE:HD11	2:M:344:PHE:CE2	2.40	0.56
2:M:230:ARG:HG3	2:M:231:PRO:HD2	1.88	0.56
2:M:56:GLU:HG2	2:M:359:MET:HE3	1.88	0.56
2:M:1110:ASP:OD2	2:M:1114:GLY:N	2.34	0.56
1:A:220:GLU:O	1:A:223:THR:HB	2.07	0.55
2:C:118:ILE:HD11	2:C:344:PHE:CE2	2.40	0.55
2:C:717:LEU:CD2	2:C:763:GLY:HA2	2.35	0.55
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.42	0.55
3:D:939:PHE:O	3:D:942:SER:OG	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1263:PHE:HD2	3:D:1375:MET:CE	2.17	0.55
1:K:70:GLY:N	2:M:607:ASP:OD1	2.38	0.55
2:M:154:ARG:NH2	2:M:178:PRO:N	2.53	0.55
2:M:157:ARG:HH11	2:M:157:ARG:CG	2.15	0.55
3:N:1263:PHE:HD2	3:N:1375:MET:HE1	1.71	0.55
5:P:153:PRO:HA	5:P:156:VAL:HG22	1.88	0.55
3:D:1258:ARG:HH21	3:D:1351:GLU:CG	2.19	0.55
5:F:354:LEU:O	5:F:358:LEU:HG	2.06	0.55
1:K:25:LEU:HD11	1:L:224:TYR:O	2.07	0.55
3:N:478:LEU:O	3:N:481:MET:HB2	2.06	0.55
1:A:30:ARG:HD3	1:A:191:ASP:CG	2.26	0.55
2:C:164:PRO:HA	2:C:269:LEU:HD12	1.88	0.55
2:C:858:MET:HG3	2:C:867:VAL:HG23	1.88	0.55
1:L:4:SER:O	1:L:189:ARG:NH1	2.39	0.55
2:M:637:LEU:HD23	2:M:659:PRO:HG2	1.88	0.55
3:N:835:SER:CB	3:N:838:ARG:CG	2.82	0.55
5:P:144:ILE:HB	5:P:147:LEU:HB2	1.88	0.55
1:B:102:LYS:HA	1:B:138:LEU:O	2.06	0.55
5:F:259:ARG:HG2	5:F:259:ARG:HH11	1.72	0.55
1:L:102:LYS:HA	1:L:138:LEU:O	2.07	0.55
2:M:157:ARG:HG3	2:M:176:VAL:HG12	1.88	0.55
3:N:553:ARG:HD2	3:N:570:GLU:OE2	2.06	0.55
3:N:1380:GLU:HB2	3:N:1420:LEU:HD22	1.88	0.55
2:C:524:VAL:CG1	2:C:528:GLU:HB2	2.36	0.55
2:C:858:MET:HG2	2:C:867:VAL:O	2.06	0.55
3:D:16:GLU:OE2	3:D:16:GLU:N	2.34	0.55
2:M:224:GLU:OE2	2:M:224:GLU:N	2.30	0.55
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.47	0.55
3:D:274:ARG:HH22	3:D:279:VAL:HG21	1.70	0.55
3:D:372:ASP:OD1	3:D:372:ASP:N	2.40	0.55
2:M:598:GLU:O	2:M:651:LYS:HG3	2.06	0.55
2:C:151:ASP:OD1	2:C:153:ALA:N	2.39	0.55
3:D:149:LYS:O	3:D:150:ARG:HB2	2.05	0.55
3:D:1331:ASP:C	3:D:1331:ASP:OD1	2.45	0.55
1:K:39:PRO:CG	1:L:39:PRO:HG3	2.36	0.55
2:M:141:HIS:CE1	2:M:334:ARG:HD2	2.42	0.55
2:M:1097:LEU:HD11	3:N:103:TRP:HZ3	1.72	0.55
5:P:364:ARG:NH1	5:P:392:VAL:HG11	2.22	0.55
3:N:32:ILE:O	5:P:258:ILE:HG23	2.07	0.55
3:N:56:TYR:CE1	3:N:69:GLU:HG3	2.38	0.55
3:N:1100:ASP:CG	3:N:1440:PHE:HB2	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1237:THR:CG2	3:N:1238:MET:N	2.57	0.55
3:N:1264:GLU:OE1	3:N:1264:GLU:HA	2.07	0.55
5:P:364:ARG:HH12	5:P:392:VAL:HG11	1.72	0.55
2:C:325:ILE:H	2:C:330:ASN:HD22	1.55	0.55
2:C:593:ALA:HB1	2:C:659:PRO:HD2	1.89	0.55
2:C:719:PRO:HB3	2:C:820:ARG:CZ	2.36	0.55
3:D:696:HIS:CD2	4:E:57:ASP:OD1	2.60	0.55
3:D:1312:LEU:CD2	3:D:1327:ARG:HG3	2.30	0.55
1:L:211:LEU:O	1:L:215:VAL:HG13	2.07	0.55
2:M:680:ASP:OD2	2:M:978:ARG:NH2	2.39	0.55
2:M:922:PHE:CE2	2:M:964:LYS:HB2	2.42	0.55
3:N:685:ASP:HA	3:N:688:TRP:HD1	1.72	0.55
3:N:1156:LEU:HD23	3:N:1182:GLU:OE2	2.07	0.55
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.40	0.55
5:P:125:ASP:N	5:P:125:ASP:OD1	2.40	0.55
1:B:18:ARG:O	1:B:207:PRO:HD3	2.07	0.54
1:B:211:LEU:O	1:B:215:VAL:HG13	2.06	0.54
2:C:35:PRO:CG	2:C:38:LYS:HD2	2.36	0.54
3:D:56:TYR:HE1	3:D:69:GLU:HG3	1.71	0.54
3:N:227:LEU:O	3:N:227:LEU:HD23	2.07	0.54
3:N:1410:GLU:HG2	3:N:1410:GLU:O	2.06	0.54
5:P:299:TRP:CE3	5:P:303:ARG:HD3	2.41	0.54
5:P:358:LEU:HD23	5:P:370:LYS:HE2	1.88	0.54
3:D:241:ILE:HA	3:D:312:ARG:HB3	1.89	0.54
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.07	0.54
3:N:771:SER:O	3:N:775:GLY:HA2	2.07	0.54
2:C:164:PRO:CD	2:C:171:TRP:HD1	2.16	0.54
2:M:151:ASP:OD1	2:M:153:ALA:N	2.39	0.54
2:M:236:ILE:HD12	2:M:248:PRO:HB3	1.90	0.54
3:N:1292:VAL:HG21	3:N:1305:LEU:HD11	1.88	0.54
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.42	0.54
3:D:478:LEU:O	3:D:481:MET:HB2	2.07	0.54
3:D:658:LEU:HD23	3:D:661:MET:CE	2.37	0.54
1:K:133:GLU:HG2	1:K:134:GLU:N	2.22	0.54
1:L:92:PRO:O	1:L:146:ARG:NH1	2.35	0.54
2:M:174:LEU:CD1	2:M:174:LEU:N	2.70	0.54
3:N:274:ARG:O	3:N:275:GLU:HB2	2.06	0.54
2:C:176:VAL:O	2:C:177:GLU:CB	2.56	0.54
3:D:478:LEU:O	3:D:481:MET:N	2.41	0.54
3:D:536:ALA:HA	5:F:315:VAL:O	2.08	0.54
2:M:324:ASP:HB3	2:M:327:HIS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1482:ARG:HH21	3:N:1483:PHE:HZ	1.55	0.54
5:P:382:THR:HG23	5:P:384:GLU:HG2	1.89	0.54
5:P:383:LEU:H	5:P:383:LEU:CD2	2.17	0.54
1:K:220:GLU:O	1:K:223:THR:HB	2.08	0.54
2:M:988:VAL:HG21	3:N:949:ILE:O	2.08	0.54
3:N:143:ASN:OD1	3:N:144:GLY:N	2.40	0.54
3:N:800:LYS:HB3	3:N:822:ALA:HB2	1.90	0.54
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.89	0.54
1:K:184:THR:O	1:K:192:LEU:HB2	2.08	0.54
2:M:437:ARG:CZ	2:M:491:GLU:OE2	2.55	0.54
2:M:545:ASN:HB3	2:M:583:LEU:HD22	1.90	0.54
2:M:704:HIS:CD2	2:M:831:ARG:HD2	2.42	0.54
3:N:1282:ARG:CG	3:N:1282:ARG:NH1	2.66	0.54
3:N:1400:VAL:HG21	3:N:1417:TRP:HD1	1.70	0.54
5:P:125:ASP:O	5:P:129:GLU:HG2	2.08	0.54
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.90	0.54
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.89	0.54
3:D:433:GLY:HA3	3:D:446:VAL:HG13	1.89	0.54
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.89	0.54
2:M:206:THR:CA	2:M:209:ARG:HD2	2.38	0.54
3:N:372:ASP:N	3:N:372:ASP:OD1	2.36	0.54
3:N:475:LYS:O	3:N:479:GLU:HG2	2.08	0.54
5:P:383:LEU:HD23	5:P:383:LEU:N	2.18	0.54
2:C:758:ARG:H	2:C:789:SER:HB3	1.72	0.54
2:C:983:ILE:HG21	2:C:987:ILE:HD11	1.89	0.54
5:F:270:LYS:HG2	5:F:295:MET:HE1	1.90	0.54
3:N:573:MET:CE	5:P:214:GLN:HG3	2.38	0.54
3:N:1213:ARG:HB2	3:N:1214:PRO:HD2	1.89	0.54
2:C:198:ARG:CZ	2:C:230:ARG:HA	2.38	0.54
5:F:155:THR:O	5:F:159:ILE:HG12	2.07	0.54
5:F:231:ARG:O	5:F:232:ARG:CB	2.56	0.54
2:M:395:LYS:HE2	2:M:403:SER:HB2	1.90	0.54
3:N:1292:VAL:HG23	3:N:1305:LEU:HD11	1.89	0.54
3:N:1314:LYS:O	3:N:1317:ASP:HB2	2.07	0.54
1:B:92:PRO:O	1:B:146:ARG:NH1	2.33	0.53
2:C:86:LYS:HB2	2:C:88:LEU:HG	1.90	0.53
2:C:184:MET:HE3	2:C:186:VAL:CG2	2.37	0.53
2:C:598:GLU:O	2:C:651:LYS:HG3	2.08	0.53
2:C:999:HIS:HB3	2:C:1004:LYS:HE3	1.90	0.53
3:D:1283:ILE:CG1	3:D:1315:ASP:HB2	2.35	0.53
2:M:242:LEU:HD12	2:M:256:TYR:OH	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:581:THR:N	2:M:584:GLU:OE2	2.40	0.53
2:M:966:LEU:HD13	2:M:986:PRO:HB3	1.90	0.53
3:N:259:VAL:HG13	3:N:270:LEU:CD1	2.37	0.53
3:N:1312:LEU:HD22	3:N:1327:ARG:HG2	1.90	0.53
2:C:184:MET:HE3	2:C:186:VAL:HG21	1.90	0.53
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.91	0.53
3:D:1310:ARG:CD	3:D:1327:ARG:HB2	2.37	0.53
3:N:187:LYS:N	3:N:200:ASP:HB3	2.23	0.53
3:N:433:GLY:HA3	3:N:446:VAL:CG1	2.39	0.53
3:N:654:LYS:HB3	3:N:655:PRO:HD3	1.89	0.53
4:O:40:LEU:HG	4:O:67:GLU:HG2	1.89	0.53
5:P:140:ARG:HH11	5:P:140:ARG:HG2	1.73	0.53
1:A:201:THR:HG22	1:A:202:ASP:N	2.23	0.53
2:C:581:THR:N	2:C:584:GLU:OE2	2.41	0.53
3:D:187:LYS:N	3:D:200:ASP:HB3	2.23	0.53
1:L:18:ARG:O	1:L:207:PRO:HD3	2.09	0.53
2:M:419:THR:HB	2:M:422:ARG:HG2	1.91	0.53
3:N:1046:GLN:HA	3:N:1052:THR:HA	1.89	0.53
2:C:177:GLU:CG	2:C:178:PRO:HD2	2.30	0.53
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.90	0.53
3:D:580:ALA:HA	3:D:584:ASN:HA	1.88	0.53
3:D:685:ASP:HA	3:D:688:TRP:HD1	1.74	0.53
2:M:740:GLU:HB3	2:M:805:ARG:NH1	2.23	0.53
2:C:640:ARG:HH11	2:C:642:ARG:NH2	2.07	0.53
3:D:143:ASN:OD1	3:D:144:GLY:N	2.40	0.53
3:D:270:LEU:HD12	3:D:284:LEU:HD11	1.89	0.53
3:D:1468:LEU:HB3	3:D:1470:ARG:HG3	1.91	0.53
2:M:184:MET:HE3	2:M:186:VAL:HG21	1.90	0.53
3:N:840:LYS:HE3	3:N:841:TYR:OH	2.09	0.53
3:N:1263:PHE:HA	3:N:1375:MET:HE1	1.89	0.53
2:C:229:MET:O	2:C:230:ARG:CB	2.55	0.53
2:C:944:LEU:HD21	2:C:963:LEU:HD23	1.90	0.53
3:D:1386:ASP:CB	3:D:1412:LYS:HD2	2.39	0.53
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.09	0.53
3:N:1232:PRO:HG2	3:N:1356:TYR:HE2	1.73	0.53
1:A:9:PRO:CD	1:B:224:TYR:CD2	2.92	0.53
2:C:55:GLU:HG3	2:C:56:GLU:H	1.73	0.53
2:C:191:PHE:HB2	2:C:192:PRO:HD2	1.90	0.53
2:C:224:GLU:OE2	2:C:224:GLU:N	2.30	0.53
2:M:157:ARG:HH12	2:M:176:VAL:HG13	1.71	0.53
1:A:58:ILE:HB	1:A:61:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:419:THR:HB	2:C:422:ARG:HG2	1.91	0.53
3:D:192:ALA:HB1	3:D:193:PRO:HD2	1.90	0.53
5:F:394:ARG:O	5:F:397:ILE:HG22	2.08	0.53
2:M:419:THR:N	2:M:422:ARG:HG3	2.21	0.53
5:P:152:ASP:OD1	5:P:152:ASP:N	2.42	0.53
5:P:343:ASP:O	5:P:346:THR:HB	2.09	0.53
1:A:30:ARG:CD	1:A:191:ASP:OD2	2.57	0.53
2:C:560:MET:O	2:C:564:MET:HG3	2.09	0.53
2:C:580:MET:HB3	2:C:584:GLU:CD	2.29	0.53
2:M:156:GLY:C	2:M:157:ARG:HD3	2.29	0.53
2:M:535:SER:O	2:M:538:GLN:HG2	2.08	0.53
2:M:759:THR:HB	2:M:785:VAL:HB	1.90	0.53
3:N:478:LEU:O	3:N:481:MET:N	2.42	0.53
3:N:1462:LEU:O	3:N:1466:VAL:HG23	2.08	0.53
5:P:368:VAL:HG11	5:P:397:ILE:HD11	1.91	0.53
3:D:405:ASP:CG	3:D:406:ASP:H	2.11	0.53
3:D:897:TRP:CH2	3:D:902:LEU:HD22	2.44	0.53
3:D:1280:VAL:HG12	3:D:1295:GLU:O	2.10	0.53
4:E:95:VAL:HG23	4:E:95:VAL:O	2.08	0.53
2:M:164:PRO:HA	2:M:269:LEU:HD12	1.91	0.53
3:N:405:ASP:CG	3:N:406:ASP:H	2.11	0.53
4:O:14:ASP:OD1	4:O:18:ARG:NH1	2.42	0.53
1:A:112:ARG:HB3	1:A:125:PRO:HB2	1.91	0.52
2:C:1065:ALA:HB1	2:C:1077:PRO:HG3	1.90	0.52
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.09	0.52
3:D:881:LEU:O	3:D:885:ILE:HG13	2.09	0.52
3:D:1044:LEU:HD12	3:D:1044:LEU:N	2.23	0.52
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.91	0.52
5:F:365:GLU:HB2	5:F:404:ALA:HB2	1.91	0.52
2:M:363:SER:O	2:M:367:LEU:HD21	2.09	0.52
3:N:32:ILE:CD1	5:P:258:ILE:HD11	2.33	0.52
4:O:43:GLU:OE1	4:O:43:GLU:N	2.36	0.52
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.90	0.52
3:D:801:GLY:HA3	3:D:825:ALA:CB	2.40	0.52
3:D:945:SER:OG	3:D:947:ILE:HG12	2.09	0.52
2:M:15:LEU:HD12	2:M:458:TYR:CZ	2.44	0.52
2:M:55:GLU:HG3	2:M:56:GLU:H	1.72	0.52
3:N:255:GLU:HB3	3:N:279:VAL:HG11	1.91	0.52
5:P:366:ALA:O	5:P:370:LYS:HG3	2.09	0.52
5:P:395:GLU:HA	5:P:398:ARG:HG2	1.90	0.52
1:B:110:LYS:NZ	1:B:128:HIS:CB	2.67	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:182:VAL:HG23	2:C:193:LEU:HB2	1.90	0.52
2:C:712:ALA:HB3	2:C:821:GLU:HG3	1.91	0.52
3:D:786:ILE:CG2	3:D:1026:SER:HB2	2.39	0.52
3:D:1282:ARG:HB3	3:D:1293:PHE:HB2	1.90	0.52
3:D:1326:THR:HG22	3:D:1327:ARG:H	1.74	0.52
5:F:390:PHE:HD1	5:F:397:ILE:HD11	1.74	0.52
2:M:858:MET:HG2	2:M:867:VAL:O	2.09	0.52
3:N:945:SER:OG	3:N:947:ILE:HG12	2.09	0.52
3:N:1044:LEU:HD12	3:N:1044:LEU:N	2.22	0.52
1:B:67:THR:O	1:B:69:PRO:HD3	2.10	0.52
2:M:191:PHE:HB2	2:M:192:PRO:HD2	1.90	0.52
2:M:999:HIS:HB3	2:M:1004:LYS:HE3	1.92	0.52
3:N:260:GLU:OE1	3:N:273:ARG:NH2	2.42	0.52
3:N:407:VAL:HG23	3:N:422:ALA:HB2	1.91	0.52
3:N:601:ARG:HD3	5:P:318:GLU:HG2	1.92	0.52
3:N:669:ASN:HD22	5:P:417:LYS:HD3	1.73	0.52
3:N:1311:LEU:N	3:N:1311:LEU:HD23	2.18	0.52
5:P:361:LEU:CD1	5:P:362:SER:H	2.16	0.52
2:C:292:ARG:HG3	2:C:299:LYS:CB	2.39	0.52
2:C:807:ARG:NH2	2:C:810:ASP:OD2	2.43	0.52
3:D:1495:ILE:HD13	4:E:80:VAL:HG21	1.92	0.52
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.90	0.52
1:K:201:THR:HG22	1:K:202:ASP:N	2.25	0.52
3:N:192:ALA:HB1	3:N:193:PRO:HD2	1.91	0.52
3:N:860:LEU:O	3:N:876:SER:HB2	2.09	0.52
1:A:133:GLU:HG2	1:A:134:GLU:N	2.24	0.52
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.92	0.52
1:K:112:ARG:HB3	1:K:125:PRO:HB2	1.92	0.52
2:M:954:THR:OG1	2:M:957:LYS:HE3	2.10	0.52
2:M:1090:LYS:HD3	2:M:1112:PHE:CZ	2.44	0.52
3:N:277:GLU:OE1	3:N:277:GLU:N	2.42	0.52
3:N:1310:ARG:HD3	3:N:1327:ARG:CD	2.35	0.52
2:C:948:GLU:HB3	2:C:953:VAL:HG23	1.92	0.52
3:D:371:ILE:CD1	5:F:230:LYS:HA	2.40	0.52
3:D:399:ARG:HB2	3:D:401:TYR:CE1	2.45	0.52
3:D:475:LYS:O	3:D:479:GLU:HG2	2.09	0.52
3:D:1364:HIS:ND1	3:D:1366:LYS:HB2	2.25	0.52
2:M:757:GLY:HA2	2:M:789:SER:CB	2.36	0.52
2:M:787:ASP:OD1	2:M:789:SER:OG	2.26	0.52
3:N:801:GLY:HA3	3:N:825:ALA:CB	2.40	0.52
3:N:1267:ARG:HG2	3:N:1331:ASP:OD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:372:ARG:HD2	5:P:381:HIS:O	2.09	0.52
1:A:209:GLU:O	1:A:213:GLN:HG3	2.10	0.52
1:B:80:LEU:HD11	3:D:842:VAL:HG12	1.91	0.52
3:D:1282:ARG:NE	3:D:1295:GLU:OE2	2.41	0.52
2:M:1037:VAL:HG13	2:M:1049:LEU:HD11	1.90	0.52
2:M:1097:LEU:HD11	3:N:103:TRP:CZ3	2.45	0.52
3:N:114:THR:HG23	3:N:495:ARG:HG2	1.91	0.52
3:N:399:ARG:HB2	3:N:401:TYR:CE1	2.45	0.52
2:C:156:GLY:C	2:C:157:ARG:HD3	2.29	0.52
2:C:424:GLY:O	2:C:428:ARG:HG3	2.09	0.52
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.45	0.52
1:K:4:SER:HA	1:K:189:ARG:HH21	1.74	0.52
2:M:248:PRO:C	2:M:250:ARG:H	2.12	0.52
2:M:550:LEU:HB3	2:M:905:ILE:HG23	1.92	0.52
2:M:768:THR:HB	2:M:771:GLU:HB2	1.91	0.52
2:M:808:ARG:NH2	5:P:305:GLU:OE2	2.43	0.52
2:M:876:VAL:N	2:M:877:PRO:HD2	2.25	0.52
2:M:1053:LEU:HA	3:N:621:LYS:HD2	1.91	0.52
3:N:786:ILE:CG2	3:N:1026:SER:HB2	2.39	0.52
5:P:231:ARG:O	5:P:232:ARG:CB	2.56	0.52
2:C:954:THR:OG1	2:C:957:LYS:HE3	2.10	0.52
2:C:966:LEU:HD13	2:C:986:PRO:HB3	1.92	0.52
2:M:229:MET:O	2:M:230:ARG:CB	2.58	0.52
2:M:294:GLU:O	2:M:295:ASP:C	2.48	0.52
2:M:580:MET:HB3	2:M:584:GLU:OE2	2.10	0.52
3:N:693:GLU:HA	4:O:48:MET:CE	2.40	0.52
3:N:835:SER:H	3:N:838:ARG:NE	2.07	0.52
3:N:881:LEU:O	3:N:885:ILE:HG13	2.09	0.52
5:P:402:ASN:O	5:P:406:ARG:HG3	2.09	0.52
3:D:860:LEU:O	3:D:876:SER:HB2	2.09	0.51
2:M:212:GLY:HA2	2:M:218:VAL:HG21	1.91	0.51
3:N:897:TRP:CH2	3:N:902:LEU:HD22	2.44	0.51
3:N:1336:LEU:HB2	3:N:1344:VAL:HG21	1.92	0.51
2:C:1090:LYS:HD3	2:C:1112:PHE:CZ	2.45	0.51
3:D:706:PRO:HB2	3:D:708:LEU:HD21	1.91	0.51
2:M:983:ILE:HG21	2:M:987:ILE:CD1	2.40	0.51
3:N:890:VAL:CG1	3:N:922:LEU:CD1	2.88	0.51
3:N:1283:ILE:CD1	3:N:1283:ILE:H	2.23	0.51
3:N:1290:LEU:CG	3:N:1307:LYS:CE	2.64	0.51
5:P:404:ALA:O	5:P:408:LEU:HB2	2.11	0.51
2:C:983:ILE:HG21	2:C:987:ILE:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:804:LEU:O	3:D:827:ILE:HG23	2.11	0.51
3:D:895:VAL:HG11	3:D:922:LEU:CD2	2.40	0.51
5:F:95:THR:HG22	5:F:96:LEU:N	2.25	0.51
2:M:66:LEU:HD11	2:M:98:LEU:HB3	1.92	0.51
2:M:194:VAL:HA	2:M:197:LEU:HD12	1.92	0.51
2:M:323:ASP:O	2:M:325:ILE:CG2	2.59	0.51
2:M:807:ARG:NH2	2:M:810:ASP:OD2	2.43	0.51
2:M:948:GLU:HB3	2:M:953:VAL:HG23	1.92	0.51
3:N:46:ASP:OD2	3:N:48:ARG:CG	2.53	0.51
3:N:147:VAL:HG21	3:N:161:LEU:HD21	1.93	0.51
5:P:83:GLN:O	5:P:87:GLU:HG3	2.09	0.51
4:E:40:LEU:HG	4:E:67:GLU:HG2	1.91	0.51
2:M:170:PRO:HA	7:R:13:DT:H3	1.74	0.51
2:M:290:LEU:HD23	2:M:302:VAL:HG21	1.91	0.51
2:M:669:GLY:H	2:M:993:PHE:HZ	1.56	0.51
5:P:419:ARG:HD2	5:P:422:LEU:HD11	1.92	0.51
1:A:180:GLN:NE2	2:C:935:GLY:O	2.43	0.51
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.91	0.51
1:K:209:GLU:O	1:K:213:GLN:HG3	2.09	0.51
2:M:184:MET:HE3	2:M:186:VAL:CG2	2.40	0.51
2:M:470:PRO:HB2	2:M:534:VAL:HG21	1.93	0.51
2:M:861:LEU:HD23	2:M:974:LEU:CD1	2.40	0.51
3:N:693:GLU:HA	4:O:48:MET:HE1	1.92	0.51
3:N:1258:ARG:HH21	3:N:1351:GLU:HG2	1.73	0.51
5:P:399:GLN:O	5:P:402:ASN:HB2	2.11	0.51
1:A:47:SER:O	1:A:49:PRO:HD3	2.11	0.51
2:C:97:ARG:HD3	2:C:110:GLU:OE1	2.11	0.51
3:D:614:PHE:HA	3:D:618:LEU:HD23	1.93	0.51
6:G:11:DT:H2"	6:G:12:DG:H5"	1.92	0.51
2:M:154:ARG:NH2	2:M:178:PRO:HA	2.26	0.51
2:M:1065:ALA:HB1	2:M:1077:PRO:HG3	1.91	0.51
3:N:823:LEU:HD11	3:N:837:GLY:CA	2.37	0.51
3:N:823:LEU:CD1	3:N:837:GLY:HA2	2.37	0.51
3:N:834:THR:HG23	3:N:835:SER:O	2.11	0.51
3:N:959:GLU:HB3	3:N:963:TYR:CE1	2.45	0.51
5:P:386:VAL:CG1	5:P:397:ILE:HG21	2.41	0.51
2:C:48:PHE:HA	2:C:348:LEU:HD21	1.93	0.51
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.46	0.51
3:D:646:LYS:HB3	3:D:688:TRP:CZ3	2.46	0.51
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.44	0.51
3:D:1312:LEU:HD21	3:D:1327:ARG:CG	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:267:TYR:CE2	2:M:290:LEU:HG	2.46	0.51
3:N:709:HIS:HA	3:N:1227:GLN:HB3	1.92	0.51
3:N:1481:VAL:HG23	4:O:21:VAL:HG21	1.93	0.51
3:D:619:LEU:HD11	3:D:1439:SER:HB3	1.93	0.51
3:N:71:LYS:HG3	3:N:72:VAL:N	2.25	0.51
3:N:218:LYS:HA	3:N:337:LEU:O	2.11	0.51
3:N:566:ILE:HD13	5:P:217:ASN:HB3	1.91	0.51
2:C:223:ASP:O	2:C:227:PHE:HD2	1.94	0.51
2:C:1103:ASP:OD2	2:C:1107:ASN:HB2	2.10	0.51
2:M:97:ARG:HD3	2:M:110:GLU:OE1	2.11	0.51
2:M:171:TRP:HZ3	7:R:14:DG:OP1	1.94	0.51
2:M:250:ARG:HG3	2:M:250:ARG:HH11	1.76	0.51
2:M:325:ILE:H	2:M:330:ASN:HD22	1.57	0.51
2:M:503:LEU:CD2	2:M:508:ILE:HD13	2.41	0.51
3:N:44:LEU:HB3	3:N:525:ARG:HH21	1.76	0.51
3:N:566:ILE:HD11	5:P:192:LEU:HD21	1.92	0.51
3:N:573:MET:SD	5:P:210:LEU:HB3	2.51	0.51
3:N:1231:GLU:N	3:N:1232:PRO:HD2	2.26	0.51
3:N:1386:ASP:OD2	3:N:1413:THR:OG1	2.17	0.51
2:C:637:LEU:HD23	2:C:659:PRO:HG3	1.91	0.51
5:F:377:ASP:OD1	5:F:377:ASP:C	2.50	0.51
5:F:418:LEU:HD12	5:F:418:LEU:N	2.25	0.51
1:K:90:LEU:O	1:K:92:PRO:HD3	2.11	0.51
1:L:83:LYS:HE2	1:L:168:ASP:HB2	1.93	0.51
3:N:1099:VAL:O	3:N:1103:HIS:HB3	2.11	0.51
1:B:156:HIS:ND1	1:B:158:ILE:HG23	2.26	0.50
2:C:12:VAL:HG11	2:C:472:ARG:HD3	1.93	0.50
2:C:56:GLU:HG2	2:C:359:MET:HE3	1.92	0.50
2:C:66:LEU:HD11	2:C:98:LEU:HB3	1.93	0.50
2:M:1103:ASP:OD2	2:M:1107:ASN:HB2	2.11	0.50
3:N:111:LYS:HG3	3:N:1452:ILE:HD11	1.93	0.50
3:N:646:LYS:HB3	3:N:688:TRP:CZ3	2.46	0.50
5:P:380:GLU:H	5:P:380:GLU:CD	2.14	0.50
2:C:878:SER:HA	3:D:1034:GLN:OE1	2.11	0.50
3:D:258:VAL:HG12	3:D:297:ILE:HD13	1.92	0.50
3:D:376:GLU:HG3	3:D:376:GLU:O	2.11	0.50
2:M:223:ASP:O	2:M:227:PHE:HD2	1.94	0.50
2:M:758:ARG:H	2:M:789:SER:HB3	1.76	0.50
2:M:1065:ALA:CB	2:M:1077:PRO:HG3	2.41	0.50
5:P:261:PRO:O	5:P:265:VAL:HG23	2.11	0.50
1:A:27:PRO:HB2	1:A:192:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:THR:CG2	2:C:105:THR:O	2.58	0.50
2:C:418:LEU:HD21	7:H:14:DG:C8	2.46	0.50
3:D:47:GLU:CB	3:D:78:VAL:CG2	2.87	0.50
3:D:1232:PRO:HG2	3:D:1356:TYR:HE2	1.75	0.50
3:D:1263:PHE:HA	3:D:1375:MET:HE2	1.94	0.50
2:M:189:ARG:HH12	2:M:244:PRO:CD	2.20	0.50
3:N:114:THR:HG21	3:N:498:VAL:HG21	1.94	0.50
1:B:94:LEU:HD22	1:B:96:THR:H	1.76	0.50
2:C:15:LEU:HD12	2:C:458:TYR:CZ	2.46	0.50
3:D:1339:LYS:HG2	3:D:1343:ALA:HB2	1.91	0.50
3:D:1465:ASN:HB3	3:D:1470:ARG:HB2	1.92	0.50
4:E:67:GLU:O	4:E:70:THR:OG1	2.29	0.50
1:L:156:HIS:ND1	1:L:158:ILE:HG23	2.26	0.50
2:M:12:VAL:HG11	2:M:472:ARG:HD3	1.93	0.50
3:N:279:VAL:HG13	3:N:279:VAL:O	2.10	0.50
3:N:323:GLU:HB2	3:N:334:THR:HB	1.93	0.50
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.93	0.50
2:M:171:TRP:CH2	7:R:13:DT:H2"	2.45	0.50
