Full wwPDB X-ray Structure Validation Report ⓘ

Aug 15, 2023 – 09:17 PM EDT

PDB ID	:	1XDO
Title	:	Crystal Structure of Escherichia coli Polyphosphate Kinase
Authors	:	Zhu, Y.; Huang, W.; Lee, S.S.; Xu, W.
Deposited on	:	2004-09-07
Resolution	:	3.00 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 ⓘ 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 ⓘ) were used in the production of this report:

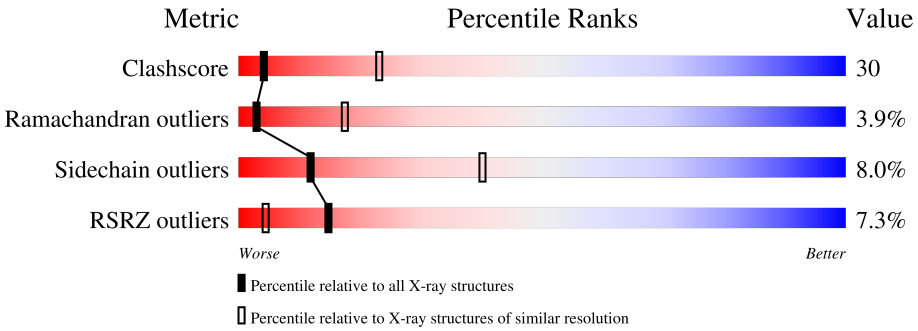
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	687	7% 51% 42% 7%
1	B	687	8% 50% 43% 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 11234 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 Polyphosphate kinase.

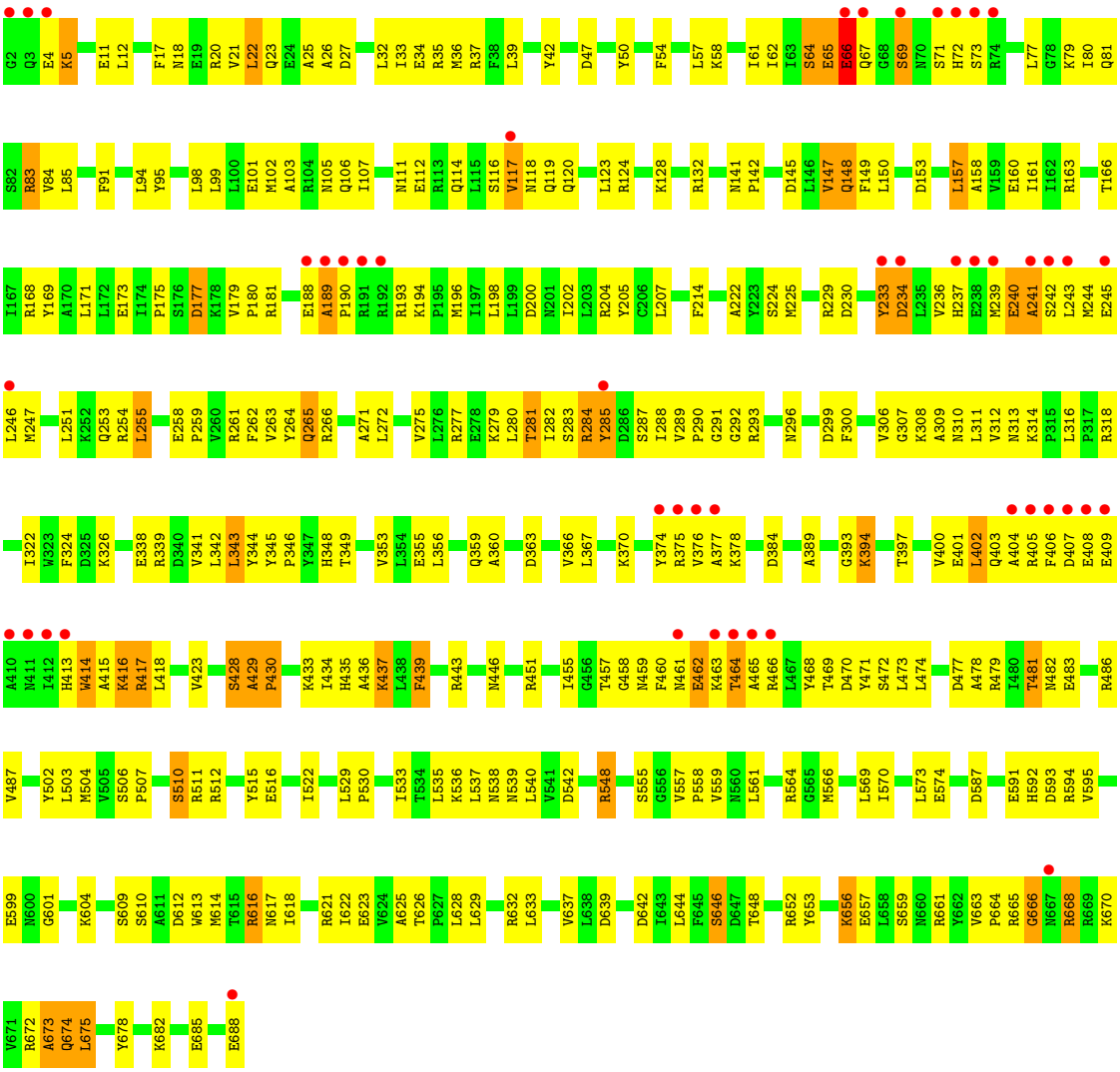
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5617	3568	1008	1025	16			
1	B	687	Total	C	N	O	S	0	0	0
			5617	3568	1008	1025	16			

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.

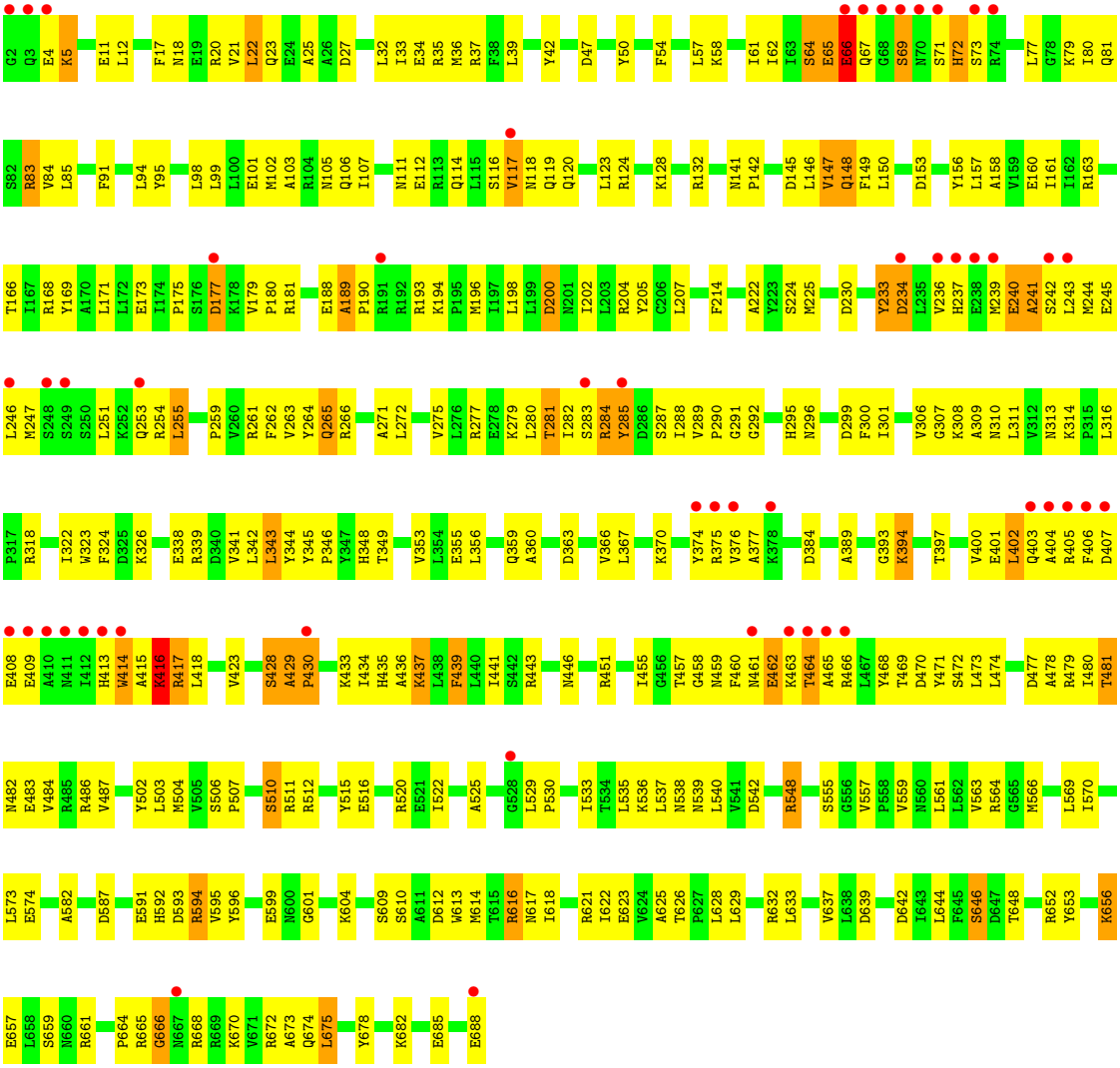
• Molecule 1: Polyphosphate kinase

Chain A:



• Molecule 1: Polyphosphate kinase

Chain B:


G2 Q3 E4 K5 E11 L12 F17 N18 E19 R20 V21 L22 Q23 E24 A25 A26 D27 L32 I33 E34 R35 M36 R37 F38 L39 Y42 D47 Y50 F54 L57 K58 I61 I62 I63 S64 E65 E66 Q67 G68 S69 N70 S71 H72 S73 R74 L77 G78 K79 I80 Q81
S82 R83 V84 L85 F91 L94 Y95 L98 L99 L100 E101 M102 A103 R104 N105 Q106 I107 N111 E112 R113 Q114 L115 S116 V117 N118 Q119 Q120 L123 R124 K128 R132 N141 P142 D145 L146 V147 Q148 F149 L150 D153 Y156 L157 A158 V159 E160 I161 I162 R163
T166 I167 R168 Y169 A170 L171 L172 E173 I174 P175 S176 D177 K178 V179 P180 R181 E188 A189 P190 R191 R192 R193 K194 P195 M196 I197 L198 L199 D200 N201 I202 L203 R204 Y205 G206 L207 F214 A222 Y223 S224 M225 D230 Y233 D234 L235 V236 H237 E238 M239 E240 A241 S242 L243 M244 E245
L246 M247 S248 S249 S250 L251 K252 Q253 R254 L255 P259 V260 R261 F262 V263 Y264 Q265 R266 A271 L272 V275 L276 R277 E278 K279 L280 T281 I282 S283 R284 Y285 D286 S287 I288 V289 P290 G291 G292 H295 N296 D299 F300 I301 V306 G307 K308 A309 N310 L311 V312 N313 K314 P315 L316
P317 R318 I322 W323 F324 D325 K326 E338 R339 D340 V341 L342 L343 Y344 Y345 P346 Y347 H348 T349 V353 L354 E355 L356 Q359 A360 D363 V366 L367 K370 Y374 R375 V376 A377 K378 D384 A389 G393 K394 T397 V400 E401 L402 Q403 A404 R405 F406 D407
E408 E409 A410 N411 I412 H413 W414 A415 K416 R417 L418 V423 S428 A429 P430 K433 I434 H435 A436 K437 L438 F439 L440 I441 S442 R443 N446 R451 I455 C456 T457 G458 N459 F460 N461 E462 K463 T464 A465 R466 L467 Y468 T469 D470 Y471 S472 L473 L474 D477 A478 R479 I480 T481
N482 E483 V484 R485 R486 V487 Y502 L503 M504 V505 S506 P507 S510 R511 R512 Y515 E516 R520 E521 I522 A525 G528 L529 P530 I533 T534 L535 K536 L537 N538 N539 L540 V541 D542 R548 S555 G556 V557 P558 V559 N560 L561 L562 V563 R564 G565 M566 L569 I570
L573 E574 A582 D587 E591 H592 D593 R594 V595 Y596 E599 N600 G601 K604 S609 S610 A611 D612 W613 M614 T615 R616 N617 I618 R621 I622 E623 V624 A625 T626 P627 L628 L629 R632 L633 V637 L638 D639 D642 I643 L644 F645 S646 D647 T648 R652 Y653 K656
E657 L658 S659 N660 R661 P664 R665 G666 N667 R668 R669 K670 V671 R672 A673 Q674 L675 Y678 K682 E685 E688

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	154.00Å 154.00Å 155.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.79 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.00-3.00) 86.2 (19.79-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.31 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.273 0.267 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k 0.017 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	11234	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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

5.1 Standard geometry

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	0.45	0/5735	0.69	1/7772 (0.0%)
1	B	0.46	0/5735	0.70	2/7772 (0.0%)
All	All	0.46	0/11470	0.69	3/15544 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	595	VAL	CA-CB-CG2	5.36	118.94	110.90
1	A	595	VAL	CA-CB-CG2	5.29	118.84	110.90
1	B	596	TYR	CB-CG-CD2	5.03	124.02	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5617	0	5456	326	0
1	B	5617	0	5456	333	0
All	All	11234	0	10912	656	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 30.

