W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:34 PM GMT

PDB ID	:	1UAA
Title	:	E. COLI REP HELICASE/DNA COMPLEX
Authors	:	Korolev, S.; Waksman, G.
Deposited on	:	1997-06-30
Resolution	:	3.00 Å(reported)

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

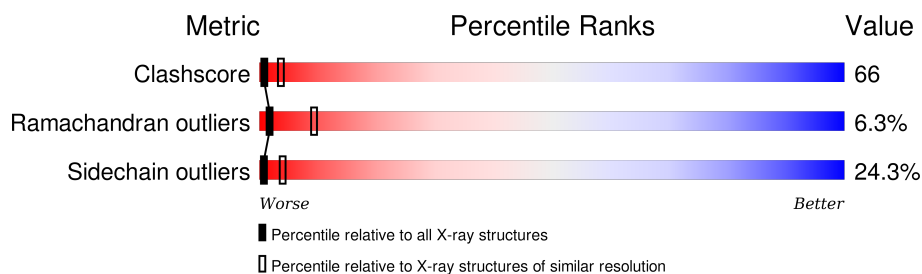|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	Percentile Ranks	Value
Clashscore		66
Ramachandran outliers		6.3%
Sidechain outliers		24.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	16	6% 94%
2	A	673	24% 51% 18% • 5%
2	B	673	24% 51% 17% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10404 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 DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP* TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	16	Total 317	C 160	N 32	O 110	P 15	0	0	0

- Molecule 2 is a protein called PROTEIN (ATP-DEPENDENT DNA HELICASE REP.).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	636	Total 5032	C 3186	N 881	O 942	S 23	0	0	0
2	B	633	Total 5055	C 3203	N 886	O 945	S 21	0	0	0

3 Residue-property plots ⓘ

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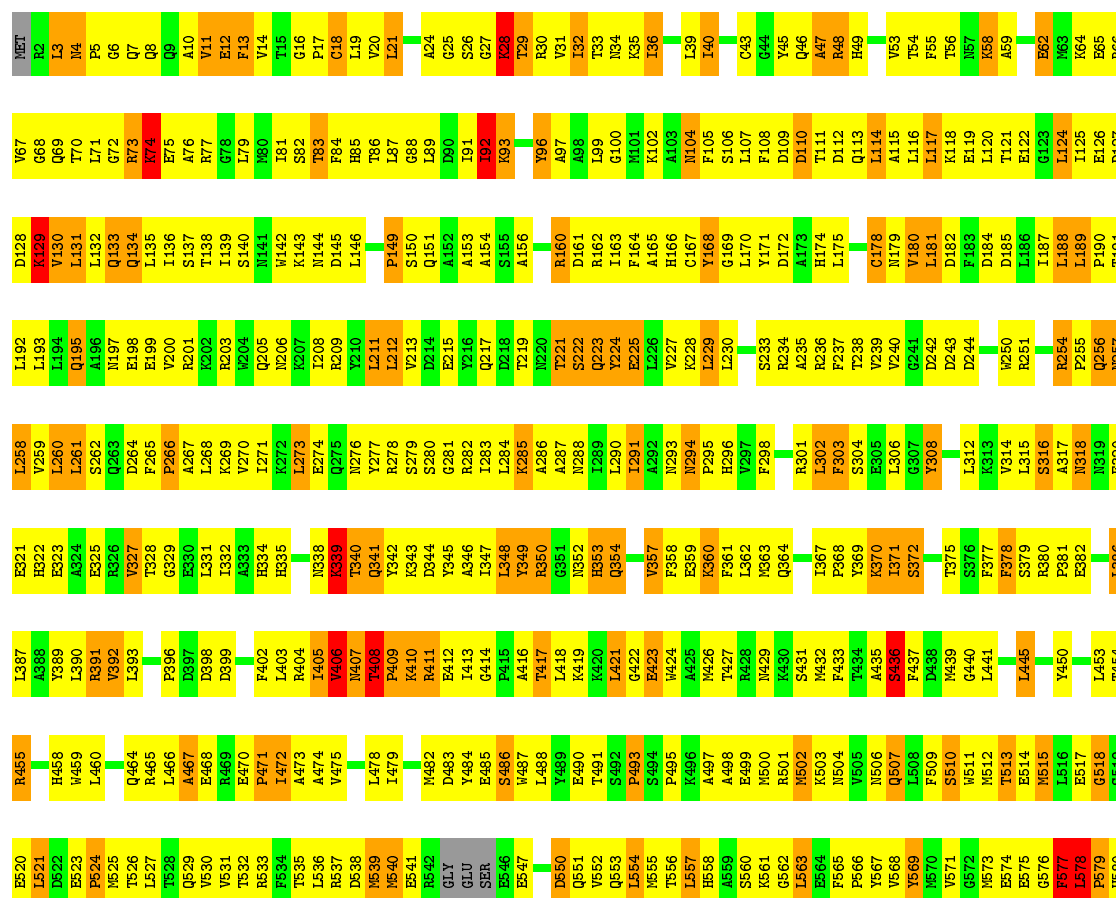
Note EDS was not executed.

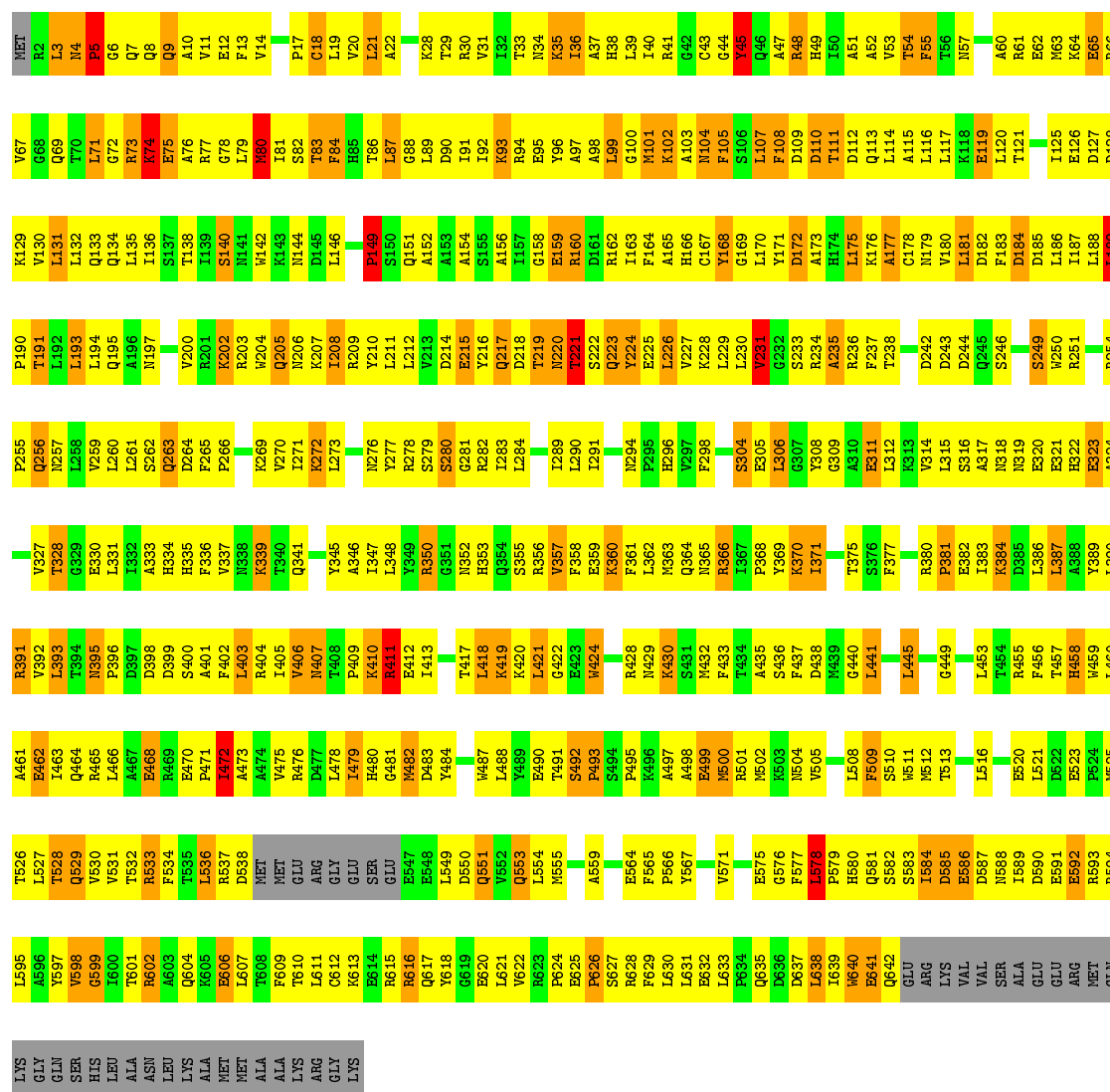• Molecule 1: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')

Chain C:

• Molecule 2: PROTEIN (ATP-DEPENDENT DNA HELICASE REP.)

Chain A:

Q581 S582 S583 I584 D585 E586 D587 N588 I589 D590 E591 E592 R593 R594 L595 A596 Y597 V598 G599 I600 T601 R602 A603 Q604 K605 E606 L607 T608 F609 T610 L611 C612 K613 R616 V622 R623 P624 S627 R628 F629 L630 L631 E632 Q635 D636 D637 L638 I639 W640 GLU GLN GLU ARG LYS VAL VAL

SER ALA GLU ARG MET GLN LYS GLY GLN SER HIS LEU ALA ASN LEU LYS ALA MET ALA ALA LYS ARG GLY LYS

- **Molecule 2: PROTEIN (ATP-DEPENDENT DNA HELICASE REP.)**

Chain B:

24%   51%   17%   6%

MET R2 L3 N4 P5 G6 Q7 Q8 Q9 A10 V11 E12 F13 V14 P17 C18 L19 V20 L21 A22 K28 T29 R30 V31 I32 T33 N34 K35 I36 A37 H38 L39 I40 R41 G42 C43 G44 Y45 Q46 A47 R48 H49 I50 A51 A52 V53 T54 F55 T56 N57 A60 R61 E62 M63 K64 E65 R66

V67 G68 Q69 T70 L71 G72 R73 K74 E75 A76 R77 G78 L79 M80 I81 S82 T83 F84 H85 T86 L87 G88 L89 D90 I91 I92 K93 R94 E95 Y96 A97 A98 L99 G100 M101 K102 A103 N104 F105 S106 L107 F108 D109 D110 T111 D112 Q113 L114 A115 L116 L117 K118 E119 L120 T121 I125 E126 D127 D128

K129 V130 L131 L132 Q133 Q134 L135 I136 S137 T138 I139 S140 N141 W142 K143 N144 D145 L146 P149 S150 Q151 A152 A153 A154 S155 A156 I157 G158 E159 R160 D161 R162 I163 F164 A165 H166 C167 Y168 G169 L170 Y171 D172 A173 H174 L175 K176 A177 C178 N179 V180 L181 D182 F183 D184 D185 L186 I187 L188 L189

P190 T191 L192 L193 L194 Q195 A196 N197 V200 R201 K202 R203 W204 Q205 N206 K207 I208 R209 Y210 L211 L212 V213 D214 E215 Y216 Q217 D218 T219 N220 T221 S222 Q223 Y224 E225 L226 V227 K228 L229 L230 V231 G232 S233 R234 A235 R236 F237 T238 D242 D243 D244 Q245 S246 S249 W250 R251 R254

P255 Q256 N257 L258 V259 L260 L261 S262 Q263 D264 F265 P266 K269 V270 I271 K272 L273 N276 Y277 R278 S279 S280 G281 E282 I283 L284 I289 L290 I291 N294 P295 H296 V297 F298 S304 E305 L306 G307 Y308 G309 A310 E311 L312 K313 V314 L315 S316 A317 N318 N319 E320 E321 H322 E323 A324

V327 T328 G329 E330 L331 I332 A333 H334 H335 F336 V337 N338 K339 T340 Q341 Y345 A346 I347 L348 Y349 R350 G351 N352 H353 Q354 S355 R356 V357 F358 E359 K360 F361 L362 M363 Q364 N365 R366 I367 P368 Y369 K370 I371 T375 S376 F377 R380 P381 E382 I383 K384 D385 L386 L387 A388 Y389 L390

R391 V392 L393 T394 N395 P396 D397 D398 D399 S400 A401 F402 L403 R404 I405 V406 N407 T408 P409 K410 R411 E412 I413 T417 L418 K419 K420 L421 G422 E423 W424 R428 N429 K430 S431 M432 F433 T434 A435 S436 F437 D438 M439 G440 L441 L445 G449 L453 T454 R455 F456 T457 H458 W459 L460

A461 E462 I463 Q464 R465 L466 A467 E468 R469 E470 P471 I472 A473 A474 V475 R476 D477 L478 I479 H480 G481 M482 D483 Y484 W487 L488 Y489 E490 T491 S492 P493 S494 P495 K496 A497 A498 E499 M500 R501 M502 K503 N504 V505 L508 F509 S510 W511 M512 T513 L516 E520 L521 D522 E523 P524 M525

T526 L527 S528 Q529 V530 V531 T532 R533 F534 T535 L536 R537 D538 MET MET GLU ARG GLY GLU GLY SER GLU E547 E548 L549 D550 Q551 V552 Q553 L554 M555 A559 E564 F565 P566 Y567 V571 E575 G576 F577 L578 P579 H580 Q581 S582 S583 I584 D585 E586 D587 N588 I589 D590 E591 E592 R593 R594

L595 A596 Y597 V598 G599 I600 T601 R602 A603 Q604 K605 E606 L607 T608 F609 T610 L611 C612 K613 E614 R615 R616 Q617 Y618 G619 E620 L621 V622 R623 P624 P626 S627 R628 F629 L630 L631 E632 L633 P634 Q635 D636 D637 L638 I639 W640 E641 Q642 GLU ARG LYS VAL VAL SER ALA GLU GLU ARG MET GLN

LYS GLY GLN SER HIS LEU ALA ASN LEU LYS ALA MET ALA ALA LYS ARG GLY LYS

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	141.80Å 141.80Å 284.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00	Depositor
% Data completeness (in resolution range)	88.0 (15.00-3.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.228 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10404	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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	C	1.08	0/348	1.07	0/536
2	A	0.83	0/5127	0.96	7/6932 (0.1%)
2	B	0.92	4/5151 (0.1%)	0.97	7/6961 (0.1%)
All	All	0.88	4/10626 (0.0%)	0.97	14/14429 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	18	CYS	CB-SG	-6.21	1.71	1.82
2	B	612	CYS	CB-SG	-6.15	1.71	1.82
2	B	337	VAL	CB-CG1	-6.13	1.40	1.52
2	B	65	GLU	CG-CD	5.24	1.59	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	410	LYS	N-CA-C	8.50	133.94	111.00
2	B	411	ARG	NE-CZ-NH2	7.69	124.14	120.30
2	A	3	LEU	N-CA-C	-5.65	95.74	111.00
2	B	266	PRO	CB-CA-C	-5.52	98.21	112.00
2	B	149	PRO	N-CA-CB	5.52	109.92	103.30
2	B	231	VAL	N-CA-C	-5.37	96.49	111.00
2	B	266	PRO	N-CA-C	5.26	125.77	112.10
2	A	28	LYS	CB-CA-C	-5.19	100.03	110.40
2	A	178	CYS	CA-CB-SG	-5.18	104.67	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	536	LEU	CA-CB-CG	5.17	127.19	115.30
2	B	131	LEU	CA-CB-CG	-5.17	103.42	115.30
2	A	579	PRO	N-CA-C	-5.09	98.85	112.10
2	A	149	PRO	N-CA-CB	5.08	109.40	103.30
2	A	554	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	308	TYR	Sidechain
2	A	569	TYR	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	C	317	0	194	68	0
2	A	5032	0	4953	650	0
2	B	5055	0	5014	660	0
All	All	10404	0	10161	1353	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 66.