3:N:558:LEU:HD23	3:N:567:ILE:HD12	1.93	0.50
1:A:184:THR:N	1:A:192:LEU:O	2.38	0.50
2:C:198:ARG:HH11	2:C:230:ARG:CA	2.24	0.50
3:D:147:VAL:HG21	3:D:161:LEU:HD21	1.94	0.50
3:D:291:LEU:HD12	3:D:303:PRO:HB2	1.94	0.50
3:D:596:SER:O	3:D:597:ASP:OD2	2.30	0.50
3:D:693:GLU:CA	4:E:48:MET:HE1	2.41	0.50
3:D:829:VAL:O	3:D:830:ALA:HB3	2.11	0.50
2:M:580:MET:HB3	2:M:584:GLU:CD	2.32	0.50
3:D:69:GLU:HA	3:D:80:VAL:HG23	1.92	0.50
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.46	0.50
2:M:327:HIS:CE1	2:M:488:ALA:HB1	2.46	0.50
3:N:1480:PHE:O	4:O:18:ARG:NH2	2.45	0.50
2:C:48:PHE:O	2:C:52:PHE:HD2	1.94	0.50
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.46	0.50
2:C:550:LEU:HB3	2:C:905:ILE:HG23	1.94	0.50
2:C:787:ASP:OD1	2:C:789:SER:OG	2.30	0.50
3:D:407:VAL:HG23	3:D:422:ALA:HB2	1.94	0.50
3:D:483:HIS:ND1	3:D:484:PRO:HD2	2.27	0.50
3:D:1097:LYS:O	3:D:1101:VAL:HG23	2.12	0.50
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.93	0.50
2:M:843:HIS:NE2	2:M:887:GLU:OE2	2.45	0.50
3:N:44:LEU:O	3:N:525:ARG:NH2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:412:GLY:N	3:N:435:VAL:HG12	2.26	0.50
3:N:483:HIS:ND1	3:N:484:PRO:HD2	2.27	0.50
1:B:176:ARG:HG2	1:B:200:TRP:CE3	2.47	0.50
2:C:524:VAL:HG12	2:C:525:SER:N	2.27	0.50
2:C:1097:LEU:HD11	3:D:103:TRP:HZ3	1.75	0.50
3:D:23:TYR:CD2	3:D:89:ARG:HD3	2.47	0.50
3:D:970:LYS:O	3:D:974:ILE:HG13	2.11	0.50
1:K:47:SER:O	1:K:49:PRO:HD3	2.11	0.50
1:K:153:ALA:N	1:K:168:ASP:OD1	2.33	0.50
2:M:690:ILE:CD1	2:M:869:VAL:HG22	2.42	0.50
2:M:926:PHE:HE1	2:M:929:ARG:HH11	1.59	0.50
3:N:1208:ASP:HB2	3:N:1215:VAL:HA	1.94	0.50
3:N:1440:PHE:O	3:N:1441:GLN:HG3	2.12	0.50
2:C:82:GLU:O	2:C:86:LYS:HG3	2.12	0.49
2:C:194:VAL:HA	2:C:197:LEU:HD12	1.94	0.49
2:M:460:ARG:HD2	2:M:485:TYR:CZ	2.46	0.49
3:N:368:VAL:HB	3:N:377:VAL:HB	1.94	0.49
3:N:661:MET:CE	3:N:677:LEU:HD11	2.42	0.49
5:P:152:ASP:HB2	5:P:153:PRO:HD2	1.92	0.49
5:P:398:ARG:O	5:P:401:GLU:HG2	2.10	0.49
1:A:90:LEU:O	1:A:92:PRO:HD3	2.11	0.49
2:C:535:SER:OG	2:C:537:LYS:HG3	2.12	0.49
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.60	0.49
3:D:33:ASN:HB2	3:D:40:GLU:OE1	2.11	0.49
3:D:217:LYS:HB2	3:D:339:TRP:CE2	2.47	0.49
3:D:595:GLY:O	3:D:597:ASP:OD2	2.30	0.49
3:D:1347:TYR:O	3:D:1351:GLU:HB2	2.11	0.49
2:M:211:LEU:HD23	2:M:311:PHE:HD2	1.76	0.49
2:M:524:VAL:HG12	2:M:525:SER:N	2.27	0.49
3:N:274:ARG:CZ	3:N:279:VAL:HG21	2.42	0.49
5:P:403:LYS:NZ	5:P:406:ARG:HH12	2.10	0.49
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.93	0.49
2:C:289:THR:HG22	2:C:291:ALA:H	1.76	0.49
2:C:660:ALA:O	2:C:667:ALA:N	2.39	0.49
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.93	0.49
3:D:567:ILE:HG22	3:D:571:LYS:HE3	1.94	0.49
3:D:916:TYR:CE1	3:D:920:LEU:HD11	2.46	0.49
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.94	0.49
5:F:372:ARG:HE	5:F:383:LEU:HG	1.77	0.49
1:K:47:SER:HG	1:L:32:PHE:HE1	1.60	0.49
2:M:425:PHE:CZ	3:N:1086:LEU:HD12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1090:LYS:HD3	2:M:1112:PHE:CE2	2.47	0.49
3:N:315:ARG:O	3:N:316:GLN:HB3	2.12	0.49
5:P:140:ARG:HG2	5:P:140:ARG:NH1	2.27	0.49
1:A:39:PRO:CG	1:B:39:PRO:HG3	2.42	0.49
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.47	0.49
2:C:436:GLY:HA2	2:C:538:GLN:O	2.12	0.49
3:D:230:TRP:CZ2	3:D:232:GLU:HA	2.47	0.49
3:N:619:LEU:HD11	3:N:1439:SER:HB3	1.92	0.49
3:N:806:PHE:HB2	3:N:829:VAL:HG22	1.94	0.49
2:C:711:GLU:HB2	2:C:713:ARG:NH1	2.28	0.49
3:D:128:TYR:CZ	3:D:587:ARG:HD3	2.47	0.49
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.92	0.49
4:E:43:GLU:OE1	4:E:43:GLU:N	2.37	0.49
1:K:34:VAL:CG2	1:L:42:ARG:CZ	2.90	0.49
1:L:176:ARG:HG2	1:L:200:TRP:CE3	2.47	0.49
2:M:157:ARG:NH1	2:M:157:ARG:CG	2.74	0.49
2:M:229:MET:HE2	2:M:234:ALA:HA	1.87	0.49
3:N:473:LEU:HD21	3:N:495:ARG:NH2	2.27	0.49
3:D:661:MET:CE	3:D:677:LEU:HD11	2.43	0.49
3:D:1305:LEU:HD23	3:D:1305:LEU:H	1.66	0.49
1:L:80:LEU:HD11	3:N:842:VAL:HG12	1.95	0.49
2:M:86:LYS:HB2	2:M:88:LEU:HG	1.94	0.49
2:M:289:THR:CG2	2:M:291:ALA:O	2.61	0.49
2:M:327:HIS:CE1	2:M:433:THR:HG21	2.47	0.49
3:N:614:PHE:HA	3:N:618:LEU:HD23	1.94	0.49
5:P:391:GLY:O	5:P:392:VAL:O	2.31	0.49
2:M:23:VAL:HG12	2:M:24:GLU:N	2.26	0.49
2:M:136:ILE:HB	2:M:336:VAL:CG1	2.43	0.49
2:M:261:ILE:HG22	2:M:291:ALA:HB3	1.94	0.49
2:M:424:GLY:O	2:M:428:ARG:HG3	2.12	0.49
3:N:671:LYS:NZ	5:P:420:ASP:O	2.40	0.49
3:N:1238:MET:CG	3:N:1359:GLN:OE1	2.61	0.49
2:C:23:VAL:HG12	2:C:24:GLU:N	2.27	0.49
3:D:473:LEU:HD21	3:D:495:ARG:NH2	2.27	0.49
3:D:1264:GLU:OE2	3:D:1425:THR:OG1	2.31	0.49
5:F:123:ASP:HB3	5:F:125:ASP:OD1	2.12	0.49
2:M:5:ARG:HB3	2:M:902:ILE:HB	1.95	0.49
2:M:685:GLU:OE1	2:M:685:GLU:HA	2.12	0.49
3:N:595:GLY:C	3:N:597:ASP:OD2	2.48	0.49
3:N:729:HIS:ND1	3:N:730:PRO:HD2	2.28	0.49
3:N:832:ARG:HD2	3:N:833:GLU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HD3	1:B:224:TYR:CE2	2.47	0.49
1:A:25:LEU:HD22	1:B:225:PHE:CZ	2.47	0.49
2:C:470:PRO:HB2	2:C:534:VAL:HG21	1.95	0.49
3:D:272:LEU:O	3:D:279:VAL:N	2.43	0.49
3:D:431:VAL:HG12	3:D:432:TYR:N	2.27	0.49
5:F:156:VAL:O	5:F:160:ASP:HB2	2.13	0.49
2:M:238:LEU:HD11	2:M:242:LEU:CD2	2.43	0.49
2:M:878:SER:HA	3:N:1034:GLN:OE1	2.13	0.49
3:N:433:GLY:HA3	3:N:446:VAL:HG13	1.95	0.49
3:N:1237:THR:O	3:N:1238:MET:O	2.30	0.49
2:C:50:GLU:OE1	2:C:345:ARG:NE	2.46	0.49
2:C:290:LEU:HD23	2:C:302:VAL:HG21	1.95	0.49
2:C:1065:ALA:CB	2:C:1077:PRO:HG3	2.42	0.49
3:D:74:GLU:CD	3:D:74:GLU:H	2.17	0.49
1:L:48:ILE:HG22	1:L:173:PRO:HD2	1.95	0.49
2:M:560:MET:O	2:M:564:MET:HG3	2.13	0.49
2:M:660:ALA:O	2:M:667:ALA:N	2.41	0.49
3:N:80:VAL:O	3:N:80:VAL:HG23	2.13	0.49
3:N:313:MET:HG3	3:N:314:PRO:HD2	1.95	0.49
3:N:437:VAL:HG11	5:P:175:HIS:HD2	1.78	0.49
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.13	0.48
2:M:740:GLU:HB3	2:M:805:ARG:HH12	1.77	0.48
3:N:219:GLU:N	3:N:339:TRP:CH2	2.81	0.48
3:N:286:VAL:HG13	3:N:312:ARG:O	2.13	0.48
3:N:770:LEU:HD23	3:N:777:PRO:HA	1.95	0.48
3:N:850:LEU:HD12	3:N:884:ARG:NH2	2.28	0.48
3:N:890:VAL:HG21	3:N:922:LEU:HD11	1.95	0.48
3:N:1283:ILE:H	3:N:1283:ILE:HD12	1.78	0.48
2:M:858:MET:HG3	2:M:867:VAL:CG2	2.43	0.48
2:M:1043:TYR:CG	3:N:763:MET:HG2	2.49	0.48
3:N:890:VAL:CB	3:N:922:LEU:HD11	2.41	0.48
5:P:89:GLY:HA3	7:R:7:DG:C6	2.48	0.48
1:B:48:ILE:HG22	1:B:173:PRO:HD2	1.95	0.48
2:C:685:GLU:OE1	2:C:685:GLU:HA	2.12	0.48
2:C:876:VAL:N	2:C:877:PRO:HD2	2.28	0.48
3:D:371:ILE:HG23	5:F:230:LYS:HD2	1.95	0.48
5:F:226:LYS:HD2	7:H:1:DT:H72	1.95	0.48
2:M:99:GLN:NE2	2:M:101:ILE:HD11	2.28	0.48
2:M:154:ARG:HH22	2:M:178:PRO:HA	1.77	0.48
2:M:810:ASP:HB2	2:M:811:PRO:HD2	1.95	0.48
2:M:850:ALA:HA	3:N:632:VAL:HG21	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:874:LEU:HD23	3:N:1023:MET:SD	2.53	0.48
1:L:60:ASP:O	1:L:62:LEU:HD12	2.13	0.48
2:M:553:ASP:OD1	2:M:843:HIS:ND1	2.38	0.48
2:M:1053:LEU:HD11	3:N:1466:VAL:HG13	1.94	0.48
3:N:574:LEU:O	3:N:578:VAL:HG23	2.13	0.48
1:B:54:THR:OG1	1:B:145:ASP:OD1	2.28	0.48
2:C:511:GLU:HG3	2:C:512:ARG:HG2	1.96	0.48
2:C:810:ASP:HB2	2:C:811:PRO:HD2	1.94	0.48
3:D:770:LEU:HD23	3:D:777:PRO:HA	1.96	0.48
3:D:1263:PHE:HA	3:D:1375:MET:CE	2.43	0.48
1:K:180:GLN:NE2	2:M:935:GLY:O	2.47	0.48
2:M:805:ARG:HG3	2:M:823:VAL:HG22	1.96	0.48
3:N:255:GLU:HA	3:N:300:LYS:HE2	1.95	0.48
3:N:1400:VAL:CG2	3:N:1417:TRP:CD1	2.96	0.48
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.13	0.48
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.94	0.48
2:M:76:PRO:HG3	2:M:120:LEU:CD1	2.44	0.48
2:M:511:GLU:HG3	2:M:512:ARG:HG2	1.96	0.48
3:N:314:PRO:HG2	3:N:317:VAL:HG12	1.95	0.48
3:N:315:ARG:H	3:N:315:ARG:HD3	1.78	0.48
3:N:835:SER:CB	3:N:838:ARG:NE	2.37	0.48
3:N:936:TYR:O	3:N:940:THR:OG1	2.28	0.48
2:C:174:LEU:CD1	2:C:184:MET:HG3	2.43	0.48
2:C:936:VAL:HG11	2:C:959:PRO:CB	2.44	0.48
3:D:999:THR:O	3:D:1003:VAL:HG13	2.13	0.48
5:F:164:LYS:HA	5:F:171:LYS:HE3	1.94	0.48
5:F:295:MET:HA	5:F:295:MET:CE	2.44	0.48
3:N:394:LEU:HG	3:N:396:VAL:HG23	1.95	0.48
5:P:361:LEU:HD21	5:P:408:LEU:HD12	1.96	0.48
1:B:58:ILE:HG22	1:B:61:VAL:CG1	2.40	0.48
2:C:76:PRO:HG3	2:C:120:LEU:CD1	2.44	0.48
2:C:211:LEU:HD23	2:C:311:PHE:HD2	1.79	0.48
3:D:465:LEU:HD12	3:D:513:ILE:HD13	1.96	0.48
2:M:925:TYR:CD1	2:M:967:PHE:CE1	3.02	0.48
3:N:270:LEU:HD23	3:N:284:LEU:HD11	1.96	0.48
3:N:567:ILE:HG22	3:N:571:LYS:HE3	1.96	0.48
3:N:1049:SER:OG	3:N:1051:GLU:HG2	2.12	0.48
3:N:1258:ARG:NH2	3:N:1351:GLU:HG2	2.29	0.48
1:A:185:ARG:HE	1:A:187:GLY:HA2	1.79	0.48
2:C:141:HIS:CE1	2:C:334:ARG:HD2	2.49	0.48
2:C:157:ARG:NH1	2:C:157:ARG:CG	2.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:845:ASN:C	2:C:845:ASN:HD22	2.17	0.48
2:C:1056:LYS:O	3:D:624:ASP:N	2.43	0.48
3:D:208:PRO:HA	3:D:390:PRO:HA	1.95	0.48
3:D:832:ARG:HD2	3:D:833:GLU:H	1.77	0.48
2:M:92:ALA:HB2	2:M:120:LEU:HD11	1.94	0.48
2:M:172:ILE:HA	2:M:185:LYS:O	2.14	0.48
2:M:177:GLU:CB	2:M:178:PRO:HD2	2.44	0.48
2:M:351:LEU:HD12	2:M:374:ASN:O	2.14	0.48
2:M:404:LEU:O	2:M:408:ARG:HG3	2.14	0.48
3:N:250:LEU:H	3:N:250:LEU:HD12	1.78	0.48
3:N:255:GLU:HB3	3:N:279:VAL:CG1	2.44	0.48
1:A:34:VAL:CG2	1:B:42:ARG:CZ	2.92	0.48
2:C:136:ILE:HB	2:C:336:VAL:CG1	2.44	0.48
2:C:425:PHE:CZ	3:D:1086:LEU:HD12	2.49	0.48
2:C:580:MET:SD	2:C:584:GLU:HG3	2.54	0.48
2:C:925:TYR:CD1	2:C:967:PHE:CE1	3.01	0.48
3:D:71:LYS:HG3	3:D:72:VAL:N	2.28	0.48
3:D:529:GLN:HG2	3:D:535:PHE:CE1	2.49	0.48
3:D:1258:ARG:HH21	3:D:1351:GLU:HG2	1.78	0.48
3:D:1403:LEU:HD12	3:D:1406:ARG:HH11	1.78	0.48
5:F:365:GLU:O	5:F:369:LEU:HD13	2.14	0.48
1:K:219:ARG:HG3	1:K:220:GLU:H	1.78	0.48
2:M:121:MET:HE1	2:M:336:VAL:HG21	1.96	0.48
2:M:182:VAL:HG21	2:M:193:LEU:CB	2.22	0.48
2:M:944:LEU:HD21	2:M:963:LEU:HD23	1.94	0.48
3:N:465:LEU:HD12	3:N:513:ILE:HD13	1.96	0.48
3:N:493:ARG:NH1	11:N:2121:HOH:O	2.47	0.48
3:N:706:PRO:HB2	3:N:708:LEU:HD21	1.96	0.48
3:N:1282:ARG:CD	3:N:1295:GLU:CD	2.75	0.48
5:P:97:GLU:H	5:P:97:GLU:CD	2.18	0.48
1:A:188:GLN:HG2	1:A:189:ARG:N	2.29	0.47
2:C:569:VAL:HG21	2:C:1000:MET:CE	2.44	0.47
2:C:757:GLY:HA2	2:C:789:SER:CB	2.42	0.47
3:D:729:HIS:ND1	3:D:730:PRO:HD2	2.29	0.47
3:D:1104:GLU:O	3:D:1106:VAL:HG23	2.13	0.47
2:M:168:ARG:HH11	2:M:168:ARG:CG	2.27	0.47
3:N:1413:THR:HG22	3:N:1414:PRO:HD2	1.94	0.47
2:M:685:GLU:O	2:M:686:ASP:HB2	2.15	0.47
3:N:134:VAL:HG23	3:N:150:ARG:N	2.29	0.47
5:P:205:ARG:HH11	5:P:205:ARG:HG2	1.72	0.47
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:404:LEU:O	2:C:408:ARG:HG3	2.14	0.47
2:C:419:THR:N	2:C:422:ARG:HG3	2.21	0.47
2:C:850:ALA:HA	3:D:632:VAL:HG22	1.93	0.47
3:D:394:LEU:HG	3:D:396:VAL:HG23	1.96	0.47
3:D:574:LEU:O	3:D:578:VAL:HG23	2.13	0.47
3:D:868:TYR:CE2	3:D:869:MET:HG3	2.49	0.47
1:L:175:ARG:N	1:L:200:TRP:O	2.44	0.47
3:N:840:LYS:HE3	3:N:841:TYR:CZ	2.49	0.47
1:A:72:LYS:HE3	2:C:643:VAL:O	2.14	0.47
3:D:219:GLU:CB	3:D:339:TRP:CH2	2.97	0.47
3:D:1140:ILE:HG22	3:D:1144:LEU:HD12	1.96	0.47
5:F:279:GLN:HA	5:F:284:ARG:O	2.15	0.47
1:K:32:PHE:HA	1:K:35:THR:HB	1.95	0.47
3:N:431:VAL:HG12	3:N:432:TYR:N	2.29	0.47
3:N:536:ALA:HA	5:P:315:VAL:O	2.13	0.47
3:N:868:TYR:CE2	3:N:869:MET:HG3	2.50	0.47
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.50	0.47
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.14	0.47
3:D:1112:CYS:HB3	3:D:1196:THR:OG1	2.14	0.47
1:K:57:TYR:CG	1:K:161:ARG:HD2	2.49	0.47
2:M:418:LEU:HD21	7:R:14:DG:C8	2.48	0.47
2:M:680:ASP:OD1	3:N:943:THR:HG21	2.15	0.47
3:N:650:LEU:HD12	3:N:657:LEU:CD2	2.45	0.47
1:A:9:PRO:CD	1:B:224:TYR:CE2	2.98	0.47
1:A:159:LYS:HE3	1:A:164:ALA:O	2.14	0.47
1:A:219:ARG:HG3	1:A:220:GLU:H	1.79	0.47
2:C:128:ILE:O	2:C:129:ILE:HD13	2.15	0.47
3:D:214:GLU:HG2	3:D:342:PRO:HB3	1.97	0.47
3:D:890:VAL:O	3:D:926:LYS:NZ	2.47	0.47
5:F:234:LYS:HD3	7:H:5:DA:OP2	2.15	0.47
1:K:8:ALA:HA	1:K:9:PRO:HD3	1.65	0.47
1:K:39:PRO:HG3	1:L:39:PRO:CG	2.44	0.47
2:M:173:ASP:O	2:M:174:LEU:HD12	2.14	0.47
3:N:204:LEU:HD23	3:N:441:ARG:NH2	2.29	0.47
3:N:273:ARG:CG	3:N:278:PRO:HA	2.44	0.47
1:B:91:ASN:HB3	1:B:94:LEU:HB2	1.97	0.47
1:B:206:THR:H	1:B:209:GLU:HB2	1.80	0.47
2:C:35:PRO:HG2	2:C:38:LYS:CD	2.44	0.47
2:C:56:GLU:HA	2:C:56:GLU:OE2	2.14	0.47
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.95	0.47
2:C:1090:LYS:HD3	2:C:1112:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:47:GLU:HA	3:D:51:GLY:O	2.15	0.47
3:D:134:VAL:HG23	3:D:150:ARG:N	2.29	0.47
3:D:1100:ASP:OD2	3:D:1440:PHE:HB2	2.13	0.47
1:L:101:LEU:HD11	1:L:113:ASP:HB2	1.96	0.47
2:M:580:MET:SD	2:M:584:GLU:HG3	2.54	0.47
2:M:711:GLU:HB2	2:M:713:ARG:NH1	2.30	0.47
2:M:850:ALA:HA	3:N:632:VAL:HG22	1.92	0.47
3:N:134:VAL:HG23	3:N:150:ARG:H	1.80	0.47
3:N:208:PRO:HA	3:N:390:PRO:HA	1.95	0.47
3:N:271:VAL:HG22	3:N:281:THR:HG23	1.96	0.47
3:N:693:GLU:CB	4:O:48:MET:HE1	2.45	0.47
3:N:1068:LEU:O	3:N:1072:ILE:HG12	2.15	0.47
3:N:1347:TYR:O	3:N:1351:GLU:HB2	2.15	0.47
5:P:247:ILE:O	5:P:251:ILE:HG13	2.14	0.47
5:P:365:GLU:O	5:P:368:VAL:HG22	2.15	0.47
2:C:150:PRO:CD	2:C:322:VAL:HG11	2.42	0.47
2:C:229:MET:C	2:C:230:ARG:CG	2.74	0.47
2:C:535:SER:O	2:C:538:GLN:HG2	2.14	0.47
3:D:131:LYS:O	3:D:456:MET:HG2	2.15	0.47
3:D:265:GLU:HB3	3:D:266:GLU:H	1.51	0.47
3:D:936:TYR:O	3:D:940:THR:OG1	2.30	0.47
3:N:310:LEU:HD23	3:N:310:LEU:H	1.80	0.47
3:N:1407:LEU:O	3:N:1410:GLU:N	2.44	0.47
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.97	0.47
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.30	0.47
3:D:1128:VAL:HG22	3:D:1129:THR:HG23	1.96	0.47
3:D:1216:SER:HB3	4:E:15:SER:HA	1.97	0.47
1:K:58:ILE:HG21	1:K:68:ILE:HD11	1.97	0.47
1:K:159:LYS:HE3	1:K:164:ALA:O	2.15	0.47
2:M:436:GLY:HA2	2:M:538:GLN:O	2.15	0.47
2:M:550:LEU:HD23	2:M:905:ILE:HG21	1.97	0.47
2:M:571:LEU:HD23	2:M:702:SER:HB3	1.97	0.47
2:M:936:VAL:HG11	2:M:959:PRO:CB	2.44	0.47
3:N:1005:GLN:O	3:N:1009:LYS:HG2	2.14	0.47
3:N:1101:VAL:HG12	3:N:1374:GLN:HB3	1.96	0.47
3:N:1284:GLU:OE1	3:N:1285:GLU:CA	2.63	0.47
6:Q:14:DG:H5'	6:Q:14:DG:H8	1.80	0.47
2:C:164:PRO:CD	2:C:171:TRP:CD1	2.85	0.47
2:C:261:ILE:O	2:C:289:THR:HG23	2.15	0.47
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.50	0.47
3:D:596:SER:C	3:D:597:ASP:OD2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:816:LYS:HA	2:M:816:LYS:HD2	1.61	0.47
3:N:37:LEU:HD13	3:N:535:PHE:HZ	1.79	0.47
3:N:434:ARG:O	3:N:447:VAL:HG23	2.15	0.47
3:N:970:LYS:O	3:N:974:ILE:HG13	2.14	0.47
5:P:153:PRO:O	5:P:156:VAL:HG22	2.14	0.47
2:C:77:PRO:HB2	2:C:78:PHE:CD1	2.50	0.46
2:C:685:GLU:O	2:C:686:ASP:HB2	2.15	0.46
2:C:850:ALA:HA	3:D:632:VAL:HG21	1.95	0.46
2:M:168:ARG:HG3	2:M:268:ASP:HB3	1.97	0.46
2:M:229:MET:C	2:M:233:GLU:HB2	2.33	0.46
2:M:577:PRO:HB3	2:M:993:PHE:CG	2.50	0.46
3:N:17:LYS:O	3:N:20:SER:HB3	2.15	0.46
3:N:356:PRO:HG2	3:N:359:ALA:HB2	1.97	0.46
3:N:1283:ILE:HG22	3:N:1315:ASP:HB2	1.92	0.46
3:N:1290:LEU:HD21	3:N:1307:LYS:CE	2.43	0.46
3:D:242:LEU:HD23	3:D:285:PRO:HG3	1.96	0.46
3:D:368:VAL:HB	3:D:377:VAL:HB	1.97	0.46
3:D:1208:ASP:C	3:D:1208:ASP:OD1	2.52	0.46
3:D:1252:ILE:HG23	3:D:1253:THR:HG23	1.96	0.46
2:M:154:ARG:NH2	2:M:177:GLU:O	2.47	0.46
3:N:675:ARG:HH12	5:P:420:ASP:CG	2.18	0.46
3:N:1248:GLY:C	3:N:1250:ALA:H	2.18	0.46
3:N:1276:GLU:O	3:N:1277:ILE:HD13	2.15	0.46
3:N:1404:ASN:OD1	3:N:1415:VAL:HB	2.14	0.46
2:C:680:ASP:OD2	2:C:978:ARG:NH2	2.48	0.46
2:C:690:ILE:HB	2:C:852:ILE:HD13	1.97	0.46
2:C:843:HIS:NE2	2:C:887:GLU:OE2	2.49	0.46
3:D:558:LEU:HD23	3:D:567:ILE:HD12	1.96	0.46
3:D:843:PHE:CD1	3:D:864:VAL:HG11	2.50	0.46
1:K:34:VAL:HG22	1:L:42:ARG:NH2	2.31	0.46
1:L:54:THR:OG1	1:L:145:ASP:OD1	2.28	0.46
2:M:503:LEU:HD23	2:M:508:ILE:HA	1.97	0.46
2:M:541:SER:O	2:M:545:ASN:ND2	2.41	0.46
3:N:84:ILE:CD1	3:N:87:ARG:HD3	2.45	0.46
3:N:136:ASP:H	3:N:453:ASP:HB3	1.78	0.46
3:N:1284:GLU:O	3:N:1285:GLU:OE2	2.33	0.46
3:N:1486:VAL:HG22	4:O:75:PHE:HB3	1.97	0.46
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.96	0.46
2:C:690:ILE:HD13	2:C:690:ILE:HA	1.74	0.46
2:C:1071:ILE:O	3:D:659:LYS:HD3	2.14	0.46
2:C:1095:LEU:O	2:C:1096:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:58:CYS:HA	3:D:78:VAL:CG1	2.45	0.46
2:M:52:PHE:HB3	2:M:53:PRO:HA	1.97	0.46
2:M:135:VAL:HG23	2:M:395:LYS:HG3	1.96	0.46
2:M:289:THR:HG22	2:M:291:ALA:H	1.80	0.46
2:M:366:SER:O	2:M:367:LEU:HD23	2.15	0.46
2:M:605:LYS:HB2	2:M:612:VAL:HB	1.98	0.46
2:M:690:ILE:HD13	2:M:690:ILE:HA	1.74	0.46
3:N:892:ASP:OD1	3:N:894:LYS:HD2	2.12	0.46
3:N:1310:ARG:CD	3:N:1327:ARG:NH1	2.47	0.46
1:A:32:PHE:HA	1:A:35:THR:HB	1.97	0.46
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.97	0.46
2:C:102:HIS:CB	2:C:105:THR:HG21	2.45	0.46
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.30	0.46
3:D:373:PRO:HA	3:D:376:GLU:OE2	2.16	0.46
3:D:1231:GLU:N	3:D:1232:PRO:CD	2.79	0.46
2:M:845:ASN:HD22	2:M:845:ASN:C	2.18	0.46
3:N:134:VAL:CG2	3:N:151:GLN:H	2.28	0.46
3:N:999:THR:O	3:N:1003:VAL:HG13	2.16	0.46
3:N:1353:GLN:O	3:N:1357:ARG:HG3	2.15	0.46
7:R:2:DA:H5'	7:R:2:DA:C8	2.50	0.46
1:B:175:ARG:N	1:B:200:TRP:O	2.43	0.46
3:D:56:TYR:CE1	3:D:69:GLU:HG3	2.49	0.46
3:D:243:ALA:HB3	3:D:311:LEU:HD21	1.97	0.46
3:D:1283:ILE:CD1	3:D:1315:ASP:OD2	2.64	0.46
2:M:1001:VAL:HG11	3:N:725:SER:HB3	1.97	0.46
3:N:90:MET:HE3	3:N:519:VAL:O	2.16	0.46
3:N:204:LEU:HD21	3:N:445:ARG:NH1	2.31	0.46
3:N:1326:THR:HG22	3:N:1327:ARG:N	2.28	0.46
3:N:1472:ILE:O	3:N:1477:GLY:HA3	2.16	0.46
2:C:102:HIS:CG	2:C:105:THR:HB	2.50	0.46
2:C:236:ILE:O	2:C:240:THR:HG23	2.16	0.46
2:C:550:LEU:HD23	2:C:905:ILE:HG21	1.97	0.46
3:D:274:ARG:CZ	3:D:279:VAL:HG21	2.46	0.46
7:H:18:DC:H2'	7:H:19:DG:C8	2.51	0.46
2:M:1056:LYS:O	3:N:624:ASP:N	2.44	0.46
3:N:47:GLU:C	3:N:78:VAL:HG22	2.36	0.46
3:N:829:VAL:O	3:N:830:ALA:HB3	2.15	0.46
4:O:68:LEU:HD12	4:O:68:LEU:HA	1.79	0.46
5:P:220:LEU:HD11	5:P:235:PHE:HE2	1.81	0.46
6:Q:18:DA:H2"	6:Q:19:DG:H5'	1.98	0.46
3:D:134:VAL:HG23	3:D:150:ARG:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:907:GLU:OE1	3:D:909:ASN:N	2.48	0.46
5:F:393:THR:O	5:F:396:ARG:HB3	2.16	0.46
1:L:94:LEU:HD12	1:L:96:THR:H	1.81	0.46
2:M:444:PRO:CG	2:M:452:ILE:HB	2.45	0.46
3:N:135:LEU:HD23	3:N:463:GLN:HG2	1.98	0.46
3:N:474:GLU:HG3	3:N:496:LEU:HD11	1.97	0.46
