Full wwPDB X-ray Structure Validation Report (i)

Oct 19, 2023 – 04:50 AM EDT

PDB ID	:	2QZP
Title	:	Crystal structure of mutation of an acylptide hydrolase/esterase from Aeropyrum pernix K1
Authors	:	Zhang, H.F.; Zheng, B.S.; Rao, Z.
Deposited on	:	2007-08-17
Resolution	:	2.70 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:

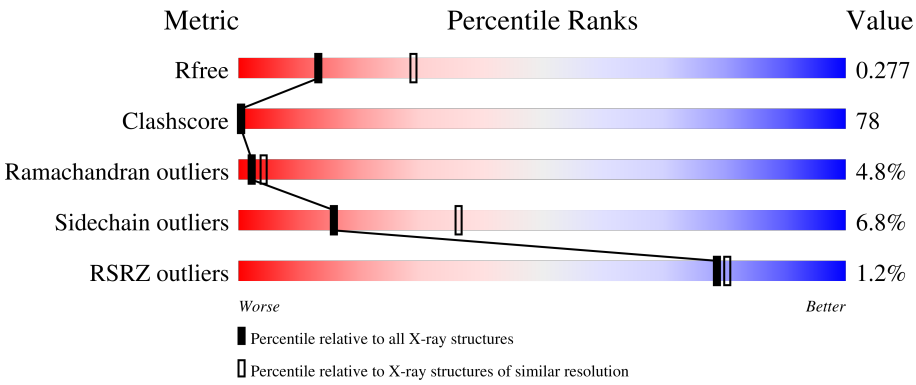
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

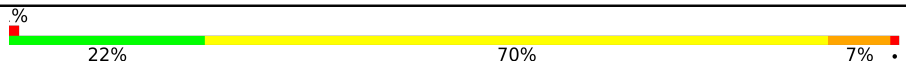
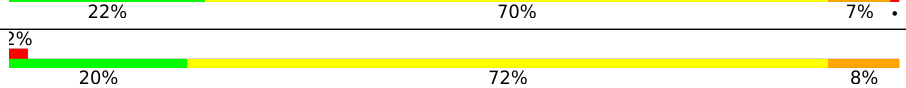
The reported resolution of this entry is 2.70 Å.

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	562	
1	B	562	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8881 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 Acylamino-acid-releasing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	560	4255	2685	750	808	12	0	0	0
1	B	561	4260	2688	751	809	12	0	0	0

- Molecule 2 is water.

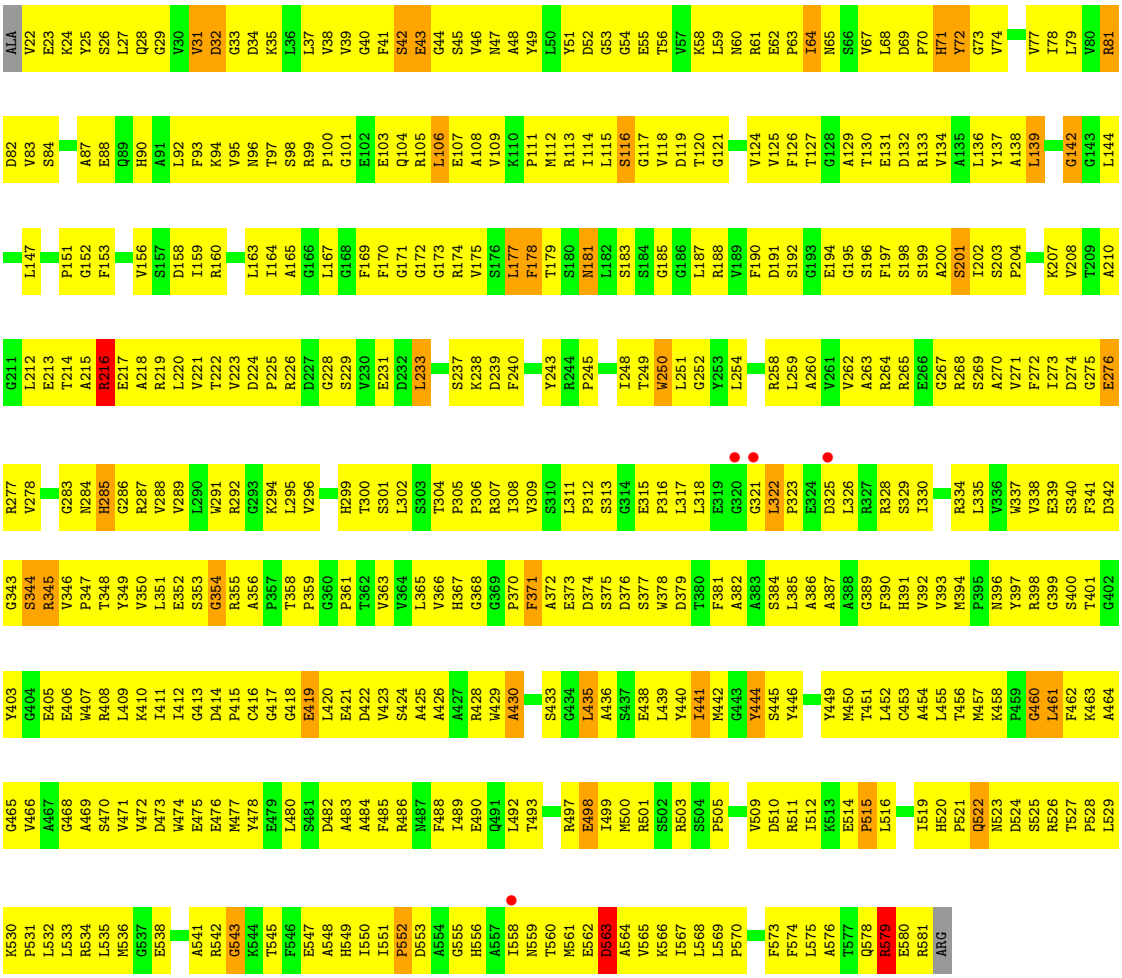
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	154	154	154	0	0
2	B	212	212	212	0	0

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.

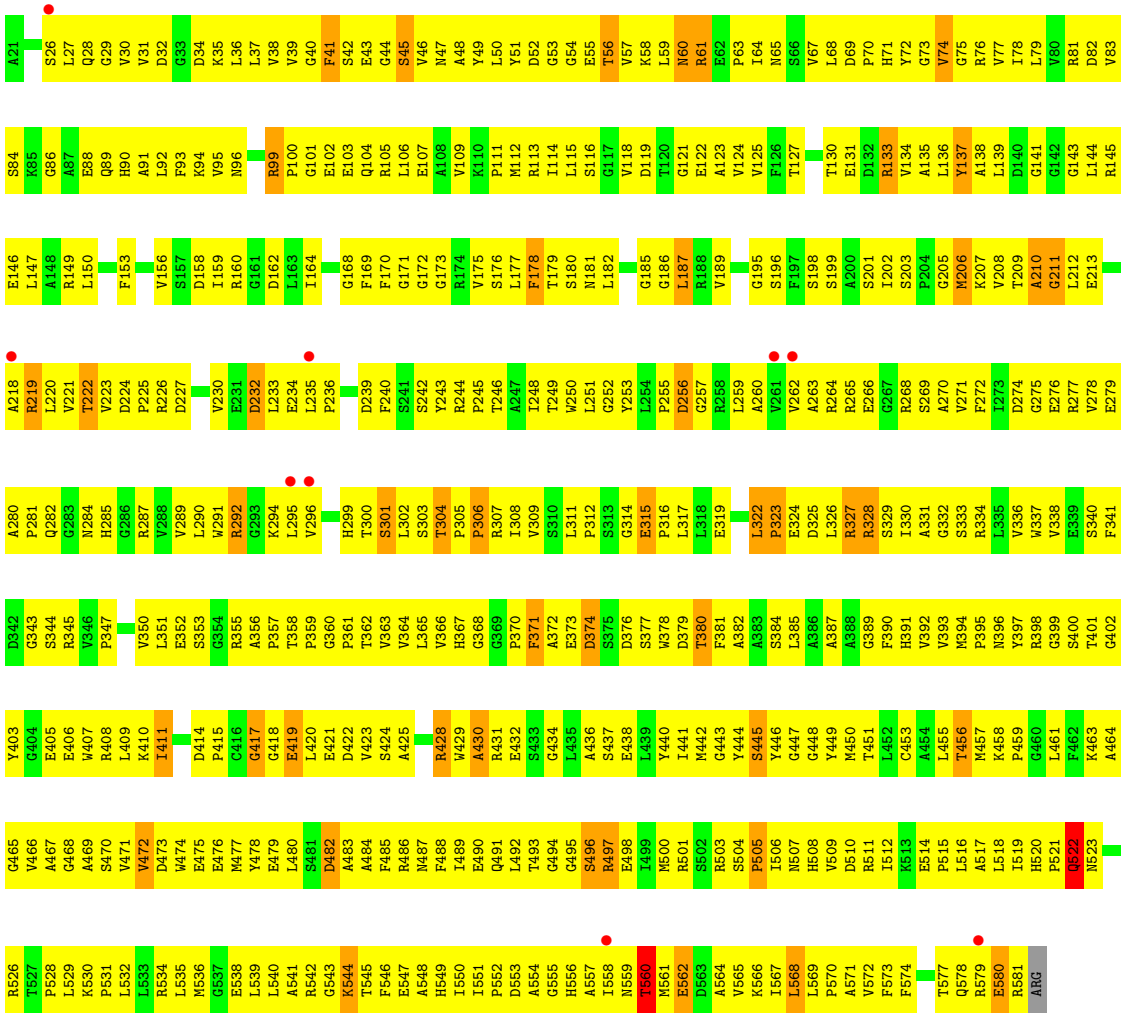
• Molecule 1: Acylamino-acid-releasing enzyme

Chain A:



• Molecule 1: Acylamino-acid-releasing enzyme

Chain B:


A21 S26 L27 Q28 G29 V30 V31 D32 G33 D34 K35 L36 L37 V38 V39 G40 F41 S42 E43 G44 S45 V46 N47 A48 Y49 L50 Y51 D52 G53 G54 E55 T56 V57 K58 L59 N60 R61 E62 P63 I64 N65 S66 V67 L68 D69 P70 H71 Y72 G73 V74 G75 R76 V77 I78 L79 V80 R81 D82 V83
S84 K85 G86 A87 E88 Q89 H90 A91 L92 F93 K94 V95 N96 R99 P100 G101 E102 E103 Q104 R105 L106 E107 A108 V109 K110 P111 M112 R113 I114 L115 S116 G117 V118 D119 T120 G121 E122 A123 V124 V125 F126 T127 T130 E131 D132 R133 V134 A135 L136 Y137 A138 L139 D140 G141 G142 G143 L144 R145
E146 L147 A148 R149 L150 F153 V156 S157 D158 I159 R160 G161 D162 L163 I164 G168 F169 F170 G171 G172 G173 R174 V175 S176 L177 F178 T179 S180 N181 L182 G185 G186 L187 R188 V189 G195 S196 F197 S198 S199 A200 S201 I202 S203 P204 G205 M206 K207 V208 T209 A210 G211 L212 E213
A218 R219 L220 V221 T222 V223 D224 P225 R226 D227 V230 E231 D232 L233 E234 L235 P236 D239 F240 S241 S242 Y243 R244 P245 T246 A247 I248 T249 W250 L251 G252 Y253 L254 P255 D256 G257 R258 L259 A260 V261 V262 A263 R264 R265 E266 G267 R268 S269 A270 V271 F272 I273 D274 G275 E276 R277 V278 E279
A280 P281 Q282 G283 N284 H285 G286 R287 V288 V289 L290 W291 R292 G293 K294 L295 V296 H299 T300 S301 L302 S303 T304 P305 P306 R307 I308 V309 S310 L311 P312 S313 G314 E315 P316 L317 L318 E319 L322 P323 E324 D325 L326 R327 R328 S329 I330 A331 G332 S333 R334 L335 V336 W337 V338 E339 S340 F341
D342 G343 S344 R345 V346 P347 V350 L351 E352 S353 G354 R355 A356 P357 T358 P359 G360 P361 T362 V363 V364 L365 V366 H367 G368 G369 P370 F371 A372 E373 D374 S375 D376 S377 W378 D379 T380 F381 A382 A383 S384 L385 A386 A387 A388 G389 F390 H391 V392 V393 M394 P395 N396 Y397 R398 G399 S400 T401 G402
Y403 G404 E405 E406 W407 R408 L409 K410 I411 D414 P415 G416 G417 G418 E419 L420 E421 D422 V423 S424 A425 R428 W429 A430 R431 E432 S433 G434 L435 A436 S437 E438 L439 Y440 I441 M442 G443 Y444 S445 Y446 G447 G448 Y449 M450 T451 L452 C453 A454 L455 T456 M457 K458 P459 G460 L461 F462 K463 A464
G465 V466 A467 G468 A469 S470 V471 V472 D473 W474 E475 E476 M477 Y478 E479 L480 S481 D482 A483 A484 F485 R486 M487 F488 I489 E490 Q491 L492 T493 G494 G495 S496 R497 E498 I499 M500 R501 S502 R503 S504 P505 I506 N507 H508 V509 D510 R511 I512 K513 E514 P515 L516 A517 L518 I519 H520 P521 Q522 N523
R526 T527 P528 L529 K530 P531 L532 L533 R534 L535 M536 G537 E538 L539 L540 A541 R542 G543 K544 T545 F546 E547 A548 H549 I550 I551 P552 D553 A554 G555 H556 A557 I558 N559 T560 M561 E562 D563 A564 V565 K566 I567 L568 L569 P570 A571 V572 F573 F574 T577 Q578 R579 E580 R581 ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.12Å 102.18Å 163.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.11 – 2.70 48.11 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.0 (48.11-2.70) 90.3 (48.11-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.277 0.226 , 0.277	Depositor DCC
R_{free} test set	1393 reflections (3.96%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 81.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8881	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.47	0/4346	0.76	0/5892
1	B	0.46	0/4351	0.75	1/5899 (0.0%)
All	All	0.46	0/8697	0.75	1/11791 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	374	ASP	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4255	0	4219	642	0
1	B	4260	0	4224	704	0
2	A	154	0	0	93	0
2	B	212	0	0	137	0
All	All	8881	0	8443	1329	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 78.