All (1353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:DT:C6	1:C:10:DT:H5'	1.73	1.24
1:C:10:DT:H3'	1:C:10:DT:OP1	1.41	1.20
1:C:4:DT:H2"	1:C:5:DT:C5'	1.79	1.12
1:C:11:DT:H2'	1:C:11:DT:OP2	1.49	1.11
1:C:10:DT:C5'	1:C:10:DT:H6	1.66	1.09
2:B:602:ARG:HG3	2:B:602:ARG:HH11	1.13	1.08
1:C:4:DT:H2"	1:C:5:DT:H5'	1.37	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:370:LYS:HZ1	2:A:554:LEU:N	1.54	1.04
2:B:92:ILE:HG12	2:B:189:LEU:HD12	1.37	1.03
2:A:121:THR:HA	2:A:124:LEU:HD11	1.38	1.03
2:A:211:LEU:HD11	2:A:213:VAL:HG23	1.41	1.03
2:A:197:ASN:HD22	2:A:200:VAL:HG12	1.23	1.00
2:B:189:LEU:HB3	2:B:190:PRO:HD3	1.43	1.00
2:B:406:VAL:HG23	2:B:407:ASN:H	1.28	0.99
2:A:36:ILE:HA	2:A:39:LEU:HD12	1.42	0.98
2:A:83:THR:HG22	2:A:86:THR:H	1.28	0.98
2:B:391:ARG:HD2	2:B:401:ALA:HB2	1.44	0.97
2:A:381:PRO:HB2	2:A:501:ARG:NH2	1.80	0.97
1:C:10:DT:H6	1:C:10:DT:H5'	0.80	0.95
2:B:92:ILE:HG13	2:B:190:PRO:HG3	1.48	0.95
2:B:436:SER:HB2	2:B:453:LEU:HD21	1.49	0.94
2:B:578:LEU:HB3	2:B:579:PRO:HD3	1.46	0.93
2:B:472:ILE:HG12	2:B:473:ALA:H	1.31	0.93
2:B:103:ALA:HB1	2:B:105:PHE:CE1	2.03	0.93
2:A:102:LYS:NZ	2:A:104:ASN:HB3	1.82	0.93
2:B:74:LYS:HZ1	2:B:75:GLU:H	1.10	0.93
2:A:320:GLU:HA	2:A:612:CYS:SG	2.07	0.93
2:A:586:GLU:O	2:A:587:ASP:HB3	1.69	0.92
2:A:124:LEU:H	2:A:124:LEU:HD23	1.32	0.91
2:A:578:LEU:HB3	2:A:579:PRO:HD3	1.53	0.90
2:B:272:LYS:HD2	2:B:272:LYS:H	1.35	0.90
2:B:89:LEU:HB2	2:B:186:LEU:HD23	1.52	0.90
2:A:102:LYS:HZ3	2:A:104:ASN:HB3	1.35	0.89
2:A:160:ARG:HA	2:A:163:ILE:HD12	1.54	0.89
1:C:4:DT:H2"	1:C:5:DT:H5"	1.52	0.88
2:B:410:LYS:HG2	2:B:410:LYS:O	1.73	0.88
2:A:211:LEU:HD12	2:A:212:LEU:N	1.88	0.88
2:B:74:LYS:NZ	2:B:75:GLU:H	1.71	0.88
2:A:54:THR:HG22	2:A:55:PHE:H	1.37	0.88
2:B:407:ASN:HA	2:B:411:ARG:HG2	1.54	0.88
2:A:358:PHE:O	2:A:362:LEU:HG	1.74	0.88
2:A:362:LEU:HA	2:A:367:ILE:HD12	1.56	0.86
1:C:3:DT:H2"	1:C:4:DT:OP2	1.73	0.86
2:A:411:ARG:HG3	2:A:412:GLU:H	1.40	0.86
2:A:211:LEU:HD11	2:A:213:VAL:CG2	2.06	0.85
2:A:139:ILE:HD11	2:A:168:TYR:HA	1.57	0.85
2:A:441:LEU:HD11	2:A:445:LEU:HD22	1.58	0.85
2:B:158:GLY:O	2:B:162:ARG:HG3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:ASN:ND2	2:B:223:GLN:HG2	1.91	0.85
2:A:590:ASP:O	2:A:593:ARG:HB2	1.77	0.84
2:B:602:ARG:NH1	2:B:602:ARG:HG3	1.90	0.84
2:A:433:PHE:O	2:A:436:SER:HB3	1.77	0.84
2:A:294:ASN:HD21	2:A:590:ASP:HA	1.41	0.83
2:B:598:VAL:HG12	2:B:602:ARG:HD3	1.60	0.83
2:B:350:ARG:HG3	2:B:350:ARG:HH11	1.42	0.83
1:C:12:DT:H2"	1:C:13:DT:OP2	1.79	0.82
2:B:74:LYS:HD3	2:B:74:LYS:H	1.44	0.82
2:A:257:ASN:HA	2:A:260:LEU:HD22	1.61	0.82
2:A:139:ILE:HA	2:A:142:TRP:CE3	2.14	0.82
1:C:7:DT:O2	1:C:7:DT:H2'	1.80	0.81
2:A:86:THR:HG22	2:A:533:ARG:HH12	1.43	0.81
2:B:92:ILE:HD11	2:B:190:PRO:HD3	1.62	0.81
2:A:213:VAL:HB	2:A:239:VAL:HG12	1.62	0.81
2:B:389:TYR:HE1	2:B:405:ILE:HB	1.45	0.81
2:A:212:LEU:N	2:A:212:LEU:HD12	1.96	0.81
2:B:160:ARG:HA	2:B:163:ILE:HD12	1.60	0.81
2:B:389:TYR:CE1	2:B:405:ILE:HB	2.16	0.81
2:A:121:THR:HA	2:A:124:LEU:CD1	2.10	0.81
2:A:33:THR:O	2:A:36:ILE:HG12	1.81	0.81
2:A:135:LEU:HD13	2:A:164:PHE:CD1	2.15	0.81
2:B:105:PHE:N	2:B:105:PHE:CD1	2.45	0.81
2:A:244:ASP:HB3	2:A:597:TYR:CE2	2.16	0.80
2:B:223:GLN:O	2:B:227:VAL:HG23	1.81	0.80
2:B:91:ILE:HG21	2:B:190:PRO:HB3	1.63	0.80
1:C:13:DT:C2	2:A:350:ARG:NH2	2.49	0.80
2:B:465:ARG:O	2:B:468:GLU:HB2	1.81	0.80
1:C:16:DT:H1'	2:A:85:HIS:CE1	2.17	0.80
2:A:197:ASN:ND2	2:A:200:VAL:HG12	1.97	0.79
2:A:281:GLY:HA2	2:A:284:LEU:HD12	1.63	0.79
2:B:424:TRP:HD1	2:B:441:LEU:HA	1.45	0.79
2:A:83:THR:CG2	2:A:86:THR:H	1.96	0.79
2:B:220:ASN:ND2	2:B:223:GLN:H	1.80	0.79
2:A:3:LEU:CD1	2:A:30:ARG:HE	1.96	0.79
2:B:389:TYR:CE2	2:B:482:MET:SD	2.75	0.79
2:B:175:LEU:HG	2:B:180:VAL:HG23	1.62	0.79
2:A:278:ARG:HH22	2:A:602:ARG:HH22	1.31	0.79
2:B:22:ALA:HB2	2:B:273:LEU:HD12	1.64	0.79
2:A:335:HIS:CD2	2:A:340:THR:H	2.00	0.79
2:B:384:LYS:HA	2:B:384:LYS:HE2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:GLN:HA	2:B:136:ILE:HD12	1.65	0.78
2:B:92:ILE:HD11	2:B:189:LEU:HB3	1.66	0.78
2:B:220:ASN:HD21	2:B:223:GLN:H	1.31	0.78
2:B:622:VAL:O	2:B:624:PRO:HD3	1.84	0.78
2:A:527:LEU:O	2:A:531:VAL:HG23	1.83	0.78
2:B:578:LEU:HB3	2:B:579:PRO:CD	2.13	0.78
2:A:276:ASN:HB2	2:A:302:LEU:HD23	1.66	0.78
2:A:104:ASN:HD22	2:A:104:ASN:H	1.32	0.78
2:A:372:SER:HB2	2:A:555:MET:HA	1.66	0.78
1:C:10:DT:H3'	1:C:10:DT:P	2.24	0.77
2:A:396:PRO:HG3	2:A:464:GLN:HE22	1.49	0.77
2:A:28:LYS:O	2:A:32:ILE:HG12	1.83	0.77
2:A:254:ARG:HD3	2:A:260:LEU:HD23	1.67	0.77
2:A:160:ARG:HH21	2:A:161:ASP:CG	1.88	0.77
2:B:459:TRP:HA	2:B:462:GLU:OE1	1.84	0.77
2:A:72:GLY:HA3	2:A:74:LYS:NZ	1.98	0.77
2:A:261:LEU:HD13	2:A:268:LEU:HD22	1.65	0.76
2:B:410:LYS:HB2	2:B:487:TRP:CE3	2.20	0.76
2:B:97:ALA:HA	2:B:101:MET:O	1.84	0.76
2:B:472:ILE:HG12	2:B:473:ALA:N	1.99	0.76
1:C:1:DT:O2	1:C:2:DT:C2	2.38	0.76
2:A:192:LEU:HA	2:A:195:GLN:HE21	1.51	0.76
2:B:125:ILE:HG13	2:B:131:LEU:HD21	1.68	0.76
2:A:407:ASN:O	2:A:410:LYS:HA	1.86	0.76
2:B:526:THR:OG1	2:B:528:THR:HG23	1.85	0.76
2:B:616:ARG:NH2	2:B:621:LEU:HG	2.02	0.75
2:B:220:ASN:H	2:B:223:GLN:HG3	1.49	0.75
2:A:290:LEU:HD13	2:A:600:ILE:HD11	1.66	0.75
2:A:472:ILE:HD13	2:A:473:ALA:N	2.01	0.75
2:B:135:LEU:HD13	2:B:164:PHE:HD1	1.51	0.75
2:B:525:MET:HB3	2:B:529:GLN:HG3	1.69	0.75
2:A:254:ARG:HH11	2:A:254:ARG:HG2	1.50	0.75
2:B:602:ARG:HH11	2:B:602:ARG:CG	1.98	0.74
2:B:393:LEU:HD23	2:B:464:GLN:HA	1.66	0.74
2:B:618:TYR:C	2:B:620:GLU:H	1.89	0.74
2:B:74:LYS:CE	2:B:75:GLU:H	2.00	0.74
2:A:135:LEU:HD13	2:A:164:PHE:HD1	1.51	0.74
2:A:635:GLN:HA	2:A:638:LEU:HD22	1.68	0.74
2:B:126:GLU:HG2	2:B:131:LEU:HD22	1.69	0.74
2:B:484:TYR:CE2	2:B:488:LEU:HD21	2.21	0.74
2:A:526:THR:OG1	2:A:529:GLN:HG3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:ALA:HB1	2:B:105:PHE:CZ	2.23	0.74
2:A:81:ILE:HD12	2:A:81:ILE:H	1.53	0.74
2:B:74:LYS:HZ1	2:B:75:GLU:N	1.84	0.74
2:A:244:ASP:HB3	2:A:597:TYR:HE2	1.52	0.74
2:A:497:ALA:O	2:A:501:ARG:HG3	1.87	0.74
2:A:105:PHE:CD1	2:A:181:LEU:HD11	2.22	0.74
1:C:11:DT:H5"	2:A:353:HIS:CE1	2.23	0.74
2:B:135:LEU:HB2	2:B:164:PHE:HE1	1.53	0.74
2:A:282:ARG:O	2:A:285:LYS:HB3	1.88	0.74
2:B:135:LEU:HD13	2:B:164:PHE:CD1	2.23	0.73
2:A:77:ARG:HB2	2:A:521:LEU:O	1.88	0.73
1:C:4:DT:C2'	1:C:5:DT:H5"	2.18	0.73
2:B:133:GLN:OE1	2:B:134:GLN:HG3	1.88	0.73
2:A:370:LYS:HZ1	2:A:554:LEU:H	1.35	0.73
2:B:424:TRP:HA	2:B:424:TRP:CE3	2.24	0.73
2:A:573:MET:SD	2:A:578:LEU:HD12	2.28	0.73
2:B:350:ARG:HH11	2:B:350:ARG:CG	2.01	0.73
2:B:132:LEU:O	2:B:136:ILE:HG13	1.88	0.73
1:C:6:DT:H2"	1:C:7:DT:OP2	1.88	0.73
2:A:381:PRO:HB2	2:A:501:ARG:HH22	1.51	0.73
2:A:132:LEU:O	2:A:135:LEU:HB3	1.89	0.73
2:A:512:MET:HG3	2:A:530:VAL:HG11	1.69	0.73
2:B:411:ARG:N	2:B:411:ARG:HD2	2.02	0.73
2:B:459:TRP:CZ2	2:B:481:GLY:HA3	2.24	0.73
2:A:200:VAL:O	2:A:203:ARG:HB2	1.89	0.72
2:A:556:THR:HG22	2:A:557:LEU:N	2.04	0.72
2:A:174:HIS:CE1	2:A:178:CYS:SG	2.83	0.72
2:A:136:ILE:O	2:A:139:ILE:HG22	1.89	0.72
2:B:581:GLN:HA	2:B:584:ILE:HG13	1.71	0.72
2:B:579:PRO:HA	2:B:592:GLU:HG2	1.71	0.72
2:A:411:ARG:HG3	2:A:412:GLU:N	2.04	0.72
2:B:51:ALA:O	2:B:211:LEU:HD12	1.90	0.72
2:A:629:PHE:HA	2:A:632:GLU:OE1	1.90	0.72
2:B:602:ARG:N	2:B:602:ARG:HD2	2.03	0.72
2:B:165:ALA:O	2:B:168:TYR:HB3	1.90	0.71
2:A:33:THR:HA	2:A:36:ILE:HD11	1.71	0.71
2:A:25:GLY:HA2	2:A:278:ARG:HE	1.55	0.71
2:B:336:PHE:O	2:B:339:LYS:HE3	1.91	0.71
2:B:263:GLN:O	2:B:265:PHE:N	2.23	0.71
2:A:278:ARG:HH12	2:A:602:ARG:HH12	1.38	0.71
2:A:116:LEU:O	2:A:120:LEU:HG	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:TYR:CD2	2:B:478:LEU:HD11	2.26	0.71
2:A:408:THR:O	2:A:410:LYS:N	2.23	0.71
2:B:220:ASN:HD22	2:B:220:ASN:C	1.93	0.71
2:B:107:LEU:HD13	2:B:107:LEU:H	1.56	0.71
2:A:77:ARG:HD2	2:A:523:GLU:HG2	1.70	0.71
2:B:189:LEU:HB3	2:B:190:PRO:CD	2.13	0.71
2:B:389:TYR:OH	2:B:409:PRO:CG	2.39	0.71
2:B:105:PHE:HB3	2:B:179:ASN:O	1.91	0.71
2:A:160:ARG:HH11	2:A:160:ARG:HB3	1.55	0.71
2:B:424:TRP:CD1	2:B:441:LEU:HD22	2.26	0.70
2:B:3:LEU:HD23	2:B:8:GLN:N	2.06	0.70
2:A:291:ILE:HD11	2:A:296:HIS:NE2	2.07	0.70
2:B:194:LEU:HD21	2:B:204:TRP:CD1	2.27	0.70
2:B:182:ASP:O	2:B:185:ASP:HB2	1.91	0.70
2:B:417:THR:HG21	2:B:449:GLY:HA3	1.74	0.70
2:A:203:ARG:NH1	2:A:203:ARG:HB3	2.06	0.70
2:A:280:SER:OG	2:A:283:ILE:HG12	1.91	0.70
2:A:29:THR:O	2:A:33:THR:HG23	1.90	0.70
2:A:596:ALA:O	2:A:600:ILE:HG13	1.91	0.70
2:A:493:PRO:HD2	2:B:99:LEU:HD11	1.74	0.70
2:A:86:THR:CG2	2:A:533:ARG:HH12	2.04	0.70
2:B:117:LEU:HA	2:B:120:LEU:HD12	1.73	0.70
2:B:616:ARG:HA	2:B:621:LEU:HD23	1.73	0.70
2:B:93:LYS:HG3	2:B:94:ARG:N	2.06	0.70
2:A:369:TYR:CB	2:A:552:VAL:HB	2.23	0.69
1:C:4:DT:C2'	1:C:5:DT:C5'	2.66	0.69
2:A:503:LYS:HA	2:A:506:ASN:HD22	1.58	0.69
2:A:139:ILE:HA	2:A:142:TRP:CZ3	2.27	0.69
2:B:428:ARG:HH22	2:B:440:GLY:HA3	1.57	0.69
2:A:26:SER:CB	2:A:273:LEU:HG	2.22	0.69
2:A:635:GLN:HE21	2:A:638:LEU:HD22	1.56	0.69
2:A:219:THR:HB	2:A:257:ASN:OD1	1.91	0.69
1:C:11:DT:C2'	1:C:11:DT:OP2	2.35	0.69
2:A:370:LYS:HE3	2:A:553:GLN:HA	1.74	0.69
2:B:74:LYS:H	2:B:74:LYS:CD	2.03	0.69
2:B:525:MET:HE3	2:B:533:ARG:NH1	2.08	0.69
2:A:49:HIS:CE1	2:A:209:ARG:HE	2.11	0.69
2:A:293:ASN:OD1	2:A:632:GLU:HB3	1.92	0.69
2:B:92:ILE:HG13	2:B:190:PRO:CG	2.23	0.69
2:A:200:VAL:HG13	2:A:201:ARG:H	1.57	0.69
2:A:321:GLU:HG2	2:A:361:PHE:CE2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:343:LYS:HA	2:A:553:GLN:OE1	1.92	0.68
2:A:64:LYS:HG2	2:A:81:ILE:HD13	1.73	0.68
2:B:125:ILE:CG1	2:B:131:LEU:HD21	2.23	0.68
2:B:163:ILE:HG22	2:B:167:CYS:SG	2.34	0.68
2:B:107:LEU:N	2:B:107:LEU:HD22	2.07	0.68
2:A:360:LYS:O	2:A:363:MET:HG2	1.93	0.68
2:B:159:GLU:HG3	2:B:160:ARG:H	1.58	0.68
2:B:260:LEU:HA	2:B:263:GLN:NE2	2.08	0.68
2:A:25:GLY:CA	2:A:278:ARG:HE	2.07	0.68
2:B:424:TRP:HE3	2:B:424:TRP:HA	1.57	0.68
2:B:389:TYR:HD2	2:B:478:LEU:HD21	1.59	0.68
2:A:334:HIS:O	2:A:338:ASN:HB2	1.94	0.68
2:A:342:TYR:HA	2:A:345:TYR:HD2	1.57	0.67
2:B:280:SER:HB3	2:B:283:ILE:HD13	1.76	0.67
2:B:98:ALA:C	2:B:100:GLY:H	1.96	0.67
2:A:556:THR:HG22	2:A:558:HIS:H	1.59	0.67
2:B:383:ILE:HG23	2:B:508:LEU:HD22	1.77	0.67
2:B:278:ARG:HD3	2:B:564:GLU:OE1	1.93	0.67
2:B:389:TYR:CD1	2:B:405:ILE:HD12	2.30	0.67
2:B:63:MET:O	2:B:67:VAL:HG23	1.95	0.67
2:B:396:PRO:HG2	2:B:464:GLN:HE22	1.60	0.67
2:A:160:ARG:NH1	2:A:160:ARG:HB3	2.09	0.67