All (656) 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:A:594:ARG:HD3	1:A:612:ASP:OD1	1.47	1.13
1:B:461:ASN:HB3	1:B:464:THR:HB	1.31	1.09
1:A:437:LYS:HG2	1:A:459:ASN:HA	1.14	1.06
1:B:437:LYS:HG2	1:B:459:ASN:HA	1.12	1.06
1:A:402:LEU:HD23	1:A:402:LEU:H	1.20	1.06
1:A:461:ASN:HB3	1:A:464:THR:HB	1.34	1.06
1:B:437:LYS:HZ2	1:B:459:ASN:HB3	1.16	1.06
1:B:376:VAL:HG12	1:B:460:PHE:HB2	1.35	1.05
1:B:402:LEU:HD23	1:B:402:LEU:H	1.22	1.04
1:A:376:VAL:HG12	1:A:460:PHE:HB2	1.34	1.02
1:A:318:ARG:HH22	1:A:465:ALA:HB1	1.25	1.01
1:A:437:LYS:HZ2	1:A:459:ASN:HB3	1.19	1.01
1:B:318:ARG:HH22	1:B:465:ALA:HB1	1.23	0.99
1:A:436:ALA:C	1:A:437:LYS:HD2	1.84	0.98
1:B:436:ALA:C	1:B:437:LYS:HD2	1.86	0.95
1:A:344:TYR:H	1:A:348:HIS:HD2	1.10	0.95
1:A:470:ASP:OD2	1:A:592:HIS:HB3	1.66	0.94
1:B:470:ASP:OD2	1:B:592:HIS:HB3	1.68	0.93
1:B:111:ASN:H	1:B:114:GLN:HE21	1.11	0.93
1:B:284:ARG:HG3	1:B:285:TYR:H	1.34	0.92
1:B:240:GLU:HB3	1:B:244:MET:H	1.35	0.92
1:A:111:ASN:H	1:A:114:GLN:HE21	1.11	0.92
1:A:240:GLU:HB3	1:A:244:MET:H	1.34	0.91
1:B:665:ARG:HH21	1:B:670:LYS:HG3	1.36	0.91
1:B:344:TYR:H	1:B:348:HIS:HD2	1.11	0.91
1:A:408:GLU:HG3	1:A:409:GLU:H	1.38	0.89
1:A:548:ARG:HG2	1:A:548:ARG:HH11	1.34	0.89
1:B:548:ARG:HG2	1:B:548:ARG:HH11	1.35	0.88
1:A:264:TYR:CZ	1:A:290:PRO:HB3	2.09	0.88
1:A:12:LEU:HD22	1:A:83:ARG:NH1	1.88	0.88
1:B:12:LEU:HD22	1:B:83:ARG:NH1	1.88	0.88
1:B:429:ALA:HB1	1:B:430:PRO:HD2	1.56	0.87
1:B:408:GLU:HG3	1:B:409:GLU:H	1.39	0.87
1:A:284:ARG:HG3	1:A:285:TYR:H	1.35	0.87
1:A:429:ALA:HB1	1:A:430:PRO:HD2	1.57	0.86
1:A:437:LYS:NZ	1:A:459:ASN:HB3	1.90	0.86
1:A:537:LEU:HA	1:A:594:ARG:HG2	1.54	0.86
1:B:437:LYS:HE3	1:B:458:GLY:C	1.96	0.85
1:A:284:ARG:HG3	1:A:285:TYR:HD1	1.41	0.85
1:A:665:ARG:HH21	1:A:670:LYS:HG3	1.40	0.84
1:B:437:LYS:NZ	1:B:459:ASN:HB3	1.91	0.84
1:B:284:ARG:HG3	1:B:285:TYR:HD1	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:MET:HE1	1:B:306:VAL:HG21	1.59	0.84
1:B:264:TYR:CZ	1:B:290:PRO:HB3	2.13	0.84
1:A:437:LYS:HE3	1:A:458:GLY:C	1.98	0.83
1:B:594:ARG:HD3	1:B:612:ASP:OD1	1.77	0.83
1:A:437:LYS:HG2	1:A:459:ASN:CA	2.05	0.82
1:A:458:GLY:HA3	1:A:470:ASP:OD1	1.79	0.81
1:B:458:GLY:HA3	1:B:470:ASP:OD1	1.80	0.81
1:A:196:MET:HE1	1:A:306:VAL:HG21	1.63	0.81
1:A:464:THR:O	1:A:468:TYR:HB2	1.82	0.80
1:B:64:SER:HB3	1:B:69:SER:HB3	1.64	0.80
1:B:437:LYS:HG2	1:B:459:ASN:CA	2.03	0.80
1:A:360:ALA:HA	1:A:366:VAL:HG21	1.65	0.79
1:A:65:GLU:HA	1:A:69:SER:OG	1.81	0.79
1:A:32:LEU:HD13	1:A:101:GLU:OE2	1.83	0.78
1:A:437:LYS:CG	1:A:459:ASN:HA	2.08	0.78
1:A:242:SER:O	1:A:246:LEU:HG	1.82	0.78
1:B:116:SER:O	1:B:120:GLN:HG3	1.82	0.78
1:A:116:SER:O	1:A:120:GLN:HG3	1.82	0.78
1:B:242:SER:O	1:B:246:LEU:HG	1.83	0.78
1:B:179:VAL:HG13	1:B:180:PRO:HD2	1.65	0.77
1:B:464:THR:O	1:B:468:TYR:HB2	1.84	0.77
1:B:65:GLU:O	1:B:67:GLN:N	2.17	0.77
1:B:402:LEU:HD23	1:B:402:LEU:N	1.99	0.77
1:B:65:GLU:HA	1:B:69:SER:OG	1.84	0.77
1:A:65:GLU:O	1:A:67:GLN:N	2.17	0.76
1:B:32:LEU:HD13	1:B:101:GLU:OE2	1.85	0.76
1:A:402:LEU:HD23	1:A:402:LEU:N	1.98	0.76
1:B:437:LYS:CG	1:B:459:ASN:HA	2.06	0.76
1:A:179:VAL:HG13	1:A:180:PRO:HD2	1.67	0.76
1:A:116:SER:OG	1:A:119:GLN:HG3	1.86	0.76
1:A:64:SER:HB3	1:A:69:SER:HB3	1.65	0.75
1:B:665:ARG:NH2	1:B:670:LYS:HG3	2.02	0.75
1:B:360:ALA:HA	1:B:366:VAL:HG21	1.67	0.75
1:A:112:GLU:HB2	1:A:205:TYR:HB2	1.69	0.74
1:B:111:ASN:N	1:B:114:GLN:HE21	1.86	0.74
1:A:181:ARG:HH12	1:A:296:ASN:HB2	1.53	0.74
1:B:537:LEU:HA	1:B:594:ARG:HG2	1.69	0.73
1:B:112:GLU:HB2	1:B:205:TYR:HB2	1.70	0.73
1:A:237:HIS:HB2	1:A:244:MET:SD	2.29	0.73
1:A:266:ARG:NH1	1:A:291:GLY:HA2	2.03	0.73
1:A:224:SER:H	1:A:265:GLN:NE2	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:SER:OG	1:B:119:GLN:HG3	1.89	0.73
1:A:307:GLY:HA3	1:A:311:LEU:HD12	1.71	0.72
1:A:429:ALA:HB1	1:A:430:PRO:CD	2.19	0.72
1:B:429:ALA:HB1	1:B:430:PRO:CD	2.18	0.72
1:B:307:GLY:HA3	1:B:311:LEU:HD12	1.72	0.72
1:B:266:ARG:NH1	1:B:291:GLY:HA2	2.05	0.72
1:B:344:TYR:HE2	1:B:593:ASP:OD1	1.73	0.72
1:A:344:TYR:H	1:A:348:HIS:CD2	2.01	0.72
1:A:594:ARG:HH11	1:A:612:ASP:CG	1.94	0.72
1:B:659:SER:OG	1:B:661:ARG:HG3	1.90	0.72
1:B:665:ARG:O	1:B:665:ARG:HG3	1.89	0.72
1:B:237:HIS:HB2	1:B:244:MET:SD	2.30	0.71
1:B:181:ARG:HH12	1:B:296:ASN:HB2	1.54	0.71
1:B:437:LYS:HD3	1:B:458:GLY:O	1.91	0.71
1:A:111:ASN:N	1:A:114:GLN:HE21	1.86	0.71
1:B:224:SER:H	1:B:265:GLN:NE2	1.88	0.70
1:B:326:LYS:HE2	1:B:688:GLU:OE2	1.91	0.70
1:B:344:TYR:H	1:B:348:HIS:CD2	2.02	0.70
1:A:665:ARG:O	1:A:665:ARG:HG3	1.89	0.70
1:B:204:ARG:HH12	1:B:265:GLN:HE22	1.40	0.70
1:B:402:LEU:O	1:B:403:GLN:HG3	1.92	0.69
1:A:326:LYS:HE2	1:A:688:GLU:OE2	1.91	0.69
1:A:207:LEU:HD11	1:A:222:ALA:HB2	1.75	0.69
1:A:587:ASP:HB3	1:A:674:GLN:OE1	1.92	0.69
1:A:22:LEU:HD22	1:A:94:LEU:HD12	1.75	0.69
1:B:207:LEU:HD11	1:B:222:ALA:HB2	1.74	0.69
1:A:659:SER:OG	1:A:661:ARG:HG3	1.93	0.69
1:A:251:LEU:O	1:A:255:LEU:HB2	1.93	0.69
1:A:339:ARG:HD2	1:A:632:ARG:NH1	2.07	0.69
1:B:240:GLU:HB3	1:B:244:MET:N	2.07	0.69
1:A:111:ASN:H	1:A:114:GLN:NE2	1.89	0.69
1:A:402:LEU:HD21	1:A:428:SER:O	1.93	0.69
1:B:402:LEU:H	1:B:402:LEU:CD2	2.04	0.69
1:A:402:LEU:O	1:A:403:GLN:HG3	1.92	0.68
1:A:470:ASP:CG	1:A:592:HIS:HB3	2.14	0.68
1:B:587:ASP:HB3	1:B:674:GLN:OE1	1.93	0.68
1:A:665:ARG:NH2	1:A:670:LYS:HG3	2.06	0.68
1:B:402:LEU:HD21	1:B:428:SER:O	1.93	0.68
1:B:251:LEU:O	1:B:255:LEU:HB2	1.93	0.68
1:A:163:ARG:O	1:A:166:THR:HB	1.92	0.68
1:A:402:LEU:H	1:A:402:LEU:CD2	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:ASP:CG	1:B:592:HIS:HB3	2.13	0.67
1:A:318:ARG:HH22	1:A:465:ALA:CB	2.05	0.67
1:A:204:ARG:HH12	1:A:265:GLN:HE22	1.43	0.67
1:A:318:ARG:NH2	1:A:465:ALA:HB1	2.05	0.67
1:B:163:ARG:O	1:B:166:THR:HB	1.93	0.67
1:B:318:ARG:NH2	1:B:465:ALA:HB1	2.04	0.67
1:A:483:GLU:HB3	1:A:503:LEU:HD22	1.76	0.67
1:B:504:MET:HB3	1:B:625:ALA:HB3	1.77	0.67
1:A:240:GLU:HB3	1:A:244:MET:N	2.06	0.66
1:B:65:GLU:N	1:B:69:SER:HB3	2.10	0.66
1:B:111:ASN:H	1:B:114:GLN:NE2	1.89	0.66
1:A:240:GLU:CB	1:A:244:MET:HB2	2.24	0.66
1:B:240:GLU:CB	1:B:244:MET:HB2	2.25	0.66
1:B:141:ASN:HB3	1:B:142:PRO:HD2	1.78	0.66
1:A:141:ASN:HB3	1:A:142:PRO:HD2	1.77	0.65
1:A:65:GLU:N	1:A:69:SER:HB3	2.11	0.65
1:A:594:ARG:NH1	1:A:612:ASP:OD2	2.29	0.65
1:B:339:ARG:HD2	1:B:632:ARG:NH1	2.11	0.65
1:A:504:MET:HB3	1:A:625:ALA:HB3	1.78	0.65
1:A:181:ARG:HH12	1:A:296:ASN:CB	2.10	0.65
1:A:376:VAL:CG1	1:A:460:PHE:HB2	2.18	0.65
1:B:181:ARG:HH12	1:B:296:ASN:CB	2.10	0.65
1:A:405:ARG:HG2	1:A:433:LYS:NZ	2.12	0.64
1:A:35:ARG:NH2	1:A:101:GLU:OE2	2.30	0.64
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.62	0.64
1:B:95:TYR:CE2	1:B:99:LEU:HD11	2.32	0.64
1:B:266:ARG:HH11	1:B:266:ARG:HG2	1.62	0.64
1:B:318:ARG:HH22	1:B:465:ALA:CB	2.05	0.64
1:B:644:LEU:HD23	1:B:673:ALA:HB1	1.79	0.64
1:A:644:LEU:HD23	1:A:673:ALA:HB1	1.80	0.64
1:A:437:LYS:HD3	1:A:458:GLY:O	1.97	0.64
1:A:408:GLU:HG3	1:A:409:GLU:N	2.12	0.64
1:A:284:ARG:HG3	1:A:285:TYR:N	2.11	0.64
1:B:22:LEU:HD22	1:B:94:LEU:HD12	1.78	0.63
1:B:344:TYR:CE2	1:B:593:ASP:OD1	2.50	0.63
1:A:405:ARG:HE	1:A:621:ARG:HH22	1.47	0.63
1:A:196:MET:CE	1:A:306:VAL:HG21	2.28	0.63
1:A:548:ARG:HH11	1:A:548:ARG:CG	2.11	0.63
1:B:405:ARG:HG2	1:B:433:LYS:NZ	2.14	0.63
1:A:80:ILE:O	1:A:84:VAL:HG23	1.99	0.63
1:A:569:LEU:C	1:A:569:LEU:HD23	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLU:HG3	1:B:313:ASN:ND2	2.14	0.63
1:A:262:PHE:HD2	1:A:288:ILE:HG23	1.64	0.62
1:B:483:GLU:HB3	1:B:503:LEU:HD22	1.80	0.62
1:A:95:TYR:CE2	1:A:99:LEU:HD11	2.34	0.62
1:B:284:ARG:HG3	1:B:285:TYR:N	2.10	0.62
1:A:437:LYS:HE3	1:A:459:ASN:N	2.13	0.62
1:B:413:HIS:HA	1:B:416:LYS:HE3	1.81	0.62
1:B:262:PHE:HD2	1:B:288:ILE:HG23	1.65	0.62
1:B:437:LYS:HE3	1:B:459:ASN:N	2.14	0.62
1:A:34:GLU:HG3	1:A:313:ASN:ND2	2.14	0.61
1:A:413:HIS:HA	1:A:416:LYS:HE3	1.81	0.61
1:B:376:VAL:CG1	1:B:460:PHE:HB2	2.20	0.61
1:B:483:GLU:O	1:B:487:VAL:HG23	2.00	0.61
1:A:266:ARG:CZ	1:A:291:GLY:HA2	2.30	0.61
1:A:20:ARG:HG2	1:A:652:ARG:HD2	1.82	0.61
1:B:569:LEU:HD23	1:B:569:LEU:C	2.20	0.61
1:B:95:TYR:CZ	1:B:99:LEU:HD11	2.36	0.61
1:A:483:GLU:O	1:A:487:VAL:HG23	2.01	0.60
1:B:64:SER:OG	1:B:69:SER:HA	2.01	0.60
1:A:22:LEU:HD22	1:A:94:LEU:CD1	2.31	0.60
1:A:27:ASP:O	1:A:35:ARG:HD3	2.01	0.60
1:B:437:LYS:HB3	1:B:460:PHE:CE1	2.36	0.60
1:A:240:GLU:HB2	1:A:244:MET:HB2	1.82	0.60
1:B:173:GLU:O	1:B:175:PRO:HD3	2.02	0.60
1:B:240:GLU:HB2	1:B:244:MET:HB2	1.82	0.60
1:B:20:ARG:HG2	1:B:652:ARG:HD2	1.83	0.60
1:B:266:ARG:CZ	1:B:291:GLY:HA2	2.32	0.60
1:B:405:ARG:HE	1:B:621:ARG:HH22	1.48	0.60
1:A:370:LYS:HG2	1:A:397:THR:HB	1.84	0.60
1:A:506:SER:O	1:A:622:ILE:HA	2.02	0.60
1:B:437:LYS:CD	1:B:458:GLY:O	2.49	0.60
1:A:393:GLY:O	1:A:394:LYS:O	2.19	0.60
1:B:80:ILE:O	1:B:84:VAL:HG23	2.01	0.60
1:B:241:ALA:O	1:B:245:GLU:HG3	2.02	0.60
1:A:241:ALA:O	1:A:245:GLU:HG3	2.02	0.60
1:A:66:GLU:HG3	1:A:251:LEU:HD22	1.84	0.60
1:B:196:MET:CE	1:B:306:VAL:HG21	2.30	0.60
1:A:478:ALA:HA	1:A:481:THR:HB	1.83	0.60
1:B:370:LYS:HG2	1:B:397:THR:HB	1.84	0.60
1:A:120:GLN:HB3	1:A:205:TYR:OH	2.02	0.59
1:A:266:ARG:NH1	1:A:266:ARG:HG2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:HIS:HE1	1:A:685:GLU:OE1	1.84	0.59
1:A:437:LYS:HB3	1:A:460:PHE:CE1	2.37	0.59
1:B:266:ARG:NH1	1:B:266:ARG:HG2	2.16	0.59
1:B:533:ILE:HB	1:B:559:VAL:HG22	1.85	0.59
1:A:539:ASN:ND2	1:A:566:MET:H	2.01	0.59
1:A:189:ALA:HB3	1:A:190:PRO:CD	2.33	0.59
1:B:402:LEU:N	1:B:402:LEU:CD2	2.66	0.59
1:A:339:ARG:HD2	1:A:632:ARG:HH12	1.66	0.58
1:B:437:LYS:HD2	1:B:437:LYS:N	2.18	0.58
1:B:27:ASP:O	1:B:35:ARG:HD3	2.03	0.58
1:B:120:GLN:HB3	1:B:205:TYR:OH	2.02	0.58
1:B:348:HIS:HE1	1:B:685:GLU:OE1	1.85	0.58