3:N:613:ARG:HG3	3:N:618:LEU:CD2	2.46	0.46
3:N:1339:LYS:HG2	3:N:1343:ALA:HB2	1.97	0.46
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.98	0.46
2:C:764:GLU:OE1	2:C:764:GLU:N	2.42	0.46
3:D:36:THR:O	3:D:37:LEU:CB	2.58	0.46
3:D:46:ASP:OD2	3:D:48:ARG:NE	2.46	0.46
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.27	0.46
1:K:206:THR:O	1:K:207:PRO:C	2.54	0.46
1:L:97:VAL:HG12	1:L:98:THR:N	2.31	0.46
2:M:77:PRO:HB2	2:M:78:PHE:CD1	2.51	0.46
2:M:173:ASP:C	2:M:174:LEU:CD1	2.85	0.46
3:N:222:GLY:HA2	3:N:333:LEU:O	2.16	0.46
3:N:1280:VAL:HG22	3:N:1281:VAL:N	2.31	0.46
3:N:1305:LEU:O	3:N:1306:PRO:C	2.55	0.46
5:P:114:LYS:O	5:P:117:SER:OG	2.24	0.46
2:C:5:ARG:HB3	2:C:902:ILE:HB	1.98	0.46
2:C:1081:VAL:HA	2:C:1082:PRO:HD3	1.85	0.46
3:D:134:VAL:CG2	3:D:151:GLN:H	2.29	0.46
3:D:331:VAL:O	3:D:331:VAL:HG13	2.16	0.46
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.97	0.46
3:D:1314:LYS:HG3	3:D:1317:ASP:OD2	2.16	0.46
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.97	0.46
5:F:281:GLU:OE2	5:F:282:LEU:HD21	2.15	0.46
1:L:38:ASN:HB2	1:L:39:PRO:HD3	1.97	0.46
1:L:154:GLU:H	1:L:154:GLU:CD	2.19	0.46
2:M:198:ARG:HH11	2:M:230:ARG:CA	2.28	0.46
2:M:404:LEU:O	2:M:404:LEU:HG	2.15	0.46
3:N:472:ALA:O	3:N:476:GLU:HG3	2.16	0.46
3:N:778:LEU:HD23	3:N:778:LEU:HA	1.63	0.46
3:N:890:VAL:HG11	3:N:922:LEU:CD1	2.46	0.46
3:N:916:TYR:CE1	3:N:920:LEU:HD11	2.51	0.46
3:N:1400:VAL:CG2	3:N:1417:TRP:HD1	2.29	0.46
2:C:150:PRO:HD3	2:C:322:VAL:HG13	1.96	0.45
2:C:1008:ARG:NH1	2:C:1028:GLY:HA2	2.29	0.45
3:D:564:GLU:OE2	5:F:140:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:650:LEU:HD12	3:D:657:LEU:CD2	2.46	0.45
3:D:808:THR:HG22	3:D:810:GLU:N	2.31	0.45
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.50	0.45
1:L:138:LEU:HD11	1:L:140:MET:HE2	1.98	0.45
1:L:206:THR:H	1:L:209:GLU:HB2	1.81	0.45
2:M:604:ALA:O	2:M:645:VAL:HG13	2.16	0.45
2:M:644:VAL:HG22	2:M:645:VAL:N	2.32	0.45
2:M:675:ALA:HB2	2:M:867:VAL:HG11	1.98	0.45
1:A:201:THR:CG2	1:A:202:ASP:N	2.79	0.45
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.51	0.45
3:D:38:LYS:HD2	3:D:38:LYS:HA	1.68	0.45
3:D:145:VAL:HB	3:D:146:PRO:HD2	1.98	0.45
3:D:1136:LYS:O	3:D:1140:ILE:HG13	2.16	0.45
5:F:374:GLY:HA2	5:F:379:ARG:O	2.15	0.45
1:K:193:ASP:HB3	2:M:938:LYS:CE	2.45	0.45
3:N:1100:ASP:OD1	3:N:1440:PHE:HB2	2.16	0.45
3:N:1107:VAL:HA	3:N:1200:VAL:O	2.16	0.45
3:N:1459:LEU:HD12	3:N:1464:GLU:HB3	1.99	0.45
5:P:260:ILE:HG22	5:P:265:VAL:HG23	1.99	0.45
5:P:273:ARG:HA	5:P:276:ARG:NH1	2.31	0.45
2:C:439:CYS:HA	2:C:440:PRO:HD3	1.82	0.45
2:C:571:LEU:HD23	2:C:702:SER:HB3	1.97	0.45
2:C:1053:LEU:HA	3:D:621:LYS:HD2	1.97	0.45
3:D:355:VAL:HG13	3:D:359:ALA:HB3	1.98	0.45
3:D:922:LEU:N	3:D:922:LEU:HD23	2.32	0.45
3:D:1102:THR:CG2	3:D:1371:VAL:HG22	2.47	0.45
2:M:56:GLU:OE2	2:M:56:GLU:HA	2.16	0.45
2:M:419:THR:HB	2:M:422:ARG:CG	2.47	0.45
2:M:469:THR:HG23	2:M:471:TYR:CE1	2.51	0.45
3:N:904:VAL:HG23	3:N:905:PRO:HD2	1.98	0.45
3:N:1248:GLY:O	3:N:1249:ALA:HB3	2.16	0.45
3:N:1276:GLU:OE2	3:N:1301:LYS:CE	2.64	0.45
3:N:1283:ILE:CD1	3:N:1283:ILE:N	2.79	0.45
3:N:1304:LYS:CA	3:N:1305:LEU:HD23	2.45	0.45
2:C:229:MET:O	2:C:230:ARG:CD	2.58	0.45
3:D:573:MET:SD	5:F:210:LEU:HB3	2.56	0.45
3:D:778:LEU:HA	3:D:778:LEU:HD23	1.63	0.45
2:M:86:LYS:O	2:M:87:ASP:HB2	2.17	0.45
2:M:157:ARG:NH1	2:M:176:VAL:HG12	2.09	0.45
3:N:890:VAL:O	3:N:926:LYS:NZ	2.48	0.45
2:C:229:MET:HE2	2:C:234:ALA:CA	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:230:ARG:HD3	2:C:233:GLU:OE1	2.16	0.45
2:C:323:ASP:O	2:C:325:ILE:CG2	2.65	0.45
2:C:444:PRO:CG	2:C:452:ILE:HB	2.47	0.45
3:D:106:LYS:HD2	3:D:106:LYS:HA	1.60	0.45
3:D:1267:ARG:HG2	3:D:1331:ASP:OD2	2.16	0.45
3:D:1439:SER:HB2	3:D:1463:LYS:HZ1	1.77	0.45
3:D:1440:PHE:O	3:D:1441:GLN:CG	2.65	0.45
5:F:162:LYS:HE3	5:F:162:LYS:HB2	1.53	0.45
5:F:278:LEU:O	5:F:282:LEU:HG	2.17	0.45
5:F:372:ARG:HD3	5:F:401:GLU:OE2	2.17	0.45
5:F:418:LEU:HD12	5:F:418:LEU:H	1.81	0.45
1:L:123:MET:C	1:L:125:PRO:HD3	2.37	0.45
2:M:52:PHE:CD2	2:M:68:PHE:HB2	2.52	0.45
2:M:230:ARG:HG3	2:M:231:PRO:CD	2.46	0.45
3:N:843:PHE:CD1	3:N:864:VAL:HG11	2.50	0.45
1:B:201:THR:HG22	1:B:202:ASP:N	2.32	0.45
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.99	0.45
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.98	0.45
3:D:1440:PHE:O	3:D:1441:GLN:HG3	2.17	0.45
2:M:582:GLY:N	2:M:584:GLU:OE2	2.44	0.45
3:N:30:GLU:OE1	3:N:40:GLU:HG2	2.16	0.45
3:N:693:GLU:CA	4:O:48:MET:HE1	2.46	0.45
3:N:1237:THR:HG21	3:N:1246:VAL:CG1	2.42	0.45
3:N:1309:ALA:O	3:N:1310:ARG:HB3	2.16	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.64	0.45
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.98	0.45
5:F:88:ILE:HD12	5:F:88:ILE:HA	1.78	0.45
5:F:394:ARG:HG3	5:F:395:GLU:N	2.32	0.45
2:M:87:ASP:HA	2:M:131:GLY:HA3	1.98	0.45
5:P:401:GLU:HG3	5:P:402:ASN:N	2.32	0.45
2:C:717:LEU:HD12	2:C:717:LEU:N	2.32	0.45
3:D:1386:ASP:HB3	3:D:1412:LYS:HD2	1.98	0.45
3:D:1460:ILE:N	3:D:1460:ILE:HD13	2.30	0.45
5:F:390:PHE:CD1	5:F:397:ILE:HD11	2.51	0.45
1:L:64:GLU:O	1:L:75:VAL:HB	2.16	0.45
1:L:201:THR:HG22	1:L:202:ASP:N	2.31	0.45
2:M:302:VAL:C	2:M:305:PRO:HD2	2.37	0.45
2:M:680:ASP:H	3:N:943:THR:CG2	2.30	0.45
3:N:355:VAL:HG13	3:N:359:ALA:HB3	1.99	0.45
3:N:640:HIS:ND1	3:N:641:GLN:HG3	2.32	0.45
5:P:80:PRO:HB2	5:P:210:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:222:ARG:HA	5:P:222:ARG:HE	1.82	0.45
2:C:419:THR:HB	2:C:422:ARG:CG	2.47	0.45
2:C:858:MET:HG3	2:C:867:VAL:CG2	2.46	0.45
3:D:534:ARG:HH21	3:D:534:ARG:HG3	1.82	0.45
3:D:805:GLU:HA	3:D:828:LYS:O	2.17	0.45
1:L:190:THR:O	1:L:190:THR:HG22	2.17	0.45
2:M:261:ILE:O	2:M:289:THR:HG23	2.16	0.45
2:M:281:LEU:HD11	2:M:306:THR:HG22	1.98	0.45
5:P:237:THR:OG1	7:R:4:DA:H8	2.00	0.45
5:P:358:LEU:HD23	5:P:370:LYS:CE	2.47	0.45
1:B:91:ASN:HA	1:B:92:PRO:HD2	1.88	0.45
1:B:97:VAL:HG12	1:B:99:LEU:HD12	1.98	0.45
1:B:123:MET:C	1:B:125:PRO:HD3	2.36	0.45
1:B:143:ARG:HD3	1:B:158:ILE:HD13	1.99	0.45
1:B:190:THR:O	1:B:190:THR:HG22	2.17	0.45
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.52	0.45
2:C:1104:GLU:HB3	3:D:6:ARG:HG3	1.98	0.45
5:F:96:LEU:O	5:F:100:VAL:HG23	2.17	0.45
2:M:35:PRO:HG2	2:M:38:LYS:HB2	1.99	0.45
2:M:154:ARG:NH2	2:M:178:PRO:CA	2.80	0.45
2:M:1101:THR:HB	3:N:5:VAL:HG13	1.99	0.45
3:N:806:PHE:O	3:N:830:ALA:N	2.48	0.45
3:N:1123:PHE:CE1	3:N:1134:LEU:HD12	2.51	0.45
3:N:1478:SER:O	3:N:1482:ARG:HB2	2.17	0.45
5:P:338:LEU:HA	5:P:339:PRO:HD3	1.84	0.45
1:A:153:ALA:N	1:A:168:ASP:OD1	2.33	0.44
2:C:231:PRO:HG2	2:C:232:GLU:CD	2.37	0.44
2:C:1071:ILE:HG23	3:D:670:VAL:HG21	1.99	0.44
3:D:32:ILE:HG23	3:D:37:LEU:C	2.36	0.44
3:D:84:ILE:CD1	3:D:87:ARG:HD3	2.47	0.44
3:D:596:SER:C	3:D:597:ASP:CG	2.76	0.44
3:D:791:TYR:CD1	3:D:945:SER:HB2	2.52	0.44
3:D:1031:ASN:C	3:D:1031:ASN:OD1	2.56	0.44
3:D:1310:ARG:O	3:D:1310:ARG:HG2	2.17	0.44
2:M:280:LYS:HE3	2:M:309:TYR:CZ	2.52	0.44
2:M:480:THR:HG22	2:M:481:ASP:N	2.32	0.44
2:M:684:PHE:HE1	3:N:783:ARG:HB2	1.81	0.44
3:N:47:GLU:HG2	3:N:51:GLY:O	2.17	0.44
3:N:241:ILE:HD13	3:N:312:ARG:HB3	1.99	0.44
3:N:634:GLY:O	3:N:637:LEU:CD1	2.65	0.44
2:C:604:ALA:O	2:C:645:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1200:VAL:CG1	3:D:1201:CYS:N	2.80	0.44
3:N:97:THR:HG22	3:N:98:PRO:O	2.17	0.44
3:N:313:MET:HE1	3:N:319:ALA:HB2	1.99	0.44
3:N:661:MET:HE2	3:N:677:LEU:HD11	1.98	0.44
1:A:34:VAL:HG22	1:B:42:ARG:NH2	2.33	0.44
1:B:38:ASN:HB2	1:B:39:PRO:HD3	1.98	0.44
2:C:1060:ILE:HD13	5:F:338:LEU:HD13	1.98	0.44
3:D:1213:ARG:HB2	3:D:1214:PRO:HD2	1.98	0.44
3:D:1406:ARG:O	3:D:1410:GLU:HB3	2.17	0.44
1:L:56:VAL:HG21	1:L:82:LEU:CD1	2.47	0.44
2:M:639:GLN:HA	2:M:657:ASP:O	2.18	0.44
2:M:767:PRO:HB2	2:M:772:ARG:HD2	1.99	0.44
3:N:14:SER:HB3	3:N:511:TRP:CZ2	2.53	0.44
3:N:46:ASP:OD1	3:N:48:ARG:HG2	2.18	0.44
3:N:213:VAL:HG21	3:N:367:ILE:CD1	2.44	0.44
3:N:1126:ASP:OD2	3:N:1126:ASP:N	2.49	0.44
3:N:1255:GLY:O	3:N:1258:ARG:HB3	2.16	0.44
3:N:1439:SER:OG	3:N:1467:ILE:HD11	2.17	0.44
5:P:202:TYR:HB2	5:P:212:LEU:HD13	1.98	0.44
5:P:286:PRO:HB2	5:P:291:ILE:HG13	1.99	0.44
2:C:144:PRO:HG2	2:C:165:LEU:HD23	1.98	0.44
2:C:639:GLN:HA	2:C:657:ASP:O	2.18	0.44
2:C:873:PRO:HB2	3:D:949:ILE:CD1	2.48	0.44
3:D:133:ILE:HD12	3:D:152:LEU:HD23	2.00	0.44
3:D:237:LYS:N	3:D:240:GLU:OE1	2.49	0.44
1:K:30:ARG:HD3	1:K:191:ASP:OD1	2.17	0.44
2:M:229:MET:HE2	2:M:229:MET:HB3	1.86	0.44
2:M:323:ASP:O	2:M:325:ILE:HG22	2.17	0.44
3:N:71:LYS:O	3:N:80:VAL:HG22	2.17	0.44
3:N:215:TYR:CE1	3:N:380:GLU:O	2.70	0.44
3:N:252:ARG:NH2	3:N:303:PRO:HD3	2.32	0.44
3:N:808:THR:HG22	3:N:810:GLU:N	2.30	0.44
3:N:1477:GLY:O	3:N:1482:ARG:HD3	2.17	0.44
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.53	0.44
2:C:644:VAL:HG22	2:C:645:VAL:N	2.33	0.44
2:C:862:PRO:HA	2:C:975:TYR:CE2	2.52	0.44
2:C:1059:ASP:OD2	2:C:1062:GLY:HA3	2.18	0.44
2:M:237:ARG:HD2	2:M:241:LEU:HD21	1.99	0.44
2:M:439:CYS:HA	2:M:440:PRO:HD3	1.82	0.44
3:N:142:LEU:HG	3:N:143:ASN:H	1.82	0.44
3:N:170:PRO:HA	3:N:392:SER:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:1282:ARG:HB3	3:N:1293:PHE:HB2	1.98	0.44
3:N:1304:LYS:C	3:N:1305:LEU:CD2	2.78	0.44
3:N:1321:ALA:O	3:N:1339:LYS:HD3	2.17	0.44
5:P:412:GLU:O	5:P:416:ARG:HG3	2.18	0.44
1:B:58:ILE:HD13	1:B:140:MET:HB2	2.00	0.44
2:C:86:LYS:O	2:C:87:ASP:HB2	2.18	0.44
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.82	0.44
3:D:775:GLY:HA2	3:D:1209:LEU:O	2.17	0.44
5:F:259:ARG:HH11	5:F:259:ARG:CG	2.31	0.44
1:L:97:VAL:HG12	1:L:99:LEU:HD12	1.99	0.44
2:M:202:TYR:CE1	2:M:304:LEU:HD22	2.53	0.44
2:M:1008:ARG:NH1	2:M:1028:GLY:HA2	2.29	0.44
3:N:264:LEU:O	3:N:264:LEU:HD12	2.17	0.44
3:N:679:ARG:HD3	3:N:682:ASP:OD2	2.18	0.44
3:D:170:PRO:HA	3:D:392:SER:HB3	1.98	0.44
3:D:230:TRP:CD1	3:D:331:VAL:HG11	2.52	0.44
3:D:629:SER:O	3:D:744:GLN:HG2	2.17	0.44
3:D:661:MET:HE2	3:D:677:LEU:HD11	1.99	0.44
3:D:679:ARG:HD3	3:D:682:ASP:OD2	2.18	0.44
1:K:201:THR:CG2	1:K:202:ASP:N	2.81	0.44
2:M:167:LYS:HD3	2:M:167:LYS:HA	1.72	0.44
2:M:422:ARG:HH22	7:R:13:DT:H5”	1.82	0.44
2:M:437:ARG:HH22	2:M:491:GLU:HB2	1.83	0.44
2:M:535:SER:OG	2:M:537:LYS:HG3	2.18	0.44
2:M:604:ALA:HB3	2:M:612:VAL:HG12	1.99	0.44
3:N:145:VAL:HB	3:N:146:PRO:HD2	1.99	0.44
3:N:411:THR:CA	3:N:435:VAL:HG12	2.40	0.44
2:C:351:LEU:HD12	2:C:374:ASN:O	2.18	0.44
3:D:890:VAL:CG2	3:D:922:LEU:HD11	2.48	0.44
1:L:123:MET:O	1:L:125:PRO:HD3	2.17	0.44
3:N:989:TYR:CZ	3:N:993:LEU:HD11	2.53	0.44
5:P:393:THR:HG23	5:P:396:ARG:HB3	1.99	0.44
1:B:58:ILE:C	1:B:61:VAL:HG13	2.39	0.44
2:C:712:ALA:HB3	2:C:821:GLU:CG	2.47	0.44
2:C:1056:LYS:HE2	3:D:751:LEU:HG	1.99	0.44
2:C:1058:ASP:OD2	2:C:1084:SER:HB2	2.18	0.44
3:D:792:ILE:HD13	3:D:941:PHE:CE1	2.53	0.44
3:D:823:LEU:HD11	3:D:837:GLY:CA	2.44	0.44
3:D:904:VAL:HG23	3:D:905:PRO:HD2	1.99	0.44
3:D:1353:GLN:OE1	3:D:1353:GLN:HA	2.17	0.44
1:K:206:THR:HG22	1:K:208:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:74:ASP:O	1:L:78:ILE:HG13	2.18	0.44
2:M:206:THR:O	2:M:209:ARG:HD2	2.18	0.44
2:M:717:LEU:N	2:M:717:LEU:HD12	2.32	0.44
2:M:1095:LEU:O	2:M:1096:ALA:HB3	2.18	0.44
3:N:669:ASN:HD22	5:P:417:LYS:CD	2.30	0.44
3:N:1311:LEU:HD22	3:N:1311:LEU:H	1.71	0.44
3:N:1386:ASP:HB2	3:N:1412:LYS:HD2	2.00	0.44
3:N:1487:VAL:CG2	3:N:1491:THR:HB	2.47	0.44
4:O:57:ASP:HA	4:O:58:PRO:HD3	1.85	0.44
1:A:206:THR:O	1:A:207:PRO:C	2.54	0.43
1:B:80:LEU:HB3	3:D:867:ARG:NH2	2.33	0.43
2:C:281:LEU:HD11	2:C:306:THR:HG22	2.00	0.43
2:C:572:ILE:HG13	2:C:573:ARG:HG3	2.00	0.43
2:C:680:ASP:H	3:D:943:THR:CG2	2.32	0.43
2:C:836:GLY:C	2:C:1001:VAL:HG22	2.39	0.43
3:D:314:PRO:HD2	3:D:317:VAL:CG1	2.48	0.43
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.99	0.43
3:D:709:HIS:HA	3:D:1227:GLN:HB3	1.99	0.43
5:F:278:LEU:HD11	5:F:294:ALA:CB	2.47	0.43
1:L:161:ARG:HE	1:L:161:ARG:HB2	1.63	0.43
1:L:185:ARG:CG	1:L:190:THR:HG23	2.48	0.43
2:M:223:ASP:HA	2:M:224:GLU:OE2	2.18	0.43
2:M:376:ARG:HB2	2:M:377:PRO:HD3	2.00	0.43
2:M:684:PHE:HB3	3:N:633:VAL:HG21	2.00	0.43
3:N:314:PRO:HG2	3:N:317:VAL:HG11	1.99	0.43
3:N:598:ARG:NH2	5:P:316:SER:OG	2.51	0.43
3:N:835:SER:HB2	3:N:838:ARG:HE	1.66	0.43
3:N:907:GLU:OE1	3:N:909:ASN:N	2.51	0.43
2:C:176:VAL:HG12	2:C:177:GLU:O	2.19	0.43
2:C:541:SER:O	2:C:545:ASN:ND2	2.40	0.43
2:C:841:ASN:C	2:C:841:ASN:OD1	2.56	0.43
5:F:81:VAL:O	5:F:85:LEU:HG	2.18	0.43
5:F:376:ILE:C	5:F:378:GLY:H	2.21	0.43
1:K:83:LYS:CE	1:K:168:ASP:HB2	2.46	0.43
1:L:58:ILE:HD13	1:L:140:MET:HB2	2.00	0.43
1:L:88:ARG:HD2	1:L:123:MET:HE2	2.00	0.43
2:M:572:ILE:HG13	2:M:573:ARG:HG3	2.00	0.43
2:M:637:LEU:HA	2:M:659:PRO:HG3	2.00	0.43
3:N:597:ASP:HB2	3:N:598:ARG:H	1.56	0.43
3:N:1284:GLU:O	3:N:1285:GLU:CD	2.57	0.43
3:N:1353:GLN:HG2	3:N:1368:ILE:HD12	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:350:LEU:O	5:P:354:LEU:HG	2.18	0.43
1:A:57:TYR:CZ	1:A:161:ARG:HD2	2.52	0.43
1:B:117:VAL:O	1:B:118:ALA:C	2.57	0.43
2:C:469:THR:HG23	2:C:471:TYR:CE1	2.54	0.43
2:C:706:GLU:OE1	2:C:706:GLU:HA	2.18	0.43
2:C:911:GLU:N	2:C:912:PRO:CD	2.81	0.43
2:C:937:ASP:OD1	2:C:939:ARG:CG	2.66	0.43
3:D:142:LEU:HG	3:D:143:ASN:H	1.84	0.43
3:D:1373:ARG:HE	3:D:1373:ARG:HB2	1.55	0.43
2:M:1058:ASP:OD2	2:M:1084:SER:HB2	2.19	0.43
3:N:204:LEU:HD23	3:N:441:ARG:CZ	2.49	0.43
3:N:648:MET:O	3:N:652:LEU:HG	2.18	0.43
3:N:1171:VAL:O	3:N:1175:ILE:HG13	2.18	0.43
5:P:371:LEU:HA	5:P:381:HIS:HD2	1.83	0.43
5:P:372:ARG:O	5:P:380:GLU:HB2	2.17	0.43
1:B:138:LEU:HD11	1:B:140:MET:HE2	2.00	0.43
1:B:185:ARG:CG	1:B:190:THR:HG23	2.49	0.43
2:C:223:ASP:HA	2:C:224:GLU:OE2	2.19	0.43
2:C:480:THR:HG22	2:C:481:ASP:N	2.32	0.43
2:C:699:PHE:O	2:C:700:TYR:HB2	2.18	0.43
2:C:719:PRO:HD2	2:C:761:PHE:HE1	1.82	0.43
2:C:937:ASP:OD1	2:C:939:ARG:HG3	2.17	0.43
7:H:2:DA:H5'	7:H:2:DA:C8	2.53	0.43
2:M:375:SER:O	2:M:378:LEU:N	2.51	0.43
3:N:827:ILE:CG2	3:N:828:LYS:N	2.80	0.43
1:B:56:VAL:HG21	1:B:82:LEU:CD1	2.48	0.43
1:B:58:ILE:HG21	1:B:61:VAL:CG1	2.37	0.43
3:D:314:PRO:HD2	3:D:317:VAL:HG11	1.99	0.43
3:D:529:GLN:HA	3:D:534:ARG:O	2.18	0.43
3:D:629:SER:C	3:D:744:GLN:HG2	2.39	0.43
3:D:1313:VAL:HG23	3:D:1313:VAL:O	2.19	0.43
5:F:95:THR:HG22	5:F:96:LEU:H	1.82	0.43
5:F:144:ILE:HB	5:F:147:LEU:HB2	2.01	0.43
5:F:228:GLU:OE2	5:F:231:ARG:NE	2.49	0.43
5:F:295:MET:HA	5:F:295:MET:HE3	2.00	0.43
2:M:90:TYR:CD2	2:M:120:LEU:HB2	2.54	0.43
2:M:308:ARG:HE	2:M:308:ARG:HB3	1.70	0.43
2:M:524:VAL:HG11	2:M:528:GLU:HB2	1.99	0.43
2:M:706:GLU:OE1	2:M:706:GLU:HA	2.18	0.43
3:N:315:ARG:O	3:N:316:GLN:CB	2.65	0.43
3:N:1403:LEU:O	3:N:1406:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:172:ARG:O	5:P:176:ILE:HG12	2.18	0.43
1:B:123:MET:O	1:B:125:PRO:HD3	2.18	0.43
2:C:35:PRO:HG2	2:C:38:LYS:HB2	2.00	0.43
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.01	0.43
2:C:376:ARG:HB2	2:C:377:PRO:HD3	2.01	0.43
2:C:910:LYS:HB3	2:C:912:PRO:HD2	2.00	0.43
3:D:1277:ILE:HG22	3:D:1278:ASP:N	2.27	0.43
3:D:1429:LEU:HD21	3:D:1441:GLN:HB2	2.01	0.43
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.81	0.43
1:K:36:LEU:HD23	1:K:36:LEU:HA	1.85	0.43
2:M:905:ILE:C	2:M:907:ASP:H	2.22	0.43
2:M:910:LYS:HB3	2:M:912:PRO:HD2	1.99	0.43
2:M:1092:LEU:HD13	2:M:1099:VAL:HG21	2.00	0.43
3:N:68:PHE:O	3:N:80:VAL:HG21	2.17	0.43
3:N:570:GLU:OE2	5:P:214:GLN:NE2	2.48	0.43
3:N:900:ILE:H	3:N:900:ILE:HG13	1.63	0.43
3:N:959:GLU:HB3	3:N:963:TYR:HE1	1.84	0.43
1:B:88:ARG:HD2	1:B:123:MET:HE2	2.00	0.43
2:C:561:GLY:O	2:C:565:GLN:HG3	2.19	0.43
3:D:613:ARG:HG3	3:D:618:LEU:CD2	2.48	0.43
3:D:696:HIS:HD2	4:E:57:ASP:OD1	2.00	0.43
5:F:383:LEU:O	5:F:397:ILE:HG21	2.19	0.43
1:K:89:PHE:HB2	1:K:146:ARG:NH2	2.33	0.43
1:L:143:ARG:HD3	1:L:158:ILE:HD13	1.99	0.43
2:M:136:ILE:HD13	2:M:392:SER:HA	2.01	0.43
2:M:176:VAL:CG1	2:M:177:GLU:O	2.67	0.43
2:M:911:GLU:N	2:M:912:PRO:CD	2.81	0.43
3:N:367:ILE:HB	3:N:377:VAL:HG12	2.01	0.43
3:N:1462:LEU:HD23	3:N:1473:PRO:HG2	2.00	0.43
2:C:260:LEU:C	2:C:261:ILE:HD12	2.39	0.43
2:C:524:VAL:HG11	2:C:528:GLU:HB2	1.99	0.43
3:D:145:VAL:HB	3:D:146:PRO:CD	2.48	0.43
3:D:207:PHE:HB2	3:D:391:ALA:HB2	2.01	0.43
3:D:356:PRO:HB3	3:D:441:ARG:HA	2.01	0.43
3:D:729:HIS:HA	3:D:730:PRO:HD3	1.91	0.43
3:D:1267:ARG:HA	3:D:1268:PRO:HD3	1.86	0.43
3:D:1403:LEU:O	3:D:1406:ARG:HB2	2.18	0.43
2:M:12:VAL:HG11	2:M:472:ARG:NH1	2.34	0.43
2:M:48:PHE:O	2:M:52:PHE:CD2	2.61	0.43
2:M:164:PRO:HB2	2:M:168:ARG:O	2.19	0.43
2:M:171:TRP:CE3	7:R:14:DG:OP1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:177:GLU:HG3	2:M:178:PRO:HD2	2.00	0.43
2:M:428:ARG:HB3	2:M:450:GLY:HA3	2.00	0.43
2:M:708:TYR:HB3	2:M:790:LEU:HD21	2.00	0.43
2:M:937:ASP:OD1	2:M:939:ARG:CG	2.66	0.43
3:N:245:LEU:HD22	3:N:249:TYR:HB3	2.01	0.43
3:N:520:LEU:HD12	3:N:521:PRO:HD2	1.99	0.43
3:N:1082:ALA:O	3:N:1086:LEU:HG	2.18	0.43
2:C:302:VAL:C	2:C:305:PRO:HD2	2.38	0.43
2:C:807:ARG:HE	2:C:807:ARG:HB2	1.56	0.43
3:D:1005:GLN:O	3:D:1009:LYS:HG2	2.19	0.43
3:D:1188:VAL:HG13	3:D:1189:ARG:O	2.19	0.43
1:L:48:ILE:HA	1:L:49:PRO:HD3	1.71	0.43
1:L:117:VAL:O	1:L:118:ALA:C	2.57	0.43
2:M:1032:PHE:HZ	2:M:1040:LEU:HG	1.84	0.43
2:M:1059:ASP:OD2	2:M:1062:GLY:HA3	2.19	0.43
3:N:133:ILE:CG2	3:N:460:ALA:HB1	2.48	0.43
3:N:801:GLY:HA2	3:N:821:VAL:HG13	2.01	0.43
3:N:1208:ASP:C	3:N:1208:ASP:OD1	2.57	0.43
3:N:1309:ALA:O	3:N:1310:ARG:HB2	2.18	0.43
5:P:78:SER:O	5:P:79:ASP:C	2.58	0.43
5:P:362:SER:HB3	5:P:365:GLU:CG	2.49	0.43
2:C:36:PRO:HA	2:C:39:ARG:HG3	2.01	0.43
3:D:634:GLY:O	3:D:637:LEU:CD1	2.66	0.43
3:D:984:THR:HG22	3:D:985:ASP:N	2.34	0.43
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.51	0.43
1:L:124:ASN:N	1:L:124:ASN:OD1	2.52	0.43
2:M:304:LEU:HB3	2:M:305:PRO:HD3	2.01	0.43
2:M:841:ASN:C	2:M:841:ASN:OD1	2.57	0.43
1:B:97:VAL:HG12	1:B:98:THR:N	2.33	0.42
2:C:202:TYR:CE1	2:C:304:LEU:HD22	2.53	0.42
3:D:155:ASP:O	3:D:159:ARG:HG3	2.18	0.42
3:N:269:PHE:CE2	3:N:283:PHE:HD1	2.37	0.42
3:N:959:GLU:OE1	3:N:959:GLU:N	2.45	0.42
3:N:1495:ILE:HG21	4:O:80:VAL:HG21	2.00	0.42
5:P:101:GLU:CG	5:P:105:LYS:HE2	2.49	0.42
1:B:101:LEU:HD21	1:B:109:VAL:HG11	2.01	0.42
2:C:292:ARG:NE	2:C:299:LYS:HD3	2.34	0.42
2:C:474:VAL:HG22	2:C:479:VAL:HG22	2.01	0.42