2:A:501:ARG:HA	2:A:504:ASN:HD22	1.59	0.67
2:A:278:ARG:HH12	2:A:602:ARG:NH1	1.93	0.67
2:B:419:LYS:HZ1	2:B:422:GLY:HA3	1.60	0.67
2:B:420:LYS:HB2	2:B:445:LEU:HD23	1.76	0.67
2:A:565:PHE:O	2:A:604:GLN:HG2	1.95	0.66
2:B:635:GLN:OE1	2:B:640:TRP:CZ3	2.48	0.66
2:A:581:GLN:HA	2:A:584:ILE:HB	1.78	0.66
1:C:11:DT:H5"	2:A:353:HIS:ND1	2.09	0.66
2:A:88:GLY:O	2:A:92:ILE:HG12	1.95	0.66
1:C:9:DT:H1'	1:C:10:DT:H4'	1.77	0.66
2:B:476:ARG:HB2	2:B:476:ARG:HH11	1.60	0.66
2:A:28:LYS:O	2:A:32:ILE:CD1	2.43	0.66
2:A:28:LYS:O	2:A:32:ILE:CG1	2.44	0.66
2:B:170:LEU:O	2:B:173:ALA:HB3	1.94	0.66
2:B:365:ASN:O	2:B:366:ARG:HG2	1.95	0.66
2:B:208:ILE:O	2:B:208:ILE:HG22	1.97	0.66
2:A:19:LEU:HD22	2:A:270:VAL:HG13	1.77	0.65
2:B:359:GLU:HG2	2:B:369:TYR:OH	1.95	0.65
2:A:3:LEU:HG	2:A:7:GLN:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:LEU:HD22	2:B:135:LEU:HG	1.77	0.65
2:A:407:ASN:HD22	2:A:410:LYS:HD2	1.61	0.65
2:B:419:LYS:HA	2:B:419:LYS:NZ	2.10	0.65
2:B:479:ILE:HG22	2:B:480:HIS:N	2.11	0.65
2:A:573:MET:SD	2:A:578:LEU:CD1	2.84	0.65
2:B:526:THR:OG1	2:B:529:GLN:HG2	1.97	0.65
2:B:389:TYR:OH	2:B:409:PRO:HG3	1.96	0.65
2:B:459:TRP:HZ2	2:B:481:GLY:HA3	1.61	0.65
2:B:312:LEU:HB2	2:B:638:LEU:HD13	1.77	0.65
2:A:396:PRO:HG3	2:A:464:GLN:NE2	2.11	0.65
2:A:513:THR:HG22	2:A:517:GLU:HG3	1.79	0.65
2:A:579:PRO:HG3	2:A:629:PHE:CE2	2.31	0.65
2:A:328:THR:HG21	2:A:361:PHE:HB3	1.79	0.65
2:A:211:LEU:C	2:A:212:LEU:HD12	2.17	0.65
2:B:436:SER:OG	2:B:457:THR:HG21	1.96	0.65
2:A:389:TYR:HB3	2:A:478:LEU:HD21	1.78	0.65
2:B:263:GLN:C	2:B:265:PHE:H	2.01	0.65
2:B:555:MET:HG3	2:B:559:ALA:HB3	1.79	0.65
2:B:176:LYS:HG3	2:B:177:ALA:N	2.12	0.64
2:B:377:PHE:O	2:B:380:ARG:HG3	1.96	0.64
2:B:363:MET:SD	2:B:364:GLN:N	2.70	0.64
2:A:368:PRO:HB2	2:A:551:GLN:HE21	1.62	0.64
2:B:578:LEU:O	2:B:580:HIS:N	2.29	0.64
2:A:347:ILE:C	2:A:348:LEU:HD23	2.17	0.64
2:A:335:HIS:O	2:A:339:LYS:N	2.30	0.64
2:A:370:LYS:NZ	2:A:554:LEU:N	2.38	0.64
2:A:589:ILE:HD12	2:A:590:ASP:N	2.13	0.64
2:B:617:GLN:HB2	2:B:622:VAL:CG1	2.28	0.64
2:B:49:HIS:HB3	2:B:209:ARG:HG3	1.79	0.64
2:A:200:VAL:HG13	2:A:201:ARG:N	2.12	0.64
2:B:424:TRP:CD1	2:B:441:LEU:HA	2.30	0.64
2:B:576:GLY:O	2:B:580:HIS:HA	1.97	0.64
2:B:363:MET:SD	2:B:363:MET:C	2.76	0.64
2:A:3:LEU:HD13	2:A:30:ARG:HE	1.61	0.64
2:B:472:ILE:O	2:B:475:VAL:HG12	1.98	0.64
2:B:135:LEU:HB2	2:B:164:PHE:CE1	2.33	0.64
2:B:74:LYS:HE3	2:B:75:GLU:H	1.62	0.64
2:B:428:ARG:NH1	2:B:438:ASP:HB3	2.12	0.63
2:B:441:LEU:HD12	2:B:445:LEU:HD11	1.79	0.63
2:A:484:TYR:O	2:A:487:TRP:HB3	1.98	0.63
2:B:28:LYS:HG3	2:B:29:THR:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:560:SER:O	2:A:563:LEU:HB2	1.97	0.63
2:B:428:ARG:NH2	2:B:440:GLY:HA3	2.13	0.63
2:A:321:GLU:HG2	2:A:361:PHE:HE2	1.63	0.63
2:A:382:GLU:OE2	2:A:501:ARG:HA	1.97	0.63
2:B:581:GLN:O	2:B:584:ILE:HB	1.98	0.63
2:A:441:LEU:HD11	2:A:445:LEU:CD2	2.27	0.63
2:B:571:VAL:HA	2:B:610:THR:OG1	1.99	0.63
2:A:188:LEU:N	2:A:188:LEU:HD23	2.12	0.63
2:B:433:PHE:HZ	2:B:461:ALA:HB2	1.64	0.63
2:A:83:THR:HG23	2:A:85:HIS:N	2.13	0.63
2:A:380:ARG:HH11	2:A:380:ARG:HG3	1.64	0.63
2:A:255:PRO:HG2	2:A:256:GLN:HG2	1.78	0.63
2:B:9:GLN:HG2	2:B:271:ILE:HD13	1.81	0.63
2:A:611:LEU:HD22	2:A:611:LEU:O	1.99	0.63
2:B:194:LEU:HD21	2:B:204:TRP:HD1	1.64	0.63
2:A:203:ARG:CZ	2:A:203:ARG:HB3	2.28	0.63
2:A:168:TYR:HE1	2:A:172:ASP:HB2	1.64	0.63
2:A:104:ASN:ND2	2:A:104:ASN:H	1.96	0.62
2:A:187:ILE:O	2:A:190:PRO:HD2	1.99	0.62
2:B:181:LEU:H	2:B:181:LEU:HD12	1.64	0.62
2:A:24:ALA:O	2:A:276:ASN:ND2	2.32	0.62
2:B:315:LEU:HB2	2:B:610:THR:HG22	1.79	0.62
2:B:53:VAL:HG11	2:B:84:PHE:CD1	2.34	0.62
1:C:15:DT:H2"	1:C:16:DT:C5'	2.29	0.62
2:B:350:ARG:HD3	2:B:350:ARG:O	1.99	0.62
2:A:224:TYR:HD2	2:A:257:ASN:HD21	1.44	0.62
2:B:492:SER:HB3	2:B:498:ALA:HB2	1.81	0.62
2:A:487:TRP:O	2:A:491:THR:HG22	1.98	0.62
2:A:54:THR:HG22	2:A:55:PHE:N	2.11	0.62
2:B:456:PHE:CZ	2:B:460:LEU:HD11	2.34	0.62
2:A:234:ARG:HB3	2:A:236:ARG:HG2	1.79	0.62
2:A:278:ARG:HH22	2:A:602:ARG:NH2	1.98	0.62
2:B:500:MET:HG3	2:B:501:ARG:N	2.14	0.62
2:B:272:LYS:N	2:B:272:LYS:HD2	2.04	0.62
2:B:389:TYR:HB3	2:B:478:LEU:HD21	1.82	0.61
2:B:567:TYR:HD1	2:B:606:GLU:HG3	1.65	0.61
2:B:76:ALA:O	2:B:79:LEU:HD23	1.99	0.61
1:C:12:DT:H5'	2:A:580:HIS:CE1	2.36	0.61
2:B:183:PHE:HA	2:B:186:LEU:HD13	1.81	0.61
2:A:20:VAL:HB	2:A:240:VAL:HG22	1.82	0.61
2:B:270:VAL:HG21	2:B:298:PHE:HE2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:181:LEU:HD12	2:A:181:LEU:N	2.15	0.61
2:B:210:TYR:CE1	2:B:237:PHE:HA	2.35	0.61
2:A:184:ASP:O	2:A:188:LEU:HG	2.00	0.61
2:A:414:GLY:O	2:A:417:THR:HG23	2.00	0.61
2:A:600:ILE:HG23	2:A:607:LEU:CD2	2.31	0.61
2:A:116:LEU:HD11	2:A:174:HIS:CD2	2.35	0.61
2:B:74:LYS:HE3	2:B:75:GLU:N	2.16	0.61
2:B:617:GLN:HB2	2:B:622:VAL:HG13	1.83	0.61
2:B:324:ALA:O	2:B:328:THR:OG1	2.19	0.61
2:A:407:ASN:ND2	2:A:410:LYS:HD2	2.16	0.61
2:B:419:LYS:NZ	2:B:422:GLY:HA3	2.15	0.61
2:A:370:LYS:NZ	2:A:554:LEU:H	1.97	0.61
2:B:389:TYR:CD2	2:B:478:LEU:HD21	2.36	0.61
2:B:220:ASN:ND2	2:B:220:ASN:C	2.53	0.61
2:A:197:ASN:HD22	2:A:200:VAL:CG1	2.05	0.61
2:B:134:GLN:O	2:B:138:THR:HG22	2.01	0.61
2:A:28:LYS:O	2:A:32:ILE:HD11	2.01	0.61
2:B:359:GLU:HG2	2:B:369:TYR:CZ	2.35	0.61
2:A:635:GLN:HA	2:A:635:GLN:HE21	1.66	0.61
2:A:327:VAL:HG12	2:A:328:THR:N	2.16	0.61
2:B:419:LYS:HZ3	2:B:419:LYS:HA	1.64	0.61
2:B:234:ARG:HH11	2:B:234:ARG:HG3	1.65	0.61
2:B:406:VAL:CG2	2:B:407:ASN:H	2.06	0.60
2:A:484:TYR:CE2	2:A:488:LEU:HD21	2.36	0.60
2:B:79:LEU:HB3	2:B:81:ILE:HG13	1.82	0.60
1:C:10:DT:H2"	1:C:11:DT:N3	2.15	0.60
2:B:128:ASP:O	2:B:132:LEU:HG	2.01	0.60
2:A:589:ILE:HD12	2:A:590:ASP:H	1.65	0.60
2:B:181:LEU:HD12	2:B:181:LEU:N	2.16	0.60
1:C:10:DT:C3'	1:C:10:DT:P	2.89	0.60
2:B:618:TYR:C	2:B:620:GLU:N	2.55	0.60
2:A:386:LEU:HD11	2:A:479:ILE:CD1	2.32	0.60
1:C:10:DT:C6	1:C:10:DT:C5'	2.57	0.60
2:A:160:ARG:O	2:A:163:ILE:HB	2.02	0.60
2:A:181:LEU:HD12	2:A:181:LEU:H	1.66	0.60
2:B:152:ALA:O	2:B:156:ALA:HB2	2.02	0.60
2:A:370:LYS:HE3	2:A:553:GLN:HG3	1.84	0.60
2:B:193:LEU:O	2:B:193:LEU:HD12	2.02	0.60
2:A:72:GLY:HA3	2:A:74:LYS:HZ1	1.67	0.60
2:B:22:ALA:CB	2:B:273:LEU:HD12	2.29	0.60
2:A:486:SER:O	2:A:490:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:DT:H2"	1:C:10:DT:H4'	1.82	0.60
2:A:533:ARG:NH2	2:A:538:ASP:HB2	2.17	0.60
2:A:87:LEU:O	2:A:91:ILE:HD12	2.02	0.60
2:A:58:LYS:NZ	2:A:58:LYS:HB2	2.16	0.60
1:C:9:DT:H2"	1:C:10:DT:O5'	2.02	0.59
2:B:402:PHE:O	2:B:406:VAL:HG13	2.02	0.59
2:A:279:SER:HB2	2:A:284:LEU:HD21	1.84	0.59
2:A:368:PRO:C	2:A:551:GLN:HB2	2.23	0.59
2:A:261:LEU:HD13	2:A:268:LEU:CD2	2.32	0.59
2:A:555:MET:HG3	2:A:556:THR:O	2.00	0.59
2:B:132:LEU:O	2:B:135:LEU:HB3	2.02	0.59
2:A:102:LYS:HZ2	2:A:104:ASN:HB3	1.65	0.59
2:A:256:GLN:HA	2:A:256:GLN:HE21	1.67	0.59
2:A:369:TYR:HB2	2:A:552:VAL:HB	1.84	0.59
1:C:9:DT:C2	1:C:11:DT:H71	2.37	0.59
2:B:389:TYR:HE2	2:B:482:MET:SD	2.25	0.59
2:A:500:MET:SD	2:A:504:ASN:ND2	2.72	0.59
2:B:216:TYR:CE2	2:B:257:ASN:HB3	2.37	0.59
2:B:433:PHE:CE1	2:B:457:THR:HG23	2.37	0.59
2:A:408:THR:C	2:A:410:LYS:H	2.05	0.59
2:A:122:GLU:H	2:A:124:LEU:HD21	1.67	0.59
2:B:328:THR:CG2	2:B:362:LEU:HD23	2.32	0.59
2:A:217:GLN:N	2:A:217:GLN:OE1	2.33	0.59
2:A:19:LEU:C	2:A:19:LEU:HD23	2.22	0.59
2:A:339:LYS:NZ	2:A:341:GLN:H	2.01	0.59
2:A:165:ALA:O	2:A:168:TYR:HB3	2.02	0.58
2:A:419:LYS:HD2	2:A:423:GLU:OE1	2.03	0.58
2:B:331:LEU:HD23	2:B:331:LEU:C	2.23	0.58
2:A:557:LEU:HB3	2:A:595:LEU:CD2	2.33	0.58
2:B:185:ASP:O	2:B:189:LEU:HB2	2.02	0.58
2:B:476:ARG:HB2	2:B:476:ARG:NH1	2.17	0.58
2:A:594:ARG:O	2:A:597:TYR:HB3	2.03	0.58
1:C:10:DT:H2"	1:C:11:DT:C2	2.38	0.58
2:A:14:VAL:HG21	2:A:43:CYS:SG	2.43	0.58
2:A:328:THR:O	2:A:332:ILE:HG13	2.03	0.58
2:A:509:PHE:O	2:A:512:MET:HB3	2.04	0.58
2:A:256:GLN:O	2:A:260:LEU:HD13	2.03	0.58
2:B:111:THR:HG23	2:B:112:ASP:H	1.68	0.58
2:B:456:PHE:CE2	2:B:460:LEU:HD11	2.39	0.58
2:B:328:THR:HG22	2:B:362:LEU:HD23	1.84	0.58
2:B:45:TYR:CE1	2:B:210:TYR:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:126:GLU:O	2:A:128:ASP:N	2.37	0.58
2:A:278:ARG:NH2	2:A:602:ARG:HH22	2.00	0.58
2:B:460:LEU:O	2:B:463:ILE:HG22	2.03	0.58
2:B:592:GLU:O	2:B:595:LEU:HB3	2.04	0.58
2:B:142:TRP:HE3	2:B:168:TYR:CD2	2.22	0.58
2:B:49:HIS:HB3	2:B:209:ARG:CG	2.34	0.58
2:B:40:ILE:HG22	2:B:41:ARG:N	2.19	0.58
2:B:594:ARG:O	2:B:598:VAL:HG23	2.04	0.58
2:B:177:ALA:O	2:B:179:ASN:N	2.37	0.58
2:B:314:VAL:HG23	2:B:638:LEU:HD11	1.85	0.58
2:A:238:THR:HG22	2:A:238:THR:O	2.04	0.58
2:B:324:ALA:HA	2:B:358:PHE:CE1	2.39	0.58
2:A:576:GLY:O	2:A:580:HIS:HA	2.04	0.57
2:A:582:SER:O	2:A:586:GLU:HB2	2.04	0.57
2:B:291:ILE:HB	2:B:597:TYR:CD2	2.39	0.57
2:B:391:ARG:HD3	2:B:398:ASP:CG	2.25	0.57
2:B:208:ILE:HD13	2:B:230:LEU:HD22	1.85	0.57
1:C:15:DT:O2	1:C:15:DT:O5'	2.21	0.57
2:A:334:HIS:CE1	2:A:338:ASN:HD22	2.22	0.57
2:A:83:THR:HG23	2:A:84:PHE:N	2.19	0.57
2:A:459:TRP:CH2	2:A:478:LEU:HD12	2.40	0.57
2:B:184:ASP:OD1	2:B:184:ASP:N	2.35	0.57
1:C:1:DT:N3	1:C:2:DT:N3	2.52	0.57
2:B:208:ILE:CD1	2:B:230:LEU:HD22	2.34	0.57
2:A:369:TYR:HB3	2:A:552:VAL:HB	1.85	0.57
2:A:87:LEU:HG	2:A:91:ILE:CD1	2.35	0.57
2:B:206:ASN:O	2:B:209:ARG:NE	2.37	0.57
2:B:384:LYS:HA	2:B:384:LYS:CE	2.33	0.57
2:A:188:LEU:H	2:A:188:LEU:HD23	1.69	0.57
2:B:61:ARG:O	2:B:65:GLU:HG3	2.05	0.57
2:A:25:GLY:HA2	2:A:278:ARG:NE	2.18	0.57
2:A:143:LYS:O	2:A:145:ASP:N	2.37	0.57
2:A:243:ASP:HB3	2:A:258:LEU:HG	1.86	0.57
2:B:406:VAL:HG23	2:B:407:ASN:N	2.10	0.57
2:B:320:GLU:HG3	2:B:615:ARG:NH1	2.20	0.57
2:A:279:SER:HA	2:A:604:GLN:HA	1.86	0.57
2:B:171:TYR:OH	2:B:182:ASP:HB3	2.04	0.57
2:A:488:LEU:HA	2:A:491:THR:CG2	2.34	0.57
2:B:108:PHE:HE2	2:B:116:LEU:HD22	1.69	0.57
2:B:488:LEU:HD22	2:B:501:ARG:NE	2.20	0.57
2:B:55:PHE:HD1	2:B:55:PHE:N	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:399:ASP:O	2:B:403:LEU:HB2	2.05	0.57
2:A:382:GLU:HA	2:A:484:TYR:OH	2.04	0.57
2:A:224:TYR:CZ	2:A:228:LYS:NZ	2.72	0.57
2:A:381:PRO:HB2	2:A:501:ARG:HH21	1.65	0.56
2:A:320:GLU:CA	2:A:612:CYS:SG	2.90	0.56
2:B:226:LEU:HD22	2:B:230:LEU:CD1	2.34	0.56
2:A:224:TYR:CD2	2:A:257:ASN:ND2	2.73	0.56
2:B:259:VAL:HG12	2:B:260:LEU:N	2.20	0.56
2:B:9:GLN:CG	2:B:271:ILE:HD13	2.34	0.56
2:B:12:GLU:O	2:B:14:VAL:HG13	2.05	0.56
2:B:407:ASN:O	2:B:410:LYS:N	2.34	0.56
2:B:116:LEU:HG	2:B:120:LEU:CD1	2.36	0.56
2:A:136:ILE:HG22	2:A:137:SER:N	2.19	0.56