1:A:95:TYR:CZ	1:A:99:LEU:HD11	2.38	0.58
1:B:189:ALA:HB3	1:B:190:PRO:CD	2.33	0.58
1:A:307:GLY:HA3	1:A:311:LEU:CD1	2.34	0.58
1:B:529:LEU:HB3	1:B:530:PRO:HD2	1.85	0.58
1:B:539:ASN:ND2	1:B:566:MET:H	2.01	0.58
1:B:233:TYR:O	1:B:234:ASP:HB2	2.04	0.58
1:B:478:ALA:HA	1:B:481:THR:HB	1.85	0.58
1:B:506:SER:HB2	1:B:623:GLU:HB2	1.86	0.58
1:A:437:LYS:HD2	1:A:437:LYS:N	2.19	0.58
1:B:377:ALA:HB2	1:B:462:GLU:H	1.69	0.58
1:B:506:SER:O	1:B:622:ILE:HA	2.04	0.58
1:A:64:SER:OG	1:A:69:SER:HA	2.03	0.57
1:A:377:ALA:HB2	1:A:462:GLU:H	1.69	0.57
1:A:512:ARG:HG2	1:A:516:GLU:OE2	2.04	0.57
1:B:402:LEU:HG	1:B:403:GLN:OE1	2.03	0.57
1:B:539:ASN:HD22	1:B:566:MET:H	1.52	0.57
1:A:173:GLU:O	1:A:175:PRO:HD3	2.04	0.57
1:A:402:LEU:HG	1:A:403:GLN:OE1	2.04	0.57
1:A:405:ARG:HG2	1:A:433:LYS:HZ3	1.68	0.57
1:A:529:LEU:HB3	1:A:530:PRO:HD2	1.86	0.57
1:B:307:GLY:HA3	1:B:311:LEU:CD1	2.35	0.57
1:A:435:HIS:O	1:A:437:LYS:HE2	2.04	0.57
1:B:512:ARG:HG2	1:B:516:GLU:OE2	2.04	0.57
1:B:515:TYR:CD2	1:B:548:ARG:HG3	2.39	0.57
1:A:436:ALA:CA	1:A:437:LYS:HD2	2.34	0.57
1:B:405:ARG:HG2	1:B:433:LYS:HZ2	1.68	0.57
1:B:408:GLU:HG3	1:B:409:GLU:N	2.14	0.57
1:A:285:TYR:H	1:A:285:TYR:HD1	1.52	0.56
1:A:345:TYR:CE1	1:A:472:SER:HB2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:TYR:O	1:A:234:ASP:HB2	2.05	0.56
1:A:240:GLU:HA	1:A:243:LEU:HB2	1.86	0.56
1:A:515:TYR:CD2	1:A:548:ARG:HG3	2.40	0.56
1:A:539:ASN:HD22	1:A:566:MET:H	1.52	0.56
1:A:570:ILE:HG23	1:A:656:LYS:HB3	1.86	0.56
1:B:17:PHE:HA	1:B:20:ARG:CZ	2.35	0.56
1:B:116:SER:C	1:B:118:ASN:H	2.09	0.56
1:B:548:ARG:HH11	1:B:548:ARG:CG	2.12	0.56
1:A:116:SER:C	1:A:118:ASN:H	2.09	0.56
1:A:355:GLU:O	1:A:359:GLN:HG3	2.05	0.56
1:A:179:VAL:CG1	1:A:180:PRO:HD2	2.36	0.56
1:A:537:LEU:HA	1:A:594:ARG:CG	2.31	0.56
1:B:435:HIS:O	1:B:437:LYS:HE2	2.04	0.56
1:B:22:LEU:HD22	1:B:94:LEU:CD1	2.35	0.56
1:A:17:PHE:HA	1:A:20:ARG:CZ	2.36	0.56
1:A:25:ALA:O	1:A:35:ARG:HD2	2.05	0.56
1:B:25:ALA:O	1:B:35:ARG:HD2	2.06	0.56
1:A:204:ARG:HH12	1:A:265:GLN:NE2	2.04	0.56
1:B:81:GLN:O	1:B:85:LEU:HG	2.07	0.56
1:B:35:ARG:NH2	1:B:101:GLU:OE2	2.38	0.55
1:B:179:VAL:CG1	1:B:180:PRO:HD2	2.34	0.55
1:B:204:ARG:HH12	1:B:265:GLN:NE2	2.02	0.55
1:A:477:ASP:OD1	1:A:479:ARG:HB2	2.06	0.55
1:B:271:ALA:O	1:B:275:VAL:HG23	2.07	0.55
1:B:285:TYR:H	1:B:285:TYR:HD1	1.52	0.55
1:A:437:LYS:N	1:A:437:LYS:CD	2.69	0.55
1:A:473:LEU:C	1:A:474:LEU:HD22	2.26	0.55
1:A:62:ILE:HA	1:A:65:GLU:OE1	2.07	0.55
1:A:377:ALA:N	1:A:461:ASN:HA	2.21	0.55
1:A:437:LYS:CD	1:A:458:GLY:O	2.55	0.55
1:B:437:LYS:CD	1:B:437:LYS:N	2.70	0.55
1:B:599:GLU:OE2	1:B:604:LYS:NZ	2.34	0.55
1:B:240:GLU:HA	1:B:243:LEU:HB2	1.88	0.55
1:B:468:TYR:HD2	1:B:592:HIS:HB2	1.72	0.55
1:B:570:ILE:HG23	1:B:656:LYS:HB3	1.88	0.55
1:A:436:ALA:C	1:A:437:LYS:CD	2.69	0.55
1:B:37:ARG:HA	1:B:300:PHE:O	2.08	0.55
1:B:393:GLY:O	1:B:394:LYS:O	2.25	0.55
1:A:468:TYR:HD2	1:A:592:HIS:HB2	1.71	0.54
1:A:338:GLU:HG3	1:A:339:ARG:HG3	1.90	0.54
1:B:66:GLU:HG3	1:B:251:LEU:HD22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ALA:O	1:A:275:VAL:HG23	2.07	0.54
1:B:339:ARG:HD2	1:B:632:ARG:HH12	1.71	0.54
1:A:160:GLU:HG3	1:A:169:TYR:HE2	1.72	0.54
1:B:160:GLU:HG3	1:B:169:TYR:HE2	1.72	0.54
1:B:254:ARG:O	1:B:254:ARG:HD3	2.07	0.54
1:B:377:ALA:N	1:B:461:ASN:HA	2.22	0.54
1:B:455:ILE:HG21	1:B:626:THR:OG1	2.08	0.54
1:A:254:ARG:O	1:A:254:ARG:HD3	2.08	0.54
1:B:345:TYR:CE1	1:B:472:SER:HB2	2.42	0.54
1:A:594:ARG:HD3	1:A:612:ASP:CG	2.26	0.53
1:A:67:GLN:HE22	1:A:246:LEU:CD1	2.22	0.53
1:B:436:ALA:CA	1:B:437:LYS:HD2	2.37	0.53
1:B:477:ASP:OD1	1:B:479:ARG:HB2	2.08	0.53
1:A:375:ARG:HG2	1:A:407:ASP:HB2	1.90	0.53
1:B:375:ARG:CD	1:B:407:ASP:HB2	2.38	0.53
1:B:511:ARG:HD2	1:B:515:TYR:CZ	2.44	0.53
1:A:656:LYS:HG3	1:A:657:GLU:OE1	2.08	0.53
1:B:510:SER:HB3	1:B:618:ILE:HG23	1.90	0.53
1:B:665:ARG:HG2	1:B:665:ARG:HH11	1.72	0.53
1:A:375:ARG:CD	1:A:407:ASP:HB2	2.37	0.53
1:A:510:SER:HB3	1:A:618:ILE:HG23	1.89	0.53
1:A:533:ILE:HB	1:A:559:VAL:HG22	1.89	0.53
1:A:81:GLN:O	1:A:85:LEU:HG	2.09	0.53
1:B:39:LEU:HD11	1:B:98:LEU:HD12	1.91	0.53
1:B:338:GLU:HG3	1:B:339:ARG:HG3	1.91	0.53
1:A:402:LEU:N	1:A:402:LEU:CD2	2.64	0.52
1:B:263:VAL:HA	1:B:289:VAL:O	2.09	0.52
1:A:61:ILE:HG23	1:A:73:SER:CB	2.39	0.52
1:B:239:MET:O	1:B:241:ALA:N	2.39	0.52
1:B:539:ASN:HD22	1:B:566:MET:HB2	1.74	0.52
1:B:628:LEU:CD1	1:B:637:VAL:HG21	2.39	0.52
1:A:375:ARG:CG	1:A:407:ASP:HB2	2.39	0.52
1:B:469:THR:C	1:B:470:ASP:OD2	2.48	0.52
1:A:37:ARG:HA	1:A:300:PHE:O	2.10	0.52
1:B:61:ILE:HG23	1:B:73:SER:CB	2.39	0.52
1:B:247:MET:SD	1:B:251:LEU:HD23	2.49	0.52
1:A:455:ILE:HG21	1:A:626:THR:OG1	2.10	0.52
1:B:62:ILE:HA	1:B:65:GLU:OE1	2.09	0.52
1:B:284:ARG:NH1	1:B:284:ARG:HB2	2.25	0.52
1:B:642:ASP:O	1:B:646:SER:HB3	2.10	0.52
1:A:123:LEU:HD22	1:A:202:ILE:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:LEU:HD22	1:B:83:ARG:HH11	1.70	0.52
1:B:656:LYS:HG3	1:B:657:GLU:OE1	2.10	0.52
1:A:359:GLN:HB3	1:B:214:PHE:CZ	2.45	0.51
1:A:628:LEU:CD1	1:A:637:VAL:HG21	2.40	0.51
1:A:66:GLU:CG	1:A:251:LEU:HD22	2.40	0.51
1:A:284:ARG:HB2	1:A:284:ARG:NH1	2.25	0.51
1:B:403:GLN:OE1	1:B:430:PRO:O	2.28	0.51
1:A:469:THR:O	1:A:470:ASP:OD2	2.28	0.51
1:B:67:GLN:HE22	1:B:246:LEU:CD1	2.23	0.51
1:A:665:ARG:HG2	1:A:665:ARG:HH11	1.74	0.51
1:B:473:LEU:C	1:B:474:LEU:HD22	2.30	0.51
1:B:639:ASP:O	1:B:642:ASP:HB2	2.11	0.51
1:A:239:MET:O	1:A:241:ALA:N	2.39	0.51
1:B:177:ASP:N	1:B:177:ASP:OD1	2.41	0.51
1:B:281:THR:O	1:B:281:THR:HG22	2.11	0.51
1:B:375:ARG:HD3	1:B:404:ALA:HB1	1.92	0.51
1:B:375:ARG:CG	1:B:407:ASP:HB2	2.40	0.51
1:B:672:ARG:HD3	1:B:675:LEU:HD12	1.91	0.51
1:A:23:GLN:OE1	1:A:652:ARG:HD3	2.11	0.51
1:A:263:VAL:HA	1:A:289:VAL:O	2.11	0.51
1:A:609:SER:OG	1:A:610:SER:N	2.43	0.51
1:A:247:MET:SD	1:A:251:LEU:HD23	2.51	0.51
1:B:117:VAL:HG12	1:B:117:VAL:O	2.11	0.51
1:A:628:LEU:HD11	1:A:637:VAL:HG21	1.92	0.51
1:A:599:GLU:OE2	1:A:604:LYS:NZ	2.36	0.51
1:B:79:LYS:O	1:B:83:ARG:HD3	2.11	0.50
1:B:628:LEU:HD11	1:B:637:VAL:HG21	1.91	0.50
1:A:111:ASN:OD1	1:A:114:GLN:HG3	2.10	0.50
1:A:506:SER:HB2	1:A:623:GLU:HB2	1.94	0.50
1:B:194:LYS:HD2	1:B:306:VAL:CG1	2.42	0.50
1:A:103:ALA:HA	1:A:107:ILE:O	2.11	0.50
1:A:614:MET:HB2	1:A:617:ASN:HD22	1.77	0.50
1:A:672:ARG:HD3	1:A:675:LEU:HD12	1.91	0.50
1:B:609:SER:OG	1:B:610:SER:N	2.44	0.50
1:A:236:VAL:HG12	1:A:236:VAL:O	2.12	0.50
1:A:469:THR:C	1:A:470:ASP:OD2	2.50	0.50
1:A:642:ASP:O	1:A:646:SER:HB3	2.12	0.50
1:B:375:ARG:HG2	1:B:407:ASP:HB2	1.92	0.50
1:B:614:MET:HB2	1:B:617:ASN:HD22	1.77	0.50
1:A:418:LEU:HB3	1:A:423:VAL:HB	1.94	0.50
1:A:39:LEU:HD22	1:A:91:PHE:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ASP:O	1:A:642:ASP:HB2	2.11	0.50
1:B:73:SER:O	1:B:77:LEU:HD23	2.11	0.50
1:B:236:VAL:O	1:B:236:VAL:HG12	2.12	0.50
1:B:71:SER:O	1:B:73:SER:N	2.40	0.49
1:B:233:TYR:CG	1:B:234:ASP:N	2.80	0.49
1:A:281:THR:HG22	1:A:281:THR:O	2.12	0.49
1:B:469:THR:O	1:B:470:ASP:OD2	2.30	0.49
1:A:194:LYS:HD2	1:A:306:VAL:CG1	2.42	0.49
1:B:355:GLU:O	1:B:359:GLN:HG3	2.11	0.49
1:B:434:ILE:HA	1:B:622:ILE:HB	1.94	0.49
1:B:457:THR:CG2	1:B:471:TYR:HB2	2.42	0.49
1:A:240:GLU:HB3	1:A:244:MET:HB2	1.94	0.49
1:A:479:ARG:NH1	1:A:629:LEU:HD13	2.27	0.49
1:B:161:ILE:HB	1:B:168:ARG:HB2	1.94	0.49
1:B:418:LEU:HB3	1:B:423:VAL:HB	1.95	0.49
1:B:105:ASN:O	1:B:106:GLN:HB2	2.13	0.49
1:B:367:LEU:O	1:B:394:LYS:HA	2.13	0.49
1:A:264:TYR:CE2	1:A:290:PRO:HB3	2.47	0.49
1:A:79:LYS:O	1:A:83:ARG:HD3	2.12	0.49
1:A:233:TYR:CG	1:A:234:ASP:N	2.80	0.49
1:A:540:LEU:CD2	1:A:561:LEU:HD13	2.42	0.49
1:B:61:ILE:HG23	1:B:73:SER:HB2	1.95	0.49
1:B:66:GLU:CG	1:B:251:LEU:HD22	2.43	0.49
1:B:400:VAL:HG23	1:B:400:VAL:O	2.13	0.49
1:B:111:ASN:OD1	1:B:114:GLN:HG3	2.13	0.49
1:A:117:VAL:HG12	1:A:117:VAL:O	2.13	0.49
1:A:344:TYR:N	1:A:348:HIS:HD2	1.94	0.49
1:A:457:THR:CG2	1:A:471:TYR:HB2	2.43	0.49
1:B:405:ARG:HH22	1:B:616:ARG:HE	1.60	0.49
1:B:413:HIS:O	1:B:415:ALA:N	2.41	0.48
1:A:161:ILE:HB	1:A:168:ARG:HB2	1.96	0.48
1:B:240:GLU:HB3	1:B:244:MET:HB2	1.94	0.48
1:A:479:ARG:HG2	1:A:502:TYR:OH	2.14	0.48
1:B:103:ALA:HA	1:B:107:ILE:O	2.13	0.48
1:B:648:THR:HG22	1:B:668:ARG:HH21	1.79	0.48
1:B:61:ILE:CG2	1:B:73:SER:HB2	2.43	0.48
1:B:233:TYR:CD1	1:B:234:ASP:N	2.82	0.48
1:B:306:VAL:HG12	1:B:306:VAL:O	2.13	0.48
1:A:61:ILE:CG2	1:A:73:SER:HB2	2.44	0.48
1:A:158:ALA:HA	1:A:171:LEU:HD23	1.96	0.48
1:A:177:ASP:OD1	1:A:177:ASP:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:TYR:CD2	1:B:437:LYS:NZ	2.82	0.48
1:B:401:GLU:HA	1:B:428:SER:HB3	1.96	0.48
1:B:451:ARG:HB2	1:B:481:THR:CG2	2.43	0.48
1:A:12:LEU:HD22	1:A:83:ARG:HH11	1.70	0.48
1:A:403:GLN:OE1	1:A:430:PRO:O	2.31	0.48
1:A:405:ARG:HH22	1:A:616:ARG:HE	1.59	0.48
1:B:468:TYR:HD2	1:B:592:HIS:CG	2.32	0.48
1:B:587:ASP:HB3	1:B:674:GLN:CD	2.34	0.48
1:A:36:MET:O	1:A:39:LEU:HB2	2.14	0.48
1:B:538:ASN:HB2	1:B:612:ASP:OD1	2.14	0.48
1:A:548:ARG:HG2	1:A:548:ARG:NH1	2.12	0.48
1:B:81:GLN:O	1:B:81:GLN:HG2	2.14	0.48
1:A:73:SER:O	1:A:77:LEU:HD23	2.13	0.47
1:A:214:PHE:CZ	1:B:359:GLN:HB3	2.49	0.47
1:B:461:ASN:OD1	1:B:463:LYS:HB2	2.14	0.47
1:B:536:LYS:NZ	1:B:591:GLU:OE1	2.42	0.47
1:A:401:GLU:HA	1:A:428:SER:HB3	1.97	0.47
1:B:39:LEU:HD22	1:B:91:PHE:CE1	2.50	0.47
1:B:436:ALA:C	1:B:437:LYS:CD	2.72	0.47
1:A:375:ARG:HD3	1:A:404:ALA:HB1	1.95	0.47
1:B:194:LYS:HD2	1:B:306:VAL:HG11	1.95	0.47
1:B:301:ILE:HG22	1:B:301:ILE:O	2.14	0.47
1:A:233:TYR:CD1	1:A:234:ASP:N	2.82	0.47
1:A:511:ARG:HD2	1:A:515:TYR:CZ	2.50	0.47
1:A:389:ALA:HB1	1:A:394:LYS:HG3	1.96	0.47
1:A:39:LEU:HD11	1:A:98:LEU:HD12	1.96	0.47
1:A:461:ASN:OD1	1:A:463:LYS:HB2	2.15	0.47
1:A:71:SER:O	1:A:73:SER:N	2.41	0.47
1:A:400:VAL:HG23	1:A:400:VAL:O	2.14	0.47