3:D:434:ARG:NH1	5:F:135:ILE:O	2.52	0.42
3:D:618:LEU:HG	3:D:1467:ILE:HG23	2.01	0.42
5:F:114:LYS:O	5:F:118:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:133:GLU:HG2	1:K:134:GLU:H	1.83	0.42
2:M:51:THR:HG21	2:M:352:ALA:HB2	2.01	0.42
2:M:552:HIS:CD2	2:M:886:LEU:HD12	2.54	0.42
2:M:879:ARG:N	2:M:879:ARG:HD2	2.34	0.42
2:M:1056:LYS:HE2	3:N:751:LEU:HG	2.01	0.42
3:N:108:VAL:HB	3:N:109:PRO:CD	2.46	0.42
3:N:367:ILE:HD11	3:N:379:ALA:HB2	2.01	0.42
3:N:593:ASN:OD1	3:N:594:PRO:HD3	2.20	0.42
3:N:719:VAL:O	3:N:721:VAL:HG13	2.20	0.42
3:N:890:VAL:HG11	3:N:922:LEU:HD12	2.01	0.42
3:N:1101:VAL:HG21	3:N:1424:VAL:CB	2.49	0.42
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.33	0.42
2:C:231:PRO:CG	2:C:232:GLU:OE2	2.59	0.42
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.34	0.42
2:C:1001:VAL:HG13	3:D:630:VAL:HB	2.00	0.42
3:D:65:ARG:HG3	5:F:378:GLY:O	2.19	0.42
3:D:142:LEU:HD13	3:D:161:LEU:CD1	2.48	0.42
3:D:758:GLU:OE1	3:D:1476:THR:OG1	2.26	0.42
3:D:827:ILE:CG2	3:D:828:LYS:N	2.82	0.42
3:D:894:LYS:N	3:D:894:LYS:CD	2.30	0.42
3:D:957:PRO:HG3	3:D:1007:VAL:HA	2.01	0.42
1:L:5:LYS:HE3	1:L:6:LEU:H	1.84	0.42
3:N:791:TYR:CD1	3:N:945:SER:HB2	2.53	0.42
3:N:957:PRO:HG3	3:N:1007:VAL:HA	2.02	0.42
3:D:275:GLU:HB3	3:D:276:ASP:H	1.57	0.42
3:D:553:ARG:HD3	5:F:214:GLN:HB3	2.02	0.42
3:D:890:VAL:CB	3:D:922:LEU:HD11	2.45	0.42
3:D:959:GLU:HB3	3:D:963:TYR:HE1	1.85	0.42
5:F:127:ILE:O	5:F:131:VAL:HG23	2.19	0.42
5:F:350:LEU:HD13	5:F:421:PHE:CD1	2.55	0.42
5:F:418:LEU:H	5:F:418:LEU:CD1	2.32	0.42
1:K:34:VAL:HG22	1:L:42:ARG:CZ	2.49	0.42
1:L:124:ASN:HD22	1:L:127:LEU:HB2	1.84	0.42
2:M:54:ILE:HG23	2:M:356:ARG:HG3	2.01	0.42
2:M:105:THR:CG2	2:M:107:LEU:N	2.60	0.42
2:M:470:PRO:HD3	2:M:485:TYR:CE2	2.55	0.42
2:M:836:GLY:C	2:M:1001:VAL:HG22	2.39	0.42
2:M:937:ASP:OD1	2:M:939:ARG:HG3	2.18	0.42
2:M:998:TYR:CG	2:M:998:TYR:O	2.73	0.42
3:N:138:LYS:HB2	3:N:451:ASP:O	2.17	0.42
3:N:598:ARG:NH2	5:P:316:SER:CB	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:827:ILE:O	3:N:834:THR:N	2.45	0.42
3:N:1286:THR:HG22	3:N:1288:GLU:N	2.32	0.42
1:A:44:LEU:HA	1:A:48:ILE:HG12	2.01	0.42
2:C:64:LEU:CD1	2:C:367:LEU:HD12	2.50	0.42
2:C:236:ILE:HG23	2:C:248:PRO:CB	2.50	0.42
2:C:559:LEU:C	2:C:559:LEU:HD23	2.39	0.42
3:D:128:TYR:CZ	3:D:587:ARG:HD2	2.55	0.42
3:D:367:ILE:HD11	3:D:379:ALA:HB2	2.01	0.42
3:D:520:LEU:HD12	3:D:521:PRO:HD2	2.00	0.42
3:D:1106:VAL:O	3:D:1108:ARG:HG3	2.20	0.42
3:D:1373:ARG:HG3	3:D:1374:GLN:N	2.35	0.42
1:L:201:THR:CG2	1:L:202:ASP:N	2.82	0.42
2:M:151:ASP:OD2	2:M:175:GLU:OE2	2.38	0.42
2:M:1071:ILE:HG23	3:N:670:VAL:HG21	2.02	0.42
2:M:1081:VAL:HA	2:M:1082:PRO:HD3	1.85	0.42
3:N:1031:ASN:C	3:N:1031:ASN:OD1	2.58	0.42
3:N:1312:LEU:CD2	3:N:1327:ARG:CG	2.90	0.42
1:B:201:THR:CG2	1:B:202:ASP:N	2.83	0.42
2:C:229:MET:CE	2:C:234:ALA:CA	2.96	0.42
2:C:774:LEU:HD21	5:F:418:LEU:HB3	2.02	0.42
3:D:187:LYS:HG3	3:D:198:ARG:O	2.20	0.42
3:D:259:VAL:O	3:D:295:GLY:N	2.44	0.42
3:D:640:HIS:ND1	3:D:641:GLN:HG3	2.34	0.42
4:E:34:GLY:O	4:E:35:PHE:HB2	2.19	0.42
2:M:187:ASN:HD22	2:M:187:ASN:HA	1.63	0.42
2:M:918:LEU:HD23	2:M:918:LEU:HA	1.95	0.42
3:N:48:ARG:CZ	3:N:76:CYS:O	2.68	0.42
3:N:266:GLU:HG2	3:N:286:VAL:HB	2.01	0.42
3:N:553:ARG:HD3	5:P:214:GLN:HB3	2.01	0.42
3:N:801:GLY:HA3	3:N:825:ALA:HB1	2.01	0.42
3:N:1003:VAL:O	3:N:1007:VAL:HG23	2.20	0.42
5:P:222:ARG:HA	5:P:222:ARG:NE	2.34	0.42
2:C:690:ILE:HG23	2:C:694:LEU:HD12	2.01	0.42
2:C:1001:VAL:HG11	3:D:725:SER:HB3	2.01	0.42
3:D:47:GLU:C	3:D:78:VAL:CG2	2.88	0.42
3:D:67:ARG:CZ	5:F:379:ARG:HB2	2.50	0.42
3:D:231:VAL:O	3:D:231:VAL:HG22	2.20	0.42
3:D:1321:ALA:O	3:D:1339:LYS:HD3	2.19	0.42
5:F:230:LYS:O	5:F:232:ARG:CG	2.67	0.42
2:M:289:THR:HG21	2:M:291:ALA:O	2.19	0.42
2:M:327:HIS:HE1	2:M:488:ALA:C	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:717:LEU:HD23	2:M:763:GLY:CA	2.43	0.42
2:M:1001:VAL:HG13	3:N:630:VAL:HB	2.02	0.42
3:N:33:ASN:CB	3:N:36:THR:HG23	2.43	0.42
3:N:35:ARG:CB	3:N:35:ARG:HH11	2.32	0.42
3:N:111:LYS:HG3	3:N:1452:ILE:CD1	2.49	0.42
3:N:134:VAL:HG22	3:N:151:GLN:O	2.20	0.42
3:N:568:ARG:HD2	5:P:87:GLU:OE1	2.20	0.42
3:N:784:ASP:HB2	3:N:939:PHE:HE2	1.84	0.42
3:N:827:ILE:HG23	3:N:828:LYS:N	2.34	0.42
3:N:1256:LEU:O	3:N:1260:ILE:HG13	2.19	0.42
3:N:1283:ILE:O	3:N:1283:ILE:CG1	2.67	0.42
1:B:74:ASP:O	1:B:78:ILE:HG13	2.20	0.42
1:B:179:PHE:CB	1:B:197:LEU:HD13	2.49	0.42
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.02	0.42
2:C:118:ILE:HD11	2:C:344:PHE:HE2	1.80	0.42
2:C:604:ALA:HB3	2:C:612:VAL:HG12	2.01	0.42
3:D:560:GLN:HE22	5:F:222:ARG:HH11	1.68	0.42
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.55	0.42
5:F:270:LYS:HE2	5:F:295:MET:CE	2.50	0.42
2:M:48:PHE:HA	2:M:348:LEU:HD21	2.02	0.42
2:M:289:THR:HG22	2:M:291:ALA:O	2.20	0.42
2:M:695:LEU:HD23	2:M:695:LEU:N	2.34	0.42
3:N:33:ASN:OD1	3:N:36:THR:CG2	2.67	0.42
3:N:140:ALA:HA	3:N:450:TYR:CG	2.55	0.42
3:N:187:LYS:HG3	3:N:198:ARG:O	2.20	0.42
3:N:230:TRP:HA	3:N:243:ALA:HB2	2.01	0.42
3:N:530:VAL:HG22	3:N:534:ARG:O	2.20	0.42
4:O:61:VAL:O	4:O:65:MET:HG3	2.20	0.42
5:P:368:VAL:HG23	5:P:369:LEU:N	2.35	0.42
1:B:58:ILE:O	1:B:61:VAL:HG13	2.20	0.42
2:C:988:VAL:HG21	3:D:949:ILE:C	2.40	0.42
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	0.42
3:D:530:VAL:HG22	3:D:534:ARG:HB3	2.01	0.42
3:D:637:LEU:HD22	3:D:642:CYS:HA	2.02	0.42
3:D:794:GLN:OE1	3:D:794:GLN:HA	2.19	0.42
3:D:1285:GLU:HA	3:D:1290:LEU:HD22	2.02	0.42
5:F:102:LEU:O	5:F:106:VAL:HG23	2.20	0.42
5:F:260:ILE:HG22	5:F:265:VAL:HG23	2.01	0.42
2:M:118:ILE:HD11	2:M:344:PHE:HE2	1.81	0.42
2:M:260:LEU:C	2:M:261:ILE:HD12	2.39	0.42
2:M:693:GLU:HA	2:M:696:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:751:PRO:HB2	3:N:680:GLN:HB2	2.02	0.42
3:N:36:THR:OG1	3:N:38:LYS:HB2	2.20	0.42
3:N:44:LEU:HB3	3:N:525:ARG:NH2	2.35	0.42
3:N:580:ALA:HA	3:N:584:ASN:HA	2.02	0.42
2:C:675:ALA:HB2	2:C:867:VAL:HG11	2.01	0.42
2:C:786:LYS:HB3	2:C:786:LYS:HZ3	1.84	0.42
3:D:437:VAL:HG11	5:F:175:HIS:CE1	2.55	0.42
3:D:801:GLY:HA3	3:D:825:ALA:HB1	2.01	0.42
4:E:70:THR:HB	4:E:72:ARG:HG3	2.02	0.42
2:M:98:LEU:HD12	2:M:113:VAL:HG21	2.02	0.42
2:M:248:PRO:O	2:M:250:ARG:N	2.53	0.42
2:M:690:ILE:HG23	2:M:694:LEU:HD12	2.02	0.42
2:M:736:ASP:O	2:M:744:ARG:HG2	2.20	0.42
3:N:145:VAL:HB	3:N:146:PRO:CD	2.49	0.42
3:N:317:VAL:CG2	3:N:339:TRP:HB3	2.49	0.42
3:N:602:SER:O	3:N:606:ILE:HG13	2.19	0.42
3:N:1394:VAL:HG12	3:N:1395:LEU:N	2.34	0.42
2:C:54:ILE:HG23	2:C:356:ARG:HG3	2.02	0.41
2:C:64:LEU:HD11	2:C:367:LEU:HD12	2.02	0.41
2:C:289:THR:HG22	2:C:290:LEU:N	2.34	0.41
2:C:592:LEU:N	2:C:592:LEU:HD23	2.35	0.41
2:C:642:ARG:HD3	2:C:642:ARG:HA	1.90	0.41
2:C:1090:LYS:HA	2:C:1090:LYS:HD2	1.88	0.41
3:D:1420:LEU:HD12	3:D:1420:LEU:HA	1.89	0.41
1:L:101:LEU:HD21	1:L:109:VAL:HG11	2.02	0.41
1:L:128:HIS:HE1	1:L:131:THR:CG2	2.33	0.41
2:M:102:HIS:O	2:M:106:GLY:CA	2.68	0.41
2:M:820:ARG:HE	2:M:820:ARG:HB2	1.59	0.41
2:M:999:HIS:HB3	2:M:1004:LYS:CE	2.49	0.41
3:N:36:THR:HG1	3:N:38:LYS:HB2	1.84	0.41
3:N:133:ILE:HD12	3:N:152:LEU:HD23	2.02	0.41
3:N:326:GLU:HG2	3:N:331:VAL:HG12	2.02	0.41
3:N:1374:GLN:HA	3:N:1374:GLN:OE1	2.19	0.41
5:P:228:GLU:OE2	5:P:231:ARG:NH2	2.53	0.41
1:A:23:PHE:HE1	1:A:208:LEU:HD12	1.85	0.41
2:C:258:TYR:CD2	2:C:262:ALA:HB3	2.56	0.41
2:C:404:LEU:O	2:C:404:LEU:HG	2.20	0.41
3:D:80:VAL:HG23	3:D:80:VAL:O	2.20	0.41
3:D:261:LEU:HD12	3:D:269:PHE:O	2.20	0.41
3:D:801:GLY:O	3:D:804:LEU:HG	2.21	0.41
5:F:228:GLU:OE2	5:F:231:ARG:NH2	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:14:DG:H5'	6:G:14:DG:H8	1.85	0.41
1:K:150:TYR:CD1	2:M:696:LYS:HG2	2.55	0.41
2:M:100:LEU:HD23	2:M:367:LEU:O	2.20	0.41
2:M:487:THR:HG23	2:M:490:GLU:HB2	1.96	0.41
2:M:571:LEU:HD22	2:M:700:TYR:HA	2.01	0.41
2:M:776:SER:O	5:P:405:LEU:HD21	2.21	0.41
3:N:483:HIS:HA	3:N:484:PRO:HD3	1.85	0.41
3:N:794:GLN:HA	3:N:794:GLN:OE1	2.19	0.41
5:P:263:HIS:HA	5:P:266:GLU:HG2	2.01	0.41
1:B:124:ASN:OD1	1:B:124:ASN:N	2.54	0.41
2:C:736:ASP:O	2:C:744:ARG:HG2	2.19	0.41
2:C:999:HIS:HB3	2:C:1004:LYS:CE	2.49	0.41
3:D:1353:GLN:O	3:D:1357:ARG:HG3	2.20	0.41
2:M:163:ILE:HA	2:M:164:PRO:HD2	1.93	0.41
3:N:468:LEU:HD23	3:N:468:LEU:HA	1.86	0.41
3:N:890:VAL:CG2	3:N:922:LEU:HD11	2.49	0.41
1:B:185:ARG:HA	1:B:189:ARG:O	2.21	0.41
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.89	0.41
2:C:340:MET:SD	2:C:340:MET:C	2.98	0.41
2:C:905:ILE:C	2:C:907:ASP:H	2.23	0.41
2:C:1032:PHE:HZ	2:C:1040:LEU:HG	1.85	0.41
3:D:243:ALA:O	3:D:311:LEU:HD23	2.20	0.41
3:D:288:MET:CE	3:D:305:ALA:HB3	2.50	0.41
4:E:36:LYS:HE3	4:E:36:LYS:HB3	1.76	0.41
2:M:184:MET:HE1	2:M:191:PHE:CZ	2.56	0.41
2:M:325:ILE:O	2:M:325:ILE:HG13	2.13	0.41
2:M:394:PHE:CE2	2:M:632:ASN:HB3	2.55	0.41
3:N:37:LEU:HD13	3:N:535:PHE:CE1	2.54	0.41
3:N:103:TRP:CZ2	3:N:1444:THR:HG22	2.55	0.41
3:N:116:LEU:HD21	3:N:465:LEU:HD23	2.02	0.41
3:N:273:ARG:HG2	3:N:277:GLU:C	2.41	0.41
3:N:785:ILE:HD13	3:N:935:LYS:HA	2.02	0.41
5:P:135:ILE:HD13	5:P:135:ILE:HA	1.96	0.41
5:P:408:LEU:O	5:P:408:LEU:HD23	2.20	0.41
6:Q:11:DT:H2"	6:Q:12:DG:C8	2.55	0.41
1:A:184:THR:CG2	1:A:192:LEU:CB	2.81	0.41
1:A:184:THR:CG2	1:A:192:LEU:HB2	2.45	0.41
2:C:918:LEU:HD23	2:C:918:LEU:HA	1.94	0.41
3:D:207:PHE:HB2	3:D:391:ALA:CB	2.51	0.41
3:D:472:ALA:O	3:D:476:GLU:HG3	2.19	0.41
3:D:849:ALA:O	3:D:852:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:959:GLU:OE1	3:D:959:GLU:N	2.44	0.41
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.20	0.41
5:F:256:ARG:NH2	5:F:311:ALA:O	2.53	0.41
1:K:44:LEU:HA	1:K:48:ILE:HG12	2.02	0.41
2:M:569:VAL:HG21	2:M:1000:MET:HE1	2.02	0.41
3:N:356:PRO:HB3	3:N:441:ARG:HA	2.02	0.41
3:N:410:SER:O	3:N:435:VAL:HG11	2.19	0.41
3:N:487:ALA:O	3:N:491:LYS:HG2	2.19	0.41
3:N:632:VAL:O	3:N:727:GLN:HA	2.20	0.41
3:N:792:ILE:HD13	3:N:941:PHE:CE1	2.56	0.41
3:N:823:LEU:CD1	3:N:837:GLY:CA	2.98	0.41
3:N:1267:ARG:HA	3:N:1268:PRO:HD3	1.90	0.41
5:P:384:GLU:HB3	5:P:394:ARG:CD	2.47	0.41
2:C:182:VAL:HG21	2:C:193:LEU:CB	2.27	0.41
2:C:864:GLY:O	2:C:866:PRO:HD3	2.20	0.41
3:D:437:VAL:HG11	5:F:175:HIS:ND1	2.36	0.41
3:D:801:GLY:HA2	3:D:821:VAL:HG13	2.02	0.41
3:D:1464:GLU:OE1	3:D:1464:GLU:N	2.36	0.41
5:F:264:MET:O	5:F:268:ILE:HG13	2.20	0.41
1:L:224:TYR:N	1:L:224:TYR:CD1	2.86	0.41
2:M:559:LEU:HD23	2:M:559:LEU:C	2.40	0.41
3:N:1102:THR:HG21	3:N:1371:VAL:HG22	2.02	0.41
3:N:1238:MET:HG2	3:N:1359:GLN:OE1	2.21	0.41
5:P:367:MET:HB3	5:P:390:PHE:HZ	1.85	0.41
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.87	0.41
1:A:206:THR:HG22	1:A:208:LEU:N	2.34	0.41
1:B:48:ILE:HA	1:B:49:PRO:HD3	1.71	0.41
1:B:128:HIS:HE1	1:B:131:THR:CG2	2.34	0.41
1:B:154:GLU:H	1:B:154:GLU:CD	2.20	0.41
2:C:786:LYS:CB	2:C:786:LYS:HZ3	2.32	0.41
3:D:255:GLU:OE1	3:D:274:ARG:NH2	2.54	0.41
2:M:223:ASP:O	2:M:227:PHE:CD2	2.73	0.41
2:M:1102:LEU:HB2	3:N:7:LYS:HB2	2.03	0.41
3:N:275:GLU:HB3	3:N:276:ASP:H	1.60	0.41
3:N:984:THR:HG22	3:N:985:ASP:N	2.36	0.41
3:N:1100:ASP:OD2	3:N:1440:PHE:HB2	2.21	0.41
3:N:1263:PHE:HD2	3:N:1375:MET:HE3	1.80	0.41
3:N:1353:GLN:HG2	3:N:1368:ILE:CD1	2.51	0.41
3:N:1495:ILE:HG21	4:O:80:VAL:CG2	2.51	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.92	0.41
1:B:124:ASN:HD22	1:B:127:LEU:HB2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:394:PHE:CE2	2:C:632:ASN:HB3	2.55	0.41
2:C:976:ASP:OD2	2:C:978:ARG:NH1	2.54	0.41
3:D:567:ILE:CG2	3:D:571:LYS:HE3	2.50	0.41
3:D:586:ARG:HH12	6:G:10:DG:H5"	1.86	0.41
3:D:648:MET:O	3:D:652:LEU:HG	2.21	0.41
3:D:806:PHE:HB2	3:D:829:VAL:HG23	1.98	0.41
3:D:1011:PHE:HB3	3:D:1021:TYR:CG	2.55	0.41
3:D:1082:ALA:O	3:D:1086:LEU:HG	2.20	0.41
5:F:195:VAL:HG13	5:F:216:GLY:HA3	2.01	0.41
2:M:238:LEU:HD12	2:M:238:LEU:C	2.40	0.41
2:M:976:ASP:OD2	2:M:978:ARG:NH1	2.54	0.41
3:N:132:TYR:HB2	3:N:153:LEU:CD1	2.50	0.41
3:N:232:GLU:O	3:N:232:GLU:HG2	2.21	0.41
3:N:939:PHE:O	3:N:942:SER:OG	2.23	0.41
3:N:1011:PHE:HB3	3:N:1021:TYR:CG	2.56	0.41
5:P:126:LEU:O	5:P:130:VAL:HG23	2.21	0.41
1:B:80:LEU:O	1:B:83:LYS:HB2	2.21	0.41
1:B:227:ASN:HA	1:B:228:PRO:HD3	1.90	0.41
2:C:163:ILE:HG23	2:C:171:TRP:CD1	2.55	0.41
2:C:204:GLN:HB2	2:C:227:PHE:CD1	2.56	0.41
2:C:372:LEU:HD12	2:C:372:LEU:HA	1.88	0.41
2:C:494:TYR:HD1	2:C:530:GLU:OE2	2.04	0.41
2:C:679:PHE:HA	3:D:943:THR:HB	2.03	0.41
2:C:786:LYS:NZ	2:C:786:LYS:HB3	2.33	0.41
2:C:998:TYR:O	2:C:998:TYR:CG	2.74	0.41
2:C:1105:LYS:O	2:C:1106:ASP:HB2	2.20	0.41
3:D:90:MET:HE3	3:D:519:VAL:O	2.21	0.41
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.56	0.41
3:D:1000:THR:O	3:D:1003:VAL:HG22	2.21	0.41
3:D:1107:VAL:CG1	3:D:1217:ILE:HA	2.51	0.41
3:D:1323:GLN:HA	3:D:1324:PRO:HD3	1.94	0.41
3:D:1468:LEU:HD22	3:D:1468:LEU:HA	1.79	0.41
5:F:259:ARG:CG	5:F:259:ARG:NH1	2.83	0.41
5:F:278:LEU:HD11	5:F:294:ALA:HB3	2.02	0.41
5:F:338:LEU:HD23	5:F:339:PRO:HD2	2.03	0.41
7:H:13:DT:H6	7:H:13:DT:H2'	1.70	0.41
1:K:57:TYR:CE1	1:K:161:ARG:HD2	2.55	0.41
2:M:230:ARG:HG3	2:M:232:GLU:H	1.86	0.41
2:M:561:GLY:O	2:M:565:GLN:HG3	2.21	0.41
2:M:944:LEU:HD22	2:M:962:GLN:HB3	2.03	0.41
2:M:1071:ILE:O	3:N:659:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:132:TYR:HE2	3:N:155:ASP:HB3	1.86	0.41
3:N:155:ASP:O	3:N:159:ARG:HG3	2.21	0.41
3:N:230:TRP:HA	3:N:243:ALA:CB	2.50	0.41
3:N:567:ILE:CG2	3:N:571:LYS:HE3	2.51	0.41
3:N:597:ASP:OD2	3:N:597:ASP:N	2.54	0.41
3:N:731:LEU:CD1	3:N:931:LEU:HB3	2.51	0.41
3:N:784:ASP:HB2	3:N:939:PHE:CE2	2.56	0.41
3:N:1290:LEU:CD2	3:N:1307:LYS:CE	2.85	0.41
5:P:101:GLU:O	5:P:105:LYS:HG3	2.21	0.41
5:P:120:THR:HG22	5:P:122:LEU:HD13	2.02	0.41
5:P:391:GLY:O	5:P:392:VAL:C	2.58	0.41
2:C:6:PHE:CD2	2:C:909:ALA:HB2	2.56	0.41
2:C:226:VAL:HA	2:C:229:MET:HG3	2.03	0.41
2:C:229:MET:HB3	2:C:233:GLU:CB	2.47	0.41
2:C:375:SER:O	2:C:378:LEU:N	2.53	0.41
2:C:682:TYR:CD1	3:D:635:PRO:HG2	2.56	0.41
2:C:879:ARG:N	2:C:879:ARG:HD2	2.35	0.41
3:D:215:TYR:CE1	3:D:380:GLU:O	2.74	0.41
3:D:561:GLY:HA3	5:F:132:ARG:HD3	2.03	0.41
3:D:1060:SER:OG	3:D:1063:GLU:HG3	2.21	0.41
2:M:258:TYR:CD2	2:M:262:ALA:HB3	2.56	0.41
2:M:1105:LYS:O	2:M:1106:ASP:HB2	2.20	0.41
3:N:1342:GLU:H	3:N:1342:GLU:CD	2.25	0.41
5:P:195:VAL:HG13	5:P:216:GLY:HA3	2.02	0.41
5:P:369:LEU:HD12	5:P:401:GLU:HB2	2.03	0.41
1:B:184:THR:O	1:B:192:LEU:HB2	2.21	0.40
2:C:229:MET:O	2:C:233:GLU:HB2	2.21	0.40
2:C:1027:PHE:CD2	2:C:1027:PHE:O	2.74	0.40
2:C:1056:LYS:NZ	3:D:749:VAL:O	2.38	0.40
3:D:47:GLU:C	3:D:78:VAL:HG23	2.42	0.40
3:D:134:VAL:HG22	3:D:151:GLN:O	2.21	0.40
3:D:632:VAL:O	3:D:727:GLN:HA	2.21	0.40
3:D:1258:ARG:NH2	3:D:1351:GLU:HG2	2.35	0.40
5:F:324:GLU:HB2	5:F:326:ASP:OD1	2.21	0.40
1:L:80:LEU:O	1:L:83:LYS:HB2	2.22	0.40
3:N:1310:ARG:CG	3:N:1327:ARG:NH1	2.84	0.40
1:A:30:ARG:CD	1:A:191:ASP:CG	2.89	0.40
2:C:501:THR:HG21	2:C:513:VAL:HB	2.03	0.40
3:D:106:LYS:HE3	3:D:587:ARG:HG3	2.03	0.40
3:D:486:ARG:H	3:D:486:ARG:HG3	1.58	0.40
3:D:634:GLY:O	3:D:637:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:771:SER:O	3:D:775:GLY:HA2	2.21	0.40
4:E:61:VAL:O	4:E:65:MET:HG3	2.21	0.40
4:E:70:THR:CB	4:E:72:ARG:HG3	2.52	0.40
5:F:281:GLU:CG	5:F:282:LEU:CD2	2.86	0.40
1:L:94:LEU:HD21	1:L:97:VAL:CG2	2.51	0.40
2:M:395:LYS:HE2	2:M:403:SER:CB	2.51	0.40
2:M:474:VAL:HG22	2:M:479:VAL:HG22	2.03	0.40
2:M:707:ARG:NE	2:M:824:ARG:HD3	2.37	0.40
2:M:708:TYR:OH	2:M:796:GLU:OE1	2.21	0.40
2:M:729:LEU:HD23	2:M:729:LEU:HA	1.91	0.40
2:M:1053:LEU:CD1	3:N:1466:VAL:HG13	2.51	0.40
3:N:90:MET:HE3	3:N:520:LEU:HA	2.02	0.40
3:N:138:LYS:CB	3:N:451:ASP:O	2.69	0.40
3:N:483:HIS:CG	3:N:484:PRO:HD2	2.57	0.40
3:N:637:LEU:HD22	3:N:642:CYS:HA	2.03	0.40
3:N:1289:LYS:O	3:N:1290:LEU:HD23	2.20	0.40
5:P:285:GLU:HA	5:P:286:PRO:HD3	1.78	0.40
5:P:325:LYS:HE2	5:P:325:LYS:HB2	1.80	0.40
1:A:39:PRO:O	1:A:43:ILE:HG13	2.22	0.40
2:C:229:MET:HE2	2:C:229:MET:HB2	1.91	0.40
2:C:626:ARG:HG3	2:C:629:TYR:CG	2.56	0.40
2:C:718:GLY:HA3	2:C:761:PHE:CD1	2.56	0.40
2:C:830:LYS:HB3	2:C:830:LYS:HE2	1.89	0.40
3:D:132:TYR:HB2	3:D:153:LEU:CD1	2.51	0.40
3:D:900:ILE:H	3:D:900:ILE:HG13	1.62	0.40
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	2.03	0.40
1:K:23:PHE:HE1	1:K:208:LEU:HD12	1.85	0.40
2:M:557:ARG:HG3	2:M:844:GLY:HA3	2.02	0.40
2:M:864:GLY:O	2:M:866:PRO:HD3	2.20	0.40
2:M:899:GLN:HE21	2:M:901:TYR:HE2	1.67	0.40
2:M:1012:PRO:HB2	2:M:1021:LEU:HD12	2.03	0.40
3:N:121:THR:O	3:N:124:GLU:HB3	2.21	0.40
3:N:622:ARG:NH1	6:Q:17:DG:OP1	2.43	0.40
3:N:801:GLY:O	3:N:804:LEU:HG	2.21	0.40
3:N:1258:ARG:NH2	3:N:1262:LEU:HD21	2.36	0.40
5:P:295:MET:HE2	5:P:295:MET:HA	2.02	0.40
1:A:97:VAL:HG12	1:A:98:THR:N	2.36	0.40
2:C:223:ASP:O	2:C:227:PHE:CD2	2.73	0.40
2:C:717:LEU:N	2:C:717:LEU:CD1	2.84	0.40
3:D:23:TYR:CE2	3:D:89:ARG:HD3	2.57	0.40
3:D:208:PRO:HA	3:D:389:GLU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:260:ILE:HG23	5:F:261:PRO:HD2	2.03	0.40
1:L:184:THR:O	1:L:192:LEU:HB2	2.22	0.40
1:L:185:ARG:HA	1:L:189:ARG:O	2.21	0.40
1:L:205:VAL:HG12	1:L:206:THR:H	1.86	0.40
2:M:385:PHE:O	2:M:389:SER:HB3	2.21	0.40
3:N:252:ARG:HD3	3:N:301:GLY:O	2.21	0.40
3:N:832:ARG:HD2	3:N:833:GLU:N	2.37	0.40
3:N:899:LEU:HD22	3:N:917:GLN:HB3	2.02	0.40
3:N:1102:THR:CG2	3:N:1371:VAL:HG22	2.52	0.40
3:N:1293:PHE:CE2	3:N:1302:GLU:HG3	2.54	0.40
5:P:101:GLU:HG3	5:P:105:LYS:HE2	2.02	0.40
7:R:18:DC:H2'	7:R:19:DG:C8	2.57	0.40
1:A:73:GLU:OE1	1:A:73:GLU:N	2.54	0.40
2:C:103:LYS:H	2:C:103:LYS:HG3	1.55	0.40
2:C:176:VAL:O	2:C:181:VAL:O	2.39	0.40
2:C:758:ARG:N	2:C:789:SER:HB3	2.36	0.40
2:C:1071:ILE:CG2	3:D:670:VAL:HG21	2.52	0.40
3:D:285:PRO:HG2	3:D:311:LEU:HD12	2.04	0.40
3:D:899:LEU:HD22	3:D:917:GLN:HB3	2.03	0.40
1:K:97:VAL:HG12	1:K:98:THR:N	2.35	0.40
2:M:328:LEU:HD12	2:M:433:THR:O	2.22	0.40
2:M:719:PRO:HD2	2:M:761:PHE:CE1	2.57	0.40
3:N:39:PRO:HB3	3:N:45:PHE:O	2.22	0.40
3:N:223:LEU:HD21	3:N:225:LEU:HD21	2.03	0.40
3:N:245:LEU:HD12	3:N:245:LEU:N	2.35	0.40
3:N:1258:ARG:HH21	3:N:1351:GLU:HG3	1.86	0.40
3:N:1406:ARG:HB3	3:N:1406:ARG:NH2	2.36	0.40
4:O:67:GLU:O	4:O:70:THR:OG1	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1314:LYS:NZ	2:M:784:ASP:OD2[1_445]	1.83	0.37
2:M:40:GLU:OE1	5:P:364:ARG:NH1[1_545]	2.03	0.17