2:B:382:GLU:CD	2:B:501:ARG:HG3	2.26	0.56
2:A:638:LEU:O	2:A:639:ILE:HD13	2.05	0.56
2:B:149:PRO:CB	2:B:169:GLY:HA2	2.35	0.56
2:A:124:LEU:H	2:A:124:LEU:CD2	2.04	0.56
2:B:433:PHE:CD1	2:B:457:THR:HG23	2.40	0.56
2:A:7:GLN:HG2	2:A:273:LEU:CD2	2.36	0.56
2:B:98:ALA:C	2:B:100:GLY:N	2.58	0.56
2:B:55:PHE:CD1	2:B:55:PHE:N	2.74	0.56
2:B:383:ILE:O	2:B:383:ILE:HG22	2.05	0.56
2:B:501:ARG:O	2:B:505:VAL:HG23	2.06	0.56
2:A:556:THR:HG22	2:A:557:LEU:H	1.70	0.56
2:A:578:LEU:HB3	2:A:579:PRO:CD	2.27	0.56
2:B:91:ILE:CG2	2:B:190:PRO:HB3	2.35	0.56
1:C:1:DT:O4'	2:B:580:HIS:NE2	2.38	0.56
2:B:616:ARG:HA	2:B:621:LEU:CD2	2.36	0.56
2:A:64:LYS:HE2	2:A:77:ARG:HA	1.88	0.56
2:A:578:LEU:O	2:A:580:HIS:N	2.38	0.56
2:B:202:LYS:HE3	2:B:205:GLN:HB3	1.88	0.56
2:B:403:LEU:O	2:B:406:VAL:HG22	2.05	0.56
2:B:509:PHE:CD1	2:B:510:SER:N	2.73	0.56
2:A:553:GLN:HG2	2:A:565:PHE:HE1	1.70	0.56
1:C:3:DT:C2'	1:C:4:DT:OP2	2.51	0.56
2:B:193:LEU:HG	2:B:194:LEU:HD12	1.88	0.56
2:A:7:GLN:HG2	2:A:273:LEU:HD22	1.88	0.56
2:A:370:LYS:HE3	2:A:553:GLN:CA	2.35	0.56
2:A:382:GLU:H	2:A:501:ARG:HH21	1.52	0.56
2:A:257:ASN:CA	2:A:260:LEU:HD22	2.35	0.56
2:B:314:VAL:HG23	2:B:638:LEU:CD1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:234:ARG:HG2	2:B:236:ARG:HG2	1.88	0.55
2:B:628:ARG:HA	2:B:631:LEU:HD23	1.88	0.55
2:A:344:ASP:O	2:A:566:PRO:HG2	2.06	0.55
2:B:208:ILE:O	2:B:208:ILE:CG2	2.54	0.55
2:A:8:GLN:O	2:A:12:GLU:HG2	2.05	0.55
2:B:472:ILE:HD13	2:B:472:ILE:N	2.22	0.55
2:A:82:SER:HB2	2:A:86:THR:OG1	2.07	0.55
2:A:591:GLU:HA	2:A:594:ARG:HH11	1.72	0.55
2:B:91:ILE:HB	2:B:190:PRO:CG	2.36	0.55
2:A:119:GLU:HG3	2:A:120:LEU:N	2.21	0.55
2:A:168:TYR:CD1	2:A:168:TYR:C	2.78	0.55
2:B:159:GLU:HA	2:B:162:ARG:CZ	2.37	0.55
1:C:9:DT:C1'	1:C:10:DT:H4'	2.37	0.55
2:B:79:LEU:O	2:B:81:ILE:N	2.40	0.55
2:A:290:LEU:HD13	2:A:600:ILE:CD1	2.36	0.55
2:B:472:ILE:HD13	2:B:472:ILE:H	1.72	0.55
2:B:350:ARG:CG	2:B:350:ARG:NH1	2.68	0.55
2:B:304:SER:OG	2:B:306:LEU:HD12	2.06	0.55
2:B:528:THR:O	2:B:532:THR:HG23	2.06	0.55
2:A:402:PHE:CD2	2:A:432:MET:HB2	2.42	0.55
2:B:217:GLN:NE2	2:B:217:GLN:H	2.04	0.55
1:C:13:DT:O4'	2:A:350:ARG:NH2	2.40	0.55
2:A:237:PHE:HE1	2:A:239:VAL:HG22	1.72	0.55
2:A:107:LEU:HB2	2:A:535:THR:HG21	1.87	0.55
2:A:361:PHE:HA	2:A:364:GLN:HB3	1.88	0.55
2:B:202:LYS:HE2	2:B:206:ASN:HB2	1.89	0.55
2:B:20:VAL:HA	2:B:271:ILE:O	2.06	0.55
2:B:61:ARG:HA	2:B:64:LYS:HG3	1.88	0.55
2:A:279:SER:O	2:A:284:LEU:HD11	2.07	0.55
2:A:294:ASN:ND2	2:A:593:ARG:HH11	2.05	0.55
2:A:342:TYR:HA	2:A:345:TYR:CD2	2.42	0.55
2:B:114:LEU:O	2:B:117:LEU:HB2	2.06	0.55
2:A:54:THR:HG21	2:A:59:ALA:HB3	1.89	0.55
2:A:622:VAL:O	2:A:624:PRO:HD3	2.06	0.55
2:A:556:THR:CG2	2:A:557:LEU:N	2.70	0.55
2:B:424:TRP:HB3	2:B:441:LEU:CD1	2.37	0.55
2:B:74:LYS:O	2:B:76:ALA:N	2.39	0.55
2:A:135:LEU:HB2	2:A:164:PHE:HE1	1.70	0.55
2:A:160:ARG:HH21	2:A:161:ASP:CB	2.19	0.55
2:B:641:GLU:HG2	2:B:642:GLN:N	2.22	0.55
2:B:151:GLN:O	2:B:154:ALA:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:GLU:OE2	2:B:200:VAL:HG13	2.07	0.54
2:A:342:TYR:HB3	2:A:552:VAL:HG22	1.89	0.54
2:A:493:PRO:CD	2:B:99:LEU:HD11	2.37	0.54
2:A:378:PHE:CE2	2:A:539:MET:HB3	2.42	0.54
2:A:288:ASN:ND2	2:A:302:LEU:N	2.55	0.54
2:B:88:GLY:O	2:B:190:PRO:HG2	2.07	0.54
2:B:71:LEU:HB3	2:B:76:ALA:HB2	1.89	0.54
2:A:139:ILE:HA	2:A:142:TRP:HE3	1.68	0.54
2:A:354:GLN:O	2:A:358:PHE:CD1	2.59	0.54
2:B:468:GLU:HA	2:B:468:GLU:OE2	2.08	0.54
2:B:346:ALA:HA	2:B:553:GLN:O	2.07	0.54
2:A:40:ILE:HA	2:A:45:TYR:O	2.08	0.54
2:A:70:THR:O	2:A:71:LEU:HD23	2.08	0.54
2:B:323:GLU:O	2:B:327:VAL:HG23	2.07	0.54
2:A:342:TYR:HB2	2:A:551:GLN:C	2.27	0.54
1:C:7:DT:O4	2:B:105:PHE:CD1	2.60	0.54
2:A:259:VAL:O	2:A:262:SER:N	2.41	0.54
2:B:3:LEU:HD23	2:B:7:GLN:C	2.28	0.54
2:A:341:GLN:HB2	2:A:343:LYS:HG2	1.90	0.54
2:A:484:TYR:HE2	2:A:488:LEU:HD21	1.72	0.54
2:B:105:PHE:N	2:B:105:PHE:HD1	2.03	0.54
2:A:124:LEU:N	2:A:124:LEU:HD23	2.13	0.54
2:A:39:LEU:O	2:A:43:CYS:HB2	2.08	0.54
2:B:105:PHE:H	2:B:105:PHE:HD1	1.54	0.54
2:B:164:PHE:O	2:B:168:TYR:HB2	2.07	0.54
2:B:531:VAL:HG12	2:B:532:THR:N	2.22	0.54
2:B:585:ASP:O	2:B:586:GLU:HG3	2.07	0.54
2:B:187:ILE:C	2:B:189:LEU:H	2.11	0.54
2:B:391:ARG:CD	2:B:401:ALA:HB2	2.26	0.54
2:B:508:LEU:HD11	2:B:534:PHE:CE2	2.43	0.54
2:A:64:LYS:CG	2:A:81:ILE:HD13	2.36	0.54
2:B:598:VAL:O	2:B:601:THR:N	2.41	0.54
2:B:126:GLU:OE2	2:B:131:LEU:HD13	2.08	0.54
2:B:105:PHE:HB2	2:B:180:VAL:HA	1.89	0.54
2:A:288:ASN:HD21	2:A:301:ARG:CA	2.21	0.54
2:A:370:LYS:CE	2:A:553:GLN:HA	2.37	0.54
2:A:370:LYS:NZ	2:A:554:LEU:O	2.41	0.54
2:A:607:LEU:HD12	2:A:608:THR:H	1.73	0.54
2:B:91:ILE:HB	2:B:190:PRO:HG2	1.89	0.54
2:B:516:LEU:HD21	2:B:527:LEU:HD12	1.90	0.54
2:B:128:ASP:O	2:B:131:LEU:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:DT:O2	1:C:7:DT:C2'	2.53	0.54
2:B:226:LEU:HD22	2:B:230:LEU:HD12	1.90	0.54
2:A:635:GLN:HA	2:A:635:GLN:NE2	2.22	0.54
2:A:284:LEU:HD13	2:A:304:SER:H	1.73	0.54
2:B:74:LYS:HB2	2:B:74:LYS:NZ	2.22	0.54
2:B:13:PHE:CE2	2:B:269:LYS:CB	2.91	0.54
2:A:7:GLN:O	2:A:11:VAL:HG23	2.07	0.53
2:B:369:TYR:CE1	2:B:371:ILE:HD11	2.42	0.53
2:A:104:ASN:HD22	2:A:104:ASN:N	1.96	0.53
2:B:554:LEU:C	2:B:554:LEU:HD23	2.29	0.53
2:A:392:VAL:HG12	2:A:393:LEU:N	2.23	0.53
2:B:435:ALA:C	2:B:437:PHE:H	2.11	0.53
2:A:286:ALA:HB2	2:A:312:LEU:HD11	1.90	0.53
2:A:211:LEU:HD12	2:A:212:LEU:C	2.29	0.53
2:B:575:GLU:OE2	2:B:579:PRO:HG2	2.07	0.53
2:B:74:LYS:O	2:B:77:ARG:HG3	2.07	0.53
2:A:408:THR:HB	2:A:409:PRO:HD3	1.89	0.53
2:B:525:MET:CE	2:B:529:GLN:HB2	2.38	0.53
2:A:318:ASN:HA	2:A:613:LYS:CB	2.38	0.53
2:A:254:ARG:HG3	2:A:257:ASN:CG	2.29	0.53
2:A:426:MET:C	2:A:426:MET:SD	2.87	0.53
2:B:72:GLY:O	2:B:74:LYS:HE3	2.08	0.53
2:A:574:GLU:HG3	2:A:577:PHE:CD1	2.43	0.53
2:A:389:TYR:OH	2:A:409:PRO:HG2	2.07	0.53
2:B:84:PHE:CE2	2:B:223:GLN:HB3	2.43	0.53
2:A:81:ILE:HD12	2:A:81:ILE:N	2.23	0.53
2:A:416:ALA:O	2:A:419:LYS:N	2.41	0.53
2:A:33:THR:HA	2:A:36:ILE:CD1	2.36	0.53
2:B:350:ARG:HD3	2:B:350:ARG:C	2.29	0.53
2:B:173:ALA:O	2:B:176:LYS:HG2	2.09	0.53
1:C:7:DT:O4	2:B:105:PHE:HD1	1.92	0.53
2:A:224:TYR:O	2:A:227:VAL:HB	2.08	0.53
2:B:617:GLN:N	2:B:620:GLU:O	2.42	0.53
2:A:105:PHE:HD1	2:A:181:LEU:HD11	1.73	0.53
2:A:573:MET:N	2:A:610:THR:O	2.39	0.53
2:B:312:LEU:O	2:B:638:LEU:HD12	2.09	0.53
2:B:476:ARG:HH11	2:B:476:ARG:CB	2.19	0.53
2:A:378:PHE:HE2	2:A:539:MET:CB	2.22	0.53
2:B:441:LEU:O	2:B:445:LEU:HD12	2.08	0.53
2:B:108:PHE:CE2	2:B:116:LEU:HD22	2.44	0.53
2:B:47:ALA:HB2	2:B:75:GLU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:PRO:O	2:B:498:ALA:N	2.41	0.53
2:B:217:GLN:HE21	2:B:242:ASP:H	1.57	0.53
2:A:174:HIS:CE1	2:A:178:CYS:HG	2.25	0.53
2:B:417:THR:CG2	2:B:449:GLY:HA3	2.38	0.53
2:A:406:VAL:HG23	2:A:407:ASN:H	1.74	0.53
2:B:160:ARG:O	2:B:163:ILE:HB	2.09	0.53
2:B:357:VAL:O	2:B:360:LYS:HB3	2.08	0.53
2:B:107:LEU:HD22	2:B:107:LEU:H	1.72	0.53
2:B:276:ASN:OD1	2:B:277:TYR:N	2.41	0.53
2:B:370:LYS:HG3	2:B:551:GLN:OE1	2.09	0.53
1:C:9:DT:C2'	1:C:10:DT:H4'	2.39	0.52
2:B:19:LEU:HD12	2:B:20:VAL:N	2.23	0.52
2:A:435:ALA:O	2:A:437:PHE:N	2.42	0.52
2:A:86:THR:HG22	2:A:533:ARG:NH1	2.19	0.52
2:B:217:GLN:H	2:B:217:GLN:CD	2.12	0.52
2:A:541:GLU:H	2:A:541:GLU:CD	2.12	0.52
2:B:350:ARG:NH1	2:B:580:HIS:HB2	2.24	0.52
2:A:7:GLN:O	2:A:10:ALA:HB3	2.10	0.52
2:A:79:LEU:O	2:A:81:ILE:HD12	2.10	0.52
2:A:143:LYS:O	2:A:146:LEU:N	2.43	0.52
2:B:28:LYS:CG	2:B:29:THR:N	2.72	0.52
1:C:13:DT:O2	2:A:350:ARG:NH2	2.43	0.52
2:B:389:TYR:CZ	2:B:482:MET:SD	3.03	0.52
2:B:224:TYR:C	2:B:224:TYR:CD1	2.83	0.52
2:B:622:VAL:HG23	2:B:624:PRO:HG3	1.92	0.52
2:B:13:PHE:HE2	2:B:269:LYS:CB	2.23	0.52
2:B:471:PRO:HB3	2:B:527:LEU:HD13	1.92	0.52
2:A:254:ARG:HD3	2:A:260:LEU:CD2	2.38	0.52
2:B:4:ASN:OD1	2:B:7:GLN:HG3	2.10	0.52
2:A:89:LEU:HA	2:A:92:ILE:HG13	1.92	0.52
2:A:135:LEU:HB2	2:A:164:PHE:CE1	2.44	0.52
2:A:635:GLN:NE2	2:A:638:LEU:HD22	2.24	0.52
2:A:573:MET:HG3	2:A:609:PHE:HB3	1.92	0.52
2:A:62:GLU:O	2:A:66:ARG:HD2	2.10	0.52
2:B:407:ASN:OD1	2:B:413:ILE:N	2.42	0.52
2:B:420:LYS:HD2	2:B:445:LEU:HB3	1.91	0.52
2:A:515:MET:HG2	2:A:525:MET:CE	2.40	0.52
2:B:98:ALA:O	2:B:100:GLY:N	2.43	0.52
1:C:13:DT:H4'	2:A:556:THR:HG21	1.92	0.51
2:A:212:LEU:N	2:A:212:LEU:CD1	2.67	0.51
2:A:237:PHE:CD1	2:A:238:THR:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:LEU:HD21	2:B:463:ILE:HG23	1.92	0.51
2:A:87:LEU:HG	2:A:91:ILE:HD11	1.92	0.51
2:B:249:SER:HB3	2:B:591:GLU:OE1	2.10	0.51
1:C:1:DT:H3	1:C:2:DT:H3	1.58	0.51
2:B:22:ALA:HA	2:B:273:LEU:HB2	1.92	0.51
2:A:117:LEU:O	2:A:121:THR:N	2.43	0.51
2:B:392:VAL:HG12	2:B:393:LEU:N	2.25	0.51
2:B:455:ARG:O	2:B:458:HIS:HB3	2.10	0.51
2:B:459:TRP:CH2	2:B:478:LEU:HD12	2.45	0.51
2:A:224:TYR:OH	2:A:261:LEU:HA	2.10	0.51
2:B:202:LYS:O	2:B:202:LYS:HD3	2.10	0.51
2:B:60:ALA:O	2:B:64:LYS:HG3	2.10	0.51
2:A:413:ILE:O	2:A:413:ILE:HG22	2.10	0.51
2:B:89:LEU:HD23	2:B:90:ASP:N	2.25	0.51
2:A:91:ILE:HG21	2:A:190:PRO:HB3	1.92	0.51
2:B:575:GLU:O	2:B:579:PRO:O	2.29	0.51
2:A:405:ILE:HA	2:A:408:THR:OG1	2.11	0.51
2:A:128:ASP:HB3	2:A:131:LEU:HD23	1.91	0.51
2:A:285:LYS:HD2	2:A:308:TYR:OH	2.10	0.51
2:B:254:ARG:NH1	2:B:260:LEU:HD23	2.25	0.51
2:A:342:TYR:HB2	2:A:551:GLN:HA	1.92	0.51
2:A:598:VAL:O	2:A:602:ARG:HG2	2.10	0.51
2:B:120:LEU:CD2	2:B:170:LEU:HG	2.41	0.51
2:A:3:LEU:HD23	2:A:8:GLN:HG2	1.91	0.51
2:B:284:LEU:CD1	2:B:304:SER:HB3	2.41	0.51
2:B:215:GLU:HG3	2:B:218:ASP:OD2	2.11	0.51
2:A:573:MET:HE3	2:A:627:SER:HB2	1.93	0.51
2:B:598:VAL:O	2:B:599:GLY:C	2.48	0.51
2:B:403:LEU:HG	2:B:432:MET:HE1	1.93	0.51
1:C:1:DT:C2	1:C:2:DT:N3	2.78	0.51
2:B:53:VAL:HG11	2:B:84:PHE:CE1	2.46	0.51
2:A:416:ALA:O	2:A:417:THR:C	2.49	0.51
2:A:422:GLY:O	2:A:426:MET:N	2.41	0.51
2:A:408:THR:CB	2:A:409:PRO:HD3	2.40	0.51
2:B:220:ASN:CG	2:B:223:GLN:HG2	2.31	0.51
2:A:639:ILE:HG22	2:A:640:TRP:N	2.26	0.51
2:A:303:PHE:O	2:A:303:PHE:CD1	2.64	0.51
2:A:237:PHE:C	2:A:237:PHE:CD1	2.83	0.51
2:B:487:TRP:O	2:B:490:GLU:HG2	2.11	0.51
2:B:220:ASN:HD21	2:B:222:SER:HB3	1.75	0.51
2:B:226:LEU:O	2:B:226:LEU:HD22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:20:VAL:HA	2:A:271:ILE:O	2.10	0.51
2:A:105:PHE:HA	2:A:179:ASN:OD1	2.11	0.51
2:B:353:HIS:C	2:B:355:SER:N	2.63	0.51
2:B:410:LYS:O	2:B:410:LYS:CG	2.45	0.51
2:B:99:LEU:HB2	2:B:101:MET:HG2	1.93	0.51
2:A:411:ARG:CG	2:A:412:GLU:H	2.18	0.51