1:A:539:ASN:HD22	1:A:566:MET:HB2	1.80	0.47
1:A:587:ASP:HB3	1:A:674:GLN:CD	2.34	0.47
1:B:207:LEU:HD11	1:B:222:ALA:CB	2.42	0.47
1:B:344:TYR:N	1:B:348:HIS:HD2	1.95	0.47
1:A:557:VAL:HA	1:A:558:PRO:HD3	1.73	0.47
1:B:120:GLN:O	1:B:124:ARG:HG3	2.14	0.47
1:B:439:PHE:CD1	1:B:439:PHE:C	2.88	0.47
1:A:538:ASN:HB2	1:A:612:ASP:OD1	2.15	0.47
1:B:23:GLN:OE1	1:B:652:ARG:HD3	2.14	0.47
1:B:405:ARG:HH21	1:B:616:ARG:HD2	1.80	0.47
1:A:194:LYS:HD2	1:A:306:VAL:HG11	1.96	0.47
1:A:207:LEU:HD11	1:A:222:ALA:CB	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:TYR:CG	1:A:375:ARG:N	2.82	0.47
1:A:648:THR:HG22	1:A:668:ARG:HH21	1.79	0.47
1:B:548:ARG:CG	1:B:548:ARG:NH1	2.75	0.46
1:A:105:ASN:O	1:A:106:GLN:HB2	2.16	0.46
1:A:511:ARG:NH1	1:A:542:ASP:OD1	2.44	0.46
1:B:285:TYR:N	1:B:285:TYR:CD1	2.83	0.46
1:B:540:LEU:CD2	1:B:561:LEU:HD13	2.45	0.46
1:A:413:HIS:O	1:A:415:ALA:N	2.39	0.46
1:A:11:GLU:HG2	1:A:57:LEU:HD22	1.98	0.46
1:A:308:LYS:O	1:A:310:ASN:N	2.49	0.46
1:B:363:ASP:OD2	1:B:443:ARG:NH1	2.45	0.46
1:B:415:ALA:O	1:B:417:ARG:N	2.47	0.46
1:A:61:ILE:HG23	1:A:73:SER:HB2	1.97	0.46
1:A:416:LYS:H	1:A:416:LYS:HG2	1.61	0.46
1:B:18:ASN:O	1:B:21:VAL:HB	2.16	0.46
1:B:374:TYR:CG	1:B:375:ARG:N	2.83	0.46
1:A:18:ASN:O	1:A:21:VAL:HB	2.16	0.46
1:B:415:ALA:O	1:B:416:LYS:C	2.54	0.46
1:A:318:ARG:NH1	1:A:466:ARG:HG2	2.30	0.46
1:A:477:ASP:OD2	1:A:479:ARG:NH2	2.48	0.46
1:B:261:ARG:HG2	1:B:287:SER:HB3	1.98	0.46
1:B:570:ILE:HG22	1:B:573:LEU:HG	1.96	0.46
1:A:111:ASN:CG	1:A:114:GLN:HG3	2.36	0.46
1:A:363:ASP:O	1:A:394:LYS:NZ	2.48	0.46
1:A:415:ALA:O	1:A:417:ARG:N	2.48	0.46
1:B:345:TYR:O	1:B:469:THR:HA	2.15	0.46
1:B:128:LYS:HG2	1:B:132:ARG:HH21	1.81	0.46
1:B:506:SER:HA	1:B:507:PRO:HA	1.72	0.46
1:A:405:ARG:NH2	1:A:616:ARG:HE	2.14	0.45
1:A:405:ARG:NH2	1:A:616:ARG:NE	2.64	0.45
1:B:405:ARG:NH2	1:B:616:ARG:NE	2.64	0.45
1:A:374:TYR:CD2	1:A:437:LYS:NZ	2.84	0.45
1:A:405:ARG:HH21	1:A:616:ARG:HD2	1.81	0.45
1:B:64:SER:CB	1:B:69:SER:HA	2.46	0.45
1:B:83:ARG:HH11	1:B:83:ARG:HG2	1.81	0.45
1:B:158:ALA:HA	1:B:171:LEU:HD23	1.97	0.45
1:B:470:ASP:OD1	1:B:592:HIS:HB3	2.16	0.45
1:A:644:LEU:HD23	1:A:673:ALA:CB	2.46	0.45
1:B:264:TYR:CE2	1:B:290:PRO:HB3	2.51	0.45
1:B:405:ARG:NH2	1:B:616:ARG:HE	2.14	0.45
1:A:66:GLU:HB2	1:A:251:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:VAL:O	1:A:306:VAL:HG12	2.16	0.45
1:B:548:ARG:HG2	1:B:548:ARG:NH1	2.14	0.45
1:A:265:GLN:HG3	1:A:292:GLY:O	2.17	0.45
1:B:36:MET:O	1:B:39:LEU:HB2	2.16	0.45
1:B:111:ASN:CG	1:B:114:GLN:HG3	2.37	0.45
1:B:190:PRO:HG2	1:B:193:ARG:HD2	1.98	0.45
1:B:592:HIS:HD2	1:B:594:ARG:HH22	1.65	0.45
1:A:345:TYR:O	1:A:469:THR:HA	2.17	0.45
1:A:522:ILE:HG23	1:A:555:SER:CB	2.46	0.45
1:B:451:ARG:HG2	1:B:451:ARG:HH11	1.81	0.45
1:B:533:ILE:O	1:B:559:VAL:HA	2.17	0.45
1:A:64:SER:CB	1:A:69:SER:HA	2.47	0.45
1:B:11:GLU:HG2	1:B:57:LEU:HD22	1.98	0.45
1:A:393:GLY:O	1:A:394:LYS:C	2.56	0.44
1:A:439:PHE:CD1	1:A:439:PHE:C	2.90	0.44
1:A:451:ARG:HB2	1:A:481:THR:CG2	2.46	0.44
1:B:477:ASP:OD2	1:B:479:ARG:NH2	2.49	0.44
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.81	0.44
1:B:22:LEU:HG	1:B:42:TYR:CE1	2.53	0.44
1:B:308:LYS:O	1:B:310:ASN:N	2.50	0.44
1:B:339:ARG:HE	1:B:339:ARG:HB3	1.44	0.44
1:B:341:VAL:HG12	1:B:343:LEU:HD13	1.99	0.44
1:A:190:PRO:HG2	1:A:193:ARG:HD2	1.99	0.44
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.81	0.44
1:A:150:LEU:HD22	1:A:280:LEU:HD21	1.98	0.44
1:A:262:PHE:HD2	1:A:288:ILE:CG2	2.31	0.44
1:A:506:SER:HA	1:A:507:PRO:HA	1.70	0.44
1:B:389:ALA:HB1	1:B:394:LYS:HG3	1.98	0.44
1:B:666:GLY:C	1:B:668:ARG:H	2.21	0.44
1:A:367:LEU:O	1:A:394:LYS:HA	2.18	0.44
1:B:4:GLU:O	1:B:5:LYS:C	2.56	0.44
1:A:533:ILE:O	1:A:559:VAL:HA	2.17	0.44
1:A:599:GLU:HG3	1:A:601:GLY:O	2.16	0.44
1:B:318:ARG:NH1	1:B:466:ARG:HG2	2.32	0.44
1:A:266:ARG:HG2	1:A:291:GLY:HA2	2.00	0.44
1:A:285:TYR:N	1:A:285:TYR:CD1	2.83	0.44
1:A:415:ALA:O	1:A:416:LYS:C	2.56	0.44
1:A:434:ILE:HA	1:A:622:ILE:HB	1.99	0.44
1:B:32:LEU:HD21	1:B:102:MET:HA	2.00	0.44
1:B:64:SER:HB3	1:B:69:SER:CB	2.44	0.44
1:A:341:VAL:HG12	1:A:343:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASP:OD2	1:A:443:ARG:NH1	2.49	0.44
1:A:377:ALA:HB2	1:A:462:GLU:N	2.32	0.44
1:A:481:THR:HG22	1:A:482:ASN:N	2.32	0.44
1:B:262:PHE:HD2	1:B:288:ILE:CG2	2.31	0.44
1:B:377:ALA:HB2	1:B:462:GLU:N	2.33	0.44
1:A:120:GLN:O	1:A:124:ARG:HG3	2.18	0.44
1:A:470:ASP:OD1	1:A:592:HIS:HB3	2.18	0.44
1:B:50:TYR:OH	1:B:84:VAL:HG11	2.18	0.44
1:A:230:ASP:OD1	1:A:259:PRO:HG2	2.18	0.43
1:A:536:LYS:NZ	1:A:591:GLU:OE1	2.45	0.43
1:B:324:PHE:CE1	1:B:341:VAL:HG11	2.53	0.43
1:B:599:GLU:HG3	1:B:601:GLY:O	2.18	0.43
1:B:653:TYR:CE1	1:B:664:PRO:HD3	2.53	0.43
1:A:50:TYR:OH	1:A:84:VAL:HG11	2.18	0.43
1:A:284:ARG:HG3	1:A:285:TYR:CD1	2.34	0.43
1:A:429:ALA:O	1:A:430:PRO:C	2.57	0.43
1:B:67:GLN:HE22	1:B:246:LEU:HD13	1.83	0.43
1:B:265:GLN:HG3	1:B:292:GLY:O	2.19	0.43
1:A:4:GLU:O	1:A:5:LYS:C	2.56	0.43
1:A:67:GLN:HE22	1:A:246:LEU:HD13	1.82	0.43
1:B:457:THR:HG21	1:B:471:TYR:HB2	2.00	0.43
1:B:480:ILE:O	1:B:484:VAL:HG23	2.18	0.43
1:A:33:ILE:HB	1:A:311:LEU:O	2.18	0.43
1:A:81:GLN:O	1:A:81:GLN:HG2	2.18	0.43
1:B:150:LEU:HD22	1:B:280:LEU:HD21	2.00	0.43
1:B:437:LYS:HB3	1:B:460:PHE:CD1	2.53	0.43
1:A:261:ARG:HG2	1:A:287:SER:HB3	1.98	0.43
1:A:548:ARG:CG	1:A:548:ARG:NH1	2.73	0.43
1:B:181:ARG:O	1:B:198:LEU:HD23	2.19	0.43
1:B:266:ARG:HG2	1:B:291:GLY:HA2	2.01	0.43
1:B:644:LEU:HD23	1:B:673:ALA:CB	2.46	0.43
1:A:324:PHE:CE1	1:A:341:VAL:HG11	2.54	0.43
1:A:344:TYR:HE2	1:A:593:ASP:OD1	2.01	0.43
1:A:128:LYS:HG2	1:A:132:ARG:HH21	1.84	0.43
1:B:295:HIS:O	1:B:296:ASN:HB2	2.19	0.43
1:B:522:ILE:HG23	1:B:555:SER:CB	2.49	0.43
1:A:160:GLU:HG3	1:A:169:TYR:CE2	2.54	0.43
1:A:339:ARG:HE	1:A:339:ARG:HB3	1.46	0.43
1:B:123:LEU:HD22	1:B:202:ILE:HG23	2.00	0.43
1:B:479:ARG:HG2	1:B:502:TYR:OH	2.18	0.43
1:A:54:PHE:CD2	1:A:58:LYS:HE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASP:HB2	1:B:214:PHE:CD2	2.54	0.43
1:A:653:TYR:CE1	1:A:664:PRO:HD3	2.54	0.43
1:B:66:GLU:HB2	1:B:251:LEU:HD22	2.00	0.43
1:B:393:GLY:O	1:B:394:LYS:C	2.57	0.43
1:B:308:LYS:HB2	1:B:310:ASN:ND2	2.33	0.43
1:B:353:VAL:HG13	1:B:439:PHE:HE2	1.84	0.43
1:B:451:ARG:HB2	1:B:481:THR:HG21	2.01	0.43
1:B:537:LEU:O	1:B:563:VAL:HA	2.18	0.43
1:A:32:LEU:HD21	1:A:102:MET:HA	2.01	0.42
1:B:17:PHE:HA	1:B:20:ARG:NH2	2.34	0.42
1:B:512:ARG:O	1:B:516:GLU:HG3	2.19	0.42
1:A:147:VAL:HG22	1:A:279:LYS:O	2.19	0.42
1:B:323:TRP:CH2	1:B:339:ARG:HD3	2.55	0.42
1:A:181:ARG:O	1:A:198:LEU:HD23	2.20	0.42
1:A:415:ALA:C	1:A:417:ARG:N	2.73	0.42
1:A:666:GLY:C	1:A:668:ARG:H	2.21	0.42
1:B:656:LYS:HB2	1:B:656:LYS:HE2	1.79	0.42
1:A:233:TYR:HE1	1:A:236:VAL:HB	1.85	0.42
1:A:312:VAL:HG12	1:A:313:ASN:N	2.35	0.42
1:A:429:ALA:O	1:A:430:PRO:O	2.38	0.42
1:B:64:SER:O	1:B:69:SER:N	2.53	0.42
1:B:233:TYR:HE1	1:B:236:VAL:HB	1.85	0.42
1:B:415:ALA:C	1:B:417:ARG:N	2.72	0.42
1:B:525:ALA:HB2	1:B:557:VAL:HG22	2.01	0.42
1:B:479:ARG:NH1	1:B:629:LEU:HD13	2.34	0.42
1:B:511:ARG:NH1	1:B:542:ASP:OD1	2.45	0.42
1:B:561:LEU:HB2	1:B:582:ALA:CB	2.49	0.42
1:A:22:LEU:HG	1:A:42:TYR:CE1	2.55	0.42
1:A:570:ILE:HG22	1:A:573:LEU:HG	2.02	0.42
1:A:64:SER:O	1:A:69:SER:N	2.53	0.41
1:B:200:ASP:OD2	1:B:200:ASP:N	2.53	0.41
1:A:656:LYS:HB2	1:A:656:LYS:HE2	1.81	0.41
1:B:22:LEU:HG	1:B:42:TYR:CD1	2.55	0.41
1:B:147:VAL:HG22	1:B:279:LYS:O	2.20	0.41
1:B:342:LEU:HB3	1:B:633:LEU:HD22	2.02	0.41
1:B:160:GLU:HG3	1:B:169:TYR:CE2	2.54	0.41
1:B:429:ALA:O	1:B:430:PRO:C	2.59	0.41
1:A:265:GLN:HG3	1:A:293:ARG:HA	2.02	0.41
1:A:342:LEU:HB3	1:A:633:LEU:HD22	2.03	0.41
1:B:54:PHE:CD2	1:B:58:LYS:HE3	2.54	0.41
1:B:441:ILE:O	1:B:451:ARG:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:SER:HA	1:B:625:ALA:HA	2.01	0.41
1:A:345:TYR:HE1	1:A:472:SER:HB2	1.86	0.41
1:A:437:LYS:HB3	1:A:460:PHE:CD1	2.55	0.41
1:B:481:THR:HG22	1:B:482:ASN:N	2.35	0.41
1:B:535:LEU:HD11	1:B:613:TRP:CH2	2.55	0.41
1:A:378:LYS:HE2	1:A:378:LYS:HB3	1.92	0.41
1:B:561:LEU:HB2	1:B:582:ALA:HB2	2.03	0.41
1:B:95:TYR:O	1:B:99:LEU:HG	2.19	0.41
1:B:156:TYR:CE2	1:B:173:GLU:HB2	2.55	0.41
1:B:375:ARG:HD2	1:B:407:ASP:HB2	2.03	0.41
1:A:148:GLN:O	1:A:150:LEU:N	2.53	0.41
1:B:540:LEU:HD23	1:B:561:LEU:HD13	2.03	0.41
1:A:240:GLU:HB3	1:A:244:MET:CB	2.51	0.41
1:A:281:THR:O	1:A:283:SER:N	2.54	0.41
1:A:457:THR:HG21	1:A:471:TYR:HB2	2.02	0.41
1:B:281:THR:O	1:B:283:SER:N	2.54	0.41
1:B:346:PRO:HD2	1:B:469:THR:HG22	2.01	0.41
1:A:26:ALA:HA	1:A:94:LEU:HD21	2.03	0.41
1:A:535:LEU:HD11	1:A:613:TRP:CH2	2.55	0.41
1:B:33:ILE:HB	1:B:311:LEU:O	2.20	0.41
1:B:678:TYR:CE1	1:B:682:LYS:HD3	2.57	0.41
1:A:67:GLN:HE22	1:A:246:LEU:HD12	1.86	0.40
1:B:148:GLN:O	1:B:150:LEU:N	2.54	0.40
1:B:375:ARG:CD	1:B:404:ALA:HB1	2.51	0.40
1:B:506:SER:HB2	1:B:623:GLU:CB	2.52	0.40
1:A:157:LEU:HA	1:A:157:LEU:HD12	1.87	0.40
1:A:229:ARG:HE	1:A:258:GLU:HG3	1.86	0.40
1:A:308:LYS:HB2	1:A:310:ASN:ND2	2.36	0.40
1:A:346:PRO:HD2	1:A:469:THR:HG22	2.04	0.40
1:B:145:ASP:O	1:B:146:LEU:C	2.59	0.40
1:B:416:LYS:H	1:B:416:LYS:HG2	1.59	0.40
1:B:194:LYS:CE	1:B:306:VAL:HG12	2.51	0.40
1:A:479:ARG:HG2	1:A:502:TYR:CZ	2.56	0.40
1:A:663:VAL:HA	1:A:664:PRO:HD3	1.87	0.40
1:A:678:TYR:CZ	1:A:682:LYS:HD3	2.57	0.40
1:B:230:ASP:OD1	1:B:259:PRO:HG2	2.21	0.40
1:B:520:ARG:HB2	1:B:520:ARG:NH1	2.36	0.40
1:A:145:ASP:O	1:A:145:ASP:CG	2.60	0.40
1:A:353:VAL:HG13	1:A:439:PHE:HE2	1.86	0.40
1:A:375:ARG:HD2	1:A:407:ASP:HB2	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	685/687 (100%)	585 (85%)	73 (11%)	27 (4%)	3 17
1	B	685/687 (100%)	582 (85%)	77 (11%)	26 (4%)	3 18
All	All	1370/1374 (100%)	1167 (85%)	150 (11%)	53 (4%)	3 17