All (1329) 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:B:497:ARG:HH11	1:B:497:ARG:HB2	0.94	1.11
1:A:552:PRO:HD3	1:B:547:GLU:HB2	1.30	1.11
1:A:346:VAL:HG21	1:A:422:ASP:HB3	1.32	1.09
1:B:334:ARG:HH21	1:B:350:VAL:HG11	1.03	1.09
1:A:547:GLU:HB3	1:B:552:PRO:HD3	1.18	1.07
1:B:92:LEU:HD12	1:B:109:VAL:HG21	1.34	1.03
1:B:90:HIS:HB2	1:B:114:ILE:HD13	1.42	1.00
1:A:530:LYS:HB3	1:A:531:PRO:HD3	1.41	1.00
1:B:376:ASP:HA	2:B:791:HOH:O	1.60	1.00
1:B:323:PRO:HB2	1:B:326:LEU:HB2	1.42	0.99
1:B:497:ARG:HB2	1:B:497:ARG:NH1	1.79	0.98
1:B:347:PRO:O	1:B:396:ASN:HB2	1.63	0.98
1:B:212:LEU:HD23	1:B:219:ARG:HH12	1.26	0.96
1:B:201:SER:HB3	2:B:767:HOH:O	1.65	0.96
1:A:558:ILE:HD12	1:A:563:ASP:HB3	1.45	0.95
1:B:322:LEU:HD12	1:B:323:PRO:HD2	1.49	0.94
1:B:567:ILE:HD12	1:B:568:LEU:N	1.82	0.94
1:B:497:ARG:HH11	1:B:497:ARG:CB	1.81	0.93
1:A:522:GLN:HA	1:A:529:LEU:HD22	1.45	0.93
1:A:471:VAL:HG12	2:A:657:HOH:O	1.68	0.92
1:A:558:ILE:HG23	1:A:563:ASP:HB2	1.51	0.92
1:B:212:LEU:HD23	1:B:219:ARG:NH1	1.85	0.91
1:A:529:LEU:HD11	1:A:550:ILE:HD12	1.51	0.90
1:B:530:LYS:HB3	1:B:531:PRO:HD3	1.51	0.90
1:B:42:SER:HA	1:B:561:MET:SD	2.12	0.90
1:B:88:GLU:HG2	1:B:113:ARG:NH1	1.85	0.90
1:B:363:VAL:HG22	1:B:440:TYR:HB2	1.52	0.89
1:A:449:TYR:HA	2:A:709:HOH:O	1.71	0.88
1:A:69:ASP:HB2	1:A:118:VAL:HG22	1.56	0.88
1:A:68:LEU:HD12	1:A:78:ILE:HG21	1.52	0.88
1:B:325:ASP:HA	1:B:328:ARG:HB2	1.56	0.88
1:A:65:ASN:HD21	1:A:82:ASP:HB2	1.37	0.88
1:A:547:GLU:CB	1:B:552:PRO:HD3	2.03	0.88
1:B:334:ARG:NH2	1:B:350:VAL:HG11	1.87	0.88
1:B:509:VAL:HA	1:B:512:ILE:HD13	1.56	0.87
1:A:574:PHE:HA	2:A:602:HOH:O	1.74	0.87
1:A:127:THR:HB	2:A:677:HOH:O	1.73	0.87
1:B:208:VAL:HB	1:B:223:VAL:HB	1.56	0.87
1:B:528:PRO:HG3	2:B:756:HOH:O	1.75	0.86
1:A:545:THR:HB	2:A:613:HOH:O	1.73	0.86
1:A:457:MET:HB2	2:A:696:HOH:O	1.75	0.86
1:B:49:TYR:HA	1:B:57:VAL:O	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:PRO:HG2	2:B:731:HOH:O	1.76	0.86
1:B:520:HIS:HD2	1:B:521:PRO:HD2	1.40	0.86
1:B:539:LEU:HB2	2:B:678:HOH:O	1.75	0.86
1:A:515:PRO:HA	2:A:613:HOH:O	1.76	0.85
1:B:303:SER:O	1:B:304:THR:HG23	1.74	0.85
1:B:26:SER:HB3	1:B:39:VAL:HB	1.58	0.85
1:A:569:LEU:HB3	1:A:570:PRO:HD3	1.57	0.85
1:A:412:ILE:HB	2:A:721:HOH:O	1.77	0.84
1:B:127:THR:HG23	1:B:156:VAL:HG23	1.59	0.84
1:B:278:VAL:HG11	1:B:295:LEU:HD12	1.56	0.84
1:A:215:ALA:HB1	1:A:406:GLU:HB2	1.57	0.84
1:A:558:ILE:HG22	1:A:560:THR:O	1.78	0.84
1:A:547:GLU:HB3	1:B:552:PRO:CD	2.07	0.84
1:A:273:ILE:O	1:A:276:GLU:HB2	1.77	0.83
1:B:561:MET:HA	2:B:589:HOH:O	1.76	0.83
1:B:338:VAL:HG11	1:B:425:ALA:O	1.78	0.83
1:B:484:ALA:HB3	2:B:604:HOH:O	1.79	0.83
1:A:194:GLU:HB2	1:A:212:LEU:HD21	1.60	0.83
1:A:548:ALA:HB3	1:B:550:ILE:HD13	1.58	0.83
1:B:463:LYS:HB2	2:B:658:HOH:O	1.77	0.82
1:B:458:LYS:HE3	2:B:778:HOH:O	1.79	0.82
1:A:116:SER:N	2:A:677:HOH:O	2.13	0.82
1:A:452:LEU:HD22	2:A:709:HOH:O	1.78	0.82
1:A:532:LEU:HD13	1:A:532:LEU:O	1.79	0.82
1:B:70:PRO:HB2	1:B:74:VAL:HG21	1.61	0.82
1:A:94:LYS:O	1:A:94:LYS:HG3	1.79	0.82
1:B:420:LEU:HD21	1:B:458:LYS:HD3	1.59	0.82
1:B:284:ASN:HD22	1:B:376:ASP:C	1.83	0.81
1:B:302:LEU:HG	2:B:600:HOH:O	1.79	0.81
1:A:177:LEU:HD21	1:A:208:VAL:HG11	1.62	0.81
1:A:138:ALA:HB2	1:A:147:LEU:HD21	1.63	0.81
1:A:458:LYS:HD3	1:A:461:LEU:HD13	1.63	0.80
1:B:102:GLU:HA	2:B:621:HOH:O	1.79	0.80
1:A:322:LEU:HD23	1:A:323:PRO:HD2	1.63	0.80
1:A:23:GLU:HA	2:A:730:HOH:O	1.80	0.80
1:B:158:ASP:O	1:B:159:ILE:HD13	1.80	0.80
1:B:374:ASP:CG	1:B:394:MET:HB3	2.01	0.80
1:B:406:GLU:HG2	1:B:410:LYS:HE2	1.64	0.80
1:A:545:THR:HG23	1:B:553:ASP:OD1	1.80	0.80
1:B:570:PRO:HD2	2:B:594:HOH:O	1.82	0.79
1:B:44:GLY:O	1:B:560:THR:HG22	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:HD13	1:B:124:VAL:HG13	1.63	0.79
1:A:38:VAL:HG12	1:A:39:VAL:N	1.97	0.79
1:B:281:PRO:O	1:B:285:HIS:HE1	1.66	0.78
1:A:238:LYS:HG2	2:A:614:HOH:O	1.84	0.78
1:B:376:ASP:HB2	2:B:616:HOH:O	1.82	0.78
1:A:558:ILE:HG23	1:A:563:ASP:CB	2.14	0.78
1:A:32:ASP:HB2	1:A:35:LYS:HB2	1.64	0.78
1:A:44:GLY:HA2	1:A:561:MET:H	1.49	0.78
1:B:353:SER:HB3	1:B:356:ALA:HB3	1.66	0.78
1:A:406:GLU:O	1:A:410:LYS:HG3	1.85	0.77
1:A:469:ALA:O	1:A:527:THR:HG21	1.84	0.77
1:B:522:GLN:HA	1:B:529:LEU:HD22	1.64	0.77
1:B:569:LEU:HB3	1:B:570:PRO:HD3	1.66	0.77
1:B:574:PHE:HA	2:B:784:HOH:O	1.84	0.77
1:A:83:VAL:HA	2:A:717:HOH:O	1.84	0.77
1:B:406:GLU:O	1:B:410:LYS:HG3	1.85	0.77
1:A:138:ALA:CB	1:A:147:LEU:HD21	2.13	0.77
1:A:562:GLU:O	1:A:564:ALA:N	2.17	0.77
1:B:268:ARG:HA	2:B:614:HOH:O	1.83	0.77
1:A:61:ARG:NH1	1:A:101:GLY:HA3	1.99	0.77
1:A:519:ILE:HA	1:A:549:HIS:HB2	1.66	0.77
1:A:523:ASN:ND2	1:A:553:ASP:HA	1.99	0.77
1:A:417:GLY:N	1:A:419:GLU:OE2	2.18	0.77
1:B:323:PRO:HG2	1:B:326:LEU:HD12	1.67	0.77
1:B:387:ALA:HB2	2:B:643:HOH:O	1.83	0.77
1:A:334:ARG:HH21	1:A:350:VAL:HG11	1.50	0.76
1:A:90:HIS:HD2	1:A:114:ILE:H	1.32	0.76
1:A:215:ALA:N	1:A:405:GLU:HB3	2.01	0.75
1:A:420:LEU:HD21	2:A:696:HOH:O	1.84	0.75
1:B:567:ILE:HD11	1:B:568:LEU:HD22	1.69	0.75
1:B:520:HIS:ND1	1:B:532:LEU:HG	2.01	0.75
1:A:552:PRO:CD	1:B:547:GLU:HB2	2.14	0.75
1:A:411:ILE:HD11	1:A:446:TYR:OH	1.87	0.74
1:A:194:GLU:HB3	1:A:214:THR:CG2	2.16	0.74
1:B:139:LEU:HD13	1:B:144:LEU:HB2	1.69	0.74
1:B:542:ARG:HG3	1:B:542:ARG:HH11	1.49	0.74
1:A:428:ARG:HG3	2:A:622:HOH:O	1.87	0.74
1:B:480:LEU:HB2	2:B:756:HOH:O	1.88	0.74
1:A:534:ARG:O	1:A:538:GLU:HG2	1.88	0.74
1:A:309:VAL:HA	1:A:316:PRO:HA	1.68	0.73
1:B:59:LEU:O	1:B:95:VAL:HG11	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:HG	2:A:670:HOH:O	1.87	0.73
1:B:239:ASP:HB2	1:B:275:GLY:O	1.87	0.73
1:B:579:ARG:C	1:B:581:ARG:H	1.91	0.73
1:A:136:LEU:HD21	1:A:164:ILE:HG21	1.70	0.73
1:A:526:ARG:HH11	1:A:556:HIS:HD2	1.34	0.73
1:B:265:ARG:HB3	2:B:696:HOH:O	1.87	0.73
1:A:194:GLU:HB3	1:A:214:THR:HG21	1.70	0.73
1:B:428:ARG:HG2	2:B:592:HOH:O	1.88	0.73
1:B:445:SER:H	1:B:469:ALA:HB3	1.54	0.73
1:A:529:LEU:HD23	1:B:540:LEU:HD13	1.70	0.72
1:A:65:ASN:ND2	1:A:82:ASP:HB2	2.04	0.72
1:B:90:HIS:CB	1:B:114:ILE:HD13	2.20	0.72
1:B:477:MET:HG3	1:B:528:PRO:HD2	1.72	0.72
1:B:485:PHE:HA	1:B:488:PHE:HB3	1.72	0.72
1:B:503:ARG:O	1:B:505:PRO:HD3	1.89	0.72
1:B:133:ARG:HD3	1:B:149:ARG:HE	1.54	0.72
1:B:177:LEU:CD2	1:B:223:VAL:HG21	2.19	0.72
1:B:496:SER:HB3	2:B:619:HOH:O	1.89	0.72
1:A:251:LEU:HD13	1:A:259:LEU:HD11	1.71	0.71
1:B:71:HIS:O	1:B:74:VAL:HG13	1.89	0.71
1:B:519:ILE:HD13	2:B:594:HOH:O	1.90	0.71
1:A:271:VAL:HB	1:A:278:VAL:HB	1.71	0.71
1:A:419:GLU:HG3	2:A:643:HOH:O	1.90	0.71
1:B:95:VAL:HA	2:B:742:HOH:O	1.90	0.71
1:B:347:PRO:O	1:B:396:ASN:CB	2.38	0.71
1:B:573:PHE:HB2	2:B:653:HOH:O	1.90	0.71
1:A:549:HIS:CE1	1:A:570:PRO:HB3	2.26	0.71
1:A:361:PRO:HA	1:A:438:GLU:CG	2.21	0.71
1:B:374:ASP:OD2	1:B:394:MET:HB3	1.90	0.71
1:B:381:PHE:CZ	1:B:567:ILE:HD13	2.25	0.71
1:B:417:GLY:O	1:B:421:GLU:HG2	1.89	0.71
1:A:350:VAL:O	1:A:351:LEU:HD23	1.89	0.71
1:B:364:VAL:HG22	2:B:775:HOH:O	1.91	0.71
1:B:472:VAL:HG12	1:B:506:ILE:HB	1.71	0.71
1:B:475:GLU:O	1:B:479:GLU:HG3	1.88	0.71
1:B:451:THR:CG2	1:B:467:ALA:HB2	2.21	0.71
1:B:577:THR:HB	2:B:784:HOH:O	1.89	0.71
1:B:160:ARG:HB3	1:B:202:ILE:HG21	1.74	0.70
1:A:338:VAL:O	1:A:345:ARG:HA	1.91	0.70
1:A:308:ILE:HB	1:A:318:LEU:HB2	1.73	0.70
1:B:45:SER:HA	1:B:560:THR:HA	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:HIS:O	1:A:74:VAL:HG23	1.91	0.70
1:A:363:VAL:HG12	2:A:693:HOH:O	1.92	0.70
1:A:284:ASN:ND2	1:A:377:SER:OG	2.25	0.70
1:A:309:VAL:HG12	1:A:316:PRO:HA	1.73	0.70
1:B:30:VAL:HG23	1:B:289:VAL:CG1	2.21	0.70
1:B:356:ALA:HB2	1:B:389:GLY:O	1.92	0.70
1:B:362:THR:HG22	1:B:363:VAL:N	2.06	0.70
1:B:564:ALA:O	1:B:567:ILE:HD11	1.92	0.70
1:A:129:ALA:CB	1:A:134:VAL:HG22	2.21	0.70
1:B:164:ILE:HB	1:B:180:SER:HB3	1.74	0.70
1:B:373:GLU:OE2	1:B:396:ASN:HB3	1.91	0.70
1:B:331:ALA:HB3	1:B:352:GLU:HB3	1.73	0.69
1:A:335:LEU:HD12	1:A:348:THR:O	1.93	0.69
1:B:51:TYR:HE2	1:B:317:LEU:HB3	1.58	0.69
1:B:79:LEU:HD11	1:B:95:VAL:HG21	1.74	0.69
1:A:346:VAL:HG13	1:A:407:TRP:HZ2	1.58	0.69
1:A:90:HIS:HB2	1:A:114:ILE:HD13	1.75	0.69
1:B:565:VAL:C	1:B:567:ILE:H	1.93	0.69
1:A:441:ILE:HD13	1:A:442:MET:N	2.06	0.69
1:A:439:LEU:N	2:A:729:HOH:O	2.24	0.69
1:A:511:ARG:O	2:A:630:HOH:O	2.10	0.69
1:B:178:PHE:HB3	2:B:706:HOH:O	1.93	0.69
1:B:208:VAL:HG23	1:B:223:VAL:O	1.93	0.69
1:A:528:PRO:HD3	2:A:644:HOH:O	1.91	0.69
1:B:245:PRO:HA	2:B:696:HOH:O	1.93	0.69
1:B:324:GLU:O	1:B:327:ARG:HB3	1.92	0.69
1:A:130:THR:OG1	1:A:132:ASP:OD1	2.10	0.68
1:B:327:ARG:O	2:B:720:HOH:O	2.11	0.68
1:A:174:ARG:HE	1:A:409:LEU:HD11	1.59	0.68
1:B:35:LYS:HG2	1:B:52:ASP:OD1	1.93	0.68
1:A:200:ALA:HB3	2:A:639:HOH:O	1.92	0.68
1:A:405:GLU:OE1	1:A:409:LEU:HG	1.93	0.68
1:A:163:LEU:C	1:A:164:ILE:HD12	2.13	0.68
1:A:474:TRP:HB2	1:A:500:MET:HB3	1.75	0.68
1:A:175:VAL:HG23	1:A:196:SER:HB3	1.76	0.68
1:B:169:PHE:CZ	1:B:175:VAL:HG22	2.28	0.68
1:B:329:SER:HB2	1:B:387:ALA:HA	1.76	0.68
1:A:352:GLU:HA	1:A:391:HIS:ND1	2.09	0.68
1:A:361:PRO:HA	1:A:438:GLU:HG2	1.76	0.68
1:A:27:LEU:HD21	1:A:289:VAL:HG22	1.76	0.68
1:B:92:LEU:O	1:B:106:LEU:HD12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:MET:HA	2:B:756:HOH:O	1.93	0.68
1:B:526:ARG:NH2	1:B:557:ALA:HB2	2.08	0.68
1:B:218:ALA:HB1	1:B:248:ILE:HD11	1.76	0.67
1:B:526:ARG:HA	2:B:680:HOH:O	1.94	0.67
1:A:42:SER:HB2	2:A:649:HOH:O	1.94	0.67
1:B:222:THR:O	1:B:230:VAL:HG13	1.95	0.67
1:B:59:LEU:HD13	1:B:77:VAL:HG21	1.76	0.67
1:B:218:ALA:HB1	1:B:248:ILE:CD1	2.25	0.67
1:A:27:LEU:HD23	1:A:287:ARG:O	1.93	0.67
1:A:368:GLY:HA2	2:A:686:HOH:O	1.95	0.67
1:B:295:LEU:O	1:B:311:LEU:HG	1.95	0.67
1:B:485:PHE:O	1:B:489:ILE:HG12	1.95	0.67
1:B:91:ALA:HB3	1:B:93:PHE:CZ	2.30	0.66