2:A:251:ARG:O	2:A:251:ARG:HG3	2.11	0.51
2:A:577:PHE:H	2:A:577:PHE:HD1	1.59	0.51
2:B:276:ASN:HD22	2:B:284:LEU:HD21	1.76	0.51
1:C:9:DT:O3'	1:C:11:DT:OP1	2.29	0.50
2:B:471:PRO:HD2	2:B:472:ILE:HD13	1.93	0.50
2:B:219:THR:HG22	2:B:257:ASN:ND2	2.26	0.50
2:A:175:LEU:CD1	2:A:180:VAL:HG22	2.41	0.50
2:B:409:PRO:O	2:B:410:LYS:CB	2.59	0.50
2:B:409:PRO:O	2:B:410:LYS:HB3	2.11	0.50
2:A:506:ASN:O	2:A:507:GLN:C	2.46	0.50
2:B:237:PHE:C	2:B:237:PHE:CD1	2.85	0.50
2:B:69:GLN:NE2	2:B:69:GLN:HA	2.26	0.50
2:B:424:TRP:HB3	2:B:441:LEU:CD2	2.41	0.50
2:B:188:LEU:C	2:B:188:LEU:HD12	2.32	0.50
2:B:282:ARG:HE	2:B:637:ASP:HB3	1.77	0.50
2:B:599:GLY:O	2:B:602:ARG:HB2	2.12	0.50
2:A:166:HIS:O	2:A:169:GLY:N	2.45	0.50
2:A:389:TYR:CB	2:A:478:LEU:HD21	2.42	0.50
2:B:10:ALA:HA	2:B:271:ILE:CD1	2.41	0.50
2:A:611:LEU:HD13	2:A:611:LEU:N	2.26	0.50
2:A:206:ASN:O	2:A:206:ASN:ND2	2.44	0.50
2:A:84:PHE:HB3	2:A:187:ILE:HD11	1.94	0.50
2:A:77:ARG:HH11	2:A:523:GLU:CG	2.24	0.50
2:A:316:SER:OG	2:A:611:LEU:HD21	2.12	0.50
2:A:122:GLU:N	2:A:124:LEU:HD21	2.26	0.50
2:B:641:GLU:HG2	2:B:642:GLN:H	1.77	0.50
2:B:51:ALA:HA	2:B:80:MET:HB2	1.93	0.50
2:A:565:PHE:O	2:A:603:ALA:HA	2.12	0.50
2:B:125:ILE:HG13	2:B:131:LEU:CD2	2.41	0.50
2:A:161:ASP:O	2:A:164:PHE:HB2	2.12	0.50
2:B:225:GLU:O	2:B:226:LEU:C	2.48	0.50
2:B:48:ARG:HA	2:B:78:GLY:O	2.11	0.50
2:B:353:HIS:O	2:B:355:SER:N	2.45	0.50
2:A:267:ALA:O	2:A:269:LYS:HG2	2.12	0.50
1:C:12:DT:H5'	2:A:580:HIS:HE1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:DT:OP1	2:A:352:ASN:ND2	2.43	0.49
2:B:594:ARG:HH11	2:B:594:ARG:HG3	1.77	0.49
2:A:114:LEU:O	2:A:117:LEU:HB2	2.11	0.49
2:B:433:PHE:CZ	2:B:461:ALA:HB2	2.44	0.49
2:A:533:ARG:HH21	2:A:538:ASP:HB2	1.77	0.49
2:B:175:LEU:HD23	2:B:181:LEU:HA	1.94	0.49
2:B:74:LYS:N	2:B:74:LYS:CD	2.74	0.49
2:A:346:ALA:HA	2:A:553:GLN:O	2.11	0.49
2:A:579:PRO:HD3	2:A:627:SER:OG	2.12	0.49
2:B:411:ARG:HB2	2:B:413:ILE:CD1	2.42	0.49
2:B:108:PHE:O	2:B:113:GLN:HG3	2.11	0.49
2:B:365:ASN:N	2:B:365:ASN:HD22	2.10	0.49
2:B:371:ILE:HD12	2:B:554:LEU:HD22	1.94	0.49
2:B:635:GLN:OE1	2:B:640:TRP:HZ3	1.93	0.49
2:A:586:GLU:O	2:A:587:ASP:CB	2.51	0.49
2:A:506:ASN:O	2:A:509:PHE:HB3	2.12	0.49
2:A:323:GLU:OE2	2:A:571:VAL:HB	2.11	0.49
2:B:371:ILE:O	2:B:371:ILE:HG22	2.12	0.49
2:B:21:LEU:CD1	2:B:242:ASP:HA	2.42	0.49
2:A:341:GLN:CB	2:A:343:LYS:HG2	2.43	0.49
2:A:278:ARG:NH1	2:A:602:ARG:HH12	2.08	0.49
2:A:185:ASP:O	2:A:189:LEU:HB2	2.13	0.49
2:B:575:GLU:O	2:B:576:GLY:C	2.47	0.49
2:B:52:ALA:O	2:B:81:ILE:HA	2.12	0.49
2:B:224:TYR:HD1	2:B:224:TYR:C	2.14	0.49
2:A:46:GLN:O	2:A:48:ARG:N	2.46	0.49
2:A:532:THR:O	2:A:535:THR:HB	2.11	0.49
2:A:254:ARG:HD3	2:A:257:ASN:ND2	2.28	0.49
2:B:361:PHE:H	2:B:361:PHE:HD1	1.59	0.49
2:B:593:ARG:HA	2:B:629:PHE:CZ	2.47	0.49
2:B:589:ILE:O	2:B:590:ASP:C	2.50	0.49
2:B:117:LEU:HD13	2:B:136:ILE:HG12	1.93	0.49
2:B:74:LYS:O	2:B:77:ARG:N	2.33	0.49
2:B:617:GLN:HG3	2:B:618:TYR:CD2	2.48	0.49
2:A:342:TYR:HD2	2:A:550:ASP:O	1.95	0.49
2:A:597:TYR:HA	2:A:600:ILE:HD12	1.94	0.49
1:C:2:DT:OP1	2:B:352:ASN:ND2	2.41	0.49
2:A:320:GLU:HG3	2:A:616:ARG:CB	2.43	0.49
2:A:168:TYR:C	2:A:168:TYR:HD1	2.15	0.49
2:B:421:LEU:HA	2:B:441:LEU:HD11	1.95	0.49
2:B:319:ASN:OD1	2:B:319:ASN:C	2.49	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:ARG:NH1	2:B:564:GLU:OE1	2.45	0.49
2:B:350:ARG:HH12	2:B:592:GLU:CD	2.15	0.49
2:B:261:LEU:HA	2:B:261:LEU:HD12	1.63	0.49
2:B:36:ILE:O	2:B:37:ALA:C	2.51	0.49
2:B:226:LEU:O	2:B:230:LEU:HD12	2.13	0.49
2:A:4:ASN:ND2	2:A:7:GLN:HG3	2.28	0.49
2:B:631:LEU:N	2:B:631:LEU:HD22	2.28	0.49
2:B:589:ILE:O	2:B:592:GLU:N	2.46	0.48
2:A:110:ASP:O	2:A:113:GLN:HB3	2.13	0.48
2:B:625:GLU:HG3	2:B:626:PRO:HD2	1.94	0.48
2:B:626:PRO:O	2:B:627:SER:C	2.52	0.48
2:B:430:LYS:CG	2:B:435:ALA:HB2	2.42	0.48
2:A:168:TYR:O	2:A:168:TYR:HD1	1.96	0.48
2:B:593:ARG:HA	2:B:629:PHE:CE2	2.49	0.48
2:A:244:ASP:OD1	2:A:296:HIS:CE1	2.66	0.48
2:A:368:PRO:O	2:A:551:GLN:HB2	2.13	0.48
2:A:553:GLN:HG2	2:A:565:PHE:CE1	2.47	0.48
2:A:579:PRO:HG3	2:A:629:PHE:CD2	2.48	0.48
2:B:597:TYR:O	2:B:601:THR:HG23	2.13	0.48
2:B:432:MET:O	2:B:436:SER:N	2.44	0.48
2:A:515:MET:HB3	2:A:530:VAL:HG22	1.95	0.48
2:B:583:SER:O	2:B:584:ILE:C	2.52	0.48
1:C:7:DT:H73	2:B:103:ALA:C	2.33	0.48
2:B:508:LEU:O	2:B:511:TRP:HB2	2.13	0.48
2:A:349:TYR:N	2:A:349:TYR:CD1	2.79	0.48
2:B:92:ILE:HD11	2:B:189:LEU:CB	2.41	0.48
2:B:312:LEU:HD22	2:B:607:LEU:HB3	1.94	0.48
2:B:33:THR:HG22	2:B:34:ASN:N	2.27	0.48
2:B:317:ALA:O	2:B:613:LYS:N	2.43	0.48
1:C:15:DT:O2	1:C:15:DT:H2'	2.13	0.48
2:A:129:LYS:O	2:A:131:LEU:N	2.47	0.48
2:B:204:TRP:HA	2:B:204:TRP:CE3	2.47	0.48
2:A:163:ILE:O	2:A:166:HIS:HB3	2.14	0.48
2:A:639:ILE:CG2	2:A:640:TRP:N	2.77	0.48
2:A:348:LEU:N	2:A:348:LEU:HD23	2.29	0.48
2:B:31:VAL:O	2:B:35:LYS:N	2.42	0.48
2:A:581:GLN:O	2:A:582:SER:C	2.51	0.48
2:B:580:HIS:CD2	2:B:582:SER:OG	2.67	0.48
2:B:170:LEU:HA	2:B:173:ALA:HB3	1.96	0.48
2:B:47:ALA:HB1	2:B:79:LEU:HD21	1.93	0.48
2:B:3:LEU:HD23	2:B:8:GLN:CA	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:74:LYS:CG	2:A:75:GLU:H	2.27	0.48
2:A:378:PHE:HE2	2:A:539:MET:HB3	1.78	0.48
2:A:567:TYR:CD1	2:A:606:GLU:HG2	2.49	0.48
2:A:335:HIS:NE2	2:A:339:LYS:HE2	2.29	0.48
2:A:380:ARG:HB3	2:A:382:GLU:OE1	2.14	0.48
2:A:160:ARG:HA	2:A:163:ILE:CD1	2.36	0.48
2:A:26:SER:HB3	2:A:273:LEU:HG	1.95	0.48
2:A:340:THR:O	2:A:345:TYR:CE2	2.67	0.48
2:B:411:ARG:HB3	2:B:455:ARG:HH21	1.79	0.48
2:B:131:LEU:HD23	2:B:132:LEU:HD23	1.95	0.48
2:B:382:GLU:HG2	2:B:383:ILE:N	2.29	0.48
2:A:322:HIS:HA	2:A:325:GLU:HB2	1.96	0.48
2:B:598:VAL:O	2:B:602:ARG:HD2	2.14	0.47
2:B:424:TRP:HB3	2:B:441:LEU:HD11	1.96	0.47
2:B:133:GLN:CD	2:B:134:GLN:N	2.66	0.47
2:A:404:ARG:O	2:A:404:ARG:HG3	2.13	0.47
2:B:10:ALA:HA	2:B:271:ILE:HD12	1.94	0.47
2:A:302:LEU:O	2:A:303:PHE:HB3	2.14	0.47
2:B:353:HIS:HE2	2:B:577:PHE:HE1	1.62	0.47
2:A:495:PRO:O	2:A:498:ALA:HB3	2.14	0.47
2:A:237:PHE:HD1	2:A:238:THR:N	2.11	0.47
2:B:413:ILE:HG23	2:B:417:THR:OG1	2.14	0.47
2:B:130:VAL:O	2:B:133:GLN:OE1	2.32	0.47
2:B:206:ASN:ND2	2:B:209:ARG:HE	2.12	0.47
2:A:294:ASN:HD22	2:A:593:ARG:HH11	1.63	0.47
2:A:288:ASN:HD21	2:A:302:LEU:N	2.11	0.47
2:A:254:ARG:CD	2:A:257:ASN:ND2	2.77	0.47
2:A:143:LYS:C	2:A:145:ASP:H	2.15	0.47
2:B:279:SER:HB2	2:B:284:LEU:HD21	1.95	0.47
2:B:33:THR:O	2:B:36:ILE:HB	2.14	0.47
2:A:244:ASP:CB	2:A:597:TYR:HE2	2.24	0.47
2:B:472:ILE:CG1	2:B:473:ALA:H	2.16	0.47
2:B:79:LEU:C	2:B:81:ILE:H	2.17	0.47
2:A:135:LEU:O	2:A:139:ILE:HB	2.15	0.47
2:A:404:ARG:O	2:A:408:THR:OG1	2.22	0.47
2:B:223:GLN:HG2	2:B:223:GLN:H	1.46	0.47
2:B:5:PRO:O	2:B:8:GLN:HB3	2.14	0.47
2:A:359:GLU:O	2:A:363:MET:HG2	2.13	0.47
2:A:130:VAL:O	2:A:134:GLN:HG2	2.15	0.47
2:A:315:LEU:N	2:A:315:LEU:CD2	2.77	0.47
1:C:9:DT:H2"	1:C:10:DT:C5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ALA:HB1	2:B:79:LEU:CD2	2.44	0.47
2:A:111:THR:OG1	2:A:112:ASP:N	2.48	0.47
2:A:598:VAL:O	2:A:599:GLY:C	2.52	0.47
2:A:33:THR:OG1	2:A:34:ASN:N	2.48	0.47
2:B:410:LYS:HB2	2:B:487:TRP:CZ3	2.49	0.47
2:A:190:PRO:O	2:A:191:THR:C	2.53	0.47
2:A:82:SER:HB2	2:A:86:THR:HG1	1.77	0.47
2:B:391:ARG:HD2	2:B:401:ALA:CB	2.31	0.47
2:B:224:TYR:HD1	2:B:224:TYR:O	1.98	0.47
2:A:3:LEU:CD1	2:A:30:ARG:NE	2.72	0.47
2:B:256:GLN:O	2:B:260:LEU:HD13	2.14	0.47
2:B:19:LEU:HD23	2:B:270:VAL:HG22	1.96	0.47
2:A:341:GLN:O	2:A:343:LYS:N	2.47	0.47
2:A:119:GLU:HG3	2:A:120:LEU:HD23	1.97	0.47
1:C:15:DT:H2”	1:C:16:DT:O5'	2.14	0.47
2:B:142:TRP:HE3	2:B:168:TYR:HD2	1.63	0.47
2:A:260:LEU:H	2:A:260:LEU:HD13	1.80	0.47
2:B:17:PRO:HB3	2:B:235:ALA:HB1	1.97	0.47
2:B:553:GLN:HG2	2:B:565:PHE:CE2	2.50	0.47
2:B:334:HIS:ND1	2:B:345:TYR:OH	2.38	0.47
2:A:256:GLN:HE21	2:A:256:GLN:CA	2.28	0.47
2:B:13:PHE:HE2	2:B:269:LYS:HB3	1.79	0.47
2:A:354:GLN:O	2:A:358:PHE:HD1	1.97	0.47
2:B:221:THR:O	2:B:224:TYR:N	2.48	0.47
2:B:361:PHE:O	2:B:362:LEU:C	2.53	0.47
2:A:421:LEU:HD13	2:A:432:MET:HB3	1.97	0.47
2:B:537:ARG:O	2:B:538:ASP:O	2.33	0.47
2:B:92:ILE:CD1	2:B:190:PRO:HD3	2.39	0.46
2:B:421:LEU:HD21	2:B:436:SER:HA	1.97	0.46
2:B:581:GLN:O	2:B:582:SER:C	2.52	0.46
2:A:167:CYS:O	2:A:170:LEU:HB2	2.15	0.46
2:A:19:LEU:HD23	2:A:20:VAL:N	2.30	0.46
2:B:533:ARG:O	2:B:534:PHE:C	2.52	0.46
2:A:347:ILE:N	2:A:347:ILE:HD12	2.29	0.46
2:B:87:LEU:O	2:B:90:ASP:N	2.48	0.46
2:B:411:ARG:N	2:B:411:ARG:CD	2.69	0.46
2:B:413:ILE:N	2:B:413:ILE:HD12	2.31	0.46
2:A:482:MET:HE2	2:A:484:TYR:HB2	1.97	0.46
2:A:321:GLU:CG	2:A:357:VAL:HG23	2.45	0.46
2:B:420:LYS:CB	2:B:445:LEU:HD23	2.43	0.46
2:B:255:PRO:HB2	2:B:256:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:265:PHE:HA	2:A:266:PRO:HD2	1.63	0.46
2:A:290:LEU:C	2:A:290:LEU:HD23	2.35	0.46
2:A:370:LYS:HE3	2:A:553:GLN:CG	2.45	0.46
2:B:171:TYR:C	2:B:171:TYR:CD1	2.88	0.46
2:A:197:ASN:ND2	2:A:200:VAL:H	2.13	0.46
2:A:382:GLU:H	2:A:501:ARG:NH2	2.12	0.46
2:A:284:LEU:O	2:A:288:ASN:HB2	2.15	0.46
2:B:424:TRP:HB3	2:B:441:LEU:HD21	1.97	0.46
2:A:72:GLY:HA3	2:A:74:LYS:CE	2.45	0.46
2:B:235:ALA:HB2	2:B:265:PHE:HE1	1.80	0.46
2:A:386:LEU:HD11	2:A:479:ILE:HD11	1.98	0.46
2:B:13:PHE:CE2	2:B:269:LYS:HB3	2.48	0.46
2:A:488:LEU:HA	2:A:491:THR:HG22	1.98	0.46
2:A:221:THR:OG1	2:A:254:ARG:NH2	2.49	0.46
2:B:324:ALA:HB2	2:B:357:VAL:HG13	1.98	0.46
2:A:465:ARG:O	2:A:468:GLU:HB2	2.16	0.46
2:A:278:ARG:O	2:A:604:GLN:HB2	2.15	0.46
2:A:279:SER:HB2	2:A:284:LEU:CD2	2.46	0.46
2:A:174:HIS:ND1	2:A:178:CYS:SG	2.80	0.46
2:A:65:GLU:O	2:A:66:ARG:C	2.54	0.46
2:B:428:ARG:HB3	2:B:430:LYS:NZ	2.30	0.46
2:A:254:ARG:NH1	2:A:254:ARG:HG2	2.27	0.46
2:A:635:GLN:NE2	2:A:635:GLN:CA	2.76	0.46
2:A:106:SER:H	2:A:180:VAL:HA	1.80	0.46
2:A:46:GLN:O	2:A:47:ALA:C	2.54	0.46
2:B:499:GLU:O	2:B:502:MET:HB3	2.16	0.46
2:A:36:ILE:HD11	2:A:67:VAL:CG2	2.45	0.46
2:A:389:TYR:CE2	2:A:409:PRO:HG2	2.50	0.46
2:B:361:PHE:O	2:B:364:GLN:N	2.49	0.46
2:B:3:LEU:HD23	2:B:8:GLN:HA	1.97	0.46
2:B:282:ARG:CZ	2:B:308:TYR:HE2	2.29	0.46
2:A:335:HIS:HD2	2:A:340:THR:H	1.60	0.46
2:A:117:LEU:O	2:A:118:LYS:C	2.53	0.46
2:A:211:LEU:HD12	2:A:212:LEU:O	2.16	0.46
2:B:511:TRP:O	2:B:512:MET:C	2.54	0.46
2:A:639:ILE:CG2	2:A:640:TRP:H	2.28	0.46
2:B:347:ILE:C	2:B:348:LEU:HD23	2.36	0.46
2:A:315:LEU:N	2:A:315:LEU:HD22	2.30	0.46
2:A:17:PRO:HB3	2:A:235:ALA:HB1	1.98	0.46
2:A:340:THR:O	2:A:341:GLN:O	2.34	0.46
2:A:370:LYS:HE3	2:A:553:GLN:CB	2.46	0.46