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
1	A	66	GLU
1	A	234	ASP
1	A	241	ALA
1	A	394	LYS
1	A	414	TRP
1	A	430	PRO
1	B	65	GLU
1	B	66	GLU
1	B	241	ALA
1	B	394	LYS
1	B	414	TRP
1	B	430	PRO
1	A	117	VAL
1	A	147	VAL
1	A	149	PHE
1	A	188	GLU
1	A	189	ALA
1	A	309	ALA
1	A	510	SER
1	B	117	VAL
1	B	147	VAL
1	B	149	PHE
1	B	188	GLU
1	B	189	ALA

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Mol	Chain	Res	Type
1	B	234	ASP
1	B	309	ALA
1	A	281	THR
1	A	446	ASN
1	B	281	THR
1	B	446	ASN
1	B	510	SER
1	A	5	LYS
1	A	148	GLN
1	A	240	GLU
1	A	282	ILE
1	A	416	LYS
1	A	574	GLU
1	B	5	LYS
1	B	240	GLU
1	B	282	ILE
1	B	416	LYS
1	B	574	GLU
1	A	429	ALA
1	A	674	GLN
1	B	72	HIS
1	B	148	GLN
1	B	322	ILE
1	B	429	ALA
1	A	673	ALA
1	A	322	ILE
1	A	666	GLY
1	B	666	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	566/619 (91%)	521 (92%)	45 (8%)	12 40
1	B	566/619 (91%)	520 (92%)	46 (8%)	11 40
All	All	1132/1238 (91%)	1041 (92%)	91 (8%)	12 40