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	224/315 (71%)	218 (97%)	5 (2%)	1 (0%)	34	72
1	B	220/315 (70%)	212 (96%)	6 (3%)	2 (1%)	17	55
1	K	224/315 (71%)	218 (97%)	6 (3%)	0	100	100
1	L	223/315 (71%)	213 (96%)	8 (4%)	2 (1%)	17	55
2	C	1107/1119 (99%)	1066 (96%)	37 (3%)	4 (0%)	34	72
2	M	1107/1119 (99%)	1063 (96%)	39 (4%)	5 (0%)	29	68
3	D	1478/1524 (97%)	1423 (96%)	53 (4%)	2 (0%)	51	85
3	N	1485/1524 (97%)	1423 (96%)	57 (4%)	5 (0%)	41	76
4	E	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
4	O	92/99 (93%)	88 (96%)	4 (4%)	0	100	100
5	F	344/443 (78%)	335 (97%)	9 (3%)	0	100	100
5	P	345/443 (78%)	329 (95%)	12 (4%)	4 (1%)	13	48
All	All	6941/7630 (91%)	6677 (96%)	239 (3%)	25 (0%)	34	72

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	325	ILE
2	M	325	ILE
5	P	78	SER
5	P	417	LYS
3	D	1310	ARG
3	N	1310	ARG
5	P	392	VAL
3	N	1237	THR
5	P	79	ASP
1	A	60	ASP
1	B	59	GLU
1	B	118	ALA