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:594:ARG:HG3	2:B:594:ARG:NH1	2.31	0.46
2:B:130:VAL:O	2:B:133:GLN:HB3	2.16	0.46
2:B:225:GLU:O	2:B:228:LYS:N	2.49	0.46
2:A:151:GLN:O	2:A:154:ALA:HB3	2.15	0.46
2:B:321:GLU:O	2:B:322:HIS:C	2.54	0.46
2:A:566:PRO:HA	2:A:604:GLN:HG3	1.98	0.45
2:B:428:ARG:HH12	2:B:441:LEU:N	2.14	0.45
2:B:160:ARG:HD3	2:B:160:ARG:H	1.81	0.45
2:A:259:VAL:O	2:A:260:LEU:C	2.54	0.45
2:A:26:SER:OG	2:A:273:LEU:HG	2.16	0.45
2:B:512:MET:HG2	2:B:530:VAL:HG11	1.98	0.45
2:B:254:ARG:O	2:B:257:ASN:ND2	2.49	0.45
2:B:263:GLN:C	2:B:265:PHE:N	2.68	0.45
2:B:368:PRO:HB2	2:B:551:GLN:HB3	1.98	0.45
1:C:13:DT:C2	2:A:250:TRP:CZ2	3.04	0.45
2:B:389:TYR:HD2	2:B:478:LEU:CD2	2.25	0.45
2:A:423:GLU:O	2:A:427:THR:HG23	2.16	0.45
2:B:87:LEU:O	2:B:88:GLY:C	2.54	0.45
2:A:36:ILE:HG23	2:A:212:LEU:HD22	1.98	0.45
2:B:428:ARG:HH22	2:B:440:GLY:CA	2.28	0.45
2:B:487:TRP:CZ2	2:B:491:THR:HG21	2.52	0.45
2:B:110:ASP:O	2:B:113:GLN:HB2	2.16	0.45
2:A:102:LYS:HZ2	2:A:104:ASN:CB	2.28	0.45
2:A:254:ARG:HH11	2:A:254:ARG:CG	2.21	0.45
2:A:435:ALA:C	2:A:437:PHE:H	2.20	0.45
2:B:200:VAL:HG22	2:B:203:ARG:NH2	2.31	0.45
2:A:589:ILE:O	2:A:592:GLU:N	2.49	0.45
2:B:186:LEU:H	2:B:186:LEU:HD12	1.80	0.45
2:B:187:ILE:O	2:B:189:LEU:N	2.49	0.45
2:A:66:ARG:O	2:A:69:GLN:NE2	2.47	0.45
2:B:389:TYR:OH	2:B:482:MET:SD	2.68	0.45
2:A:64:LYS:HG2	2:A:81:ILE:CD1	2.43	0.45
2:A:73:ARG:HD2	2:A:521:LEU:N	2.30	0.45
2:B:246:SER:O	2:B:246:SER:OG	2.34	0.45
2:B:389:TYR:HD2	2:B:478:LEU:CG	2.30	0.45
1:C:1:DT:C6	2:B:580:HIS:NE2	2.84	0.45
2:B:224:TYR:CE1	2:B:228:LYS:HD3	2.51	0.45
2:B:314:VAL:CG2	2:B:638:LEU:HD11	2.46	0.45
2:A:294:ASN:ND2	2:A:593:ARG:HG3	2.32	0.45
2:A:291:ILE:HD11	2:A:296:HIS:CD2	2.52	0.45
2:B:525:MET:SD	2:B:533:ARG:NH1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:107:LEU:HA	2:A:107:LEU:HD13	1.70	0.45
2:B:221:THR:O	2:B:224:TYR:HB3	2.17	0.45
2:A:392:VAL:HG11	2:A:460:LEU:HD21	1.98	0.45
2:B:333:ALA:O	2:B:334:HIS:C	2.55	0.45
2:A:370:LYS:O	2:A:554:LEU:HB3	2.17	0.45
2:B:244:ASP:HA	2:B:594:ARG:HD3	1.98	0.45
2:B:190:PRO:O	2:B:191:THR:C	2.55	0.45
2:B:389:TYR:CB	2:B:478:LEU:HD21	2.47	0.45
2:B:466:LEU:HD11	2:B:470:GLU:HB2	1.98	0.45
2:B:359:GLU:HG2	2:B:369:TYR:HH	1.82	0.45
2:B:525:MET:HE3	2:B:533:ARG:HH11	1.82	0.45
2:A:399:ASP:OD1	2:A:432:MET:HG2	2.17	0.45
2:A:435:ALA:C	2:A:437:PHE:N	2.70	0.45
2:A:24:ALA:O	2:A:302:LEU:HD21	2.17	0.45
2:A:506:ASN:O	2:A:509:PHE:N	2.50	0.45
2:A:92:ILE:HD13	2:A:189:LEU:HB3	1.99	0.45
2:B:578:LEU:O	2:B:578:LEU:HD12	2.16	0.45
2:B:112:ASP:O	2:B:115:ALA:HB3	2.17	0.45
2:A:110:ASP:CG	2:A:111:THR:N	2.70	0.45
2:A:466:LEU:O	2:A:468:GLU:N	2.50	0.45
2:A:257:ASN:HA	2:A:257:ASN:HD22	1.51	0.45
2:B:28:LYS:HD3	2:B:214:ASP:OD1	2.17	0.45
2:A:62:GLU:HA	2:A:65:GLU:OE1	2.16	0.44
2:A:511:TRP:O	2:A:512:MET:C	2.56	0.44
2:B:43:CYS:O	2:B:45:TYR:N	2.47	0.44
2:B:202:LYS:HD3	2:B:202:LYS:C	2.36	0.44
2:B:212:LEU:N	2:B:212:LEU:HD12	2.32	0.44
2:A:341:GLN:C	2:A:343:LYS:N	2.70	0.44
2:A:575:GLU:HA	2:A:575:GLU:OE1	2.16	0.44
2:B:389:TYR:O	2:B:392:VAL:HB	2.17	0.44
2:A:529:GLN:O	2:A:530:VAL:C	2.56	0.44
2:B:160:ARG:HA	2:B:163:ILE:CD1	2.41	0.44
2:A:273:LEU:HD12	2:A:274:GLU:N	2.33	0.44
2:B:186:LEU:HD12	2:B:186:LEU:N	2.32	0.44
2:B:348:LEU:HA	2:B:555:MET:O	2.17	0.44
2:A:518:GLY:HA3	2:A:524:PRO:HB3	1.98	0.44
2:A:288:ASN:HD21	2:A:301:ARG:C	2.20	0.44
2:A:342:TYR:HB2	2:A:551:GLN:CA	2.47	0.44
2:A:529:GLN:C	2:A:531:VAL:N	2.70	0.44
2:B:176:LYS:CG	2:B:177:ALA:N	2.79	0.44
2:B:221:THR:O	2:B:222:SER:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:618:TYR:O	2:B:620:GLU:N	2.51	0.44
2:B:525:MET:CE	2:B:533:ARG:NH1	2.79	0.44
2:B:210:TYR:OH	2:B:238:THR:OG1	2.35	0.44
2:A:510:SER:O	2:A:513:THR:HB	2.18	0.44
2:B:304:SER:CB	2:B:306:LEU:HD12	2.48	0.44
2:B:353:HIS:C	2:B:355:SER:H	2.20	0.44
2:B:617:GLN:OE1	2:B:617:GLN:HA	2.18	0.44
2:B:255:PRO:C	2:B:257:ASN:H	2.21	0.44
2:A:115:ALA:O	2:A:118:LYS:HB2	2.17	0.44
2:B:407:ASN:HA	2:B:411:ARG:CG	2.37	0.44
2:B:410:LYS:HB2	2:B:487:TRP:HE3	1.80	0.44
2:B:386:LEU:HD13	2:B:386:LEU:C	2.38	0.44
2:A:465:ARG:O	2:A:468:GLU:HG2	2.17	0.44
1:C:10:DT:C6	1:C:10:DT:C4'	3.00	0.44
2:B:190:PRO:O	2:B:194:LEU:N	2.49	0.44
2:B:103:ALA:HB1	2:B:105:PHE:HE1	1.76	0.44
2:B:363:MET:HE1	2:B:534:PHE:CE1	2.52	0.44
2:B:380:ARG:O	2:B:383:ILE:N	2.49	0.44
2:B:54:THR:OG1	2:B:55:PHE:N	2.49	0.44
2:A:21:LEU:HD13	2:A:242:ASP:HA	1.99	0.44
2:A:551:GLN:O	2:A:553:GLN:OE1	2.35	0.44
2:A:18:CYS:O	2:A:238:THR:HA	2.18	0.44
2:B:135:LEU:HA	2:B:164:PHE:CE1	2.52	0.44
2:A:72:GLY:O	2:A:74:LYS:N	2.50	0.44
2:A:472:ILE:HD13	2:A:473:ALA:CA	2.48	0.44
1:C:14:DT:O4	2:A:133:GLN:HG2	2.17	0.44
2:A:590:ASP:O	2:A:594:ARG:HG3	2.17	0.44
1:C:13:DT:H2'	1:C:13:DT:H6	1.70	0.44
2:B:243:ASP:O	2:B:594:ARG:HD3	2.17	0.44
2:A:389:TYR:CZ	2:A:405:ILE:HG23	2.52	0.44
2:B:389:TYR:CD1	2:B:405:ILE:CD1	3.01	0.43
2:A:221:THR:O	2:A:222:SER:C	2.56	0.43
2:B:377:PHE:HA	2:B:380:ARG:HD2	2.00	0.43
2:B:261:LEU:O	2:B:265:PHE:HB2	2.19	0.43
2:B:83:THR:HG23	2:B:86:THR:OG1	2.18	0.43
2:B:140:SER:O	2:B:144:ASN:ND2	2.51	0.43
2:A:280:SER:O	2:A:284:LEU:HG	2.17	0.43
1:C:12:DT:H5"	2:A:353:HIS:CE1	2.53	0.43
2:B:170:LEU:HD12	2:B:173:ALA:HB3	2.00	0.43
2:B:220:ASN:HD22	2:B:221:THR:N	2.15	0.43
2:A:19:LEU:HD23	2:A:20:VAL:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:VAL:O	2:B:262:SER:N	2.51	0.43
2:A:321:GLU:HG2	2:A:361:PHE:CZ	2.52	0.43
2:A:225:GLU:O	2:A:229:LEU:HD23	2.19	0.43
2:A:230:LEU:HA	2:A:230:LEU:HD23	1.76	0.43
2:A:568:VAL:HB	2:A:603:ALA:HB2	1.99	0.43
2:B:74:LYS:HB2	2:B:74:LYS:HZ1	1.82	0.43
2:A:407:ASN:ND2	2:A:411:ARG:O	2.42	0.43
2:A:611:LEU:H	2:A:611:LEU:HD13	1.82	0.43
2:A:134:GLN:HG2	2:A:134:GLN:H	1.48	0.43
2:A:276:ASN:OD1	2:A:278:ARG:N	2.36	0.43
2:A:284:LEU:HG	2:A:284:LEU:H	1.60	0.43
2:A:594:ARG:O	2:A:595:LEU:C	2.57	0.43
2:A:197:ASN:HD21	2:A:199:GLU:HB3	1.82	0.43
2:A:531:VAL:O	2:A:532:THR:C	2.54	0.43
2:A:499:GLU:O	2:A:502:MET:HB3	2.18	0.43
2:A:358:PHE:CE2	2:A:571:VAL:HG11	2.53	0.43
2:B:227:VAL:O	2:B:228:LYS:C	2.56	0.43
2:B:283:ILE:N	2:B:283:ILE:HD12	2.33	0.43
2:A:153:ALA:O	2:A:156:ALA:HB3	2.18	0.43
2:B:121:THR:HB	2:B:125:ILE:HG22	2.00	0.43
2:B:170:LEU:HA	2:B:173:ALA:CB	2.49	0.43
2:B:105:PHE:CB	2:B:179:ASN:O	2.65	0.43
2:B:466:LEU:C	2:B:468:GLU:N	2.71	0.43
2:B:356:ARG:CZ	2:B:377:PHE:HD2	2.30	0.43
2:B:362:LEU:HD23	2:B:362:LEU:HA	1.64	0.43
2:B:363:MET:SD	2:B:364:GLN:HA	2.59	0.43
2:B:9:GLN:HG2	2:B:271:ILE:CG2	2.49	0.43
2:A:68:GLY:O	2:A:71:LEU:O	2.36	0.43
2:A:536:LEU:HD23	2:A:536:LEU:HA	1.56	0.43
2:A:287:ALA:O	2:A:291:ILE:HG22	2.19	0.43
2:A:604:GLN:H	2:A:604:GLN:HG2	1.70	0.43
2:B:278:ARG:HH21	2:B:602:ARG:NH2	2.15	0.43
2:A:35:LYS:O	2:A:39:LEU:HG	2.18	0.43
1:C:1:DT:N3	1:C:2:DT:C4	2.86	0.43
2:A:138:THR:O	2:A:142:TRP:CE3	2.72	0.43
2:A:168:TYR:O	2:A:171:TYR:N	2.51	0.43
2:B:511:TRP:O	2:B:513:THR:N	2.52	0.43
2:B:95:GLU:HA	2:B:95:GLU:OE1	2.19	0.43
2:A:371:ILE:HG12	2:A:371:ILE:O	2.18	0.43
2:A:450:TYR:CE1	2:A:454:THR:HG21	2.53	0.43
2:A:573:MET:CE	2:A:627:SER:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:200:VAL:O	2:A:201:ARG:C	2.57	0.43
2:B:402:PHE:HA	2:B:405:ILE:HG12	2.01	0.43
2:B:108:PHE:HE2	2:B:116:LEU:CD2	2.30	0.43
2:B:382:GLU:OE1	2:B:382:GLU:N	2.37	0.43
2:A:328:THR:HG23	2:A:329:GLY:N	2.34	0.43
2:A:188:LEU:N	2:A:188:LEU:CD2	2.81	0.43
2:B:36:ILE:HG22	2:B:37:ALA:N	2.33	0.43
2:B:318:ASN:HA	2:B:613:LYS:HB2	2.00	0.43
2:A:342:TYR:HB3	2:A:552:VAL:CG2	2.49	0.43
2:A:575:GLU:O	2:A:579:PRO:O	2.37	0.43
2:A:182:ASP:N	2:A:185:ASP:OD2	2.51	0.43
2:A:485:GLU:HB2	2:A:502:MET:HE2	1.99	0.43
2:A:72:GLY:O	2:A:74:LYS:HG2	2.18	0.43
2:B:211:LEU:O	2:B:237:PHE:HB2	2.19	0.43
2:B:282:ARG:CZ	2:B:308:TYR:CE2	3.01	0.43
2:A:46:GLN:OE1	2:A:47:ALA:N	2.52	0.43
2:A:341:GLN:O	2:A:344:ASP:N	2.41	0.43
2:A:533:ARG:HA	2:A:533:ARG:HD2	1.62	0.43
2:A:91:ILE:H	2:A:91:ILE:HD12	1.84	0.43
2:B:116:LEU:O	2:B:119:GLU:HG3	2.18	0.43
2:A:335:HIS:HD2	2:A:339:LYS:HA	1.83	0.43
2:B:392:VAL:HG21	2:B:405:ILE:HD11	1.99	0.43
2:A:574:GLU:OE2	2:A:612:CYS:HB2	2.19	0.43
2:A:4:ASN:HB3	2:A:277:TYR:OH	2.19	0.43
2:B:497:ALA:HA	2:B:500:MET:HG2	2.01	0.43
2:B:363:MET:HE1	2:B:534:PHE:HE1	1.83	0.43
2:B:280:SER:OG	2:B:281:GLY:N	2.51	0.43
2:A:258:LEU:HB3	2:A:298:PHE:CE2	2.54	0.43
2:B:550:ASP:C	2:B:551:GLN:HG2	2.40	0.43
2:A:21:LEU:CD1	2:A:242:ASP:HA	2.48	0.43
2:B:433:PHE:O	2:B:436:SER:OG	2.33	0.42
2:B:459:TRP:HH2	2:B:478:LEU:O	2.02	0.42
2:B:475:VAL:O	2:B:478:LEU:HB3	2.19	0.42
1:C:1:DT:H73	2:B:582:SER:HB2	2.00	0.42
2:B:81:ILE:O	2:B:82:SER:HB3	2.19	0.42
2:A:135:LEU:CD1	2:A:164:PHE:CD1	2.96	0.42
2:A:458:HIS:O	2:A:459:TRP:C	2.54	0.42
2:A:221:THR:N	2:A:254:ARG:NH1	2.67	0.42
2:B:78:GLY:O	2:B:80:MET:HE3	2.19	0.42
2:B:405:ILE:O	2:B:409:PRO:HD2	2.18	0.42
2:A:515:MET:HG2	2:A:525:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:DT:H2"	1:C:16:DT:H5'	2.00	0.42
2:B:228:LYS:O	2:B:229:LEU:C	2.58	0.42
2:B:362:LEU:CD1	2:B:554:LEU:HD12	2.48	0.42
2:A:421:LEU:HD21	2:A:435:ALA:HB3	2.01	0.42
2:A:377:PHE:C	2:A:379:SER:H	2.23	0.42
1:C:9:DT:H2"	1:C:10:DT:C4'	2.49	0.42
2:B:244:ASP:O	2:B:594:ARG:HG2	2.19	0.42
2:A:121:THR:HA	2:A:124:LEU:CG	2.50	0.42
2:B:314:VAL:HB	2:B:640:TRP:HA	2.01	0.42
2:A:258:LEU:HB3	2:A:298:PHE:HE2	1.84	0.42
2:B:21:LEU:HD12	2:B:21:LEU:C	2.39	0.42
2:A:322:HIS:O	2:A:325:GLU:HB2	2.19	0.42
2:A:314:VAL:O	2:A:314:VAL:HG12	2.20	0.42
2:B:183:PHE:O	2:B:186:LEU:HD13	2.20	0.42
2:B:392:VAL:O	2:B:393:LEU:C	2.57	0.42
2:A:19:LEU:C	2:A:19:LEU:CD2	2.88	0.42
2:A:229:LEU:HD13	2:A:229:LEU:HA	1.69	0.42
2:B:311:GLU:OE1	2:B:639:ILE:HD11	2.19	0.42
2:A:474:ALA:O	2:A:475:VAL:C	2.57	0.42
2:B:400:SER:O	2:B:404:ARG:HG2	2.19	0.42
2:B:392:VAL:O	2:B:395:ASN:N	2.50	0.42
2:B:405:ILE:O	2:B:409:PRO:CD	2.68	0.42
1:C:16:DT:C1'	2:A:85:HIS:CE1	2.98	0.42
2:B:220:ASN:HD21	2:B:223:GLN:N	2.08	0.42
2:B:341:GLN:HB3	2:B:550:ASP:OD1	2.19	0.42
2:B:187:ILE:C	2:B:189:LEU:N	2.73	0.42
2:A:62:GLU:HB3	2:A:66:ARG:NH1	2.35	0.42
2:B:393:LEU:HD23	2:B:464:GLN:CA	2.43	0.42
2:A:515:MET:HE2	2:A:533:ARG:CB	2.50	0.42
2:A:497:ALA:HB1	2:B:101:MET:SD	2.59	0.42
2:B:383:ILE:HD11	2:B:504:ASN:HB3	2.02	0.42
2:A:386:LEU:O	2:A:390:LEU:HG	2.19	0.42
2:B:311:GLU:HG3	2:B:639:ILE:HD12	2.00	0.42
2:B:289:ILE:O	2:B:290:LEU:C	2.58	0.42
2:B:189:LEU:HD22	2:B:189:LEU:HA	1.48	0.42
2:A:211:LEU:CD1	2:A:213:VAL:HG23	2.30	0.42
2:A:407:ASN:O	2:A:410:LYS:N	2.48	0.42
2:A:254:ARG:HG3	2:A:257:ASN:OD1	2.19	0.42
2:A:3:LEU:HD23	2:A:8:GLN:CG	2.49	0.42
2:A:32:ILE:H	2:A:32:ILE:HG12	1.59	0.42
2:B:107:LEU:N	2:B:107:LEU:CD2	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:ASN:O	2:B:304:SER:HB2	2.20	0.42
2:A:460:LEU:HA	2:A:460:LEU:HD12	1.65	0.42
2:A:133:GLN:O	2:A:134:GLN:C	2.56	0.42
2:A:454:THR:O	2:A:455:ARG:C	2.58	0.42
2:A:540:MET:HG3	2:A:540:MET:O	2.19	0.42
2:A:294:ASN:OD1	2:A:295:PRO:HD2	2.20	0.42
2:A:211:LEU:CA	2:A:212:LEU:HD12	2.50	0.42
2:B:406:VAL:HG11	2:B:418:LEU:CD1	2.50	0.42
2:A:189:LEU:HD22	2:A:189:LEU:HA	1.70	0.42
2:A:533:ARG:HH21	2:A:538:ASP:CB	2.33	0.42
2:B:116:LEU:O	2:B:120:LEU:HG	2.20	0.42
2:A:53:VAL:CG1	2:A:54:THR:N	2.83	0.42
2:A:27:GLY:O	2:A:30:ARG:HB3	2.19	0.42
2:B:531:VAL:O	2:B:534:PHE:N	2.53	0.42
2:B:3:LEU:CD2	2:B:8:GLN:HA	2.50	0.42
2:A:567:TYR:HD1	2:A:606:GLU:HG2	1.84	0.42
2:A:120:LEU:O	2:A:124:LEU:HD11	2.20	0.42
2:A:515:MET:HG2	2:A:525:MET:HE1	2.02	0.42
2:A:382:GLU:HG3	2:A:501:ARG:O	2.19	0.42
2:B:220:ASN:HD22	2:B:222:SER:N	2.17	0.42
2:B:219:THR:HG22	2:B:257:ASN:HD21	1.85	0.42
2:B:4:ASN:C	2:B:4:ASN:ND2	2.73	0.42
2:B:6:GLY:O	2:B:7:GLN:C	2.58	0.42
2:A:143:LYS:C	2:A:145:ASP:N	2.74	0.42
2:A:391:ARG:HG2	2:A:398:ASP:OD2	2.20	0.42
2:A:600:ILE:O	2:A:602:ARG:N	2.53	0.41
2:B:189:LEU:O	2:B:190:PRO:C	2.54	0.41
2:B:114:LEU:HA	2:B:117:LEU:HD12	2.02	0.41
2:A:327:VAL:CG1	2:A:328:THR:N	2.83	0.41
2:A:416:ALA:O	2:A:418:LEU:N	2.53	0.41
2:A:470:GLU:O	2:A:471:PRO:C	2.57	0.41
2:A:580:HIS:O	2:A:584:ILE:HG13	2.20	0.41
2:B:578:LEU:HD13	2:B:578:LEU:HA	1.85	0.41
2:A:54:THR:CG2	2:A:55:PHE:H	2.21	0.41
2:A:4:ASN:C	2:A:4:ASN:HD22	2.23	0.41
2:B:237:PHE:HD1	2:B:238:THR:N	2.18	0.41
2:A:514:GLU:HA	2:A:517:GLU:HB2	2.02	0.41
2:A:97:ALA:C	2:A:100:GLY:H	2.23	0.41
2:A:568:VAL:CG1	2:A:569:TYR:N	2.83	0.41
2:B:424:TRP:CG	2:B:441:LEU:HD22	2.54	0.41
2:A:166:HIS:CE1	2:A:170:LEU:HD21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:6:GLY:O	2:A:7:GLN:C	2.59	0.41
2:B:512:MET:HB2	2:B:534:PHE:CE2	2.55	0.41
2:B:311:GLU:HG3	2:B:639:ILE:CD1	2.50	0.41
2:A:580:HIS:HD2	2:A:582:SER:H	1.69	0.41
1:C:9:DT:O4'	1:C:9:DT:O2	2.38	0.41
1:C:1:DT:C2	1:C:2:DT:C2	3.07	0.41
2:A:389:TYR:CG	2:A:478:LEU:HD21	2.55	0.41
2:B:525:MET:HE1	2:B:529:GLN:HB2	2.01	0.41
2:B:566:PRO:HB2	2:B:567:TYR:CD2	2.54	0.41
2:B:311:GLU:H	2:B:311:GLU:HG2	1.49	0.41
2:A:349:TYR:OH	2:A:554:LEU:HD23	2.20	0.41
2:A:556:THR:CG2	2:A:557:LEU:H	2.29	0.41
2:A:596:ALA:O	2:A:597:TYR:C	2.59	0.41
2:A:66:ARG:O	2:A:69:GLN:HG3	2.19	0.41
2:A:88:GLY:O	2:A:190:PRO:HG2	2.21	0.41
2:A:526:THR:HG23	2:A:529:GLN:OE1	2.21	0.41
2:A:485:GLU:CB	2:A:502:MET:HE2	2.50	0.41
2:B:135:LEU:CB	2:B:164:PHE:CE1	3.02	0.41
2:A:10:ALA:HA	2:A:271:ILE:CD1	2.51	0.41
2:B:476:ARG:O	2:B:479:ILE:HB	2.21	0.41
2:B:54:THR:O	2:B:83:THR:HA	2.21	0.41
2:A:589:ILE:O	2:A:590:ASP:C	2.59	0.41
2:A:211:LEU:HD12	2:A:212:LEU:H	1.79	0.41
2:A:200:VAL:CG1	2:A:201:ARG:N	2.81	0.41
2:B:421:LEU:HD22	2:B:441:LEU:HD12	2.01	0.41
2:B:581:GLN:HA	2:B:584:ILE:CG1	2.46	0.41
2:A:192:LEU:HD23	2:A:195:GLN:NE2	2.36	0.41
2:B:386:LEU:HD12	2:B:508:LEU:HD23	2.02	0.41
2:B:500:MET:HG3	2:B:501:ARG:H	1.84	0.41
2:B:630:LEU:HB3	2:B:640:TRP:CZ2	2.56	0.41
2:B:202:LYS:HA	2:B:205:GLN:HB2	2.03	0.41
2:B:492:SER:HA	2:B:493:PRO:HD3	1.91	0.41
2:B:38:HIS:O	2:B:39:LEU:C	2.57	0.41
2:A:453:LEU:HD12	2:A:453:LEU:HA	1.76	0.41
2:A:566:PRO:O	2:A:605:LYS:HB2	2.19	0.41
2:B:89:LEU:HD23	2:B:89:LEU:C	2.41	0.41
2:B:210:TYR:CD1	2:B:211:LEU:N	2.88	0.41
2:B:21:LEU:HD13	2:B:242:ASP:HA	2.02	0.41
2:B:387:LEU:HA	2:B:387:LEU:HD12	1.84	0.41
2:A:424:TRP:CH2	2:A:440:GLY:HA3	2.56	0.41
2:A:568:VAL:CG2	2:A:603:ALA:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:SER:C	2:B:251:ARG:H	2.24	0.41
2:B:164:PHE:O	2:B:168:TYR:CB	2.68	0.41
2:B:172:ASP:O	2:B:176:LYS:HG2	2.19	0.41
2:B:177:ALA:C	2:B:179:ASN:H	2.23	0.41
2:B:159:GLU:HA	2:B:162:ARG:NE	2.34	0.41
2:A:179:ASN:O	2:A:179:ASN:CG	2.58	0.41
2:B:237:PHE:HD1	2:B:237:PHE:C	2.24	0.41
2:B:104:ASN:CG	2:B:104:ASN:O	2.57	0.41
2:A:288:ASN:HD21	2:A:301:ARG:HB2	1.86	0.41
2:B:389:TYR:HD1	2:B:405:ILE:HG21	1.86	0.41
2:A:484:TYR:O	2:A:485:GLU:C	2.59	0.41
2:A:485:GLU:HB2	2:A:502:MET:CE	2.51	0.41
2:B:589:ILE:O	2:B:591:GLU:N	2.54	0.41
2:A:160:ARG:NH2	2:A:161:ASP:H	2.19	0.41
2:A:222:SER:O	2:A:223:GLN:C	2.59	0.41
2:A:3:LEU:HD23	2:A:8:GLN:HA	2.02	0.41
2:A:105:PHE:HB3	2:A:179:ASN:HD21	1.86	0.41
2:B:479:ILE:CG2	2:B:480:HIS:N	2.80	0.41
2:B:553:GLN:HG3	2:B:555:MET:CE	2.50	0.41
2:A:317:ALA:O	2:A:613:LYS:CB	2.68	0.41
2:A:314:VAL:HG21	2:A:630:LEU:HD11	2.02	0.41
2:A:13:PHE:C	2:A:13:PHE:CD1	2.95	0.41
2:A:200:VAL:CG1	2:A:201:ARG:H	2.31	0.41
2:B:116:LEU:HG	2:B:120:LEU:HD11	2.02	0.41
2:B:621:LEU:HD23	2:B:621:LEU:HA	1.85	0.41
2:B:93:LYS:HG3	2:B:94:ARG:H	1.84	0.41
2:A:16:GLY:HA3	2:A:17:PRO:HD2	1.93	0.41
2:A:225:GLU:O	2:A:229:LEU:CD2	2.69	0.41
2:A:31:VAL:H	2:A:31:VAL:HG23	1.60	0.41
2:A:566:PRO:HA	2:A:604:GLN:CG	2.51	0.40
2:A:525:MET:HA	2:A:529:GLN:OE1	2.21	0.40
2:B:159:GLU:HG3	2:B:160:ARG:N	2.32	0.40
2:B:220:ASN:O	2:B:221:THR:C	2.60	0.40
2:A:254:ARG:CG	2:A:254:ARG:NH1	2.81	0.40
2:B:361:PHE:HA	2:B:364:GLN:HB2	2.02	0.40
2:B:335:HIS:O	2:B:336:PHE:C	2.59	0.40
2:B:276:ASN:ND2	2:B:284:LEU:HD21	2.36	0.40
2:A:125:ILE:HA	2:A:125:ILE:HD12	1.97	0.40
2:A:119:GLU:O	2:A:121:THR:N	2.54	0.40
2:A:66:ARG:O	2:A:67:VAL:C	2.58	0.40
1:C:7:DT:C7	2:B:103:ALA:HB3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:LEU:CD1	2:B:181:LEU:N	2.84	0.40
2:B:567:TYR:HD1	2:B:606:GLU:CG	2.32	0.40
2:A:48:ARG:HG3	2:A:48:ARG:O	2.21	0.40
2:A:93:LYS:O	2:A:96:TYR:HB2	2.20	0.40
2:A:278:ARG:HH22	2:A:602:ARG:HH12	1.68	0.40
2:A:343:LYS:HB3	2:A:550:ASP:HA	2.03	0.40
1:C:11:DT:O5'	1:C:11:DT:C6	2.75	0.40
2:B:204:TRP:O	2:B:207:LYS:N	2.45	0.40
2:B:391:ARG:HD3	2:B:398:ASP:OD2	2.22	0.40
2:A:149:PRO:CB	2:A:169:GLY:HA2	2.51	0.40
2:A:12:GLU:H	2:A:12:GLU:HG2	1.63	0.40
2:B:364:GLN:C	2:B:365:ASN:HD22	2.25	0.40
2:B:280:SER:OG	2:B:309:GLY:N	2.54	0.40
2:B:284:LEU:HA	2:B:284:LEU:HD23	1.81	0.40
2:B:102:LYS:HD3	2:B:102:LYS:N	2.36	0.40
2:B:204:TRP:CZ3	2:B:207:LYS:HG3	2.57	0.40
2:B:403:LEU:HG	2:B:432:MET:CE	2.51	0.40
2:B:389:TYR:CZ	2:B:409:PRO:HG3	2.57	0.40
2:B:453:LEU:O	2:B:457:THR:HB	2.22	0.40
2:A:83:THR:HG22	2:A:86:THR:N	2.12	0.40
2:A:168:TYR:O	2:A:169:GLY:C	2.57	0.40
2:A:396:PRO:HB3	2:A:433:PHE:HD2	1.86	0.40
2:A:10:ALA:HA	2:A:271:ILE:HD12	2.02	0.40
2:B:607:LEU:HD21	2:B:609:PHE:CZ	2.56	0.40
2:A:600:ILE:H	2:A:600:ILE:HG13	1.64	0.40
2:B:602:ARG:CD	2:B:602:ARG:N	2.79	0.40
2:B:389:TYR:CD1	2:B:405:ILE:HB	2.54	0.40
2:B:250:TRP:CE3	2:B:251:ARG:HG2	2.57	0.40
2:A:56:THR:HG23	2:A:59:ALA:H	1.87	0.40
2:A:227:VAL:O	2:A:228:LYS:C	2.59	0.40
2:B:529:GLN:HG2	2:B:529:GLN:H	1.74	0.40
2:B:210:TYR:C	2:B:210:TYR:CD1	2.95	0.40
2:A:466:LEU:O	2:A:467:ALA:C	2.60	0.40
2:A:208:ILE:HD12	2:A:230:LEU:HD13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	632/673 (94%)	449 (71%)	142 (22%)	41 (6%)	1	8
2	B	629/673 (94%)	443 (70%)	148 (24%)	38 (6%)	2	11
All	All	1261/1346 (94%)	892 (71%)	290 (23%)	79 (6%)	2	9