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	47	ASP
1	A	64	SER
1	A	66	GLU
1	A	69	SER
1	A	72	HIS
1	A	83	ARG
1	A	153	ASP
1	A	157	LEU
1	A	177	ASP
1	A	200	ASP
1	A	225	MET
1	A	233	TYR
1	A	253	GLN
1	A	255	LEU
1	A	265	GLN
1	A	272	LEU
1	A	277	ARG
1	A	284	ARG
1	A	285	TYR
1	A	299	ASP
1	A	314	LYS
1	A	316	LEU
1	A	343	LEU
1	A	349	THR
1	A	356	LEU
1	A	384	ASP
1	A	402	LEU
1	A	406	PHE
1	A	414	TRP
1	A	417	ARG
1	A	428	SER
1	A	437	LYS
1	A	439	PHE
1	A	462	GLU
1	A	464	THR
1	A	481	THR
1	A	486	ARG
1	A	548	ARG
1	A	564	ARG
1	A	616	ARG
1	A	646	SER

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Mol	Chain	Res	Type
1	A	656	LYS
1	A	668	ARG
1	A	675	LEU
1	B	22	LEU
1	B	47	ASP
1	B	64	SER
1	B	66	GLU
1	B	69	SER
1	B	72	HIS
1	B	83	ARG
1	B	153	ASP
1	B	157	LEU
1	B	177	ASP
1	B	200	ASP
1	B	225	MET
1	B	233	TYR
1	B	253	GLN
1	B	255	LEU
1	B	265	GLN
1	B	272	LEU
1	B	277	ARG
1	B	284	ARG
1	B	285	TYR
1	B	299	ASP
1	B	314	LYS
1	B	316	LEU
1	B	343	LEU
1	B	349	THR
1	B	356	LEU
1	B	384	ASP
1	B	402	LEU
1	B	406	PHE
1	B	414	TRP
1	B	416	LYS
1	B	417	ARG
1	B	428	SER
1	B	437	LYS
1	B	439	PHE
1	B	462	GLU
1	B	464	THR
1	B	481	THR
1	B	486	ARG