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Mol	Chain	Res	Type
2	C	429	ASP
1	L	118	ALA
2	M	230	ARG
2	C	230	ARG
2	M	249	LYS
3	N	1137	ARG
3	N	1306	PRO
1	L	59	GLU
2	C	177	GLU
2	M	170	PRO
3	D	530	VAL
3	N	530	VAL
2	M	177	GLU

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	199/273 (73%)	189 (95%)	10 (5%)	24	60
1	B	195/273 (71%)	182 (93%)	13 (7%)	16	49
1	K	199/273 (73%)	189 (95%)	10 (5%)	24	60
1	L	198/273 (72%)	188 (95%)	10 (5%)	24	60
2	C	936/941 (100%)	880 (94%)	56 (6%)	19	53
2	M	936/941 (100%)	873 (93%)	63 (7%)	16	49
3	D	1250/1279 (98%)	1165 (93%)	85 (7%)	16	48
3	N	1253/1279 (98%)	1169 (93%)	84 (7%)	16	49
4	E	83/88 (94%)	80 (96%)	3 (4%)	35	70
4	O	83/88 (94%)	81 (98%)	2 (2%)	49	79
5	F	301/388 (78%)	287 (95%)	14 (5%)	26	63
5	P	302/388 (78%)	280 (93%)	22 (7%)	14	44
All	All	5935/6484 (92%)	5563 (94%)	372 (6%)	18	51