1:B:440:TYR:OH	1:B:463:LYS:HD3	1.94	0.66
1:B:221:VAL:HB	1:B:230:VAL:HG12	1.77	0.66
1:A:90:HIS:O	1:A:111:PRO:HA	1.96	0.66
1:A:386:ALA:HA	1:A:390:PHE:O	1.95	0.66
1:B:438:GLU:HA	2:B:714:HOH:O	1.95	0.66
1:B:449:TYR:HB2	2:B:685:HOH:O	1.94	0.66
1:A:498:GLU:HA	1:A:501:ARG:HD2	1.77	0.66
1:B:559:ASN:O	1:B:560:THR:HG23	1.95	0.66
1:A:58:LYS:O	1:A:100:PRO:HB3	1.96	0.66
1:A:81:ARG:HB2	1:A:81:ARG:HH11	1.61	0.66
1:A:423:VAL:HA	2:A:651:HOH:O	1.95	0.66
1:A:353:SER:O	1:A:356:ALA:N	2.29	0.66
1:A:529:LEU:HD11	1:A:550:ILE:CD1	2.25	0.66
1:B:159:ILE:HD12	1:B:164:ILE:HG23	1.78	0.66
1:A:322:LEU:HD23	1:A:323:PRO:CD	2.25	0.66
1:A:548:ALA:O	1:B:549:HIS:HA	1.95	0.66
1:A:551:ILE:HG23	1:A:552:PRO:HD2	1.77	0.66
1:B:421:GLU:OE2	1:B:421:GLU:HA	1.96	0.66
1:B:574:PHE:O	1:B:577:THR:HB	1.96	0.66
1:A:480:LEU:HD21	1:A:530:LYS:HD2	1.78	0.66
1:A:567:ILE:HG13	1:A:567:ILE:O	1.95	0.66
1:B:424:SER:HB3	1:B:428:ARG:NH1	2.11	0.66
1:A:45:SER:HB2	1:A:63:PRO:HB3	1.76	0.65
1:A:125:VAL:HA	1:A:137:TYR:O	1.96	0.65
1:A:392:VAL:HG22	2:A:720:HOH:O	1.95	0.65
1:B:153:PHE:HE1	1:B:488:PHE:HB2	1.61	0.65
1:A:308:ILE:O	1:A:318:LEU:N	2.23	0.65
1:B:171:GLY:O	1:B:173:GLY:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:HIS:N	1:A:112:MET:O	2.21	0.65
1:A:555:GLY:HA3	2:A:663:HOH:O	1.96	0.65
1:B:99:ARG:HB2	1:B:102:GLU:OE2	1.96	0.65
1:B:410:LYS:HG2	2:B:695:HOH:O	1.95	0.65
1:A:302:LEU:HD13	1:A:351:LEU:HD21	1.78	0.65
1:B:523:ASN:ND2	1:B:553:ASP:HA	2.11	0.65
1:A:579:ARG:NH1	1:A:579:ARG:HB2	2.12	0.65
1:B:103:GLU:HB2	2:B:687:HOH:O	1.97	0.65
1:B:458:LYS:HB3	1:B:461:LEU:HD22	1.79	0.65
1:B:532:LEU:O	1:B:536:MET:HG3	1.97	0.65
1:B:469:ALA:HB1	1:B:556:HIS:CE1	2.31	0.65
1:A:563:ASP:HA	1:A:566:LYS:CG	2.27	0.65
1:A:63:PRO:HA	2:A:595:HOH:O	1.97	0.65
1:B:278:VAL:HG11	1:B:295:LEU:CD1	2.27	0.64
1:B:29:GLY:CA	1:B:289:VAL:HG21	2.28	0.64
1:B:136:LEU:O	1:B:147:LEU:N	2.31	0.64
1:A:353:SER:O	1:A:355:ARG:N	2.30	0.64
1:B:100:PRO:O	1:B:102:GLU:HG3	1.96	0.64
1:B:133:ARG:HA	1:B:483:ALA:CB	2.27	0.64
1:B:137:TYR:HA	1:B:146:GLU:HA	1.80	0.64
1:B:362:THR:CG2	1:B:363:VAL:N	2.60	0.64
1:A:88:GLU:HG3	1:A:113:ARG:HH12	1.61	0.64
1:A:223:VAL:HA	1:A:229:SER:O	1.98	0.64
1:A:263:ALA:O	1:A:269:SER:HB2	1.97	0.64
1:A:325:ASP:HA	1:A:328:ARG:HB3	1.79	0.64
1:A:337:TRP:CZ3	1:A:347:PRO:HB3	2.33	0.64
1:B:69:ASP:O	1:B:118:VAL:HG13	1.97	0.64
1:B:201:SER:N	2:B:652:HOH:O	2.30	0.64
1:A:61:ARG:HH12	1:A:101:GLY:HA3	1.62	0.64
1:A:438:GLU:HB2	2:A:729:HOH:O	1.96	0.64
1:A:525:SER:C	2:A:644:HOH:O	2.35	0.64
1:A:526:ARG:HD2	1:A:556:HIS:CD2	2.32	0.64
1:B:181:ASN:HB2	1:B:185:GLY:O	1.97	0.64
1:A:38:VAL:CG1	1:A:39:VAL:N	2.61	0.64
1:A:272:PHE:CE2	1:A:277:ARG:HD3	2.33	0.64
1:A:415:PRO:O	1:A:503:ARG:HD2	1.98	0.64
1:B:46:VAL:HG23	2:B:764:HOH:O	1.98	0.64
1:A:172:GLY:O	1:A:409:LEU:HD22	1.98	0.64
1:B:90:HIS:HB2	1:B:114:ILE:CD1	2.23	0.64
1:B:201:SER:CB	1:B:252:GLY:HA2	2.28	0.64
1:B:251:LEU:HG	2:B:652:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ILE:CD1	1:B:419:GLU:HG2	2.27	0.64
1:A:129:ALA:HB2	1:A:134:VAL:HG22	1.80	0.64
1:A:200:ALA:CB	2:A:639:HOH:O	2.46	0.64
1:A:214:THR:C	1:A:405:GLU:HB3	2.18	0.64
1:B:361:PRO:HA	1:B:438:GLU:HG2	1.80	0.64
1:B:373:GLU:OE1	1:B:396:ASN:ND2	2.31	0.64
1:A:164:ILE:HD13	1:A:181:ASN:C	2.18	0.63
1:A:370:PRO:O	1:A:372:ALA:N	2.29	0.63
1:A:511:ARG:HG2	2:A:630:HOH:O	1.98	0.63
1:B:137:TYR:CD2	1:B:146:GLU:HG3	2.32	0.63
1:A:493:THR:O	1:A:499:ILE:HD12	1.97	0.63
1:B:90:HIS:HD2	1:B:114:ILE:H	1.47	0.63
1:B:92:LEU:HD12	1:B:109:VAL:CG2	2.22	0.63
1:B:180:SER:HA	2:B:750:HOH:O	1.98	0.63
1:B:104:GLN:HG2	2:B:620:HOH:O	1.98	0.63
1:B:428:ARG:O	1:B:431:ARG:HB2	1.98	0.63
1:B:471:VAL:HG11	1:B:474:TRP:CH2	2.33	0.63
1:A:93:PHE:C	2:A:589:HOH:O	2.36	0.63
1:A:133:ARG:HA	1:A:483:ALA:CB	2.28	0.63
1:B:411:ILE:HD11	1:B:446:TYR:OH	1.99	0.63
1:B:441:ILE:HG21	2:B:615:HOH:O	1.96	0.63
1:A:62:GLU:HB2	1:A:81:ARG:HH21	1.64	0.63
1:B:186:GLY:O	1:B:187:LEU:HB2	1.98	0.63
1:B:171:GLY:C	1:B:173:GLY:H	2.00	0.63
1:B:472:VAL:CG1	1:B:506:ILE:HB	2.29	0.63
1:B:542:ARG:HG3	1:B:542:ARG:NH1	2.14	0.63
1:B:61:ARG:HB2	1:B:103:GLU:OE1	1.99	0.62
1:B:278:VAL:HG13	1:B:312:PRO:HB3	1.80	0.62
1:B:340:SER:HB3	2:B:722:HOH:O	1.98	0.62
1:A:109:VAL:HG12	2:A:594:HOH:O	1.99	0.62
1:A:475:GLU:HB3	2:A:627:HOH:O	2.00	0.62
1:B:99:ARG:NH2	1:B:102:GLU:HB3	2.13	0.62
1:B:264:ARG:O	1:B:264:ARG:HG3	1.97	0.62
1:B:78:ILE:HD13	1:B:124:VAL:CG1	2.30	0.62
1:A:523:ASN:HD21	1:A:553:ASP:HA	1.61	0.62
1:B:91:ALA:HB1	1:B:105:ARG:HE	1.65	0.62
1:B:116:SER:C	2:B:596:HOH:O	2.38	0.62
1:A:45:SER:OG	1:A:47:ASN:ND2	2.30	0.62
1:B:523:ASN:HB2	1:B:554:ALA:O	1.99	0.62
1:A:58:LYS:HE2	1:A:60:ASN:O	1.99	0.62
1:B:68:LEU:O	1:B:70:PRO:HD3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ARG:HD2	2:B:684:HOH:O	2.00	0.62
1:B:539:LEU:HD13	1:B:546:PHE:CG	2.34	0.62
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.64	0.62
1:B:29:GLY:HA2	1:B:289:VAL:HG21	1.82	0.62
1:B:420:LEU:CD2	1:B:458:LYS:HD3	2.29	0.62
1:A:90:HIS:HB2	1:A:114:ILE:CD1	2.30	0.62
1:B:133:ARG:NH1	1:B:146:GLU:OE2	2.32	0.62
1:A:45:SER:HB2	2:A:595:HOH:O	1.99	0.61
1:A:251:LEU:HD12	1:A:252:GLY:N	2.13	0.61
1:A:283:GLY:HA2	1:A:376:ASP:OD2	2.00	0.61
1:A:470:SER:O	1:A:527:THR:HB	2.00	0.61
1:B:115:LEU:HB2	1:B:127:THR:OG1	2.00	0.61
1:A:341:PHE:CD2	1:A:421:GLU:HB3	2.35	0.61
1:A:346:VAL:HG22	1:A:407:TRP:CH2	2.36	0.61
1:B:373:GLU:OE1	1:B:373:GLU:HA	1.99	0.61
1:A:273:ILE:HG13	1:A:295:LEU:HD11	1.82	0.61
1:A:499:ILE:HD11	2:A:732:HOH:O	2.01	0.61
1:B:160:ARG:NH2	2:B:715:HOH:O	2.33	0.61
1:A:419:GLU:CD	1:A:420:LEU:H	2.03	0.61
1:B:370:PRO:O	1:B:372:ALA:N	2.33	0.61
1:A:340:SER:HB2	1:A:344:SER:O	1.99	0.61
1:B:31:VAL:HG12	1:B:32:ASP:N	2.15	0.61
1:B:559:ASN:HB2	2:B:762:HOH:O	2.00	0.61
1:A:547:GLU:OE2	1:A:574:PHE:HB2	2.00	0.61
1:A:558:ILE:HG12	2:A:583:HOH:O	2.01	0.61
1:A:533:LEU:CD1	1:B:536:MET:HB3	2.30	0.61
1:B:323:PRO:CG	1:B:326:LEU:HD12	2.31	0.61
1:A:497:ARG:O	1:A:499:ILE:N	2.34	0.61
1:B:55:GLU:C	2:B:735:HOH:O	2.38	0.61
1:B:399:GLY:HA2	1:B:408:ARG:O	2.01	0.61
1:A:533:LEU:HD11	1:B:536:MET:HB3	1.81	0.61
1:B:45:SER:HB2	1:B:63:PRO:HB3	1.83	0.60
1:B:127:THR:HG23	1:B:156:VAL:CG2	2.29	0.60
1:B:347:PRO:HG2	1:B:396:ASN:HB2	1.83	0.60
1:B:282:GLN:HB3	2:B:700:HOH:O	1.99	0.60
1:B:567:ILE:CD1	1:B:568:LEU:HD22	2.32	0.60
1:A:264:ARG:NH2	1:A:373:GLU:OE2	2.33	0.60
1:A:562:GLU:C	1:A:564:ALA:H	2.05	0.60
1:B:26:SER:O	1:B:308:ILE:HD11	2.01	0.60
1:B:30:VAL:H	1:B:289:VAL:HG11	1.64	0.60
1:A:296:VAL:HG13	1:A:309:VAL:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PHE:CE2	1:A:561:MET:HA	2.37	0.60
1:A:160:ARG:N	1:A:202:ILE:HD12	2.16	0.60
1:B:90:HIS:CD2	1:B:114:ILE:HD13	2.35	0.60
1:A:533:LEU:HD21	1:B:536:MET:SD	2.42	0.60
1:A:41:PHE:CZ	1:A:561:MET:HA	2.35	0.60
1:A:309:VAL:HG12	1:A:316:PRO:CA	2.32	0.60
1:A:468:GLY:HA2	1:A:519:ILE:O	2.02	0.60
1:B:135:ALA:HB3	1:B:137:TYR:CZ	2.37	0.60
1:B:517:ALA:HB2	1:B:574:PHE:CD1	2.37	0.60
1:B:530:LYS:HB3	1:B:531:PRO:CD	2.27	0.60
1:A:334:ARG:HG3	2:A:694:HOH:O	2.01	0.60
1:B:330:ILE:HD12	2:B:720:HOH:O	2.02	0.60
1:A:385:LEU:HD13	2:A:720:HOH:O	2.00	0.60
1:B:361:PRO:O	1:B:390:PHE:HA	2.02	0.59
1:B:325:ASP:CA	1:B:328:ARG:HB2	2.30	0.59
1:B:410:LYS:HE3	2:B:786:HOH:O	2.02	0.59
1:A:171:GLY:O	1:A:174:ARG:HB2	2.02	0.59
1:B:175:VAL:HB	1:B:196:SER:HB3	1.84	0.59
1:A:55:GLU:HA	2:A:604:HOH:O	2.03	0.59
1:A:267:GLY:HA2	1:A:375:SER:HB2	1.83	0.59
1:A:356:ALA:HB2	1:A:389:GLY:O	2.01	0.59
1:B:451:THR:HG21	1:B:467:ALA:HB2	1.85	0.59
1:A:558:ILE:CG2	1:A:560:THR:O	2.51	0.59
1:B:361:PRO:HG3	1:B:438:GLU:CD	2.23	0.59
1:B:471:VAL:HG11	1:B:474:TRP:CZ3	2.37	0.59
1:A:37:LEU:HD23	1:A:70:PRO:HG3	1.85	0.59
1:A:480:LEU:HD21	1:A:530:LYS:CD	2.32	0.59
1:A:530:LYS:CB	1:A:531:PRO:HD3	2.24	0.59
1:A:109:VAL:HG12	1:A:109:VAL:O	2.02	0.59
1:A:306:PRO:HD3	1:A:378:TRP:HB3	1.83	0.59
1:B:565:VAL:C	1:B:567:ILE:N	2.56	0.59
1:A:526:ARG:HH11	1:A:556:HIS:CD2	2.18	0.59
1:B:145:ARG:HG3	2:B:748:HOH:O	2.01	0.58
1:B:302:LEU:HD13	1:B:351:LEU:CD1	2.33	0.58
1:B:46:VAL:HB	1:B:64:ILE:O	2.03	0.58
1:B:246:THR:HG22	1:B:264:ARG:O	2.03	0.58
1:B:251:LEU:CD1	1:B:259:LEU:HD11	2.33	0.58
1:B:456:THR:CG2	1:B:512:ILE:HD11	2.32	0.58
1:A:475:GLU:HA	1:A:500:MET:HE2	1.85	0.58
1:B:414:ASP:HA	1:B:503:ARG:HH12	1.66	0.58
1:B:210:ALA:HA	1:B:251:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ARG:NH2	2:B:595:HOH:O	2.33	0.58
1:A:165:ALA:CB	2:A:653:HOH:O	2.51	0.58
1:A:455:LEU:HD23	2:A:682:HOH:O	2.03	0.58
1:A:465:GLY:O	1:A:516:LEU:HA	2.04	0.58
1:B:28:GLN:HG3	1:B:67:VAL:CG2	2.33	0.58
1:B:61:ARG:HB2	1:B:103:GLU:CD	2.24	0.58
1:B:250:TRP:HZ3	1:B:260:ALA:HB3	1.67	0.58
1:B:324:GLU:OE2	1:B:327:ARG:NH1	2.33	0.58
1:B:390:PHE:CE1	1:B:579:ARG:NH2	2.72	0.58
1:A:177:LEU:HB3	1:A:190:PHE:HB2	1.86	0.58
1:B:248:ILE:HD12	1:B:248:ILE:H	1.69	0.58
1:A:40:GLY:C	1:A:42:SER:H	2.07	0.58
1:B:27:LEU:CD1	1:B:38:VAL:HG12	2.33	0.58
1:B:284:ASN:ND2	1:B:376:ASP:C	2.54	0.58
1:B:528:PRO:O	1:B:532:LEU:HD23	2.03	0.58
1:A:159:ILE:HG23	1:A:163:LEU:O	2.03	0.58
1:A:38:VAL:CG1	1:A:39:VAL:H	2.17	0.58
1:A:160:ARG:HD3	1:A:202:ILE:HG22	1.85	0.58
1:B:133:ARG:HA	1:B:483:ALA:HB2	1.85	0.58
1:B:497:ARG:O	1:B:500:MET:N	2.37	0.58
1:A:120:THR:HB	2:A:617:HOH:O	2.04	0.57
1:A:403:TYR:HD1	2:A:618:HOH:O	1.87	0.57
1:B:60:ASN:O	1:B:101:GLY:HA2	2.05	0.57
1:B:201:SER:HB2	1:B:252:GLY:HA2	1.86	0.57
1:A:217:GLU:HG2	1:A:245:PRO:O	2.05	0.57
1:B:295:LEU:HB2	1:B:311:LEU:HB2	1.85	0.57
1:B:343:GLY:N	2:B:722:HOH:O	2.37	0.57
1:A:44:GLY:HA2	1:A:561:MET:CB	2.34	0.57
1:A:51:TYR:CZ	1:A:53:GLY:HA2	2.39	0.57
1:B:266:GLU:HG2	1:B:337:TRP:HZ2	1.69	0.57
1:B:477:MET:HB3	2:B:642:HOH:O	2.05	0.57