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	127	ASP
2	A	341	GLN
2	A	357	VAL
2	A	372	SER
2	A	375	THR
2	A	493	PRO
2	A	521	LEU
2	A	577	PHE
2	A	578	LEU
2	B	110	ASP
2	B	177	ALA
2	B	406	VAL
2	B	410	LYS
2	B	493	PRO
2	B	641	GLU
2	A	47	ALA
2	A	73	ARG
2	A	129	LYS
2	A	130	VAL
2	A	144	ASN
2	A	303	PHE
2	A	360	LYS
2	A	467	ALA
2	A	561	LYS
2	B	45	TYR

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Mol	Chain	Res	Type
2	B	73	ARG
2	B	74	LYS
2	B	75	GLU
2	B	104	ASN
2	B	146	LEU
2	B	159	GLU
2	B	178	CYS
2	B	235	ALA
2	B	264	ASP
2	B	479	ILE
2	B	586	GLU
2	A	28	LYS
2	A	74	LYS
2	A	76	ALA
2	A	339	LYS
2	A	378	PHE
2	A	436	SER
2	A	518	GLY
2	A	540	MET
2	A	601	THR
2	B	5	PRO
2	B	48	ARG
2	B	80	MET
2	B	99	LEU
2	B	189	LEU
2	B	429	ASN
2	B	536	LEU
2	B	599	GLY
2	A	406	VAL
2	A	513	THR
2	A	562	GLY
2	A	266	PRO
2	A	285	LYS
2	A	429	ASN
2	A	547	GLU
2	A	587	ASP
2	B	221	THR
2	B	256	GLN
2	B	360	LYS
2	A	409	PRO
2	B	44	GLY
2	B	231	VAL