All (372) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	58	ILE
1	A	86	VAL
1	A	87	VAL
1	A	126	ASP
1	A	142	VAL
1	A	184	THR
1	A	186	LEU
1	A	198	ARG
1	A	215	VAL
1	B	54	THR
1	B	61	VAL
1	B	63	HIS
1	B	66	SER
1	B	94	LEU
1	B	96	THR
1	B	165	ILE
1	B	191	ASP
1	B	192	LEU
1	B	197	LEU
1	B	205	VAL
1	B	206	THR
1	B	215	VAL
2	C	11	GLU
2	C	81	ASP
2	C	85	GLU
2	C	103	LYS
2	C	105	THR
2	C	107	LEU
2	C	108	ILE
2	C	141	HIS
2	C	149	THR
2	C	154	ARG
2	C	157	ARG
2	C	168	ARG
2	C	177	GLU
2	C	182	VAL
2	C	196	LEU
2	C	216	GLU
2	C	218	VAL
2	C	221	LEU
2	C	223	ASP

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Mol	Chain	Res	Type
2	C	229	MET
2	C	230	ARG
2	C	232	GLU
2	C	233	GLU
2	C	251	ASP
2	C	325	ILE
2	C	353	ARG
2	C	359	MET
2	C	361	MET
2	C	372	LEU
2	C	402	SER
2	C	427	VAL
2	C	434	HIS
2	C	454	SER
2	C	527	GLU
2	C	575	GLN
2	C	584	GLU
2	C	585	GLU
2	C	610	ARG
2	C	617	ASP
2	C	633	GLN
2	C	640	ARG
2	C	650	ARG
2	C	670	GLN
2	C	774	LEU
2	C	775	ARG
2	C	786	LYS
2	C	807	ARG
2	C	815	LEU
2	C	845	ASN
2	C	848	VAL
2	C	930	LYS
2	C	939	ARG
2	C	968	LEU
2	C	978	ARG
2	C	1001	VAL
2	C	1080	SER
3	D	36	THR
3	D	38	LYS
3	D	40	GLU
3	D	67	ARG
3	D	68	PHE