1:B:477:MET:CE	1:B:489:ILE:HD11	2.34	0.57
1:B:326:LEU:HA	1:B:355:ARG:HH11	1.67	0.57
1:A:187:LEU:HD12	1:A:188:ARG:H	1.68	0.57
1:A:412:ILE:HD13	1:A:492:LEU:HD12	1.86	0.57
1:B:233:LEU:HD23	1:B:234:GLU:N	2.20	0.57
1:A:38:VAL:HG12	1:A:39:VAL:H	1.65	0.57
1:A:187:LEU:HD12	1:A:188:ARG:N	2.20	0.57
1:A:267:GLY:HA2	1:A:375:SER:CB	2.34	0.57
1:A:372:ALA:O	1:A:401:THR:N	2.34	0.57
1:B:271:VAL:O	1:B:277:ARG:HA	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:ASN:HA	2:B:679:HOH:O	2.04	0.57
1:B:198:SER:HB3	1:B:213:GLU:OE2	2.04	0.57
1:B:551:ILE:HB	1:B:554:ALA:HB2	1.87	0.57
1:A:251:LEU:HD12	1:A:251:LEU:C	2.24	0.57
1:A:323:PRO:HD2	1:A:326:LEU:HD12	1.86	0.57
1:A:569:LEU:HG	1:A:573:PHE:HE2	1.70	0.57
1:B:329:SER:HB3	1:B:355:ARG:HE	1.69	0.57
1:B:464:ALA:CB	1:B:578:GLN:HG3	2.35	0.57
1:A:169:PHE:HE2	1:A:371:PHE:CD1	2.22	0.57
1:A:449:TYR:HB2	1:A:471:VAL:HG23	1.86	0.57
1:A:113:ARG:NH2	1:A:525:SER:OG	2.38	0.56
1:A:446:TYR:HB3	2:A:686:HOH:O	2.05	0.56
1:B:68:LEU:HG	1:B:78:ILE:HB	1.87	0.56
1:A:174:ARG:HH21	1:A:405:GLU:CD	2.08	0.56
1:A:342:ASP:CG	1:A:398:ARG:HH22	2.08	0.56
1:A:419:GLU:O	1:A:423:VAL:HG23	2.06	0.56
1:A:473:ASP:N	2:A:657:HOH:O	2.38	0.56
1:A:526:ARG:HD2	1:A:556:HIS:CG	2.40	0.56
1:B:127:THR:HA	1:B:135:ALA:O	2.06	0.56
1:B:304:THR:O	1:B:378:TRP:HB2	2.06	0.56
1:A:363:VAL:HA	1:A:440:TYR:O	2.05	0.56
1:B:420:LEU:HD22	1:B:453:CYS:SG	2.46	0.56
1:A:305:PRO:HA	1:A:378:TRP:CG	2.41	0.56
1:A:429:TRP:CD1	1:A:433:SER:HB2	2.40	0.56
1:B:240:PHE:HE1	1:B:263:ALA:HB2	1.70	0.56
1:B:361:PRO:HA	1:B:438:GLU:CG	2.34	0.56
1:B:516:LEU:HD12	1:B:517:ALA:H	1.70	0.56
1:A:519:ILE:HG12	1:A:549:HIS:CD2	2.40	0.56
1:B:99:ARG:CZ	1:B:102:GLU:HB3	2.36	0.56
1:B:198:SER:HB3	1:B:213:GLU:CD	2.26	0.56
1:B:455:LEU:HD22	1:B:514:GLU:HB2	1.88	0.56
1:A:393:VAL:HG11	1:A:426:ALA:HB1	1.88	0.56
1:A:441:ILE:HB	1:A:462:PHE:CD1	2.41	0.56
1:A:486:ARG:HH11	1:A:486:ARG:HG3	1.71	0.56
1:B:90:HIS:O	1:B:111:PRO:HA	2.05	0.56
1:B:517:ALA:HB2	1:B:574:PHE:CE1	2.41	0.56
1:A:305:PRO:HD3	1:A:322:LEU:HD12	1.88	0.56
1:B:456:THR:HG23	1:B:512:ILE:HD11	1.87	0.56
1:A:46:VAL:N	2:A:595:HOH:O	2.38	0.56
1:A:106:LEU:HA	2:A:698:HOH:O	2.04	0.56
1:A:164:ILE:O	1:A:179:THR:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PRO:HG3	1:A:403:TYR:CD2	2.41	0.56
1:A:458:LYS:O	1:A:460:GLY:N	2.39	0.56
1:B:271:VAL:O	1:B:277:ARG:HD2	2.06	0.56
1:B:331:ALA:HB3	1:B:352:GLU:CB	2.36	0.56
1:A:550:ILE:O	1:B:547:GLU:HA	2.06	0.55
1:A:219:ARG:HG3	1:A:219:ARG:HH11	1.71	0.55
1:A:445:SER:HA	1:A:469:ALA:O	2.06	0.55
1:A:520:HIS:O	1:A:550:ILE:HA	2.06	0.55
1:B:350:VAL:HG21	1:B:429:TRP:CH2	2.41	0.55
1:B:453:CYS:HB2	2:B:731:HOH:O	2.07	0.55
1:A:92:LEU:O	1:A:106:LEU:HG	2.04	0.55
1:A:178:PHE:CD1	1:A:178:PHE:C	2.80	0.55
1:A:563:ASP:OD2	2:A:585:HOH:O	2.18	0.55
1:B:471:VAL:HG23	2:B:685:HOH:O	2.05	0.55
1:A:25:TYR:HB3	1:A:38:VAL:HG11	1.88	0.55
1:A:426:ALA:HB2	2:A:651:HOH:O	2.06	0.55
1:B:123:ALA:HA	1:B:139:LEU:O	2.06	0.55
1:B:268:ARG:NH1	1:B:282:GLN:CD	2.60	0.55
1:B:326:LEU:HB3	2:B:794:HOH:O	2.05	0.55
1:B:455:LEU:CD2	1:B:514:GLU:HB2	2.37	0.55
1:A:399:GLY:O	1:A:408:ARG:HG3	2.06	0.55
1:A:478:TYR:HE1	1:A:486:ARG:O	1.90	0.55
1:A:499:ILE:HG23	1:A:503:ARG:HG3	1.89	0.55
1:A:532:LEU:HD13	1:A:532:LEU:C	2.26	0.55
1:A:541:ALA:C	1:A:543:GLY:H	2.09	0.55
1:B:51:TYR:CZ	1:B:53:GLY:HA2	2.42	0.55
1:A:379:ASP:OD1	1:A:381:PHE:N	2.38	0.55
1:A:474:TRP:CD1	1:A:500:MET:HA	2.42	0.55
1:B:59:LEU:HD22	2:B:727:HOH:O	2.07	0.55
1:B:255:PRO:O	1:B:257:GLY:N	2.39	0.55
1:B:496:SER:CB	2:B:619:HOH:O	2.52	0.55
1:A:579:ARG:HG2	1:A:580:GLU:HG3	1.88	0.55
1:B:169:PHE:CE2	1:B:175:VAL:HG22	2.40	0.55
1:B:246:THR:CG2	1:B:402:GLY:O	2.55	0.55
1:B:259:LEU:HD11	2:B:767:HOH:O	2.06	0.55
1:A:169:PHE:HE2	1:A:371:PHE:HD1	1.54	0.55
1:A:215:ALA:CB	1:A:406:GLU:HB2	2.35	0.55
1:A:418:GLY:O	1:A:421:GLU:HB2	2.07	0.55
1:A:550:ILE:HB	1:B:548:ALA:H	1.71	0.55
1:B:219:ARG:HG3	1:B:220:LEU:N	2.22	0.55
1:A:237:SER:HB3	1:A:276:GLU:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ASP:CG	1:A:542:ARG:HE	2.10	0.55
1:B:373:GLU:HB3	2:B:739:HOH:O	2.05	0.55
1:B:451:THR:HG21	1:B:466:VAL:C	2.27	0.55
1:A:173:GLY:O	1:A:408:ARG:NH1	2.38	0.55
1:A:449:TYR:HB2	1:A:471:VAL:CG2	2.36	0.55
1:A:472:VAL:HG21	1:A:535:LEU:HD13	1.88	0.55
1:A:159:ILE:HD12	1:A:164:ILE:HG13	1.89	0.54
1:A:269:SER:OG	1:A:285:HIS:CD2	2.60	0.54
1:A:563:ASP:HA	1:A:566:LYS:HB2	1.88	0.54
1:B:220:LEU:HG	1:B:240:PHE:CE2	2.43	0.54
1:B:250:TRP:CD2	1:B:287:ARG:HA	2.42	0.54
1:B:355:ARG:HG3	1:B:387:ALA:HA	1.88	0.54
1:B:406:GLU:HA	2:B:763:HOH:O	2.07	0.54
1:A:284:ASN:HB2	1:A:300:THR:HG23	1.89	0.54
1:A:519:ILE:HG22	1:A:567:ILE:HG22	1.89	0.54
1:B:90:HIS:CD2	1:B:114:ILE:H	2.25	0.54
1:B:300:THR:O	1:B:301:SER:HB2	2.06	0.54
1:B:357:PRO:O	1:B:360:GLY:HA3	2.07	0.54
1:B:359:PRO:HB3	1:B:434:GLY:O	2.07	0.54
1:B:458:LYS:O	1:B:461:LEU:HB2	2.07	0.54
1:A:322:LEU:HD22	1:A:323:PRO:O	2.07	0.54
1:B:35:LYS:HE2	1:B:52:ASP:OD2	2.07	0.54
1:B:52:ASP:C	1:B:54:GLY:H	2.11	0.54
1:B:411:ILE:HD12	1:B:419:GLU:HG2	1.87	0.54
1:A:307:ARG:HB2	1:A:318:LEU:O	2.08	0.54
1:A:346:VAL:HG13	1:A:407:TRP:CZ2	2.40	0.54
1:A:353:SER:O	1:A:354:GLY:C	2.45	0.54
1:A:220:LEU:HB3	1:A:233:LEU:HD12	1.89	0.54
1:A:549:HIS:HD1	1:B:549:HIS:CE1	2.25	0.54
1:B:91:ALA:HB1	1:B:105:ARG:NE	2.22	0.54
1:B:562:GLU:HG3	2:B:724:HOH:O	2.07	0.54
1:A:24:LYS:O	1:A:40:GLY:HA2	2.08	0.54
1:A:59:LEU:O	1:A:101:GLY:N	2.41	0.54
1:A:249:THR:HG22	1:A:250:TRP:HB3	1.88	0.54
1:A:175:VAL:HB	1:A:197:PHE:H	1.73	0.54
1:A:309:VAL:HG12	1:A:316:PRO:HB3	1.90	0.54
1:A:379:ASP:OD1	1:A:381:PHE:CD1	2.61	0.54
1:B:60:ASN:CG	2:B:679:HOH:O	2.46	0.54
1:B:171:GLY:C	1:B:173:GLY:N	2.61	0.54
1:B:376:ASP:CB	2:B:616:HOH:O	2.46	0.54
1:B:397:TYR:HD1	1:B:419:GLU:HB3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:O	1:A:107:GLU:N	2.40	0.54
1:B:245:PRO:HB2	1:B:263:ALA:HB1	1.90	0.54
1:B:323:PRO:CB	1:B:326:LEU:HD12	2.37	0.54
1:A:308:ILE:N	1:A:318:LEU:O	2.33	0.54
1:B:408:ARG:O	1:B:411:ILE:HG22	2.08	0.54
1:B:421:GLU:O	1:B:425:ALA:N	2.39	0.54
1:B:570:PRO:HA	2:B:653:HOH:O	2.07	0.54
1:B:164:ILE:HD11	1:B:182:LEU:HA	1.89	0.54
1:B:565:VAL:O	1:B:568:LEU:N	2.40	0.54
1:A:23:GLU:HG2	2:A:600:HOH:O	2.08	0.53
1:A:536:MET:HE1	1:A:550:ILE:HD11	1.89	0.53
1:A:578:GLN:O	1:A:579:ARG:C	2.46	0.53
1:B:30:VAL:N	1:B:289:VAL:HG11	2.23	0.53
1:B:205:GLY:O	1:B:206:MET:HB2	2.08	0.53
1:A:258:ARG:HD2	1:A:273:ILE:CG2	2.38	0.53
1:B:177:LEU:HD22	1:B:223:VAL:HG21	1.89	0.53
1:B:178:PHE:C	1:B:178:PHE:CD1	2.81	0.53
1:B:490:GLU:O	1:B:495:GLY:N	2.27	0.53
1:B:522:GLN:HB3	1:B:551:ILE:O	2.07	0.53
1:A:96:ASN:HD21	1:A:98:SER:HB2	1.73	0.53
1:A:175:VAL:CG2	1:A:196:SER:HB3	2.38	0.53
1:B:114:ILE:N	1:B:114:ILE:HD12	2.23	0.53
1:B:249:THR:N	1:B:262:VAL:O	2.42	0.53
1:A:37:LEU:HD12	1:A:49:TYR:O	2.08	0.53
1:A:292:ARG:O	1:A:294:LYS:HD2	2.08	0.53
1:A:334:ARG:NH2	1:A:350:VAL:HG11	2.22	0.53
1:A:579:ARG:HG2	1:A:580:GLU:N	2.22	0.53
1:A:46:VAL:O	1:A:64:ILE:HG12	2.09	0.53
1:A:115:LEU:O	1:A:116:SER:HB3	2.07	0.53
1:A:174:ARG:NH2	1:A:405:GLU:OE2	2.41	0.53
1:A:351:LEU:CD1	1:A:382:ALA:HB1	2.38	0.53
1:A:469:ALA:HA	1:A:520:HIS:CE1	2.44	0.53
1:B:92:LEU:C	1:B:106:LEU:HD12	2.29	0.53
1:B:195:GLY:HA3	1:B:213:GLU:O	2.08	0.53
1:A:22:VAL:HG21	1:A:323:PRO:HD3	1.90	0.53
1:A:442:MET:HG3	1:A:466:VAL:HB	1.89	0.53
1:A:456:THR:HG22	1:A:512:ILE:HG12	1.90	0.53
1:A:524:ASP:OD1	1:A:556:HIS:HB2	2.09	0.53
1:B:509:VAL:HA	1:B:512:ILE:CD1	2.35	0.53
1:A:58:LYS:HD3	2:A:736:HOH:O	2.08	0.53
1:A:62:GLU:HB2	1:A:81:ARG:NH2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HB2	2:A:677:HOH:O	2.08	0.53
1:A:379:ASP:OD1	1:A:381:PHE:HD1	1.92	0.53
1:B:423:VAL:HG21	1:B:450:MET:HG2	1.90	0.53
1:A:194:GLU:HB3	1:A:214:THR:HG22	1.91	0.53
1:A:348:THR:HG21	1:A:393:VAL:HG13	1.90	0.53
1:B:31:VAL:CG1	1:B:32:ASP:N	2.71	0.53
1:B:42:SER:OG	1:B:43:GLU:N	2.42	0.53
1:A:151:PRO:HB2	1:A:170:PHE:CD2	2.44	0.53
1:A:169:PHE:CE2	1:A:371:PHE:HD1	2.27	0.53
1:A:497:ARG:C	1:A:499:ILE:H	2.13	0.53
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.23	0.52
1:A:350:VAL:HA	2:A:652:HOH:O	2.09	0.52
1:A:84:SER:OG	1:A:87:ALA:HB3	2.10	0.52
1:A:125:VAL:HG13	1:A:137:TYR:O	2.09	0.52
1:B:493:THR:O	1:B:494:GLY:C	2.47	0.52
1:B:133:ARG:HD2	1:B:146:GLU:OE2	2.09	0.52
1:B:539:LEU:HD13	1:B:546:PHE:CD1	2.44	0.52
1:A:106:LEU:HD11	2:A:589:HOH:O	2.09	0.52
1:A:551:ILE:N	1:A:551:ILE:HD12	2.25	0.52
1:B:209:THR:O	1:B:210:ALA:HB2	2.09	0.52
1:B:366:VAL:HG12	2:B:588:HOH:O	2.07	0.52
1:A:198:SER:HB3	1:A:213:GLU:OE2	2.09	0.52
1:A:392:VAL:HG12	1:A:393:VAL:N	2.25	0.52
1:A:441:ILE:HB	1:A:462:PHE:CE1	2.45	0.52
1:A:442:MET:HE2	1:A:444:TYR:HE1	1.74	0.52
1:A:463:LYS:HB2	2:A:729:HOH:O	2.09	0.52
1:B:59:LEU:HA	1:B:100:PRO:HB3	1.90	0.52
1:B:325:ASP:HA	1:B:328:ARG:NE	2.24	0.52
1:B:579:ARG:C	1:B:581:ARG:N	2.59	0.52
1:A:132:ASP:O	1:A:133:ARG:HB3	2.09	0.52
1:A:415:PRO:HD3	1:A:492:LEU:O	2.08	0.52
1:B:246:THR:HG21	1:B:402:GLY:O	2.10	0.52
1:A:309:VAL:HG12	1:A:316:PRO:CB	2.39	0.52
1:A:353:SER:HB2	1:A:386:ALA:HA	1.92	0.52
1:B:501:ARG:O	1:B:507:ASN:OD1	2.27	0.52
1:A:304:THR:HG23	2:A:654:HOH:O	2.10	0.52
1:A:339:GLU:OE2	1:A:343:GLY:HA2	2.09	0.52
1:A:463:LYS:O	1:A:514:GLU:HB3	2.09	0.52
1:A:530:LYS:HB3	1:A:531:PRO:CD	2.28	0.52
1:B:159:ILE:CD1	1:B:164:ILE:HG23	2.39	0.52
1:B:472:VAL:HG23	1:B:532:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ALA:HB2	2:B:729:HOH:O	2.10	0.52
1:B:246:THR:HG22	1:B:265:ARG:HA	1.91	0.52
1:A:202:ILE:HG13	2:A:653:HOH:O	2.09	0.51
1:B:37:LEU:HD23	1:B:70:PRO:HG3	1.91	0.51
1:B:145:ARG:HD3	2:B:664:HOH:O	2.09	0.51
1:B:281:PRO:HG3	2:B:595:HOH:O	2.09	0.51
1:A:129:ALA:HB1	1:A:134:VAL:HG22	1.91	0.51