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Mol	Chain	Res	Type
1	B	548	ARG
1	B	564	ARG
1	B	594	ARG
1	B	616	ARG
1	B	646	SER
1	B	656	LYS
1	B	675	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	72	HIS
1	A	75	HIS
1	A	114	GLN
1	A	253	GLN
1	A	265	GLN
1	A	295	HIS
1	A	310	ASN
1	A	313	ASN
1	A	348	HIS
1	A	446	ASN
1	A	459	ASN
1	A	527	GLN
1	A	539	ASN
1	A	617	ASN
1	B	67	GLN
1	B	72	HIS
1	B	75	HIS
1	B	114	GLN
1	B	253	GLN
1	B	265	GLN
1	B	295	HIS
1	B	310	ASN
1	B	313	ASN
1	B	348	HIS
1	B	446	ASN
1	B	459	ASN
1	B	527	GLN
1	B	539	ASN
1	B	592	HIS
1	B	617	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	687/687 (100%)	-0.01	48 (6%)	16	5	7, 35, 95, 135	0
1	B	687/687 (100%)	0.01	52 (7%)	13	4	12, 35, 97, 133	0
All	All	1374/1374 (100%)	0.00	100 (7%)	15	4	7, 35, 97, 135	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	410	ALA	11.2
1	A	412	ILE	8.1
1	B	3	GLN	7.5
1	A	73	SER	6.7
1	B	406	PHE	6.6
1	B	2	GLY	6.6
1	A	411	ASN	6.4
1	A	407	ASP	6.3
1	B	376	VAL	6.3
1	B	69	SER	6.2
1	B	405	ARG	5.9
1	B	464	THR	5.6
1	A	242	SER	5.5
1	A	69	SER	5.4
1	B	238	GLU	5.3
1	B	242	SER	5.3
1	A	375	ARG	5.3
1	A	464	THR	5.3
1	A	465	ALA	5.0
1	B	408	GLU	4.9
1	B	409	GLU	4.9
1	A	461	ASN	4.7
1	A	404	ALA	4.7
1	A	238	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	73	SER	4.6
1	A	406	PHE	4.6
1	A	688	GLU	4.6
1	A	408	GLU	4.5
1	A	67	GLN	4.5
1	B	67	GLN	4.4
1	B	404	ALA	4.2
1	B	407	ASP	4.2
1	B	4	GLU	4.2
1	A	74	ARG	4.2
1	B	375	ARG	4.1
1	A	376	VAL	4.1
1	B	465	ALA	4.1
1	A	189	ALA	4.0
1	B	466	ARG	3.9
1	A	234	ASP	3.8
1	B	234	ASP	3.8
1	B	413	HIS	3.7
1	A	413	HIS	3.7
1	B	461	ASN	3.7
1	B	410	ALA	3.7
1	A	66	GLU	3.6
1	B	246	LEU	3.6
1	B	411	ASN	3.6
1	A	72	HIS	3.6
1	A	239	MET	3.5
1	B	66	GLU	3.5
1	A	2	GLY	3.4
1	B	412	ILE	3.3
1	B	463	LYS	3.3
1	A	463	LYS	3.2
1	B	70	ASN	3.2
1	A	3	GLN	3.2
1	A	409	GLU	3.1
1	A	71	SER	3.1
1	A	188	GLU	3.0
1	A	374	TYR	2.9
1	B	688	GLU	2.9
1	A	667	ASN	2.9
1	A	192	ARG	2.8
1	B	378	LYS	2.8
1	A	241	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	403	GLN	2.7
1	B	191	ARG	2.7
1	A	4	GLU	2.7
1	A	233	TYR	2.7
1	A	191	ARG	2.6
1	B	243	LEU	2.6
1	A	285	TYR	2.6
1	A	117	VAL	2.5
1	B	430	PRO	2.5
1	B	374	TYR	2.5
1	A	243	LEU	2.5
1	B	248	SER	2.5
1	B	74	ARG	2.5
1	B	528	GLY	2.4
1	B	71	SER	2.4
1	B	285	TYR	2.4
1	A	237	HIS	2.4
1	B	68	GLY	2.4
1	B	253	GLN	2.4
1	A	190	PRO	2.3
1	A	246	LEU	2.3
1	A	377	ALA	2.3
1	B	667	ASN	2.3
1	A	405	ARG	2.2
1	B	239	MET	2.2
1	B	117	VAL	2.2
1	B	236	VAL	2.2
1	B	414	TRP	2.2
1	B	283	SER	2.1
1	A	466	ARG	2.1
1	A	245	GLU	2.1
1	B	237	HIS	2.0
1	B	177	ASP	2.0
1	B	249	SER	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.