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Mol	Chain	Res	Type
3	D	69	GLU
3	D	78	VAL
3	D	81	THR
3	D	106	LYS
3	D	141	ILE
3	D	154	THR
3	D	184	GLU
3	D	199	LEU
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	265	GLU
3	D	270	LEU
3	D	273	ARG
3	D	274	ARG
3	D	275	GLU
3	D	335	LEU
3	D	354	VAL
3	D	372	ASP
3	D	374	GLU
3	D	411	THR
3	D	445	ARG
3	D	486	ARG
3	D	488	ARG
3	D	525	ARG
3	D	534	ARG
3	D	596	SER
3	D	623	VAL
3	D	637	LEU
3	D	640	HIS
3	D	709	HIS
3	D	717	GLN
3	D	754	PHE
3	D	784	ASP
3	D	785	ILE
3	D	817	GLU
3	D	829	VAL
3	D	832	ARG
3	D	833	GLU
3	D	858	VAL
3	D	867	ARG
3	D	894	LYS

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Mol	Chain	Res	Type
3	D	922	LEU
3	D	924	MET
3	D	940	THR
3	D	943	THR
3	D	969	ARG
3	D	1041	LEU
3	D	1044	LEU
3	D	1046	GLN
3	D	1083	ASP
3	D	1100	ASP
3	D	1128	VAL
3	D	1130	ARG
3	D	1132	LEU
3	D	1133	ARG
3	D	1152	GLU
3	D	1208	ASP
3	D	1219	GLU
3	D	1234	THR
3	D	1283	ILE
3	D	1284	GLU
3	D	1287	GLU
3	D	1288	GLU
3	D	1289	LYS
3	D	1290	LEU
3	D	1305	LEU
3	D	1308	GLU
3	D	1310	ARG
3	D	1311	LEU
3	D	1312	LEU
3	D	1317	ASP
3	D	1373	ARG
3	D	1382	THR
3	D	1383	ASP
3	D	1389	LEU
3	D	1393	GLN
3	D	1406	ARG
3	D	1456	LYS
3	D	1468	LEU
4	E	50	THR
4	E	92	LEU
4	E	95	VAL
5	F	88	ILE

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Mol	Chain	Res	Type
5	F	117	SER
5	F	125	ASP
5	F	186	HIS
5	F	203	THR
5	F	205	ARG
5	F	218	GLN
5	F	259	ARG
5	F	287	THR
5	F	295	MET
5	F	315	VAL
5	F	325	LYS
5	F	376	ILE
5	F	377	ASP
1	K	6	LEU
1	K	58	ILE
1	K	86	VAL
1	K	87	VAL
1	K	126	ASP
1	K	142	VAL
1	K	184	THR
1	K	185	ARG
1	K	188	GLN
1	K	215	VAL
1	L	5	LYS
1	L	54	THR
1	L	96	THR
1	L	191	ASP
1	L	192	LEU
1	L	197	LEU
1	L	205	VAL
1	L	206	THR
1	L	215	VAL
1	L	223	THR
2	M	11	GLU
2	M	38	LYS
2	M	50	GLU
2	M	81	ASP
2	M	85	GLU
2	M	103	LYS
2	M	105	THR
2	M	107	LEU
2	M	133	ASP

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Mol	Chain	Res	Type
2	M	141	HIS
2	M	149	THR
2	M	154	ARG
2	M	157	ARG
2	M	167	LYS
2	M	168	ARG
2	M	174	LEU
2	M	176	VAL
2	M	182	VAL
2	M	196	LEU
2	M	209	ARG
2	M	216	GLU
2	M	218	VAL
2	M	221	LEU
2	M	223	ASP
2	M	230	ARG
2	M	233	GLU
2	M	237	ARG
2	M	238	LEU
2	M	240	THR
2	M	297	GLU
2	M	299	LYS
2	M	325	ILE
2	M	353	ARG
2	M	359	MET
2	M	361	MET
2	M	372	LEU
2	M	427	VAL
2	M	434	HIS
2	M	454	SER
2	M	490	GLU
2	M	493	ARG
2	M	527	GLU
2	M	575	GLN
2	M	584	GLU
2	M	585	GLU
2	M	610	ARG
2	M	617	ASP
2	M	633	GLN
2	M	640	ARG
2	M	650	ARG
2	M	670	GLN

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Mol	Chain	Res	Type
2	M	781	LYS
2	M	807	ARG
2	M	815	LEU
2	M	816	LYS
2	M	845	ASN
2	M	848	VAL
2	M	930	LYS
2	M	939	ARG
2	M	968	LEU
2	M	978	ARG
2	M	1001	VAL
2	M	1080	SER
3	N	35	ARG
3	N	36	THR
3	N	48	ARG
3	N	106	LYS
3	N	107	ASP
3	N	141	ILE
3	N	154	THR
3	N	184	GLU
3	N	199	LEU
3	N	230	TRP
3	N	264	LEU
3	N	266	GLU
3	N	270	LEU
3	N	277	GLU
3	N	279	VAL
3	N	286	VAL
3	N	298	VAL
3	N	306	GLU
3	N	311	LEU
3	N	315	ARG
3	N	354	VAL
3	N	411	THR
3	N	434	ARG
3	N	445	ARG
3	N	486	ARG
3	N	488	ARG
3	N	518	PRO
3	N	525	ARG
3	N	587	ARG
3	N	591	VAL

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Mol	Chain	Res	Type
3	N	597	ASP
3	N	598	ARG
3	N	623	VAL
3	N	637	LEU
3	N	640	HIS
3	N	709	HIS
3	N	717	GLN
3	N	754	PHE
3	N	817	GLU
3	N	820	GLU
3	N	827	ILE
3	N	832	ARG
3	N	833	GLU
3	N	834	THR
3	N	838	ARG
3	N	858	VAL
3	N	867	ARG
3	N	894	LYS
3	N	940	THR
3	N	943	THR
3	N	1020	LEU
3	N	1041	LEU
3	N	1044	LEU
3	N	1046	GLN
3	N	1083	ASP
3	N	1100	ASP
3	N	1128	VAL
3	N	1129	THR
3	N	1130	ARG
3	N	1131	SER
3	N	1132	LEU
3	N	1159	ARG
3	N	1188	VAL
3	N	1219	GLU
3	N	1234	THR
3	N	1238	MET
3	N	1282	ARG
3	N	1283	ILE
3	N	1284	GLU
3	N	1291	SER
3	N	1301	LYS
3	N	1305	LEU

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Mol	Chain	Res	Type
3	N	1308	GLU
3	N	1311	LEU
3	N	1312	LEU
3	N	1317	ASP
3	N	1373	ARG
3	N	1382	THR
3	N	1383	ASP
3	N	1389	LEU
3	N	1393	GLN
3	N	1413	THR
3	N	1418	LYS
3	N	1459	LEU
4	O	50	THR
4	O	93	TYR
5	P	77	THR
5	P	82	ARG
5	P	123	ASP
5	P	140	ARG
5	P	186	HIS
5	P	205	ARG
5	P	222	ARG
5	P	244	ARG
5	P	287	THR
5	P	315	VAL
5	P	325	LYS
5	P	361	LEU
5	P	362	SER
5	P	377	ASP
5	P	379	ARG
5	P	383	LEU
5	P	386	VAL
5	P	393	THR
5	P	414	ARG
5	P	416	ARG
5	P	417	LYS
5	P	418	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	187	ASN
2	C	330	ASN

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Mol	Chain	Res	Type
2	C	845	ASN
2	C	884	GLN
3	D	483	HIS
3	D	1046	GLN
3	D	1172	HIS
1	L	221	HIS
2	M	187	ASN
2	M	330	ASN
2	M	845	ASN
2	M	884	GLN
3	N	483	HIS
3	N	1046	GLN
3	N	1195	GLN
3	N	1202	GLN
3	N	1441	GLN
5	P	381	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	1/2 (50%)	0	0
8	S	1/2 (50%)	0	0
All	All	2/4 (50%)	0	0

There are no RNA backbone outliers to report.

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	226/315 (71%)	-0.28	0 100 100	47, 67, 98, 118	0
1	B	222/315 (70%)	-0.17	2 (0%) 84 63	50, 79, 119, 142	0
1	K	226/315 (71%)	-0.21	0 100 100	49, 73, 103, 122	0
1	L	225/315 (71%)	-0.14	3 (1%) 77 51	51, 81, 126, 148	0
2	C	1111/1119 (99%)	-0.03	29 (2%) 56 27	34, 62, 122, 168	0
2	M	1111/1119 (99%)	0.24	82 (7%) 14 4	38, 76, 142, 179	0
3	D	1482/1524 (97%)	0.02	47 (3%) 47 20	32, 66, 130, 178	1 (0%)
3	N	1489/1524 (97%)	0.06	55 (3%) 41 17	34, 69, 129, 201	1 (0%)
4	E	94/99 (94%)	-0.08	3 (3%) 47 20	44, 66, 113, 121	0
4	O	94/99 (94%)	-0.10	3 (3%) 47 20	49, 72, 116, 130	0
5	F	346/443 (78%)	-0.14	6 (1%) 70 41	42, 70, 124, 147	0
5	P	347/443 (78%)	0.04	19 (5%) 25 9	46, 83, 156, 214	0
6	G	16/21 (76%)	-0.49	0 100 100	42, 78, 172, 179	0
6	Q	16/21 (76%)	-0.63	0 100 100	53, 80, 182, 183	0
7	H	24/27 (88%)	-0.39	0 100 100	67, 95, 146, 201	0
7	R	24/27 (88%)	-0.39	0 100 100	65, 106, 160, 210	0
8	I	2/2 (100%)	-0.43	0 100 100	50, 50, 50, 55	0
8	S	2/2 (100%)	-0.41	0 100 100	62, 62, 62, 63	0
All	All	7057/7730 (91%)	0.01	249 (3%) 44 18	32, 71, 132, 214	2 (0%)

All (249) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	363	SER	6.5
5	P	392	VAL	6.1
5	P	411	HIS	6.0

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Mol	Chain	Res	Type	RSRZ
2	M	191	PHE	5.9
5	P	375	LEU	5.6
2	M	367	LEU	5.5
2	M	196	LEU	5.5
2	M	200	LEU	5.3
2	M	362	GLY	5.3
3	D	241	ILE	5.0
5	P	389	PHE	5.0
3	N	1247	ALA	5.0
2	M	311	PHE	4.8
5	P	410	TYR	4.8
3	D	991	GLN	4.7
3	N	1246	VAL	4.4
2	M	211	LEU	4.4
5	P	415	THR	4.4
2	M	199	VAL	4.3
2	M	226	VAL	4.3
2	M	778	PHE	4.3
2	M	296	GLY	4.2
2	M	221	LEU	4.2
3	D	980	MET	4.1
5	P	393	THR	4.1
3	N	355	VAL	4.1
5	P	373	LYS	4.1
2	C	364	GLU	4.0
2	M	364	GLU	4.0
3	D	1297	GLU	4.0
3	N	367	ILE	4.0
2	C	365	ASP	3.9
5	P	423	ASP	3.8
3	N	978	TYR	3.8
3	N	1128	VAL	3.8
3	D	335	LEU	3.8
3	N	311	LEU	3.8
2	C	188	LYS	3.7
3	D	995	LEU	3.7
2	M	207	LEU	3.7
3	N	378	ILE	3.7
2	M	777	ILE	3.7
2	M	295	ASP	3.6
2	M	368	THR	3.7
2	C	176	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
2	M	172	ILE	3.6
5	P	391	GLY	3.6
5	F	423	ASP	3.6
2	M	188	LYS	3.6
2	M	231	PRO	3.6
3	D	1279	GLY	3.6
2	M	184	MET	3.6
2	M	181	VAL	3.6
2	M	64	LEU	3.6
3	D	367	ILE	3.6
2	M	68	PHE	3.6
3	N	191	LEU	3.6
2	M	109	LYS	3.5
3	D	1128	VAL	3.5
3	N	202	VAL	3.5
5	P	390	PHE	3.5
2	C	366	SER	3.5
3	D	343	LYS	3.5
2	M	649	VAL	3.5
3	D	203	ALA	3.4
2	M	365	ASP	3.4
3	N	1250	ALA	3.4
3	D	982	PHE	3.4
5	P	414	ARG	3.3
3	N	177	ALA	3.3
3	N	1249	ALA	3.3
2	C	219	GLN	3.3
1	L	65	PHE	3.3
4	O	85	LEU	3.3
3	N	371	ILE	3.3
2	M	98	LEU	3.3
3	D	371	ILE	3.2
2	M	107	LEU	3.2
2	C	814	GLU	3.2
3	N	1129	THR	3.2
2	M	104	ASP	3.2
4	O	84	ARG	3.2
3	D	977	ALA	3.2
2	C	101	ILE	3.1
3	D	976	GLN	3.1
2	M	222	MET	3.1
3	D	1130	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	257	VAL	3.1
2	M	297	GLU	3.1
2	M	764	GLU	3.1
3	D	988	ARG	3.1
2	M	769	PRO	3.0
3	N	974	ILE	3.0
2	C	616	GLU	3.0
2	M	300	ASP	3.0
3	N	1408	ILE	3.0
3	D	213	VAL	3.0
2	M	201	GLY	2.9
3	N	1304	LYS	2.9
2	C	811	PRO	2.9
2	M	152	PRO	2.9
5	P	416	ARG	2.9
3	N	394	LEU	2.9
3	N	232	GLU	2.9
3	N	1409	ALA	2.9
3	D	1318	TYR	2.9
2	M	344	PHE	2.9
3	N	406	ASP	2.9
3	N	1281	VAL	2.9
5	P	386	VAL	2.9
3	N	213	VAL	2.8
2	M	762	LYS	2.8
2	M	175	GLU	2.8
3	D	360	ARG	2.8
3	D	198	ARG	2.8
3	D	309	GLY	2.8
4	E	52	GLU	2.8
5	P	406	ARG	2.8
2	M	811	PRO	2.8
3	D	1495	ILE	2.8
3	N	388	HIS	2.8
5	P	359	SER	2.8
3	D	983	LEU	2.8
2	M	44	ILE	2.8
2	C	181	VAL	2.7
2	M	307	LEU	2.7
2	M	30	LEU	2.7
2	M	645	VAL	2.7
3	N	352	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
2	M	265	ARG	2.7
2	C	650	ARG	2.7
2	M	66	LEU	2.7
2	M	766	GLU	2.7
3	N	212	ARG	2.7
2	C	815	LEU	2.7
2	M	655	LEU	2.7
3	N	1299	PHE	2.7
2	M	102	HIS	2.7
2	M	111	ASP	2.6
2	M	219	GLN	2.6
3	N	971	LEU	2.6
3	N	1497	GLU	2.6
3	D	345	TYR	2.6
2	M	254	VAL	2.6
3	D	388	HIS	2.6
3	D	406	ASP	2.6
3	N	426	LYS	2.6
3	N	1319	VAL	2.6
3	D	212	ARG	2.6
2	M	372	LEU	2.6
3	N	353	VAL	2.6
2	M	153	ALA	2.6
3	D	310	LEU	2.6
2	M	48	PHE	2.6
3	D	1294	VAL	2.5
2	M	108	ILE	2.5
2	M	197	LEU	2.5
2	M	595	LEU	2.5
3	D	839	LEU	2.5
3	N	1313	VAL	2.5
3	D	992	ILE	2.5
3	N	1251	ASP	2.5
3	N	218	LYS	2.5
2	M	106	GLY	2.5
3	D	973	GLN	2.5
2	M	1	MET	2.5
3	N	68	PHE	2.5
2	M	594	ALA	2.5
2	M	190	LYS	2.5
3	D	322	VAL	2.5
2	M	354	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	65	VAL	2.4
2	C	55	GLU	2.4
2	C	66	LEU	2.4
3	N	1248	GLY	2.4
2	M	101	ILE	2.4
3	N	197	SER	2.4
4	O	95	VAL	2.4
3	D	355	VAL	2.3
3	N	396	VAL	2.3
3	D	197	SER	2.3
2	M	235	LEU	2.3
3	N	63	TYR	2.3
3	N	236	TYR	2.3
3	N	1495	ILE	2.3
2	M	614	ARG	2.3
2	M	644	VAL	2.3
3	D	1498	ALA	2.3
2	C	729	LEU	2.3
2	C	764	GLU	2.3
2	C	157	ARG	2.2
3	N	407	VAL	2.2
3	D	470	LEU	2.2
2	M	629	TYR	2.2
2	M	65	VAL	2.2
2	M	785	VAL	2.2
3	D	161	LEU	2.2
2	M	351	LEU	2.2
2	C	629	TYR	2.2
2	M	371	LYS	2.2
2	M	176	VAL	2.2
3	N	1314	LYS	2.2
2	C	254	VAL	2.2
5	F	379	ARG	2.2
5	F	422	LEU	2.2
2	C	778	PHE	2.2
5	F	388	ALA	2.2
3	D	1319	VAL	2.2
3	N	1292	VAL	2.2
3	N	235	ALA	2.2
3	D	76	CYS	2.2
3	N	1253	THR	2.2
5	F	232	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	69	LEU	2.1
3	N	807	ALA	2.1
3	N	318	ARG	2.1
1	L	165	ILE	2.1
2	M	814	GLU	2.1
2	C	170	PRO	2.1
2	M	293	PHE	2.1
4	E	51	LEU	2.1
3	N	203	ALA	2.1
3	D	339	TRP	2.1
2	C	92	ALA	2.1
3	N	316	GLN	2.1
1	L	4	SER	2.1
2	M	220	GLY	2.1
3	N	279	VAL	2.1
3	D	409	VAL	2.1
3	D	1041	LEU	2.1
3	D	1408	ILE	2.1
3	N	1493	LYS	2.1
2	M	203	ASP	2.0
3	N	393	ILE	2.0
5	P	382	THR	2.0
2	M	170	PRO	2.0
2	C	8	ARG	2.0
2	C	172	ILE	2.0
3	D	666	ILE	2.0
5	F	380	GLU	2.0
2	C	100	LEU	2.0
2	M	648	ARG	2.0
1	B	66	SER	2.0
5	P	232	ARG	2.0
4	E	87	LYS	2.0
1	B	64	GLU	2.0
5	P	413	SER	2.0
2	M	621	VAL	2.0
3	D	165	LYS	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
10	MG	N	2003	1/1	0.78	0.20	46,46,46,46	0
10	MG	N	2004	1/1	0.82	0.37	65,65,65,65	0
10	MG	K	1001	1/1	0.89	0.66	69,69,69,69	0
10	MG	D	2003	1/1	0.94	0.24	40,40,40,40	0
10	MG	D	2004	1/1	0.97	0.44	63,63,63,63	0
9	ZN	N	2001	1/1	0.98	0.20	62,62,62,62	0
9	ZN	D	2002	1/1	0.98	0.07	83,83,83,83	0
9	ZN	N	2002	1/1	0.99	0.05	107,107,107,107	0
9	ZN	D	2001	1/1	0.99	0.13	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.