1:A:133:ARG:HD2	2:A:609:HOH:O	2.10	0.51
1:A:341:PHE:C	1:A:343:GLY:H	2.13	0.51
1:A:497:ARG:O	1:A:500:MET:N	2.43	0.51
1:A:471:VAL:HG11	1:A:474:TRP:CZ3	2.46	0.51
1:B:397:TYR:CD1	1:B:419:GLU:HB3	2.45	0.51
1:B:497:ARG:N	2:B:648:HOH:O	2.42	0.51
1:A:482:ASP:OD1	1:A:485:PHE:HD1	1.93	0.51
1:A:172:GLY:C	1:A:174:ARG:N	2.63	0.51
1:A:181:ASN:HB3	1:A:185:GLY:H	1.75	0.51
1:A:299:HIS:CG	1:A:300:THR:N	2.77	0.51
1:B:72:TYR:CE2	1:B:289:VAL:HG13	2.46	0.51
1:B:136:LEU:O	1:B:147:LEU:HB2	2.10	0.51
1:B:463:LYS:O	2:B:689:HOH:O	2.19	0.51
1:B:579:ARG:O	1:B:581:ARG:N	2.43	0.51
1:A:87:ALA:HA	1:A:523:ASN:O	2.11	0.51
1:A:202:ILE:HG22	1:A:203:SER:N	2.26	0.51
1:A:284:ASN:ND2	1:A:376:ASP:O	2.43	0.51
1:B:78:ILE:HD11	1:B:124:VAL:HG22	1.93	0.51
1:B:139:LEU:HD12	1:B:143:GLY:C	2.31	0.51
1:B:411:ILE:HD12	1:B:419:GLU:CG	2.41	0.51
1:B:487:ASN:O	1:B:491:GLN:HG3	2.10	0.51
1:A:27:LEU:HB3	2:A:605:HOH:O	2.10	0.51
1:A:286:GLY:O	1:A:287:ARG:C	2.48	0.51
1:B:225:PRO:HB2	2:B:738:HOH:O	2.11	0.51
1:A:399:GLY:HA2	1:A:408:ARG:O	2.10	0.51
1:A:350:VAL:HG12	1:A:351:LEU:N	2.26	0.51
1:B:344:SER:N	2:B:722:HOH:O	2.43	0.51
1:A:63:PRO:HB3	2:A:595:HOH:O	2.11	0.51
1:A:81:ARG:O	1:A:90:HIS:HA	2.11	0.51
1:A:174:ARG:HH21	1:A:405:GLU:CG	2.23	0.51
1:A:385:LEU:HB3	2:A:720:HOH:O	2.11	0.51
1:A:474:TRP:CB	1:A:500:MET:HB3	2.40	0.51
1:B:362:THR:CG2	1:B:363:VAL:H	2.23	0.51
1:B:401:THR:HG22	1:B:408:ARG:CD	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:MET:HE1	1:B:489:ILE:HD11	1.91	0.51
1:B:82:ASP:OD1	1:B:84:SER:OG	2.22	0.50
1:A:371:PHE:N	1:A:371:PHE:CD2	2.78	0.50
1:B:139:LEU:HD12	1:B:143:GLY:O	2.11	0.50
1:B:430:ALA:O	1:B:436:ALA:N	2.38	0.50
1:A:202:ILE:CG1	2:A:653:HOH:O	2.58	0.50
1:A:415:PRO:O	1:A:416:CYS:HB3	2.11	0.50
1:A:472:VAL:HG21	1:A:535:LEU:HD22	1.93	0.50
1:A:551:ILE:CG2	1:A:552:PRO:HD2	2.41	0.50
1:B:451:THR:O	2:B:615:HOH:O	2.18	0.50
1:B:476:GLU:HA	1:B:479:GLU:CD	2.31	0.50
1:B:482:ASP:HB2	2:B:604:HOH:O	2.12	0.50
1:A:29:GLY:O	1:A:37:LEU:HB3	2.11	0.50
1:A:207:LYS:HE2	1:A:224:ASP:HB2	1.93	0.50
1:A:569:LEU:O	1:A:573:PHE:CD2	2.65	0.50
1:B:109:VAL:CG2	1:B:139:LEU:HD22	2.41	0.50
1:B:314:GLY:HA3	2:B:595:HOH:O	2.09	0.50
1:B:353:SER:HB3	1:B:356:ALA:CB	2.38	0.50
1:A:160:ARG:NH1	1:A:203:SER:HA	2.27	0.50
1:A:268:ARG:HA	1:A:283:GLY:O	2.11	0.50
1:B:76:ARG:NH2	2:B:725:HOH:O	2.32	0.50
1:B:362:THR:OG1	1:B:391:HIS:HB2	2.11	0.50
1:B:35:LYS:HB2	1:B:50:LEU:HD22	1.93	0.50
1:B:56:THR:N	2:B:735:HOH:O	2.43	0.50
1:B:81:ARG:HB3	1:B:93:PHE:CE1	2.47	0.50
1:B:393:VAL:HB	2:B:775:HOH:O	2.11	0.50
1:B:476:GLU:O	1:B:480:LEU:HG	2.12	0.50
1:A:365:LEU:HB2	2:A:693:HOH:O	2.12	0.50
1:A:399:GLY:N	1:A:407:TRP:O	2.45	0.50
1:B:35:LYS:CG	1:B:52:ASP:OD1	2.60	0.50
1:B:250:TRP:CZ3	1:B:260:ALA:HB3	2.46	0.50
1:B:371:PHE:CE2	1:B:408:ARG:NH1	2.79	0.50
1:A:249:THR:HG22	1:A:250:TRP:N	2.25	0.50
1:A:294:LYS:O	1:A:296:VAL:HG23	2.12	0.50
1:A:366:VAL:HG12	1:A:367:HIS:O	2.12	0.50
1:B:34:ASP:O	1:B:35:LYS:HG2	2.10	0.50
1:B:455:LEU:CD1	1:B:516:LEU:HD13	2.42	0.50
1:A:94:LYS:HB3	1:A:106:LEU:HD21	1.94	0.50
1:A:413:GLY:HA2	1:A:493:THR:HA	1.93	0.50
1:A:308:ILE:O	1:A:317:LEU:N	2.44	0.49
1:A:536:MET:CE	1:A:550:ILE:HD11	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:HIS:C	1:B:510:ASP:N	2.64	0.49
1:A:441:ILE:HD13	1:A:441:ILE:C	2.31	0.49
1:A:529:LEU:CD1	1:A:550:ILE:HD12	2.33	0.49
1:B:268:ARG:HH12	1:B:282:GLN:CD	2.15	0.49
1:B:431:ARG:HG3	1:B:431:ARG:HH11	1.77	0.49
1:A:60:ASN:ND2	1:A:62:GLU:O	2.37	0.49
1:A:240:PHE:HD1	1:A:272:PHE:CD1	2.31	0.49
1:B:251:LEU:HD11	1:B:259:LEU:HD11	1.93	0.49
1:B:543:GLY:O	1:B:544:LYS:C	2.50	0.49
1:A:71:HIS:HB2	1:A:119:ASP:O	2.11	0.49
1:A:468:GLY:C	1:A:470:SER:N	2.61	0.49
1:A:522:GLN:HG2	1:A:552:PRO:HA	1.94	0.49
1:B:49:TYR:CA	1:B:57:VAL:O	2.54	0.49
1:B:405:GLU:HG3	1:B:409:LEU:HG	1.95	0.49
1:B:451:THR:HG21	1:B:466:VAL:O	2.12	0.49
1:A:68:LEU:HB2	1:A:78:ILE:HB	1.94	0.49
1:A:408:ARG:O	1:A:411:ILE:HG22	2.13	0.49
1:A:416:CYS:SG	1:A:416:CYS:O	2.70	0.49
1:B:153:PHE:CE1	1:B:488:PHE:HB2	2.45	0.49
1:B:311:LEU:HB3	1:B:312:PRO:HA	1.95	0.49
1:B:486:ARG:O	1:B:490:GLU:HG3	2.12	0.49
1:A:44:GLY:HA2	1:A:561:MET:N	2.22	0.49
1:B:243:TYR:CZ	1:B:270:ALA:HB2	2.47	0.49
1:B:431:ARG:HG3	1:B:431:ARG:NH1	2.28	0.49
1:A:87:ALA:O	1:A:525:SER:OG	2.24	0.49
1:A:160:ARG:HH22	1:A:204:PRO:HG3	1.78	0.49
1:A:309:VAL:HA	1:A:317:LEU:H	1.77	0.49
1:B:242:SER:C	1:B:244:ARG:H	2.15	0.49
1:B:365:LEU:HD23	1:B:394:MET:HG2	1.94	0.49
1:A:142:GLY:HA3	2:A:636:HOH:O	2.11	0.49
1:B:90:HIS:CG	1:B:114:ILE:HD13	2.46	0.49
1:A:174:ARG:NE	1:A:409:LEU:HD11	2.25	0.49
1:A:489:ILE:O	1:A:490:GLU:C	2.50	0.49
1:B:36:LEU:HD11	1:B:296:VAL:HG11	1.94	0.49
1:B:209:THR:HG23	1:B:233:LEU:HD12	1.95	0.49
1:A:124:VAL:N	1:A:139:LEU:O	2.38	0.49
1:A:224:ASP:OD1	1:A:225:PRO:HD2	2.12	0.49
1:A:475:GLU:OE1	1:A:497:ARG:HG3	2.13	0.49
1:B:65:ASN:HD21	1:B:82:ASP:HB2	1.77	0.49
1:B:280:ALA:CB	1:B:285:HIS:CE1	2.96	0.49
1:B:506:ILE:CD1	1:B:535:LEU:HA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:GLN:HG3	1:B:523:ASN:N	2.27	0.49
1:A:74:VAL:HG11	1:A:121:GLY:CA	2.43	0.48
1:A:240:PHE:CE1	1:A:245:PRO:HG3	2.47	0.48
1:A:305:PRO:HD2	2:A:654:HOH:O	2.11	0.48
1:B:71:HIS:HA	2:B:666:HOH:O	2.13	0.48
1:B:411:ILE:HD13	1:B:419:GLU:HG2	1.94	0.48
1:A:194:GLU:CB	1:A:212:LEU:HD21	2.38	0.48
1:A:277:ARG:HD2	1:A:278:VAL:H	1.77	0.48
1:B:239:ASP:HA	1:B:242:SER:OG	2.13	0.48
1:A:341:PHE:CG	1:A:342:ASP:N	2.82	0.48
1:A:579:ARG:NH1	1:A:579:ARG:CB	2.75	0.48
1:B:379:ASP:HB3	1:B:382:ALA:CB	2.43	0.48
1:B:459:PRO:HG3	2:B:605:HOH:O	2.13	0.48
1:B:516:LEU:HD21	1:B:518:LEU:HD21	1.94	0.48
1:A:136:LEU:HD11	1:A:156:VAL:HG22	1.96	0.48
1:A:194:GLU:OE2	1:A:219:ARG:NH2	2.47	0.48
1:A:274:ASP:C	1:A:276:GLU:H	2.17	0.48
1:B:68:LEU:HD12	1:B:78:ILE:CD1	2.43	0.48
1:B:453:CYS:N	2:B:731:HOH:O	2.46	0.48
1:A:563:ASP:HA	1:A:566:LYS:CB	2.43	0.48
1:B:40:GLY:HA3	1:B:49:TYR:HE1	1.79	0.48
1:B:272:PHE:CE2	1:B:277:ARG:HB2	2.48	0.48
1:B:445:SER:C	1:B:447:GLY:N	2.66	0.48
1:A:361:PRO:HB3	1:A:438:GLU:OE2	2.14	0.48
1:A:384:SER:O	1:A:387:ALA:HB3	2.13	0.48
1:B:68:LEU:HD12	1:B:124:VAL:HG13	1.95	0.48
1:A:26:SER:OG	1:A:28:GLN:NE2	2.46	0.48
1:A:192:SER:HB3	1:A:195:GLY:O	2.13	0.48
1:A:258:ARG:HB3	1:A:273:ILE:HG23	1.96	0.48
1:A:264:ARG:NE	1:A:373:GLU:OE2	2.45	0.48
1:A:374:ASP:N	1:A:396:ASN:OD1	2.35	0.48
1:B:376:ASP:HA	2:B:600:HOH:O	2.12	0.48
1:A:129:ALA:CB	1:A:484:ALA:HB2	2.43	0.48
1:A:330:ILE:HD12	1:A:330:ILE:N	2.29	0.48
1:A:452:LEU:HB3	1:A:505:PRO:HG2	1.95	0.48
1:A:549:HIS:ND1	1:A:570:PRO:HB3	2.29	0.48
1:B:28:GLN:HG3	1:B:67:VAL:HG21	1.96	0.48
1:B:449:TYR:N	2:B:685:HOH:O	2.47	0.48
1:B:519:ILE:HD13	1:B:567:ILE:O	2.13	0.48
1:A:173:GLY:O	1:A:408:ARG:NH2	2.47	0.48
1:A:174:ARG:NH2	1:A:195:GLY:HA2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HB	1:A:231:GLU:CG	2.43	0.48
1:A:414:ASP:CG	1:A:414:ASP:O	2.51	0.48
1:A:553:ASP:OD1	1:B:545:THR:CG2	2.61	0.48
1:B:365:LEU:HD11	1:B:381:PHE:HB3	1.96	0.48
1:B:367:HIS:CE1	1:B:400:SER:OG	2.67	0.48
1:B:442:MET:HG3	1:B:466:VAL:CG1	2.44	0.48
1:B:457:MET:C	1:B:459:PRO:HD2	2.34	0.48
1:B:468:GLY:HA2	1:B:519:ILE:O	2.13	0.48
1:A:497:ARG:C	1:A:499:ILE:N	2.67	0.48
1:B:38:VAL:CG1	1:B:308:ILE:HD13	2.44	0.48
1:B:282:GLN:NE2	2:B:660:HOH:O	2.46	0.48
1:B:294:LYS:HG2	2:B:705:HOH:O	2.13	0.48
1:B:411:ILE:HG12	1:B:492:LEU:HD11	1.95	0.48
1:B:458:LYS:N	1:B:459:PRO:CD	2.77	0.48
1:B:568:LEU:O	1:B:572:VAL:HG23	2.14	0.48
1:A:90:HIS:HD2	1:A:114:ILE:N	2.08	0.47
1:A:415:PRO:HG3	1:A:493:THR:HG22	1.95	0.47
1:A:474:TRP:HD1	1:A:500:MET:HA	1.79	0.47
1:A:569:LEU:HB3	1:A:570:PRO:CD	2.36	0.47
1:B:325:ASP:C	1:B:328:ARG:H	2.17	0.47
1:B:333:SER:HA	1:B:350:VAL:O	2.14	0.47
1:B:520:HIS:CB	2:B:744:HOH:O	2.62	0.47
1:A:372:ALA:O	1:A:373:GLU:HB3	2.14	0.47
1:A:521:PRO:CB	1:A:555:GLY:O	2.62	0.47
1:A:532:LEU:HD12	1:A:536:MET:HE3	1.96	0.47
1:B:406:GLU:HG2	1:B:410:LYS:CE	2.41	0.47
1:B:451:THR:HA	2:B:615:HOH:O	2.14	0.47
1:B:27:LEU:HD12	1:B:38:VAL:HG12	1.94	0.47
1:B:158:ASP:C	1:B:159:ILE:HD13	2.34	0.47
1:B:322:LEU:O	1:B:323:PRO:O	2.33	0.47
1:B:475:GLU:O	1:B:478:TYR:HB3	2.14	0.47
1:A:224:ASP:O	1:A:228:GLY:HA2	2.14	0.47
1:A:515:PRO:CA	2:A:613:HOH:O	2.47	0.47
1:B:212:LEU:CD2	1:B:219:ARG:HH12	2.12	0.47
1:B:550:ILE:N	1:B:550:ILE:HD12	2.29	0.47
1:A:309:VAL:CA	1:A:316:PRO:HA	2.41	0.47
1:B:70:PRO:HA	1:B:119:ASP:HB3	1.97	0.47
1:B:248:ILE:HD12	1:B:248:ILE:N	2.28	0.47
1:B:504:SER:O	1:B:506:ILE:N	2.48	0.47
1:B:520:HIS:CE1	2:B:618:HOH:O	2.67	0.47
1:B:551:ILE:HB	1:B:554:ALA:CB	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:LEU:O	1:B:390:PHE:N	2.45	0.47
1:B:477:MET:HA	1:B:528:PRO:HG3	1.96	0.47
1:A:104:GLN:NE2	2:A:699:HOH:O	2.47	0.47
1:A:219:ARG:HH12	1:A:221:VAL:CG1	2.27	0.47
1:A:254:LEU:HD11	1:A:295:LEU:HD21	1.96	0.47
1:A:430:ALA:HB1	1:A:436:ALA:HB2	1.97	0.47
1:A:468:GLY:O	1:A:469:ALA:C	2.53	0.47
1:B:112:MET:HB2	1:B:130:THR:HG22	1.97	0.47
1:B:250:TRP:CE3	1:B:287:ARG:HA	2.50	0.47
1:B:309:VAL:HG12	1:B:316:PRO:CA	2.45	0.47
1:B:477:MET:CA	2:B:756:HOH:O	2.58	0.47
1:B:480:LEU:CB	2:B:756:HOH:O	2.52	0.47
1:A:258:ARG:HD2	1:A:273:ILE:HG21	1.97	0.47
1:A:346:VAL:HG22	1:A:407:TRP:CZ2	2.50	0.47
1:A:367:HIS:HE1	1:A:396:ASN:HA	1.80	0.47
1:B:476:GLU:CG	1:B:531:PRO:HG3	2.45	0.47
1:B:495:GLY:O	1:B:496:SER:O	2.33	0.47
1:A:237:SER:O	1:A:275:GLY:HA3	2.14	0.47
1:A:267:GLY:CA	1:A:375:SER:HB2	2.45	0.47
1:A:452:LEU:HB2	2:A:709:HOH:O	2.14	0.47
1:B:445:SER:HA	1:B:469:ALA:O	2.15	0.47
1:B:472:VAL:HG23	2:B:683:HOH:O	2.14	0.47
1:A:62:GLU:HB2	1:A:81:ARG:HE	1.80	0.47
1:A:519:ILE:CG2	1:A:567:ILE:HG22	2.44	0.47
1:B:47:ASN:HB2	2:B:656:HOH:O	2.15	0.47
1:B:89:GLN:HA	1:B:112:MET:O	2.15	0.47