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Mol	Chain	Res	Type
2	A	598	VAL
2	A	524	PRO
2	B	149	PRO
2	B	381	PRO
2	A	92	ILE
2	A	408	THR
2	B	472	ILE
2	B	578	LEU
2	B	598	VAL
2	A	40	ILE
2	B	36	ILE
2	B	371	ILE

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	
2	A	528/580 (91%)	402 (76%)	126 (24%)	1	4
2	B	536/580 (92%)	403 (75%)	133 (25%)	1	3
All	All	1064/1160 (92%)	805 (76%)	259 (24%)	1	4

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4	ASN
2	A	5	PRO
2	A	11	VAL
2	A	12	GLU
2	A	13	PHE
2	A	18	CYS
2	A	21	LEU
2	A	29	THR
2	A	32	ILE
2	A	36	ILE
2	A	48	ARG

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Mol	Chain	Res	Type
2	A	58	LYS
2	A	62	GLU
2	A	74	LYS
2	A	83	THR
2	A	92	ILE
2	A	93	LYS
2	A	96	TYR
2	A	99	LEU
2	A	104	ASN
2	A	108	PHE
2	A	109	ASP
2	A	110	ASP
2	A	114	LEU
2	A	117	LEU
2	A	124	LEU
2	A	129	LYS
2	A	131	LEU
2	A	133	GLN
2	A	134	GLN
2	A	140	SER
2	A	150	SER
2	A	160	ARG
2	A	162	ARG
2	A	168	TYR
2	A	180	VAL
2	A	181	LEU
2	A	188	LEU
2	A	189	LEU
2	A	193	LEU
2	A	195	GLN
2	A	198	GLU
2	A	205	GLN
2	A	211	LEU
2	A	212	LEU
2	A	215	GLU
2	A	221	THR
2	A	222	SER
2	A	223	GLN
2	A	224	TYR
2	A	225	GLU
2	A	229	LEU
2	A	233	SER

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Mol	Chain	Res	Type
2	A	254	ARG
2	A	256	GLN
2	A	257	ASN
2	A	258	LEU
2	A	260	LEU
2	A	261	LEU
2	A	264	ASP
2	A	273	LEU
2	A	291	ILE
2	A	294	ASN
2	A	302	LEU
2	A	306	LEU
2	A	316	SER
2	A	318	ASN
2	A	327	VAL
2	A	331	LEU
2	A	339	LYS
2	A	340	THR
2	A	348	LEU
2	A	349	TYR
2	A	350	ARG
2	A	353	HIS
2	A	354	GLN
2	A	370	LYS
2	A	371	ILE
2	A	386	LEU
2	A	387	LEU
2	A	391	ARG
2	A	392	VAL
2	A	403	LEU
2	A	405	ILE
2	A	406	VAL
2	A	407	ASN
2	A	408	THR
2	A	411	ARG
2	A	417	THR
2	A	421	LEU
2	A	423	GLU
2	A	431	SER
2	A	436	SER
2	A	439	MET
2	A	445	LEU

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Mol	Chain	Res	Type
2	A	455	ARG
2	A	471	PRO
2	A	472	ILE
2	A	483	ASP
2	A	486	SER
2	A	502	MET
2	A	507	GLN
2	A	510	SER
2	A	515	MET
2	A	520	GLU
2	A	537	ARG
2	A	539	MET
2	A	550	ASP
2	A	557	LEU
2	A	563	LEU
2	A	577	PHE
2	A	578	LEU
2	A	585	ASP
2	A	587	ASP
2	A	589	ILE
2	A	595	LEU
2	A	597	TYR
2	A	601	THR
2	A	602	ARG
2	A	610	THR
2	A	611	LEU
2	A	612	CYS
2	A	623	ARG
2	A	630	LEU
2	A	637	ASP
2	A	638	LEU
2	B	3	LEU
2	B	4	ASN
2	B	5	PRO
2	B	9	GLN
2	B	11	VAL
2	B	18	CYS
2	B	21	LEU
2	B	30	ARG
2	B	35	LYS
2	B	45	TYR
2	B	54	THR

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Mol	Chain	Res	Type
2	B	55	PHE
2	B	57	ASN
2	B	62	GLU
2	B	66	ARG
2	B	71	LEU
2	B	73	ARG
2	B	74	LYS
2	B	80	MET
2	B	83	THR
2	B	84	PHE
2	B	87	LEU
2	B	93	LYS
2	B	96	TYR
2	B	101	MET
2	B	102	LYS
2	B	105	PHE
2	B	107	LEU
2	B	108	PHE
2	B	109	ASP
2	B	111	THR
2	B	119	GLU
2	B	127	ASP
2	B	129	LYS
2	B	140	SER
2	B	160	ARG
2	B	166	HIS
2	B	168	TYR
2	B	172	ASP
2	B	175	LEU
2	B	181	LEU
2	B	184	ASP
2	B	189	LEU
2	B	191	THR
2	B	193	LEU
2	B	195	GLN
2	B	197	ASN
2	B	202	LYS
2	B	205	GLN
2	B	208	ILE
2	B	215	GLU
2	B	217	GLN
2	B	219	THR

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Mol	Chain	Res	Type
2	B	220	ASN
2	B	221	THR
2	B	223	GLN
2	B	224	TYR
2	B	226	LEU
2	B	231	VAL
2	B	233	SER
2	B	249	SER
2	B	263	GLN
2	B	272	LYS
2	B	280	SER
2	B	294	ASN
2	B	296	HIS
2	B	304	SER
2	B	305	GLU
2	B	306	LEU
2	B	311	GLU
2	B	316	SER
2	B	323	GLU
2	B	328	THR
2	B	330	GLU
2	B	339	LYS
2	B	350	ARG
2	B	357	VAL
2	B	366	ARG
2	B	370	LYS
2	B	375	THR
2	B	381	PRO
2	B	384	LYS
2	B	387	LEU
2	B	390	LEU
2	B	391	ARG
2	B	393	LEU
2	B	395	ASN
2	B	403	LEU
2	B	407	ASN
2	B	411	ARG
2	B	412	GLU
2	B	418	LEU
2	B	419	LYS
2	B	421	LEU
2	B	424	TRP

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Mol	Chain	Res	Type
2	B	430	LYS
2	B	441	LEU
2	B	445	LEU
2	B	458	HIS
2	B	462	GLU
2	B	468	GLU
2	B	472	ILE
2	B	482	MET
2	B	483	ASP
2	B	492	SER
2	B	499	GLU
2	B	500	MET
2	B	509	PHE
2	B	520	GLU
2	B	521	LEU
2	B	523	GLU
2	B	528	THR
2	B	529	GLN
2	B	533	ARG
2	B	549	LEU
2	B	551	GLN
2	B	553	GLN
2	B	578	LEU
2	B	584	ILE
2	B	585	ASP
2	B	587	ASP
2	B	588	ASN
2	B	592	GLU
2	B	602	ARG
2	B	604	GLN
2	B	606	GLU
2	B	611	LEU
2	B	616	ARG
2	B	626	PRO
2	B	632	GLU
2	B	633	LEU
2	B	638	LEU
2	B	640	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	4	ASN
2	A	8	GLN
2	A	57	ASN
2	A	104	ASN
2	A	144	ASN
2	A	166	HIS
2	A	195	GLN
2	A	197	ASN
2	A	206	ASN
2	A	223	GLN
2	A	256	GLN
2	A	257	ASN
2	A	288	ASN
2	A	294	ASN
2	A	335	HIS
2	A	338	ASN
2	A	464	GLN
2	A	506	ASN
2	A	551	GLN
2	A	553	GLN
2	A	558	HIS
2	A	580	HIS
2	A	635	GLN
2	B	69	GLN
2	B	144	ASN
2	B	174	HIS
2	B	195	GLN
2	B	205	GLN
2	B	206	ASN
2	B	217	GLN
2	B	220	ASN
2	B	223	GLN
2	B	263	GLN
2	B	318	ASN
2	B	338	ASN
2	B	354	GLN
2	B	364	GLN
2	B	365	ASN
2	B	464	GLN
2	B	507	GLN
2	B	553	GLN
2	B	558	HIS
2	B	604	GLN

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Mol	Chain	Res	Type
2	B	635	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.