1:B:280:ALA:HB3	1:B:285:HIS:CE1	2.50	0.47
1:B:367:HIS:HD2	1:B:368:GLY:O	1.98	0.47
1:B:441:ILE:HD13	2:B:615:HOH:O	2.15	0.47
1:B:495:GLY:O	1:B:496:SER:C	2.54	0.47
1:A:151:PRO:HD2	1:A:170:PHE:CZ	2.49	0.46
1:A:366:VAL:HG13	1:A:397:TYR:CE2	2.50	0.46
1:B:141:GLY:C	1:B:143:GLY:H	2.18	0.46
1:B:431:ARG:HA	1:B:436:ALA:HB3	1.98	0.46
1:A:45:SER:CB	2:A:595:HOH:O	2.59	0.46
1:A:160:ARG:NH2	1:A:204:PRO:HG3	2.30	0.46
1:B:133:ARG:HD2	2:B:608:HOH:O	2.16	0.46
1:B:567:ILE:HD12	1:B:567:ILE:C	2.32	0.46
1:A:302:LEU:HG	1:A:376:ASP:OD1	2.15	0.46
1:A:305:PRO:O	1:A:306:PRO:C	2.52	0.46
1:A:532:LEU:O	1:A:536:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:GLY:H	1:B:352:GLU:HB2	1.80	0.46
1:B:520:HIS:CD2	1:B:521:PRO:HD2	2.32	0.46
1:A:88:GLU:HG3	1:A:113:ARG:NH1	2.29	0.46
1:A:270:ALA:HB3	2:A:588:HOH:O	2.15	0.46
1:A:399:GLY:CA	1:A:408:ARG:HA	2.46	0.46
1:B:41:PHE:HZ	1:B:558:ILE:HG22	1.80	0.46
1:B:134:VAL:HB	1:B:150:LEU:HB2	1.97	0.46
1:B:178:PHE:HB2	1:B:187:LEU:HD11	1.96	0.46
1:B:251:LEU:HD12	1:B:259:LEU:HD11	1.97	0.46
1:B:458:LYS:O	1:B:461:LEU:CB	2.63	0.46
1:A:172:GLY:C	1:A:174:ARG:H	2.18	0.46
1:A:486:ARG:HG3	1:A:486:ARG:NH1	2.29	0.46
1:A:510:ASP:HB2	2:A:607:HOH:O	2.16	0.46
1:B:160:ARG:HD2	1:B:202:ILE:CG2	2.46	0.46
1:A:93:PHE:HA	1:A:104:GLN:O	2.16	0.46
1:A:272:PHE:HD2	1:A:277:ARG:HA	1.80	0.46
1:A:398:ARG:HD3	1:A:410:LYS:HB3	1.97	0.46
1:B:51:TYR:CE2	1:B:53:GLY:HA2	2.51	0.46
1:B:88:GLU:HG2	1:B:113:ARG:HH12	1.74	0.46
1:B:323:PRO:HG2	1:B:326:LEU:CD1	2.43	0.46
1:A:138:ALA:HB2	1:A:147:LEU:CD2	2.38	0.46
1:A:222:THR:HG22	1:A:222:THR:O	2.16	0.46
1:A:240:PHE:CZ	1:A:245:PRO:HG3	2.51	0.46
1:A:265:ARG:HD3	2:A:598:HOH:O	2.15	0.46
1:A:579:ARG:CB	1:A:579:ARG:HH11	2.28	0.46
1:B:125:VAL:HA	1:B:138:ALA:HA	1.96	0.46
1:B:379:ASP:O	1:B:380:THR:C	2.53	0.46
1:A:277:ARG:HD2	1:A:278:VAL:N	2.31	0.46
1:A:444:TYR:O	1:A:445:SER:HB3	2.16	0.46
1:A:474:TRP:HZ3	1:A:477:MET:HE1	1.80	0.46
1:B:51:TYR:CE2	1:B:317:LEU:HB3	2.43	0.46
1:B:448:GLY:HA3	1:B:470:SER:HB3	1.97	0.46
1:B:464:ALA:HB2	1:B:578:GLN:HG3	1.98	0.46
1:B:577:THR:CB	2:B:784:HOH:O	2.57	0.46
1:A:354:GLY:C	1:A:356:ALA:H	2.18	0.46
1:A:574:PHE:O	1:A:578:GLN:HG2	2.15	0.46
1:B:30:VAL:CG2	1:B:290:LEU:O	2.64	0.46
1:B:75:GLY:O	1:B:96:ASN:OD1	2.34	0.46
1:B:347:PRO:HG2	1:B:396:ASN:CB	2.45	0.46
1:B:458:LYS:HB3	1:B:461:LEU:CD2	2.45	0.46
1:A:95:VAL:CG2	1:A:103:GLU:HG2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:SER:C	2:A:618:HOH:O	2.53	0.45
1:B:48:ALA:O	1:B:58:LYS:HA	2.17	0.45
1:B:235:LEU:HD13	1:B:274:ASP:C	2.37	0.45
1:B:251:LEU:HD11	1:B:259:LEU:HD21	1.98	0.45
1:B:279:GLU:HB2	1:B:312:PRO:O	2.15	0.45
1:B:334:ARG:NH2	1:B:429:TRP:HH2	2.14	0.45
1:A:47:ASN:HB3	1:A:60:ASN:OD1	2.17	0.45
1:A:178:PHE:CD1	1:A:178:PHE:O	2.70	0.45
1:A:420:LEU:HD11	1:A:454:ALA:HA	1.97	0.45
1:A:558:ILE:HD12	1:A:563:ASP:CB	2.31	0.45
1:B:178:PHE:HD2	2:B:706:HOH:O	1.99	0.45
1:B:307:ARG:HB2	1:B:319:GLU:CB	2.46	0.45
1:A:446:TYR:O	1:A:449:TYR:HB3	2.15	0.45
1:B:255:PRO:C	1:B:257:GLY:H	2.19	0.45
1:B:326:LEU:HD23	1:B:355:ARG:NH1	2.31	0.45
1:A:129:ALA:HA	1:A:134:VAL:HA	1.99	0.45
1:B:327:ARG:NH2	2:B:651:HOH:O	2.48	0.45
1:B:445:SER:C	1:B:447:GLY:H	2.19	0.45
1:B:482:ASP:O	1:B:486:ARG:HG3	2.17	0.45
1:A:475:GLU:HG2	1:A:500:MET:HB2	1.98	0.45
1:B:27:LEU:HD13	1:B:38:VAL:HG12	1.98	0.45
1:B:61:ARG:N	1:B:103:GLU:OE2	2.50	0.45
1:B:91:ALA:CB	1:B:105:ARG:NE	2.79	0.45
1:B:92:LEU:CD1	1:B:109:VAL:HG11	2.46	0.45
1:B:95:VAL:HG13	2:B:742:HOH:O	2.15	0.45
1:B:551:ILE:HD11	1:B:567:ILE:HG22	1.98	0.45
1:A:44:GLY:CA	1:A:561:MET:H	2.24	0.45
1:A:160:ARG:HD3	1:A:202:ILE:CG2	2.46	0.45
1:A:346:VAL:HG22	1:A:407:TRP:HH2	1.81	0.45
1:A:463:LYS:CB	2:A:729:HOH:O	2.63	0.45
1:A:579:ARG:HB2	1:A:579:ARG:CZ	2.46	0.45
1:B:164:ILE:O	1:B:179:THR:HA	2.16	0.45
1:B:233:LEU:HD22	1:B:235:LEU:HG	1.99	0.45
1:B:444:TYR:HA	1:B:468:GLY:O	2.17	0.45
1:A:34:ASP:O	1:A:291:TRP:NE1	2.50	0.45
1:A:251:LEU:HA	1:A:260:ALA:O	2.17	0.45
1:A:440:TYR:HE2	1:A:578:GLN:HB3	1.82	0.45
1:B:219:ARG:HD2	1:B:232:ASP:OD1	2.16	0.45
1:B:376:ASP:C	2:B:600:HOH:O	2.55	0.45
1:B:424:SER:CB	2:B:778:HOH:O	2.65	0.45
1:B:522:GLN:HE21	1:B:523:ASN:CG	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG12	1:A:23:GLU:N	2.32	0.45
1:A:68:LEU:HD12	1:A:78:ILE:CG2	2.35	0.45
1:A:239:ASP:O	1:A:243:TYR:N	2.48	0.45
1:A:370:PRO:HG3	1:A:411:ILE:HD13	1.99	0.45
1:A:421:GLU:OE2	1:A:458:LYS:CE	2.65	0.45
1:A:475:GLU:HA	1:A:500:MET:CE	2.47	0.45
1:A:547:GLU:HB2	1:B:550:ILE:O	2.17	0.45
1:B:29:GLY:HA3	1:B:289:VAL:HG21	1.99	0.45
1:B:398:ARG:NH2	1:B:407:TRP:HZ3	2.13	0.45
1:B:411:ILE:CG1	1:B:492:LEU:HD11	2.46	0.45
1:B:479:GLU:HG2	2:B:617:HOH:O	2.16	0.45
1:B:520:HIS:HD2	1:B:521:PRO:CD	2.21	0.45
1:B:520:HIS:HB2	2:B:744:HOH:O	2.17	0.45
1:A:125:VAL:O	1:A:126:PHE:HB3	2.16	0.45
1:A:262:VAL:O	1:A:262:VAL:HG12	2.17	0.45
1:A:263:ALA:O	1:A:269:SER:CB	2.65	0.45
1:A:335:LEU:HD13	1:A:349:TYR:CE1	2.51	0.45
1:B:226:ARG:NE	2:B:769:HOH:O	2.49	0.45
1:B:476:GLU:HA	1:B:479:GLU:CG	2.47	0.45
1:B:476:GLU:HA	1:B:479:GLU:HG3	1.99	0.45
1:B:565:VAL:O	1:B:567:ILE:N	2.50	0.45
1:B:569:LEU:CB	1:B:570:PRO:HD3	2.42	0.45
1:A:179:THR:H	1:A:187:LEU:CD1	2.30	0.45
1:B:415:PRO:O	1:B:503:ARG:HG3	2.17	0.45
1:B:448:GLY:HA3	1:B:470:SER:HA	1.99	0.45
1:A:163:LEU:HB3	1:A:202:ILE:HD13	1.98	0.44
1:A:417:GLY:H	1:A:419:GLU:CD	2.19	0.44
1:B:38:VAL:HG11	1:B:308:ILE:HD13	1.99	0.44
1:B:156:VAL:HG23	2:B:596:HOH:O	2.16	0.44
1:A:25:TYR:HB3	1:A:38:VAL:CG1	2.46	0.44
1:B:330:ILE:HG23	1:B:351:LEU:HD21	1.99	0.44
1:B:364:VAL:HA	1:B:393:VAL:O	2.17	0.44
1:A:224:ASP:HA	1:A:225:PRO:HD3	1.83	0.44
1:A:520:HIS:N	1:A:549:HIS:O	2.35	0.44
1:B:340:SER:CA	2:B:722:HOH:O	2.65	0.44
1:B:551:ILE:HG23	1:B:566:LYS:HD3	1.98	0.44
1:A:109:VAL:HA	2:A:728:HOH:O	2.17	0.44
1:A:217:GLU:HG2	1:A:218:ALA:H	1.82	0.44
1:A:393:VAL:HG22	2:A:652:HOH:O	2.16	0.44
1:A:424:SER:HB3	1:A:461:LEU:HD21	1.99	0.44
1:B:40:GLY:N	1:B:47:ASN:O	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:VAL:HG12	1:B:232:ASP:HA	2.00	0.44
1:B:401:THR:HG22	1:B:408:ARG:HD3	1.97	0.44
1:B:571:ALA:HA	2:B:723:HOH:O	2.16	0.44
1:A:304:THR:HA	1:A:305:PRO:HD3	1.82	0.44
1:A:488:PHE:HZ	2:A:672:HOH:O	2.00	0.44
1:A:509:VAL:O	1:A:509:VAL:HG12	2.17	0.44
1:B:226:ARG:HG3	1:B:226:ARG:HH11	1.82	0.44
1:B:240:PHE:CE1	1:B:263:ALA:HB2	2.52	0.44
1:B:340:SER:N	2:B:722:HOH:O	2.43	0.44
1:A:31:VAL:HB	1:A:74:VAL:O	2.16	0.44
1:A:219:ARG:NH1	1:A:221:VAL:HG12	2.33	0.44
1:A:367:HIS:HD2	1:A:372:ALA:HB3	1.81	0.44
1:A:499:ILE:O	1:A:503:ARG:HB2	2.17	0.44
1:A:576:ALA:O	1:A:579:ARG:HB3	2.18	0.44
1:B:135:ALA:HB2	2:B:608:HOH:O	2.17	0.44
1:B:239:ASP:HA	1:B:242:SER:HG	1.82	0.44
1:B:243:TYR:O	1:B:244:ARG:C	2.56	0.44
1:B:456:THR:HG22	1:B:512:ILE:CD1	2.47	0.44
1:A:379:ASP:OD1	1:A:379:ASP:C	2.56	0.44
1:A:451:THR:O	1:A:455:LEU:HG	2.18	0.44
1:B:59:LEU:HB3	2:B:727:HOH:O	2.17	0.44
1:B:301:SER:HA	1:B:376:ASP:O	2.18	0.44
1:B:371:PHE:HD2	1:B:408:ARG:HH11	1.61	0.44
1:A:51:TYR:CE2	1:A:53:GLY:HA2	2.53	0.44
1:A:374:ASP:CG	1:A:394:MET:HB3	2.39	0.44
1:A:442:MET:CE	1:A:444:TYR:HE1	2.31	0.44
1:B:465:GLY:O	1:B:516:LEU:HD12	2.18	0.44
1:B:549:HIS:CE1	2:B:686:HOH:O	2.70	0.44
1:A:72:TYR:OH	1:A:289:VAL:HG12	2.18	0.44
1:A:117:GLY:HA2	1:A:126:PHE:HA	2.00	0.44
1:A:430:ALA:HB3	1:A:439:LEU:HD11	2.00	0.44
1:A:440:TYR:HD2	1:A:464:ALA:HB3	1.82	0.44
1:A:475:GLU:CA	1:A:500:MET:HE2	2.48	0.44
1:B:523:ASN:ND2	1:B:553:ASP:CA	2.81	0.44
1:A:61:ARG:NH1	1:A:101:GLY:CA	2.74	0.43
1:A:174:ARG:NH2	1:A:405:GLU:HG2	2.33	0.43
1:A:195:GLY:HA3	1:A:213:GLU:O	2.18	0.43
1:A:309:VAL:HB	1:A:315:GLU:O	2.18	0.43
1:A:499:ILE:CD1	2:A:732:HOH:O	2.63	0.43
1:A:503:ARG:HA	2:A:601:HOH:O	2.17	0.43
1:B:48:ALA:N	2:B:679:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:VAL:HG21	1:B:159:ILE:HG12	1.99	0.43
1:B:264:ARG:HA	1:B:269:SER:HA	2.00	0.43
1:A:62:GLU:CB	1:A:81:ARG:HH21	2.31	0.43
1:B:86:GLY:CA	1:B:555:GLY:HA3	2.48	0.43
1:B:169:PHE:CZ	1:B:175:VAL:CG2	2.99	0.43
1:B:170:PHE:HD1	1:B:189:VAL:HG11	1.83	0.43
1:B:251:LEU:CD2	2:B:652:HOH:O	2.66	0.43
1:B:477:MET:HE2	1:B:489:ILE:HD11	2.00	0.43
1:A:79:LEU:HD11	1:A:95:VAL:HG21	1.99	0.43
1:A:165:ALA:HB2	2:A:653:HOH:O	2.16	0.43
1:A:438:GLU:HG3	1:A:440:TYR:HE1	1.83	0.43
1:A:565:VAL:O	1:A:569:LEU:HB2	2.18	0.43
1:B:198:SER:HB2	1:B:248:ILE:O	2.18	0.43
1:B:209:THR:CA	1:B:222:THR:HG22	2.48	0.43
1:B:210:ALA:O	1:B:211:GLY:C	2.55	0.43
1:B:270:ALA:HB1	1:B:277:ARG:CZ	2.48	0.43
1:B:431:ARG:NH2	2:B:714:HOH:O	2.47	0.43
1:B:472:VAL:CG2	1:B:532:LEU:HD22	2.48	0.43
1:B:487:ASN:HA	1:B:490:GLU:OE1	2.17	0.43
1:B:580:GLU:O	1:B:581:ARG:HB2	2.18	0.43
1:A:40:GLY:C	1:A:42:SER:N	2.72	0.43
1:A:130:THR:O	1:A:131:GLU:C	2.56	0.43
1:A:164:ILE:HD13	1:A:181:ASN:CA	2.47	0.43
1:A:248:ILE:N	1:A:248:ILE:HD12	2.33	0.43
1:A:469:ALA:HB1	1:A:556:HIS:CE1	2.54	0.43
1:A:469:ALA:HB1	1:A:556:HIS:ND1	2.32	0.43
1:B:224:ASP:HB3	1:B:227:ASP:OD1	2.18	0.43
1:B:487:ASN:O	1:B:487:ASN:OD1	2.37	0.43
1:A:277:ARG:NH1	1:A:277:ARG:HG2	2.33	0.43
1:A:366:VAL:HG11	1:A:450:MET:HG3	2.00	0.43
1:A:578:GLN:O	1:A:581:ARG:N	2.52	0.43
1:B:42:SER:HA	1:B:561:MET:CE	2.48	0.43
1:B:79:LEU:HD11	1:B:95:VAL:CG2	2.45	0.43
1:B:207:LYS:HG2	1:B:222:THR:HB	1.99	0.43
1:B:371:PHE:HA	1:B:399:GLY:O	2.19	0.43
1:B:414:ASP:OD2	1:B:418:GLY:N	2.30	0.43
1:B:493:THR:HA	2:B:629:HOH:O	2.18	0.43
1:A:33:GLY:H	1:A:73:GLY:HA2	1.83	0.43
1:A:74:VAL:HG11	1:A:121:GLY:HA3	2.00	0.43
1:A:421:GLU:O	1:A:424:SER:HB2	2.19	0.43
1:A:509:VAL:O	1:A:509:VAL:CG1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:ALA:HB3	1:B:352:GLU:C	2.38	0.43
1:B:472:VAL:HG21	1:B:532:LEU:HA	2.01	0.43
1:B:472:VAL:O	1:B:505:PRO:HD2	2.18	0.43
1:B:473:ASP:OD1	1:B:475:GLU:N	2.49	0.43
1:B:494:GLY:O	1:B:496:SER:N	2.51	0.43
1:B:522:GLN:HB3	1:B:550:ILE:HG22	1.99	0.43
1:B:523:ASN:HD21	1:B:553:ASP:HA	1.82	0.43
1:A:106:LEU:CD2	2:A:698:HOH:O	2.66	0.43
1:A:178:PHE:HB2	1:A:187:LEU:HD11	2.01	0.43
1:B:240:PHE:O	1:B:245:PRO:CD	2.67	0.43
1:B:419:GLU:O	1:B:423:VAL:HG23	2.19	0.43
1:A:77:VAL:HG23	1:A:97:THR:CG2	2.49	0.43
1:A:197:PHE:HD2	1:A:210:ALA:HB1	1.84	0.43
1:A:214:THR:C	1:A:216:ARG:N	2.70	0.43
1:A:381:PHE:O	1:A:385:LEU:HB2	2.18	0.43
1:A:460:GLY:O	1:A:461:LEU:C	2.57	0.43
1:B:137:TYR:CD1	1:B:137:TYR:N	2.86	0.43
1:B:209:THR:OG1	1:B:253:TYR:OH	2.32	0.43
1:B:246:THR:CG2	1:B:265:ARG:HA	2.49	0.43
1:B:299:HIS:CG	1:B:300:THR:N	2.86	0.43
1:B:300:THR:O	1:B:301:SER:CB	2.67	0.43
1:B:377:SER:N	2:B:600:HOH:O	2.51	0.43
1:B:520:HIS:CE1	1:B:529:LEU:HA	2.54	0.43
1:B:30:VAL:HG23	1:B:289:VAL:HG12	1.99	0.43
1:A:71:HIS:HB2	1:A:120:THR:HA	2.01	0.43
1:A:78:ILE:HG23	2:A:589:HOH:O	2.19	0.43
1:A:167:LEU:CD2	1:A:197:PHE:HB2	2.49	0.43
1:B:59:LEU:CD1	1:B:77:VAL:HG21	2.46	0.43
1:B:73:GLY:O	1:B:74:VAL:C	2.57	0.43
1:B:205:GLY:O	1:B:206:MET:CB	2.67	0.43
1:B:334:ARG:NH2	1:B:429:TRP:CH2	2.87	0.43
1:B:489:ILE:HG13	2:B:642:HOH:O	2.18	0.43
1:A:138:ALA:HB3	1:A:147:LEU:HD21	1.98	0.42
1:A:167:LEU:HD11	1:A:199:SER:HA	2.01	0.42
1:A:188:ARG:HG3	1:A:188:ARG:HH11	1.84	0.42
1:A:350:VAL:HG22	2:A:652:HOH:O	2.19	0.42
1:B:31:VAL:HG21	1:B:37:LEU:HD22	2.00	0.42
1:B:203:SER:O	1:B:206:MET:N	2.46	0.42
1:B:324:GLU:HA	1:B:324:GLU:OE1	2.19	0.42
1:A:32:ASP:CB	1:A:35:LYS:HD2	2.49	0.42
1:A:120:THR:HG22	1:A:120:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:SER:OG	1:B:28:GLN:NE2	2.51	0.42
1:B:50:LEU:CD1	1:B:59:LEU:HD21	2.48	0.42
1:B:218:ALA:HB1	1:B:248:ILE:HD12	1.97	0.42
1:B:401:THR:HG22	1:B:408:ARG:HD2	2.01	0.42
1:B:526:ARG:HH21	1:B:557:ALA:HB2	1.81	0.42
1:A:203:SER:CB	1:A:204:PRO:CD	2.97	0.42
1:A:288:VAL:CG1	1:A:295:LEU:HD22	2.49	0.42
1:A:351:LEU:HD12	1:A:382:ALA:HB1	2.00	0.42
1:B:84:SER:HB3	1:B:89:GLN:HB2	2.01	0.42
1:B:428:ARG:O	1:B:431:ARG:N	2.49	0.42
1:B:450:MET:HA	1:B:453:CYS:HB3	2.01	0.42
1:A:203:SER:HB2	1:A:204:PRO:CD	2.49	0.42
1:A:312:PRO:O	1:A:313:SER:C	2.58	0.42
1:A:342:ASP:N	1:A:342:ASP:OD1	2.50	0.42
1:A:440:TYR:HE2	1:A:578:GLN:CB	2.32	0.42
1:B:330:ILE:HB	2:B:720:HOH:O	2.19	0.42
1:B:536:MET:HA	2:B:678:HOH:O	2.19	0.42
1:A:35:LYS:HG2	1:A:52:ASP:OD2	2.20	0.42
1:A:96:ASN:HD22	1:A:99:ARG:HG3	1.84	0.42
1:A:196:SER:OG	1:A:405:GLU:OE2	2.36	0.42
1:B:123:ALA:CB	1:B:182:LEU:HD11	2.50	0.42
1:B:359:PRO:O	1:B:437:SER:HB3	2.19	0.42
1:B:574:PHE:CB	2:B:723:HOH:O	2.67	0.42
1:A:158:ASP:HB2	1:A:201:SER:HA	2.02	0.42
1:A:170:PHE:HB2	2:A:662:HOH:O	2.20	0.42
1:B:70:PRO:HB2	1:B:74:VAL:CG2	2.41	0.42
1:B:501:ARG:NH1	2:B:749:HOH:O	2.52	0.42
1:A:29:GLY:HA2	1:A:289:VAL:HG11	2.02	0.42
1:A:48:ALA:HB2	1:A:67:VAL:HG21	2.01	0.42
1:A:98:SER:C	1:A:100:PRO:HD3	2.39	0.42
1:A:152:GLY:O	1:A:153:PHE:C	2.57	0.42
1:A:359:PRO:HA	1:A:435:LEU:HA	2.02	0.42
1:A:393:VAL:CG1	1:A:426:ALA:HB1	2.49	0.42
1:A:532:LEU:CD1	1:A:536:MET:CE	2.98	0.42
1:A:579:ARG:CG	1:A:580:GLU:N	2.82	0.42
1:B:476:GLU:OE1	1:B:531:PRO:HA	2.20	0.42
1:A:371:PHE:CE1	1:A:408:ARG:NH1	2.88	0.42
1:B:392:VAL:HG12	1:B:394:MET:HG3	2.02	0.42
1:B:418:GLY:O	1:B:421:GLU:HB2	2.19	0.42
1:A:44:GLY:HA2	1:A:561:MET:HB3	2.01	0.42
1:A:84:SER:CB	1:A:87:ALA:HB3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:GLU:OE1	1:A:315:GLU:HA	2.18	0.42
1:A:469:ALA:HB1	1:A:556:HIS:HD1	1.85	0.42
1:B:79:LEU:N	1:B:93:PHE:O	2.43	0.42
1:B:209:THR:HA	1:B:222:THR:HG22	2.02	0.42
1:B:305:PRO:HA	1:B:306:PRO:HD3	1.92	0.42
1:B:428:ARG:O	1:B:429:TRP:C	2.58	0.42
1:B:443:GLY:HA2	2:B:601:HOH:O	2.19	0.42
1:A:212:LEU:HG	1:A:214:THR:HG23	2.01	0.42
1:A:367:HIS:N	2:A:584:HOH:O	2.53	0.42
1:B:76:ARG:HA	1:B:96:ASN:HA	2.01	0.42
1:B:133:ARG:NE	1:B:149:ARG:HH21	2.18	0.42
1:B:322:LEU:O	1:B:323:PRO:C	2.59	0.42
1:A:92:LEU:HB3	1:A:106:LEU:HD12	2.02	0.41
1:B:168:GLY:HA3	2:B:706:HOH:O	2.20	0.41
1:B:240:PHE:HD1	1:B:272:PHE:CD1	2.37	0.41
1:B:569:LEU:HD12	1:B:569:LEU:HA	1.83	0.41
1:A:264:ARG:HA	1:A:269:SER:HA	2.02	0.41
1:B:71:HIS:O	1:B:72:TYR:C	2.58	0.41
1:B:176:SER:HA	2:B:746:HOH:O	2.19	0.41
1:B:300:THR:OG1	1:B:301:SER:N	2.53	0.41
1:B:302:LEU:HD13	1:B:351:LEU:HD13	2.02	0.41
1:B:315:GLU:HA	1:B:316:PRO:HD2	1.75	0.41
1:B:520:HIS:HA	1:B:521:PRO:HD3	1.81	0.41
1:A:296:VAL:HA	2:A:670:HOH:O	2.20	0.41
1:A:532:LEU:CD1	1:A:536:MET:HE3	2.50	0.41
1:B:201:SER:HB3	2:B:652:HOH:O	2.20	0.41
1:B:227:ASP:OD1	1:B:227:ASP:N	2.42	0.41
1:B:264:ARG:HH11	1:B:264:ARG:HG2	1.85	0.41
1:B:419:GLU:OE2	1:B:420:LEU:N	2.45	0.41
1:A:373:GLU:HB2	1:A:396:ASN:OD1	2.20	0.41
1:B:457:MET:O	1:B:459:PRO:HD2	2.20	0.41
1:A:169:PHE:CE2	1:A:371:PHE:CD1	3.04	0.41
1:A:219:ARG:NH1	1:A:221:VAL:CG1	2.84	0.41
1:B:86:GLY:O	1:B:555:GLY:HA3	2.21	0.41
1:B:133:ARG:HE	1:B:133:ARG:HB3	1.50	0.41
1:B:291:TRP:O	1:B:292:ARG:HB2	2.19	0.41
1:B:309:VAL:HA	1:B:316:PRO:HA	2.02	0.41
1:B:397:TYR:CB	1:B:422:ASP:HB2	2.49	0.41
1:B:567:ILE:HD12	1:B:568:LEU:CA	2.47	0.41
1:B:569:LEU:HB3	1:B:570:PRO:CD	2.43	0.41
1:A:108:ALA:O	1:A:144:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:SER:CB	1:A:213:GLU:OE2	2.68	0.41
1:A:421:GLU:O	1:A:425:ALA:N	2.53	0.41
1:B:30:VAL:H	1:B:289:VAL:CG1	2.33	0.41
1:B:31:VAL:HG22	1:B:74:VAL:CG2	2.51	0.41
1:B:325:ASP:O	1:B:328:ARG:HB2	2.21	0.41
1:B:411:ILE:O	1:B:411:ILE:HG13	2.21	0.41
1:B:456:THR:HG22	1:B:512:ILE:HD11	2.00	0.41
1:A:25:TYR:HA	1:A:39:VAL:O	2.20	0.41
1:A:226:ARG:HA	1:A:226:ARG:HD3	1.93	0.41
1:A:569:LEU:H	1:A:570:PRO:CD	2.33	0.41
1:B:78:ILE:CD1	1:B:124:VAL:HG22	2.50	0.41
1:B:328:ARG:NH1	2:B:682:HOH:O	2.54	0.41
1:B:444:TYR:OH	1:B:521:PRO:HG2	2.21	0.41
1:A:26:SER:HA	2:A:725:HOH:O	2.21	0.41
1:A:367:HIS:CE1	1:A:396:ASN:HA	2.56	0.41
1:A:393:VAL:HA	2:A:652:HOH:O	2.21	0.41
1:A:551:ILE:HD13	1:A:567:ILE:HG22	2.03	0.41
1:B:125:VAL:HG13	1:B:137:TYR:O	2.20	0.41
1:B:263:ALA:O	1:B:269:SER:HA	2.21	0.41
1:B:476:GLU:CD	1:B:531:PRO:HG3	2.41	0.41
1:B:514:GLU:HA	1:B:515:PRO:HD3	1.90	0.41
1:A:158:ASP:CB	1:A:201:SER:HA	2.50	0.41
1:A:190:PHE:CD1	1:A:190:PHE:N	2.88	0.41
1:A:194:GLU:CB	1:A:214:THR:HG22	2.51	0.41
1:A:224:ASP:O	1:A:228:GLY:N	2.53	0.41
1:A:322:LEU:HB2	2:A:697:HOH:O	2.21	0.41
1:A:329:SER:HB2	1:A:387:ALA:HA	2.02	0.41
1:A:358:THR:HA	1:A:359:PRO:C	2.39	0.41
1:A:398:ARG:HB2	1:A:410:LYS:HB2	2.03	0.41
1:A:451:THR:HG21	1:A:466:VAL:C	2.42	0.41
1:A:562:GLU:O	1:A:565:VAL:N	2.52	0.41
1:B:29:GLY:HA2	1:B:289:VAL:HG11	2.03	0.41
1:B:31:VAL:CG1	1:B:32:ASP:H	2.34	0.41
1:B:145:ARG:NH1	2:B:624:HOH:O	2.53	0.41
1:B:272:PHE:HA	1:B:276:GLU:O	2.21	0.41
1:B:491:GLN:NE2	2:B:747:HOH:O	2.53	0.41
1:B:504:SER:C	1:B:506:ILE:H	2.24	0.41
1:B:522:GLN:NE2	2:B:663:HOH:O	2.53	0.41
1:B:522:GLN:OE1	1:B:552:PRO:HA	2.21	0.41
1:A:59:LEU:O	1:A:101:GLY:HA2	2.20	0.41
1:A:119:ASP:OD1	1:A:120:THR:N	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ALA:HB1	1:A:277:ARG:NE	2.36	0.41
1:A:309:VAL:CG1	1:A:316:PRO:HA	2.46	0.41
1:A:476:GLU:C	1:A:478:TYR:N	2.74	0.41
1:B:77:VAL:O	1:B:94:LYS:HA	2.20	0.41
1:B:156:VAL:CG1	1:B:159:ILE:HD11	2.51	0.41
1:B:280:ALA:HB1	1:B:285:HIS:CE1	2.56	0.41
1:B:357:PRO:O	1:B:360:GLY:CA	2.69	0.41
1:B:511:ARG:NH1	2:B:605:HOH:O	2.37	0.41
1:B:520:HIS:O	1:B:550:ILE:HA	2.21	0.41
1:B:534:ARG:HD3	1:B:534:ARG:HA	1.80	0.41
1:B:538:GLU:O	1:B:541:ALA:N	2.54	0.41
1:A:136:LEU:CD1	1:A:156:VAL:HG22	2.51	0.40
1:A:413:GLY:H	1:A:492:LEU:C	2.24	0.40
1:A:474:TRP:CZ3	1:A:477:MET:HE1	2.56	0.40
1:A:520:HIS:HA	1:A:521:PRO:HD3	1.80	0.40
1:A:521:PRO:HG2	1:A:555:GLY:O	2.21	0.40
1:B:93:PHE:CD1	1:B:93:PHE:N	2.89	0.40
1:B:364:VAL:CG1	1:B:395:PRO:HD3	2.51	0.40
1:B:453:CYS:CB	2:B:731:HOH:O	2.66	0.40
1:A:95:VAL:O	1:A:95:VAL:HG12	2.22	0.40
1:A:163:LEU:HD23	1:A:202:ILE:HD13	2.03	0.40
1:A:249:THR:HB	1:A:262:VAL:O	2.21	0.40
1:A:284:ASN:ND2	1:A:376:ASP:C	2.75	0.40
1:B:95:VAL:HB	2:B:727:HOH:O	2.20	0.40
1:B:199:SER:OG	1:B:251:LEU:HB3	2.22	0.40
1:B:210:ALA:HA	1:B:251:LEU:CD2	2.51	0.40
1:B:278:VAL:CG1	1:B:312:PRO:HB3	2.49	0.40
1:B:397:TYR:HB2	1:B:422:ASP:HB2	2.03	0.40
1:B:440:TYR:CZ	1:B:463:LYS:HD3	2.56	0.40
1:B:567:ILE:HA	2:B:594:HOH:O	2.21	0.40
1:A:117:GLY:HA3	1:A:126:PHE:CB	2.51	0.40
1:A:147:LEU:HD22	2:A:695:HOH:O	2.21	0.40
1:A:219:ARG:HG3	1:A:219:ARG:NH1	2.36	0.40
1:A:428:ARG:CG	2:A:622:HOH:O	2.58	0.40
1:A:497:ARG:HD3	1:A:501:ARG:HE	1.85	0.40
1:B:371:PHE:CD2	1:B:408:ARG:NH1	2.79	0.40
1:B:379:ASP:HB3	1:B:382:ALA:HB3	2.03	0.40
1:B:398:ARG:HG2	1:B:419:GLU:HA	2.02	0.40
1:B:429:TRP:O	1:B:431:ARG:N	2.54	0.40
1:A:23:GLU:H	1:A:23:GLU:HG3	1.69	0.40
1:A:188:ARG:HH11	1:A:188:ARG:CG	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LEU:O	1:A:424:SER:N	2.54	0.40
1:B:60:ASN:O	1:B:61:ARG:HG2	2.21	0.40
1:B:432:GLU:HG3	2:B:759:HOH:O	2.21	0.40
1:B:444:TYR:O	1:B:447:GLY:N	2.50	0.40
1:A:98:SER:O	1:A:100:PRO:HD3	2.21	0.40
1:A:305:PRO:CD	1:A:322:LEU:HD12	2.50	0.40
1:A:444:TYR:CD1	1:A:444:TYR:N	2.90	0.40
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.93	0.40
1:B:131:GLU:OE2	1:B:131:GLU:O	2.40	0.40
1:B:133:ARG:CD	2:B:608:HOH:O	2.70	0.40
1:B:266:GLU:HA	1:B:403:TYR:CE2	2.57	0.40
1:B:281:PRO:HB2	1:B:299:HIS:CE1	2.57	0.40
1:B:334:ARG:HD2	2:B:661:HOH:O	2.22	0.40
1:B:385:LEU:HD11	1:B:442:MET:CE	2.51	0.40
1:B:520:HIS:O	1:B:550:ILE:HG23	2.21	0.40
1:B:521:PRO:HA	1:B:554:ALA:HB3	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
1	A	558/562 (99%)	445 (80%)	90 (16%)	23 (4%)	3 6
1	B	559/562 (100%)	432 (77%)	96 (17%)	31 (6%)	2 3
All	All	1117/1124 (99%)	877 (78%)	186 (17%)	54 (5%)	2 4

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	72	TYR

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Mol	Chain	Res	Type
1	A	563	ASP
1	B	206	MET
1	B	232	ASP
1	B	371	PHE
1	B	496	SER
1	A	106	LEU
1	A	321	GLY
1	A	354	GLY
1	A	371	PHE
1	A	498	GLU
1	A	543	GLY
1	A	568	LEU
1	B	45	SER
1	B	60	ASN
1	B	107	GLU
1	B	172	GLY
1	B	187	LEU
1	B	210	ALA
1	B	211	GLY
1	B	256	ASP
1	B	580	GLU
1	A	42	SER
1	A	216	ARG
1	B	323	PRO
1	B	498	GLU
1	B	505	PRO
1	B	522	GLN
1	B	544	LYS
1	A	116	SER
1	B	61	ARG
1	B	74	VAL
1	B	121	GLY
1	B	122	GLU
1	B	380	THR
1	B	430	ALA
1	B	560	THR
1	B	562	GLU
1	A	31	VAL
1	A	32	ASP
1	A	276	GLU
1	A	579	ARG
1	B	292	ARG

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Mol	Chain	Res	Type
1	A	430	ALA
1	B	301	SER
1	B	417	GLY
1	A	54	GLY
1	A	64	ILE
1	A	142	GLY
1	A	460	GLY
1	A	515	PRO
1	B	306	PRO
1	B	472	VAL

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	448/449 (100%)	418 (93%)	30 (7%)	16	37
1	B	448/449 (100%)	417 (93%)	31 (7%)	15	35
All	All	896/898 (100%)	835 (93%)	61 (7%)	16	36

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	56	THR
1	A	71	HIS
1	A	81	ARG
1	A	139	LEU
1	A	177	LEU
1	A	178	PHE
1	A	181	ASN
1	A	183	SER
1	A	191	ASP
1	A	201	SER
1	A	216	ARG
1	A	233	LEU

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Mol	Chain	Res	Type
1	A	250	TRP
1	A	285	HIS
1	A	301	SER
1	A	322	LEU
1	A	344	SER
1	A	345	ARG
1	A	419	GLU
1	A	435	LEU
1	A	441	ILE
1	A	444	TYR
1	A	453	CYS
1	A	461	LEU
1	A	522	GLN
1	A	552	PRO
1	A	559	ASN
1	A	563	ASP
1	A	579	ARG
1	B	41	PHE
1	B	56	THR
1	B	83	VAL
1	B	99	ARG
1	B	133	ARG
1	B	137	TYR
1	B	162	ASP
1	B	178	PHE
1	B	219	ARG
1	B	222	THR
1	B	236	PRO
1	B	256	ASP
1	B	304	THR
1	B	315	GLU
1	B	322	LEU
1	B	327	ARG
1	B	328	ARG
1	B	336	VAL
1	B	341	PHE
1	B	358	THR
1	B	384	SER
1	B	411	ILE
1	B	419	GLU
1	B	428	ARG
1	B	445	SER

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Mol	Chain	Res	Type
1	B	456	THR
1	B	482	ASP
1	B	497	ARG
1	B	522	GLN
1	B	560	THR
1	B	568	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	90	HIS
1	A	96	ASN
1	A	104	GLN
1	A	284	ASN
1	A	285	HIS
1	A	523	ASN
1	B	28	GLN
1	B	65	ASN
1	B	90	HIS
1	B	96	ASN
1	B	104	GLN
1	B	284	ASN
1	B	299	HIS
1	B	367	HIS
1	B	396	ASN
1	B	507	ASN
1	B	520	HIS
1	B	522	GLN
1	B	523	ASN

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 monosaccharides 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)

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	560/562 (99%)	-0.10	4 (0%)	87	89	7, 26, 44, 73	0
1	B	561/562 (99%)	0.13	9 (1%)	72	74	9, 32, 51, 71	0
All	All	1121/1124 (99%)	0.02	13 (1%)	79	80	7, 28, 49, 73	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	295	LEU	3.9
1	A	558	ILE	3.9
1	A	325	ASP	2.9
1	B	261	VAL	2.8
1	B	296	VAL	2.7
1	B	558	ILE	2.7
1	B	579	ARG	2.6
1	A	320	GLY	2.6
1	A	321	GLY	2.1
1	B	262	VAL	2.1
1	B	235	LEU	2.1
1	B	26	SER	2.1
1	B	218	ALA	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.